Full wwPDB EM Validation Report

Mar 20, 2026 – 11:12 AM UTC

PDB ID	:	9UEN / pdb_00009uen
EMDB ID	:	EMD-64087
Title	:	Cryo-EM structure of coccolithophore photosystem I
Authors	:	Zhao, L.S.; Sun, X.M.; Li, K.; Zhang, Y.Z.; Liu, L.N.
Deposited on	:	2025-04-08
Resolution	:	3.10 Å(reported)

This is a Full wwPDB EM Validation 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 ⓘ 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 ⓘ) were used in the production of this report:

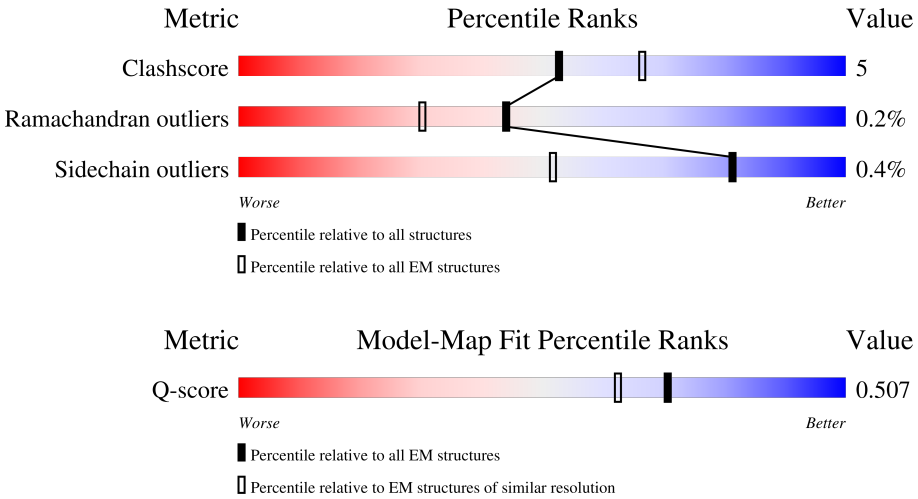
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

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



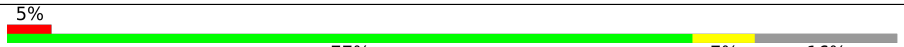
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	A	201	85% 6% 9%
2	B	219	21% 61% 6% 32%
3	C	208	9% 75% 11% 14%
4	D	255	62% 11% 26%

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Mol	Chain	Length	Quality of chain
5	E	217	
6	F	239	
7	G	198	
8	H	199	
9	I	196	
10	J	208	
11	K	204	
12	L	228	
13	M	224	
13	P	224	
13	W	224	
14	N	225	
15	O	210	
15	R	210	
15	T	210	
16	Q	187	
17	S	245	
18	U	198	
19	V	123	
20	X	253	
21	Y	244	
22	Z	254	
23	a	752	
24	b	734	
25	c	81	

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Mol	Chain	Length	Quality of chain
26	d	142	91% 7%
27	e	131	44% 5% 52%
28	f	184	72% 14% 12%
29	i	36	78% 8% 14%
30	j	40	82% 18%
31	k	112	55% 7% 38%
32	l	145	92% 6%
33	m	30	80% 20%
34	o	273	76% 10% 14%
35	p	255	38% 79% 10% 11%
35	u	255	80% 9% 11%
35	x	255	77% 13% 11%
36	q	268	77% 11% 11%
36	v	268	76% 12% 11%
37	r	133	63% 5% 32%
38	t	260	31% 73% 8% 19%
38	w	260	52% 73% 8% 19%
38	y	260	22% 73% 23%
39	z	257	81% 6% 14%

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
40	CLA	A	301	X	-	-	-
40	CLA	A	302	X	-	-	-
40	CLA	A	303	X	-	-	-
40	CLA	A	304	X	-	-	-
40	CLA	A	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	A	306	X	-	-	-
40	CLA	A	307	X	-	-	-
40	CLA	A	308	X	-	-	-
40	CLA	A	309	X	-	-	-
40	CLA	A	311	X	-	-	-
40	CLA	B	301	X	-	-	-
40	CLA	B	302	X	-	-	-
40	CLA	B	303	X	-	-	-
40	CLA	B	304	X	-	-	-
40	CLA	B	306	X	-	-	-
40	CLA	B	307	X	-	-	-
40	CLA	C	301	X	-	-	-
40	CLA	C	302	X	-	-	-
40	CLA	C	304	X	-	-	-
40	CLA	C	305	X	-	-	-
40	CLA	C	306	X	-	-	-
40	CLA	C	307	X	-	-	-
40	CLA	C	308	X	-	-	-
40	CLA	C	309	X	-	-	-
40	CLA	D	301	X	-	-	-
40	CLA	D	302	X	-	-	-
40	CLA	D	303	X	-	-	-
40	CLA	D	304	X	-	-	-
40	CLA	D	305	X	-	-	-
40	CLA	D	306	X	-	-	-
40	CLA	D	307	X	-	-	-
40	CLA	D	308	X	-	-	-
40	CLA	D	309	X	-	-	-
40	CLA	D	310	X	-	-	-
40	CLA	D	311	X	-	-	-
40	CLA	D	312	X	-	-	-
40	CLA	E	302	X	-	-	-
40	CLA	E	303	X	-	-	-
40	CLA	E	304	X	-	-	-
40	CLA	E	305	X	-	-	-
40	CLA	E	306	X	-	-	-
40	CLA	E	307	X	-	-	-
40	CLA	E	308	X	-	-	-
40	CLA	E	309	X	-	-	-
40	CLA	E	310	X	-	-	-
40	CLA	E	311	X	-	-	-
40	CLA	E	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	E	313	X	-	-	-
40	CLA	E	314	X	-	-	-
40	CLA	F	301	X	-	-	-
40	CLA	F	303	X	-	-	-
40	CLA	F	304	X	-	-	-
40	CLA	F	305	X	-	-	-
40	CLA	F	306	X	-	-	-
40	CLA	F	307	X	-	-	-
40	CLA	F	308	X	-	-	-
40	CLA	F	310	X	-	-	-
40	CLA	F	311	X	-	-	-
40	CLA	F	321	X	-	-	-
40	CLA	G	201	X	-	-	-
40	CLA	G	203	X	-	-	-
40	CLA	G	204	X	-	-	-
40	CLA	G	205	X	-	-	-
40	CLA	G	206	X	-	-	-
40	CLA	G	207	X	-	-	-
40	CLA	G	213	X	-	-	-
40	CLA	H	301	X	-	-	-
40	CLA	H	302	X	-	-	-
40	CLA	H	304	X	-	-	-
40	CLA	H	305	X	-	-	-
40	CLA	H	306	X	-	-	-
40	CLA	H	307	X	-	-	-
40	CLA	H	308	X	-	-	-
40	CLA	H	309	X	-	-	-
40	CLA	H	310	X	-	-	-
40	CLA	H	311	X	-	-	-
40	CLA	I	201	X	-	-	-
40	CLA	I	202	X	-	-	-
40	CLA	I	203	X	-	-	-
40	CLA	I	204	X	-	-	-
40	CLA	I	205	X	-	-	-
40	CLA	I	206	X	-	-	-
40	CLA	I	207	X	-	-	-
40	CLA	I	208	X	-	-	-
40	CLA	J	302	X	-	-	-
40	CLA	J	303	X	-	-	-
40	CLA	J	305	X	-	-	-
40	CLA	J	306	X	-	-	-
40	CLA	J	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	J	308	X	-	-	-
40	CLA	J	309	X	-	-	-
40	CLA	J	310	X	-	-	-
40	CLA	J	311	X	-	-	-
40	CLA	J	312	X	-	-	-
40	CLA	J	318	X	-	-	-
40	CLA	K	301	X	-	-	-
40	CLA	K	304	X	-	-	-
40	CLA	K	306	X	-	-	-
40	CLA	K	307	X	-	-	-
40	CLA	K	308	X	-	-	-
40	CLA	K	312	X	-	-	-
40	CLA	L	301	X	-	-	-
40	CLA	L	304	X	-	-	-
40	CLA	L	305	X	-	-	-
40	CLA	L	306	X	-	-	-
40	CLA	L	307	X	-	-	-
40	CLA	L	310	X	-	-	-
40	CLA	L	311	X	-	-	-
40	CLA	L	312	X	-	-	-
40	CLA	M	304	X	-	-	-
40	CLA	M	305	X	-	-	-
40	CLA	M	306	X	-	-	-
40	CLA	M	307	X	-	-	-
40	CLA	M	310	X	-	-	-
40	CLA	M	311	X	-	-	-
40	CLA	M	312	X	-	-	-
40	CLA	N	304	X	-	-	-
40	CLA	N	305	X	-	-	-
40	CLA	N	306	X	-	-	-
40	CLA	N	307	X	-	-	-
40	CLA	N	310	X	-	-	-
40	CLA	N	311	X	-	-	-
40	CLA	O	304	X	-	-	-
40	CLA	O	305	X	-	-	-
40	CLA	O	306	X	-	-	-
40	CLA	O	307	X	-	-	-
40	CLA	O	310	X	-	-	-
40	CLA	O	316	X	-	-	-
40	CLA	P	305	X	-	-	-
40	CLA	P	306	X	-	-	-
40	CLA	P	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	P	308	X	-	-	-
40	CLA	P	311	X	-	-	-
40	CLA	P	312	X	-	-	-
40	CLA	P	313	X	-	-	-
40	CLA	Q	202	X	-	-	-
40	CLA	Q	203	X	-	-	-
40	CLA	Q	204	X	-	-	-
40	CLA	Q	205	X	-	-	-
40	CLA	Q	206	X	-	-	-
40	CLA	Q	207	X	-	-	-
40	CLA	Q	208	X	-	-	-
40	CLA	Q	209	X	-	-	-
40	CLA	R	304	X	-	-	-
40	CLA	R	305	X	-	-	-
40	CLA	R	306	X	-	-	-
40	CLA	R	307	X	-	-	-
40	CLA	R	310	X	-	-	-
40	CLA	R	316	X	-	-	-
40	CLA	S	301	X	-	-	-
40	CLA	S	302	X	-	-	-
40	CLA	S	305	X	-	-	-
40	CLA	S	306	X	-	-	-
40	CLA	S	307	X	-	-	-
40	CLA	S	308	X	-	-	-
40	CLA	S	311	X	-	-	-
40	CLA	S	312	X	-	-	-
40	CLA	S	313	X	-	-	-
40	CLA	S	314	X	-	-	-
40	CLA	S	319	X	-	-	-
40	CLA	T	304	X	-	-	-
40	CLA	T	305	X	-	-	-
40	CLA	T	306	X	-	-	-
40	CLA	T	307	X	-	-	-
40	CLA	T	310	X	-	-	-
40	CLA	T	317	X	-	-	-
40	CLA	U	202	X	-	-	-
40	CLA	U	203	X	-	-	-
40	CLA	U	204	X	-	-	-
40	CLA	U	205	X	-	-	-
40	CLA	U	206	X	-	-	-
40	CLA	U	207	X	-	-	-
40	CLA	U	208	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	V	201	X	-	-	-
40	CLA	V	202	X	-	-	-
40	CLA	W	305	X	-	-	-
40	CLA	W	306	X	-	-	-
40	CLA	W	307	X	-	-	-
40	CLA	W	308	X	-	-	-
40	CLA	W	311	X	-	-	-
40	CLA	W	312	X	-	-	-
40	CLA	W	313	X	-	-	-
40	CLA	X	301	X	-	-	-
40	CLA	X	304	X	-	-	-
40	CLA	X	305	X	-	-	-
40	CLA	X	306	X	-	-	-
40	CLA	X	307	X	-	-	-
40	CLA	X	310	X	-	-	-
40	CLA	X	311	X	-	-	-
40	CLA	X	312	X	-	-	-
40	CLA	X	313	X	-	-	-
40	CLA	Y	301	X	-	-	-
40	CLA	Y	304	X	-	-	-
40	CLA	Y	305	X	-	-	-
40	CLA	Y	306	X	-	-	-
40	CLA	Y	307	X	-	-	-
40	CLA	Y	310	X	-	-	-
40	CLA	Y	311	X	-	-	-
40	CLA	Y	312	X	-	-	-
40	CLA	Y	313	X	-	-	-
40	CLA	Z	301	X	-	-	-
40	CLA	Z	304	X	-	-	-
40	CLA	Z	305	X	-	-	-
40	CLA	Z	306	X	-	-	-
40	CLA	Z	307	X	-	-	-
40	CLA	Z	310	X	-	-	-
40	CLA	Z	311	X	-	-	-
40	CLA	Z	312	X	-	-	-
40	CLA	Z	313	X	-	-	-
40	CLA	a	803	X	-	-	-
40	CLA	a	804	X	-	-	-
40	CLA	a	805	X	-	-	-
40	CLA	a	806	X	-	-	-
40	CLA	a	807	X	-	-	-
40	CLA	a	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	a	809	X	-	-	-
40	CLA	a	810	X	-	-	-
40	CLA	a	811	X	-	-	-
40	CLA	a	812	X	-	-	-
40	CLA	a	813	X	-	-	-
40	CLA	a	814	X	-	-	-
40	CLA	a	815	X	-	-	-
40	CLA	a	816	X	-	-	-
40	CLA	a	817	X	-	-	-
40	CLA	a	818	X	-	-	-
40	CLA	a	819	X	-	X	-
40	CLA	a	820	X	-	-	-
40	CLA	a	821	X	-	-	-
40	CLA	a	822	X	-	-	-
40	CLA	a	823	X	-	-	-
40	CLA	a	824	X	-	-	-
40	CLA	a	825	X	-	-	-
40	CLA	a	826	X	-	-	-
40	CLA	a	827	X	-	-	-
40	CLA	a	828	X	-	-	-
40	CLA	a	829	X	-	-	-
40	CLA	a	830	X	-	-	-
40	CLA	a	831	X	-	-	-
40	CLA	a	832	X	-	-	-
40	CLA	a	833	X	-	-	-
40	CLA	a	834	X	-	-	-
40	CLA	a	835	X	-	-	-
40	CLA	a	836	X	-	-	-
40	CLA	a	837	X	-	-	-
40	CLA	a	838	X	-	-	-
40	CLA	a	839	X	-	-	-
40	CLA	a	840	X	-	-	-
40	CLA	a	841	X	-	-	-
40	CLA	a	842	X	-	-	-
40	CLA	a	850	X	-	-	-
40	CLA	a	851	X	-	-	-
40	CLA	a	852	X	-	-	-
40	CLA	b	801	X	-	-	-
40	CLA	b	802	X	-	-	-
40	CLA	b	803	X	-	-	-
40	CLA	b	805	X	-	-	-
40	CLA	b	806	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	b	807	X	-	-	-
40	CLA	b	808	X	-	-	-
40	CLA	b	809	X	-	-	-
40	CLA	b	810	X	-	-	-
40	CLA	b	811	X	-	-	-
40	CLA	b	812	X	-	-	-
40	CLA	b	813	X	-	-	-
40	CLA	b	814	X	-	-	-
40	CLA	b	815	X	-	-	-
40	CLA	b	816	X	-	-	-
40	CLA	b	817	X	-	-	-
40	CLA	b	818	X	-	-	-
40	CLA	b	819	X	-	-	-
40	CLA	b	820	X	-	-	-
40	CLA	b	821	X	-	-	-
40	CLA	b	822	X	-	-	-
40	CLA	b	823	X	-	-	-
40	CLA	b	824	X	-	-	-
40	CLA	b	825	X	-	-	-
40	CLA	b	826	X	-	-	-
40	CLA	b	827	X	-	-	-
40	CLA	b	828	X	-	-	-
40	CLA	b	829	X	-	-	-
40	CLA	b	830	X	-	-	-
40	CLA	b	831	X	-	-	-
40	CLA	b	832	X	-	-	-
40	CLA	b	833	X	-	-	-
40	CLA	b	834	X	-	-	-
40	CLA	b	835	X	-	-	-
40	CLA	b	836	X	-	-	-
40	CLA	b	837	X	-	-	-
40	CLA	b	838	X	-	-	-
40	CLA	b	839	X	-	-	-
40	CLA	b	840	X	-	-	-
40	CLA	b	841	X	-	-	-
40	CLA	b	842	X	-	-	-
40	CLA	f	201	X	-	-	-
40	CLA	f	202	X	-	-	-
40	CLA	f	204	X	-	-	-
40	CLA	f	205	X	-	-	-
40	CLA	i	101	X	-	-	-
40	CLA	j	102	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	k	201	X	-	-	-
40	CLA	k	202	X	-	-	-
40	CLA	l	202	X	-	-	-
40	CLA	l	203	X	-	-	-
40	CLA	l	204	X	-	-	-
40	CLA	l	205	X	-	-	-
40	CLA	o	301	X	-	-	-
40	CLA	o	304	X	-	-	-
40	CLA	o	305	X	-	-	-
40	CLA	o	306	X	-	-	-
40	CLA	o	307	X	-	-	-
40	CLA	o	310	X	-	-	-
40	CLA	o	311	X	-	-	-
40	CLA	o	312	X	-	-	-
40	CLA	o	313	X	-	-	-
40	CLA	p	302	X	-	-	-
40	CLA	p	305	X	-	-	-
40	CLA	p	306	X	-	-	-
40	CLA	p	307	X	-	-	-
40	CLA	p	308	X	-	-	-
40	CLA	p	311	X	-	-	-
40	CLA	p	312	X	-	-	-
40	CLA	p	313	X	-	-	-
40	CLA	p	314	X	-	-	-
40	CLA	q	301	X	-	-	-
40	CLA	q	304	X	-	-	-
40	CLA	q	305	X	-	-	-
40	CLA	q	306	X	-	-	-
40	CLA	q	307	X	-	-	-
40	CLA	q	310	X	-	-	-
40	CLA	q	311	X	-	-	-
40	CLA	q	312	X	-	-	-
40	CLA	q	313	X	-	-	-
40	CLA	t	302	X	-	-	-
40	CLA	t	303	X	-	-	-
40	CLA	t	304	X	-	-	-
40	CLA	t	305	X	-	-	-
40	CLA	t	307	X	-	-	-
40	CLA	t	309	X	-	-	-
40	CLA	u	302	X	-	-	-
40	CLA	u	305	X	-	-	-
40	CLA	u	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	u	307	X	-	-	-
40	CLA	u	308	X	-	-	-
40	CLA	u	311	X	-	-	-
40	CLA	u	312	X	-	-	-
40	CLA	u	313	X	-	-	-
40	CLA	u	314	X	-	-	-
40	CLA	v	301	X	-	-	-
40	CLA	v	304	X	-	-	-
40	CLA	v	305	X	-	-	-
40	CLA	v	306	X	-	-	-
40	CLA	v	307	X	-	-	-
40	CLA	v	310	X	-	-	-
40	CLA	v	311	X	-	-	-
40	CLA	v	312	X	-	-	-
40	CLA	v	313	X	-	-	-
40	CLA	w	302	X	-	-	-
40	CLA	w	303	X	-	-	-
40	CLA	w	304	X	-	-	-
40	CLA	w	305	X	-	-	-
40	CLA	w	308	X	-	-	-
40	CLA	w	309	X	-	-	-
40	CLA	x	302	X	-	-	-
40	CLA	x	305	X	-	-	-
40	CLA	x	306	X	-	-	-
40	CLA	x	307	X	-	-	-
40	CLA	x	308	X	-	-	-
40	CLA	x	311	X	-	-	-
40	CLA	x	312	X	-	-	-
40	CLA	x	313	X	-	-	-
40	CLA	x	314	X	-	-	-
40	CLA	y	302	X	-	-	-
40	CLA	y	303	X	-	-	-
40	CLA	y	304	X	-	-	-
40	CLA	y	305	X	-	-	-
40	CLA	y	308	X	-	-	-
40	CLA	y	309	X	-	-	-
40	CLA	z	302	X	-	-	-
40	CLA	z	305	X	-	-	-
40	CLA	z	306	X	-	-	-
40	CLA	z	307	X	-	-	-
40	CLA	z	308	X	-	-	-
40	CLA	z	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CLA	z	312	X	-	-	-
40	CLA	z	313	X	-	-	-
40	CLA	z	314	X	-	-	-
40	CLA	z	324	X	-	-	-
42	DD6	P	315	X	-	-	-
42	DD6	t	312	-	-	X	-
42	DD6	w	312	-	-	X	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 110086 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 Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	183	1419	916	229	264	10	0	0

- Molecule 2 is a protein called EFCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	148	1108	711	186	205	6	0	0

- Molecule 3 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	178	1352	874	225	244	9	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	103	ALA	VAL	conflict	UNP A0A6V2SE28
C	104	GLU	ASP	conflict	UNP A0A6V2SE28

- Molecule 4 is a protein called EFCPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	188	1446	943	232	265	6	1	0

- Molecule 5 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	187	1383	896	222	257	8	0	0

- Molecule 6 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	188	Total	C	N	O	S	0	0
			1414	909	244	252	9		

- Molecule 7 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	168	Total	C	N	O	S	0	0
			1248	803	206	231	8		

- Molecule 8 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	167	Total	C	N	O	S	0	0
			1251	802	205	232	12		

- Molecule 9 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	155	Total	C	N	O	S	0	0
			1195	773	199	214	9		

- Molecule 10 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	166	Total	C	N	O	S	0	0
			1231	783	216	225	7		

- Molecule 11 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	171	Total	C	N	O	S	0	0
			1333	868	226	232	7		

- Molecule 12 is a protein called EFCPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	189	Total	C	N	O	S	0	0
			1419	927	236	250	6		

- Molecule 13 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	193	Total	C	N	O	S	0	0
			1455	940	247	263	5		
13	P	193	Total	C	N	O	S	0	0
			1455	940	247	263	5		
13	W	193	Total	C	N	O	S	0	0
			1455	940	247	263	5		

- Molecule 14 is a protein called EFCPI-17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	194	Total	C	N	O	S	0	0
			1454	943	245	257	9		

- Molecule 15 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	179	Total	C	N	O	S	0	0
			1325	858	221	240	6		
15	R	179	Total	C	N	O	S	0	0
			1325	858	221	240	6		
15	T	179	Total	C	N	O	S	0	0
			1325	858	221	240	6		

- Molecule 16 is a protein called EFCPI-18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	156	Total	C	N	O	S	0	0
			1192	763	202	219	8		

- Molecule 17 is a protein called EFCPI-22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	210	Total	C	N	O	S	0	0
			1640	1082	264	288	6		

- Molecule 18 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	144	Total	C	N	O	S	0	0
			1130	728	190	206	6		

- Molecule 19 is a protein called LEFP.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	47	Total	C	N	O	S	0	0
			351	225	59	65	2		

- Molecule 20 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	211	Total	C	N	O	S	0	0
			1643	1069	273	294	7		

- Molecule 21 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	213	Total	C	N	O	S	0	0
			1660	1090	278	284	8		

- Molecule 22 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	219	Total	C	N	O	S	0	0
			1714	1121	279	309	5		

- Molecule 23 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	741	Total	C	N	O	S	0	0
			5832	3815	993	994	30		

- Molecule 24 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	731	Total	C	N	O	S	0	0
			5807	3822	980	984	21		

- Molecule 25 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	80	Total	C	N	O	S	0	0
			597	365	105	116	11		

- Molecule 26 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	140	Total	C	N	O	S	0	0
			1103	710	184	206	3		

- Molecule 27 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	63	Total	C	N	O	S	0	0
			493	313	86	93	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	81	ALA	PRO	conflict	UNP R1EZZ6
e	85	THR	PRO	conflict	UNP R1EZZ6

- Molecule 28 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	161	Total	C	N	O	S	0	0
			1238	800	210	224	4		

- Molecule 29 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	i	31	Total	C	N	O	S	0	0
			243	170	32	40	1		

- Molecule 30 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	j	40	Total	C	N	O	S	0	0
			317	211	47	56	3		

- Molecule 31 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	k	70	Total	C	N	O	S	0	0
			510	331	83	90	6		

- Molecule 32 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	l	143	Total	C	N	O	S	0	0
			1084	716	172	195	1		

- Molecule 33 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	m	30	Total	C	N	O	S	0	0
			224	149	35	38	2		

- Molecule 34 is a protein called EFCPI-30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	o	236	Total	C	N	O	S	0	0
			1760	1142	290	318	10		

- Molecule 35 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	p	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		
35	u	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		
35	x	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		

- Molecule 36 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	q	238	Total	C	N	O	S	0	0
			1790	1163	296	323	8		
36	v	238	Total	C	N	O	S	0	0
			1790	1163	296	323	8		

- Molecule 37 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	r	91	Total	C	N	O	S	0	0
			681	443	111	126	1		

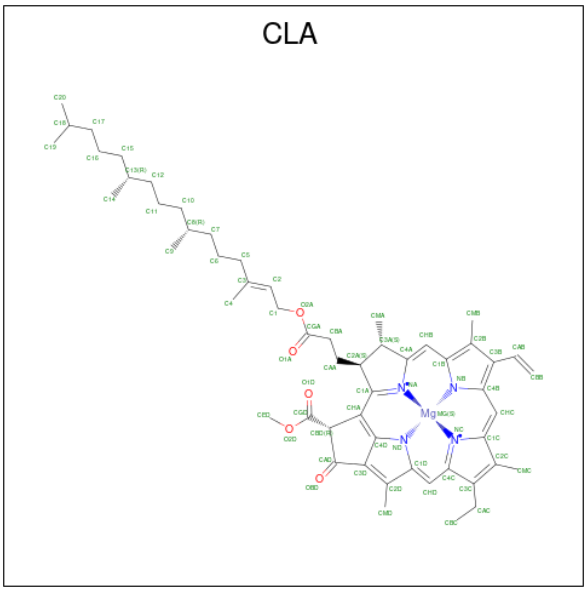
- Molecule 38 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	t	211	Total	C	N	O	S	0	0
			1631	1057	272	295	7		
38	w	211	Total	C	N	O	S	0	0
			1631	1057	272	295	7		
38	y	201	Total	C	N	O	S	0	0
			1546	1001	261	277	7		

- Molecule 39 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	z	222	Total	C	N	O	S	0	0
			1718	1126	280	307	5		

- Molecule 40 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
40	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
40	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
40	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	C	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	C	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	C	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
40	C	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	C	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	C	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	C	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	D	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	D	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	D	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	D	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
40	D	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
40	D	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	D	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	D	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
40	D	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	D	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	D	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	E	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	E	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	E	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	E	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	E	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	E	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
40	E	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	E	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
40	E	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	E	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	E	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	F	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
40	F	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
40	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	F	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	F	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	F	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
40	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	F	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	F	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	F	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	G	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
40	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
40	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
40	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
40	G	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	H	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
40	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	H	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
40	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	I	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	I	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
40	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	I	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	J	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	J	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	J	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	J	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
40	J	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	J	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	J	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	J	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	J	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	J	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
40	J	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	K	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	K	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
40	K	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
40	K	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	L	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	L	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
40	L	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	L	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	L	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	L	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	L	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	M	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	M	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	M	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
40	M	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	M	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
40	M	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
40	M	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	N	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
40	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	O	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	O	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	O	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
40	O	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	O	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	P	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	P	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	P	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	Q	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
40	Q	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
40	Q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
40	Q	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
40	Q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	Q	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	Q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	Q	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	R	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
40	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	R	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	R	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	S	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	S	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
40	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
40	S	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	S	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	S	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	S	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	T	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
40	T	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	T	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	T	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
40	T	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	U	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	U	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	U	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	U	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	U	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	U	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	V	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
40	V	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	X	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	X	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
40	X	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	X	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	X	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
40	X	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	X	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	Y	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	Y	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	Y	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	Y	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	Z	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
40	Z	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	Z	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
40	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	f	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	f	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	i	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	j	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	k	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	k	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	l	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
40	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	o	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	o	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	o	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	o	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	o	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	o	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	o	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
40	o	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	o	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	p	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	p	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	p	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	p	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	p	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	q	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
40	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	q	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
40	q	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
40	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	q	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	t	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	t	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	t	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	t	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
40	t	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	t	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	u	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	u	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	u	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	u	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	u	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	v	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	v	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
40	v	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	v	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	v	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	v	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
40	v	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
40	v	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	v	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	w	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	w	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	w	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	w	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
40	w	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	w	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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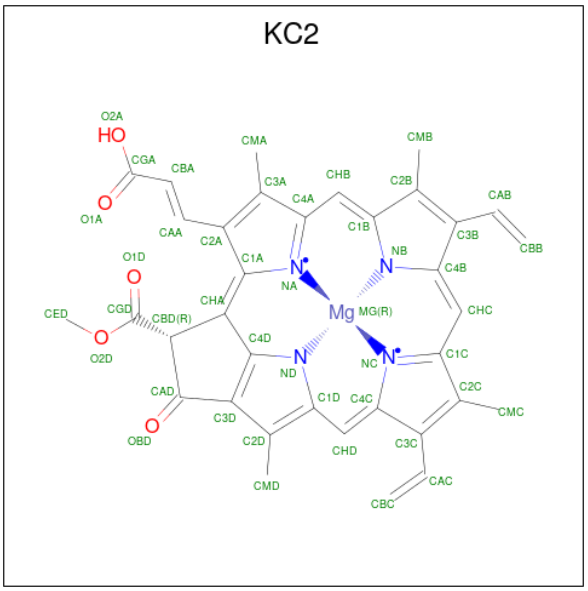
Mol	Chain	Residues	Atoms					AltConf
40	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	x	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
40	x	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	x	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	x	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	x	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	x	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	x	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	x	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	y	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	y	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	y	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
40	y	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	z	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	z	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	z	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

- Molecule 41 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
41	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
41	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
41	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
41	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
41	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	o	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	o	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	o	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	o	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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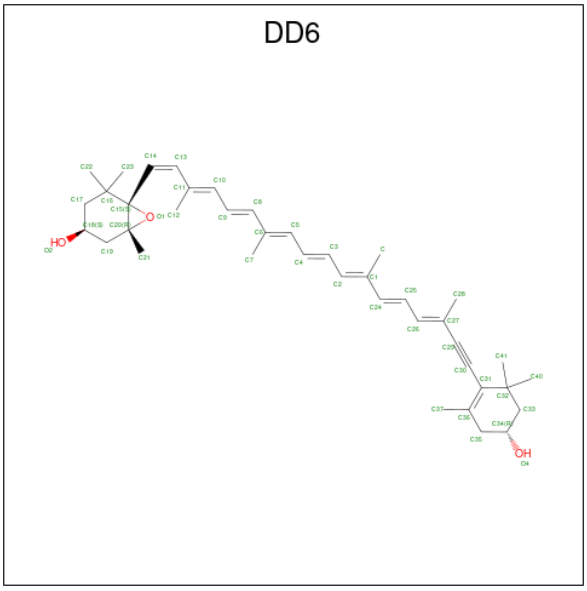
Mol	Chain	Residues	Atoms					AltConf
41	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	t	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	w	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	w	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	w	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
41	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 42 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
42	A	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
42	A	1	Total	C	O	0
			43	40	3	
42	A	1	Total	C	O	0
			43	40	3	
42	A	1	Total	C	O	0
			43	40	3	
42	A	1	Total	C	O	0
			43	40	3	
42	B	1	Total	C	O	0
			43	40	3	
42	C	1	Total	C	O	0
			43	40	3	
42	C	1	Total	C	O	0
			43	40	3	
42	C	1	Total	C	O	0
			43	40	3	
42	D	1	Total	C	O	0
			43	40	3	
42	D	1	Total	C	O	0
			43	40	3	
42	D	1	Total	C	O	0
			43	40	3	
42	D	1	Total	C	O	0
			43	40	3	
42	D	1	Total	C	O	0
			43	40	3	
42	E	1	Total	C	O	0
			43	40	3	
42	E	1	Total	C	O	0
			43	40	3	
42	E	1	Total	C	O	0
			43	40	3	
42	E	1	Total	C	O	0
			43	40	3	
42	F	1	Total	C	O	0
			43	40	3	
42	F	1	Total	C	O	0
			43	40	3	
42	F	1	Total	C	O	0
			43	40	3	
42	G	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
42	H	1	Total	C	O	0
			43	40	3	
42	H	1	Total	C	O	0
			43	40	3	
42	H	1	Total	C	O	0
			43	40	3	
42	I	1	Total	C	O	0
			43	40	3	
42	I	1	Total	C	O	0
			43	40	3	
42	I	1	Total	C	O	0
			43	40	3	
42	I	1	Total	C	O	0
			43	40	3	
42	J	1	Total	C	O	0
			43	40	3	
42	J	1	Total	C	O	0
			43	40	3	
42	J	1	Total	C	O	0
			43	40	3	
42	J	1	Total	C	O	0
			43	40	3	
42	J	1	Total	C	O	0
			43	40	3	
42	J	1	Total	C	O	0
			43	40	3	
42	K	1	Total	C	O	0
			43	40	3	
42	K	1	Total	C	O	0
			43	40	3	
42	L	1	Total	C	O	0
			43	40	3	
42	L	1	Total	C	O	0
			43	40	3	
42	M	1	Total	C	O	0
			43	40	3	
42	N	1	Total	C	O	0
			43	40	3	
42	N	1	Total	C	O	0
			43	40	3	
42	N	1	Total	C	O	0
			43	40	3	

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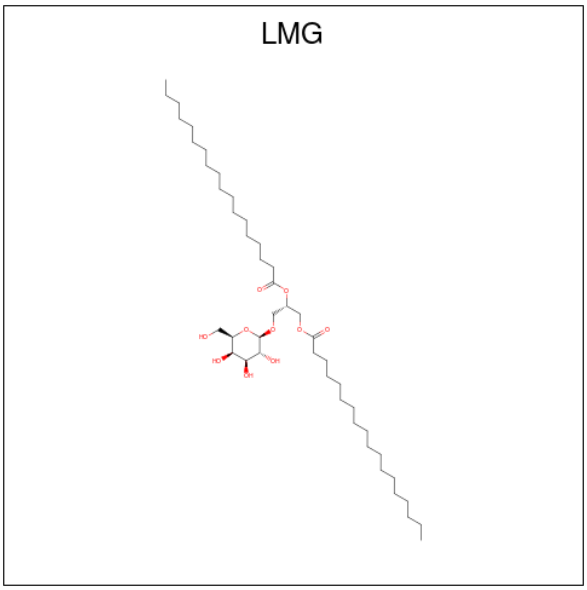
Mol	Chain	Residues	Atoms			AltConf
42	O	1	Total	C	O	0
			43	40	3	
42	P	1	Total	C	O	0
			43	40	3	
42	Q	1	Total	C	O	0
			43	40	3	
42	Q	1	Total	C	O	0
			43	40	3	
42	Q	1	Total	C	O	0
			43	40	3	
42	Q	1	Total	C	O	0
			43	40	3	
42	R	1	Total	C	O	0
			43	40	3	
42	T	1	Total	C	O	0
			43	40	3	
42	U	1	Total	C	O	0
			43	40	3	
42	U	1	Total	C	O	0
			43	40	3	
42	W	1	Total	C	O	0
			43	40	3	
42	X	1	Total	C	O	0
			43	40	3	
42	Y	1	Total	C	O	0
			43	40	3	
42	Z	1	Total	C	O	0
			43	40	3	
42	j	1	Total	C	O	0
			43	40	3	
42	k	1	Total	C	O	0
			43	40	3	
42	o	1	Total	C	O	0
			43	40	3	
42	o	1	Total	C	O	0
			43	40	3	
42	p	1	Total	C	O	0
			43	40	3	
42	q	1	Total	C	O	0
			43	40	3	
42	q	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms	AltConf
42	t	1	Total C O 43 40 3	0
42	u	1	Total C O 43 40 3	0
42	v	1	Total C O 43 40 3	0
42	v	1	Total C O 43 40 3	0
42	w	1	Total C O 43 40 3	0
42	x	1	Total C O 43 40 3	0
42	y	1	Total C O 43 40 3	0
42	z	1	Total C O 43 40 3	0
42	z	1	Total C O 43 40 3	0

- Molecule 43 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



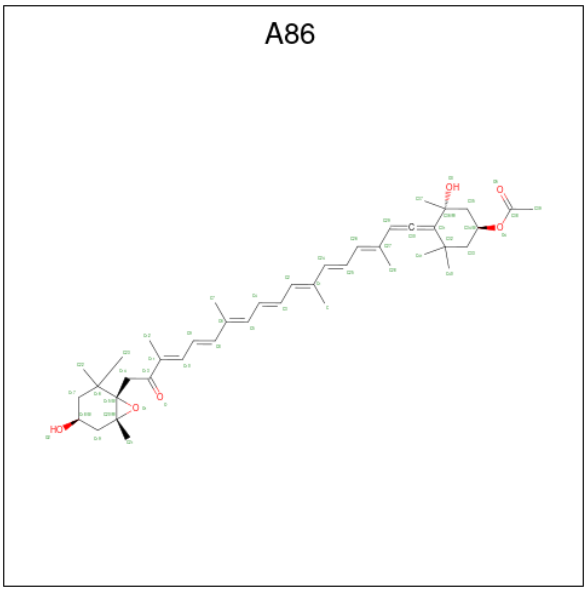
Mol	Chain	Residues	Atoms	AltConf
43	A	1	Total C O 40 30 10	0
43	D	1	Total C O 40 30 10	0

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Mol	Chain	Residues	Atoms			AltConf
43	E	1	Total	C	O	0
			31	21	10	
43	E	1	Total	C	O	0
			31	21	10	
43	E	1	Total	C	O	0
			40	30	10	
43	F	1	Total	C	O	0
			39	29	10	
43	L	1	Total	C	O	0
			37	27	10	
43	M	1	Total	C	O	0
			39	29	10	
43	P	1	Total	C	O	0
			39	29	10	
43	S	1	Total	C	O	0
			39	29	10	
43	T	1	Total	C	O	0
			40	30	10	
43	W	1	Total	C	O	0
			39	29	10	
43	a	1	Total	C	O	0
			35	25	10	
43	a	1	Total	C	O	0
			35	25	10	
43	j	1	Total	C	O	0
			30	20	10	
43	l	1	Total	C	O	0
			39	29	10	
43	p	1	Total	C	O	0
			39	29	10	
43	u	1	Total	C	O	0
			39	29	10	
43	x	1	Total	C	O	0
			39	29	10	

- Molecule 44 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (CCD ID: A86) (formula: $C_{42}H_{58}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
44	C	1	Total C O 48 42 6	0
44	D	1	Total C O 48 42 6	0
44	D	1	Total C O 48 42 6	0
44	F	1	Total C O 48 42 6	0
44	F	1	Total C O 48 42 6	0
44	F	1	Total C O 48 42 6	0
44	G	1	Total C O 48 42 6	0
44	G	1	Total C O 48 42 6	0
44	H	1	Total C O 48 42 6	0
44	K	1	Total C O 48 42 6	0
44	L	1	Total C O 48 42 6	0
44	M	1	Total C O 48 42 6	0
44	M	1	Total C O 48 42 6	0
44	M	1	Total C O 48 42 6	0

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Mol	Chain	Residues	Atoms			AltConf
44	M	1	Total	C	O	0
			48	42	6	
44	N	1	Total	C	O	0
			48	42	6	
44	N	1	Total	C	O	0
			48	42	6	
44	N	1	Total	C	O	0
			48	42	6	
44	N	1	Total	C	O	0
			48	42	6	
44	O	1	Total	C	O	0
			48	42	6	
44	O	1	Total	C	O	0
			48	42	6	
44	O	1	Total	C	O	0
			48	42	6	
44	P	1	Total	C	O	0
			48	42	6	
44	P	1	Total	C	O	0
			48	42	6	
44	P	1	Total	C	O	0
			48	42	6	
44	P	1	Total	C	O	0
			48	42	6	
44	Q	1	Total	C	O	0
			48	42	6	
44	Q	1	Total	C	O	0
			48	42	6	
44	R	1	Total	C	O	0
			48	42	6	
44	R	1	Total	C	O	0
			48	42	6	
44	R	1	Total	C	O	0
			48	42	6	
44	S	1	Total	C	O	0
			48	42	6	
44	S	1	Total	C	O	0
			48	42	6	
44	S	1	Total	C	O	0
			48	42	6	
44	S	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
44	T	1	Total	C	O	0
			48	42	6	
44	T	1	Total	C	O	0
			48	42	6	
44	T	1	Total	C	O	0
			48	42	6	
44	T	1	Total	C	O	0
			48	42	6	
44	U	1	Total	C	O	0
			48	42	6	
44	W	1	Total	C	O	0
			48	42	6	
44	W	1	Total	C	O	0
			48	42	6	
44	W	1	Total	C	O	0
			48	42	6	
44	X	1	Total	C	O	0
			48	42	6	
44	X	1	Total	C	O	0
			48	42	6	
44	X	1	Total	C	O	0
			48	42	6	
44	X	1	Total	C	O	0
			48	42	6	
44	X	1	Total	C	O	0
			48	42	6	
44	X	1	Total	C	O	0
			48	42	6	
44	X	1	Total	C	O	0
			48	42	6	
44	X	1	Total	C	O	0
			48	42	6	
44	Y	1	Total	C	O	0
			48	42	6	
44	Y	1	Total	C	O	0
			48	42	6	
44	Y	1	Total	C	O	0
			48	42	6	
44	Y	1	Total	C	O	0
			48	42	6	
44	Y	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms	AltConf
44	Y	1	Total C O 48 42 6	0
44	Y	1	Total C O 48 42 6	0
44	Z	1	Total C O 48 42 6	0
44	Z	1	Total C O 48 42 6	0
44	Z	1	Total C O 48 42 6	0
44	Z	1	Total C O 48 42 6	0
44	o	1	Total C O 48 42 6	0
44	o	1	Total C O 48 42 6	0
44	o	1	Total C O 48 42 6	0
44	o	1	Total C O 48 42 6	0
44	o	1	Total C O 48 42 6	0
44	p	1	Total C O 48 42 6	0
44	p	1	Total C O 48 42 6	0
44	p	1	Total C O 48 42 6	0
44	p	1	Total C O 48 42 6	0
44	p	1	Total C O 48 42 6	0
44	p	1	Total C O 48 42 6	0
44	q	1	Total C O 48 42 6	0
44	q	1	Total C O 48 42 6	0
44	q	1	Total C O 48 42 6	0
44	q	1	Total C O 48 42 6	0

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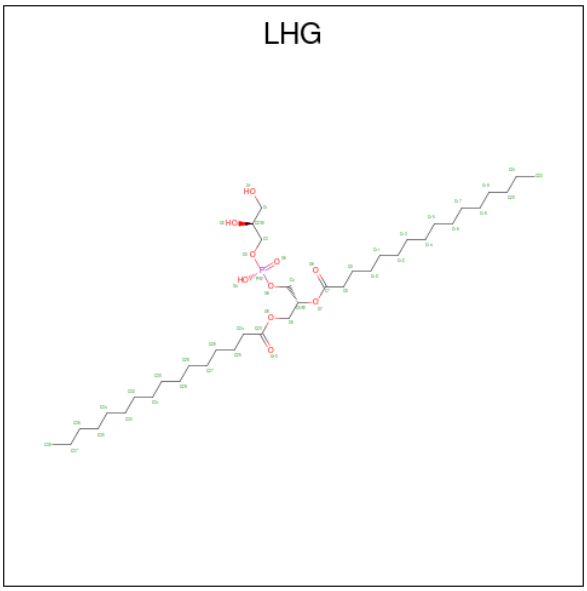
Mol	Chain	Residues	Atoms			AltConf
44	q	1	Total	C	O	0
			48	42	6	
44	q	1	Total	C	O	0
			48	42	6	
44	t	1	Total	C	O	0
			48	42	6	
44	t	1	Total	C	O	0
			48	42	6	
44	t	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			48	42	6	
44	v	1	Total	C	O	0
			48	42	6	
44	v	1	Total	C	O	0
			48	42	6	
44	v	1	Total	C	O	0
			48	42	6	
44	v	1	Total	C	O	0
			48	42	6	
44	v	1	Total	C	O	0
			48	42	6	
44	v	1	Total	C	O	0
			48	42	6	
44	w	1	Total	C	O	0
			48	42	6	
44	w	1	Total	C	O	0
			48	42	6	
44	w	1	Total	C	O	0
			48	42	6	
44	w	1	Total	C	O	0
			48	42	6	
44	x	1	Total	C	O	0
			48	42	6	

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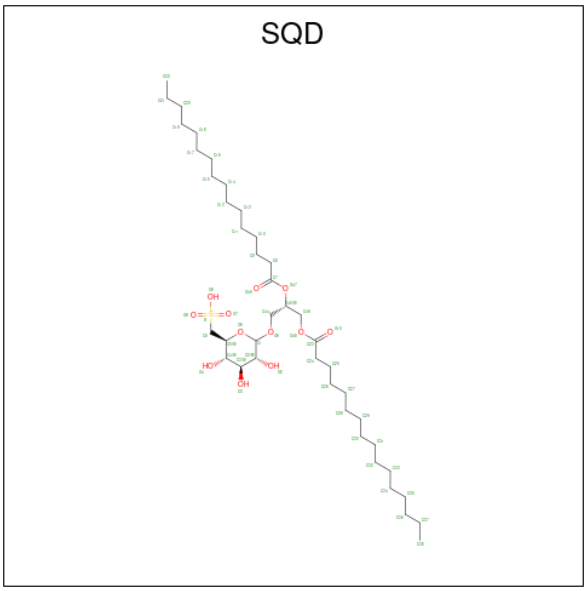
Mol	Chain	Residues	Atoms	AltConf
44	x	1	Total C O 48 42 6	0
44	x	1	Total C O 48 42 6	0
44	x	1	Total C O 48 42 6	0
44	y	1	Total C O 48 42 6	0
44	z	1	Total C O 48 42 6	0
44	z	1	Total C O 48 42 6	0
44	z	1	Total C O 48 42 6	0
44	z	1	Total C O 48 42 6	0
44	z	1	Total C O 48 42 6	0
44	z	1	Total C O 48 42 6	0
44	z	1	Total C O 48 42 6	0

- Molecule 45 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
45	F	1	Total	C	O	P	0
			40	29	10	1	
45	S	1	Total	C	O	P	0
			40	29	10	1	
45	a	1	Total	C	O	P	0
			48	37	10	1	
45	a	1	Total	C	O	P	0
			30	19	10	1	

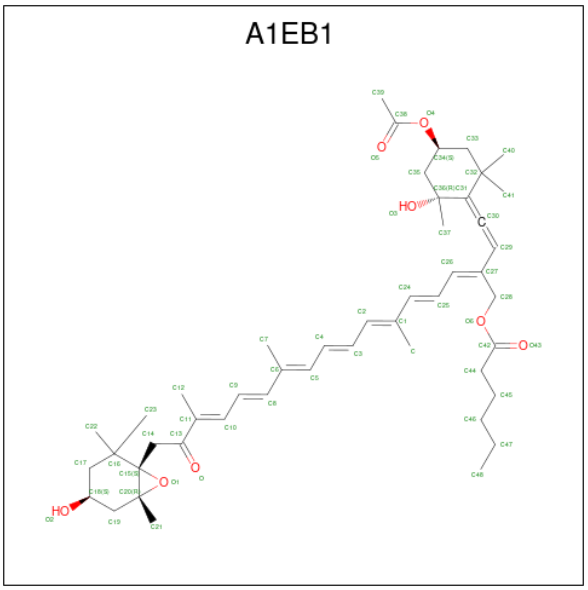
- Molecule 46 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
46	F	1	Total	C	O	S	0
			36	23	12	1	
46	I	1	Total	C	O	S	0
			54	41	12	1	
46	M	1	Total	C	O	S	0
			32	19	12	1	
46	P	1	Total	C	O	S	0
			32	19	12	1	
46	W	1	Total	C	O	S	0
			32	19	12	1	
46	k	1	Total	C	O	S	0
			36	23	12	1	

- Molecule 47 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-2-[2-[(4 {S},6 {R})-4-acety

loxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]ethenyl]-6,11,15-trimethyl-16-oxidanylidene -17-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]heptadec a-2,4,6,8,10,12,14-heptaenyl] hexanoate (CCD ID: A1EB1) (formula: $C_{48}H_{68}O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
47	F	1	Total	C	O	0
			56	48	8	
47	G	1	Total	C	O	0
			56	48	8	
47	K	1	Total	C	O	0
			56	48	8	
47	K	1	Total	C	O	0
			56	48	8	
47	L	1	Total	C	O	0
			56	48	8	
47	L	1	Total	C	O	0
			56	48	8	
47	N	1	Total	C	O	0
			56	48	8	
47	O	1	Total	C	O	0
			56	48	8	
47	P	1	Total	C	O	0
			56	48	8	
47	R	1	Total	C	O	0
			56	48	8	
47	S	1	Total	C	O	0
			56	48	8	

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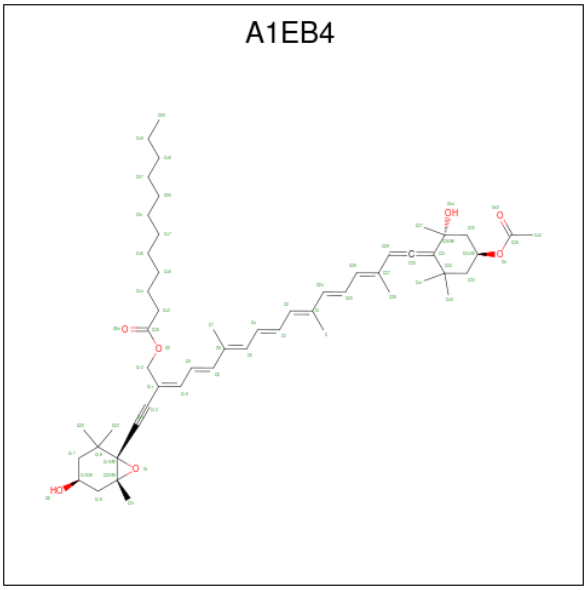
Mol	Chain	Residues	Atoms	AltConf
47	S	1	Total C O 56 48 8	0
47	T	1	Total C O 56 48 8	0
47	T	1	Total C O 56 48 8	0
47	Y	1	Total C O 56 48 8	0
47	Z	1	Total C O 56 48 8	0
47	Z	1	Total C O 56 48 8	0
47	Z	1	Total C O 56 48 8	0
47	o	1	Total C O 56 48 8	0
47	o	1	Total C O 56 48 8	0
47	p	1	Total C O 56 48 8	0
47	p	1	Total C O 56 48 8	0
47	q	1	Total C O 56 48 8	0
47	q	1	Total C O 56 48 8	0
47	q	1	Total C O 56 48 8	0
47	t	1	Total C O 56 48 8	0
47	t	1	Total C O 56 48 8	0
47	t	1	Total C O 56 48 8	0
47	u	1	Total C O 56 48 8	0
47	u	1	Total C O 56 48 8	0
47	v	1	Total C O 56 48 8	0
47	v	1	Total C O 56 48 8	0

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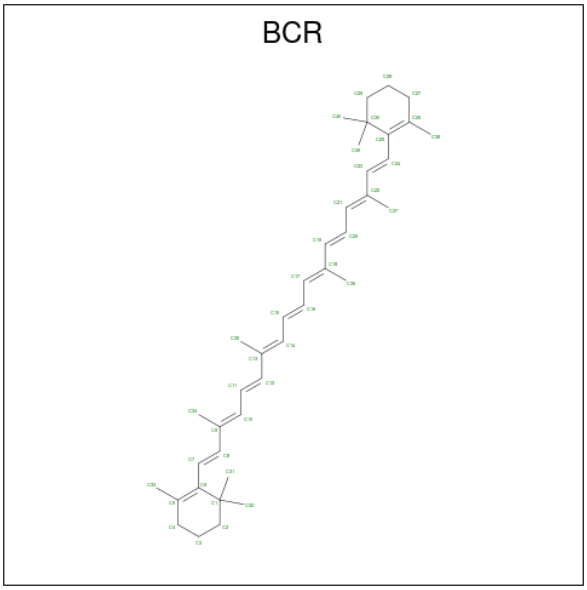
Mol	Chain	Residues	Atoms	AltConf
47	v	1	Total C O 56 48 8	0
47	v	1	Total C O 56 48 8	0
47	w	1	Total C O 56 48 8	0
47	w	1	Total C O 56 48 8	0
47	x	1	Total C O 56 48 8	0
47	x	1	Total C O 56 48 8	0
47	y	1	Total C O 56 48 8	0
47	y	1	Total C O 56 48 8	0
47	y	1	Total C O 56 48 8	0
47	z	1	Total C O 56 48 8	0

- Molecule 48 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyloxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]-6,11,15-trimethyl-2-[2-[(1 {R},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]ethynyl]heptadeca-2,4,6,8,10,12,14,16-octaenyl] dodecanoate (CCD ID: A1EB4) (formula: $C_{54}H_{78}O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
48	M	1	Total C O 56 49 7	0
48	P	1	Total C O 56 49 7	0
48	W	1	Total C O 56 49 7	0

- Molecule 49 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



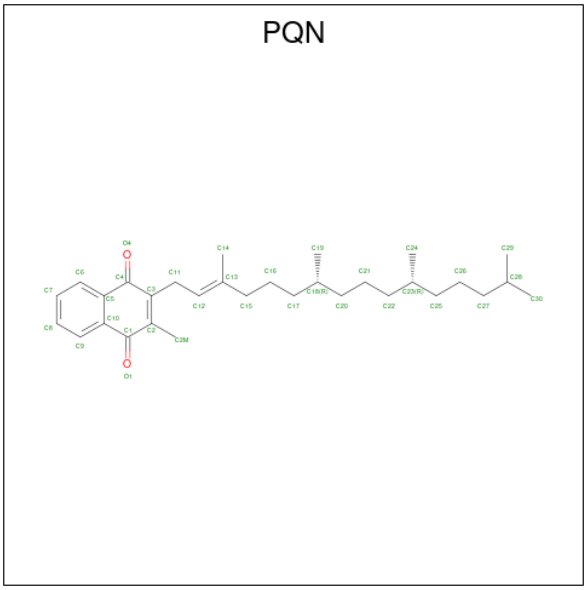
Mol	Chain	Residues	Atoms	AltConf
49	a	1	Total C 40 40	0
49	a	1	Total C 40 40	0
49	a	1	Total C 40 40	0
49	a	1	Total C 40 40	0
49	b	1	Total C 40 40	0
49	b	1	Total C 40 40	0
49	b	1	Total C 40 40	0
49	b	1	Total C 40 40	0

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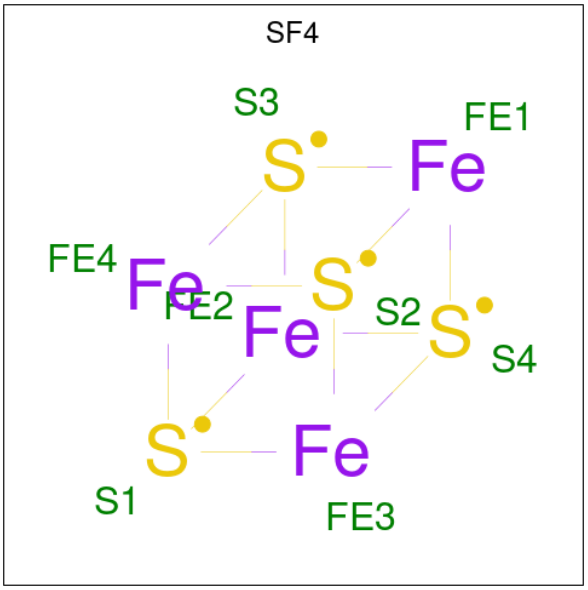
Mol	Chain	Residues	Atoms	AltConf
49	b	1	Total C 40 40	0
49	b	1	Total C 40 40	0
49	f	1	Total C 40 40	0
49	f	1	Total C 40 40	0
49	i	1	Total C 40 40	0
49	j	1	Total C 40 40	0
49	k	1	Total C 40 40	0
49	l	1	Total C 40 40	0
49	l	1	Total C 40 40	0
49	l	1	Total C 40 40	0
49	m	1	Total C 40 40	0
49	r	1	Total C 40 40	0

- Molecule 50 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



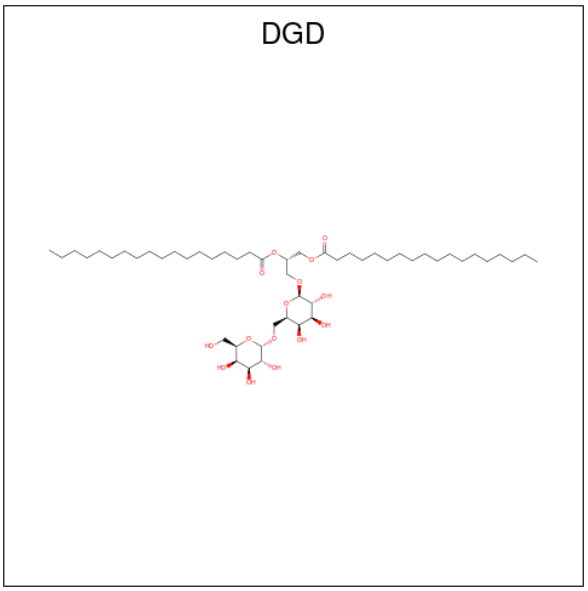
Mol	Chain	Residues	Atoms	AltConf
50	a	1	Total C O 28 26 2	0
50	b	1	Total C O 28 26 2	0

- Molecule 51 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
51	b	1	Total Fe S 8 4 4	0
51	c	1	Total Fe S 8 4 4	0
51	c	1	Total Fe S 8 4 4	0

- Molecule 52 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



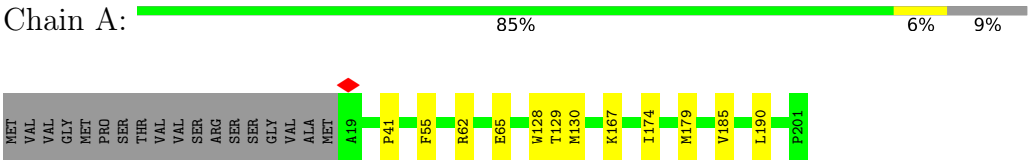
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
52	b	1	56	41	15	0

3 Residue-property plots (i)

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

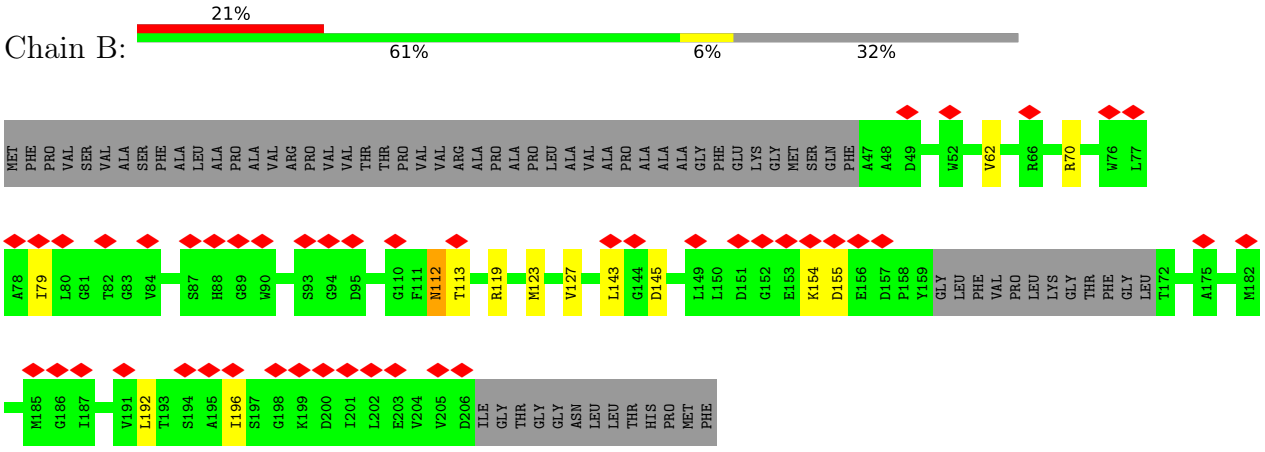
• Molecule 1: Light harvesting protein

Chain A:



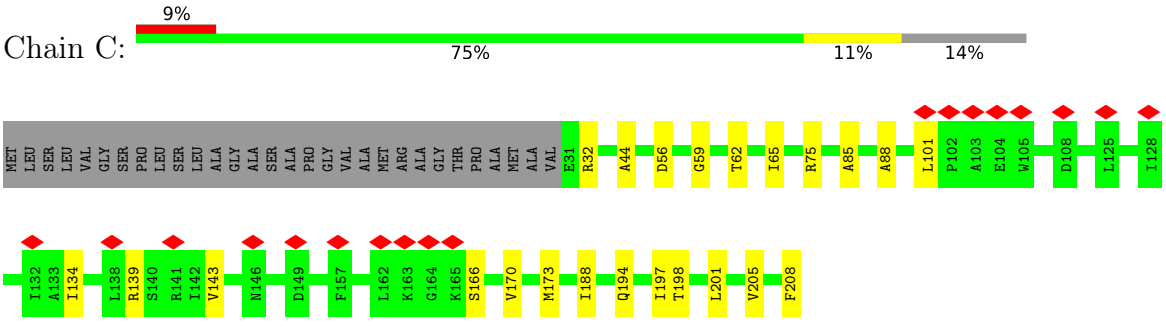
• Molecule 2: EFCPI-1

Chain B:



• Molecule 3: Light harvesting protein

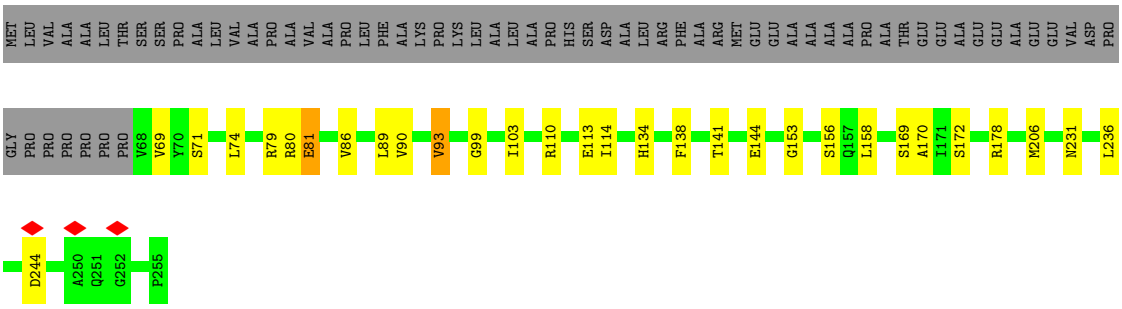
Chain C:



• Molecule 4: EFCPI-6

Chain D:

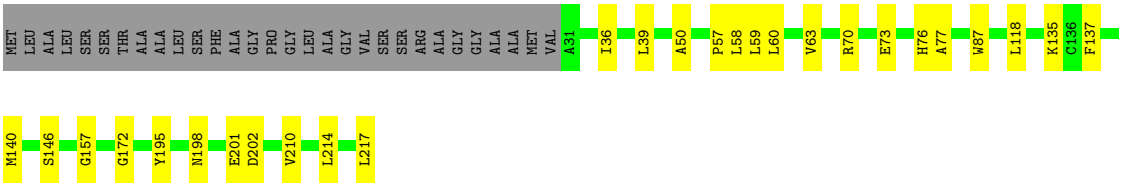




• Molecule 5: Light harvesting protein

Chain E:

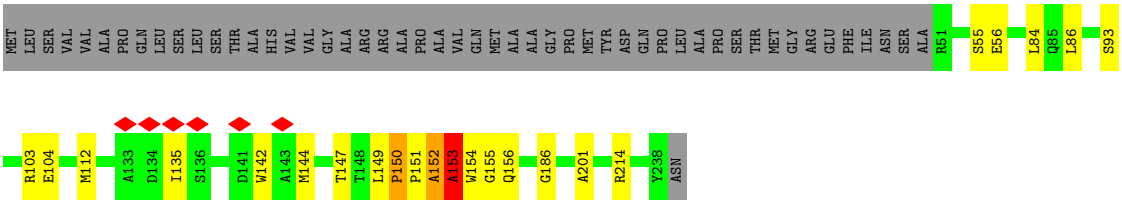




• Molecule 6: Light harvesting protein

Chain F:

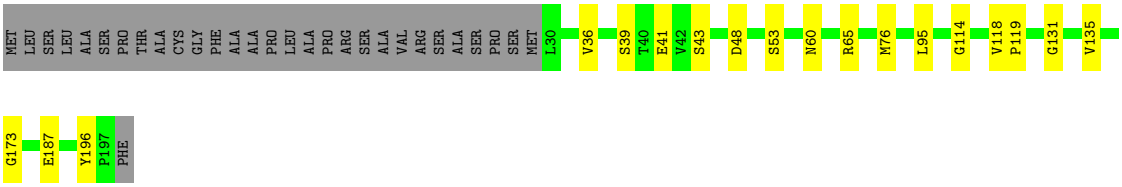




• Molecule 7: Light harvesting protein

Chain G:

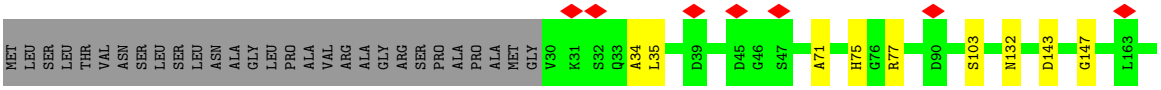


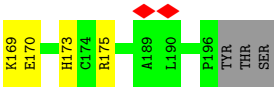


• Molecule 8: Light harvesting protein

Chain H:



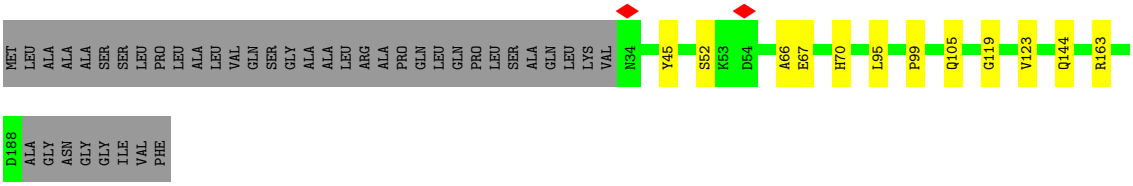




• Molecule 9: Light harvesting protein

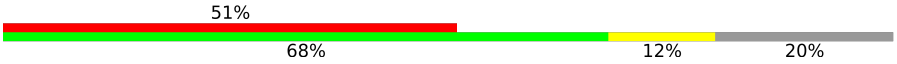
Chain I:





• Molecule 10: Light harvesting protein

Chain J:

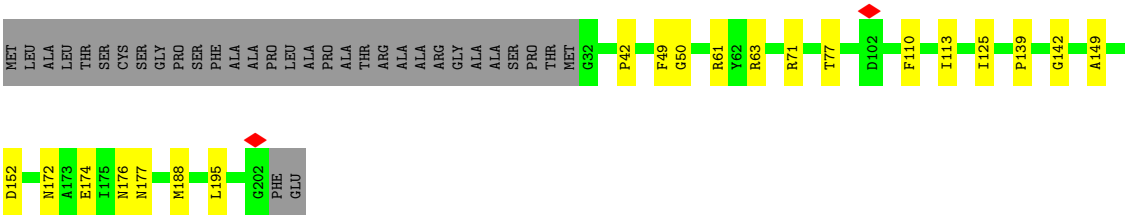




• Molecule 11: Light harvesting protein

Chain K:

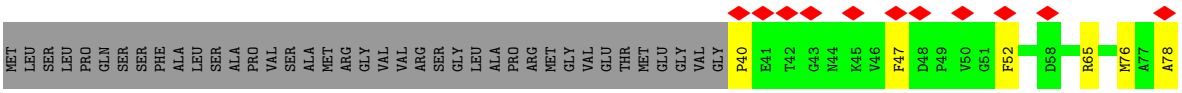


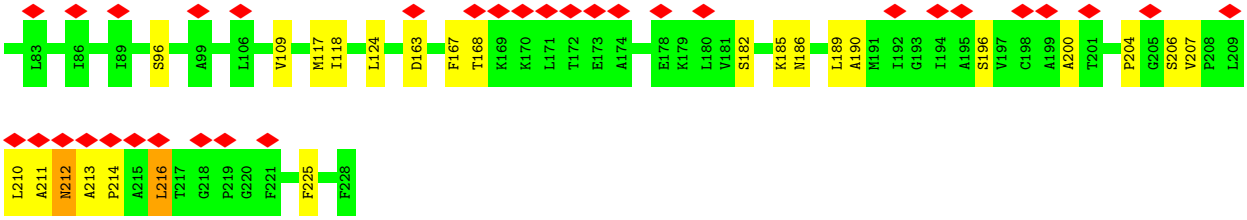


• Molecule 12: EFCPI-12

Chain L:



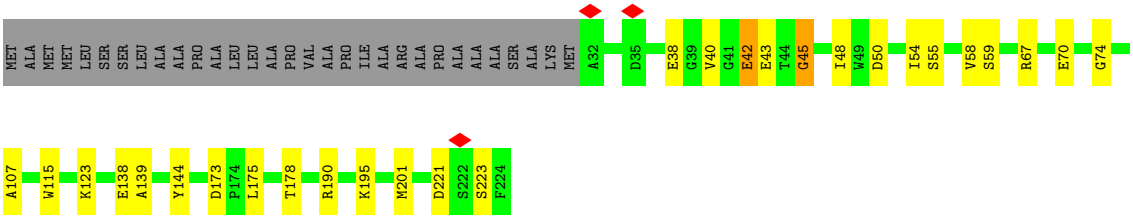




• Molecule 13: Light harvesting protein

Chain M:

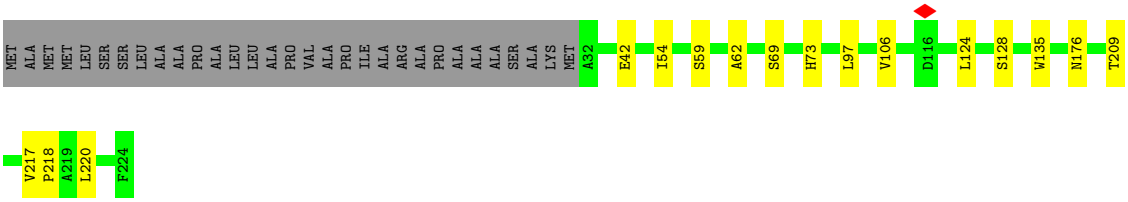




• Molecule 13: Light harvesting protein

Chain P:

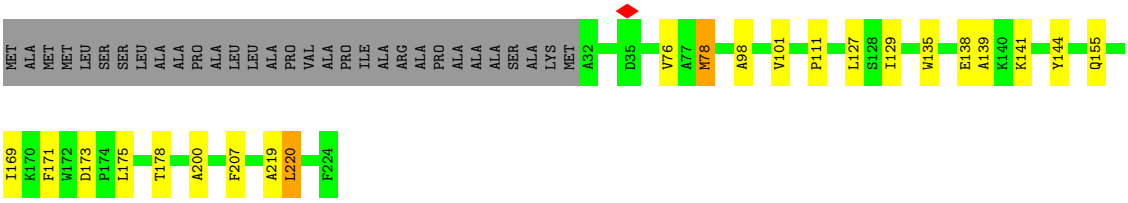




• Molecule 13: Light harvesting protein

Chain W:

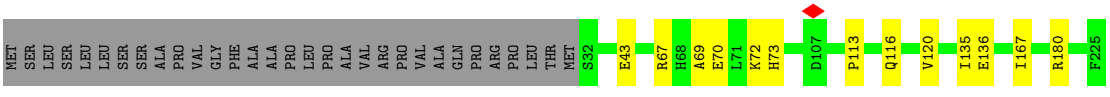




• Molecule 14: EFCPI-17

Chain N:

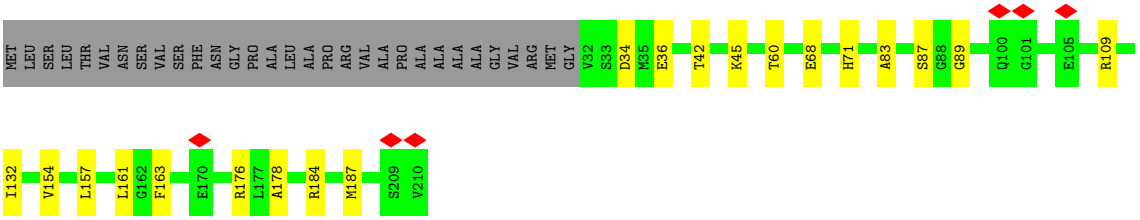




• Molecule 15: Light harvesting protein

Chain O:

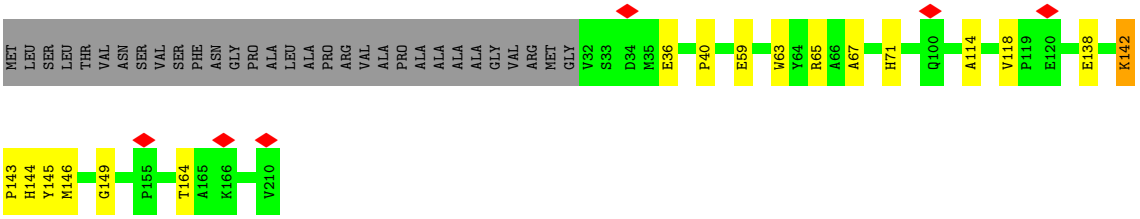




• Molecule 15: Light harvesting protein

Chain R:

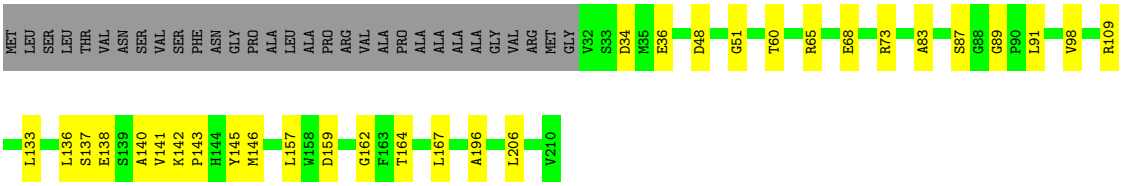




• Molecule 15: Light harvesting protein

Chain T:

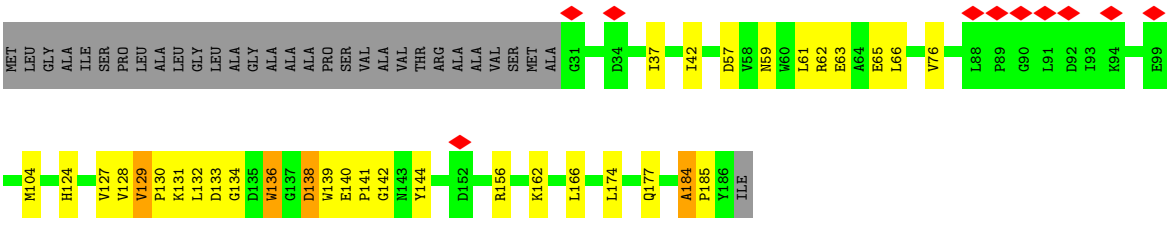




• Molecule 16: EFCPI-18

Chain Q:

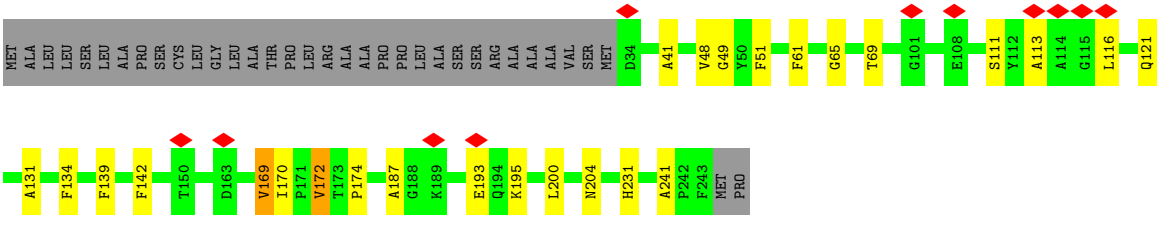




• Molecule 17: EFCPI-22

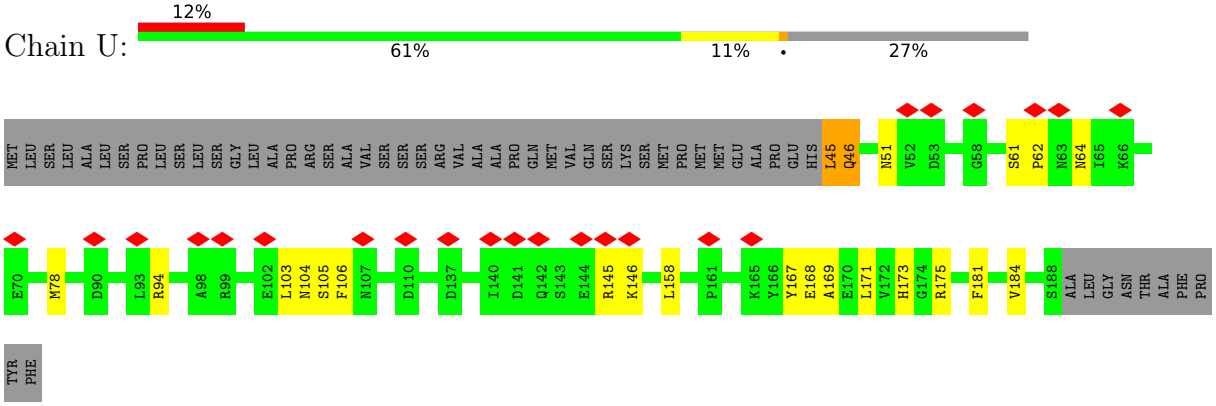
Chain S:





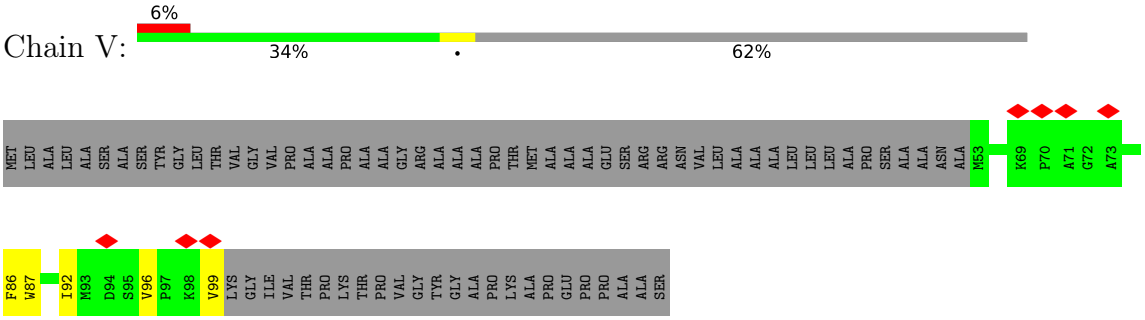
• Molecule 18: Light harvesting protein

Chain U:



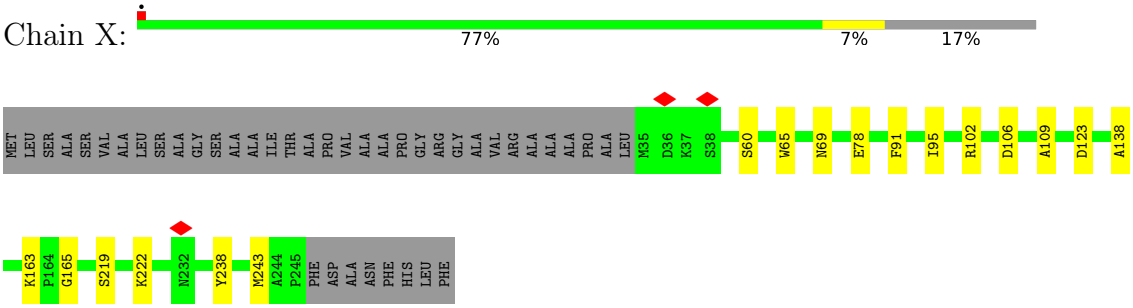
• Molecule 19: LEFP

Chain V:



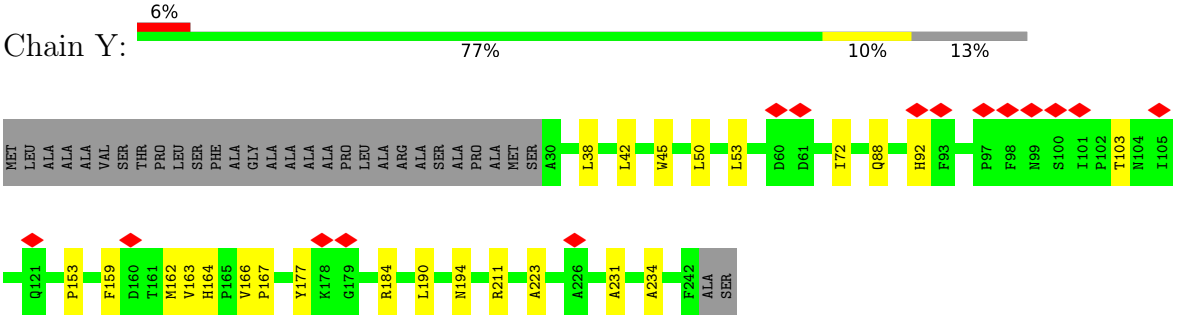
• Molecule 20: Light harvesting protein

Chain X:



• Molecule 21: Light harvesting protein

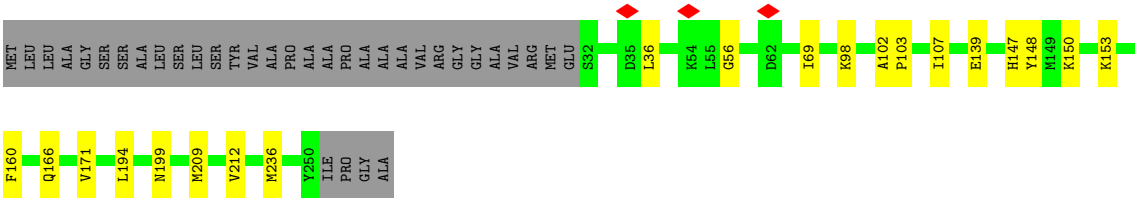
Chain Y:



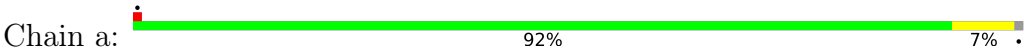
• Molecule 22: Light harvesting protein

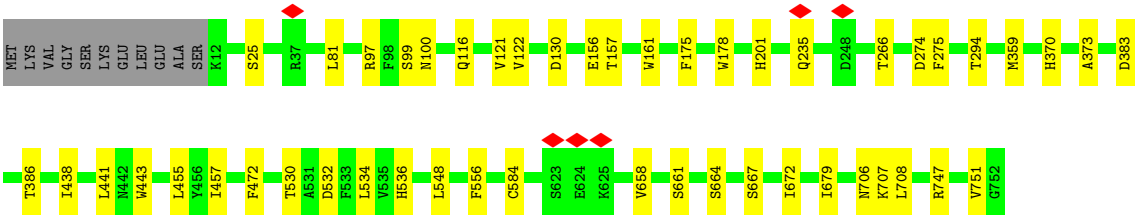
Chain Z:



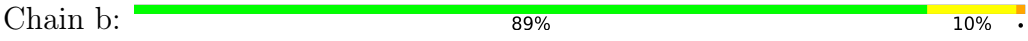


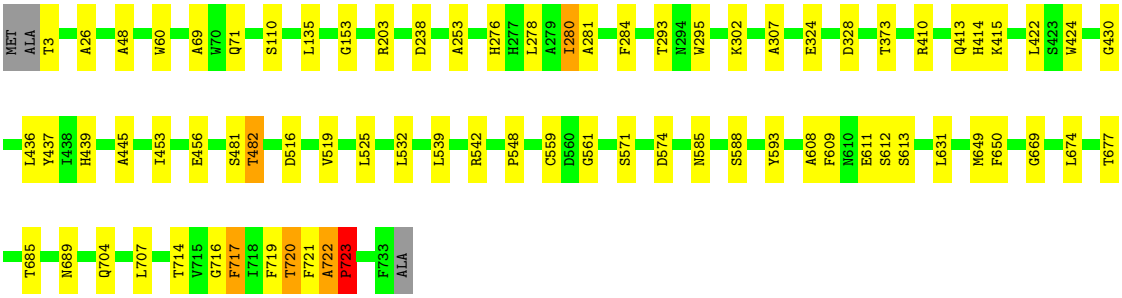
• Molecule 23: Photosystem I P700 chlorophyll a apoprotein A1



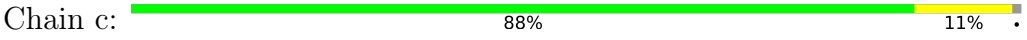


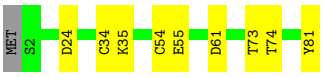
• Molecule 24: Photosystem I P700 chlorophyll a apoprotein A2



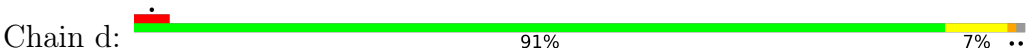


• Molecule 25: Photosystem I iron-sulfur center





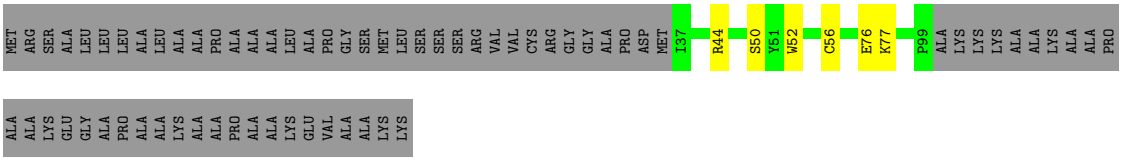
• Molecule 26: Photosystem I reaction center subunit II





• Molecule 27: Photosystem I reaction center subunit IV

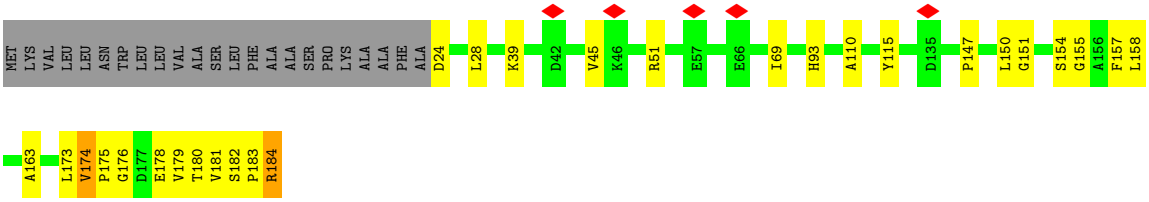




• Molecule 28: Photosystem I reaction center subunit III

Chain f:

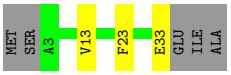




• Molecule 29: Photosystem I reaction center subunit VIII

Chain i:





• Molecule 30: Photosystem I reaction center subunit IX

Chain j:





• Molecule 31: PSI-K

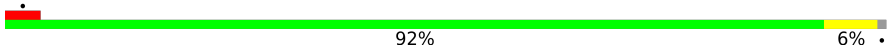
Chain k:

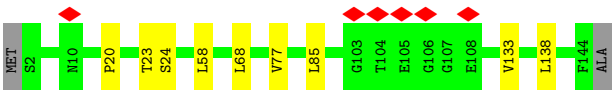




• Molecule 32: Photosystem I reaction center subunit XI

Chain l:

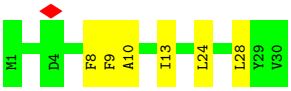




• Molecule 33: Photosystem I reaction center subunit XII

Chain m:

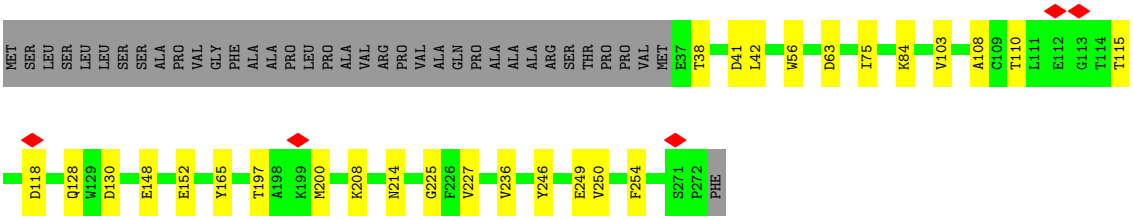




• Molecule 34: EFCPI-30

Chain o:

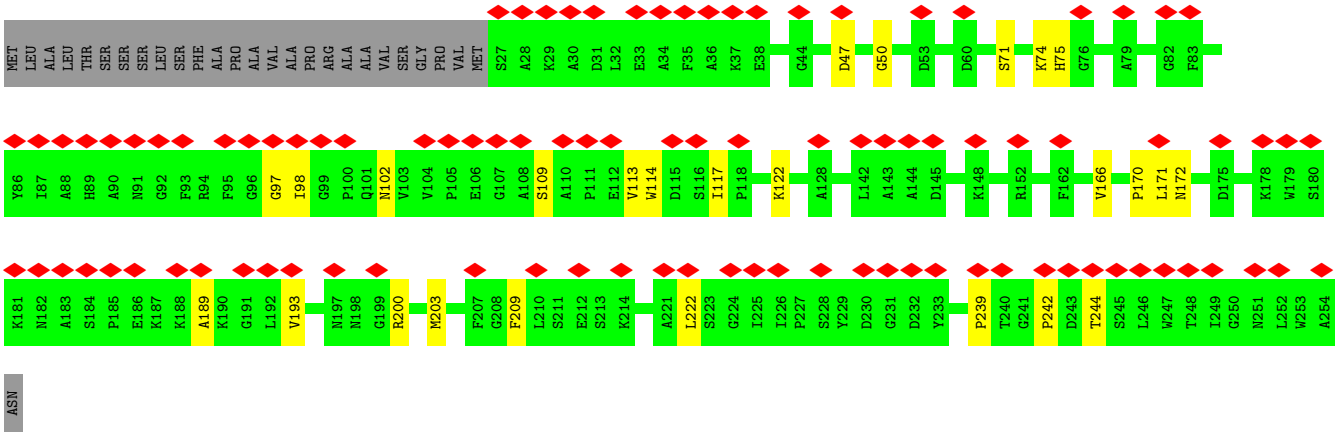




• Molecule 35: Light harvesting protein

Chain p:

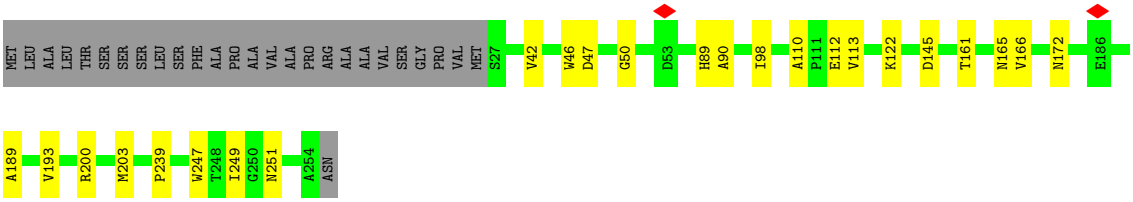




• Molecule 35: Light harvesting protein

Chain u:





• Molecule 35: Light harvesting protein

Chain x:



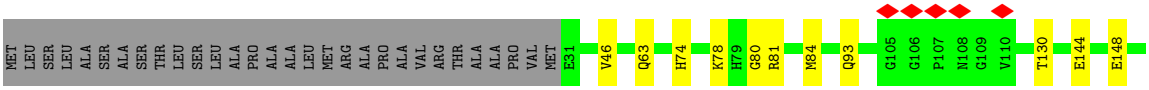




• Molecule 36: Light harvesting protein

Chain q:



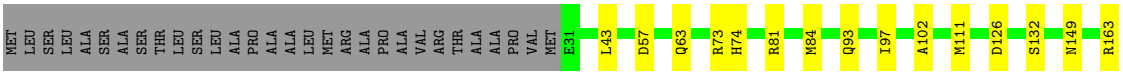


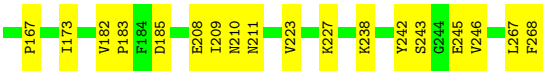


• Molecule 36: Light harvesting protein

Chain v:



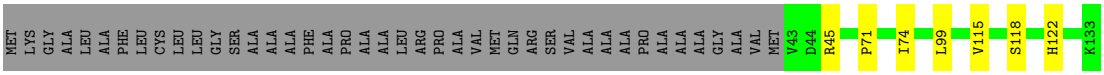




• Molecule 37: PsaR

Chain r:

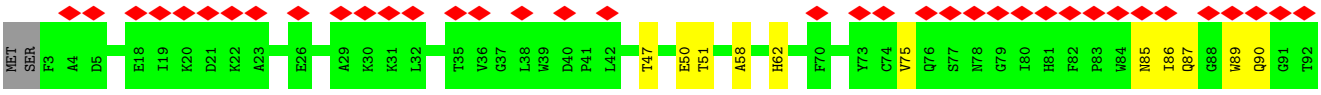


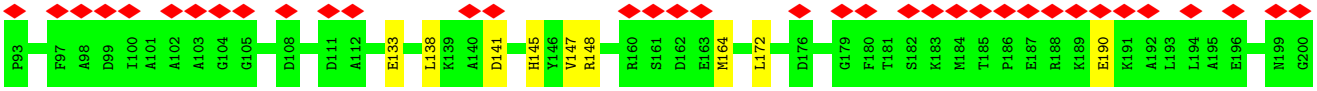


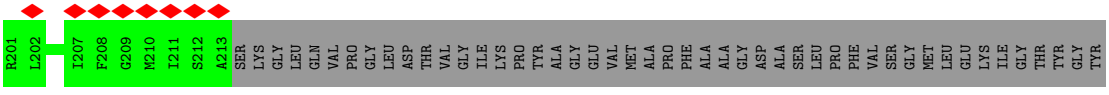
• Molecule 38: Light harvesting protein

Chain t:



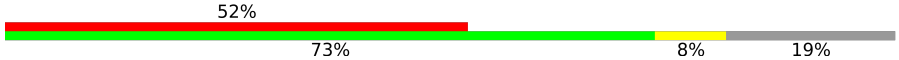


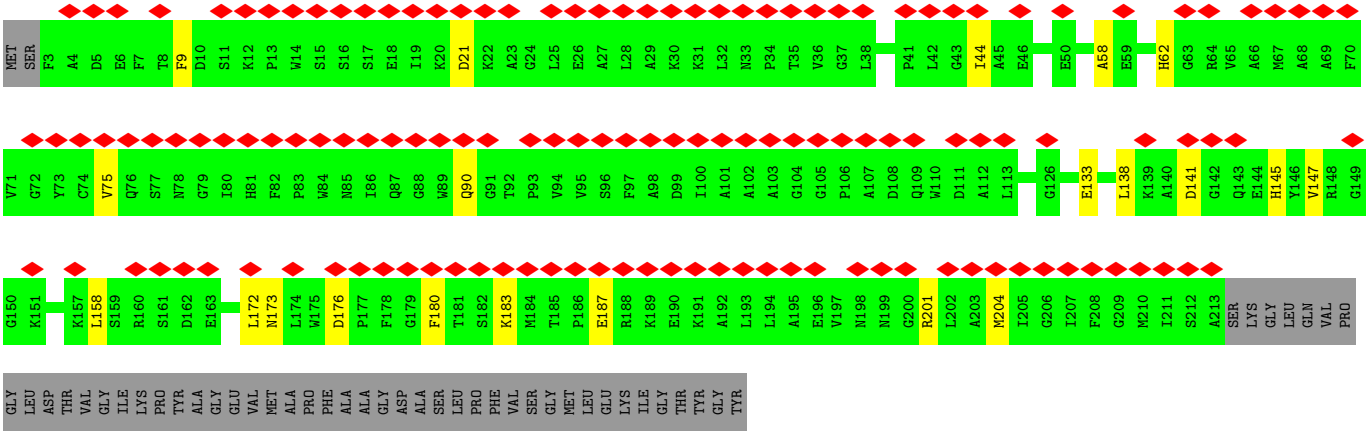




• Molecule 38: Light harvesting protein

Chain w:

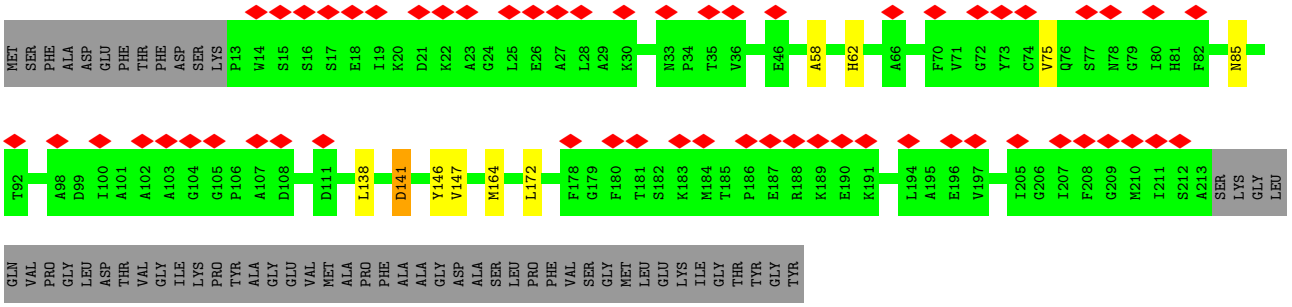




- Molecule 38: Light harvesting protein

Chain y:

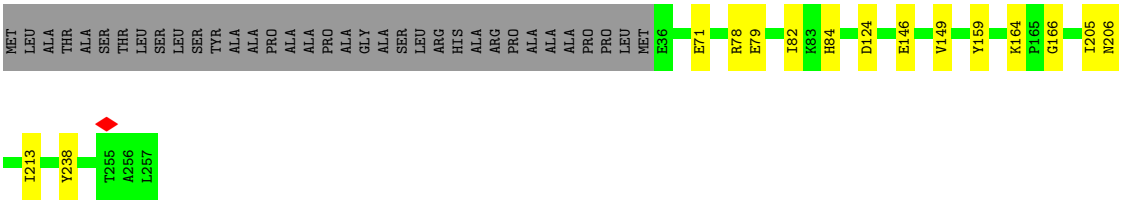




- Molecule 39: Light harvesting protein

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93213	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.457	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	530.0, 530.0, 530.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, DD6, CLA, SF4, LMG, A1EB4, A86, SQD, LHG, BCR, KC2, DGD, A1EB1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.20	0/1458	0.41	0/1979
2	B	0.30	0/1135	0.60	1/1545 (0.1%)
3	C	0.23	0/1381	0.46	0/1865
4	D	0.45	0/1486	0.52	1/2020 (0.0%)
5	E	0.21	0/1416	0.43	0/1933
6	F	0.30	0/1452	0.51	3/1970 (0.2%)
7	G	0.19	0/1277	0.37	0/1739
8	H	0.23	0/1283	0.49	0/1739
9	I	0.20	0/1225	0.40	0/1656
10	J	0.23	0/1254	0.52	0/1692
11	K	0.20	0/1378	0.41	0/1874
12	L	0.28	0/1462	0.55	1/1989 (0.1%)
13	M	0.41	0/1491	0.52	2/2020 (0.1%)
13	P	0.20	0/1491	0.43	0/2020
13	W	0.21	0/1491	0.47	0/2020
14	N	0.19	0/1494	0.43	0/2027
15	O	0.22	0/1360	0.48	0/1850
15	R	0.38	0/1360	0.53	0/1850
15	T	0.23	0/1360	0.51	0/1850
16	Q	0.47	1/1223 (0.1%)	0.64	4/1659 (0.2%)
17	S	0.21	0/1700	0.49	2/2315 (0.1%)
18	U	0.25	0/1158	0.55	1/1567 (0.1%)
19	V	0.22	0/362	0.49	0/492
20	X	0.23	0/1695	0.48	0/2300
21	Y	0.26	0/1719	0.53	0/2342
22	Z	0.24	0/1773	0.50	0/2423
23	a	0.20	0/6024	0.39	0/8200
24	b	0.38	6/6017 (0.1%)	0.46	4/8208 (0.0%)
25	c	0.22	0/607	0.45	0/824
26	d	0.20	0/1128	0.42	0/1525
27	e	0.20	0/503	0.44	0/681
28	f	0.28	0/1269	0.45	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
29	i	0.23	0/250	0.45	0/342
30	j	0.23	0/324	0.49	0/438
31	k	0.20	0/520	0.40	0/701
32	l	0.19	0/1113	0.37	0/1513
33	m	0.22	0/226	0.35	0/306
34	o	0.26	0/1809	0.54	0/2460
35	p	0.25	0/1801	0.49	0/2451
35	u	0.28	0/1801	0.49	0/2451
35	x	0.24	0/1801	0.48	0/2451
36	q	0.26	0/1843	0.48	0/2503
36	v	0.26	0/1843	0.49	0/2503
37	r	0.23	0/700	0.42	0/958
38	t	0.26	0/1682	0.49	0/2286
38	w	0.24	0/1682	0.51	0/2286
38	y	0.22	0/1594	0.47	0/2167
39	z	0.25	0/1772	0.46	0/2414
All	All	0.27	7/72193 (0.0%)	0.47	19/98125 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
15	T	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	281	ALA	CA-C	-6.35	1.44	1.52
24	b	284	PHE	C-O	-6.20	1.16	1.24
24	b	281	ALA	C-O	-5.83	1.17	1.24
16	Q	136	TRP	CA-C	-5.79	1.45	1.52
24	b	722	ALA	C-O	-5.38	1.19	1.24
24	b	281	ALA	CA-CB	-5.29	1.44	1.53
24	b	722	ALA	CA-CB	-5.06	1.47	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	722	ALA	CA-C-N	-7.89	109.97	119.84
24	b	722	ALA	C-N-CA	-7.89	109.97	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	93	VAL	N-CA-C	-7.55	103.92	111.77
6	F	152	ALA	N-CA-C	-7.37	103.18	111.07
16	Q	129	VAL	O-C-N	6.28	124.44	120.42
16	Q	136	TRP	N-CA-C	-6.27	98.95	108.67
18	U	62	PRO	CA-N-CD	-6.15	103.39	112.00
16	Q	129	VAL	CA-C-N	-5.91	112.45	119.84
16	Q	129	VAL	C-N-CA	-5.91	112.45	119.84
2	B	154	LYS	CB-CG-CD	5.90	124.87	111.30
6	F	153	ALA	CA-C-N	-5.79	111.05	120.72
6	F	153	ALA	C-N-CA	-5.79	111.05	120.72
13	M	45	GLY	N-CA-C	5.62	123.88	113.76
13	M	42	GLU	N-CA-C	-5.55	106.67	113.50
12	L	214	PRO	N-CA-C	-5.45	107.53	114.35
17	S	169	VAL	CA-C-N	5.41	132.14	122.13
17	S	169	VAL	C-N-CA	5.41	132.14	122.13
24	b	714	THR	N-CA-C	5.30	116.74	111.07
24	b	723	PRO	CA-N-CD	-5.07	104.90	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	T	142	LYS	Peptide
15	T	162	GLY	Peptide

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	A	1419	0	1408	15	0
2	B	1108	0	1082	10	0
3	C	1352	0	1383	15	0
4	D	1446	0	1404	35	0
5	E	1383	0	1399	48	0
6	F	1414	0	1411	21	0
7	G	1248	0	1251	10	0
8	H	1251	0	1225	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1195	0	1197	8	0
10	J	1231	0	1245	25	0
11	K	1333	0	1297	16	0
12	L	1419	0	1413	37	0
13	M	1455	0	1468	22	0
13	P	1455	0	1468	25	0
13	W	1455	0	1468	24	0
14	N	1454	0	1469	9	0
15	O	1325	0	1344	13	0
15	R	1325	0	1344	16	0
15	T	1325	0	1344	19	0
16	Q	1192	0	1163	39	0
17	S	1640	0	1586	22	0
18	U	1130	0	1116	12	0
19	V	351	0	350	13	0
20	X	1643	0	1607	12	0
21	Y	1660	0	1617	16	0
22	Z	1714	0	1670	14	0
23	a	5832	0	5730	59	0
24	b	5807	0	5630	63	0
25	c	597	0	581	7	0
26	d	1103	0	1113	8	0
27	e	493	0	482	4	0
28	f	1238	0	1242	40	0
29	i	243	0	255	5	0
30	j	317	0	333	15	0
31	k	510	0	520	9	0
32	l	1084	0	1090	8	0
33	m	224	0	243	5	0
34	o	1760	0	1757	18	0
35	p	1744	0	1703	16	0
35	u	1744	0	1703	16	0
35	x	1744	0	1703	24	0
36	q	1790	0	1776	27	0
36	v	1790	0	1776	26	0
37	r	681	0	667	4	0
38	t	1631	0	1593	29	0
38	w	1631	0	1593	19	0
38	y	1546	0	1523	9	0
39	z	1718	0	1701	13	0
40	A	581	0	562	24	0
40	B	287	0	218	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	C	429	0	381	4	0
40	D	668	0	613	7	0
40	E	711	0	640	35	0
40	F	544	0	482	12	0
40	G	363	0	303	4	0
40	H	521	0	442	2	0
40	I	445	0	412	0	0
40	J	549	0	441	14	0
40	K	327	0	294	6	0
40	L	394	0	312	10	0
40	M	420	0	413	3	0
40	N	345	0	324	3	0
40	O	328	0	299	0	0
40	P	393	0	364	11	0
40	Q	432	0	375	11	0
40	R	320	0	278	2	0
40	S	580	0	496	21	0
40	T	330	0	296	1	0
40	U	345	0	273	1	0
40	V	113	0	104	6	0
40	W	425	0	429	5	0
40	X	484	0	425	2	0
40	Y	478	0	415	0	0
40	Z	507	0	469	2	0
40	a	2596	0	2627	48	0
40	b	2503	0	2570	31	0
40	f	219	0	201	7	0
40	i	55	0	49	4	0
40	j	47	0	35	2	0
40	k	110	0	98	17	0
40	l	259	0	284	4	0
40	o	507	0	469	5	0
40	p	478	0	418	2	0
40	q	508	0	469	2	0
40	t	305	0	249	1	0
40	u	491	0	442	0	0
40	v	508	0	469	4	0
40	w	305	0	249	6	0
40	x	508	0	472	3	0
40	y	305	0	249	7	0
40	z	551	0	498	5	0
41	A	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	C	45	0	0	1	0
41	E	45	0	0	0	0
41	F	90	0	0	0	0
41	G	90	0	0	0	0
41	H	90	0	0	0	0
41	I	90	0	0	0	0
41	J	45	0	0	0	0
41	K	180	0	0	0	0
41	L	225	0	0	1	0
41	M	225	0	0	2	0
41	N	315	0	0	1	0
41	O	270	0	0	1	0
41	P	225	0	0	1	0
41	Q	90	0	0	10	0
41	R	270	0	0	0	0
41	S	180	0	0	0	0
41	T	270	0	0	3	0
41	U	45	0	0	0	0
41	W	225	0	0	1	0
41	X	180	0	0	1	0
41	Y	225	0	0	9	0
41	Z	180	0	0	2	0
41	o	180	0	0	1	0
41	p	225	0	0	0	0
41	q	180	0	0	0	0
41	t	135	0	0	15	0
41	u	225	0	0	0	0
41	v	180	0	0	1	0
41	w	135	0	0	13	0
41	x	225	0	0	0	0
41	y	135	0	0	8	0
41	z	180	0	0	1	0
42	A	215	0	0	10	0
42	B	43	0	0	1	0
42	C	129	0	0	1	0
42	D	215	0	0	1	0
42	E	172	0	0	0	0
42	F	129	0	0	1	0
42	G	43	0	0	0	0
42	H	129	0	0	1	0
42	I	172	0	0	2	0
42	J	258	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	K	86	0	0	0	0
42	L	86	0	0	32	0
42	M	43	0	0	1	0
42	N	129	0	0	1	0
42	O	43	0	0	1	0
42	P	43	0	0	5	0
42	Q	172	0	0	1	0
42	R	43	0	0	0	0
42	T	43	0	0	0	0
42	U	86	0	0	0	0
42	W	43	0	0	1	0
42	X	43	0	0	0	0
42	Y	43	0	0	9	0
42	Z	43	0	0	0	0
42	j	43	0	0	0	0
42	k	43	0	0	0	0
42	o	86	0	0	2	0
42	p	43	0	0	1	0
42	q	86	0	0	7	0
42	t	43	0	0	29	0
42	u	43	0	0	1	0
42	v	86	0	0	5	0
42	w	43	0	0	26	0
42	x	43	0	0	2	0
42	y	43	0	0	17	0
42	z	86	0	0	0	0
43	A	40	0	50	0	0
43	D	40	0	50	1	0
43	E	102	0	114	6	0
43	F	39	0	48	0	0
43	L	37	0	44	0	0
43	M	39	0	48	0	0
43	P	39	0	48	0	0
43	S	39	0	48	0	0
43	T	40	0	50	0	0
43	W	39	0	48	0	0
43	a	70	0	80	3	0
43	j	30	0	30	13	0
43	l	39	0	48	0	0
43	p	39	0	48	0	0
43	u	39	0	48	1	0
43	x	39	0	48	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	C	48	0	0	0	0
44	D	96	0	0	1	0
44	F	144	0	0	0	0
44	G	96	0	0	3	0
44	H	48	0	0	0	0
44	K	48	0	0	0	0
44	L	48	0	0	1	0
44	M	192	0	0	1	0
44	N	192	0	0	7	0
44	O	144	0	0	0	0
44	P	192	0	0	1	0
44	Q	96	0	0	1	0
44	R	144	0	0	0	0
44	S	192	0	0	0	0
44	T	192	0	0	0	0
44	U	48	0	0	0	0
44	W	144	0	0	2	0
44	X	384	0	0	3	0
44	Y	336	0	0	3	0
44	Z	192	0	0	1	0
44	o	240	0	0	1	0
44	p	288	0	0	1	0
44	q	288	0	0	0	0
44	t	144	0	0	1	0
44	u	240	0	0	0	0
44	v	288	0	0	0	0
44	w	192	0	0	1	0
44	x	192	0	0	0	0
44	y	48	0	0	1	0
44	z	336	0	0	1	0
45	F	40	0	50	0	0
45	S	40	0	50	2	0
45	a	78	0	99	0	0
46	F	36	0	36	2	0
46	I	54	0	78	2	0
46	M	32	0	28	1	0
46	P	32	0	28	5	0
46	W	32	0	28	4	0
46	k	36	0	36	3	0
47	F	56	0	0	0	0
47	G	56	0	0	0	0
47	K	112	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	L	112	0	0	0	0
47	N	56	0	0	0	0
47	O	56	0	0	0	0
47	P	56	0	0	9	0
47	R	56	0	0	0	0
47	S	112	0	0	0	0
47	T	112	0	0	1	0
47	Y	56	0	0	0	0
47	Z	168	0	0	1	0
47	o	112	0	0	0	0
47	p	112	0	0	2	0
47	q	168	0	0	1	0
47	t	168	0	0	2	0
47	u	112	0	0	2	0
47	v	224	0	0	5	0
47	w	112	0	0	0	0
47	x	112	0	0	2	0
47	y	168	0	0	4	0
47	z	56	0	0	0	0
48	M	56	0	0	0	0
48	P	56	0	0	4	0
48	W	56	0	0	7	0
49	a	160	0	224	7	0
49	b	240	0	336	2	0
49	f	80	0	112	4	0
49	i	40	0	56	3	0
49	j	40	0	56	0	0
49	k	40	0	56	0	0
49	l	120	0	168	4	0
49	m	40	0	56	4	0
49	r	40	0	56	1	0
50	a	28	0	33	1	0
50	b	28	0	33	2	0
51	b	8	0	0	0	0
51	c	16	0	0	0	0
52	b	56	0	70	7	0
All	All	110086	0	91890	1072	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 5.

All (1072) 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)
13:P:54:ILE:CG2	47:P:301:A1EB1:O43	1.73	1.36
30:j:1:MET:CE	43:j:101:LMG:H292	1.56	1.34
16:Q:162:LYS:NZ	41:Q:216:KC2:O2A	1.65	1.27
16:Q:42:ILE:HD12	41:Q:216:KC2:CED	1.67	1.23
4:D:103:ILE:CG2	23:a:175:PHE:CZ	2.23	1.20
40:E:307:CLA:H2	40:a:819:CLA:C9	1.70	1.20
36:q:181:PRO:HD2	42:q:318:DD6:C26	1.79	1.11
4:D:103:ILE:CG2	23:a:175:PHE:CE1	2.35	1.10
5:E:63:VAL:HG11	40:a:819:CLA:C2	1.79	1.10
24:b:548:PRO:HB3	28:f:183:PRO:HG2	1.23	1.10
13:P:54:ILE:HG22	47:P:301:A1EB1:O43	1.49	1.08
40:A:311:CLA:HED3	42:A:316:DD6:C21	1.84	1.07
4:D:103:ILE:HG21	23:a:175:PHE:CZ	1.88	1.07
12:L:47:PHE:HE1	42:L:315:DD6:C37	1.68	1.07
30:j:1:MET:HE2	43:j:101:LMG:C29	1.86	1.05
4:D:103:ILE:HG23	23:a:175:PHE:CZ	1.88	1.04
5:E:58:LEU:CD2	40:k:202:CLA:O1A	2.07	1.03
40:E:306:CLA:H51	49:a:843:BCR:HC32	1.41	1.02
5:E:58:LEU:HD22	40:k:202:CLA:O1A	1.58	1.01
30:j:1:MET:HE2	43:j:101:LMG:H292	1.01	1.00
41:w:306:KC2:C1B	42:w:312:DD6:C2	2.39	1.00
40:E:307:CLA:H2	40:a:819:CLA:H93	1.41	0.99
5:E:63:VAL:HG11	40:a:819:CLA:C3	1.93	0.98
10:J:187:MET:HE2	42:J:316:DD6:C24	1.94	0.97
5:E:63:VAL:CG1	40:a:819:CLA:C2	2.42	0.97
13:P:54:ILE:HG21	47:P:301:A1EB1:O43	1.65	0.97
13:W:219:ALA:HB2	48:W:319:A1EB4:C42	1.96	0.96
40:E:307:CLA:C2	40:a:819:CLA:C9	2.43	0.95
38:t:47:THR:HG22	42:v:318:DD6:C37	1.96	0.95
5:E:118:LEU:HD21	40:a:815:CLA:H152	1.48	0.95
40:A:306:CLA:H141	40:f:205:CLA:C2	1.97	0.94
40:E:307:CLA:C2	40:a:819:CLA:H92	1.98	0.94
40:P:308:CLA:C2B	42:P:315:DD6:C23	2.46	0.94
5:E:118:LEU:HD21	40:a:815:CLA:C15	1.99	0.93
16:Q:42:ILE:CD1	41:Q:216:KC2:CED	2.48	0.91
10:J:100:ARG:HH21	10:J:111:THR:HA	1.35	0.91
40:E:311:CLA:HAA2	40:a:815:CLA:CBA	2.02	0.90
30:j:1:MET:HE3	43:j:101:LMG:H292	1.54	0.90
40:y:308:CLA:C2C	42:y:311:DD6:C21	2.50	0.90
13:P:54:ILE:HG22	47:P:301:A1EB1:C42	2.00	0.89
47:v:324:A1EB1:C18	42:w:312:DD6:C37	2.51	0.89
12:L:167:PHE:HB2	42:L:317:DD6:C17	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:E:306:CLA:C5	49:a:843:BCR:HC32	2.03	0.88
38:t:90:GLN:HE21	42:t:312:DD6:C29	1.87	0.88
47:P:301:A1EB1:C48	40:P:306:CLA:H11	2.04	0.87
4:D:103:ILE:HG23	23:a:175:PHE:HZ	1.28	0.87
12:L:47:PHE:CE1	42:L:315:DD6:C37	2.58	0.87
24:b:719:PHE:O	24:b:723:PRO:HD2	1.76	0.86
30:j:1:MET:HG2	43:j:101:LMG:HC8	1.58	0.86
10:J:100:ARG:NH2	10:J:111:THR:HA	1.90	0.85
10:J:187:MET:CE	42:J:316:DD6:C24	2.53	0.85
12:L:167:PHE:CB	42:L:317:DD6:C17	2.53	0.85
40:A:306:CLA:H62	28:f:150:LEU:HD13	1.58	0.85
40:J:309:CLA:HBC2	42:J:316:DD6:C6	2.06	0.85
1:A:167:LYS:HG2	42:A:316:DD6:O4	1.76	0.85
38:t:90:GLN:HB3	42:t:312:DD6:C37	2.07	0.85
36:q:181:PRO:HD2	42:q:318:DD6:C29	2.07	0.84
40:E:306:CLA:C10	49:a:846:BCR:H333	2.08	0.84
5:E:63:VAL:CG1	40:a:819:CLA:C3	2.55	0.84
40:A:305:CLA:H11	28:f:154:SER:O	1.77	0.84
6:F:135:ILE:HG22	6:F:150:PRO:HG2	1.60	0.84
40:L:306:CLA:HHC	42:L:315:DD6:C26	2.08	0.83
40:Q:206:CLA:H93	40:S:305:CLA:HAB	1.61	0.83
1:A:174:ILE:HD13	42:A:316:DD6:C26	2.07	0.83
4:D:103:ILE:CG2	23:a:175:PHE:HZ	1.77	0.83
40:A:306:CLA:C14	40:f:205:CLA:C2	2.56	0.82
5:E:58:LEU:HD23	40:k:202:CLA:HAA1	1.60	0.82
19:V:92:ILE:CD1	23:a:157:THR:HA	2.10	0.82
40:V:201:CLA:C13	40:a:817:CLA:C5	2.58	0.82
5:E:58:LEU:HD23	40:k:202:CLA:CAA	2.09	0.81
41:w:306:KC2:C4C	42:w:312:DD6:C7	2.58	0.81
41:Y:308:KC2:C1B	42:Y:322:DD6:C3	2.59	0.81
13:P:54:ILE:CG2	47:P:301:A1EB1:C42	2.56	0.81
1:A:55:PHE:O	28:f:147:PRO:HB3	1.83	0.79
41:t:306:KC2:NC	42:t:312:DD6:C7	2.46	0.79
38:t:90:GLN:CB	42:t:312:DD6:C37	2.60	0.79
40:P:308:CLA:C1B	42:P:315:DD6:C23	2.60	0.79
16:Q:129:VAL:C	16:Q:131:LYS:H	1.90	0.79
16:Q:162:LYS:NZ	41:Q:216:KC2:CGA	2.45	0.79
6:F:135:ILE:HG22	6:F:150:PRO:CG	2.13	0.79
36:q:181:PRO:HD2	42:q:318:DD6:C27	2.13	0.78
16:Q:162:LYS:CE	41:Q:216:KC2:O2A	2.31	0.78
5:E:118:LEU:CD2	40:a:815:CLA:H152	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:W:219:ALA:CB	48:W:319:A1EB4:C42	2.61	0.78
40:J:309:CLA:CBC	42:J:316:DD6:C6	2.62	0.77
40:F:301:CLA:HBC3	44:N:315:A86:C10	2.14	0.77
12:L:167:PHE:CD2	42:L:317:DD6:C22	2.67	0.77
1:A:185:VAL:HG22	40:A:311:CLA:HED2	1.67	0.76
3:C:88:ALA:HB3	3:C:188:ILE:HD11	1.67	0.76
5:E:58:LEU:CD2	40:k:202:CLA:CGA	2.64	0.76
40:L:306:CLA:CHC	42:L:315:DD6:C26	2.62	0.76
41:t:306:KC2:CHB	42:t:312:DD6:C2	2.63	0.76
42:y:311:DD6:C37	47:y:313:A1EB1:C23	2.62	0.76
25:c:61:ASP:OD2	27:e:50:SER:OG	2.04	0.76
42:y:311:DD6:C37	47:y:313:A1EB1:C17	2.63	0.76
38:t:90:GLN:CG	42:t:312:DD6:C37	2.65	0.75
6:F:135:ILE:CG2	6:F:150:PRO:HG2	2.17	0.75
41:w:306:KC2:CHB	42:w:312:DD6:C2	2.64	0.75
5:E:58:LEU:HD23	40:k:202:CLA:CBA	2.17	0.74
47:T:320:A1EB1:O43	47:T:320:A1EB1:O3	2.04	0.74
38:w:90:GLN:NE2	42:w:312:DD6:C37	2.50	0.74
41:t:306:KC2:C1C	42:t:312:DD6:C7	2.66	0.74
40:E:311:CLA:HAA2	40:a:815:CLA:HBA2	1.67	0.74
12:L:167:PHE:HB3	42:L:317:DD6:C17	2.18	0.74
12:L:168:THR:HG22	42:L:317:DD6:C19	2.18	0.74
35:u:172:ASN:O	42:u:321:DD6:O4	2.06	0.73
38:t:172:LEU:HB2	42:t:312:DD6:O2	1.89	0.73
34:o:38:THR:OG1	34:o:41:ASP:OD2	2.07	0.73
5:E:50:ALA:O	5:E:70:ARG:NH2	2.22	0.73
40:w:308:CLA:CMC	42:w:312:DD6:C21	2.66	0.73
41:w:306:KC2:C1C	42:w:312:DD6:C7	2.66	0.73
40:E:311:CLA:HAA2	40:a:815:CLA:HBA1	1.67	0.73
12:L:52:PHE:HB2	42:L:315:DD6:O4	1.88	0.73
5:E:70:ARG:NH1	5:E:73:GLU:OE2	2.23	0.72
40:w:308:CLA:C2C	42:w:312:DD6:C21	2.67	0.72
36:q:181:PRO:CD	42:q:318:DD6:C26	2.65	0.72
22:Z:98:LYS:NZ	22:Z:107:ILE:O	2.23	0.71
30:j:1:MET:HG2	43:j:101:LMG:C8	2.20	0.71
1:A:41:PRO:O	1:A:62:ARG:NH2	2.23	0.71
37:r:115:VAL:O	37:r:118:SER:OG	2.07	0.71
5:E:137:PHE:CE1	43:E:321:LMG:H291	2.26	0.71
16:Q:177:GLN:OE1	44:Q:210:A86:O2	2.08	0.71
40:b:829:CLA:O1A	30:j:31:GLN:NE2	2.23	0.71
40:S:301:CLA:CHC	40:S:312:CLA:HMB1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:103:ILE:HG22	23:a:175:PHE:CE1	2.26	0.70
20:X:163:LYS:NZ	41:X:303:KC2:O1A	2.24	0.70
13:P:176:ASN:ND2	15:R:59:GLU:OE2	2.23	0.70
41:t:306:KC2:C1B	42:t:312:DD6:C2	2.68	0.70
4:D:103:ILE:CG2	23:a:175:PHE:HE1	2.00	0.70
4:D:103:ILE:HG23	23:a:175:PHE:CE1	2.18	0.70
1:A:62:ARG:NH1	1:A:65:GLU:OE1	2.24	0.70
17:S:142:PHE:HE2	40:S:301:CLA:HAB	1.57	0.70
40:E:302:CLA:HBB2	11:K:42:PRO:HB2	1.72	0.70
14:N:113:PRO:O	42:N:316:DD6:O4	2.10	0.70
35:p:172:ASN:O	42:p:322:DD6:O4	2.08	0.70
24:b:722:ALA:HB3	24:b:723:PRO:HD2	1.74	0.69
13:M:50:ASP:OD1	42:M:314:DD6:O4	2.09	0.69
24:b:422:LEU:HD13	24:b:532:LEU:HA	1.74	0.69
35:x:172:ASN:O	42:x:320:DD6:O4	2.08	0.69
40:F:301:CLA:CBC	44:N:315:A86:C11	2.69	0.69
29:i:13:VAL:HG21	40:i:101:CLA:HBC2	1.75	0.69
34:o:227:VAL:HG13	34:o:250:VAL:HG11	1.74	0.69
40:E:307:CLA:H51	40:a:819:CLA:C9	2.23	0.69
24:b:3:THR:OG1	29:i:33:GLU:OE1	2.10	0.69
41:w:306:KC2:C3C	42:w:312:DD6:C7	2.69	0.69
8:H:77:ARG:NH1	8:H:170:GLU:OE2	2.26	0.69
24:b:608:ALA:O	24:b:612:SER:OG	2.10	0.69
24:b:716:GLY:O	24:b:720:THR:HG22	1.93	0.69
32:l:133:VAL:HG21	49:l:208:BCR:H343	1.75	0.69
11:K:195:LEU:HD21	40:K:307:CLA:HED2	1.74	0.69
38:t:50:GLU:OE2	38:t:148:ARG:NH1	2.25	0.68
38:w:75:VAL:HG21	40:w:305:CLA:HBC3	1.76	0.68
35:x:247:TRP:O	35:x:251:ASN:ND2	2.26	0.68
5:E:77:ALA:HB1	5:E:172:GLY:HA3	1.75	0.68
41:w:306:KC2:C2B	42:w:312:DD6:C2	2.72	0.68
16:Q:129:VAL:C	16:Q:131:LYS:N	2.48	0.68
40:Q:206:CLA:H93	40:S:305:CLA:CAB	2.23	0.68
23:a:116:GLN:NE2	40:a:809:CLA:OBD	2.26	0.68
38:t:90:GLN:NE2	42:t:312:DD6:C29	2.56	0.68
6:F:152:ALA:C	6:F:156:GLN:HE21	2.02	0.68
40:A:308:CLA:HBC3	42:A:316:DD6:C7	2.24	0.68
12:L:196:SER:CB	42:L:317:DD6:C37	2.71	0.68
13:M:67:ARG:NH1	13:M:70:GLU:OE2	2.27	0.68
34:o:197:THR:OG1	34:o:200:MET:SD	2.45	0.67
24:b:722:ALA:HB3	24:b:723:PRO:CD	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:k:88:LEU:O	31:k:92:SER:OG	2.13	0.67
41:w:306:KC2:NC	42:w:312:DD6:C7	2.57	0.67
40:F:301:CLA:HBC2	44:N:315:A86:C11	2.24	0.67
12:L:168:THR:HA	42:L:317:DD6:O2	1.94	0.67
23:a:706:ASN:HB3	28:f:179:VAL:HG12	1.76	0.67
34:o:115:THR:OG1	34:o:118:ASP:OD1	2.05	0.67
40:L:306:CLA:HAA1	42:L:315:DD6:C37	2.25	0.67
43:E:320:LMG:O5	43:E:320:LMG:O4	2.12	0.67
18:U:78:MET:HE1	40:U:203:CLA:HBC3	1.75	0.66
41:w:306:KC2:C4B	42:w:312:DD6:C4	2.73	0.66
40:y:308:CLA:CMC	42:y:311:DD6:C21	2.73	0.66
12:L:196:SER:HB3	42:L:317:DD6:C37	2.26	0.66
35:p:74:LYS:NZ	40:p:305:CLA:O1D	2.27	0.66
15:T:89:GLY:O	15:T:109:ARG:NH2	2.29	0.66
38:w:90:GLN:CD	42:w:312:DD6:C37	2.69	0.66
11:K:177:ASN:ND2	40:K:301:CLA:OBD	2.29	0.66
16:Q:162:LYS:CE	41:Q:216:KC2:CGA	2.74	0.66
28:f:115:TYR:OH	28:f:157:PHE:O	2.09	0.66
41:t:306:KC2:C1C	42:t:312:DD6:C6	2.74	0.66
41:w:306:KC2:C2C	42:w:312:DD6:C7	2.73	0.66
20:X:78:GLU:OE1	20:X:165:GLY:N	2.29	0.66
7:G:43:SER:OG	41:Z:309:KC2:OBD	2.11	0.66
40:E:307:CLA:C3	40:a:819:CLA:H92	2.26	0.66
15:T:60:THR:OG1	13:W:175:LEU:O	2.09	0.65
41:t:306:KC2:C4C	42:t:312:DD6:C7	2.74	0.65
6:F:103:ARG:NH2	40:F:307:CLA:O1D	2.30	0.65
27:e:44:ARG:NH2	27:e:56:CYS:SG	2.69	0.65
36:q:181:PRO:CD	42:q:318:DD6:C29	2.73	0.65
25:c:24:ASP:OD1	26:d:100:HIS:ND1	2.30	0.65
31:k:75:HIS:HD1	46:k:205:SQD:HO2	1.43	0.65
4:D:110:ARG:NH1	4:D:113:GLU:OE2	2.29	0.65
15:O:42:THR:OG1	15:O:45:LYS:O	2.13	0.65
41:Y:308:KC2:C4B	42:Y:322:DD6:C2	2.75	0.65
4:D:80:ARG:HH12	43:D:318:LMG:HC8	1.61	0.65
13:P:54:ILE:HG23	47:P:301:A1EB1:O43	1.90	0.65
41:w:306:KC2:CHB	42:w:312:DD6:C24	2.75	0.65
11:K:71:ARG:NH1	11:K:174:GLU:OE2	2.30	0.64
40:Q:206:CLA:H91	40:S:305:CLA:HMB1	1.79	0.64
2:B:112:ASN:OD1	24:b:110:SER:OG	2.15	0.64
7:G:39:SER:OG	7:G:41:GLU:OE1	2.14	0.64
4:D:158:LEU:HB3	40:D:311:CLA:HBC1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:W:173:ASP:OD2	13:W:178:THR:OG1	2.09	0.64
41:t:306:KC2:C4B	42:t:312:DD6:C4	2.75	0.64
5:E:58:LEU:CD2	40:k:202:CLA:CBA	2.76	0.64
30:j:1:MET:CE	43:j:101:LMG:C29	2.52	0.64
35:u:98:ILE:O	47:u:322:A1EB1:O3	2.15	0.64
12:L:182:SER:O	12:L:186:ASN:ND2	2.31	0.63
22:Z:153:LYS:NZ	41:Z:303:KC2:O1A	2.30	0.63
35:u:42:VAL:HG13	36:v:149:ASN:ND2	2.13	0.63
16:Q:138:ASP:O	16:Q:139:TRP:C	2.39	0.63
40:b:832:CLA:H202	28:f:110:ALA:HB3	1.80	0.63
35:x:200:ARG:HA	35:x:203:MET:HE3	1.80	0.63
19:V:96:VAL:HG12	23:a:97:ARG:CZ	2.29	0.63
40:L:306:CLA:NA	42:L:315:DD6:C37	2.61	0.63
40:y:308:CLA:C3C	42:y:311:DD6:C21	2.76	0.63
40:A:306:CLA:HED2	28:f:154:SER:OG	1.98	0.63
4:D:153:GLY:O	4:D:156:SER:OG	2.16	0.63
4:D:231:ASN:ND2	4:D:236:LEU:O	2.32	0.63
6:F:144:MET:O	6:F:147:THR:OG1	2.09	0.63
24:b:307:ALA:HB3	40:b:835:CLA:HED1	1.79	0.63
10:J:105:GLU:N	10:J:105:GLU:OE2	2.32	0.63
38:y:138:LEU:O	38:y:141:ASP:C	2.42	0.62
10:J:118:ASP:OD2	42:J:315:DD6:O2	2.17	0.62
21:Y:211:ARG:O	21:Y:211:ARG:NE	2.26	0.62
24:b:707:LEU:CD2	52:b:850:DGD:HB72	2.29	0.62
38:t:89:TRP:HZ3	42:t:312:DD6:C29	2.12	0.62
6:F:151:PRO:O	6:F:155:GLY:N	2.24	0.62
15:T:146:MET:HE1	13:W:175:LEU:HA	1.80	0.62
11:K:63:ARG:NH2	40:K:306:CLA:O1D	2.32	0.62
16:Q:128:VAL:O	16:Q:131:LYS:HB2	1.99	0.62
41:Y:308:KC2:CHB	42:Y:322:DD6:C4	2.78	0.62
19:V:96:VAL:CG1	23:a:97:ARG:CZ	2.77	0.62
36:v:173:ILE:N	36:v:185:ASP:OD1	2.32	0.62
24:b:276:HIS:CE1	24:b:280:ILE:HD12	2.35	0.62
38:y:172:LEU:HB2	42:y:311:DD6:O2	1.99	0.62
16:Q:184:ALA:HB1	16:Q:185:PRO:HD2	1.82	0.62
41:Y:308:KC2:C1B	42:Y:322:DD6:C4	2.77	0.62
15:R:142:LYS:HA	15:R:142:LYS:CE	2.27	0.62
40:o:311:CLA:C18	42:o:320:DD6:C7	2.77	0.62
16:Q:127:VAL:HG13	16:Q:128:VAL:HG23	1.82	0.61
41:t:306:KC2:NB	42:t:312:DD6:C4	2.63	0.61
6:F:55:SER:OG	6:F:56:GLU:OE1	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:142:TRP:O	42:F:314:DD6:O4	2.18	0.61
35:p:98:ILE:O	47:p:323:A1EB1:O3	2.18	0.61
38:t:85:ASN:O	44:t:310:A86:O3	2.19	0.61
11:K:61:ARG:NH2	11:K:142:GLY:O	2.32	0.61
36:q:130:THR:HG21	36:q:256:LEU:HD21	1.82	0.61
36:q:221:ALA:HB1	36:q:232:VAL:HG21	1.83	0.61
3:C:44:ALA:HB1	3:C:65:ILE:HD12	1.81	0.61
5:E:63:VAL:HG11	40:a:819:CLA:C1	2.28	0.61
13:W:169:ILE:O	44:W:301:A86:O2	2.18	0.61
30:j:1:MET:HG2	43:j:101:LMG:C9	2.30	0.61
40:w:308:CLA:HMC1	42:w:312:DD6:C21	2.30	0.61
30:j:1:MET:HG2	43:j:101:LMG:HC92	1.83	0.61
15:R:138:GLU:OE2	15:R:144:HIS:NE2	2.32	0.61
40:J:309:CLA:HBC2	42:J:316:DD6:C8	2.31	0.61
40:y:308:CLA:HBC2	42:y:311:DD6:C21	2.30	0.61
40:E:307:CLA:H202	40:a:815:CLA:H43	1.82	0.61
13:W:78:MET:HB2	48:W:319:A1EB4:C4	2.31	0.61
4:D:103:ILE:HG22	23:a:175:PHE:HE1	1.62	0.60
38:w:90:GLN:OE1	42:w:312:DD6:C30	2.48	0.60
2:B:113:THR:O	2:B:113:THR:OG1	2.20	0.60
4:D:103:ILE:HG21	23:a:175:PHE:CE1	2.23	0.60
38:w:90:GLN:OE1	42:w:312:DD6:C29	2.49	0.60
6:F:86:LEU:HD13	40:F:307:CLA:H42	1.82	0.60
40:F:301:CLA:HBC1	44:N:315:A86:C21	2.31	0.60
13:P:106:VAL:HG12	40:P:308:CLA:HED1	1.84	0.60
10:J:198:LEU:HD21	42:J:316:DD6:C21	2.32	0.60
13:P:124:LEU:O	13:P:128:SER:OG	2.17	0.60
38:t:89:TRP:HZ3	42:t:312:DD6:C26	2.14	0.60
5:E:58:LEU:HD21	40:k:202:CLA:O1A	2.00	0.60
38:t:89:TRP:CZ3	42:t:312:DD6:C29	2.85	0.60
35:u:200:ARG:HA	35:u:203:MET:HE3	1.83	0.60
35:x:165:ASN:O	35:x:167:HIS:N	2.34	0.60
3:C:56:ASP:OD1	42:C:310:DD6:O2	2.20	0.60
17:S:142:PHE:CE2	40:S:301:CLA:HAB	2.37	0.60
5:E:87:TRP:CD1	5:E:195:TYR:HH	2.19	0.60
15:R:142:LYS:HA	15:R:142:LYS:HE2	1.82	0.60
40:F:301:CLA:CBC	44:N:315:A86:C10	2.79	0.59
40:E:311:CLA:O1A	40:a:815:CLA:HBA2	2.02	0.59
7:G:187:GLU:OE1	7:G:196:TYR:OH	2.13	0.59
19:V:92:ILE:HD13	23:a:157:THR:HA	1.84	0.59
23:a:370:HIS:ND1	40:a:830:CLA:OBD	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:t:90:GLN:HG2	42:t:312:DD6:C37	2.31	0.59
35:u:122:LYS:NZ	35:u:239:PRO:O	2.35	0.59
3:C:197:ILE:HG23	3:C:198:THR:HG23	1.84	0.59
34:o:152:GLU:OE2	34:o:165:TYR:OH	2.11	0.59
35:x:234:MET:HE1	40:x:306:CLA:HMC2	1.83	0.59
40:E:303:CLA:C4	46:P:319:SQD:H241	2.32	0.59
13:W:76:VAL:HG22	44:W:314:A86:O	2.02	0.59
40:E:307:CLA:H51	40:a:819:CLA:H92	1.85	0.59
11:K:77:THR:HG22	11:K:188:MET:HE3	1.85	0.59
15:T:159:ASP:OD2	15:T:164:THR:OG1	2.10	0.59
18:U:94:ARG:NH1	18:U:103:LEU:O	2.36	0.59
22:Z:56:GLY:O	22:Z:69:ILE:HD11	2.03	0.59
28:f:45:VAL:HG22	28:f:69:ILE:HD11	1.85	0.59
40:E:307:CLA:H51	40:a:819:CLA:H91	1.85	0.58
15:O:83:ALA:O	15:O:87:SER:OG	2.17	0.58
35:p:200:ARG:HA	35:p:203:MET:HE3	1.84	0.58
13:P:69:SER:OG	40:P:305:CLA:OBD	2.21	0.58
24:b:481:SER:O	24:b:482:THR:OG1	2.15	0.58
12:L:47:PHE:HE1	42:L:315:DD6:C36	2.16	0.58
24:b:719:PHE:O	24:b:723:PRO:CD	2.48	0.58
39:z:124:ASP:OD2	39:z:238:TYR:OH	2.21	0.58
5:E:198:ASN:ND2	5:E:202:ASP:OD1	2.37	0.58
5:E:118:LEU:HD21	40:a:815:CLA:H151	1.84	0.58
13:M:38:GLU:O	13:M:67:ARG:NH2	2.36	0.58
13:M:50:ASP:OD2	13:M:55:SER:OG	2.13	0.58
14:N:180:ARG:NH1	41:N:302:KC2:O1A	2.37	0.58
2:B:119:ARG:NH1	40:i:101:CLA:OBD	2.36	0.58
15:T:36:GLU:O	15:T:65:ARG:NH2	2.37	0.58
40:J:309:CLA:CBC	42:J:316:DD6:C5	2.82	0.58
28:f:176:GLY:C	28:f:178:GLU:H	2.11	0.58
6:F:135:ILE:HG22	6:F:150:PRO:CD	2.34	0.57
24:b:707:LEU:HD21	52:b:850:DGD:HB72	1.85	0.57
21:Y:38:LEU:HD23	21:Y:190:LEU:HG	1.87	0.57
36:q:238:LYS:NZ	47:t:314:A1EB1:O2	2.33	0.57
1:A:130:MET:SD	28:f:151:GLY:HA3	2.45	0.57
20:X:102:ARG:NH1	20:X:109:ALA:O	2.37	0.57
34:o:130:ASP:OD1	34:o:246:TYR:OH	2.14	0.57
39:z:79:GLU:OE1	39:z:166:GLY:N	2.37	0.57
8:H:34:ALA:O	8:H:35:LEU:HD22	2.04	0.57
23:a:81:LEU:HD22	40:a:823:CLA:HED1	1.87	0.57
34:o:84:LYS:NZ	34:o:148:GLU:OE1	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:q:81:ARG:NE	36:q:208:GLU:OE2	2.37	0.57
38:w:158:LEU:N	38:w:173:ASN:OD1	2.36	0.57
22:Z:36:LEU:CD1	22:Z:69:ILE:HD12	2.35	0.57
40:E:307:CLA:C2	40:a:819:CLA:H93	2.24	0.57
6:F:135:ILE:HG22	6:F:150:PRO:HD2	1.86	0.57
13:M:48:ILE:HD12	13:M:48:ILE:H	1.70	0.57
41:Y:308:KC2:NB	42:Y:322:DD6:C2	2.67	0.57
35:p:200:ARG:NH1	44:p:318:A86:O2	2.37	0.57
17:S:187:ALA:O	17:S:195:LYS:NZ	2.37	0.57
40:V:202:CLA:HMB1	13:W:127:LEU:HD13	1.86	0.57
4:D:134:HIS:ND1	4:D:138:PHE:O	2.38	0.57
4:D:178:ARG:NH2	43:j:101:LMG:O3	2.36	0.57
41:Y:308:KC2:CHB	42:Y:322:DD6:C3	2.83	0.57
41:Y:308:KC2:CHB	42:Y:322:DD6:C5	2.83	0.57
5:E:57:PRO:O	40:k:202:CLA:HAA2	2.05	0.56
13:P:54:ILE:HG22	47:P:301:A1EB1:C44	2.35	0.56
44:X:317:A86:C17	21:Y:177:TYR:OH	2.52	0.56
36:v:267:LEU:HD23	36:v:268:PHE:N	2.19	0.56
5:E:63:VAL:HG21	31:k:84:ILE:CG2	2.36	0.56
42:I:210:DD6:C41	46:I:215:SQD:H162	2.35	0.56
11:K:176:ASN:ND2	40:K:301:CLA:O1D	2.38	0.56
15:O:71:HIS:HB3	15:O:187:MET:HE3	1.86	0.56
24:b:430:GLY:HA2	24:b:525:LEU:HD22	1.87	0.56
36:v:93:GLN:NE2	47:v:322:A1EB1:O2	2.37	0.56
5:E:58:LEU:O	40:k:202:CLA:HED1	2.06	0.56
6:F:150:PRO:O	6:F:153:ALA:HB3	2.05	0.56
13:M:43:GLU:HG2	44:M:315:A86:C22	2.35	0.56
24:b:410:ARG:NE	40:b:828:CLA:OBD	2.33	0.56
38:w:145:HIS:ND1	38:w:147:VAL:HG22	2.21	0.56
38:y:85:ASN:O	44:y:310:A86:O3	2.23	0.56
40:P:308:CLA:CMB	42:P:315:DD6:C23	2.84	0.56
36:v:238:LYS:NZ	47:v:324:A1EB1:O2	2.24	0.56
42:y:311:DD6:C37	47:y:313:A1EB1:C16	2.84	0.56
12:L:200:ALA:HB1	12:L:216:LEU:HD13	1.87	0.56
24:b:410:ARG:O	24:b:414:HIS:ND1	2.39	0.56
40:b:810:CLA:H191	40:b:824:CLA:H193	1.87	0.56
35:u:189:ALA:O	35:u:193:VAL:HG23	2.06	0.56
5:E:157:GLY:O	13:M:59:SER:OG	2.17	0.56
21:Y:38:LEU:HD22	21:Y:194:ASN:OD1	2.06	0.56
22:Z:199:ASN:OD1	44:Z:316:A86:O2	2.24	0.56
35:x:189:ALA:O	35:x:193:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:p:170:PRO:HB2	35:p:171:LEU:HD12	1.88	0.56
13:M:107:ALA:HB2	40:M:307:CLA:HED3	1.88	0.56
24:b:571:SER:OG	24:b:574:ASP:OD2	2.24	0.56
34:o:227:VAL:CG1	34:o:250:VAL:HG11	2.36	0.56
41:y:306:KC2:C2B	42:y:311:DD6:C2	2.83	0.56
16:Q:37:ILE:O	16:Q:62:ARG:NH1	2.40	0.55
16:Q:140:GLU:O	16:Q:141:PRO:C	2.46	0.55
23:a:25:SER:OG	43:a:801:LMG:HC62	2.06	0.55
40:A:306:CLA:HED2	28:f:154:SER:CB	2.37	0.55
4:D:170:ALA:HB2	40:D:305:CLA:HMA1	1.88	0.55
32:l:20:PRO:O	32:l:24:SER:OG	2.21	0.55
32:l:85:LEU:HD11	40:l:202:CLA:C14	2.36	0.55
1:A:174:ILE:HG21	42:A:316:DD6:C24	2.37	0.55
16:Q:76:VAL:HG23	16:Q:174:LEU:HD22	1.88	0.55
16:Q:129:VAL:O	16:Q:131:LYS:N	2.39	0.55
21:Y:231:ALA:HB1	21:Y:234:ALA:HB2	1.88	0.55
25:c:81:TYR:HA	26:d:25:ALA:HB3	1.89	0.55
4:D:169:SER:O	4:D:172:SER:OG	2.20	0.55
36:v:185:ASP:O	42:v:320:DD6:O4	2.24	0.55
36:v:81:ARG:NE	36:v:208:GLU:OE2	2.37	0.55
4:D:244:ASP:OD2	13:M:123:LYS:NZ	2.37	0.55
10:J:110:ALA:H	10:J:115:THR:CG2	2.20	0.55
21:Y:88:GLN:OE1	44:Y:319:A86:O2	2.25	0.55
24:b:516:ASP:OD2	24:b:593:TYR:OH	2.16	0.55
9:I:67:GLU:OE2	9:I:163:ARG:NH1	2.39	0.55
24:b:26:ALA:HB2	52:b:850:DGD:HA32	1.89	0.55
36:v:223:VAL:CG1	36:v:246:VAL:HG11	2.37	0.55
4:D:69:VAL:HG12	4:D:79:ARG:HG3	1.88	0.54
4:D:158:LEU:CB	40:D:311:CLA:HBC1	2.37	0.54
40:v:312:CLA:H43	42:x:320:DD6:O2	2.07	0.54
38:w:172:LEU:HB2	42:w:312:DD6:O2	2.08	0.54
12:L:163:ASP:OD1	12:L:168:THR:OG1	2.25	0.54
19:V:92:ILE:HD11	23:a:157:THR:HA	1.86	0.54
40:w:308:CLA:HBC2	42:w:312:DD6:C21	2.37	0.54
35:p:189:ALA:O	35:p:193:VAL:HG23	2.07	0.54
16:Q:63:GLU:OE2	16:Q:139:TRP:NE1	2.38	0.54
40:Q:206:CLA:C9	40:S:305:CLA:HMB1	2.37	0.54
15:R:40:PRO:O	35:x:166:VAL:HG22	2.08	0.54
38:y:138:LEU:O	38:y:141:ASP:O	2.26	0.54
2:B:79:ILE:CD1	40:B:307:CLA:HMA1	2.37	0.54
44:D:319:A86:O3	40:M:305:CLA:O1D	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:156:GLU:OE1	23:a:156:GLU:N	2.40	0.54
4:D:90:VAL:O	4:D:110:ARG:NH2	2.40	0.54
16:Q:66:LEU:HD13	16:Q:142:GLY:HA3	1.90	0.54
23:a:130:ASP:OD1	28:f:51:ARG:NH2	2.40	0.54
39:z:71:GLU:OE2	39:z:71:GLU:N	2.40	0.54
32:l:58:LEU:HD22	32:l:85:LEU:HD23	1.89	0.54
38:y:75:VAL:HG21	40:y:305:CLA:HBC3	1.89	0.54
38:y:147:VAL:HG21	41:y:307:KC2:CMA	2.38	0.54
12:L:189:LEU:HG	42:L:317:DD6:C28	2.38	0.54
24:b:685:THR:O	24:b:689:ASN:ND2	2.41	0.54
40:b:833:CLA:H143	49:i:102:BCR:H362	1.90	0.54
38:t:89:TRP:CZ3	42:t:312:DD6:C26	2.90	0.54
5:E:59:LEU:HB2	40:k:202:CLA:HED1	1.90	0.53
15:R:67:ALA:O	15:R:71:HIS:ND1	2.38	0.53
20:X:123:ASP:OD2	20:X:238:TYR:OH	2.22	0.53
38:t:138:LEU:O	38:t:141:ASP:C	2.52	0.53
4:D:80:ARG:CZ	4:D:99:GLY:HA3	2.38	0.53
13:P:218:PRO:O	48:P:320:A1EB4:C42	2.57	0.53
35:x:110:ALA:O	47:x:322:A1EB1:O2	2.25	0.53
41:y:306:KC2:C1C	42:y:311:DD6:C7	2.86	0.53
40:Q:206:CLA:H43	17:S:134:PHE:CB	2.39	0.53
29:i:13:VAL:CG2	40:i:101:CLA:HBC2	2.38	0.53
14:N:135:ILE:HD13	40:N:310:CLA:HMB2	1.90	0.53
15:O:89:GLY:O	15:O:109:ARG:NH2	2.41	0.53
21:Y:159:PHE:O	21:Y:166:VAL:HG21	2.08	0.53
24:b:674:LEU:O	24:b:677:THR:OG1	2.20	0.53
44:G:209:A86:O5	40:G:213:CLA:HAB	2.09	0.53
12:L:118:ILE:HD11	40:L:307:CLA:H3A	1.91	0.53
17:S:61:PHE:H	17:S:69:THR:HG21	1.73	0.53
4:D:90:VAL:CG1	4:D:206:MET:HB2	2.39	0.53
16:Q:132:LEU:O	16:Q:133:ASP:C	2.51	0.53
20:X:106:ASP:OD1	20:X:109:ALA:N	2.37	0.53
38:t:47:THR:CG2	42:v:318:DD6:C37	2.80	0.53
41:t:306:KC2:C1B	42:t:312:DD6:C3	2.87	0.53
5:E:58:LEU:CD2	40:k:202:CLA:HAA1	2.36	0.53
5:E:201:GLU:OE1	5:E:201:GLU:N	2.41	0.53
40:K:308:CLA:HBC2	40:K:308:CLA:HHD	1.90	0.53
40:S:301:CLA:C1C	40:S:312:CLA:HMB1	2.39	0.53
35:x:98:ILE:O	47:x:321:A1EB1:O3	2.26	0.53
39:z:78:ARG:NH1	39:z:205:ILE:HD11	2.24	0.53
40:J:309:CLA:HBC3	42:J:316:DD6:C6	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:34:ASP:OD2	15:O:34:ASP:N	2.41	0.53
16:Q:132:LEU:HD23	16:Q:133:ASP:H	1.74	0.53
16:Q:162:LYS:HE3	41:Q:216:KC2:CGA	2.39	0.53
20:X:91:PHE:CE2	20:X:95:ILE:HD11	2.44	0.53
41:y:306:KC2:C1B	42:y:311:DD6:C2	2.85	0.53
39:z:78:ARG:NH1	39:z:82:ILE:HD11	2.24	0.53
43:u:301:LMG:HC91	43:u:301:LMG:O2	2.09	0.53
4:D:79:ARG:HH11	4:D:86:VAL:HG22	1.73	0.52
12:L:206:SER:HA	40:L:312:CLA:HMA3	1.91	0.52
17:S:48:VAL:HG22	45:S:323:LHG:HC82	1.90	0.52
13:W:135:TRP:NE1	46:W:318:SQD:H82	2.24	0.52
40:b:814:CLA:HBC1	33:m:10:ALA:HB1	1.91	0.52
6:F:214:ARG:HB3	40:F:307:CLA:HBC2	1.92	0.52
42:D:317:DD6:O1	43:E:301:LMG:HC61	2.09	0.52
35:u:247:TRP:O	35:u:251:ASN:ND2	2.42	0.52
24:b:611:GLU:N	24:b:611:GLU:OE1	2.42	0.52
10:J:112:SER:O	10:J:114:PHE:N	2.31	0.52
21:Y:50:LEU:HD23	21:Y:53:LEU:HD12	1.91	0.52
23:a:121:VAL:HG22	23:a:122:VAL:HG13	1.90	0.52
40:b:806:CLA:C19	49:f:206:BCR:H17C	2.39	0.52
32:l:138:LEU:HG	40:l:203:CLA:HED3	1.91	0.52
36:q:93:GLN:NE2	47:q:322:A1EB1:O2	2.42	0.52
16:Q:62:ARG:NH2	16:Q:65:GLU:OE1	2.43	0.52
40:T:305:CLA:H12	48:W:319:A1EB4:C47	2.40	0.52
9:I:66:ALA:O	9:I:70:HIS:ND1	2.42	0.52
37:r:71:PRO:HD2	37:r:74:ILE:HD12	1.92	0.52
13:P:97:LEU:HD12	13:P:106:VAL:HG21	1.92	0.52
36:v:132:SER:OG	41:v:308:KC2:OBD	2.24	0.52
35:x:122:LYS:NZ	35:x:239:PRO:O	2.41	0.52
5:E:63:VAL:HG21	31:k:84:ILE:HG22	1.92	0.52
35:x:240:THR:OG1	43:x:301:LMG:HC5	2.10	0.52
41:t:306:KC2:CHC	42:t:312:DD6:C5	2.87	0.52
3:C:173:MET:SD	41:C:303:KC2:O2A	2.68	0.51
40:E:308:CLA:H43	40:a:819:CLA:H93	1.91	0.51
35:p:97:GLY:O	35:p:102:ASN:ND2	2.43	0.51
36:v:126:ASP:OD2	36:v:242:TYR:OH	2.25	0.51
17:S:111:SER:HB2	40:S:308:CLA:HED1	1.92	0.51
13:W:135:TRP:HB3	46:W:318:SQD:H241	1.92	0.51
30:j:1:MET:CG	43:j:101:LMG:HC8	2.36	0.51
2:B:192:LEU:O	2:B:196:ILE:HD12	2.09	0.51
40:D:304:CLA:H93	40:W:306:CLA:H41	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:E:307:CLA:C5	40:a:819:CLA:H92	2.40	0.51
13:M:40:VAL:HG12	13:M:48:ILE:HA	1.92	0.51
14:N:67:ARG:NH1	14:N:70:GLU:OE2	2.44	0.51
41:Q:201:KC2:CBC	40:S:312:CLA:HBB2	2.39	0.51
28:f:176:GLY:HA2	28:f:179:VAL:HG22	1.92	0.51
42:y:311:DD6:C35	47:y:313:A1EB1:C17	2.88	0.51
12:L:168:THR:HG22	42:L:317:DD6:O2	2.10	0.51
17:S:200:LEU:O	17:S:204:ASN:ND2	2.43	0.51
23:a:679:ILE:HD11	40:a:835:CLA:HAB	1.92	0.51
39:z:146:GLU:OE2	39:z:159:TYR:OH	2.17	0.51
40:A:306:CLA:H111	40:f:205:CLA:HED3	1.92	0.51
40:Q:206:CLA:H43	17:S:134:PHE:HB3	1.91	0.51
13:W:98:ALA:HB3	13:W:101:VAL:HG22	1.92	0.51
31:k:75:HIS:ND1	46:k:205:SQD:O2	2.35	0.51
3:C:201:LEU:HD12	3:C:205:VAL:HG12	1.93	0.51
36:q:63:GLN:OE1	36:q:163:ARG:NH1	2.44	0.51
38:t:75:VAL:HG21	40:t:305:CLA:HBC3	1.91	0.51
36:v:74:HIS:ND1	36:v:167:PRO:O	2.41	0.51
40:A:305:CLA:H2	28:f:154:SER:HA	1.93	0.51
13:M:43:GLU:HG3	41:M:301:KC2:C4B	2.41	0.51
15:T:65:ARG:NH1	15:T:68:GLU:OE1	2.44	0.51
23:a:201:HIS:ND1	40:a:824:CLA:OBD	2.43	0.51
24:b:588:SER:HB3	24:b:717:PHE:HE1	1.76	0.51
1:A:185:VAL:CG2	40:A:311:CLA:HED2	2.39	0.51
16:Q:166:LEU:HD23	40:S:301:CLA:HBC1	1.94	0.51
19:V:99:VAL:HG22	40:j:102:CLA:HED1	1.93	0.51
35:u:145:ASP:OD2	35:u:161:THR:N	2.41	0.51
36:v:223:VAL:HG13	36:v:246:VAL:HG11	1.93	0.51
13:M:45:GLY:HA3	15:R:142:LYS:HE3	1.93	0.50
5:E:135:LYS:NZ	5:E:146:SER:OG	2.44	0.50
5:E:137:PHE:CE1	43:E:321:LMG:O9	2.64	0.50
10:J:114:PHE:HE1	10:J:197:ALA:HA	1.76	0.50
17:S:172:VAL:HG12	17:S:174:PRO:HD3	1.92	0.50
19:V:96:VAL:HG11	23:a:97:ARG:CZ	2.41	0.50
30:j:17:THR:O	30:j:21:SER:OG	2.19	0.50
36:q:80:GLY:O	36:q:84:MET:HG3	2.12	0.50
2:B:70:ARG:NH2	2:B:145:ASP:OD2	2.43	0.50
13:P:135:TRP:NE1	46:P:319:SQD:H92	2.25	0.50
40:S:314:CLA:H72	40:S:314:CLA:H41	1.92	0.50
40:A:306:CLA:H111	40:f:205:CLA:CED	2.42	0.50
4:D:90:VAL:HG11	4:D:206:MET:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:67:ARG:NH2	40:N:306:CLA:O1D	2.45	0.50
24:b:328:ASP:OD1	37:r:45:ARG:NH2	2.42	0.50
28:f:184:ARG:HD2	28:f:184:ARG:N	2.25	0.50
31:k:42:GLN:NE2	40:k:201:CLA:O2D	2.44	0.50
24:b:631:LEU:HD21	24:b:650:PHE:CG	2.46	0.50
40:b:809:CLA:HMB2	40:b:839:CLA:HMB2	1.93	0.50
40:J:309:CLA:HBC3	42:J:316:DD6:C5	2.41	0.50
16:Q:127:VAL:HG21	16:Q:139:TRP:CZ3	2.47	0.50
41:w:306:KC2:NB	42:w:312:DD6:C4	2.75	0.50
4:D:141:THR:OG1	4:D:144:GLU:OE1	2.24	0.50
5:E:58:LEU:HB3	31:k:84:ILE:HD13	1.94	0.50
40:E:303:CLA:O1A	46:P:319:SQD:O2	2.11	0.50
15:R:65:ARG:NH2	40:R:306:CLA:O1D	2.45	0.50
21:Y:194:ASN:ND2	44:Y:320:A86:O2	2.45	0.50
40:b:806:CLA:H192	49:f:206:BCR:H17C	1.94	0.50
36:q:185:ASP:O	42:q:320:DD6:O4	2.29	0.50
38:w:201:ARG:HA	38:w:204:MET:HE3	1.94	0.50
1:A:128:TRP:CD2	28:f:158:LEU:HD23	2.47	0.50
1:A:130:MET:SD	28:f:151:GLY:CA	3.00	0.50
5:E:217:LEU:HD21	40:P:305:CLA:C15	2.41	0.50
15:T:98:VAL:N	41:T:308:KC2:O1A	2.44	0.50
21:Y:72:ILE:HD12	21:Y:153:PRO:HB2	1.93	0.50
23:a:373:ALA:HB2	40:a:832:CLA:HBC3	1.93	0.50
43:x:301:LMG:H171	40:x:312:CLA:H121	1.94	0.50
4:D:71:SER:OG	4:D:74:LEU:O	2.30	0.49
11:K:149:ALA:HB3	11:K:152:ASP:HB2	1.94	0.49
40:b:802:CLA:HAA2	40:f:202:CLA:HMB1	1.94	0.49
38:t:145:HIS:ND1	38:t:147:VAL:HG22	2.27	0.49
36:v:211:ASN:OD1	40:v:301:CLA:HMD1	2.12	0.49
5:E:118:LEU:CD2	40:a:815:CLA:C15	2.79	0.49
10:J:100:ARG:NH2	10:J:111:THR:HG23	2.26	0.49
14:N:43:GLU:N	14:N:43:GLU:OE1	2.44	0.49
28:f:39:LYS:HD3	28:f:39:LYS:C	2.37	0.49
35:p:47:ASP:OD1	35:p:50:GLY:N	2.46	0.49
42:B:305:DD6:C37	3:C:134:ILE:HD12	2.42	0.49
6:F:104:GLU:OE1	6:F:186:GLY:N	2.42	0.49
7:G:36:VAL:O	7:G:65:ARG:NH2	2.45	0.49
13:M:139:ALA:HB1	46:M:318:SQD:H441	1.94	0.49
13:M:175:LEU:O	15:O:60:THR:OG1	2.21	0.49
19:V:99:VAL:HG21	40:j:102:CLA:O2D	2.11	0.49
22:Z:36:LEU:HD11	22:Z:69:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:w:44:ILE:HG22	44:w:316:A86:C40	2.42	0.49
23:a:266:THR:HG22	31:k:42:GLN:HB2	1.94	0.49
24:b:71:GLN:NE2	40:b:814:CLA:O1D	2.43	0.49
35:x:215:ILE:HG23	35:x:215:ILE:O	2.12	0.49
13:W:138:GLU:OE2	13:W:144:TYR:OH	2.16	0.49
43:j:101:LMG:O5	43:j:101:LMG:O4	2.18	0.49
40:A:308:CLA:HBC3	42:A:316:DD6:C6	2.42	0.49
40:S:301:CLA:CHC	40:S:312:CLA:CMB	2.90	0.49
22:Z:153:LYS:CE	22:Z:194:LEU:HD11	2.42	0.49
35:x:214:LYS:NZ	35:x:231:GLY:O	2.41	0.49
40:A:306:CLA:CED	28:f:154:SER:CB	2.91	0.49
18:U:45:LEU:O	18:U:51:ASN:ND2	2.45	0.49
21:Y:167:PRO:HG3	40:z:306:CLA:H91	1.95	0.49
26:d:35:THR:HG22	26:d:60:LEU:HD13	1.95	0.49
36:v:182:VAL:HG23	40:v:311:CLA:HED1	1.94	0.49
36:v:227:LYS:NZ	36:v:243:SER:O	2.46	0.49
9:I:99:PRO:O	42:I:212:DD6:O4	2.30	0.49
11:K:50:GLY:HA3	13:P:59:SER:OG	2.12	0.49
17:S:65:GLY:O	17:S:69:THR:HG23	2.12	0.49
36:q:267:LEU:HD22	36:q:268:PHE:H	1.77	0.49
38:w:187:GLU:OE1	38:w:187:GLU:N	2.43	0.49
7:G:60:ASN:ND2	9:I:45:TYR:O	2.46	0.49
12:L:76:MET:SD	42:L:317:DD6:C5	3.01	0.49
26:d:38:SER:OG	26:d:40:LYS:O	2.31	0.49
1:A:128:TRP:CE3	28:f:158:LEU:HD23	2.48	0.48
17:S:113:ALA:O	17:S:116:LEU:HD12	2.12	0.48
18:U:181:PHE:HA	18:U:184:VAL:HG22	1.95	0.48
23:a:99:SER:OG	23:a:100:ASN:N	2.45	0.48
24:b:722:ALA:O	24:b:723:PRO:C	2.53	0.48
40:b:809:CLA:H13	49:m:101:BCR:H14C	1.95	0.48
40:F:301:CLA:HBC2	44:N:315:A86:C12	2.43	0.48
12:L:168:THR:CA	42:L:317:DD6:O2	2.60	0.48
13:W:129:ILE:CD1	40:W:312:CLA:HBC1	2.43	0.48
34:o:225:GLY:O	34:o:236:VAL:HG21	2.13	0.48
47:v:324:A1EB1:O2	42:w:312:DD6:C37	2.61	0.48
38:y:58:ALA:O	38:y:62:HIS:ND1	2.47	0.48
16:Q:57:ASP:OD2	16:Q:136:TRP:NE1	2.33	0.48
3:C:59:GLY:O	3:C:62:THR:OG1	2.21	0.48
10:J:113:SER:O	10:J:114:PHE:C	2.56	0.48
18:U:169:ALA:O	18:U:173:HIS:ND1	2.43	0.48
23:a:455:LEU:HD23	23:a:534:LEU:CD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:542:ARG:NH2	26:d:129:ASN:OD1	2.46	0.48
29:i:13:VAL:HG22	40:i:101:CLA:HMC1	1.95	0.48
40:E:306:CLA:H52	49:a:843:BCR:H312	1.94	0.48
40:Q:206:CLA:O1A	17:S:131:ALA:HB1	2.14	0.48
40:A:306:CLA:C6	28:f:150:LEU:HD13	2.37	0.48
15:R:63:TRP:CE3	15:R:145:TYR:HE1	2.32	0.48
36:v:245:GLU:HG2	40:v:312:CLA:HMA1	1.94	0.48
5:E:58:LEU:HD21	40:k:202:CLA:CGA	2.42	0.48
15:T:137:SER:O	15:T:141:VAL:HG22	2.14	0.48
32:l:68:LEU:HD12	32:l:77:VAL:HG21	1.95	0.48
3:C:44:ALA:CB	3:C:65:ILE:HD12	2.44	0.48
12:L:109:VAL:HG21	12:L:117:MET:SD	2.54	0.48
40:b:814:CLA:H18	49:i:102:BCR:HC7	1.94	0.48
6:F:201:ALA:HB2	16:Q:133:ASP:O	2.14	0.48
19:V:92:ILE:CD1	23:a:157:THR:CA	2.89	0.48
24:b:649:MET:HB3	24:b:723:PRO:HG3	1.95	0.48
40:b:809:CLA:H112	49:m:101:BCR:H12C	1.95	0.48
10:J:153:ARG:NH1	10:J:157:GLU:O	2.45	0.47
23:a:294:THR:HG23	40:a:816:CLA:HMA3	1.95	0.47
24:b:424:TRP:HZ3	40:b:813:CLA:HBC2	1.79	0.47
40:b:826:CLA:C14	52:b:850:DGD:HAE2	2.43	0.47
40:k:202:CLA:HBB2	46:k:205:SQD:H251	1.95	0.47
49:a:845:BCR:H393	49:a:845:BCR:H23C	1.96	0.47
24:b:60:TRP:NE1	40:b:824:CLA:OBD	2.47	0.47
28:f:176:GLY:C	28:f:178:GLU:N	2.71	0.47
36:q:251:ALA:N	36:q:254:ASP:OD1	2.43	0.47
6:F:112:MET:SD	40:F:305:CLA:HBC3	2.54	0.47
15:R:144:HIS:CE1	15:R:145:TYR:CE2	3.03	0.47
23:a:532:ASP:O	23:a:536:HIS:ND1	2.44	0.47
3:C:32:ARG:NH2	8:H:143:ASP:OD2	2.47	0.47
40:E:311:CLA:O1A	40:a:815:CLA:O2A	2.33	0.47
13:W:129:ILE:HD12	40:W:312:CLA:HBC1	1.96	0.47
40:b:813:CLA:HMC3	40:f:202:CLA:HBC2	1.96	0.47
38:t:86:ILE:HG23	38:t:87:GLN:HG3	1.96	0.47
41:t:306:KC2:C4B	42:t:312:DD6:C5	2.92	0.47
40:D:306:CLA:HED3	40:D:306:CLA:O1A	2.13	0.47
12:L:76:MET:HG2	42:L:317:DD6:C3	2.44	0.47
21:Y:92:HIS:CD2	21:Y:103:THR:HG23	2.50	0.47
12:L:40:PRO:HG2	12:L:185:LYS:HE2	1.97	0.47
13:W:141:LYS:NZ	41:W:310:KC2:O2D	2.47	0.47
23:a:667:SER:HB2	24:b:445:ALA:HB1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:t:58:ALA:O	38:t:62:HIS:ND1	2.47	0.47
1:A:129:THR:HG23	28:f:155:GLY:HA3	1.96	0.47
5:E:63:VAL:HG12	40:a:819:CLA:H43	1.96	0.47
40:E:308:CLA:H41	40:a:819:CLA:H102	1.95	0.47
10:J:112:SER:C	10:J:114:PHE:N	2.73	0.47
10:J:187:MET:HE1	42:J:316:DD6:C24	2.42	0.47
12:L:168:THR:CG2	42:L:317:DD6:C19	2.90	0.47
18:U:171:LEU:HD21	18:U:175:ARG:CZ	2.45	0.47
36:q:267:LEU:HD22	36:q:268:PHE:N	2.29	0.47
37:r:99:LEU:HD21	49:r:201:BCR:H371	1.97	0.47
35:u:46:TRP:NE1	47:u:323:A1EB1:O5	2.46	0.47
35:x:240:THR:HG21	43:x:301:LMG:O6	2.15	0.47
17:S:111:SER:CB	40:S:308:CLA:HED1	2.45	0.47
7:G:48:ASP:OD2	7:G:53:SER:OG	2.30	0.47
8:H:77:ARG:NH2	8:H:147:GLY:O	2.47	0.47
9:I:119:GLY:O	9:I:123:VAL:HG13	2.15	0.47
24:b:585:ASN:O	24:b:588:SER:OG	2.29	0.47
5:E:140:MET:HE3	5:E:140:MET:HA	1.95	0.46
50:b:849:PQN:H141	40:l:202:CLA:CBB	2.45	0.46
38:t:147:VAL:HG21	41:t:308:KC2:CMA	2.45	0.46
10:J:101:ALA:CB	40:J:318:CLA:HBC3	2.46	0.46
16:Q:61:LEU:HD23	40:Q:204:CLA:O1A	2.15	0.46
21:Y:184:ARG:NH2	44:Y:315:A86:O2	2.48	0.46
38:t:89:TRP:HZ3	42:t:312:DD6:C27	2.29	0.46
36:v:183:PRO:HG2	42:v:318:DD6:C4	2.46	0.46
13:P:69:SER:O	13:P:73:HIS:ND1	2.48	0.46
40:b:832:CLA:H202	28:f:110:ALA:CB	2.44	0.46
40:b:834:CLA:CBC	40:b:835:CLA:H202	2.46	0.46
41:t:306:KC2:CHC	42:t:312:DD6:C6	2.93	0.46
35:x:106:GLU:OE1	35:x:107:GLY:N	2.45	0.46
8:H:71:ALA:O	8:H:75:HIS:ND1	2.44	0.46
9:I:144:GLN:NE2	32:l:23:THR:O	2.48	0.46
24:b:373:THR:HG21	24:b:721:PHE:CD1	2.50	0.46
52:b:850:DGD:HD2	52:b:850:DGD:HG32	1.61	0.46
34:o:108:ALA:O	44:o:315:A86:O3	2.32	0.46
40:p:306:CLA:HBC3	47:p:324:A1EB1:C7	2.45	0.46
38:t:51:THR:OG1	47:t:315:A1EB1:O2	2.11	0.46
36:v:97:ILE:HG22	36:v:97:ILE:O	2.15	0.46
3:C:139:ARG:O	3:C:143:VAL:HG23	2.15	0.46
12:L:212:ASN:O	12:L:213:ALA:C	2.58	0.46
24:b:203:ARG:NH2	24:b:238:ASP:OD2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:722:ALA:CB	24:b:723:PRO:CD	2.92	0.46
34:o:249:GLU:HG2	40:o:312:CLA:HMA1	1.97	0.46
35:p:114:TRP:CE3	35:p:117:ILE:HD11	2.51	0.46
35:u:42:VAL:HG13	36:v:149:ASN:HD22	1.79	0.46
7:G:76:MET:HE3	7:G:173:GLY:CA	2.45	0.46
18:U:45:LEU:HG	18:U:46:GLN:NE2	2.31	0.46
24:b:437:TYR:CD2	40:b:807:CLA:H203	2.51	0.46
38:t:133:GLU:OE1	38:t:145:HIS:NE2	2.47	0.46
40:A:305:CLA:H12	28:f:157:PHE:HB3	1.98	0.46
12:L:96:SER:O	12:L:96:SER:OG	2.31	0.46
2:B:123:MET:O	2:B:127:VAL:HG23	2.16	0.46
40:J:309:CLA:HBC2	42:J:316:DD6:C5	2.46	0.46
13:M:173:ASP:OD2	13:M:178:THR:OG1	2.29	0.46
24:b:69:ALA:HB2	24:b:135:LEU:HB2	1.97	0.46
28:f:24:ASP:N	28:f:28:LEU:O	2.48	0.46
38:t:172:LEU:CB	42:t:312:DD6:O2	2.62	0.46
41:L:303:KC2:CHB	42:L:317:DD6:C21	2.94	0.46
15:O:154:VAL:HG11	15:O:157:LEU:HD12	1.97	0.46
19:V:96:VAL:HG12	23:a:97:ARG:NH1	2.31	0.46
13:W:155:GLN:O	13:W:171:PHE:N	2.43	0.46
20:X:219:SER:O	20:X:222:LYS:C	2.59	0.46
24:b:293:THR:OG1	40:b:819:CLA:OBD	2.31	0.46
36:q:223:VAL:HG11	36:q:246:VAL:HG11	1.98	0.46
35:x:247:TRP:NE1	35:x:249:ILE:O	2.43	0.46
39:z:84:HIS:CD2	40:z:305:CLA:HMD3	2.50	0.46
40:A:308:CLA:CBC	42:A:316:DD6:C7	2.93	0.46
40:E:307:CLA:H43	40:E:307:CLA:HED3	1.98	0.46
13:M:221:ASP:OD1	13:M:223:SER:OG	2.32	0.46
15:O:187:MET:HE2	42:O:314:DD6:C5	2.46	0.46
24:b:439:HIS:CD2	24:b:453:ILE:HG22	2.51	0.46
38:t:190:GLU:N	38:t:190:GLU:OE1	2.49	0.46
40:E:306:CLA:HBA1	43:E:321:LMG:H361	1.96	0.45
16:Q:166:LEU:CD2	40:S:301:CLA:HBC1	2.46	0.45
21:Y:162:MET:HE1	21:Y:164:HIS:CD2	2.51	0.45
12:L:65:ARG:NH2	40:L:306:CLA:O1D	2.49	0.45
15:O:161:LEU:HD12	15:O:163:PHE:CZ	2.52	0.45
15:R:144:HIS:CE1	15:R:146:MET:HG2	2.51	0.45
17:S:51:PHE:CD1	45:S:323:LHG:HC42	2.50	0.45
17:S:193:GLU:OE1	17:S:193:GLU:N	2.50	0.45
21:Y:42:LEU:HD11	21:Y:45:TRP:CE3	2.51	0.45
24:b:415:LYS:HB2	24:b:539:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:456:GLU:OE1	28:f:93:HIS:ND1	2.49	0.45
38:w:138:LEU:O	38:w:141:ASP:C	2.59	0.45
5:E:60:LEU:HD22	40:E:308:CLA:H42	1.98	0.45
11:K:50:GLY:HA3	13:P:59:SER:CB	2.47	0.45
13:W:139:ALA:CB	46:W:318:SQD:H462	2.46	0.45
41:Y:308:KC2:C2B	42:Y:322:DD6:C4	2.94	0.45
11:K:49:PHE:HA	13:P:62:ALA:HB2	1.98	0.45
20:X:60:SER:O	20:X:69:ASN:ND2	2.49	0.45
34:o:128:GLN:OE1	40:o:307:CLA:HED3	2.16	0.45
4:D:93:VAL:HG22	40:D:307:CLA:HMD1	1.99	0.45
40:E:306:CLA:H51	49:a:843:BCR:C3	2.29	0.45
46:I:215:SQD:H442	46:I:215:SQD:O49	2.15	0.45
40:J:309:CLA:C2C	42:J:316:DD6:C3	2.95	0.45
40:Q:206:CLA:H162	17:S:139:PHE:HB2	1.99	0.45
24:b:373:THR:HG21	24:b:721:PHE:HD1	1.81	0.45
40:A:306:CLA:CED	28:f:154:SER:OG	2.63	0.45
5:E:58:LEU:HD23	40:k:202:CLA:HBA1	1.96	0.45
40:J:309:CLA:CBC	42:J:316:DD6:C7	2.95	0.45
23:a:121:VAL:HG21	30:j:28:ILE:HG23	1.98	0.45
27:e:76:GLU:OE2	27:e:76:GLU:N	2.44	0.45
35:p:122:LYS:NZ	35:p:239:PRO:O	2.49	0.45
16:Q:128:VAL:HG13	16:Q:136:TRP:CH2	2.52	0.45
34:o:214:ASN:ND2	40:o:301:CLA:O1D	2.50	0.45
8:H:175:ARG:HB3	40:H:307:CLA:HBC2	1.99	0.45
18:U:145:ARG:NH1	18:U:146:LYS:O	2.50	0.45
41:t:306:KC2:C2B	42:t:312:DD6:C3	2.94	0.45
35:u:90:ALA:HB2	35:u:110:ALA:HB2	1.98	0.45
38:w:147:VAL:HG21	41:w:307:KC2:CMA	2.47	0.45
40:y:308:CLA:HMC1	42:y:311:DD6:C21	2.47	0.45
10:J:112:SER:C	10:J:114:PHE:H	2.19	0.45
10:J:114:PHE:CE1	10:J:197:ALA:HA	2.52	0.45
15:T:167:LEU:HD12	34:o:63:ASP:OD1	2.17	0.45
40:b:810:CLA:H92	52:b:850:DGD:HBT1	1.99	0.45
27:e:52:TRP:NE1	27:e:77:LYS:O	2.43	0.45
8:H:169:LYS:O	8:H:173:HIS:ND1	2.51	0.44
12:L:47:PHE:CZ	42:L:315:DD6:C40	3.00	0.44
13:M:115:TRP:O	13:M:123:LYS:NZ	2.50	0.44
13:M:190:ARG:NH1	41:M:303:KC2:O1A	2.49	0.44
13:W:219:ALA:HB3	48:W:319:A1EB4:C42	2.45	0.44
38:w:172:LEU:CB	42:w:312:DD6:O2	2.65	0.44
10:J:107:LEU:HD13	10:J:107:LEU:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L:306:CLA:HHC	42:L:315:DD6:C25	2.48	0.44
28:f:174:VAL:HG22	28:f:175:PRO:HD2	1.97	0.44
30:j:8:TYR:O	30:j:11:THR:HG22	2.17	0.44
9:I:45:TYR:HH	9:I:52:SER:HG	1.66	0.44
25:c:81:TYR:HA	26:d:25:ALA:CB	2.47	0.44
35:x:240:THR:HG21	43:x:301:LMG:HC5	1.99	0.44
46:F:320:SQD:H111	46:F:320:SQD:O49	2.17	0.44
15:T:83:ALA:O	15:T:87:SER:OG	2.17	0.44
23:a:661:SER:O	23:a:664:SER:OG	2.33	0.44
24:b:704:GLN:HG3	52:b:850:DGD:HA31	1.99	0.44
40:w:308:CLA:CBB	42:w:312:DD6:C12	2.95	0.44
38:t:90:GLN:CD	42:t:312:DD6:C37	2.90	0.44
3:C:85:ALA:HA	3:C:188:ILE:HD12	2.00	0.44
40:L:305:CLA:CMC	42:L:315:DD6:C8	2.96	0.44
23:a:672:ILE:HD11	40:a:808:CLA:HMC3	1.98	0.44
24:b:559:CYS:SG	24:b:561:GLY:N	2.85	0.44
36:q:182:VAL:HG23	40:q:311:CLA:HED1	2.00	0.44
41:y:306:KC2:NC	42:y:311:DD6:C7	2.80	0.44
14:N:69:ALA:O	14:N:73:HIS:ND1	2.50	0.44
40:S:301:CLA:HHC	40:S:312:CLA:CMB	2.48	0.44
44:L:314:A86:C39	42:L:315:DD6:C10	2.95	0.44
13:W:200:ALA:HB2	48:W:319:A1EB4:C	2.48	0.44
40:A:306:CLA:HED2	28:f:154:SER:HB3	1.99	0.44
13:P:54:ILE:CG2	47:P:301:A1EB1:C44	2.96	0.44
15:R:144:HIS:O	15:R:146:MET:N	2.51	0.44
35:p:71:SER:O	35:p:75:HIS:ND1	2.45	0.44
10:J:129:LEU:HD23	10:J:133:CYS:SG	2.58	0.43
12:L:207:VAL:O	12:L:211:ALA:HB2	2.18	0.43
13:M:54:ILE:O	13:M:58:VAL:HG22	2.18	0.43
48:P:320:A1EB4:C47	40:R:305:CLA:H42	2.48	0.43
15:T:136:LEU:O	15:T:140:ALA:HB3	2.18	0.43
38:w:133:GLU:OE1	38:w:145:HIS:NE2	2.48	0.43
40:E:306:CLA:H52	49:a:843:BCR:HC32	1.93	0.43
14:N:116:GLN:O	14:N:120:VAL:HG23	2.19	0.43
16:Q:59:ASN:HD22	16:Q:141:PRO:HG2	1.84	0.43
18:U:158:LEU:HD22	18:U:167:TYR:CE2	2.53	0.43
23:a:438:ILE:HG13	23:a:556:PHE:HE2	1.83	0.43
23:a:441:LEU:HD23	23:a:548:LEU:HA	2.00	0.43
24:b:302:LYS:NZ	24:b:324:GLU:OE2	2.47	0.43
34:o:115:THR:N	34:o:118:ASP:OD1	2.51	0.43
36:q:46:VAL:HG22	38:t:164:MET:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:190:ALA:HB2	42:L:317:DD6:C1	2.48	0.43
41:T:301:KC2:CMB	35:p:166:VAL:HG12	2.48	0.43
22:Z:102:ALA:HB3	22:Z:103:PRO:HD3	1.98	0.43
49:m:101:BCR:H24C	49:m:101:BCR:H371	1.89	0.43
2:B:62:VAL:N	2:B:155:ASP:OD1	2.48	0.43
3:C:166:SER:O	3:C:170:VAL:HG23	2.18	0.43
5:E:63:VAL:HG12	40:a:819:CLA:C3	2.45	0.43
40:F:306:CLA:O1A	40:F:307:CLA:H43	2.19	0.43
13:P:73:HIS:CD2	40:P:305:CLA:HMD2	2.54	0.43
24:b:203:ARG:NH2	24:b:253:ALA:O	2.43	0.43
29:i:23:PHE:HZ	49:i:102:BCR:H353	1.83	0.43
49:l:207:BCR:C8	49:l:207:BCR:H331	2.48	0.43
36:q:267:LEU:CB	35:u:249:ILE:HD11	2.48	0.43
40:A:306:CLA:H92	28:f:154:SER:OG	2.17	0.43
40:J:309:CLA:HBC3	42:J:316:DD6:C7	2.47	0.43
16:Q:104:MET:HE3	40:Q:207:CLA:HED3	2.00	0.43
15:T:48:ASP:OD1	15:T:51:GLY:N	2.51	0.43
35:x:71:SER:O	35:x:75:HIS:ND1	2.44	0.43
38:y:164:MET:SD	38:y:164:MET:N	2.92	0.43
41:y:306:KC2:CHB	42:y:311:DD6:C2	2.96	0.43
40:D:303:CLA:HED2	40:D:303:CLA:H43	2.00	0.43
40:F:301:CLA:HBC3	44:N:315:A86:C11	2.39	0.43
40:V:202:CLA:H42	40:W:305:CLA:H43	2.00	0.43
24:b:436:LEU:HD21	40:b:829:CLA:HMB1	2.00	0.43
40:b:827:CLA:O1A	40:b:834:CLA:H42	2.19	0.43
38:y:146:TYR:OH	40:y:302:CLA:HED3	2.18	0.43
12:L:210:LEU:C	12:L:212:ASN:H	2.26	0.43
13:P:209:THR:HG21	40:P:313:CLA:HMD2	2.01	0.43
40:P:308:CLA:H141	48:P:320:A1EB4:C46	2.49	0.43
16:Q:132:LEU:HD23	16:Q:133:ASP:N	2.33	0.43
15:R:114:ALA:O	15:R:118:VAL:HG23	2.18	0.43
40:W:311:CLA:H11	48:W:319:A1EB4:C7	2.48	0.43
32:l:68:LEU:CD1	32:l:77:VAL:HG21	2.48	0.43
1:A:179:MET:HB3	1:A:190:LEU:HD13	2.01	0.43
17:S:121:GLN:NE2	40:S:308:CLA:HED2	2.34	0.43
40:V:201:CLA:H61	40:a:814:CLA:HBA2	2.01	0.43
23:a:443:TRP:NE1	40:a:842:CLA:OBD	2.47	0.43
36:v:43:LEU:HD22	36:v:210:ASN:OD1	2.19	0.43
4:D:79:ARG:NH1	4:D:86:VAL:HG22	2.34	0.43
4:D:80:ARG:O	4:D:81:GLU:HG2	2.19	0.43
15:T:141:VAL:O	15:T:141:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Z:160:PHE:CE2	22:Z:171:VAL:HG11	2.53	0.43
40:Z:306:CLA:H61	40:Z:306:CLA:H41	1.92	0.43
23:a:235:GLN:OE1	23:a:235:GLN:N	2.51	0.43
23:a:584:CYS:O	24:b:669:GLY:N	2.49	0.43
35:p:109:SER:O	35:p:113:VAL:HG13	2.18	0.43
35:p:209:PHE:HE1	35:p:222:LEU:HD21	1.84	0.43
35:u:247:TRP:NE1	35:u:249:ILE:O	2.48	0.43
40:A:308:CLA:CBC	42:A:316:DD6:C6	2.97	0.43
13:P:42:GLU:HA	39:z:149:VAL:HG21	2.01	0.43
13:P:217:VAL:HG13	48:P:320:A1EB4:C42	2.49	0.43
13:P:217:VAL:HB	13:P:220:LEU:HD12	2.01	0.43
15:T:196:ALA:HB2	15:T:206:LEU:HD23	2.01	0.43
21:Y:162:MET:SD	21:Y:163:VAL:N	2.92	0.43
23:a:178:TRP:CZ2	43:a:802:LMG:HC72	2.54	0.43
40:b:806:CLA:H61	40:b:806:CLA:H41	1.88	0.43
28:f:163:ALA:CB	49:f:206:BCR:H332	2.49	0.43
34:o:103:VAL:O	34:o:103:VAL:HG12	2.19	0.43
41:o:308:KC2:CAB	42:o:320:DD6:C2	2.97	0.43
36:q:148:GLU:OE2	36:q:161:TYR:OH	2.15	0.43
35:x:51:LEU:HD23	35:x:54:LEU:HD12	2.01	0.43
41:y:306:KC2:C4B	42:y:311:DD6:C4	2.96	0.43
40:E:303:CLA:H42	46:P:319:SQD:H241	2.00	0.42
8:H:132:ASN:OD1	24:b:295:TRP:NE1	2.49	0.42
40:N:304:CLA:H43	40:N:305:CLA:HMD1	2.01	0.42
17:S:231:HIS:NE2	40:S:319:CLA:HED3	2.34	0.42
20:X:65:TRP:NE1	44:X:317:A86:O1	2.51	0.42
22:Z:209:MET:HA	22:Z:212:VAL:HG22	2.01	0.42
40:Z:305:CLA:C2	40:Z:305:CLA:HMA2	2.48	0.42
23:a:383:ASP:OD2	23:a:386:THR:OG1	2.30	0.42
23:a:707:LYS:HA	28:f:174:VAL:HG12	2.00	0.42
15:T:73:ARG:NH2	41:T:303:KC2:O1D	2.52	0.42
28:f:173:LEU:HD22	40:f:202:CLA:HBA1	2.00	0.42
36:q:255:ASN:O	36:q:256:LEU:HD23	2.19	0.42
39:z:164:LYS:NZ	41:z:304:KC2:O1A	2.46	0.42
9:I:95:LEU:HD22	9:I:105:GLN:HB3	2.01	0.42
24:b:413:GLN:O	28:f:184:ARG:NH2	2.52	0.42
25:c:54:CYS:SG	25:c:55:GLU:N	2.92	0.42
28:f:175:PRO:HG2	28:f:178:GLU:CD	2.45	0.42
35:x:240:THR:HG21	43:x:301:LMG:C5	2.49	0.42
16:Q:156:ARG:NE	41:Q:201:KC2:O1A	2.52	0.42
17:S:41:ALA:HB1	17:S:49:GLY:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:359:MET:HE3	40:a:832:CLA:H43	2.02	0.42
26:d:46:MET:SD	26:d:61:LEU:HD11	2.59	0.42
35:p:242:PRO:HB2	35:p:244:THR:HG23	2.01	0.42
36:q:223:VAL:CG1	36:q:246:VAL:HG11	2.49	0.42
39:z:78:ARG:HH12	39:z:205:ILE:HD11	1.83	0.42
39:z:206:ASN:ND2	40:z:302:CLA:O1D	2.48	0.42
3:C:194:GLN:O	3:C:198:THR:OG1	2.20	0.42
40:E:311:CLA:OBD	40:a:815:CLA:H18	2.20	0.42
44:G:209:A86:C38	40:G:213:CLA:HAB	2.48	0.42
13:M:138:GLU:OE2	13:M:144:TYR:OH	2.17	0.42
41:P:303:KC2:O2A	44:P:317:A86:O3	2.38	0.42
24:b:307:ALA:CB	40:b:835:CLA:HED1	2.47	0.42
35:u:165:ASN:OD1	35:u:166:VAL:N	2.52	0.42
43:E:320:LMG:O8	43:E:320:LMG:H111	2.19	0.42
11:K:110:PHE:HA	11:K:113:ILE:HD12	2.02	0.42
15:T:34:ASP:N	15:T:34:ASP:OD1	2.53	0.42
22:Z:236:MET:HE3	47:Z:321:A1EB1:C26	2.49	0.42
23:a:658:VAL:O	23:a:661:SER:OG	2.33	0.42
40:a:841:CLA:H62	49:l:207:BCR:H363	2.02	0.42
34:o:254:PHE:HB2	40:o:312:CLA:HED1	2.02	0.42
18:U:104:ASN:O	18:U:106:PHE:N	2.52	0.42
30:j:1:MET:O	43:j:101:LMG:HC2	2.20	0.42
36:v:63:GLN:OE1	36:v:163:ARG:NH1	2.52	0.42
36:v:223:VAL:HG11	36:v:246:VAL:HG21	2.01	0.42
5:E:76:HIS:CE1	40:E:306:CLA:HMD3	2.55	0.42
40:M:311:CLA:H92	15:O:132:ILE:HG12	2.01	0.42
15:R:143:PRO:O	15:R:149:GLY:HA3	2.19	0.42
24:b:278:LEU:HD21	40:b:820:CLA:HMB2	2.01	0.42
25:c:73:THR:HG22	25:c:74:THR:H	1.85	0.42
36:q:78:LYS:NZ	36:q:144:GLU:OE1	2.43	0.42
40:B:307:CLA:HHD	40:B:307:CLA:HBC2	2.02	0.42
13:M:42:GLU:OE1	13:M:195:LYS:NZ	2.53	0.42
15:T:138:GLU:OE2	15:T:145:TYR:OH	2.28	0.42
28:f:182:SER:O	28:f:183:PRO:C	2.62	0.42
33:m:8:PHE:CD1	49:m:101:BCR:H381	2.55	0.42
1:A:174:ILE:HG21	42:A:316:DD6:C25	2.50	0.42
40:E:303:CLA:H41	46:P:319:SQD:H241	2.02	0.42
6:F:84:LEU:O	6:F:86:LEU:N	2.52	0.42
11:K:172:ASN:O	11:K:176:ASN:ND2	2.52	0.42
42:Q:214:DD6:C37	41:Q:216:KC2:C4A	2.97	0.42
24:b:48:ALA:HB3	33:m:28:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:w:183:LYS:HE2	38:w:183:LYS:HA	2.02	0.42
41:w:306:KC2:C1C	42:w:312:DD6:C6	2.97	0.42
6:F:93:SER:HB2	46:F:320:SQD:H1	2.01	0.41
16:Q:132:LEU:O	16:Q:134:GLY:N	2.53	0.41
17:S:241:ALA:HB2	40:S:313:CLA:HMA3	2.02	0.41
19:V:86:PHE:O	23:a:161:TRP:NE1	2.53	0.41
49:b:846:BCR:H271	50:b:849:PQN:H142	2.02	0.41
2:B:143:LEU:HD13	18:U:64:ASN:HA	2.02	0.41
3:C:75:ARG:NH2	40:C:307:CLA:O1D	2.53	0.41
40:C:307:CLA:H62	40:C:307:CLA:H41	1.95	0.41
11:K:125:ILE:HG23	47:K:315:A1EB1:O	2.20	0.41
40:Q:206:CLA:C9	40:S:305:CLA:HAB	2.42	0.41
23:a:457:ILE:HD12	40:a:850:CLA:H62	2.01	0.41
24:b:453:ILE:HG23	24:b:453:ILE:O	2.20	0.41
24:b:609:PHE:O	24:b:613:SER:OG	2.32	0.41
38:t:90:GLN:NE2	42:t:312:DD6:C30	2.84	0.41
35:u:89:HIS:HB3	35:u:113:VAL:HG21	2.03	0.41
36:v:183:PRO:CG	42:v:318:DD6:C4	2.98	0.41
5:E:214:LEU:HD11	42:P:315:DD6:C21	2.51	0.41
40:P:308:CLA:CHB	42:P:315:DD6:C23	2.97	0.41
16:Q:131:LYS:O	16:Q:132:LEU:C	2.62	0.41
15:T:196:ALA:CB	15:T:206:LEU:HD23	2.50	0.41
24:b:516:ASP:HA	24:b:519:VAL:HG12	2.03	0.41
38:w:58:ALA:O	38:w:62:HIS:ND1	2.52	0.41
7:G:131:GLY:O	7:G:135:VAL:HG23	2.20	0.41
16:Q:127:VAL:HG21	16:Q:139:TRP:CE3	2.56	0.41
38:w:21:ASP:OD1	38:w:21:ASP:N	2.52	0.41
40:z:305:CLA:H62	40:z:305:CLA:H41	1.90	0.41
40:A:302:CLA:H61	40:A:302:CLA:H41	1.85	0.41
5:E:36:ILE:HG21	5:E:39:LEU:HD12	2.02	0.41
10:J:74:MET:HA	10:J:74:MET:HE3	2.03	0.41
10:J:111:THR:O	10:J:111:THR:HG22	2.21	0.41
12:L:78:ALA:HA	42:L:315:DD6:C21	2.51	0.41
14:N:72:LYS:NZ	14:N:136:GLU:OE1	2.48	0.41
13:W:111:PRO:O	42:W:315:DD6:O4	2.38	0.41
22:Z:147:HIS:O	22:Z:150:LYS:N	2.48	0.41
35:x:89:HIS:HB3	35:x:113:VAL:HG21	2.03	0.41
40:C:302:CLA:CMC	40:C:302:CLA:HBC3	2.50	0.41
12:L:47:PHE:CE1	42:L:315:DD6:C36	3.00	0.41
12:L:196:SER:HB2	12:L:207:VAL:HG11	2.02	0.41
36:v:102:ALA:HB2	36:v:111:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:C:306:CLA:H92	40:C:306:CLA:HED1	2.02	0.41
8:H:103:SER:O	42:H:312:DD6:O4	2.39	0.41
40:L:306:CLA:HAA1	42:L:315:DD6:C35	2.51	0.41
13:M:74:GLY:N	13:M:201:MET:HE2	2.36	0.41
15:O:178:ALA:HB2	41:O:301:KC2:CED	2.50	0.41
13:W:207:PHE:HA	13:W:220:LEU:HD21	2.02	0.41
22:Z:139:GLU:OE2	22:Z:148:TYR:OH	2.20	0.41
23:a:747:ARG:O	23:a:751:VAL:HG22	2.21	0.41
36:q:130:THR:CG2	36:q:256:LEU:HD21	2.49	0.41
36:q:227:LYS:NZ	36:q:243:SER:O	2.54	0.41
35:u:47:ASP:OD1	35:u:50:GLY:N	2.54	0.41
40:A:302:CLA:CHD	42:A:316:DD6:C41	2.98	0.41
10:J:143:ALA:O	10:J:146:SER:OG	2.28	0.41
40:J:318:CLA:HBC2	40:J:318:CLA:HHD	2.02	0.41
50:a:847:PQN:H243	40:b:802:CLA:HBC3	2.01	0.41
36:v:57:ASP:N	36:v:57:ASP:OD1	2.54	0.41
38:w:176:ASP:OD1	38:w:180:PHE:N	2.53	0.41
4:D:80:ARG:NE	4:D:99:GLY:CA	2.84	0.41
5:E:58:LEU:CD2	40:k:202:CLA:HBA1	2.51	0.41
5:E:63:VAL:HG11	40:a:819:CLA:C5	2.45	0.41
5:E:63:VAL:HG13	40:a:819:CLA:C2	2.42	0.41
40:E:308:CLA:H41	40:E:308:CLA:H62	1.96	0.41
7:G:95:LEU:HD23	7:G:119:PRO:HD2	2.02	0.41
40:H:301:CLA:HMC1	10:J:139:VAL:HG21	2.03	0.41
10:J:190:SER:HB2	40:J:309:CLA:HMC2	2.03	0.41
40:K:308:CLA:H42	40:K:308:CLA:HBC3	2.03	0.41
40:V:202:CLA:H3A	40:V:202:CLA:HBA2	1.70	0.41
41:Y:308:KC2:NB	42:Y:322:DD6:C3	2.83	0.41
23:a:455:LEU:HD11	40:a:841:CLA:HMB1	2.02	0.41
24:b:293:THR:OG1	24:b:293:THR:O	2.39	0.41
49:b:847:BCR:H20C	49:b:847:BCR:H361	1.92	0.41
26:d:55:GLN:N	26:d:59:ASN:OD1	2.50	0.41
36:v:73:ARG:HH12	36:v:209:ILE:HD11	1.86	0.41
39:z:84:HIS:NE2	40:z:305:CLA:OBD	2.51	0.41
39:z:213:ILE:HD13	44:z:319:A86:C8	2.51	0.41
15:O:36:GLU:OE1	15:O:176:ARG:NH1	2.54	0.41
15:O:68:GLU:OE2	15:O:184:ARG:NH1	2.54	0.41
15:T:133:LEU:HD22	15:T:157:LEU:HD11	2.02	0.41
40:V:202:CLA:HMA1	13:W:127:LEU:HD11	2.02	0.41
20:X:243:MET:HE1	44:X:317:A86:C26	2.51	0.41
25:c:34:CYS:SG	25:c:35:LYS:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:l:205:CLA:NB	49:l:207:BCR:H333	2.36	0.41
40:G:201:CLA:HMB1	22:Z:166:GLN:O	2.21	0.40
11:K:50:GLY:HA3	13:P:59:SER:HB3	2.03	0.40
15:R:36:GLU:O	15:R:65:ARG:NH2	2.49	0.40
23:a:472:PHE:O	23:a:530:THR:HG21	2.20	0.40
43:a:801:LMG:O5	43:a:801:LMG:O4	2.33	0.40
35:x:74:LYS:NZ	40:x:305:CLA:O1D	2.48	0.40
35:x:109:SER:O	35:x:113:VAL:HG23	2.21	0.40
7:G:114:GLY:O	7:G:118:VAL:HG23	2.21	0.40
40:G:203:CLA:O1A	44:G:209:A86:O2	2.39	0.40
12:L:168:THR:CG2	42:L:317:DD6:O2	2.69	0.40
16:Q:128:VAL:HG13	16:Q:136:TRP:CZ3	2.57	0.40
17:S:169:VAL:O	17:S:170:ILE:HG13	2.21	0.40
40:S:301:CLA:H122	40:S:312:CLA:HMC2	2.03	0.40
20:X:138:ALA:HB2	40:X:304:CLA:CAB	2.51	0.40
23:a:359:MET:HE3	23:a:359:MET:HA	2.02	0.40
24:b:153:GLY:C	33:m:24:LEU:HD13	2.46	0.40
31:k:62:MET:CE	31:k:64:ILE:HD11	2.51	0.40
41:y:306:KC2:CMB	42:y:311:DD6:C1	2.99	0.40
2:B:79:ILE:HD12	40:B:307:CLA:HMA1	2.03	0.40
6:F:151:PRO:HA	6:F:154:TRP:NE1	2.35	0.40
6:F:152:ALA:C	6:F:156:GLN:NE2	2.77	0.40
40:J:309:CLA:HMC1	42:J:316:DD6:C2	2.51	0.40
19:V:87:TRP:HA	23:a:157:THR:OG1	2.21	0.40
23:a:274:ASP:OD1	23:a:275:PHE:N	2.54	0.40
23:a:708:LEU:HD23	28:f:173:LEU:HD23	2.02	0.40
28:f:176:GLY:O	28:f:179:VAL:HG22	2.21	0.40
40:q:311:CLA:O1D	42:q:318:DD6:C5	2.69	0.40
47:v:324:A1EB1:O	42:w:312:DD6:C27	2.69	0.40
35:x:47:ASP:OD1	35:x:50:GLY:N	2.54	0.40
4:D:110:ARG:O	4:D:114:ILE:HG13	2.21	0.40
16:Q:124:HIS:HA	16:Q:127:VAL:HG12	2.04	0.40
18:U:146:LYS:HE3	18:U:146:LYS:HA	2.04	0.40
19:V:86:PHE:HB3	23:a:161:TRP:CZ2	2.56	0.40
13:W:141:LYS:HD3	46:W:318:SQD:H61	2.03	0.40
24:b:422:LEU:HD13	24:b:532:LEU:CA	2.49	0.40
40:b:803:CLA:H62	40:b:803:CLA:H41	1.88	0.40
49:f:206:BCR:H24C	49:f:206:BCR:H371	1.91	0.40
33:m:9:PHE:CE2	33:m:13:ILE:HD11	2.57	0.40
36:q:74:HIS:ND1	36:q:167:PRO:O	2.47	0.40
41:t:306:KC2:C2B	42:t:312:DD6:C2	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:124:LEU:HD12	12:L:225:PHE:CD1	2.57	0.40
15:R:164:THR:O	15:R:164:THR:OG1	2.37	0.40
20:X:138:ALA:HB2	40:X:304:CLA:HAB	2.04	0.40
24:b:415:LYS:CB	24:b:539:LEU:HD13	2.52	0.40
34:o:42:LEU:HD11	34:o:75:ILE:HG12	2.02	0.40

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	A	181/201 (90%)	177 (98%)	4 (2%)	0	100	100
2	B	144/219 (66%)	136 (94%)	7 (5%)	1 (1%)	18	49
3	C	176/208 (85%)	166 (94%)	9 (5%)	1 (1%)	21	52
4	D	187/255 (73%)	178 (95%)	8 (4%)	1 (0%)	24	57
5	E	185/217 (85%)	176 (95%)	8 (4%)	1 (0%)	24	57
6	F	186/239 (78%)	175 (94%)	10 (5%)	1 (0%)	24	57
7	G	166/198 (84%)	161 (97%)	5 (3%)	0	100	100
8	H	165/199 (83%)	157 (95%)	8 (5%)	0	100	100
9	I	153/196 (78%)	147 (96%)	6 (4%)	0	100	100
10	J	164/208 (79%)	157 (96%)	6 (4%)	1 (1%)	21	52
11	K	169/204 (83%)	158 (94%)	10 (6%)	1 (1%)	21	52
12	L	187/228 (82%)	173 (92%)	12 (6%)	2 (1%)	11	39
13	M	191/224 (85%)	184 (96%)	7 (4%)	0	100	100
13	P	191/224 (85%)	183 (96%)	8 (4%)	0	100	100
13	W	191/224 (85%)	182 (95%)	9 (5%)	0	100	100
14	N	192/225 (85%)	182 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	177/210 (84%)	164 (93%)	13 (7%)	0	100	100
15	R	177/210 (84%)	171 (97%)	6 (3%)	0	100	100
15	T	177/210 (84%)	164 (93%)	12 (7%)	1 (1%)	21	52
16	Q	154/187 (82%)	141 (92%)	10 (6%)	3 (2%)	6	27
17	S	208/245 (85%)	189 (91%)	18 (9%)	1 (0%)	24	57
18	U	142/198 (72%)	128 (90%)	11 (8%)	3 (2%)	5	25
19	V	45/123 (37%)	43 (96%)	2 (4%)	0	100	100
20	X	209/253 (83%)	201 (96%)	8 (4%)	0	100	100
21	Y	211/244 (86%)	199 (94%)	11 (5%)	1 (0%)	24	57
22	Z	217/254 (85%)	210 (97%)	7 (3%)	0	100	100
23	a	739/752 (98%)	711 (96%)	28 (4%)	0	100	100
24	b	729/734 (99%)	706 (97%)	22 (3%)	1 (0%)	48	78
25	c	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
26	d	138/142 (97%)	132 (96%)	6 (4%)	0	100	100
27	e	61/131 (47%)	59 (97%)	2 (3%)	0	100	100
28	f	159/184 (86%)	154 (97%)	5 (3%)	0	100	100
29	i	29/36 (81%)	27 (93%)	2 (7%)	0	100	100
30	j	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
31	k	68/112 (61%)	65 (96%)	2 (3%)	1 (2%)	8	32
32	l	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
33	m	28/30 (93%)	28 (100%)	0	0	100	100
34	o	234/273 (86%)	225 (96%)	8 (3%)	1 (0%)	30	61
35	p	226/255 (89%)	223 (99%)	3 (1%)	0	100	100
35	u	226/255 (89%)	221 (98%)	5 (2%)	0	100	100
35	x	226/255 (89%)	220 (97%)	6 (3%)	0	100	100
36	q	236/268 (88%)	229 (97%)	7 (3%)	0	100	100
36	v	236/268 (88%)	224 (95%)	12 (5%)	0	100	100
37	r	89/133 (67%)	88 (99%)	1 (1%)	0	100	100
38	t	209/260 (80%)	200 (96%)	9 (4%)	0	100	100
38	w	209/260 (80%)	202 (97%)	7 (3%)	0	100	100
38	y	199/260 (76%)	194 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
39	z	220/257 (86%)	215 (98%)	5 (2%)	0	100 100
All	All	9063/10734 (84%)	8676 (96%)	366 (4%)	21 (0%)	44 73

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	81	GLU
5	E	210	VAL
10	J	71	ILE
11	K	139	PRO
12	L	204	PRO
16	Q	184	ALA
15	T	143	PRO
31	k	110	PHE
18	U	61	SER
18	U	105	SER
18	U	168	GLU
24	b	482	THR
2	B	112	ASN
17	S	172	VAL
34	o	110	THR
6	F	153	ALA
21	Y	223	ALA
12	L	212	ASN
16	Q	130	PRO
16	Q	138	ASP
3	C	101	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	155/170 (91%)	155 (100%)	0	100 100
2	B	108/160 (68%)	108 (100%)	0	100 100
3	C	142/161 (88%)	141 (99%)	1 (1%)	76 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	146/193 (76%)	145 (99%)	1 (1%)	76 82
5	E	146/163 (90%)	146 (100%)	0	100 100
6	F	140/180 (78%)	138 (99%)	2 (1%)	59 76
7	G	127/149 (85%)	127 (100%)	0	100 100
8	H	130/154 (84%)	130 (100%)	0	100 100
9	I	125/153 (82%)	125 (100%)	0	100 100
10	J	123/150 (82%)	123 (100%)	0	100 100
11	K	131/153 (86%)	131 (100%)	0	100 100
12	L	144/174 (83%)	143 (99%)	1 (1%)	76 82
13	M	146/165 (88%)	146 (100%)	0	100 100
13	P	146/165 (88%)	146 (100%)	0	100 100
13	W	146/165 (88%)	144 (99%)	2 (1%)	59 76
14	N	149/174 (86%)	148 (99%)	1 (1%)	76 82
15	O	136/157 (87%)	136 (100%)	0	100 100
15	R	136/157 (87%)	135 (99%)	1 (1%)	76 82
15	T	136/157 (87%)	135 (99%)	1 (1%)	76 82
16	Q	123/141 (87%)	122 (99%)	1 (1%)	73 81
17	S	163/188 (87%)	163 (100%)	0	100 100
18	U	118/162 (73%)	116 (98%)	2 (2%)	53 74
19	V	39/85 (46%)	39 (100%)	0	100 100
20	X	169/194 (87%)	169 (100%)	0	100 100
21	Y	166/183 (91%)	166 (100%)	0	100 100
22	Z	177/198 (89%)	177 (100%)	0	100 100
23	a	607/616 (98%)	607 (100%)	0	100 100
24	b	591/592 (100%)	587 (99%)	4 (1%)	76 82
25	c	68/69 (99%)	68 (100%)	0	100 100
26	d	120/122 (98%)	119 (99%)	1 (1%)	73 81
27	e	51/90 (57%)	51 (100%)	0	100 100
28	f	127/144 (88%)	123 (97%)	4 (3%)	35 64
29	i	28/32 (88%)	28 (100%)	0	100 100
30	j	36/36 (100%)	36 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
31	k	52/85 (61%)	52 (100%)	0	100 100
32	l	114/115 (99%)	114 (100%)	0	100 100
33	m	23/23 (100%)	23 (100%)	0	100 100
34	o	180/208 (86%)	178 (99%)	2 (1%)	65 78
35	p	179/199 (90%)	179 (100%)	0	100 100
35	u	179/199 (90%)	178 (99%)	1 (1%)	78 83
35	x	179/199 (90%)	179 (100%)	0	100 100
36	q	183/204 (90%)	182 (100%)	1 (0%)	81 85
36	v	183/204 (90%)	182 (100%)	1 (0%)	81 85
37	r	71/94 (76%)	70 (99%)	1 (1%)	59 76
38	t	168/204 (82%)	168 (100%)	0	100 100
38	w	168/204 (82%)	167 (99%)	1 (1%)	78 83
38	y	159/204 (78%)	158 (99%)	1 (1%)	78 83
39	z	177/199 (89%)	177 (100%)	0	100 100
All	All	7210/8293 (87%)	7180 (100%)	30 (0%)	81 86

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	208	PHE
4	D	89	LEU
6	F	149	LEU
6	F	150	PRO
12	L	216	LEU
14	N	167	ILE
16	Q	144	TYR
15	R	142	LYS
15	T	91	LEU
18	U	45	LEU
18	U	46	GLN
13	W	78	MET
13	W	220	LEU
24	b	280	ILE
24	b	717	PHE
24	b	720	THR
24	b	723	PRO
26	d	38	SER

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Mol	Chain	Res	Type
28	f	174	VAL
28	f	180	THR
28	f	181	VAL
28	f	184	ARG
34	o	56	TRP
34	o	208	LYS
36	q	267	LEU
37	r	122	HIS
35	u	112	GLU
36	v	84	MET
38	w	9	PHE
38	y	141	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
3	C	155	HIS
4	D	146	HIS
5	E	208	GLN
5	E	211	GLN
7	G	166	GLN
8	H	187	GLN
9	I	155	GLN
12	L	186	ASN
12	L	212	ASN
13	M	176	ASN
14	N	110	GLN
16	Q	59	ASN
17	S	121	GLN
17	S	204	ASN
17	S	220	GLN
13	W	176	ASN
21	Y	92	HIS
21	Y	195	ASN
22	Z	95	ASN
23	a	193	ASN
24	b	53	HIS
24	b	171	ASN
24	b	229	ASN
24	b	275	HIS
24	b	276	HIS

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Mol	Chain	Res	Type
34	o	153	ASN
35	p	182	ASN
36	q	44	ASN
36	q	195	ASN
38	t	87	GLN
38	t	90	GLN
35	u	140	ASN
35	u	172	ASN
38	y	85	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

790 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
40	CLA	K	301	-	51,55,73	1.96	9 (17%)	60,91,113	1.43	7 (11%)
40	CLA	Y	310	-	59,63,73	1.85	9 (15%)	70,101,113	1.41	6 (8%)
40	CLA	Q	206	-	62,68,73	1.72	9 (14%)	74,105,113	1.76	10 (13%)
41	KC2	I	209	9	49,53,53	1.83	4 (8%)	60,89,89	1.12	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	CLA	H	307	-	64,68,73	1.80	9 (14%)	76,107,113	1.47	9 (11%)
40	CLA	W	305	13	69,73,73	1.70	9 (13%)	82,113,113	1.28	8 (9%)
41	KC2	R	311	15	49,53,53	1.84	4 (8%)	60,89,89	1.07	4 (6%)
49	BCR	f	203	-	41,41,41	0.22	0	56,56,56	0.42	0
40	CLA	a	828	23	69,73,73	1.66	9 (13%)	82,113,113	1.27	6 (7%)
44	A86	D	319	-	47,50,50	0.45	1 (2%)	51,76,76	1.02	2 (3%)
40	CLA	E	304	5	59,63,73	1.84	10 (16%)	70,101,113	1.39	6 (8%)
40	CLA	b	821	-	69,73,73	1.67	9 (13%)	82,113,113	1.22	7 (8%)
40	CLA	o	307	34	64,68,73	1.78	9 (14%)	76,107,113	1.51	11 (14%)
44	A86	T	313	-	47,50,50	0.40	1 (2%)	51,76,76	0.90	3 (5%)
40	CLA	U	203	-	59,63,73	1.93	9 (15%)	70,101,113	1.49	10 (14%)
40	CLA	w	308	-	51,55,73	1.97	9 (17%)	60,91,113	1.44	5 (8%)
40	CLA	U	206	-	51,55,73	2.01	9 (17%)	60,91,113	1.39	7 (11%)
41	KC2	N	302	14	49,53,53	1.85	4 (8%)	60,89,89	1.07	5 (8%)
44	A86	N	318	-	47,50,50	0.66	1 (2%)	51,76,76	0.49	0
40	CLA	F	306	6	64,68,73	1.77	9 (14%)	76,107,113	1.33	7 (9%)
41	KC2	M	309	-	49,53,53	1.88	4 (8%)	60,89,89	1.03	3 (5%)
41	KC2	p	310	-	49,53,53	1.86	4 (8%)	60,89,89	1.05	3 (5%)
40	CLA	I	204	9	51,55,73	1.97	9 (17%)	60,91,113	1.43	6 (10%)
40	CLA	N	311	14	64,68,73	1.78	9 (14%)	76,107,113	1.45	7 (9%)
40	CLA	a	851	-	69,73,73	1.70	9 (13%)	82,113,113	1.32	7 (8%)
41	KC2	U	201	-	49,53,53	1.85	4 (8%)	60,89,89	1.08	4 (6%)
42	DD6	A	315	-	40,45,45	0.16	0	51,67,67	0.70	1 (1%)
42	DD6	x	320	-	40,45,45	0.19	0	51,67,67	0.67	2 (3%)
44	A86	P	317	-	47,50,50	0.44	1 (2%)	51,76,76	0.79	2 (3%)
41	KC2	K	303	11	49,53,53	1.85	4 (8%)	60,89,89	1.07	5 (8%)
47	A1EB1	v	323	-	54,58,58	0.51	1 (1%)	60,85,85	0.62	1 (1%)
47	A1EB1	w	313	-	54,58,58	0.43	1 (1%)	60,85,85	0.66	1 (1%)
40	CLA	T	317	47	51,55,73	1.96	8 (15%)	60,91,113	1.38	8 (13%)
40	CLA	a	840	23	59,63,73	1.83	9 (15%)	70,101,113	1.39	7 (10%)
41	KC2	x	315	-	49,53,53	1.85	4 (8%)	60,89,89	1.14	4 (6%)
42	DD6	U	211	-	40,45,45	0.20	0	51,67,67	0.71	1 (1%)
44	A86	R	312	-	47,50,50	0.76	1 (2%)	51,76,76	1.30	3 (5%)
41	KC2	R	303	-	49,53,53	1.84	4 (8%)	60,89,89	1.18	5 (8%)
40	CLA	J	318	10	51,55,73	1.99	9 (17%)	60,91,113	1.49	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	CLA	B	302	2	51,55,73	1.99	9 (17%)	60,91,113	1.38	6 (10%)
40	CLA	b	815	-	61,65,73	1.82	9 (14%)	72,103,113	1.38	6 (8%)
42	DD6	O	314	-	40,45,45	0.20	0	51,67,67	0.69	1 (1%)
40	CLA	O	304	15	69,73,73	1.69	9 (13%)	82,113,113	1.33	9 (10%)
40	CLA	V	201	-	62,66,73	1.80	9 (14%)	73,104,113	1.34	5 (6%)
40	CLA	u	306	35	51,55,73	1.98	9 (17%)	60,91,113	1.49	7 (11%)
40	CLA	S	307	17	64,68,73	1.76	10 (15%)	76,107,113	1.41	6 (7%)
47	A1EB1	K	313	-	54,58,58	0.55	1 (1%)	60,85,85	1.24	2 (3%)
40	CLA	B	306	-	56,60,73	1.99	9 (16%)	65,97,113	1.50	9 (13%)
40	CLA	J	310	-	51,55,73	2.08	9 (17%)	60,91,113	1.66	9 (15%)
40	CLA	b	837	24	64,68,73	1.74	9 (14%)	76,107,113	1.40	6 (7%)
40	CLA	u	305	35	51,55,73	1.99	9 (17%)	60,91,113	1.66	8 (13%)
47	A1EB1	w	314	-	54,58,58	0.51	1 (1%)	60,85,85	0.68	1 (1%)
41	KC2	Y	314	-	49,53,53	1.86	4 (8%)	60,89,89	1.13	5 (8%)
44	A86	q	315	-	47,50,50	0.49	1 (2%)	51,76,76	0.92	2 (3%)
44	A86	v	315	-	47,50,50	0.56	1 (2%)	51,76,76	0.85	1 (1%)
44	A86	z	316	-	47,50,50	0.52	1 (2%)	51,76,76	1.49	3 (5%)
40	CLA	a	824	-	66,70,73	1.74	9 (13%)	78,109,113	1.30	6 (7%)
40	CLA	w	302	38	51,55,73	1.97	9 (17%)	60,91,113	1.53	6 (10%)
42	DD6	z	322	-	40,45,45	0.23	0	51,67,67	1.00	4 (7%)
40	CLA	S	308	-	53,57,73	2.00	9 (16%)	65,94,113	1.56	10 (15%)
42	DD6	H	312	-	40,45,45	0.22	0	51,67,67	0.98	3 (5%)
41	KC2	O	308	15	49,53,53	1.83	4 (8%)	60,89,89	1.12	4 (6%)
42	DD6	k	204	-	40,45,45	0.20	0	51,67,67	0.82	4 (7%)
44	A86	u	320	-	47,50,50	0.38	1 (2%)	51,76,76	1.01	2 (3%)
40	CLA	M	307	-	64,68,73	1.76	9 (14%)	76,107,113	1.34	8 (10%)
47	A1EB1	x	322	-	54,58,58	0.56	1 (1%)	60,85,85	0.60	1 (1%)
40	CLA	a	809	-	54,58,73	1.98	9 (16%)	64,95,113	1.44	8 (12%)
40	CLA	l	204	-	69,73,73	1.71	9 (13%)	82,113,113	1.20	6 (7%)
40	CLA	Q	208	-	64,68,73	1.77	8 (12%)	76,107,113	1.31	8 (10%)
49	BCR	f	206	-	41,41,41	0.20	0	56,56,56	0.53	0
42	DD6	u	321	-	40,45,45	0.21	0	51,67,67	0.67	1 (1%)
40	CLA	M	310	-	60,64,73	1.78	9 (15%)	71,102,113	1.31	8 (11%)
44	A86	X	317	-	47,50,50	0.50	1 (2%)	51,76,76	0.97	3 (5%)
44	A86	v	325	-	47,50,50	0.35	0	51,76,76	1.05	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	CLA	A	305	1	65,69,73	1.76	9 (13%)	77,108,113	1.38	7 (9%)
42	DD6	J	315	-	40,45,45	0.22	0	51,67,67	0.76	3 (5%)
40	CLA	b	820	-	69,73,73	1.73	9 (13%)	82,113,113	1.33	8 (9%)
40	CLA	C	305	3	64,68,73	1.78	9 (14%)	76,107,113	1.42	8 (10%)
40	CLA	a	827	23	69,73,73	1.70	9 (13%)	82,113,113	1.27	5 (6%)
42	DD6	H	313	-	40,45,45	0.25	0	51,67,67	0.86	2 (3%)
42	DD6	I	210	-	40,45,45	0.17	0	51,67,67	0.97	3 (5%)
40	CLA	L	305	12	51,55,73	2.04	9 (17%)	60,91,113	1.50	6 (10%)
40	CLA	X	312	-	51,55,73	2.06	9 (17%)	60,91,113	1.56	8 (13%)
49	BCR	b	846	-	41,41,41	0.12	0	56,56,56	0.67	1 (1%)
40	CLA	b	805	-	65,69,73	1.77	9 (13%)	77,108,113	1.34	6 (7%)
41	KC2	w	307	-	49,53,53	1.84	4 (8%)	60,89,89	1.09	4 (6%)
40	CLA	u	311	-	59,63,73	1.94	9 (15%)	70,101,113	1.71	12 (17%)
47	A1EB1	P	301	-	54,58,58	0.52	1 (1%)	60,85,85	0.59	0
40	CLA	J	312	-	62,66,73	1.79	9 (14%)	73,104,113	1.32	6 (8%)
49	BCR	b	844	-	41,41,41	0.25	0	56,56,56	0.60	1 (1%)
40	CLA	D	310	4	64,68,73	1.73	9 (14%)	76,107,113	1.31	9 (11%)
40	CLA	b	817	24	69,73,73	1.66	9 (13%)	82,113,113	1.28	7 (8%)
47	A1EB1	t	315	-	54,58,58	0.45	1 (1%)	60,85,85	0.80	2 (3%)
40	CLA	H	310	-	64,68,73	1.78	9 (14%)	76,107,113	1.37	6 (7%)
40	CLA	Q	204	16	54,58,73	1.96	9 (16%)	62,94,113	1.88	12 (19%)
44	A86	R	313	-	47,50,50	0.60	1 (2%)	51,76,76	0.66	0
41	KC2	O	302	15	49,53,53	1.86	5 (10%)	60,89,89	1.15	4 (6%)
40	CLA	x	307	-	59,63,73	1.90	9 (15%)	70,101,113	1.64	8 (11%)
40	CLA	U	207	-	51,55,73	2.04	9 (17%)	60,91,113	1.60	8 (13%)
44	A86	M	316	-	47,50,50	0.48	1 (2%)	51,76,76	0.84	3 (5%)
40	CLA	N	304	14	64,68,73	1.76	9 (14%)	76,107,113	1.37	6 (7%)
41	KC2	Y	303	21	49,53,53	1.79	4 (8%)	60,89,89	1.01	4 (6%)
40	CLA	Y	307	21	64,68,73	1.80	9 (14%)	76,107,113	1.45	8 (10%)
40	CLA	D	304	4	60,64,73	1.84	10 (16%)	71,102,113	1.49	8 (11%)
40	CLA	a	819	23	65,69,73	1.76	9 (13%)	77,108,113	1.43	8 (10%)
42	DD6	I	213	-	40,45,45	0.26	0	51,67,67	0.80	2 (3%)
40	CLA	p	314	35	51,55,73	2.04	9 (17%)	60,91,113	1.61	7 (11%)
41	KC2	y	301	38	49,53,53	1.85	4 (8%)	60,89,89	1.07	3 (5%)
41	KC2	Y	302	-	49,53,53	1.87	4 (8%)	60,89,89	1.03	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	KC2	W	303	-	49,53,53	1.85	4 (8%)	60,89,89	1.08	5 (8%)
40	CLA	q	306	36	64,68,73	1.78	9 (14%)	76,107,113	1.39	7 (9%)
40	CLA	b	810	24	69,73,73	1.68	9 (13%)	82,113,113	1.26	8 (9%)
40	CLA	A	309	1	69,73,73	1.73	9 (13%)	82,113,113	1.28	6 (7%)
40	CLA	F	311	-	51,55,73	2.00	9 (17%)	60,91,113	1.49	6 (10%)
40	CLA	z	305	39	64,68,73	1.74	9 (14%)	76,107,113	1.42	8 (10%)
40	CLA	z	312	-	64,68,73	1.78	9 (14%)	76,107,113	1.37	7 (9%)
41	KC2	q	309	-	49,53,53	1.83	4 (8%)	60,89,89	1.07	4 (6%)
40	CLA	T	310	-	62,66,73	1.80	9 (14%)	73,104,113	1.40	7 (9%)
40	CLA	A	311	1	51,55,73	1.97	9 (17%)	60,91,113	1.49	6 (10%)
40	CLA	A	304	1	69,73,73	1.74	9 (13%)	82,113,113	1.44	10 (12%)
40	CLA	H	301	-	51,55,73	2.00	9 (17%)	60,91,113	1.48	8 (13%)
40	CLA	f	202	24	69,73,73	1.65	9 (13%)	82,113,113	1.23	6 (7%)
40	CLA	R	316	47	51,55,73	1.95	8 (15%)	60,91,113	1.34	7 (11%)
41	KC2	T	309	15	49,53,53	1.84	4 (8%)	60,89,89	1.05	3 (5%)
40	CLA	I	201	-	69,73,73	1.71	9 (13%)	82,113,113	1.30	6 (7%)
41	KC2	T	311	15	49,53,53	1.85	4 (8%)	60,89,89	1.06	4 (6%)
40	CLA	C	307	3	64,68,73	1.83	9 (14%)	76,107,113	1.52	8 (10%)
40	CLA	b	823	24	59,63,73	1.82	9 (15%)	70,101,113	1.46	7 (10%)
41	KC2	X	303	20	49,53,53	1.84	4 (8%)	60,89,89	1.04	5 (8%)
47	A1EB1	K	315	-	54,58,58	0.55	1 (1%)	60,85,85	0.50	0
40	CLA	a	815	23	69,73,73	1.73	9 (13%)	82,113,113	1.36	8 (9%)
40	CLA	t	307	-	59,63,73	1.90	9 (15%)	70,101,113	1.57	8 (11%)
41	KC2	p	309	-	49,53,53	1.84	4 (8%)	60,89,89	1.13	4 (6%)
40	CLA	Q	207	-	51,55,73	2.12	9 (17%)	60,91,113	1.73	11 (18%)
40	CLA	q	313	36	51,55,73	2.00	9 (17%)	60,91,113	1.52	7 (11%)
40	CLA	Z	310	-	59,63,73	1.94	9 (15%)	70,101,113	1.70	12 (17%)
42	DD6	p	322	-	40,45,45	0.18	0	51,67,67	0.68	0
43	LMG	D	318	-	40,40,55	0.80	0	48,48,63	1.23	5 (10%)
41	KC2	P	304	13	49,53,53	1.87	4 (8%)	60,89,89	1.08	5 (8%)
41	KC2	T	308	15	49,53,53	1.85	4 (8%)	60,89,89	1.07	4 (6%)
40	CLA	T	307	-	59,63,73	1.85	9 (15%)	70,101,113	1.46	7 (10%)
44	A86	W	301	-	47,50,50	0.43	1 (2%)	51,76,76	0.63	1 (1%)
44	A86	p	320	-	47,50,50	0.34	0	51,76,76	1.09	3 (5%)
47	A1EB1	Y	323	-	54,58,58	0.38	1 (1%)	60,85,85	0.87	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	CLA	b	826	24	68,72,73	1.72	9 (13%)	80,111,113	1.30	5 (6%)
44	A86	G	211	-	47,50,50	0.53	1 (2%)	51,76,76	0.78	1 (1%)
40	CLA	b	841	24	69,73,73	1.67	9 (13%)	82,113,113	1.26	7 (8%)
44	A86	p	321	-	47,50,50	0.35	0	51,76,76	1.00	3 (5%)
41	KC2	z	304	39	49,53,53	1.82	5 (10%)	60,89,89	1.11	5 (8%)
43	LMG	u	301	-	39,39,55	0.83	1 (2%)	47,47,63	1.29	5 (10%)
40	CLA	b	834	-	69,73,73	1.72	9 (13%)	82,113,113	1.30	5 (6%)
47	A1EB1	Z	320	-	54,58,58	0.29	0	60,85,85	0.62	0
42	DD6	J	313	-	40,45,45	0.19	0	51,67,67	0.69	1 (1%)
41	KC2	w	301	38	49,53,53	1.84	4 (8%)	60,89,89	1.06	4 (6%)
40	CLA	b	839	24	69,73,73	1.72	9 (13%)	82,113,113	1.40	6 (7%)
40	CLA	M	306	13	66,70,73	1.71	9 (13%)	78,109,113	1.30	5 (6%)
40	CLA	S	319	-	51,55,73	1.97	9 (17%)	60,91,113	1.39	6 (10%)
44	A86	X	318	-	47,50,50	0.62	1 (2%)	51,76,76	1.77	4 (7%)
47	A1EB1	v	324	-	54,58,58	0.62	1 (1%)	60,85,85	1.16	4 (6%)
41	KC2	p	303	-	49,53,53	1.87	4 (8%)	60,89,89	1.03	5 (8%)
40	CLA	L	306	12	51,55,73	2.09	9 (17%)	60,91,113	1.74	10 (16%)
40	CLA	J	308	10	59,63,73	1.84	10 (16%)	70,101,113	1.40	8 (11%)
40	CLA	a	825	-	69,73,73	1.69	9 (13%)	82,113,113	1.29	6 (7%)
40	CLA	i	101	-	59,63,73	1.93	9 (15%)	70,101,113	1.58	8 (11%)
44	A86	S	315	-	47,50,50	0.36	1 (2%)	51,76,76	1.08	2 (3%)
47	A1EB1	q	322	-	54,58,58	0.35	0	60,85,85	0.80	1 (1%)
40	CLA	D	307	4	69,73,73	1.70	9 (13%)	82,113,113	1.37	10 (12%)
41	KC2	t	308	-	49,53,53	1.86	4 (8%)	60,89,89	1.10	5 (8%)
42	DD6	N	316	-	40,45,45	0.22	0	51,67,67	0.96	2 (3%)
40	CLA	J	311	-	51,55,73	2.04	9 (17%)	60,91,113	1.60	7 (11%)
40	CLA	X	301	-	64,68,73	1.76	9 (14%)	76,107,113	1.32	6 (7%)
40	CLA	a	822	-	69,73,73	1.69	9 (13%)	82,113,113	1.34	8 (9%)
44	A86	T	312	-	47,50,50	0.46	1 (2%)	51,76,76	1.10	3 (5%)
40	CLA	E	305	5	64,68,73	1.81	9 (14%)	76,107,113	1.36	8 (10%)
42	DD6	Y	322	-	40,45,45	0.17	0	51,67,67	0.69	2 (3%)
40	CLA	D	302	43	62,66,73	1.82	9 (14%)	73,104,113	1.41	6 (8%)
40	CLA	v	311	-	67,71,73	1.78	9 (13%)	79,110,113	1.37	8 (10%)
40	CLA	B	303	-	51,55,73	1.98	9 (17%)	60,91,113	1.47	6 (10%)
44	A86	y	310	-	47,50,50	0.52	1 (2%)	51,76,76	1.09	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	KC2	P	309	13	49,53,53	1.82	4 (8%)	60,89,89	1.13	4 (6%)
49	BCR	b	843	-	41,41,41	0.13	0	56,56,56	0.44	0
40	CLA	S	312	-	51,55,73	2.05	9 (17%)	60,91,113	1.64	9 (15%)
46	SQD	P	319	-	30,32,54	1.46	3 (10%)	40,43,65	1.36	6 (15%)
40	CLA	z	306	-	59,63,73	1.84	9 (15%)	70,101,113	1.38	7 (10%)
44	A86	o	316	-	47,50,50	0.55	1 (2%)	51,76,76	1.05	3 (5%)
49	BCR	b	847	-	41,41,41	0.19	0	56,56,56	0.58	0
40	CLA	b	824	24	69,73,73	1.66	9 (13%)	82,113,113	1.31	9 (10%)
40	CLA	A	302	-	64,68,73	1.78	9 (14%)	76,107,113	1.30	6 (7%)
42	DD6	v	320	-	40,45,45	0.20	0	51,67,67	0.70	0
41	KC2	S	303	17	49,53,53	1.86	4 (8%)	60,89,89	1.10	5 (8%)
40	CLA	Z	307	22	64,68,73	1.80	9 (14%)	76,107,113	1.40	9 (11%)
40	CLA	J	303	-	51,55,73	2.07	8 (15%)	60,91,113	1.56	8 (13%)
44	A86	T	315	-	47,50,50	0.66	1 (2%)	51,76,76	0.99	1 (1%)
40	CLA	H	306	8	54,58,73	1.94	9 (16%)	64,95,113	1.43	6 (9%)
40	CLA	C	302	-	51,55,73	2.03	9 (17%)	60,91,113	1.65	7 (11%)
44	A86	z	317	-	47,50,50	0.56	1 (2%)	51,76,76	1.48	2 (3%)
40	CLA	G	213	-	51,55,73	2.04	9 (17%)	60,91,113	1.63	9 (15%)
40	CLA	a	833	23	64,68,73	1.77	9 (14%)	76,107,113	1.38	7 (9%)
40	CLA	o	311	-	67,71,73	1.76	9 (13%)	79,110,113	1.37	6 (7%)
44	A86	R	315	-	47,50,50	0.49	1 (2%)	51,76,76	1.28	3 (5%)
42	DD6	F	315	-	40,45,45	0.21	0	51,67,67	0.92	1 (1%)
41	KC2	W	310	13	49,53,53	1.88	4 (8%)	60,89,89	1.06	4 (6%)
41	KC2	L	302	-	49,53,53	1.86	4 (8%)	60,89,89	1.07	5 (8%)
44	A86	p	317	-	47,50,50	0.56	1 (2%)	51,76,76	1.11	2 (3%)
44	A86	Y	315	-	47,50,50	0.58	1 (2%)	51,76,76	1.18	2 (3%)
48	A1EB4	M	319	-	53,58,63	0.60	1 (1%)	59,84,89	0.60	1 (1%)
40	CLA	O	306	15	64,68,73	1.78	10 (15%)	76,107,113	1.45	8 (10%)
44	A86	Q	210	-	47,50,50	0.42	1 (2%)	51,76,76	0.92	1 (1%)
44	A86	z	318	-	47,50,50	0.55	1 (2%)	51,76,76	0.91	2 (3%)
49	BCR	b	848	-	41,41,41	0.14	0	56,56,56	0.34	0
44	A86	v	317	-	47,50,50	0.45	1 (2%)	51,76,76	0.73	1 (1%)
41	KC2	x	303	-	49,53,53	1.88	4 (8%)	60,89,89	1.01	4 (6%)
41	KC2	K	309	11	49,53,53	1.84	4 (8%)	60,89,89	1.11	5 (8%)
40	CLA	E	310	-	64,68,73	1.77	9 (14%)	76,107,113	1.40	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	KC2	z	310	39	49,53,53	1.83	4 (8%)	60,89,89	1.05	4 (6%)
41	KC2	R	309	15	49,53,53	1.88	4 (8%)	60,89,89	1.11	5 (8%)
40	CLA	a	850	-	69,73,73	1.67	9 (13%)	82,113,113	1.39	8 (9%)
41	KC2	N	312	14	49,53,53	1.83	4 (8%)	60,89,89	1.07	4 (6%)
40	CLA	y	303	-	51,55,73	2.06	9 (17%)	60,91,113	1.66	8 (13%)
41	KC2	v	303	36	49,53,53	1.85	4 (8%)	60,89,89	1.07	4 (6%)
40	CLA	P	311	-	51,55,73	2.02	9 (17%)	60,91,113	1.59	10 (16%)
41	KC2	x	309	-	49,53,53	1.82	4 (8%)	60,89,89	1.16	5 (8%)
44	A86	q	316	-	47,50,50	0.54	1 (2%)	51,76,76	1.29	1 (1%)
40	CLA	Y	312	-	51,55,73	2.11	9 (17%)	60,91,113	1.76	11 (18%)
42	DD6	E	318	-	40,45,45	0.20	0	51,67,67	0.76	3 (5%)
40	CLA	b	828	24	59,63,73	1.87	9 (15%)	70,101,113	1.46	8 (11%)
43	LMG	x	301	-	39,39,55	0.87	1 (2%)	47,47,63	1.23	5 (10%)
40	CLA	N	306	-	64,68,73	1.77	9 (14%)	76,107,113	1.29	7 (9%)
41	KC2	p	304	35	49,53,53	1.84	4 (8%)	60,89,89	1.06	3 (5%)
41	KC2	N	308	14	49,53,53	1.86	4 (8%)	60,89,89	1.08	4 (6%)
40	CLA	v	312	-	64,68,73	1.76	9 (14%)	76,107,113	1.34	5 (6%)
40	CLA	E	311	-	54,58,73	1.99	9 (16%)	64,95,113	1.50	7 (10%)
40	CLA	O	305	15	51,55,73	2.02	9 (17%)	60,91,113	1.52	7 (11%)
41	KC2	v	309	-	49,53,53	1.84	4 (8%)	60,89,89	1.08	4 (6%)
44	A86	U	210	-	47,50,50	0.43	1 (2%)	51,76,76	1.06	3 (5%)
43	LMG	E	321	-	40,40,55	0.86	1 (2%)	48,48,63	1.28	7 (14%)
40	CLA	E	307	-	69,73,73	1.68	9 (13%)	82,113,113	1.20	5 (6%)
40	CLA	f	204	28	51,55,73	1.94	9 (17%)	60,91,113	1.49	7 (11%)
40	CLA	H	311	-	51,55,73	2.03	9 (17%)	60,91,113	1.49	6 (10%)
40	CLA	Z	301	-	64,68,73	1.78	9 (14%)	76,107,113	1.30	5 (6%)
40	CLA	a	814	-	54,58,73	1.94	9 (16%)	64,95,113	1.46	6 (9%)
40	CLA	a	823	23	59,63,73	1.84	9 (15%)	70,101,113	1.37	6 (8%)
42	DD6	Q	213	-	40,45,45	0.21	0	51,67,67	0.76	3 (5%)
40	CLA	w	305	-	53,57,73	1.97	9 (16%)	65,94,113	1.50	5 (7%)
42	DD6	o	319	-	40,45,45	0.21	0	51,67,67	0.78	3 (5%)
47	A1EB1	y	312	-	54,58,58	0.43	1 (1%)	60,85,85	0.70	1 (1%)
49	BCR	k	203	-	41,41,41	0.17	0	56,56,56	0.47	1 (1%)
40	CLA	S	302	-	64,68,73	1.77	9 (14%)	76,107,113	1.31	7 (9%)
41	KC2	y	306	-	49,53,53	1.84	4 (8%)	60,89,89	1.02	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	CLA	x	314	35	51,55,73	1.99	9 (17%)	60,91,113	1.53	7 (11%)
44	A86	M	320	-	47,50,50	0.37	1 (2%)	51,76,76	0.64	0
40	CLA	J	302	10	51,55,73	2.00	9 (17%)	60,91,113	1.43	6 (10%)
40	CLA	G	204	7	59,63,73	1.85	9 (15%)	70,101,113	1.43	7 (10%)
44	A86	x	317	-	47,50,50	0.55	1 (2%)	51,76,76	0.89	2 (3%)
41	KC2	M	303	13	49,53,53	1.85	4 (8%)	60,89,89	1.08	5 (8%)
40	CLA	o	301	-	64,68,73	1.80	9 (14%)	76,107,113	1.31	5 (6%)
42	DD6	D	315	-	40,45,45	0.18	0	51,67,67	0.94	2 (3%)
41	KC2	T	301	-	49,53,53	1.83	4 (8%)	60,89,89	1.05	4 (6%)
43	LMG	E	320	-	31,31,55	0.98	1 (3%)	39,39,63	1.18	2 (5%)
42	DD6	N	319	-	40,45,45	0.16	0	51,67,67	1.07	4 (7%)
41	KC2	M	302	13	49,53,53	1.86	4 (8%)	60,89,89	1.06	4 (6%)
40	CLA	l	202	-	69,73,73	1.70	9 (13%)	82,113,113	1.31	8 (9%)
40	CLA	y	302	38	51,55,73	2.09	9 (17%)	60,91,113	1.59	8 (13%)
41	KC2	u	309	-	49,53,53	1.83	4 (8%)	60,89,89	1.11	4 (6%)
44	A86	L	314	-	47,50,50	0.71	1 (2%)	51,76,76	1.06	2 (3%)
40	CLA	H	302	-	51,55,73	2.04	9 (17%)	60,91,113	1.51	8 (13%)
40	CLA	C	304	3	60,64,73	1.84	10 (16%)	71,102,113	1.43	11 (15%)
42	DD6	C	313	-	40,45,45	0.19	0	51,67,67	0.59	1 (1%)
40	CLA	z	302	-	64,68,73	1.75	9 (14%)	76,107,113	1.29	5 (6%)
46	SQD	W	318	-	30,32,54	1.48	4 (13%)	40,43,65	1.30	4 (10%)
47	A1EB1	y	314	-	54,58,58	0.55	1 (1%)	60,85,85	0.44	0
42	DD6	A	313	-	40,45,45	0.17	0	51,67,67	0.67	2 (3%)
40	CLA	a	804	23	65,69,73	1.79	10 (15%)	76,107,113	1.75	10 (13%)
40	CLA	b	825	-	69,73,73	1.65	9 (13%)	82,113,113	1.30	6 (7%)
40	CLA	I	206	9	69,73,73	1.70	9 (13%)	82,113,113	1.32	8 (9%)
44	A86	t	310	-	47,50,50	0.51	1 (2%)	51,76,76	0.96	3 (5%)
40	CLA	B	304	-	51,55,73	2.04	9 (17%)	60,91,113	1.53	7 (11%)
41	KC2	O	301	15	49,53,53	1.84	4 (8%)	60,89,89	1.10	5 (8%)
44	A86	X	321	-	47,50,50	0.79	1 (2%)	51,76,76	1.16	3 (5%)
40	CLA	a	839	45	69,73,73	1.68	9 (13%)	82,113,113	1.32	6 (7%)
40	CLA	x	302	-	69,73,73	1.78	9 (13%)	82,113,113	1.43	7 (8%)
44	A86	p	316	-	47,50,50	0.44	0	51,76,76	1.16	3 (5%)
40	CLA	S	311	-	51,55,73	2.11	9 (17%)	60,91,113	1.76	10 (16%)
44	A86	u	319	-	47,50,50	0.38	1 (2%)	51,76,76	1.27	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	CLA	b	830	24	65,69,73	1.77	9 (13%)	77,108,113	1.51	9 (11%)
40	CLA	H	309	-	60,64,73	1.89	9 (15%)	71,102,113	1.64	9 (12%)
40	CLA	u	314	35	51,55,73	2.06	9 (17%)	60,91,113	1.69	8 (13%)
40	CLA	K	312	-	51,55,73	1.94	9 (17%)	60,91,113	1.47	7 (11%)
42	DD6	G	210	-	40,45,45	0.22	0	51,67,67	0.73	2 (3%)
40	CLA	I	207	9	51,55,73	2.03	9 (17%)	60,91,113	1.61	7 (11%)
40	CLA	M	304	13	64,68,73	1.74	9 (14%)	76,107,113	1.34	5 (6%)
41	KC2	Y	308	-	49,53,53	1.83	4 (8%)	60,89,89	1.09	5 (8%)
41	KC2	q	308	36	49,53,53	1.83	4 (8%)	60,89,89	1.12	4 (6%)
40	CLA	q	307	36	64,68,73	1.80	9 (14%)	76,107,113	1.50	10 (13%)
40	CLA	p	312	-	51,55,73	2.02	9 (17%)	60,91,113	1.52	7 (11%)
40	CLA	b	838	-	69,73,73	1.71	9 (13%)	82,113,113	1.38	7 (8%)
40	CLA	a	832	23	69,73,73	1.70	9 (13%)	82,113,113	1.28	7 (8%)
40	CLA	P	306	13	51,55,73	1.97	9 (17%)	60,91,113	1.43	7 (11%)
40	CLA	W	308	-	64,68,73	1.86	9 (14%)	76,107,113	1.51	9 (11%)
44	A86	u	317	-	47,50,50	0.55	1 (2%)	51,76,76	1.19	2 (3%)
42	DD6	Q	214	-	40,45,45	0.24	0	51,67,67	0.85	1 (1%)
44	A86	o	315	-	47,50,50	0.54	1 (2%)	51,76,76	1.02	3 (5%)
47	A1EB1	L	316	-	54,58,58	0.54	1 (1%)	60,85,85	0.77	1 (1%)
42	DD6	L	315	-	40,45,45	0.15	0	51,67,67	0.53	1 (1%)
40	CLA	b	816	24	51,55,73	2.00	9 (17%)	60,91,113	1.63	9 (15%)
42	DD6	z	321	-	40,45,45	0.22	0	51,67,67	0.76	1 (1%)
43	LMG	j	101	-	30,30,55	0.91	1 (3%)	38,38,63	1.30	3 (7%)
47	A1EB1	t	314	-	54,58,58	0.61	1 (1%)	60,85,85	0.91	3 (5%)
40	CLA	U	205	-	51,55,73	2.03	9 (17%)	60,91,113	1.56	8 (13%)
44	A86	x	318	-	47,50,50	0.48	1 (2%)	51,76,76	1.19	2 (3%)
41	KC2	X	309	-	49,53,53	1.88	4 (8%)	60,89,89	1.09	2 (3%)
40	CLA	x	311	-	59,63,73	1.94	9 (15%)	70,101,113	1.74	12 (17%)
40	CLA	v	301	-	59,63,73	1.87	9 (15%)	70,101,113	1.42	6 (8%)
40	CLA	z	308	39	64,68,73	1.73	9 (14%)	76,107,113	1.44	10 (13%)
40	CLA	q	312	-	64,68,73	1.76	9 (14%)	76,107,113	1.27	5 (6%)
44	A86	W	314	-	47,50,50	0.65	1 (2%)	51,76,76	0.90	2 (3%)
44	A86	Y	318	-	47,50,50	0.65	1 (2%)	51,76,76	0.94	3 (5%)
44	A86	q	319	-	47,50,50	0.35	0	51,76,76	1.34	4 (7%)
42	DD6	R	314	-	40,45,45	0.18	0	51,67,67	0.94	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	A1EB1	u	322	-	54,58,58	0.35	0	60,85,85	1.32	6 (10%)
47	A1EB1	x	321	-	54,58,58	0.52	1 (1%)	60,85,85	0.58	1 (1%)
40	CLA	F	310	-	51,55,73	1.99	10 (19%)	60,91,113	1.53	10 (16%)
40	CLA	U	202	18	59,63,73	1.91	9 (15%)	70,101,113	1.55	8 (11%)
40	CLA	Y	311	-	51,55,73	2.02	9 (17%)	60,91,113	1.46	7 (11%)
40	CLA	p	305	35	51,55,73	1.92	9 (17%)	60,91,113	1.57	7 (11%)
40	CLA	T	304	15	64,68,73	1.78	9 (14%)	76,107,113	1.36	6 (7%)
40	CLA	Z	312	-	51,55,73	2.09	9 (17%)	60,91,113	1.67	14 (23%)
40	CLA	S	301	-	64,68,73	1.82	9 (14%)	76,107,113	1.39	6 (7%)
44	A86	x	316	-	47,50,50	0.46	1 (2%)	51,76,76	1.25	3 (5%)
41	KC2	F	302	6	49,53,53	1.85	4 (8%)	60,89,89	1.07	4 (6%)
41	KC2	Z	309	-	49,53,53	1.89	4 (8%)	60,89,89	1.00	2 (3%)
44	A86	F	317	-	47,50,50	0.42	1 (2%)	51,76,76	0.83	2 (3%)
42	DD6	E	315	-	40,45,45	0.20	0	51,67,67	0.89	3 (5%)
42	DD6	P	315	-	40,45,45	0.39	0	51,67,67	0.94	2 (3%)
47	A1EB1	G	212	-	54,58,58	0.58	1 (1%)	60,85,85	0.75	1 (1%)
40	CLA	w	303	38	51,55,73	2.02	9 (17%)	60,91,113	1.52	6 (10%)
40	CLA	B	301	2	51,55,73	2.07	9 (17%)	60,91,113	1.77	9 (15%)
40	CLA	a	842	-	69,73,73	1.66	9 (13%)	82,113,113	1.26	7 (8%)
40	CLA	D	312	4	59,63,73	1.89	9 (15%)	70,101,113	1.43	6 (8%)
40	CLA	b	807	-	69,73,73	1.66	9 (13%)	82,113,113	1.23	8 (9%)
41	KC2	R	308	15	49,53,53	1.84	4 (8%)	60,89,89	1.04	4 (6%)
44	A86	u	318	-	47,50,50	0.44	1 (2%)	51,76,76	1.37	3 (5%)
47	A1EB1	z	323	-	54,58,58	0.52	1 (1%)	60,85,85	1.00	2 (3%)
47	A1EB1	t	313	-	54,58,58	0.41	1 (1%)	60,85,85	0.85	4 (6%)
40	CLA	b	811	24	51,55,73	1.93	9 (17%)	60,91,113	1.53	8 (13%)
41	KC2	T	302	-	49,53,53	1.86	5 (10%)	60,89,89	1.07	4 (6%)
41	KC2	C	303	-	49,53,53	1.86	4 (8%)	60,89,89	1.08	4 (6%)
40	CLA	Y	301	-	64,68,73	1.80	9 (14%)	76,107,113	1.31	6 (7%)
40	CLA	D	303	4	64,68,73	1.74	10 (15%)	76,107,113	1.36	7 (9%)
40	CLA	l	203	-	68,72,73	1.70	10 (14%)	80,111,113	1.51	9 (11%)
42	DD6	M	314	-	40,45,45	0.21	0	51,67,67	0.74	1 (1%)
40	CLA	a	817	23	54,58,73	1.90	9 (16%)	64,95,113	1.43	6 (9%)
40	CLA	O	316	47	51,55,73	1.97	9 (17%)	60,91,113	1.37	6 (10%)
44	A86	M	315	-	47,50,50	0.56	1 (2%)	51,76,76	1.15	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	A86	F	313	-	47,50,50	0.42	1 (2%)	51,76,76	0.80	2 (3%)
44	A86	o	317	-	47,50,50	0.47	1 (2%)	51,76,76	0.99	3 (5%)
40	CLA	Q	203	-	53,57,73	1.98	9 (16%)	62,93,113	1.89	9 (14%)
40	CLA	D	308	4	59,63,73	1.85	9 (15%)	70,101,113	1.40	7 (10%)
40	CLA	z	324	-	51,55,73	2.04	9 (17%)	60,91,113	1.56	9 (15%)
40	CLA	b	803	-	69,73,73	1.70	9 (13%)	82,113,113	1.36	8 (9%)
44	A86	Z	317	-	47,50,50	0.58	1 (2%)	51,76,76	0.82	1 (1%)
40	CLA	u	302	-	69,73,73	1.72	9 (13%)	82,113,113	1.35	8 (9%)
44	A86	G	209	-	47,50,50	0.54	1 (2%)	51,76,76	1.14	3 (5%)
40	CLA	R	305	15	64,68,73	1.78	9 (14%)	76,107,113	1.38	5 (6%)
40	CLA	A	303	1	65,69,73	1.73	9 (13%)	77,108,113	1.32	7 (9%)
51	SF4	c	102	-	0,12,12	-	-	-		
47	A1EB1	Z	321	-	54,58,58	0.51	1 (1%)	60,85,85	0.40	0
42	DD6	w	312	-	40,45,45	0.17	0	51,67,67	0.97	3 (5%)
40	CLA	M	305	13	64,68,73	1.75	9 (14%)	76,107,113	1.35	7 (9%)
41	KC2	Z	303	22	49,53,53	1.81	4 (8%)	60,89,89	1.01	4 (6%)
49	BCR	r	201	-	41,41,41	0.19	0	56,56,56	0.40	0
40	CLA	k	202	-	59,63,73	1.84	9 (15%)	70,101,113	1.38	7 (10%)
40	CLA	C	308	-	51,55,73	2.11	9 (17%)	60,91,113	1.69	10 (16%)
40	CLA	b	833	24	64,68,73	1.73	9 (14%)	76,107,113	1.37	9 (11%)
44	A86	p	318	-	47,50,50	0.47	1 (2%)	51,76,76	1.14	3 (5%)
40	CLA	o	312	-	51,55,73	2.06	9 (17%)	60,91,113	1.61	7 (11%)
41	KC2	O	309	15	49,53,53	1.83	4 (8%)	60,89,89	1.12	5 (8%)
41	KC2	t	306	-	49,53,53	1.83	4 (8%)	60,89,89	1.03	3 (5%)
49	BCR	m	101	-	41,41,41	0.17	0	56,56,56	0.34	0
51	SF4	b	804	-	0,12,12	-	-	-		
40	CLA	a	829	-	69,73,73	1.72	9 (13%)	82,113,113	1.41	9 (10%)
41	KC2	o	309	34	49,53,53	1.85	4 (8%)	60,89,89	1.04	4 (6%)
41	KC2	Q	201	16	49,53,53	1.85	4 (8%)	60,89,89	1.08	4 (6%)
40	CLA	v	305	-	64,68,73	1.79	9 (14%)	76,107,113	1.42	9 (11%)
47	A1EB1	Z	319	-	54,58,58	0.50	1 (1%)	60,85,85	0.71	1 (1%)
40	CLA	X	304	-	51,55,73	1.97	9 (17%)	60,91,113	1.46	6 (10%)
41	KC2	L	308	12	49,53,53	1.86	4 (8%)	60,89,89	0.99	3 (5%)
40	CLA	P	305	13	64,68,73	1.73	9 (14%)	76,107,113	1.35	7 (9%)
43	LMG	S	322	-	39,39,55	0.94	2 (5%)	47,47,63	1.22	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	CLA	a	816	23	69,73,73	1.68	9 (13%)	82,113,113	1.46	9 (10%)
40	CLA	p	306	35	51,55,73	2.00	9 (17%)	60,91,113	1.50	7 (11%)
41	KC2	x	304	35	49,53,53	1.83	4 (8%)	60,89,89	1.03	3 (5%)
42	DD6	C	310	-	40,45,45	0.19	0	51,67,67	0.87	3 (5%)
42	DD6	B	305	-	40,45,45	0.19	0	51,67,67	0.80	2 (3%)
47	A1EB1	v	322	-	54,58,58	0.35	0	60,85,85	0.82	1 (1%)
40	CLA	X	306	20	59,63,73	1.87	9 (15%)	70,101,113	1.53	10 (14%)
40	CLA	a	830	-	62,66,73	1.77	9 (14%)	73,104,113	1.41	9 (12%)
40	CLA	F	307	6	61,67,73	1.72	9 (14%)	74,105,113	1.49	8 (10%)
44	A86	H	315	-	47,50,50	0.48	1 (2%)	51,76,76	1.25	4 (7%)
47	A1EB1	p	324	-	54,58,58	0.49	1 (1%)	60,85,85	0.44	1 (1%)
41	KC2	A	310	1	49,53,53	1.84	4 (8%)	60,89,89	1.04	4 (6%)
40	CLA	B	307	-	51,55,73	2.04	9 (17%)	60,91,113	1.69	9 (15%)
40	CLA	P	312	13	64,68,73	1.76	9 (14%)	76,107,113	1.32	7 (9%)
42	DD6	Z	318	-	40,45,45	0.22	0	51,67,67	0.91	2 (3%)
45	LHG	a	849	40	29,29,48	0.78	0	32,35,54	1.23	2 (6%)
42	DD6	J	314	-	40,45,45	0.19	0	51,67,67	0.72	3 (5%)
40	CLA	W	312	13	64,68,73	1.76	9 (14%)	76,107,113	1.31	9 (11%)
40	CLA	J	306	10	56,60,73	1.93	9 (16%)	65,97,113	1.51	8 (12%)
40	CLA	t	302	38	51,55,73	2.01	9 (17%)	60,91,113	1.50	6 (10%)
40	CLA	p	313	-	59,63,73	1.88	9 (15%)	70,101,113	1.32	6 (8%)
41	KC2	Z	302	-	49,53,53	1.87	4 (8%)	60,89,89	1.03	4 (6%)
42	DD6	J	317	-	40,45,45	0.20	0	51,67,67	0.77	1 (1%)
40	CLA	a	838	23	59,63,73	1.90	9 (15%)	70,101,113	1.55	7 (10%)
40	CLA	Z	311	22	67,71,73	1.77	9 (13%)	79,110,113	1.40	8 (10%)
40	CLA	X	311	20	67,71,73	1.78	9 (13%)	79,110,113	1.39	7 (8%)
41	KC2	H	303	-	49,53,53	1.84	4 (8%)	60,89,89	1.08	4 (6%)
40	CLA	H	305	8	64,68,73	1.76	9 (14%)	76,107,113	1.34	10 (13%)
41	KC2	t	301	38	49,53,53	1.84	5 (10%)	60,89,89	1.05	4 (6%)
40	CLA	D	301	4	59,63,73	1.82	9 (15%)	70,101,113	1.37	6 (8%)
40	CLA	q	304	-	56,60,73	1.86	9 (16%)	65,97,113	1.39	8 (12%)
40	CLA	t	309	-	51,55,73	2.01	9 (17%)	60,91,113	1.51	6 (10%)
42	DD6	F	314	-	40,45,45	0.29	0	51,67,67	0.85	3 (5%)
47	A1EB1	o	321	-	54,58,58	0.51	1 (1%)	60,85,85	0.65	0
41	KC2	O	303	15	49,53,53	1.85	4 (8%)	60,89,89	1.06	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	CLA	D	311	-	51,55,73	2.01	9 (17%)	60,91,113	1.64	7 (11%)
44	A86	X	320	-	47,50,50	0.50	1 (2%)	51,76,76	0.92	2 (3%)
40	CLA	b	809	24	64,68,73	1.83	9 (14%)	76,107,113	1.54	9 (11%)
42	DD6	K	310	-	40,45,45	0.22	0	51,67,67	0.62	1 (1%)
40	CLA	F	304	6	59,63,73	1.93	9 (15%)	70,101,113	1.49	10 (14%)
43	LMG	W	317	-	39,39,55	0.84	0	47,47,63	1.29	6 (12%)
40	CLA	v	313	36	51,55,73	2.03	9 (17%)	60,91,113	1.61	8 (13%)
40	CLA	C	301	3	51,55,73	2.03	9 (17%)	60,91,113	1.55	7 (11%)
42	DD6	D	316	-	40,45,45	0.21	0	51,67,67	0.63	0
40	CLA	I	205	9	60,64,73	1.82	9 (15%)	71,102,113	1.36	8 (11%)
40	CLA	P	313	-	64,68,73	1.76	9 (14%)	76,107,113	1.34	6 (7%)
40	CLA	E	314	5	51,55,73	2.08	9 (17%)	60,91,113	1.95	12 (20%)
40	CLA	a	806	23	69,73,73	1.72	10 (14%)	82,113,113	1.45	7 (8%)
40	CLA	o	306	34	64,68,73	1.80	10 (15%)	76,107,113	1.40	9 (11%)
41	KC2	M	308	13	49,53,53	1.84	4 (8%)	60,89,89	1.11	5 (8%)
41	KC2	u	304	35	49,53,53	1.83	4 (8%)	60,89,89	1.07	3 (5%)
40	CLA	a	821	23	69,73,73	1.69	9 (13%)	82,113,113	1.26	7 (8%)
47	A1EB1	o	322	-	54,58,58	0.54	1 (1%)	60,85,85	0.71	1 (1%)
40	CLA	H	308	8	51,55,73	1.98	9 (17%)	60,91,113	1.46	5 (8%)
41	KC2	v	302	-	49,53,53	1.87	4 (8%)	60,89,89	1.06	4 (6%)
41	KC2	W	304	13	49,53,53	1.83	4 (8%)	60,89,89	1.07	6 (10%)
40	CLA	y	309	-	59,63,73	1.92	9 (15%)	70,101,113	1.59	8 (11%)
46	SQD	k	205	-	34,36,54	1.39	4 (11%)	44,47,65	1.25	3 (6%)
40	CLA	b	827	24	64,68,73	1.80	9 (14%)	76,107,113	1.46	7 (9%)
42	DD6	K	311	-	40,45,45	0.17	0	51,67,67	0.72	2 (3%)
45	LHG	F	319	-	39,39,48	0.68	1 (2%)	42,45,54	1.19	2 (4%)
41	KC2	Q	216	-	49,53,53	1.84	4 (8%)	60,89,89	1.08	4 (6%)
42	DD6	E	317	-	40,45,45	0.18	0	51,67,67	0.69	2 (3%)
47	A1EB1	v	321	-	54,58,58	0.52	1 (1%)	60,85,85	0.94	3 (5%)
42	DD6	A	312	-	40,45,45	0.20	0	51,67,67	0.88	1 (1%)
41	KC2	u	310	-	49,53,53	1.82	4 (8%)	60,89,89	1.04	3 (5%)
40	CLA	p	302	-	69,73,73	1.72	9 (13%)	82,113,113	1.37	8 (9%)
40	CLA	E	306	5	59,63,73	1.84	9 (15%)	70,101,113	1.40	6 (8%)
42	DD6	y	311	-	40,45,45	0.18	0	51,67,67	0.99	3 (5%)
40	CLA	a	807	-	60,64,73	1.82	9 (15%)	71,102,113	1.45	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	CLA	a	820	23	64,68,73	1.81	9 (14%)	76,107,113	1.49	8 (10%)
44	A86	X	316	-	47,50,50	0.51	1 (2%)	51,76,76	1.14	2 (3%)
44	A86	t	316	-	47,50,50	0.56	1 (2%)	51,76,76	0.52	0
40	CLA	T	306	15	64,68,73	1.76	10 (15%)	76,107,113	1.36	9 (11%)
44	A86	o	318	-	47,50,50	0.58	1 (2%)	51,76,76	0.53	0
40	CLA	S	306	17	60,64,73	1.82	9 (15%)	71,102,113	1.37	8 (11%)
42	DD6	o	320	-	40,45,45	0.18	0	51,67,67	0.59	1 (1%)
41	KC2	N	301	14	49,53,53	1.84	4 (8%)	60,89,89	1.07	2 (3%)
44	A86	z	320	-	47,50,50	0.57	1 (2%)	51,76,76	0.66	1 (1%)
41	KC2	S	304	17	49,53,53	1.83	4 (8%)	60,89,89	1.09	5 (8%)
41	KC2	K	305	11	49,53,53	1.82	4 (8%)	60,89,89	1.09	4 (6%)
40	CLA	L	310	-	51,55,73	2.04	9 (17%)	60,91,113	1.63	9 (15%)
42	DD6	C	312	-	40,45,45	0.16	0	51,67,67	1.03	2 (3%)
40	CLA	R	304	15	55,59,73	1.90	9 (16%)	64,96,113	1.58	10 (15%)
40	CLA	Z	305	22	59,63,73	1.83	9 (15%)	70,101,113	1.30	6 (8%)
42	DD6	D	313	-	40,45,45	0.18	0	51,67,67	0.85	2 (3%)
40	CLA	a	837	23	59,63,73	1.86	9 (15%)	70,101,113	1.38	6 (8%)
40	CLA	E	313	5	51,55,73	1.97	9 (17%)	60,91,113	1.50	6 (10%)
42	DD6	D	314	-	40,45,45	0.20	0	51,67,67	0.86	1 (1%)
44	A86	Y	317	41	47,50,50	0.56	1 (2%)	51,76,76	0.99	3 (5%)
49	BCR	l	208	-	41,41,41	0.20	0	56,56,56	0.67	2 (3%)
41	KC2	L	303	12	49,53,53	1.84	4 (8%)	60,89,89	1.05	5 (8%)
41	KC2	o	302	-	49,53,53	1.85	4 (8%)	60,89,89	1.08	4 (6%)
40	CLA	K	304	11	64,68,73	1.73	9 (14%)	76,107,113	1.38	6 (7%)
41	KC2	z	309	39	49,53,53	1.81	4 (8%)	60,89,89	1.06	4 (6%)
40	CLA	S	313	-	51,55,73	1.95	9 (17%)	60,91,113	1.43	7 (11%)
40	CLA	a	810	-	64,68,73	1.76	9 (14%)	76,107,113	1.40	8 (10%)
44	A86	W	316	-	47,50,50	0.42	1 (2%)	51,76,76	0.71	1 (1%)
44	A86	Z	316	-	47,50,50	0.59	1 (2%)	51,76,76	1.18	3 (5%)
40	CLA	a	852	-	59,63,73	1.84	9 (15%)	70,101,113	1.37	5 (7%)
45	LHG	S	323	-	39,39,48	0.69	2 (5%)	42,45,54	1.28	4 (9%)
40	CLA	b	818	24	66,70,73	1.71	9 (13%)	78,109,113	1.35	7 (8%)
44	A86	S	317	-	47,50,50	0.45	1 (2%)	51,76,76	0.95	2 (3%)
44	A86	Q	215	-	47,50,50	0.42	1 (2%)	51,76,76	1.20	2 (3%)
40	CLA	W	311	-	59,63,73	1.88	9 (15%)	70,101,113	1.49	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	CLA	A	308	-	59,63,73	1.85	9 (15%)	70,101,113	1.34	5 (7%)
41	KC2	q	303	36	49,53,53	1.83	4 (8%)	60,89,89	1.02	3 (5%)
40	CLA	G	201	7	51,55,73	1.98	9 (17%)	60,91,113	1.43	6 (10%)
40	CLA	L	312	-	51,55,73	2.04	9 (17%)	60,91,113	1.48	7 (11%)
41	KC2	P	310	-	49,53,53	1.84	4 (8%)	60,89,89	1.06	4 (6%)
40	CLA	u	313	-	59,63,73	1.85	9 (15%)	70,101,113	1.31	6 (8%)
42	DD6	t	312	-	40,45,45	0.15	0	51,67,67	1.04	4 (7%)
44	A86	O	315	-	47,50,50	0.39	1 (2%)	51,76,76	0.73	1 (1%)
44	A86	T	319	-	47,50,50	0.61	1 (2%)	51,76,76	0.78	2 (3%)
49	BCR	a	845	-	41,41,41	0.13	0	56,56,56	0.47	0
41	KC2	q	302	36	49,53,53	1.88	4 (8%)	60,89,89	1.09	6 (10%)
42	DD6	T	314	-	40,45,45	0.20	0	51,67,67	0.66	1 (1%)
40	CLA	R	306	15	64,68,73	1.78	9 (14%)	76,107,113	1.37	7 (9%)
40	CLA	S	314	17	59,63,73	1.88	9 (15%)	70,101,113	1.54	7 (10%)
40	CLA	q	311	-	67,71,73	1.80	9 (13%)	79,110,113	1.39	8 (10%)
44	A86	Z	315	-	47,50,50	0.48	1 (2%)	51,76,76	1.08	3 (5%)
40	CLA	k	201	31	59,63,73	1.84	9 (15%)	70,101,113	1.44	7 (10%)
42	DD6	J	301	-	40,45,45	0.22	0	51,67,67	0.69	1 (1%)
47	A1EB1	q	321	-	54,58,58	0.53	1 (1%)	60,85,85	0.97	3 (5%)
40	CLA	N	305	14	59,63,73	1.83	9 (15%)	70,101,113	1.41	6 (8%)
44	A86	O	313	-	47,50,50	0.30	0	51,76,76	0.82	2 (3%)
44	A86	Y	321	-	47,50,50	0.63	1 (2%)	51,76,76	0.75	1 (1%)
40	CLA	W	307	13	69,73,73	1.69	9 (13%)	82,113,113	1.27	8 (9%)
40	CLA	b	840	-	69,73,73	1.75	9 (13%)	82,113,113	1.39	8 (9%)
41	KC2	P	303	13	49,53,53	1.88	4 (8%)	60,89,89	1.07	3 (5%)
40	CLA	O	310	-	51,55,73	2.06	9 (17%)	60,91,113	1.70	11 (18%)
41	KC2	u	303	-	49,53,53	1.88	4 (8%)	60,89,89	1.01	4 (6%)
40	CLA	b	832	24	69,73,73	1.72	9 (13%)	82,113,113	1.45	8 (9%)
40	CLA	f	205	-	51,55,73	1.97	9 (17%)	60,91,113	1.43	7 (11%)
43	LMG	P	318	-	39,39,55	0.99	3 (7%)	47,47,63	1.32	7 (14%)
44	A86	v	316	-	47,50,50	0.56	1 (2%)	51,76,76	1.30	1 (1%)
40	CLA	Y	305	21	59,63,73	1.85	9 (15%)	70,101,113	1.41	7 (10%)
41	KC2	P	302	-	49,53,53	1.83	4 (8%)	60,89,89	1.08	5 (8%)
44	A86	u	316	-	47,50,50	0.43	1 (2%)	51,76,76	1.25	3 (5%)
40	CLA	E	302	5	51,55,73	2.02	9 (17%)	60,91,113	1.72	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	CLA	u	312	-	64,68,73	1.77	9 (14%)	76,107,113	1.31	5 (6%)
42	DD6	X	322	-	40,45,45	0.18	0	51,67,67	0.65	1 (1%)
40	CLA	o	305	34	59,63,73	1.86	9 (15%)	70,101,113	1.38	8 (11%)
41	KC2	z	303	39	49,53,53	1.85	4 (8%)	60,89,89	1.05	4 (6%)
40	CLA	A	307	1	64,68,73	1.80	10 (15%)	76,107,113	1.44	8 (10%)
40	CLA	l	205	32	69,73,73	1.75	9 (13%)	82,113,113	1.38	8 (9%)
40	CLA	z	307	-	64,68,73	1.80	9 (14%)	76,107,113	1.47	10 (13%)
40	CLA	F	308	-	59,63,73	1.88	9 (15%)	70,101,113	1.43	6 (8%)
40	CLA	a	805	23,40	58,62,73	1.82	9 (15%)	68,99,113	1.41	6 (8%)
47	A1EB1	q	323	-	54,58,58	0.54	1 (1%)	60,85,85	0.54	0
40	CLA	U	208	-	51,55,73	1.94	9 (17%)	60,91,113	1.43	9 (15%)
41	KC2	X	308	20	49,53,53	1.84	4 (8%)	60,89,89	1.02	3 (5%)
40	CLA	O	307	-	66,70,73	1.76	9 (13%)	78,109,113	1.33	6 (7%)
47	A1EB1	y	313	-	54,58,58	0.44	1 (1%)	60,85,85	0.82	2 (3%)
40	CLA	K	306	-	64,68,73	1.73	9 (14%)	76,107,113	1.39	10 (13%)
49	BCR	a	844	-	41,41,41	0.17	0	56,56,56	0.47	0
44	A86	X	315	-	47,50,50	0.50	0	51,76,76	1.66	6 (11%)
44	A86	O	312	-	47,50,50	0.46	1 (2%)	51,76,76	0.97	2 (3%)
40	CLA	E	309	-	64,68,73	1.77	9 (14%)	76,107,113	1.34	7 (9%)
44	A86	q	317	-	47,50,50	0.48	1 (2%)	51,76,76	0.87	1 (1%)
47	A1EB1	R	317	40	54,58,58	0.58	1 (1%)	60,85,85	1.15	2 (3%)
41	KC2	S	310	-	49,53,53	1.84	4 (8%)	60,89,89	1.04	3 (5%)
40	CLA	u	308	35	64,68,73	1.78	9 (14%)	76,107,113	1.42	7 (9%)
40	CLA	a	834	-	64,68,73	1.80	9 (14%)	76,107,113	1.44	8 (10%)
40	CLA	x	306	35	64,68,73	1.73	9 (14%)	76,107,113	1.32	9 (11%)
40	CLA	a	835	-	69,73,73	1.67	9 (13%)	82,113,113	1.30	7 (8%)
42	DD6	U	209	-	40,45,45	0.27	0	51,67,67	0.81	2 (3%)
40	CLA	L	307	-	59,63,73	1.84	9 (15%)	70,101,113	1.40	6 (8%)
44	A86	N	314	-	47,50,50	0.53	1 (2%)	51,76,76	1.10	4 (7%)
41	KC2	K	302	11	49,53,53	1.85	4 (8%)	60,89,89	1.07	3 (5%)
44	A86	v	319	-	47,50,50	0.36	0	51,76,76	1.32	4 (7%)
40	CLA	T	305	15	54,58,73	1.92	9 (16%)	64,95,113	1.42	6 (9%)
40	CLA	Y	306	21	64,68,73	1.79	10 (15%)	76,107,113	1.44	9 (11%)
40	CLA	S	305	-	56,60,73	1.95	9 (16%)	65,97,113	1.64	11 (16%)
40	CLA	z	313	-	51,55,73	2.06	9 (17%)	60,91,113	1.64	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	KC2	R	302	15	49,53,53	1.88	5 (10%)	60,89,89	1.07	5 (8%)
44	A86	z	319	-	47,50,50	0.53	1 (2%)	51,76,76	0.96	1 (1%)
47	A1EB1	O	317	40	54,58,58	0.54	1 (1%)	60,85,85	0.80	1 (1%)
40	CLA	b	822	-	68,72,73	1.75	9 (13%)	80,111,113	1.42	8 (10%)
40	CLA	v	306	36	64,68,73	1.77	9 (14%)	76,107,113	1.35	7 (9%)
43	LMG	a	802	-	35,35,55	0.89	1 (2%)	43,43,63	1.31	7 (16%)
40	CLA	y	304	-	64,68,73	1.79	10 (15%)	76,107,113	1.36	10 (13%)
50	PQN	b	849	-	29,29,34	0.45	0	37,39,45	0.79	1 (2%)
40	CLA	H	304	-	51,55,73	2.02	10 (19%)	60,91,113	1.53	9 (15%)
40	CLA	b	808	-	69,73,73	1.73	9 (13%)	82,113,113	1.21	9 (10%)
44	A86	o	314	-	47,50,50	0.47	1 (2%)	51,76,76	1.41	5 (9%)
40	CLA	x	313	-	59,63,73	1.85	9 (15%)	70,101,113	1.31	7 (10%)
40	CLA	b	812	24	64,68,73	1.74	9 (14%)	76,107,113	1.26	7 (9%)
44	A86	t	311	-	47,50,50	0.62	1 (2%)	51,76,76	1.22	3 (5%)
47	A1EB1	F	322	-	54,58,58	0.52	1 (1%)	60,85,85	0.42	0
41	KC2	x	310	-	49,53,53	1.84	4 (8%)	60,89,89	1.05	4 (6%)
41	KC2	S	309	17	49,53,53	1.82	4 (8%)	60,89,89	1.12	5 (8%)
44	A86	Z	314	-	47,50,50	0.50	1 (2%)	51,76,76	1.34	3 (5%)
41	KC2	O	311	-	49,53,53	1.84	4 (8%)	60,89,89	1.07	4 (6%)
40	CLA	Y	313	21	51,55,73	2.09	9 (17%)	60,91,113	1.72	9 (15%)
42	DD6	E	316	-	40,45,45	0.21	0	51,67,67	0.86	3 (5%)
47	A1EB1	L	318	-	54,58,58	0.57	1 (1%)	60,85,85	0.73	1 (1%)
40	CLA	D	309	-	62,66,73	1.81	9 (14%)	73,104,113	1.35	6 (8%)
40	CLA	Q	205	16	65,69,73	1.80	9 (13%)	76,107,113	1.74	12 (15%)
49	BCR	l	207	-	41,41,41	0.25	0	56,56,56	0.92	3 (5%)
43	LMG	M	317	-	39,39,55	0.88	2 (5%)	47,47,63	1.34	4 (8%)
41	KC2	w	306	38	49,53,53	1.84	4 (8%)	60,89,89	1.05	5 (8%)
45	LHG	a	848	-	47,47,48	0.62	0	50,53,54	1.14	3 (6%)
42	DD6	A	314	-	40,45,45	0.16	0	51,67,67	0.77	1 (1%)
40	CLA	G	203	7	56,62,73	1.75	8 (14%)	68,99,113	1.56	11 (16%)
43	LMG	F	318	-	39,39,55	0.78	0	47,47,63	1.34	6 (12%)
40	CLA	b	801	-	67,71,73	1.75	10 (14%)	79,110,113	1.42	12 (15%)
44	A86	Y	320	-	47,50,50	0.62	1 (2%)	51,76,76	1.41	3 (5%)
40	CLA	b	802	-	69,73,73	1.67	9 (13%)	82,113,113	1.29	8 (9%)
40	CLA	C	309	-	51,55,73	2.06	9 (17%)	60,91,113	1.55	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	A86	N	321	-	47,50,50	0.46	1 (2%)	51,76,76	0.87	2 (3%)
40	CLA	t	305	-	53,57,73	1.99	9 (16%)	65,94,113	1.51	6 (9%)
47	A1EB1	p	323	-	54,58,58	0.38	0	60,85,85	1.27	5 (8%)
44	A86	Y	316	-	47,50,50	0.44	1 (2%)	51,76,76	0.63	1 (1%)
41	KC2	N	313	14	49,53,53	1.84	4 (8%)	60,89,89	1.03	4 (6%)
41	KC2	J	304	-	49,53,53	1.85	4 (8%)	60,89,89	1.09	4 (6%)
40	CLA	b	829	-	51,55,73	2.02	9 (17%)	60,91,113	1.44	8 (13%)
44	A86	q	314	-	47,50,50	0.59	1 (2%)	51,76,76	1.43	5 (9%)
44	A86	v	314	-	47,50,50	0.54	1 (2%)	51,76,76	1.54	5 (9%)
42	DD6	D	317	-	40,45,45	0.19	0	51,67,67	0.79	2 (3%)
40	CLA	b	813	24	54,58,73	1.89	9 (16%)	64,95,113	1.48	8 (12%)
48	A1EB4	W	319	-	53,58,63	0.67	1 (1%)	59,84,89	0.68	1 (1%)
44	A86	C	311	-	47,50,50	0.69	1 (2%)	51,76,76	1.02	3 (5%)
41	KC2	u	315	-	49,53,53	1.84	4 (8%)	60,89,89	1.11	4 (6%)
46	SQD	I	215	-	52,54,54	1.13	3 (5%)	62,65,65	1.10	3 (4%)
41	KC2	Y	309	21,44	49,53,53	1.84	4 (8%)	60,89,89	1.01	3 (5%)
44	A86	S	316	-	47,50,50	0.53	1 (2%)	51,76,76	1.09	4 (7%)
42	DD6	I	211	-	40,45,45	0.22	0	51,67,67	1.02	3 (5%)
43	LMG	a	801	-	35,35,55	0.95	1 (2%)	43,43,63	1.18	4 (9%)
40	CLA	X	305	-	54,58,73	1.97	9 (16%)	64,95,113	1.44	8 (12%)
40	CLA	b	819	24	68,72,73	1.71	9 (13%)	80,111,113	1.31	6 (7%)
44	A86	q	324	-	47,50,50	0.34	0	51,76,76	1.06	3 (5%)
40	CLA	X	310	-	59,63,73	1.94	8 (13%)	70,101,113	1.71	11 (15%)
40	CLA	N	307	-	64,68,73	1.76	9 (14%)	76,107,113	1.34	6 (7%)
40	CLA	a	808	-	69,73,73	1.76	9 (13%)	82,113,113	1.55	10 (12%)
43	LMG	L	319	-	37,37,55	0.84	0	45,45,63	1.24	4 (8%)
44	A86	P	314	-	47,50,50	0.40	0	51,76,76	0.97	3 (5%)
40	CLA	y	305	-	53,57,73	1.99	9 (16%)	65,94,113	1.50	7 (10%)
40	CLA	K	308	11	63,67,73	1.77	9 (14%)	74,105,113	1.47	9 (12%)
47	A1EB1	S	320	-	54,58,58	0.49	1 (1%)	60,85,85	0.85	2 (3%)
41	KC2	M	301	13	49,53,53	1.84	4 (8%)	60,89,89	1.04	4 (6%)
40	CLA	J	305	10	59,63,73	1.89	10 (16%)	70,101,113	1.42	6 (8%)
40	CLA	F	321	-	64,68,73	1.78	9 (14%)	76,107,113	1.39	8 (10%)
41	KC2	y	307	-	49,53,53	1.85	4 (8%)	60,89,89	1.09	5 (8%)
40	CLA	F	301	-	57,61,73	1.90	9 (15%)	67,98,113	1.42	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	CLA	a	803	-	69,73,73	1.67	9 (13%)	82,113,113	1.25	8 (9%)
42	DD6	J	316	-	40,45,45	0.14	0	51,67,67	0.67	3 (5%)
46	SQD	F	320	-	34,36,54	1.36	3 (8%)	44,47,65	1.36	6 (13%)
40	CLA	o	313	-	51,55,73	2.08	10 (19%)	60,91,113	1.81	10 (16%)
40	CLA	p	308	-	64,68,73	1.77	9 (14%)	76,107,113	1.45	7 (9%)
40	CLA	x	305	-	55,59,73	1.86	9 (16%)	64,96,113	1.48	7 (10%)
42	DD6	I	212	-	40,45,45	0.18	0	51,67,67	0.63	1 (1%)
43	LMG	T	318	-	40,40,55	0.93	3 (7%)	48,48,63	1.24	5 (10%)
40	CLA	X	307	20	64,68,73	1.77	9 (14%)	76,107,113	1.37	7 (9%)
52	DGD	b	850	-	57,57,67	0.96	2 (3%)	71,71,81	1.47	9 (12%)
40	CLA	G	206	7	60,64,73	1.79	9 (15%)	71,102,113	1.37	8 (11%)
40	CLA	I	203	9	59,63,73	1.91	9 (15%)	70,101,113	1.48	7 (10%)
44	A86	P	321	-	47,50,50	0.51	1 (2%)	51,76,76	1.15	2 (3%)
40	CLA	Z	306	22	64,68,73	1.81	9 (14%)	76,107,113	1.44	8 (10%)
40	CLA	q	305	-	64,68,73	1.77	9 (14%)	76,107,113	1.40	8 (10%)
41	KC2	Z	308	22	49,53,53	1.82	4 (8%)	60,89,89	1.06	4 (6%)
40	CLA	t	304	-	64,68,73	1.77	9 (14%)	76,107,113	1.35	8 (10%)
42	DD6	F	316	-	40,45,45	0.20	0	51,67,67	0.89	2 (3%)
43	LMG	l	201	-	39,39,55	0.84	2 (5%)	47,47,63	1.25	4 (8%)
42	DD6	L	317	-	40,45,45	0.15	0	51,67,67	0.71	1 (1%)
41	KC2	o	303	34	49,53,53	1.87	5 (10%)	60,89,89	1.07	4 (6%)
44	A86	p	319	-	47,50,50	0.40	1 (2%)	51,76,76	1.45	4 (7%)
46	SQD	M	318	-	30,32,54	1.44	3 (10%)	40,43,65	1.18	6 (15%)
40	CLA	V	202	19	59,63,73	1.87	9 (15%)	70,101,113	1.43	9 (12%)
40	CLA	b	806	24	69,73,73	1.68	9 (13%)	82,113,113	1.26	5 (6%)
40	CLA	U	204	18	51,55,73	2.03	9 (17%)	60,91,113	1.49	6 (10%)
40	CLA	D	306	4	59,63,73	1.86	9 (15%)	70,101,113	1.40	7 (10%)
44	A86	w	316	-	47,50,50	0.59	1 (2%)	51,76,76	1.09	3 (5%)
40	CLA	b	835	24	66,72,73	1.62	8 (12%)	80,111,113	1.46	10 (12%)
40	CLA	M	312	13	64,68,73	1.76	9 (14%)	76,107,113	1.39	7 (9%)
40	CLA	a	811	23,40	65,69,73	1.81	9 (13%)	76,107,113	1.66	9 (11%)
40	CLA	f	201	-	64,68,73	1.76	9 (14%)	76,107,113	1.27	6 (7%)
44	A86	F	312	-	47,50,50	0.51	1 (2%)	51,76,76	0.88	2 (3%)
40	CLA	A	306	1	64,68,73	1.76	9 (14%)	76,107,113	1.29	6 (7%)
41	KC2	v	308	36	49,53,53	1.84	4 (8%)	60,89,89	1.13	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	BCR	j	103	-	41,41,41	0.23	0	56,56,56	0.55	0
40	CLA	L	304	12	61,65,73	1.85	9 (14%)	72,103,113	1.44	7 (9%)
40	CLA	t	303	38	51,55,73	2.00	9 (17%)	60,91,113	1.50	7 (11%)
41	KC2	G	202	-	49,53,53	1.83	4 (8%)	60,89,89	1.12	5 (8%)
40	CLA	C	306	3	69,73,73	1.71	9 (13%)	82,113,113	1.26	8 (9%)
41	KC2	T	303	-	49,53,53	1.86	4 (8%)	60,89,89	1.17	6 (10%)
42	DD6	Q	212	-	40,45,45	0.19	0	51,67,67	0.69	2 (3%)
47	A1EB1	u	323	-	54,58,58	0.49	1 (1%)	60,85,85	0.49	0
49	BCR	b	845	-	41,41,41	0.18	0	56,56,56	0.40	0
40	CLA	E	312	-	51,55,73	2.00	9 (17%)	60,91,113	1.63	6 (10%)
40	CLA	Y	304	-	51,55,73	2.05	9 (17%)	60,91,113	1.50	7 (11%)
40	CLA	Q	202	16	62,66,73	1.83	9 (14%)	73,104,113	1.47	7 (9%)
44	A86	Y	319	-	47,50,50	0.44	1 (2%)	51,76,76	1.07	3 (5%)
40	CLA	G	205	7	54,58,73	1.91	9 (16%)	64,95,113	1.43	6 (9%)
40	CLA	b	836	24	64,68,73	1.81	9 (14%)	76,107,113	1.36	7 (9%)
43	LMG	E	301	40	31,31,55	0.91	0	39,39,63	1.24	5 (12%)
40	CLA	o	304	34	64,68,73	1.75	9 (14%)	76,107,113	1.34	6 (7%)
47	A1EB1	N	320	-	54,58,58	0.42	0	60,85,85	1.12	3 (5%)
40	CLA	I	202	9	59,63,73	1.81	9 (15%)	70,101,113	1.37	5 (7%)
40	CLA	b	831	24	55,59,73	1.89	9 (16%)	64,96,113	1.43	6 (9%)
40	CLA	Z	304	-	64,68,73	1.79	9 (14%)	76,107,113	1.32	7 (9%)
44	A86	D	320	-	47,50,50	0.46	1 (2%)	51,76,76	0.89	2 (3%)
40	CLA	E	303	-	64,68,73	1.82	9 (14%)	76,107,113	1.45	7 (9%)
40	CLA	o	310	-	59,63,73	1.94	9 (15%)	70,101,113	1.57	11 (15%)
51	SF4	c	101	-	0,12,12	-	-	-		
49	BCR	a	843	-	41,41,41	0.20	0	56,56,56	0.45	0
42	DD6	A	316	-	40,45,45	0.16	0	51,67,67	0.60	2 (3%)
42	DD6	v	318	-	40,45,45	0.22	0	51,67,67	0.86	4 (7%)
41	KC2	p	315	-	49,53,53	1.84	4 (8%)	60,89,89	1.12	4 (6%)
40	CLA	u	307	35	59,63,73	1.88	9 (15%)	70,101,113	1.62	8 (11%)
40	CLA	E	308	5	62,66,73	1.79	9 (14%)	73,104,113	1.43	7 (9%)
40	CLA	P	308	-	64,68,73	1.77	9 (14%)	76,107,113	1.31	7 (9%)
40	CLA	F	305	-	51,55,73	2.00	9 (17%)	60,91,113	1.57	7 (11%)
40	CLA	L	311	12	51,55,73	2.06	9 (17%)	60,91,113	1.57	7 (11%)
40	CLA	v	304	-	56,60,73	1.86	9 (16%)	65,97,113	1.38	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	A86	K	314	-	47,50,50	0.46	1 (2%)	51,76,76	0.94	3 (5%)
41	KC2	G	208	-	49,53,53	1.83	4 (8%)	60,89,89	1.01	3 (5%)
43	LMG	A	317	-	40,40,55	0.83	0	48,48,63	1.23	4 (8%)
44	A86	N	315	-	47,50,50	0.64	1 (2%)	51,76,76	1.13	3 (5%)
40	CLA	p	311	-	59,63,73	1.98	9 (15%)	70,101,113	1.69	11 (15%)
41	KC2	o	308	34	49,53,53	1.82	4 (8%)	60,89,89	1.05	4 (6%)
40	CLA	Z	313	22	51,55,73	2.04	9 (17%)	60,91,113	1.71	9 (15%)
40	CLA	b	842	-	65,69,73	1.77	9 (13%)	77,108,113	1.34	7 (9%)
40	CLA	X	313	20	51,55,73	2.02	9 (17%)	60,91,113	1.66	9 (15%)
42	DD6	q	320	-	40,45,45	0.20	0	51,67,67	0.69	0
44	A86	w	315	-	47,50,50	0.61	1 (2%)	51,76,76	0.67	2 (3%)
44	A86	z	301	-	47,50,50	0.48	1 (2%)	51,76,76	0.99	2 (3%)
40	CLA	z	314	-	51,55,73	2.02	9 (17%)	60,91,113	1.70	9 (15%)
40	CLA	w	309	-	59,63,73	1.91	9 (15%)	70,101,113	1.57	7 (10%)
40	CLA	N	310	-	54,58,73	1.96	9 (16%)	64,95,113	1.58	10 (15%)
40	CLA	W	306	13	64,68,73	1.78	10 (15%)	76,107,113	1.40	8 (10%)
40	CLA	a	812	23	59,63,73	1.82	9 (15%)	70,101,113	1.35	8 (11%)
42	DD6	j	104	-	40,45,45	0.19	0	51,67,67	0.69	1 (1%)
41	KC2	L	313	12	49,53,53	1.86	4 (8%)	60,89,89	1.06	4 (6%)
42	DD6	H	314	-	40,45,45	0.23	0	51,67,67	0.95	4 (7%)
44	A86	w	311	-	47,50,50	0.56	2 (4%)	51,76,76	1.13	3 (5%)
40	CLA	W	313	13	64,68,73	1.78	9 (14%)	76,107,113	1.34	6 (7%)
40	CLA	I	208	-	59,63,73	1.90	9 (15%)	70,101,113	1.50	7 (10%)
40	CLA	J	307	10	51,55,73	2.02	9 (17%)	60,91,113	1.60	11 (18%)
49	BCR	a	846	-	41,41,41	0.15	0	56,56,56	0.41	0
49	BCR	i	102	-	41,41,41	0.36	0	56,56,56	0.70	0
41	KC2	X	302	-	49,53,53	1.85	4 (8%)	60,89,89	1.05	4 (6%)
40	CLA	a	831	-	64,68,73	1.79	9 (14%)	76,107,113	1.32	5 (6%)
42	DD6	Q	211	-	40,45,45	0.20	0	51,67,67	0.72	2 (3%)
40	CLA	a	826	-	65,69,73	1.71	9 (13%)	77,108,113	1.39	8 (10%)
40	CLA	D	305	4	47,51,73	1.93	10 (21%)	60,82,113	2.60	10 (16%)
40	CLA	a	813	23	64,68,73	1.81	9 (14%)	76,107,113	1.38	7 (9%)
41	KC2	N	309	-	49,53,53	1.83	4 (8%)	60,89,89	1.03	5 (8%)
43	LMG	p	301	-	39,39,55	0.80	0	47,47,63	1.19	3 (6%)
44	A86	S	318	-	47,50,50	0.41	1 (2%)	51,76,76	1.00	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	KC2	I	214	-	49,53,53	1.85	4 (8%)	60,89,89	1.05	3 (5%)
44	A86	x	319	-	47,50,50	0.29	0	51,76,76	1.27	2 (3%)
50	PQN	a	847	-	29,29,34	0.44	0	37,39,45	0.78	2 (5%)
41	KC2	E	319	-	49,53,53	1.85	4 (8%)	60,89,89	1.08	4 (6%)
42	DD6	q	318	-	40,45,45	0.20	0	51,67,67	0.91	3 (5%)
44	A86	w	310	-	47,50,50	0.44	1 (2%)	51,76,76	1.13	2 (3%)
42	DD6	W	315	-	40,45,45	0.19	0	51,67,67	0.71	2 (3%)
40	CLA	y	308	-	51,55,73	1.97	9 (17%)	60,91,113	1.44	5 (8%)
40	CLA	R	310	-	51,55,73	2.01	9 (17%)	60,91,113	1.56	7 (11%)
41	KC2	L	309	12	49,53,53	1.87	4 (8%)	60,89,89	1.00	3 (5%)
40	CLA	a	818	-	51,55,73	1.95	9 (17%)	60,91,113	1.56	8 (13%)
40	CLA	x	312	-	64,68,73	1.76	9 (14%)	76,107,113	1.37	8 (10%)
42	DD6	N	317	-	40,45,45	0.22	0	51,67,67	1.17	5 (9%)
41	KC2	W	302	-	49,53,53	1.84	4 (8%)	60,89,89	1.04	3 (5%)
40	CLA	j	102	30	51,55,73	2.07	9 (17%)	60,91,113	1.63	10 (16%)
49	BCR	l	206	-	41,41,41	0.14	0	56,56,56	0.42	0
40	CLA	x	308	35	64,68,73	1.77	9 (14%)	76,107,113	1.41	7 (9%)
40	CLA	J	309	-	51,55,73	2.01	9 (17%)	60,91,113	1.44	6 (10%)
47	A1EB1	T	316	40	54,58,58	0.48	1 (1%)	60,85,85	0.77	1 (1%)
48	A1EB4	P	320	-	53,58,63	0.79	1 (1%)	59,84,89	1.23	2 (3%)
40	CLA	K	307	11	58,62,73	1.85	9 (15%)	68,99,113	1.30	6 (8%)
40	CLA	q	310	-	55,59,73	1.92	9 (16%)	64,96,113	1.56	8 (12%)
40	CLA	v	310	-	55,59,73	1.92	9 (16%)	64,96,113	1.57	9 (14%)
44	A86	X	319	-	47,50,50	0.43	1 (2%)	51,76,76	1.32	4 (7%)
44	A86	z	315	-	47,50,50	0.40	0	51,76,76	1.44	4 (7%)
40	CLA	R	307	-	59,63,73	1.85	9 (15%)	70,101,113	1.44	6 (8%)
40	CLA	A	301	1	51,55,73	2.01	9 (17%)	60,91,113	1.52	9 (15%)
40	CLA	b	814	24	69,73,73	1.66	9 (13%)	82,113,113	1.30	5 (6%)
41	KC2	W	309	-	49,53,53	1.86	4 (8%)	60,89,89	1.12	5 (8%)
40	CLA	F	303	6	65,69,73	1.78	9 (13%)	76,107,113	1.73	10 (13%)
44	A86	M	313	-	47,50,50	0.41	1 (2%)	51,76,76	1.85	3 (5%)
40	CLA	G	207	-	58,62,73	1.88	9 (15%)	68,99,113	1.41	7 (10%)
40	CLA	z	311	-	59,63,73	1.94	9 (15%)	70,101,113	1.77	11 (15%)
44	A86	P	316	-	47,50,50	0.39	1 (2%)	51,76,76	0.99	3 (5%)
47	A1EB1	S	321	-	54,58,58	0.45	1 (1%)	60,85,85	0.75	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	CLA	p	307	35	59,63,73	1.92	9 (15%)	70,101,113	1.62	8 (11%)
41	KC2	F	309	6	49,53,53	1.83	4 (8%)	60,89,89	1.07	4 (6%)
40	CLA	a	841	23	69,73,73	1.71	9 (13%)	82,113,113	1.34	7 (8%)
41	KC2	N	303	14	49,53,53	1.80	4 (8%)	60,89,89	1.12	6 (10%)
40	CLA	L	301	-	51,55,73	2.04	8 (15%)	60,91,113	1.50	7 (11%)
40	CLA	v	307	36	64,68,73	1.80	9 (14%)	76,107,113	1.51	10 (13%)
40	CLA	M	311	13	66,70,73	1.77	9 (13%)	78,109,113	1.33	9 (11%)
44	A86	X	314	-	47,50,50	0.59	1 (2%)	51,76,76	1.11	4 (7%)
40	CLA	P	307	13	63,67,73	1.78	9 (14%)	74,105,113	1.41	7 (9%)
40	CLA	Q	209	-	51,55,73	2.04	9 (17%)	60,91,113	1.60	8 (13%)
40	CLA	w	304	-	64,68,73	1.77	9 (14%)	76,107,113	1.33	7 (9%)
41	KC2	H	316	-	49,53,53	1.81	4 (8%)	60,89,89	1.16	6 (10%)
40	CLA	a	836	23	69,73,73	1.68	9 (13%)	82,113,113	1.27	8 (9%)
47	A1EB1	T	320	-	54,58,58	0.42	1 (1%)	60,85,85	0.71	1 (1%)
40	CLA	q	301	-	59,63,73	1.87	9 (15%)	70,101,113	1.46	6 (8%)
41	KC2	R	301	15	49,53,53	1.80	4 (8%)	60,89,89	1.09	5 (8%)

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
40	CLA	K	301	-	1/1/11/20	4/18/94/115	-
40	CLA	Y	310	-	1/1/13/20	9/27/103/115	-
40	CLA	Q	206	-	1/1/14/20	7/35/112/115	-
41	KC2	I	209	9	-	8/15/71/71	-
40	CLA	H	307	-	1/1/14/20	16/33/109/115	-
40	CLA	W	305	13	1/1/15/20	6/39/115/115	-
41	KC2	R	311	15	-	8/15/71/71	-
49	BCR	f	203	-	-	0/29/63/63	0/2/2/2
40	CLA	a	828	23	1/1/15/20	13/39/115/115	-
44	A86	D	319	-	-	4/34/90/90	0/3/3/3
40	CLA	E	304	5	1/1/13/20	0/27/103/115	-
40	CLA	b	821	-	1/1/15/20	4/39/115/115	-
40	CLA	o	307	34	1/1/14/20	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	A86	T	313	-	-	2/34/90/90	0/3/3/3
40	CLA	U	203	-	1/1/13/20	8/27/103/115	-
40	CLA	w	308	-	1/1/11/20	6/18/94/115	-
40	CLA	U	206	-	1/1/11/20	1/18/94/115	-
41	KC2	N	302	14	-	5/15/71/71	-
44	A86	N	318	-	-	2/34/90/90	0/3/3/3
40	CLA	F	306	6	1/1/14/20	7/33/109/115	-
41	KC2	M	309	-	-	4/15/71/71	-
41	KC2	p	310	-	-	5/15/71/71	-
40	CLA	I	204	9	1/1/11/20	2/18/94/115	-
40	CLA	N	311	14	1/1/14/20	11/33/109/115	-
40	CLA	a	851	-	1/1/15/20	11/39/115/115	-
41	KC2	U	201	-	-	6/15/71/71	-
42	DD6	A	315	-	-	0/26/80/80	0/3/3/3
42	DD6	x	320	-	-	0/26/80/80	0/3/3/3
44	A86	P	317	-	-	3/34/90/90	0/3/3/3
41	KC2	K	303	11	-	10/15/71/71	-
47	A1EB1	v	323	-	-	16/43/100/100	1/3/3/3
47	A1EB1	w	313	-	-	12/43/100/100	0/3/3/3
40	CLA	T	317	47	1/1/11/20	4/18/94/115	-
40	CLA	a	840	23	1/1/13/20	8/27/103/115	-
41	KC2	x	315	-	-	6/15/71/71	-
42	DD6	U	211	-	-	0/26/80/80	0/3/3/3
44	A86	R	312	-	-	4/34/90/90	0/3/3/3
41	KC2	R	303	-	-	10/15/71/71	-
40	CLA	J	318	10	1/1/11/20	1/18/94/115	-
40	CLA	B	302	2	1/1/11/20	4/18/94/115	-
40	CLA	b	815	-	1/1/13/20	4/30/106/115	-
42	DD6	O	314	-	-	1/26/80/80	0/3/3/3
40	CLA	O	304	15	1/1/15/20	7/39/115/115	-
40	CLA	V	201	-	1/1/13/20	8/31/107/115	-
40	CLA	u	306	35	1/1/11/20	7/18/94/115	-
40	CLA	S	307	17	1/1/14/20	9/33/109/115	-
47	A1EB1	K	313	-	-	3/43/100/100	0/3/3/3
40	CLA	B	306	-	1/1/12/20	9/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	J	310	-	1/1/11/20	2/18/94/115	-
40	CLA	b	837	24	1/1/14/20	6/33/109/115	-
40	CLA	u	305	35	1/1/11/20	1/18/94/115	-
47	A1EB1	w	314	-	-	11/43/100/100	0/3/3/3
41	KC2	Y	314	-	-	10/15/71/71	-
44	A86	q	315	-	-	5/34/90/90	0/3/3/3
44	A86	v	315	-	-	5/34/90/90	0/3/3/3
44	A86	z	316	-	-	7/34/90/90	1/3/3/3
40	CLA	a	824	-	1/1/14/20	12/36/112/115	-
40	CLA	w	302	38	1/1/11/20	0/18/94/115	-
42	DD6	z	322	-	-	2/26/80/80	0/3/3/3
40	CLA	S	308	-	1/1/12/20	3/19/95/115	-
42	DD6	H	312	-	-	0/26/80/80	0/3/3/3
41	KC2	O	308	15	-	8/15/71/71	-
42	DD6	k	204	-	-	1/26/80/80	0/3/3/3
44	A86	u	320	-	-	5/34/90/90	0/3/3/3
40	CLA	M	307	-	1/1/14/20	7/33/109/115	-
47	A1EB1	x	322	-	-	5/43/100/100	0/3/3/3
40	CLA	a	809	-	1/1/12/20	4/21/97/115	-
40	CLA	l	204	-	1/1/15/20	11/39/115/115	-
40	CLA	Q	208	-	1/1/14/20	7/33/109/115	-
49	BCR	f	206	-	-	4/29/63/63	0/2/2/2
42	DD6	u	321	-	-	1/26/80/80	0/3/3/3
40	CLA	M	310	-	1/1/13/20	7/29/105/115	-
44	A86	X	317	-	-	6/34/90/90	0/3/3/3
44	A86	v	325	-	-	7/34/90/90	0/3/3/3
40	CLA	A	305	1	1/1/14/20	7/35/111/115	-
42	DD6	J	315	-	-	1/26/80/80	0/3/3/3
40	CLA	b	820	-	1/1/15/20	9/39/115/115	-
40	CLA	C	305	3	1/1/14/20	5/33/109/115	-
40	CLA	a	827	23	1/1/15/20	1/39/115/115	-
42	DD6	H	313	-	-	5/26/80/80	0/3/3/3
42	DD6	I	210	-	-	0/26/80/80	0/3/3/3
40	CLA	L	305	12	1/1/11/20	4/18/94/115	-
40	CLA	X	312	-	1/1/11/20	5/18/94/115	-
49	BCR	b	846	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	b	805	-	1/1/14/20	6/35/111/115	-
41	KC2	w	307	-	-	4/15/71/71	-
40	CLA	u	311	-	1/1/13/20	9/27/103/115	-
47	A1EB1	P	301	-	-	14/43/100/100	0/3/3/3
40	CLA	J	312	-	1/1/13/20	9/31/107/115	-
49	BCR	b	844	-	-	6/29/63/63	0/2/2/2
40	CLA	D	310	4	1/1/14/20	11/33/109/115	-
40	CLA	b	817	24	1/1/15/20	6/39/115/115	-
47	A1EB1	t	315	-	-	13/43/100/100	0/3/3/3
40	CLA	H	310	-	1/1/14/20	4/33/109/115	-
40	CLA	Q	204	16	1/1/12/20	2/23/99/115	-
44	A86	R	313	-	-	6/34/90/90	0/3/3/3
41	KC2	O	302	15	-	10/15/71/71	-
40	CLA	x	307	-	1/1/13/20	9/27/103/115	-
40	CLA	U	207	-	1/1/11/20	3/18/94/115	-
44	A86	M	316	-	-	2/34/90/90	0/3/3/3
40	CLA	N	304	14	1/1/14/20	10/33/109/115	-
41	KC2	Y	303	21	-	6/15/71/71	-
40	CLA	Y	307	21	1/1/14/20	9/33/109/115	-
40	CLA	D	304	4	1/1/13/20	7/29/105/115	-
40	CLA	a	819	23	1/1/14/20	9/35/111/115	-
42	DD6	I	213	-	-	1/26/80/80	0/3/3/3
40	CLA	p	314	35	1/1/11/20	8/18/94/115	-
41	KC2	y	301	38	-	10/15/71/71	-
41	KC2	Y	302	-	-	5/15/71/71	-
41	KC2	W	303	-	-	7/15/71/71	-
40	CLA	q	306	36	1/1/14/20	7/33/109/115	-
40	CLA	b	810	24	1/1/15/20	11/39/115/115	-
40	CLA	A	309	1	1/1/15/20	12/39/115/115	-
40	CLA	F	311	-	1/1/11/20	4/18/94/115	-
40	CLA	z	305	39	1/1/14/20	14/33/109/115	-
40	CLA	z	312	-	1/1/14/20	10/33/109/115	-
41	KC2	q	309	-	-	6/15/71/71	-
40	CLA	T	310	-	1/1/13/20	9/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	A	311	1	1/1/11/20	4/18/94/115	-
40	CLA	A	304	1	1/1/15/20	15/39/115/115	-
40	CLA	H	301	-	1/1/11/20	4/18/94/115	-
40	CLA	f	202	24	1/1/15/20	7/39/115/115	-
40	CLA	R	316	47	1/1/11/20	2/18/94/115	-
41	KC2	T	309	15	-	4/15/71/71	-
40	CLA	I	201	-	1/1/15/20	7/39/115/115	-
41	KC2	T	311	15	-	10/15/71/71	-
40	CLA	C	307	3	1/1/14/20	9/33/109/115	-
40	CLA	b	823	24	1/1/13/20	3/27/103/115	-
41	KC2	X	303	20	-	1/15/71/71	-
47	A1EB1	K	315	-	-	15/43/100/100	1/3/3/3
40	CLA	a	815	23	1/1/15/20	5/39/115/115	-
40	CLA	t	307	-	1/1/13/20	11/27/103/115	-
41	KC2	p	309	-	-	6/15/71/71	-
40	CLA	Q	207	-	1/1/11/20	2/18/94/115	-
40	CLA	q	313	36	1/1/11/20	7/18/94/115	-
40	CLA	Z	310	-	1/1/13/20	9/27/103/115	-
42	DD6	p	322	-	-	1/26/80/80	0/3/3/3
43	LMG	D	318	-	-	15/35/55/70	0/1/1/1
41	KC2	P	304	13	-	5/15/71/71	-
41	KC2	T	308	15	-	8/15/71/71	-
40	CLA	T	307	-	1/1/13/20	0/27/103/115	-
44	A86	W	301	-	-	1/34/90/90	0/3/3/3
44	A86	p	320	-	-	8/34/90/90	0/3/3/3
47	A1EB1	Y	323	-	-	3/43/100/100	0/3/3/3
40	CLA	b	826	24	1/1/14/20	7/38/114/115	-
44	A86	G	211	-	-	7/34/90/90	0/3/3/3
40	CLA	b	841	24	1/1/15/20	5/39/115/115	-
44	A86	p	321	-	-	7/34/90/90	0/3/3/3
41	KC2	z	304	39	-	5/15/71/71	-
43	LMG	u	301	-	-	14/34/54/70	0/1/1/1
40	CLA	b	834	-	1/1/15/20	8/39/115/115	-
47	A1EB1	Z	320	-	-	7/43/100/100	0/3/3/3
42	DD6	J	313	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	w	301	38	-	9/15/71/71	-
40	CLA	b	839	24	1/1/15/20	12/39/115/115	-
40	CLA	M	306	13	1/1/14/20	5/36/112/115	-
40	CLA	S	319	-	1/1/11/20	7/18/94/115	-
44	A86	X	318	-	-	5/34/90/90	0/3/3/3
47	A1EB1	v	324	-	-	13/43/100/100	0/3/3/3
41	KC2	p	303	-	-	6/15/71/71	-
40	CLA	L	306	12	1/1/11/20	6/18/94/115	-
40	CLA	J	308	10	1/1/13/20	8/27/103/115	-
40	CLA	a	825	-	1/1/15/20	5/39/115/115	-
40	CLA	i	101	-	1/1/13/20	12/27/103/115	-
44	A86	S	315	-	-	7/34/90/90	0/3/3/3
47	A1EB1	q	322	-	-	7/43/100/100	0/3/3/3
40	CLA	D	307	4	1/1/15/20	8/39/115/115	-
41	KC2	t	308	-	-	6/15/71/71	-
42	DD6	N	316	-	-	2/26/80/80	0/3/3/3
40	CLA	J	311	-	1/1/11/20	4/18/94/115	-
40	CLA	X	301	-	1/1/14/20	4/33/109/115	-
40	CLA	a	822	-	1/1/15/20	10/39/115/115	-
44	A86	T	312	-	-	4/34/90/90	0/3/3/3
40	CLA	E	305	5	1/1/14/20	6/33/109/115	-
42	DD6	Y	322	-	-	3/26/80/80	0/3/3/3
40	CLA	D	302	43	1/1/13/20	7/31/107/115	-
40	CLA	v	311	-	1/1/14/20	9/37/113/115	-
40	CLA	B	303	-	1/1/11/20	3/18/94/115	-
44	A86	y	310	-	-	7/34/90/90	0/3/3/3
41	KC2	P	309	13	-	5/15/71/71	-
49	BCR	b	843	-	-	0/29/63/63	0/2/2/2
40	CLA	S	312	-	1/1/11/20	4/18/94/115	-
46	SQD	P	319	-	-	7/27/47/69	0/1/1/1
40	CLA	z	306	-	1/1/13/20	5/27/103/115	-
44	A86	o	316	-	-	11/34/90/90	0/3/3/3
49	BCR	b	847	-	-	4/29/63/63	0/2/2/2
40	CLA	b	824	24	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	A	302	-	1/1/14/20	7/33/109/115	-
42	DD6	v	320	-	-	6/26/80/80	0/3/3/3
41	KC2	S	303	17	-	5/15/71/71	-
40	CLA	Z	307	22	1/1/14/20	8/33/109/115	-
40	CLA	J	303	-	1/1/11/20	4/18/94/115	-
44	A86	T	315	-	-	11/34/90/90	1/3/3/3
40	CLA	H	306	8	1/1/12/20	0/21/97/115	-
40	CLA	C	302	-	1/1/11/20	5/18/94/115	-
44	A86	z	317	-	-	6/34/90/90	0/3/3/3
40	CLA	G	213	-	1/1/11/20	8/18/94/115	-
40	CLA	a	833	23	1/1/14/20	9/33/109/115	-
40	CLA	o	311	-	1/1/14/20	8/37/113/115	-
44	A86	R	315	-	-	7/34/90/90	0/3/3/3
42	DD6	F	315	-	-	3/26/80/80	0/3/3/3
41	KC2	W	310	13	-	6/15/71/71	-
41	KC2	L	302	-	-	7/15/71/71	-
44	A86	p	317	-	-	1/34/90/90	0/3/3/3
44	A86	Y	315	-	-	8/34/90/90	0/3/3/3
48	A1EB4	M	319	-	-	6/38/98/103	0/3/3/3
40	CLA	O	306	15	1/1/14/20	7/33/109/115	-
44	A86	Q	210	-	-	5/34/90/90	0/3/3/3
44	A86	z	318	-	-	4/34/90/90	1/3/3/3
49	BCR	b	848	-	-	3/29/63/63	0/2/2/2
44	A86	v	317	-	-	1/34/90/90	0/3/3/3
41	KC2	x	303	-	-	7/15/71/71	-
41	KC2	K	309	11	-	8/15/71/71	-
40	CLA	E	310	-	1/1/14/20	6/33/109/115	-
41	KC2	z	310	39	-	8/15/71/71	-
41	KC2	R	309	15	-	7/15/71/71	-
40	CLA	a	850	-	1/1/15/20	4/39/115/115	-
41	KC2	N	312	14	-	8/15/71/71	-
40	CLA	y	303	-	1/1/11/20	4/18/94/115	-
41	KC2	v	303	36	-	6/15/71/71	-
40	CLA	P	311	-	1/1/11/20	4/18/94/115	-
41	KC2	x	309	-	-	4/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	A86	q	316	-	-	3/34/90/90	1/3/3/3
40	CLA	Y	312	-	1/1/11/20	2/18/94/115	-
42	DD6	E	318	-	-	3/26/80/80	0/3/3/3
40	CLA	b	828	24	1/1/13/20	1/27/103/115	-
43	LMG	x	301	-	-	15/34/54/70	0/1/1/1
40	CLA	N	306	-	1/1/14/20	2/33/109/115	-
41	KC2	p	304	35	-	8/15/71/71	-
41	KC2	N	308	14	-	8/15/71/71	-
40	CLA	v	312	-	1/1/14/20	7/33/109/115	-
40	CLA	E	311	-	1/1/12/20	5/21/97/115	-
40	CLA	O	305	15	1/1/11/20	2/18/94/115	-
41	KC2	v	309	-	-	6/15/71/71	-
44	A86	U	210	-	-	2/34/90/90	0/3/3/3
43	LMG	E	321	-	-	12/35/55/70	0/1/1/1
40	CLA	E	307	-	1/1/15/20	10/39/115/115	-
40	CLA	f	204	28	1/1/11/20	2/18/94/115	-
40	CLA	H	311	-	1/1/11/20	3/18/94/115	-
40	CLA	Z	301	-	1/1/14/20	6/33/109/115	-
40	CLA	a	814	-	1/1/12/20	2/21/97/115	-
40	CLA	a	823	23	1/1/13/20	5/27/103/115	-
42	DD6	Q	213	-	-	0/26/80/80	0/3/3/3
40	CLA	w	305	-	1/1/12/20	3/19/95/115	-
42	DD6	o	319	-	-	1/26/80/80	0/3/3/3
47	A1EB1	y	312	-	-	11/43/100/100	0/3/3/3
49	BCR	k	203	-	-	4/29/63/63	0/2/2/2
40	CLA	S	302	-	1/1/14/20	13/33/109/115	-
41	KC2	y	306	-	-	8/15/71/71	-
40	CLA	x	314	35	1/1/11/20	4/18/94/115	-
44	A86	M	320	-	-	5/34/90/90	0/3/3/3
40	CLA	J	302	10	1/1/11/20	8/18/94/115	-
40	CLA	G	204	7	1/1/13/20	2/27/103/115	-
44	A86	x	317	-	-	6/34/90/90	0/3/3/3
41	KC2	M	303	13	-	4/15/71/71	-
40	CLA	o	301	-	1/1/14/20	6/33/109/115	-
42	DD6	D	315	-	-	0/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	T	301	-	-	4/15/71/71	-
43	LMG	E	320	-	-	15/26/46/70	0/1/1/1
42	DD6	N	319	-	-	1/26/80/80	0/3/3/3
41	KC2	M	302	13	-	3/15/71/71	-
40	CLA	l	202	-	1/1/15/20	14/39/115/115	-
40	CLA	y	302	38	1/1/11/20	4/18/94/115	-
41	KC2	u	309	-	-	5/15/71/71	-
44	A86	L	314	-	-	4/34/90/90	0/3/3/3
40	CLA	H	302	-	1/1/11/20	8/18/94/115	-
40	CLA	C	304	3	1/1/13/20	3/29/105/115	-
42	DD6	C	313	-	-	2/26/80/80	0/3/3/3
40	CLA	z	302	-	1/1/14/20	6/33/109/115	-
46	SQD	W	318	-	-	7/27/47/69	0/1/1/1
47	A1EB1	y	314	-	-	8/43/100/100	0/3/3/3
42	DD6	A	313	-	-	1/26/80/80	0/3/3/3
40	CLA	a	804	23	1/1/14/20	8/36/112/115	-
40	CLA	b	825	-	1/1/15/20	9/39/115/115	-
40	CLA	I	206	9	1/1/15/20	7/39/115/115	-
44	A86	t	310	-	-	7/34/90/90	0/3/3/3
40	CLA	B	304	-	1/1/11/20	6/18/94/115	-
41	KC2	O	301	15	-	6/15/71/71	-
44	A86	X	321	-	-	5/34/90/90	0/3/3/3
40	CLA	a	839	45	1/1/15/20	10/39/115/115	-
40	CLA	x	302	-	1/1/15/20	8/39/115/115	-
44	A86	p	316	-	-	5/34/90/90	0/3/3/3
40	CLA	S	311	-	1/1/11/20	6/18/94/115	-
44	A86	u	319	-	-	11/34/90/90	0/3/3/3
40	CLA	b	830	24	1/1/14/20	5/35/111/115	-
40	CLA	H	309	-	1/1/13/20	6/29/105/115	-
40	CLA	u	314	35	1/1/11/20	5/18/94/115	-
40	CLA	K	312	-	1/1/11/20	2/18/94/115	-
42	DD6	G	210	-	-	1/26/80/80	0/3/3/3
40	CLA	I	207	9	1/1/11/20	4/18/94/115	-
40	CLA	M	304	13	1/1/14/20	7/33/109/115	-
41	KC2	Y	308	-	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	q	308	36	-	10/15/71/71	-
40	CLA	q	307	36	1/1/14/20	11/33/109/115	-
40	CLA	p	312	-	1/1/11/20	3/18/94/115	-
40	CLA	b	838	-	1/1/15/20	9/39/115/115	-
40	CLA	a	832	23	1/1/15/20	12/39/115/115	-
40	CLA	P	306	13	1/1/11/20	1/18/94/115	-
40	CLA	W	308	-	1/1/14/20	8/33/109/115	-
44	A86	u	317	-	-	1/34/90/90	0/3/3/3
42	DD6	Q	214	-	-	1/26/80/80	0/3/3/3
44	A86	o	315	-	-	7/34/90/90	0/3/3/3
47	A1EB1	L	316	-	-	8/43/100/100	0/3/3/3
42	DD6	L	315	-	-	0/26/80/80	0/3/3/3
40	CLA	b	816	24	1/1/11/20	5/18/94/115	-
42	DD6	z	321	-	-	1/26/80/80	0/3/3/3
43	LMG	j	101	-	-	10/25/45/70	0/1/1/1
47	A1EB1	t	314	-	-	18/43/100/100	1/3/3/3
40	CLA	U	205	-	1/1/11/20	4/18/94/115	-
44	A86	x	318	-	-	8/34/90/90	0/3/3/3
41	KC2	X	309	-	-	6/15/71/71	-
40	CLA	x	311	-	1/1/13/20	9/27/103/115	-
40	CLA	v	301	-	1/1/13/20	4/27/103/115	-
40	CLA	z	308	39	1/1/14/20	12/33/109/115	-
40	CLA	q	312	-	1/1/14/20	8/33/109/115	-
44	A86	W	314	-	-	5/34/90/90	0/3/3/3
44	A86	Y	318	-	-	9/34/90/90	0/3/3/3
44	A86	q	319	-	-	12/34/90/90	0/3/3/3
42	DD6	R	314	-	-	0/26/80/80	0/3/3/3
47	A1EB1	u	322	-	-	8/43/100/100	0/3/3/3
47	A1EB1	x	321	-	-	2/43/100/100	0/3/3/3
40	CLA	F	310	-	1/1/11/20	6/18/94/115	-
40	CLA	U	202	18	1/1/13/20	9/27/103/115	-
40	CLA	Y	311	-	1/1/11/20	5/18/94/115	-
40	CLA	p	305	35	1/1/11/20	6/18/94/115	-
40	CLA	T	304	15	1/1/14/20	4/33/109/115	-
40	CLA	Z	312	-	1/1/11/20	6/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	S	301	-	1/1/14/20	5/33/109/115	-
44	A86	x	316	-	-	5/34/90/90	0/3/3/3
41	KC2	F	302	6	-	8/15/71/71	-
41	KC2	Z	309	-	-	6/15/71/71	-
44	A86	F	317	-	-	8/34/90/90	0/3/3/3
42	DD6	P	315	-	1/1/12/24	1/26/80/80	0/3/3/3
42	DD6	E	315	-	-	1/26/80/80	0/3/3/3
47	A1EB1	G	212	-	-	14/43/100/100	0/3/3/3
40	CLA	w	303	38	1/1/11/20	4/18/94/115	-
40	CLA	B	301	2	1/1/11/20	9/18/94/115	-
40	CLA	a	842	-	1/1/15/20	14/39/115/115	-
40	CLA	D	312	4	1/1/13/20	9/27/103/115	-
40	CLA	b	807	-	1/1/15/20	9/39/115/115	-
41	KC2	R	308	15	-	8/15/71/71	-
44	A86	u	318	-	-	11/34/90/90	0/3/3/3
47	A1EB1	z	323	-	-	8/43/100/100	0/3/3/3
47	A1EB1	t	313	-	-	15/43/100/100	0/3/3/3
40	CLA	b	811	24	1/1/11/20	4/18/94/115	-
41	KC2	T	302	-	-	2/15/71/71	-
41	KC2	C	303	-	-	7/15/71/71	-
40	CLA	Y	301	-	1/1/14/20	7/33/109/115	-
40	CLA	D	303	4	1/1/14/20	12/33/109/115	-
40	CLA	l	203	-	1/1/14/20	12/38/114/115	-
42	DD6	M	314	-	-	1/26/80/80	0/3/3/3
40	CLA	a	817	23	1/1/12/20	0/21/97/115	-
40	CLA	O	316	47	1/1/11/20	2/18/94/115	-
44	A86	M	315	-	-	5/34/90/90	1/3/3/3
44	A86	F	313	-	-	6/34/90/90	0/3/3/3
44	A86	o	317	-	-	7/34/90/90	0/3/3/3
40	CLA	Q	203	-	1/1/12/20	4/21/97/115	-
40	CLA	D	308	4	1/1/13/20	2/27/103/115	-
40	CLA	z	324	-	1/1/11/20	5/18/94/115	-
40	CLA	b	803	-	1/1/15/20	13/39/115/115	-
44	A86	Z	317	-	-	2/34/90/90	1/3/3/3
40	CLA	u	302	-	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	A86	G	209	-	-	9/34/90/90	0/3/3/3
40	CLA	R	305	15	1/1/14/20	6/33/109/115	-
40	CLA	A	303	1	1/1/14/20	10/35/111/115	-
51	SF4	c	102	-	-	-	0/6/5/5
47	A1EB1	Z	321	-	-	10/43/100/100	0/3/3/3
42	DD6	w	312	-	-	1/26/80/80	0/3/3/3
40	CLA	M	305	13	1/1/14/20	10/33/109/115	-
41	KC2	Z	303	22	-	4/15/71/71	-
49	BCR	r	201	-	-	2/29/63/63	0/2/2/2
40	CLA	k	202	-	1/1/13/20	5/27/103/115	-
40	CLA	C	308	-	1/1/11/20	5/18/94/115	-
40	CLA	b	833	24	1/1/14/20	10/33/109/115	-
44	A86	p	318	-	-	10/34/90/90	0/3/3/3
40	CLA	o	312	-	1/1/11/20	5/18/94/115	-
41	KC2	O	309	15	-	9/15/71/71	-
41	KC2	t	306	-	-	8/15/71/71	-
49	BCR	m	101	-	-	0/29/63/63	0/2/2/2
51	SF4	b	804	-	-	-	0/6/5/5
40	CLA	a	829	-	1/1/15/20	15/39/115/115	-
41	KC2	o	309	34	-	10/15/71/71	-
41	KC2	Q	201	16	-	6/15/71/71	-
40	CLA	v	305	-	1/1/14/20	3/33/109/115	-
47	A1EB1	Z	319	-	-	6/43/100/100	0/3/3/3
40	CLA	X	304	-	1/1/11/20	6/18/94/115	-
41	KC2	L	308	12	-	4/15/71/71	-
40	CLA	P	305	13	1/1/14/20	9/33/109/115	-
43	LMG	S	322	-	-	9/34/54/70	0/1/1/1
40	CLA	a	816	23	1/1/15/20	6/39/115/115	-
40	CLA	p	306	35	1/1/11/20	5/18/94/115	-
41	KC2	x	304	35	-	8/15/71/71	-
42	DD6	C	310	-	-	1/26/80/80	0/3/3/3
42	DD6	B	305	-	-	3/26/80/80	0/3/3/3
47	A1EB1	v	322	-	-	7/43/100/100	0/3/3/3
40	CLA	X	306	20	1/1/13/20	7/27/103/115	-
40	CLA	a	830	-	1/1/13/20	6/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	F	307	6	1/1/14/20	6/32/109/115	-
44	A86	H	315	-	-	4/34/90/90	0/3/3/3
47	A1EB1	p	324	-	-	4/43/100/100	0/3/3/3
41	KC2	A	310	1	-	6/15/71/71	-
40	CLA	B	307	-	1/1/11/20	7/18/94/115	-
40	CLA	P	312	13	1/1/14/20	13/33/109/115	-
42	DD6	Z	318	-	-	1/26/80/80	0/3/3/3
45	LHG	a	849	40	-	17/34/34/53	-
42	DD6	J	314	-	-	0/26/80/80	0/3/3/3
40	CLA	W	312	13	1/1/14/20	9/33/109/115	-
40	CLA	J	306	10	1/1/12/20	1/24/100/115	-
40	CLA	t	302	38	1/1/11/20	0/18/94/115	-
40	CLA	p	313	-	1/1/13/20	2/27/103/115	-
41	KC2	Z	302	-	-	8/15/71/71	-
42	DD6	J	317	-	-	1/26/80/80	0/3/3/3
40	CLA	a	838	23	1/1/13/20	8/27/103/115	-
40	CLA	Z	311	22	1/1/14/20	5/37/113/115	-
40	CLA	X	311	20	1/1/14/20	11/37/113/115	-
41	KC2	H	303	-	-	4/15/71/71	-
40	CLA	H	305	8	1/1/14/20	12/33/109/115	-
41	KC2	t	301	38	-	8/15/71/71	-
40	CLA	D	301	4	1/1/13/20	6/27/103/115	-
40	CLA	q	304	-	1/1/12/20	4/24/100/115	-
40	CLA	t	309	-	1/1/11/20	4/18/94/115	-
42	DD6	F	314	-	-	1/26/80/80	0/3/3/3
47	A1EB1	o	321	-	-	9/43/100/100	1/3/3/3
41	KC2	O	303	15	-	6/15/71/71	-
40	CLA	D	311	-	1/1/11/20	4/18/94/115	-
44	A86	X	320	-	-	6/34/90/90	0/3/3/3
40	CLA	b	809	24	1/1/14/20	8/33/109/115	-
42	DD6	K	310	-	-	0/26/80/80	0/3/3/3
40	CLA	F	304	6	1/1/13/20	3/27/103/115	-
43	LMG	W	317	-	-	7/34/54/70	0/1/1/1
40	CLA	v	313	36	1/1/11/20	3/18/94/115	-
40	CLA	C	301	3	1/1/11/20	6/18/94/115	-
42	DD6	D	316	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	I	205	9	1/1/13/20	8/29/105/115	-
40	CLA	P	313	-	1/1/14/20	13/33/109/115	-
40	CLA	E	314	5	1/1/11/20	11/18/94/115	-
40	CLA	a	806	23	1/1/15/20	12/39/115/115	-
40	CLA	o	306	34	1/1/14/20	7/33/109/115	-
41	KC2	M	308	13	-	7/15/71/71	-
41	KC2	u	304	35	-	8/15/71/71	-
40	CLA	a	821	23	1/1/15/20	11/39/115/115	-
47	A1EB1	o	322	-	-	12/43/100/100	0/3/3/3
40	CLA	H	308	8	1/1/11/20	3/18/94/115	-
41	KC2	v	302	-	-	6/15/71/71	-
41	KC2	W	304	13	-	7/15/71/71	-
40	CLA	y	309	-	1/1/13/20	9/27/103/115	-
46	SQD	k	205	-	-	3/31/51/69	0/1/1/1
40	CLA	b	827	24	1/1/14/20	6/33/109/115	-
42	DD6	K	311	-	-	2/26/80/80	0/3/3/3
45	LHG	F	319	-	-	18/44/44/53	-
41	KC2	Q	216	-	-	7/15/71/71	-
42	DD6	E	317	-	-	1/26/80/80	0/3/3/3
47	A1EB1	v	321	-	-	16/43/100/100	1/3/3/3
42	DD6	A	312	-	-	0/26/80/80	0/3/3/3
41	KC2	u	310	-	-	5/15/71/71	-
40	CLA	p	302	-	1/1/15/20	7/39/115/115	-
40	CLA	E	306	5	1/1/13/20	9/27/103/115	-
42	DD6	y	311	-	-	0/26/80/80	0/3/3/3
40	CLA	a	807	-	1/1/13/20	7/29/105/115	-
40	CLA	a	820	23	1/1/14/20	13/33/109/115	-
44	A86	X	316	-	-	4/34/90/90	0/3/3/3
44	A86	t	316	-	-	7/34/90/90	0/3/3/3
40	CLA	T	306	15	1/1/14/20	3/33/109/115	-
44	A86	o	318	-	-	3/34/90/90	0/3/3/3
40	CLA	S	306	17	1/1/13/20	7/29/105/115	-
42	DD6	o	320	-	-	0/26/80/80	0/3/3/3
41	KC2	N	301	14	-	4/15/71/71	-
44	A86	z	320	-	-	2/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	S	304	17	-	6/15/71/71	-
41	KC2	K	305	11	-	6/15/71/71	-
40	CLA	L	310	-	1/1/11/20	6/18/94/115	-
42	DD6	C	312	-	-	2/26/80/80	0/3/3/3
40	CLA	R	304	15	1/1/12/20	6/23/99/115	-
40	CLA	Z	305	22	1/1/13/20	6/27/103/115	-
42	DD6	D	313	-	-	0/26/80/80	0/3/3/3
40	CLA	a	837	23	1/1/13/20	8/27/103/115	-
40	CLA	E	313	5	1/1/11/20	1/18/94/115	-
42	DD6	D	314	-	-	3/26/80/80	0/3/3/3
44	A86	Y	317	41	-	6/34/90/90	0/3/3/3
49	BCR	l	208	-	-	5/29/63/63	0/2/2/2
41	KC2	L	303	12	-	6/15/71/71	-
41	KC2	o	302	-	-	6/15/71/71	-
40	CLA	K	304	11	1/1/14/20	6/33/109/115	-
41	KC2	z	309	39	-	7/15/71/71	-
40	CLA	S	313	-	1/1/11/20	3/18/94/115	-
40	CLA	a	810	-	1/1/14/20	5/33/109/115	-
44	A86	W	316	-	-	4/34/90/90	0/3/3/3
44	A86	Z	316	-	-	5/34/90/90	1/3/3/3
40	CLA	a	852	-	1/1/13/20	7/27/103/115	-
45	LHG	S	323	-	-	19/44/44/53	-
40	CLA	b	818	24	1/1/14/20	13/36/112/115	-
44	A86	S	317	-	-	5/34/90/90	0/3/3/3
44	A86	Q	215	-	-	3/34/90/90	0/3/3/3
40	CLA	W	311	-	1/1/13/20	8/27/103/115	-
40	CLA	A	308	-	1/1/13/20	2/27/103/115	-
41	KC2	q	303	36	-	7/15/71/71	-
40	CLA	G	201	7	1/1/11/20	4/18/94/115	-
40	CLA	L	312	-	1/1/11/20	2/18/94/115	-
41	KC2	P	310	-	-	7/15/71/71	-
40	CLA	u	313	-	1/1/13/20	1/27/103/115	-
42	DD6	t	312	-	-	0/26/80/80	0/3/3/3
44	A86	O	315	-	-	5/34/90/90	0/3/3/3
44	A86	T	319	-	-	3/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	BCR	a	845	-	-	2/29/63/63	0/2/2/2
41	KC2	q	302	36	-	6/15/71/71	-
42	DD6	T	314	-	-	1/26/80/80	0/3/3/3
40	CLA	R	306	15	1/1/14/20	5/33/109/115	-
40	CLA	S	314	17	1/1/13/20	11/27/103/115	-
40	CLA	q	311	-	1/1/14/20	11/37/113/115	-
44	A86	Z	315	-	-	12/34/90/90	0/3/3/3
40	CLA	k	201	31	1/1/13/20	6/27/103/115	-
42	DD6	J	301	-	-	2/26/80/80	0/3/3/3
47	A1EB1	q	321	-	-	17/43/100/100	1/3/3/3
40	CLA	N	305	14	1/1/13/20	5/27/103/115	-
44	A86	O	313	-	-	4/34/90/90	0/3/3/3
44	A86	Y	321	-	-	4/34/90/90	0/3/3/3
40	CLA	W	307	13	1/1/15/20	10/39/115/115	-
40	CLA	b	840	-	1/1/15/20	12/39/115/115	-
41	KC2	P	303	13	-	2/15/71/71	-
40	CLA	O	310	-	1/1/11/20	6/18/94/115	-
41	KC2	u	303	-	-	6/15/71/71	-
40	CLA	b	832	24	1/1/15/20	6/39/115/115	-
40	CLA	f	205	-	1/1/11/20	1/18/94/115	-
43	LMG	P	318	-	-	11/34/54/70	0/1/1/1
44	A86	v	316	-	-	3/34/90/90	1/3/3/3
40	CLA	Y	305	21	1/1/13/20	7/27/103/115	-
41	KC2	P	302	-	-	4/15/71/71	-
44	A86	u	316	-	-	5/34/90/90	0/3/3/3
40	CLA	E	302	5	1/1/11/20	8/18/94/115	-
40	CLA	u	312	-	1/1/14/20	8/33/109/115	-
42	DD6	X	322	-	-	0/26/80/80	0/3/3/3
40	CLA	o	305	34	1/1/13/20	8/27/103/115	-
41	KC2	z	303	39	-	6/15/71/71	-
40	CLA	A	307	1	1/1/14/20	7/33/109/115	-
40	CLA	l	205	32	1/1/15/20	12/39/115/115	-
40	CLA	z	307	-	1/1/14/20	7/33/109/115	-
40	CLA	F	308	-	1/1/13/20	3/27/103/115	-
40	CLA	a	805	23,40	1/1/12/20	4/26/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	A1EB1	q	323	-	-	14/43/100/100	0/3/3/3
40	CLA	U	208	-	1/1/11/20	6/18/94/115	-
41	KC2	X	308	20	-	5/15/71/71	-
40	CLA	O	307	-	1/1/14/20	9/36/112/115	-
47	A1EB1	y	313	-	-	12/43/100/100	0/3/3/3
40	CLA	K	306	-	1/1/14/20	6/33/109/115	-
49	BCR	a	844	-	-	2/29/63/63	0/2/2/2
44	A86	X	315	-	-	5/34/90/90	0/3/3/3
44	A86	O	312	-	-	5/34/90/90	0/3/3/3
40	CLA	E	309	-	1/1/14/20	11/33/109/115	-
44	A86	q	317	-	-	1/34/90/90	0/3/3/3
47	A1EB1	R	317	40	-	9/43/100/100	0/3/3/3
41	KC2	S	310	-	-	6/15/71/71	-
40	CLA	u	308	35	1/1/14/20	7/33/109/115	-
40	CLA	a	834	-	1/1/14/20	6/33/109/115	-
40	CLA	x	306	35	1/1/14/20	14/33/109/115	-
40	CLA	a	835	-	1/1/15/20	1/39/115/115	-
42	DD6	U	209	-	-	0/26/80/80	0/3/3/3
40	CLA	L	307	-	1/1/13/20	2/27/103/115	-
44	A86	N	314	-	-	2/34/90/90	0/3/3/3
41	KC2	K	302	11	-	6/15/71/71	-
44	A86	v	319	-	-	13/34/90/90	0/3/3/3
40	CLA	T	305	15	1/1/12/20	4/21/97/115	-
40	CLA	Y	306	21	1/1/14/20	7/33/109/115	-
40	CLA	S	305	-	1/1/12/20	7/24/100/115	-
40	CLA	z	313	-	1/1/11/20	4/18/94/115	-
41	KC2	R	302	15	-	4/15/71/71	-
44	A86	z	319	-	-	5/34/90/90	0/3/3/3
47	A1EB1	O	317	40	-	9/43/100/100	1/3/3/3
40	CLA	b	822	-	1/1/14/20	9/38/114/115	-
40	CLA	v	306	36	1/1/14/20	9/33/109/115	-
43	LMG	a	802	-	-	11/30/50/70	0/1/1/1
40	CLA	y	304	-	1/1/14/20	8/33/109/115	-
50	PQN	b	849	-	-	3/17/37/43	0/2/2/2
40	CLA	H	304	-	1/1/11/20	3/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	b	808	-	1/1/15/20	8/39/115/115	-
44	A86	o	314	-	-	12/34/90/90	0/3/3/3
40	CLA	x	313	-	1/1/13/20	4/27/103/115	-
40	CLA	b	812	24	1/1/14/20	8/33/109/115	-
44	A86	t	311	-	-	12/34/90/90	1/3/3/3
47	A1EB1	F	322	-	-	7/43/100/100	0/3/3/3
41	KC2	x	310	-	-	6/15/71/71	-
41	KC2	S	309	17	-	9/15/71/71	-
44	A86	Z	314	-	-	3/34/90/90	0/3/3/3
41	KC2	O	311	-	-	6/15/71/71	-
40	CLA	Y	313	21	1/1/11/20	8/18/94/115	-
42	DD6	E	316	-	-	0/26/80/80	0/3/3/3
47	A1EB1	L	318	-	-	15/43/100/100	0/3/3/3
40	CLA	D	309	-	1/1/13/20	6/31/107/115	-
40	CLA	Q	205	16	1/1/14/20	12/36/112/115	-
49	BCR	l	207	-	-	6/29/63/63	0/2/2/2
43	LMG	M	317	-	-	9/34/54/70	0/1/1/1
41	KC2	w	306	38	-	9/15/71/71	-
45	LHG	a	848	-	-	22/52/52/53	-
42	DD6	A	314	-	-	1/26/80/80	0/3/3/3
40	CLA	G	203	7	1/1/13/20	5/26/103/115	-
43	LMG	F	318	-	-	10/34/54/70	0/1/1/1
40	CLA	b	801	-	1/1/14/20	6/37/113/115	-
44	A86	Y	320	-	-	9/34/90/90	0/3/3/3
40	CLA	b	802	-	1/1/15/20	8/39/115/115	-
40	CLA	C	309	-	1/1/11/20	1/18/94/115	-
44	A86	N	321	-	-	8/34/90/90	0/3/3/3
40	CLA	t	305	-	1/1/12/20	2/19/95/115	-
47	A1EB1	p	323	-	-	8/43/100/100	0/3/3/3
44	A86	Y	316	-	-	3/34/90/90	0/3/3/3
41	KC2	N	313	14	-	4/15/71/71	-
41	KC2	J	304	-	-	9/15/71/71	-
40	CLA	b	829	-	1/1/11/20	2/18/94/115	-
44	A86	q	314	-	-	3/34/90/90	0/3/3/3
44	A86	v	314	-	-	3/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	DD6	D	317	-	-	1/26/80/80	0/3/3/3
40	CLA	b	813	24	1/1/12/20	5/21/97/115	-
48	A1EB4	W	319	-	-	11/38/98/103	0/3/3/3
44	A86	C	311	-	-	8/34/90/90	1/3/3/3
41	KC2	u	315	-	-	8/15/71/71	-
46	SQD	I	215	-	-	17/49/69/69	0/1/1/1
41	KC2	Y	309	21,44	-	8/15/71/71	-
44	A86	S	316	-	-	8/34/90/90	0/3/3/3
42	DD6	I	211	-	-	6/26/80/80	0/3/3/3
43	LMG	a	801	-	-	13/30/50/70	0/1/1/1
40	CLA	X	305	-	1/1/12/20	8/21/97/115	-
40	CLA	b	819	24	1/1/14/20	15/38/114/115	-
44	A86	q	324	-	-	7/34/90/90	0/3/3/3
40	CLA	X	310	-	1/1/13/20	9/27/103/115	-
40	CLA	N	307	-	1/1/14/20	6/33/109/115	-
40	CLA	a	808	-	1/1/15/20	6/39/115/115	-
43	LMG	L	319	-	-	15/32/52/70	0/1/1/1
44	A86	P	314	-	-	6/34/90/90	0/3/3/3
40	CLA	y	305	-	1/1/12/20	3/19/95/115	-
40	CLA	K	308	11	1/1/13/20	9/32/108/115	-
47	A1EB1	S	320	-	-	6/43/100/100	1/3/3/3
41	KC2	M	301	13	-	6/15/71/71	-
40	CLA	J	305	10	1/1/13/20	7/27/103/115	-
40	CLA	F	321	-	1/1/14/20	12/33/109/115	-
41	KC2	y	307	-	-	6/15/71/71	-
40	CLA	F	301	-	1/1/12/20	10/25/101/115	-
40	CLA	a	803	-	1/1/15/20	4/39/115/115	-
42	DD6	J	316	-	-	0/26/80/80	0/3/3/3
46	SQD	F	320	-	-	10/31/51/69	0/1/1/1
40	CLA	o	313	-	1/1/11/20	5/18/94/115	-
40	CLA	p	308	-	1/1/14/20	7/33/109/115	-
40	CLA	x	305	-	1/1/12/20	2/23/99/115	-
42	DD6	I	212	-	-	0/26/80/80	0/3/3/3
43	LMG	T	318	-	-	15/35/55/70	0/1/1/1
40	CLA	X	307	20	1/1/14/20	5/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	DGD	b	850	-	-	19/45/85/95	0/2/2/2
40	CLA	G	206	7	1/1/13/20	9/29/105/115	-
40	CLA	I	203	9	1/1/13/20	6/27/103/115	-
44	A86	P	321	-	-	6/34/90/90	0/3/3/3
40	CLA	Z	306	22	1/1/14/20	14/33/109/115	-
40	CLA	q	305	-	1/1/14/20	3/33/109/115	-
41	KC2	Z	308	22	-	5/15/71/71	-
40	CLA	t	304	-	1/1/14/20	8/33/109/115	-
42	DD6	F	316	-	-	2/26/80/80	0/3/3/3
43	LMG	l	201	-	-	19/34/54/70	0/1/1/1
42	DD6	L	317	-	-	0/26/80/80	0/3/3/3
41	KC2	o	303	34	-	4/15/71/71	-
44	A86	p	319	-	-	11/34/90/90	0/3/3/3
46	SQD	M	318	-	-	8/27/47/69	0/1/1/1
40	CLA	V	202	19	1/1/13/20	8/27/103/115	-
40	CLA	b	806	24	1/1/15/20	14/39/115/115	-
40	CLA	U	204	18	1/1/11/20	8/18/94/115	-
40	CLA	D	306	4	1/1/13/20	6/27/103/115	-
44	A86	w	316	-	-	12/34/90/90	0/3/3/3
40	CLA	b	835	24	1/1/15/20	13/38/115/115	-
40	CLA	M	312	13	1/1/14/20	14/33/109/115	-
40	CLA	a	811	23,40	1/1/14/20	12/36/112/115	-
40	CLA	f	201	-	1/1/14/20	5/33/109/115	-
44	A86	F	312	-	-	4/34/90/90	0/3/3/3
40	CLA	A	306	1	1/1/14/20	9/33/109/115	-
41	KC2	v	308	36	-	10/15/71/71	-
49	BCR	j	103	-	-	4/29/63/63	0/2/2/2
40	CLA	L	304	12	1/1/13/20	2/30/106/115	-
40	CLA	t	303	38	1/1/11/20	3/18/94/115	-
41	KC2	G	202	-	-	10/15/71/71	-
40	CLA	C	306	3	1/1/15/20	17/39/115/115	-
41	KC2	T	303	-	-	4/15/71/71	-
42	DD6	Q	212	-	-	1/26/80/80	0/3/3/3
47	A1EB1	u	323	-	-	3/43/100/100	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	BCR	b	845	-	-	2/29/63/63	0/2/2/2
40	CLA	E	312	-	1/1/11/20	4/18/94/115	-
40	CLA	Y	304	-	1/1/11/20	1/18/94/115	-
40	CLA	Q	202	16	1/1/13/20	5/31/107/115	-
44	A86	Y	319	-	-	6/34/90/90	0/3/3/3
40	CLA	G	205	7	1/1/12/20	0/21/97/115	-
40	CLA	b	836	24	1/1/14/20	6/33/109/115	-
43	LMG	E	301	40	-	14/26/46/70	0/1/1/1
40	CLA	o	304	34	1/1/14/20	6/33/109/115	-
47	A1EB1	N	320	-	-	8/43/100/100	0/3/3/3
40	CLA	I	202	9	1/1/13/20	8/27/103/115	-
40	CLA	b	831	24	1/1/12/20	5/23/99/115	-
40	CLA	Z	304	-	1/1/14/20	4/33/109/115	-
44	A86	D	320	-	-	5/34/90/90	0/3/3/3
40	CLA	E	303	-	1/1/14/20	5/33/109/115	-
40	CLA	o	310	-	1/1/13/20	9/27/103/115	-
51	SF4	c	101	-	-	-	0/6/5/5
49	BCR	a	843	-	-	4/29/63/63	0/2/2/2
42	DD6	A	316	-	-	1/26/80/80	0/3/3/3
42	DD6	v	318	-	-	0/26/80/80	0/3/3/3
41	KC2	p	315	-	-	8/15/71/71	-
40	CLA	u	307	35	1/1/13/20	8/27/103/115	-
40	CLA	E	308	5	1/1/13/20	6/31/107/115	-
40	CLA	P	308	-	1/1/14/20	12/33/109/115	-
40	CLA	F	305	-	1/1/11/20	4/18/94/115	-
40	CLA	L	311	12	1/1/11/20	6/18/94/115	-
40	CLA	v	304	-	1/1/12/20	4/24/100/115	-
44	A86	K	314	-	-	4/34/90/90	0/3/3/3
41	KC2	G	208	-	-	4/15/71/71	-
43	LMG	A	317	-	-	22/35/55/70	0/1/1/1
44	A86	N	315	-	-	6/34/90/90	0/3/3/3
40	CLA	p	311	-	1/1/13/20	10/27/103/115	-
41	KC2	o	308	34	-	8/15/71/71	-
40	CLA	Z	313	22	1/1/11/20	5/18/94/115	-
40	CLA	b	842	-	1/1/14/20	8/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	X	313	20	1/1/11/20	1/18/94/115	-
42	DD6	q	320	-	-	6/26/80/80	0/3/3/3
44	A86	w	315	-	-	8/34/90/90	1/3/3/3
44	A86	z	301	-	-	6/34/90/90	0/3/3/3
40	CLA	z	314	-	1/1/11/20	4/18/94/115	-
40	CLA	w	309	-	1/1/13/20	9/27/103/115	-
40	CLA	N	310	-	1/1/12/20	5/21/97/115	-
40	CLA	W	306	13	1/1/14/20	12/33/109/115	-
40	CLA	a	812	23	1/1/13/20	0/27/103/115	-
42	DD6	j	104	-	-	1/26/80/80	0/3/3/3
41	KC2	L	313	12	-	8/15/71/71	-
42	DD6	H	314	-	-	2/26/80/80	0/3/3/3
44	A86	w	311	-	-	10/34/90/90	0/3/3/3
40	CLA	W	313	13	1/1/14/20	9/33/109/115	-
40	CLA	I	208	-	1/1/13/20	6/27/103/115	-
40	CLA	J	307	10	1/1/11/20	4/18/94/115	-
49	BCR	a	846	-	-	2/29/63/63	0/2/2/2
49	BCR	i	102	-	-	4/29/63/63	0/2/2/2
41	KC2	X	302	-	-	4/15/71/71	-
40	CLA	a	831	-	1/1/14/20	8/33/109/115	-
42	DD6	Q	211	-	-	1/26/80/80	0/3/3/3
40	CLA	a	826	-	1/1/14/20	11/35/111/115	-
40	CLA	D	305	4	1/1/9/20	2/18/82/115	-
40	CLA	a	813	23	1/1/14/20	6/33/109/115	-
41	KC2	N	309	-	-	4/15/71/71	-
43	LMG	p	301	-	-	9/34/54/70	0/1/1/1
44	A86	S	318	-	-	2/34/90/90	0/3/3/3
41	KC2	I	214	-	-	7/15/71/71	-
44	A86	x	319	-	-	12/34/90/90	0/3/3/3
50	PQN	a	847	-	-	3/17/37/43	0/2/2/2
41	KC2	E	319	-	-	10/15/71/71	-
42	DD6	q	318	-	-	0/26/80/80	0/3/3/3
44	A86	w	310	-	-	7/34/90/90	0/3/3/3
42	DD6	W	315	-	-	1/26/80/80	0/3/3/3
40	CLA	y	308	-	1/1/11/20	5/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	R	310	-	1/1/11/20	3/18/94/115	-
41	KC2	L	309	12	-	8/15/71/71	-
40	CLA	a	818	-	1/1/11/20	2/18/94/115	-
40	CLA	x	312	-	1/1/14/20	9/33/109/115	-
42	DD6	N	317	-	-	3/26/80/80	0/3/3/3
41	KC2	W	302	-	-	6/15/71/71	-
40	CLA	j	102	30	1/1/11/20	4/18/94/115	-
49	BCR	l	206	-	-	6/29/63/63	0/2/2/2
40	CLA	x	308	35	1/1/14/20	6/33/109/115	-
40	CLA	J	309	-	1/1/11/20	2/18/94/115	-
47	A1EB1	T	316	40	-	5/43/100/100	0/3/3/3
48	A1EB4	P	320	-	-	7/38/98/103	0/3/3/3
40	CLA	K	307	11	1/1/12/20	10/26/102/115	-
40	CLA	q	310	-	1/1/12/20	11/23/99/115	-
40	CLA	v	310	-	1/1/12/20	11/23/99/115	-
44	A86	X	319	-	-	7/34/90/90	0/3/3/3
44	A86	z	315	-	-	7/34/90/90	0/3/3/3
40	CLA	R	307	-	1/1/13/20	5/27/103/115	-
40	CLA	A	301	1	1/1/11/20	3/18/94/115	-
40	CLA	b	814	24	1/1/15/20	10/39/115/115	-
41	KC2	W	309	-	-	7/15/71/71	-
40	CLA	F	303	6	1/1/14/20	8/36/112/115	-
44	A86	M	313	-	-	3/34/90/90	0/3/3/3
40	CLA	G	207	-	1/1/12/20	5/26/102/115	-
40	CLA	z	311	-	1/1/13/20	9/27/103/115	-
44	A86	P	316	-	-	6/34/90/90	0/3/3/3
47	A1EB1	S	321	-	-	9/43/100/100	1/3/3/3
40	CLA	p	307	35	1/1/13/20	7/27/103/115	-
41	KC2	F	309	6	-	6/15/71/71	-
40	CLA	a	841	23	1/1/15/20	8/39/115/115	-
41	KC2	N	303	14	-	5/15/71/71	-
40	CLA	L	301	-	1/1/11/20	2/18/94/115	-
40	CLA	v	307	36	1/1/14/20	11/33/109/115	-
40	CLA	M	311	13	1/1/14/20	12/36/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	A86	X	314	-	-	4/34/90/90	1/3/3/3
40	CLA	P	307	13	1/1/13/20	6/32/108/115	-
40	CLA	Q	209	-	1/1/11/20	6/18/94/115	-
40	CLA	w	304	-	1/1/14/20	8/33/109/115	-
41	KC2	H	316	-	-	4/15/71/71	-
40	CLA	a	836	23	1/1/15/20	10/39/115/115	-
47	A1EB1	T	320	-	-	12/43/100/100	0/3/3/3
40	CLA	q	301	-	1/1/13/20	4/27/103/115	-
41	KC2	R	301	15	-	4/15/71/71	-

All (4168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	X	309	KC2	MG-ND	-10.40	1.85	2.05
41	Z	309	KC2	MG-ND	-10.36	1.85	2.05
41	v	303	KC2	MG-ND	-10.32	1.85	2.05
41	M	303	KC2	MG-ND	-10.26	1.85	2.05
41	P	304	KC2	MG-ND	-10.26	1.85	2.05
41	T	303	KC2	MG-ND	-10.24	1.85	2.05
41	N	301	KC2	MG-ND	-10.16	1.85	2.05
41	K	303	KC2	MG-ND	-10.16	1.85	2.05
41	W	310	KC2	MG-ND	-10.15	1.85	2.05
41	x	304	KC2	MG-ND	-10.12	1.85	2.05
41	o	303	KC2	MG-ND	-10.11	1.85	2.05
41	v	309	KC2	MG-ND	-10.11	1.85	2.05
41	N	309	KC2	MG-ND	-10.10	1.85	2.05
41	H	316	KC2	MG-ND	-10.10	1.85	2.05
41	u	309	KC2	MG-ND	-10.09	1.85	2.05
41	q	303	KC2	MG-ND	-10.08	1.85	2.05
41	O	301	KC2	MG-ND	-10.07	1.85	2.05
41	X	308	KC2	MG-ND	-10.07	1.85	2.05
41	u	304	KC2	MG-ND	-10.06	1.85	2.05
41	o	309	KC2	MG-ND	-10.05	1.85	2.05
41	p	304	KC2	MG-ND	-10.05	1.85	2.05
41	x	315	KC2	MG-ND	-10.04	1.85	2.05
41	u	315	KC2	MG-ND	-10.03	1.85	2.05
41	P	302	KC2	MG-ND	-10.03	1.85	2.05
41	L	309	KC2	MG-ND	-10.03	1.85	2.05
41	t	306	KC2	MG-ND	-10.00	1.86	2.05
41	x	309	KC2	MG-ND	-10.00	1.86	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	W	309	KC2	MG-ND	-9.99	1.86	2.05
41	W	304	KC2	MG-ND	-9.99	1.86	2.05
41	W	302	KC2	MG-ND	-9.98	1.86	2.05
41	T	309	KC2	MG-ND	-9.97	1.86	2.05
41	R	303	KC2	MG-ND	-9.97	1.86	2.05
41	x	310	KC2	MG-ND	-9.97	1.86	2.05
41	y	306	KC2	MG-ND	-9.95	1.86	2.05
41	q	309	KC2	MG-ND	-9.95	1.86	2.05
41	M	301	KC2	MG-ND	-9.94	1.86	2.05
41	Y	303	KC2	MG-ND	-9.94	1.86	2.05
41	P	310	KC2	MG-ND	-9.93	1.86	2.05
41	z	309	KC2	MG-ND	-9.93	1.86	2.05
41	F	302	KC2	MG-ND	-9.92	1.86	2.05
41	p	310	KC2	MG-ND	-9.92	1.86	2.05
41	N	308	KC2	MG-ND	-9.91	1.86	2.05
41	K	305	KC2	MG-ND	-9.91	1.86	2.05
41	M	308	KC2	MG-ND	-9.91	1.86	2.05
41	y	301	KC2	MG-ND	-9.91	1.86	2.05
41	w	301	KC2	MG-ND	-9.91	1.86	2.05
41	p	309	KC2	MG-ND	-9.91	1.86	2.05
41	S	309	KC2	MG-ND	-9.91	1.86	2.05
41	E	319	KC2	MG-ND	-9.90	1.86	2.05
41	L	313	KC2	MG-ND	-9.90	1.86	2.05
41	G	208	KC2	MG-ND	-9.90	1.86	2.05
41	M	309	KC2	MG-ND	-9.90	1.86	2.05
41	Q	216	KC2	MG-ND	-9.90	1.86	2.05
41	v	308	KC2	MG-ND	-9.90	1.86	2.05
41	L	303	KC2	MG-ND	-9.90	1.86	2.05
41	R	308	KC2	MG-ND	-9.89	1.86	2.05
41	z	310	KC2	MG-ND	-9.89	1.86	2.05
41	N	302	KC2	MG-ND	-9.89	1.86	2.05
41	K	309	KC2	MG-ND	-9.89	1.86	2.05
41	L	308	KC2	MG-ND	-9.89	1.86	2.05
41	t	301	KC2	MG-ND	-9.87	1.86	2.05
41	S	304	KC2	MG-ND	-9.87	1.86	2.05
41	T	301	KC2	MG-ND	-9.87	1.86	2.05
41	N	313	KC2	MG-ND	-9.87	1.86	2.05
41	O	303	KC2	MG-ND	-9.87	1.86	2.05
41	T	308	KC2	MG-ND	-9.87	1.86	2.05
41	T	302	KC2	MG-ND	-9.87	1.86	2.05
41	u	310	KC2	MG-ND	-9.86	1.86	2.05
41	O	309	KC2	MG-ND	-9.85	1.86	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	P	303	KC2	MG-ND	-9.85	1.86	2.05
41	R	302	KC2	MG-ND	-9.85	1.86	2.05
41	q	308	KC2	MG-ND	-9.85	1.86	2.05
41	y	307	KC2	MG-ND	-9.84	1.86	2.05
41	N	303	KC2	MG-ND	-9.84	1.86	2.05
41	Y	309	KC2	MG-ND	-9.83	1.86	2.05
41	A	310	KC2	MG-ND	-9.83	1.86	2.05
41	K	302	KC2	MG-ND	-9.83	1.86	2.05
41	W	303	KC2	MG-ND	-9.83	1.86	2.05
41	w	306	KC2	MG-ND	-9.83	1.86	2.05
41	R	309	KC2	MG-ND	-9.82	1.86	2.05
41	Z	303	KC2	MG-ND	-9.82	1.86	2.05
41	Y	314	KC2	MG-ND	-9.82	1.86	2.05
41	S	310	KC2	MG-ND	-9.81	1.86	2.05
41	Z	308	KC2	MG-ND	-9.81	1.86	2.05
41	M	302	KC2	MG-ND	-9.80	1.86	2.05
41	I	209	KC2	MG-ND	-9.80	1.86	2.05
41	N	312	KC2	MG-ND	-9.80	1.86	2.05
41	X	303	KC2	MG-ND	-9.80	1.86	2.05
41	I	214	KC2	MG-ND	-9.80	1.86	2.05
41	T	311	KC2	MG-ND	-9.79	1.86	2.05
41	G	202	KC2	MG-ND	-9.79	1.86	2.05
41	C	303	KC2	MG-ND	-9.79	1.86	2.05
41	R	301	KC2	MG-ND	-9.78	1.86	2.05
41	O	302	KC2	MG-ND	-9.78	1.86	2.05
41	L	302	KC2	MG-ND	-9.77	1.86	2.05
41	z	303	KC2	MG-ND	-9.77	1.86	2.05
41	p	315	KC2	MG-ND	-9.77	1.86	2.05
41	R	311	KC2	MG-ND	-9.77	1.86	2.05
41	x	303	KC2	MG-ND	-9.76	1.86	2.05
41	o	308	KC2	MG-ND	-9.75	1.86	2.05
41	q	302	KC2	MG-ND	-9.75	1.86	2.05
41	J	304	KC2	MG-ND	-9.75	1.86	2.05
41	H	303	KC2	MG-ND	-9.75	1.86	2.05
41	F	309	KC2	MG-ND	-9.74	1.86	2.05
41	S	303	KC2	MG-ND	-9.74	1.86	2.05
41	O	311	KC2	MG-ND	-9.74	1.86	2.05
41	t	308	KC2	MG-ND	-9.73	1.86	2.05
41	P	309	KC2	MG-ND	-9.72	1.86	2.05
41	Z	302	KC2	MG-ND	-9.71	1.86	2.05
41	u	303	KC2	MG-ND	-9.71	1.86	2.05
41	z	304	KC2	MG-ND	-9.68	1.86	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	o	302	KC2	MG-ND	-9.67	1.86	2.05
41	v	302	KC2	MG-ND	-9.67	1.86	2.05
41	Q	201	KC2	MG-ND	-9.67	1.86	2.05
41	U	201	KC2	MG-ND	-9.66	1.86	2.05
41	Y	308	KC2	MG-ND	-9.65	1.86	2.05
41	Y	302	KC2	MG-ND	-9.65	1.86	2.05
41	w	307	KC2	MG-ND	-9.65	1.86	2.05
41	O	308	KC2	MG-ND	-9.57	1.86	2.05
41	X	302	KC2	MG-ND	-9.57	1.86	2.05
41	p	303	KC2	MG-ND	-9.48	1.87	2.05
40	Q	206	CLA	C1D-ND	7.39	1.47	1.37
40	F	303	CLA	C1D-ND	7.24	1.47	1.37
40	f	205	CLA	C1D-ND	7.24	1.47	1.37
40	x	313	CLA	C1D-ND	7.20	1.47	1.37
40	u	313	CLA	C1D-ND	7.18	1.47	1.37
40	Q	208	CLA	C1D-ND	7.15	1.47	1.37
40	p	313	CLA	C1D-ND	7.13	1.47	1.37
40	J	303	CLA	C1D-ND	7.10	1.47	1.37
40	K	307	CLA	C1D-ND	7.09	1.47	1.37
40	S	319	CLA	C1D-ND	7.06	1.47	1.37
40	F	310	CLA	C1D-ND	7.05	1.47	1.37
40	E	311	CLA	C1D-ND	6.98	1.47	1.37
40	Y	311	CLA	C1D-ND	6.98	1.47	1.37
40	x	312	CLA	C1D-ND	6.98	1.47	1.37
40	V	202	CLA	C1D-ND	6.97	1.47	1.37
40	P	313	CLA	C1D-ND	6.96	1.47	1.37
40	J	309	CLA	C1D-ND	6.96	1.47	1.37
40	a	824	CLA	C1D-ND	6.95	1.47	1.37
40	W	312	CLA	C1D-ND	6.94	1.47	1.37
40	E	313	CLA	C1D-ND	6.93	1.47	1.37
40	T	317	CLA	C1D-ND	6.93	1.47	1.37
40	U	208	CLA	C1D-ND	6.93	1.47	1.37
40	G	206	CLA	C1D-ND	6.93	1.47	1.37
40	H	308	CLA	C1D-ND	6.93	1.47	1.37
40	C	308	CLA	C1D-ND	6.91	1.46	1.37
40	D	312	CLA	C1D-ND	6.90	1.46	1.37
40	F	311	CLA	C1D-ND	6.89	1.46	1.37
40	J	307	CLA	C1D-ND	6.89	1.46	1.37
40	p	312	CLA	C1D-ND	6.88	1.46	1.37
40	w	308	CLA	C1D-ND	6.88	1.46	1.37
40	A	302	CLA	C1D-ND	6.88	1.46	1.37
40	Y	301	CLA	C1D-ND	6.88	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	l	204	CLA	C1D-ND	6.87	1.46	1.37
40	a	831	CLA	C1D-ND	6.86	1.46	1.37
40	Q	204	CLA	C1D-ND	6.86	1.46	1.37
40	o	301	CLA	C1D-ND	6.86	1.46	1.37
40	a	812	CLA	C1D-ND	6.85	1.46	1.37
40	f	204	CLA	C1D-ND	6.84	1.46	1.37
40	q	313	CLA	C1D-ND	6.84	1.46	1.37
40	Q	205	CLA	C1D-ND	6.83	1.46	1.37
40	O	316	CLA	C1D-ND	6.82	1.46	1.37
40	H	301	CLA	C1D-ND	6.82	1.46	1.37
40	M	311	CLA	C1D-ND	6.81	1.46	1.37
40	l	202	CLA	C1D-ND	6.81	1.46	1.37
40	C	309	CLA	C1D-ND	6.80	1.46	1.37
40	S	302	CLA	C1D-ND	6.80	1.46	1.37
40	J	311	CLA	C1D-ND	6.80	1.46	1.37
40	O	305	CLA	C1D-ND	6.80	1.46	1.37
40	G	201	CLA	C1D-ND	6.79	1.46	1.37
40	U	204	CLA	C1D-ND	6.79	1.46	1.37
40	H	306	CLA	C1D-ND	6.79	1.46	1.37
40	w	305	CLA	C1D-ND	6.79	1.46	1.37
40	Y	313	CLA	C1D-ND	6.78	1.46	1.37
40	N	307	CLA	C1D-ND	6.77	1.46	1.37
40	X	312	CLA	C1D-ND	6.77	1.46	1.37
40	a	823	CLA	C1D-ND	6.77	1.46	1.37
40	w	304	CLA	C1D-ND	6.76	1.46	1.37
40	B	306	CLA	C1D-ND	6.76	1.46	1.37
40	P	308	CLA	C1D-ND	6.75	1.46	1.37
40	A	311	CLA	C1D-ND	6.75	1.46	1.37
40	b	831	CLA	C1D-ND	6.75	1.46	1.37
40	Z	305	CLA	C1D-ND	6.75	1.46	1.37
40	Y	305	CLA	C1D-ND	6.74	1.46	1.37
40	I	202	CLA	C1D-ND	6.74	1.46	1.37
40	L	311	CLA	C1D-ND	6.74	1.46	1.37
40	A	306	CLA	C1D-ND	6.74	1.46	1.37
40	P	312	CLA	C1D-ND	6.74	1.46	1.37
40	z	324	CLA	C1D-ND	6.74	1.46	1.37
40	I	206	CLA	C1D-ND	6.74	1.46	1.37
40	E	307	CLA	C1D-ND	6.73	1.46	1.37
40	F	321	CLA	C1D-ND	6.73	1.46	1.37
40	D	303	CLA	C1D-ND	6.73	1.46	1.37
40	D	307	CLA	C1D-ND	6.73	1.46	1.37
40	u	312	CLA	C1D-ND	6.73	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	t	305	CLA	C1D-ND	6.73	1.46	1.37
40	F	308	CLA	C1D-ND	6.72	1.46	1.37
40	a	851	CLA	C1D-ND	6.72	1.46	1.37
40	S	301	CLA	C1D-ND	6.71	1.46	1.37
40	U	206	CLA	C1D-ND	6.71	1.46	1.37
40	L	301	CLA	C1D-ND	6.71	1.46	1.37
40	Y	307	CLA	C1D-ND	6.71	1.46	1.37
40	y	305	CLA	C1D-ND	6.71	1.46	1.37
40	J	302	CLA	C1D-ND	6.70	1.46	1.37
40	T	306	CLA	C1D-ND	6.70	1.46	1.37
40	y	303	CLA	C1D-ND	6.70	1.46	1.37
40	D	301	CLA	C1D-ND	6.70	1.46	1.37
40	J	308	CLA	C1D-ND	6.70	1.46	1.37
40	y	304	CLA	C1D-ND	6.70	1.46	1.37
40	E	304	CLA	C1D-ND	6.70	1.46	1.37
40	R	304	CLA	C1D-ND	6.69	1.46	1.37
40	o	311	CLA	C1D-ND	6.69	1.46	1.37
40	J	312	CLA	C1D-ND	6.69	1.46	1.37
40	C	301	CLA	C1D-ND	6.69	1.46	1.37
40	H	302	CLA	C1D-ND	6.69	1.46	1.37
40	D	306	CLA	C1D-ND	6.68	1.46	1.37
40	G	213	CLA	C1D-ND	6.68	1.46	1.37
40	E	309	CLA	C1D-ND	6.68	1.46	1.37
40	D	308	CLA	C1D-ND	6.68	1.46	1.37
40	R	307	CLA	C1D-ND	6.68	1.46	1.37
40	a	840	CLA	C1D-ND	6.67	1.46	1.37
40	y	308	CLA	C1D-ND	6.67	1.46	1.37
40	M	312	CLA	C1D-ND	6.67	1.46	1.37
40	a	852	CLA	C1D-ND	6.67	1.46	1.37
40	J	318	CLA	C1D-ND	6.67	1.46	1.37
40	a	810	CLA	C1D-ND	6.66	1.46	1.37
40	t	303	CLA	C1D-ND	6.66	1.46	1.37
40	b	841	CLA	C1D-ND	6.66	1.46	1.37
40	p	311	CLA	MG-NA	-6.66	1.90	2.06
40	R	306	CLA	C1D-ND	6.66	1.46	1.37
40	k	201	CLA	C1D-ND	6.65	1.46	1.37
40	o	312	CLA	C1D-ND	6.65	1.46	1.37
40	N	306	CLA	C1D-ND	6.65	1.46	1.37
40	b	814	CLA	C1D-ND	6.65	1.46	1.37
40	t	309	CLA	C1D-ND	6.65	1.46	1.37
40	W	313	CLA	C1D-ND	6.65	1.46	1.37
40	A	309	CLA	C1D-ND	6.65	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	H	311	CLA	C1D-ND	6.64	1.46	1.37
40	D	309	CLA	C1D-ND	6.64	1.46	1.37
40	J	310	CLA	C1D-ND	6.64	1.46	1.37
40	t	304	CLA	C1D-ND	6.64	1.46	1.37
40	q	311	CLA	C1D-ND	6.64	1.46	1.37
40	a	817	CLA	C1D-ND	6.64	1.46	1.37
40	Z	310	CLA	MG-NA	-6.64	1.90	2.06
40	F	301	CLA	C1D-ND	6.64	1.46	1.37
40	a	811	CLA	C1D-ND	6.64	1.46	1.37
40	a	821	CLA	C1D-ND	6.63	1.46	1.37
40	R	305	CLA	C1D-ND	6.62	1.46	1.37
40	Q	209	CLA	C1D-ND	6.62	1.46	1.37
40	w	303	CLA	C1D-ND	6.62	1.46	1.37
40	b	810	CLA	C1D-ND	6.62	1.46	1.37
40	G	207	CLA	C1D-ND	6.62	1.46	1.37
40	Z	301	CLA	C1D-ND	6.61	1.46	1.37
40	X	305	CLA	C1D-ND	6.61	1.46	1.37
40	D	302	CLA	C1D-ND	6.61	1.46	1.37
40	C	306	CLA	C1D-ND	6.61	1.46	1.37
40	z	302	CLA	C1D-ND	6.61	1.46	1.37
40	M	305	CLA	C1D-ND	6.61	1.46	1.37
40	Q	203	CLA	C1D-ND	6.61	1.46	1.37
40	S	306	CLA	C1D-ND	6.61	1.46	1.37
40	a	815	CLA	C1D-ND	6.61	1.46	1.37
40	L	307	CLA	C1D-ND	6.60	1.46	1.37
40	A	308	CLA	C1D-ND	6.60	1.46	1.37
40	S	308	CLA	C1D-ND	6.60	1.46	1.37
40	b	819	CLA	C1D-ND	6.60	1.46	1.37
40	v	312	CLA	C1D-ND	6.60	1.46	1.37
40	H	310	CLA	C1D-ND	6.59	1.46	1.37
40	J	306	CLA	C1D-ND	6.59	1.46	1.37
40	a	804	CLA	C1D-ND	6.59	1.46	1.37
40	L	305	CLA	C1D-ND	6.59	1.46	1.37
40	S	313	CLA	C1D-ND	6.59	1.46	1.37
40	F	305	CLA	C1D-ND	6.59	1.46	1.37
40	A	303	CLA	C1D-ND	6.58	1.46	1.37
40	K	301	CLA	C1D-ND	6.57	1.46	1.37
40	b	836	CLA	C1D-ND	6.57	1.46	1.37
40	q	312	CLA	C1D-ND	6.57	1.46	1.37
40	G	205	CLA	C1D-ND	6.57	1.46	1.37
40	a	813	CLA	C1D-ND	6.57	1.46	1.37
40	B	303	CLA	C1D-ND	6.56	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	X	301	CLA	C1D-ND	6.55	1.46	1.37
40	E	303	CLA	C1D-ND	6.55	1.46	1.37
40	W	306	CLA	C1D-ND	6.55	1.46	1.37
40	I	201	CLA	C1D-ND	6.55	1.46	1.37
40	Y	304	CLA	C1D-ND	6.55	1.46	1.37
40	W	307	CLA	C1D-ND	6.54	1.46	1.37
40	a	833	CLA	C1D-ND	6.54	1.46	1.37
40	M	310	CLA	C1D-ND	6.54	1.46	1.37
40	b	813	CLA	C1D-ND	6.54	1.46	1.37
40	b	821	CLA	C1D-ND	6.54	1.46	1.37
40	Z	312	CLA	C1D-ND	6.54	1.46	1.37
40	S	314	CLA	C1D-ND	6.54	1.46	1.37
40	a	814	CLA	C1D-ND	6.54	1.46	1.37
40	O	306	CLA	C1D-ND	6.53	1.46	1.37
40	Z	306	CLA	C1D-ND	6.53	1.46	1.37
40	o	306	CLA	C1D-ND	6.53	1.46	1.37
40	X	311	CLA	C1D-ND	6.53	1.46	1.37
40	b	833	CLA	C1D-ND	6.53	1.46	1.37
40	a	809	CLA	C1D-ND	6.53	1.46	1.37
40	u	314	CLA	C1D-ND	6.53	1.46	1.37
40	M	306	CLA	C1D-ND	6.53	1.46	1.37
40	o	305	CLA	C1D-ND	6.53	1.46	1.37
40	P	307	CLA	C1D-ND	6.53	1.46	1.37
40	I	203	CLA	C1D-ND	6.53	1.46	1.37
40	T	305	CLA	C1D-ND	6.52	1.46	1.37
40	a	820	CLA	C1D-ND	6.52	1.46	1.37
40	A	305	CLA	C1D-ND	6.52	1.46	1.37
40	u	311	CLA	MG-NA	-6.52	1.90	2.06
40	v	311	CLA	C1D-ND	6.51	1.46	1.37
40	R	316	CLA	C1D-ND	6.51	1.46	1.37
40	z	313	CLA	C1D-ND	6.51	1.46	1.37
40	a	819	CLA	C1D-ND	6.51	1.46	1.37
40	V	201	CLA	C1D-ND	6.51	1.46	1.37
40	B	301	CLA	C1D-ND	6.51	1.46	1.37
40	A	304	CLA	C1D-ND	6.51	1.46	1.37
40	G	204	CLA	C1D-ND	6.50	1.46	1.37
40	Y	310	CLA	C1D-ND	6.50	1.46	1.37
40	b	818	CLA	C1D-ND	6.50	1.46	1.37
40	j	102	CLA	C1D-ND	6.50	1.46	1.37
40	I	207	CLA	C1D-ND	6.50	1.46	1.37
40	a	805	CLA	C1D-ND	6.50	1.46	1.37
40	x	314	CLA	C1D-ND	6.50	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	v	313	CLA	C1D-ND	6.50	1.46	1.37
40	u	308	CLA	C1D-ND	6.49	1.46	1.37
40	D	311	CLA	C1D-ND	6.49	1.46	1.37
40	F	307	CLA	C1D-ND	6.49	1.46	1.37
40	I	204	CLA	C1D-ND	6.49	1.46	1.37
40	a	829	CLA	C1D-ND	6.49	1.46	1.37
40	a	836	CLA	C1D-ND	6.49	1.46	1.37
40	M	307	CLA	C1D-ND	6.49	1.46	1.37
40	x	311	CLA	MG-NA	-6.48	1.90	2.06
40	O	304	CLA	C1D-ND	6.48	1.46	1.37
40	z	307	CLA	C1D-ND	6.48	1.46	1.37
40	a	835	CLA	C1D-ND	6.47	1.46	1.37
40	p	307	CLA	C1D-ND	6.47	1.46	1.37
40	x	302	CLA	C1D-ND	6.47	1.46	1.37
40	t	302	CLA	C1D-ND	6.47	1.46	1.37
40	i	101	CLA	C1D-ND	6.47	1.46	1.37
40	S	307	CLA	C1D-ND	6.47	1.46	1.37
40	L	310	CLA	C1D-ND	6.46	1.46	1.37
40	b	829	CLA	C1D-ND	6.46	1.46	1.37
40	o	313	CLA	C1D-ND	6.46	1.46	1.37
40	a	822	CLA	C1D-ND	6.46	1.46	1.37
40	Y	306	CLA	C1D-ND	6.46	1.46	1.37
40	p	302	CLA	C1D-ND	6.45	1.46	1.37
40	z	312	CLA	C1D-ND	6.45	1.46	1.37
40	a	827	CLA	C1D-ND	6.45	1.46	1.37
40	F	304	CLA	C1D-ND	6.45	1.46	1.37
40	K	306	CLA	C1D-ND	6.45	1.46	1.37
40	z	306	CLA	C1D-ND	6.44	1.46	1.37
40	I	205	CLA	C1D-ND	6.44	1.46	1.37
40	K	312	CLA	C1D-ND	6.44	1.46	1.37
40	P	306	CLA	C1D-ND	6.44	1.46	1.37
40	O	307	CLA	C1D-ND	6.44	1.46	1.37
40	E	310	CLA	C1D-ND	6.44	1.46	1.37
40	x	306	CLA	C1D-ND	6.44	1.46	1.37
40	p	305	CLA	C1D-ND	6.43	1.46	1.37
40	L	312	CLA	C1D-ND	6.43	1.46	1.37
40	y	309	CLA	C1D-ND	6.43	1.46	1.37
40	b	807	CLA	MG-ND	-6.43	1.93	2.05
40	Z	307	CLA	C1D-ND	6.43	1.46	1.37
40	q	306	CLA	C1D-ND	6.42	1.46	1.37
40	X	310	CLA	C1D-ND	6.42	1.46	1.37
40	U	203	CLA	C1D-ND	6.42	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	a	832	CLA	C1D-ND	6.42	1.46	1.37
40	J	305	CLA	C1D-ND	6.42	1.46	1.37
40	X	306	CLA	C1D-ND	6.41	1.46	1.37
40	X	313	CLA	C1D-ND	6.41	1.46	1.37
40	a	806	CLA	C1D-ND	6.41	1.46	1.37
40	E	302	CLA	C1D-ND	6.41	1.46	1.37
40	b	823	CLA	C1D-ND	6.41	1.46	1.37
40	b	826	CLA	C1D-ND	6.40	1.46	1.37
40	q	301	CLA	C1D-ND	6.40	1.46	1.37
40	A	307	CLA	C1D-ND	6.40	1.46	1.37
40	U	202	CLA	C1D-ND	6.40	1.46	1.37
40	N	305	CLA	C1D-ND	6.40	1.46	1.37
40	Z	313	CLA	C1D-ND	6.40	1.46	1.37
40	b	842	CLA	C1D-ND	6.39	1.46	1.37
40	t	307	CLA	C1D-ND	6.39	1.46	1.37
40	u	302	CLA	C1D-ND	6.39	1.46	1.37
40	w	309	CLA	C1D-ND	6.39	1.46	1.37
40	I	208	CLA	C1D-ND	6.39	1.46	1.37
40	q	304	CLA	C1D-ND	6.38	1.46	1.37
40	a	828	CLA	C1D-ND	6.38	1.46	1.37
40	b	811	CLA	C1D-ND	6.38	1.46	1.37
40	a	838	CLA	C1D-ND	6.38	1.46	1.37
40	o	310	CLA	C1D-ND	6.37	1.46	1.37
40	W	308	CLA	C1D-ND	6.37	1.46	1.37
40	q	305	CLA	C1D-ND	6.37	1.46	1.37
40	a	830	CLA	C1D-ND	6.37	1.46	1.37
40	U	205	CLA	C1D-ND	6.37	1.46	1.37
40	b	815	CLA	C1D-ND	6.37	1.46	1.37
40	B	307	CLA	MG-ND	-6.36	1.93	2.05
40	E	308	CLA	C1D-ND	6.36	1.46	1.37
40	E	312	CLA	C1D-ND	6.36	1.46	1.37
40	E	314	CLA	MG-ND	-6.36	1.93	2.05
40	D	304	CLA	C1D-ND	6.36	1.46	1.37
40	C	307	CLA	C1D-ND	6.36	1.46	1.37
40	L	306	CLA	C1D-ND	6.36	1.46	1.37
40	p	308	CLA	C1D-ND	6.36	1.46	1.37
40	a	839	CLA	C1D-ND	6.35	1.46	1.37
40	F	306	CLA	C1D-ND	6.35	1.46	1.37
40	a	837	CLA	C1D-ND	6.35	1.46	1.37
40	b	820	CLA	C1D-ND	6.35	1.46	1.37
40	p	306	CLA	C1D-ND	6.35	1.46	1.37
40	L	304	CLA	C1D-ND	6.34	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	U	207	CLA	C1D-ND	6.34	1.46	1.37
40	a	818	CLA	C1D-ND	6.34	1.46	1.37
40	f	202	CLA	C1D-ND	6.34	1.46	1.37
40	v	304	CLA	C1D-ND	6.34	1.46	1.37
40	C	302	CLA	C1D-ND	6.33	1.46	1.37
40	f	201	CLA	C1D-ND	6.33	1.46	1.37
40	q	307	CLA	C1D-ND	6.32	1.46	1.37
40	o	304	CLA	C1D-ND	6.32	1.46	1.37
40	v	307	CLA	C1D-ND	6.32	1.46	1.37
40	N	311	CLA	C1D-ND	6.32	1.46	1.37
40	Z	311	CLA	C1D-ND	6.32	1.46	1.37
40	a	842	CLA	C1D-ND	6.32	1.46	1.37
40	b	830	CLA	C1D-ND	6.32	1.46	1.37
40	B	302	CLA	MG-NB	-6.32	1.93	2.05
40	H	307	CLA	C1D-ND	6.31	1.46	1.37
40	v	305	CLA	C1D-ND	6.31	1.46	1.37
40	T	307	CLA	C1D-ND	6.31	1.46	1.37
40	Z	312	CLA	MG-NB	-6.31	1.93	2.05
40	a	807	CLA	C1D-ND	6.31	1.46	1.37
40	b	828	CLA	C1D-ND	6.30	1.46	1.37
40	b	835	CLA	C1D-ND	6.30	1.46	1.37
40	v	306	CLA	C1D-ND	6.30	1.46	1.37
40	T	304	CLA	C1D-ND	6.29	1.46	1.37
40	b	840	CLA	C1D-ND	6.29	1.46	1.37
40	X	307	CLA	C1D-ND	6.29	1.46	1.37
40	S	311	CLA	C1D-ND	6.29	1.46	1.37
40	z	314	CLA	C1D-ND	6.29	1.46	1.37
40	G	203	CLA	C1D-ND	6.29	1.46	1.37
40	z	311	CLA	MG-NA	-6.29	1.91	2.06
40	S	312	CLA	C1D-ND	6.29	1.46	1.37
40	W	305	CLA	C1D-ND	6.29	1.46	1.37
40	a	841	CLA	C1D-ND	6.28	1.46	1.37
40	a	834	CLA	C1D-ND	6.27	1.46	1.37
40	E	305	CLA	C1D-ND	6.27	1.46	1.37
40	Q	202	CLA	C1D-ND	6.26	1.46	1.37
40	B	304	CLA	C1D-ND	6.26	1.46	1.37
40	Q	207	CLA	C1D-ND	6.26	1.46	1.37
40	A	301	CLA	C1D-ND	6.25	1.46	1.37
40	U	203	CLA	MG-NB	-6.25	1.93	2.05
40	Y	312	CLA	MG-NA	-6.25	1.91	2.06
40	C	304	CLA	C1D-ND	6.25	1.46	1.37
41	R	309	KC2	C4B-NB	6.25	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	w	302	CLA	C1D-ND	6.24	1.46	1.37
40	a	803	CLA	MG-ND	-6.24	1.93	2.05
40	R	310	CLA	C1D-ND	6.24	1.46	1.37
40	O	310	CLA	C1D-ND	6.24	1.46	1.37
40	H	304	CLA	C1D-ND	6.23	1.46	1.37
40	H	309	CLA	C1D-ND	6.23	1.46	1.37
40	E	314	CLA	MG-NA	-6.23	1.91	2.06
40	y	309	CLA	MG-ND	-6.23	1.93	2.05
40	b	838	CLA	MG-ND	-6.23	1.93	2.05
40	H	305	CLA	C1D-ND	6.23	1.46	1.37
40	b	802	CLA	C1D-ND	6.22	1.46	1.37
40	C	305	CLA	C1D-ND	6.22	1.46	1.37
40	b	837	CLA	C1D-ND	6.22	1.46	1.37
40	p	314	CLA	C1D-ND	6.22	1.46	1.37
40	b	805	CLA	C1D-ND	6.21	1.46	1.37
40	N	304	CLA	C1D-ND	6.21	1.46	1.37
40	b	827	CLA	C1D-ND	6.21	1.46	1.37
41	q	302	KC2	C4B-NB	6.21	1.46	1.37
40	E	306	CLA	C1D-ND	6.21	1.46	1.37
40	b	816	CLA	C1D-ND	6.21	1.46	1.37
40	Y	312	CLA	C1D-ND	6.20	1.46	1.37
40	a	825	CLA	MG-ND	-6.20	1.93	2.05
40	U	203	CLA	MG-ND	-6.20	1.93	2.05
40	T	310	CLA	C1D-ND	6.19	1.46	1.37
40	b	806	CLA	C1D-ND	6.19	1.46	1.37
40	u	306	CLA	C1D-ND	6.19	1.46	1.37
40	l	203	CLA	C1D-ND	6.19	1.46	1.37
40	M	304	CLA	C1D-ND	6.19	1.46	1.37
40	a	808	CLA	MG-NA	-6.18	1.91	2.06
40	N	310	CLA	C1D-ND	6.17	1.46	1.37
40	b	809	CLA	C1D-ND	6.17	1.46	1.37
40	y	302	CLA	MG-ND	-6.17	1.93	2.05
40	X	310	CLA	MG-NA	-6.17	1.91	2.06
40	o	310	CLA	MG-NA	-6.17	1.91	2.06
40	x	308	CLA	C1D-ND	6.16	1.46	1.37
41	p	303	KC2	C4B-NB	6.16	1.46	1.37
40	a	850	CLA	MG-ND	-6.16	1.93	2.05
40	A	301	CLA	MG-ND	-6.16	1.93	2.05
40	b	803	CLA	C1D-ND	6.16	1.46	1.37
40	b	824	CLA	C1D-ND	6.16	1.46	1.37
40	x	305	CLA	C1D-ND	6.16	1.45	1.37
40	a	816	CLA	C1D-ND	6.15	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	l	205	CLA	C1D-ND	6.15	1.45	1.37
40	S	305	CLA	C1D-ND	6.15	1.45	1.37
40	Z	304	CLA	C1D-ND	6.15	1.45	1.37
40	b	822	CLA	C1D-ND	6.15	1.45	1.37
40	b	808	CLA	MG-ND	-6.14	1.93	2.05
40	u	305	CLA	C1D-ND	6.14	1.45	1.37
40	S	311	CLA	MG-NA	-6.14	1.91	2.06
41	x	303	KC2	C4B-NB	6.13	1.45	1.37
41	v	302	KC2	C4B-NB	6.13	1.45	1.37
40	w	309	CLA	MG-ND	-6.12	1.93	2.05
40	D	310	CLA	MG-ND	-6.11	1.93	2.05
40	u	307	CLA	C1D-ND	6.11	1.45	1.37
40	b	803	CLA	MG-ND	-6.11	1.93	2.05
40	q	311	CLA	MG-ND	-6.11	1.93	2.05
40	b	832	CLA	C1D-ND	6.11	1.45	1.37
40	y	302	CLA	C1D-ND	6.10	1.45	1.37
40	K	304	CLA	C1D-ND	6.09	1.45	1.37
40	B	304	CLA	MG-ND	-6.08	1.93	2.05
40	b	839	CLA	C1D-ND	6.08	1.45	1.37
40	b	812	CLA	C1D-ND	6.08	1.45	1.37
40	B	302	CLA	C1D-ND	6.08	1.45	1.37
40	Z	304	CLA	MG-ND	-6.07	1.93	2.05
41	u	303	KC2	C4B-NB	6.07	1.45	1.37
40	K	308	CLA	C1D-ND	6.06	1.45	1.37
40	x	302	CLA	MG-NB	-6.06	1.93	2.05
40	Q	207	CLA	MG-NB	-6.06	1.93	2.05
40	i	101	CLA	MG-NB	-6.06	1.93	2.05
40	x	307	CLA	C1D-ND	6.05	1.45	1.37
40	o	307	CLA	C1D-ND	6.05	1.45	1.37
40	H	309	CLA	MG-ND	-6.05	1.93	2.05
41	X	302	KC2	C4B-NB	6.05	1.45	1.37
40	L	306	CLA	MG-NB	-6.04	1.93	2.05
40	p	311	CLA	C1D-ND	6.04	1.45	1.37
40	q	310	CLA	C1D-ND	6.04	1.45	1.37
40	y	302	CLA	MG-NB	-6.04	1.93	2.05
40	P	311	CLA	C1D-ND	6.03	1.45	1.37
40	L	312	CLA	MG-ND	-6.03	1.93	2.05
40	b	840	CLA	MG-ND	-6.03	1.93	2.05
40	z	311	CLA	MG-NB	-6.03	1.93	2.05
41	P	303	KC2	C4B-NB	6.03	1.45	1.37
40	X	304	CLA	C1D-ND	6.02	1.45	1.37
40	k	202	CLA	C1D-ND	6.02	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	W	312	CLA	MG-ND	-6.02	1.93	2.05
40	a	808	CLA	C1D-ND	6.01	1.45	1.37
40	v	311	CLA	MG-ND	-6.01	1.93	2.05
40	E	314	CLA	MG-NB	-6.01	1.93	2.05
40	y	303	CLA	MG-ND	-6.00	1.93	2.05
40	P	311	CLA	MG-ND	-6.00	1.93	2.05
40	b	817	CLA	C1D-ND	6.00	1.45	1.37
40	Y	304	CLA	MG-ND	-5.99	1.93	2.05
40	X	311	CLA	MG-ND	-5.99	1.93	2.05
41	C	303	KC2	C4B-NB	5.99	1.45	1.37
41	M	302	KC2	C4B-NB	5.98	1.45	1.37
40	b	812	CLA	MG-ND	-5.98	1.93	2.05
40	F	310	CLA	MG-ND	-5.98	1.93	2.05
41	S	303	KC2	C4B-NB	5.97	1.45	1.37
40	X	304	CLA	MG-ND	-5.97	1.94	2.05
40	H	305	CLA	MG-ND	-5.97	1.94	2.05
40	o	310	CLA	MG-NB	-5.96	1.94	2.05
41	Q	201	KC2	C4B-NB	5.95	1.45	1.37
40	x	307	CLA	MG-NB	-5.95	1.94	2.05
40	u	307	CLA	MG-ND	-5.95	1.94	2.05
40	L	304	CLA	MG-ND	-5.95	1.94	2.05
40	B	301	CLA	MG-NA	-5.95	1.92	2.06
40	b	834	CLA	MG-NB	-5.94	1.94	2.05
40	C	308	CLA	MG-NB	-5.94	1.94	2.05
40	z	311	CLA	MG-ND	-5.94	1.94	2.05
41	Z	302	KC2	C4B-NB	5.94	1.45	1.37
40	x	307	CLA	MG-ND	-5.93	1.94	2.05
41	U	201	KC2	C4B-NB	5.93	1.45	1.37
40	K	308	CLA	MG-ND	-5.93	1.94	2.05
40	b	809	CLA	MG-NA	-5.93	1.92	2.06
40	b	838	CLA	C1D-ND	5.93	1.45	1.37
40	Q	207	CLA	MG-ND	-5.93	1.94	2.05
40	P	305	CLA	C1D-ND	5.93	1.45	1.37
40	J	307	CLA	MG-ND	-5.93	1.94	2.05
40	p	313	CLA	MG-NB	-5.93	1.94	2.05
40	t	307	CLA	MG-ND	-5.92	1.94	2.05
40	E	305	CLA	MG-NB	-5.92	1.94	2.05
40	a	826	CLA	C1D-ND	5.91	1.45	1.37
40	v	301	CLA	MG-ND	-5.91	1.94	2.05
40	E	306	CLA	MG-ND	-5.91	1.94	2.05
40	Q	207	CLA	MG-NA	-5.91	1.92	2.06
40	W	308	CLA	MG-NA	-5.90	1.92	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	Z	310	CLA	C1D-ND	5.90	1.45	1.37
40	N	310	CLA	MG-NA	-5.89	1.92	2.06
40	x	302	CLA	MG-ND	-5.89	1.94	2.05
40	u	302	CLA	MG-ND	-5.89	1.94	2.05
40	O	310	CLA	MG-NB	-5.88	1.94	2.05
40	T	310	CLA	MG-ND	-5.88	1.94	2.05
40	z	305	CLA	MG-ND	-5.88	1.94	2.05
40	B	307	CLA	MG-NA	-5.88	1.92	2.06
40	Y	312	CLA	MG-NB	-5.88	1.94	2.05
40	z	312	CLA	MG-ND	-5.87	1.94	2.05
41	t	308	KC2	C4B-NB	5.87	1.45	1.37
40	L	306	CLA	MG-NA	-5.87	1.92	2.06
40	z	313	CLA	MG-NB	-5.87	1.94	2.05
40	f	202	CLA	MG-ND	-5.87	1.94	2.05
41	O	308	KC2	C4B-NB	5.87	1.45	1.37
40	b	827	CLA	MG-ND	-5.87	1.94	2.05
41	L	313	KC2	C4B-NB	5.87	1.45	1.37
40	B	302	CLA	MG-NA	-5.86	1.92	2.06
40	H	301	CLA	MG-ND	-5.86	1.94	2.05
41	p	315	KC2	C4B-NB	5.86	1.45	1.37
40	l	205	CLA	MG-ND	-5.86	1.94	2.05
40	I	203	CLA	MG-NB	-5.86	1.94	2.05
40	P	305	CLA	MG-ND	-5.86	1.94	2.05
40	p	311	CLA	MG-NB	-5.86	1.94	2.05
41	O	311	KC2	C4B-NB	5.86	1.45	1.37
40	S	311	CLA	MG-NB	-5.86	1.94	2.05
40	b	842	CLA	MG-ND	-5.86	1.94	2.05
40	j	102	CLA	MG-NA	-5.86	1.92	2.06
40	S	305	CLA	MG-NA	-5.85	1.92	2.06
40	D	310	CLA	C1D-ND	5.85	1.45	1.37
40	a	825	CLA	C1D-ND	5.85	1.45	1.37
40	W	311	CLA	C1D-ND	5.85	1.45	1.37
40	l	205	CLA	MG-NB	-5.85	1.94	2.05
40	v	310	CLA	MG-NA	-5.85	1.92	2.06
40	A	301	CLA	MG-NB	-5.84	1.94	2.05
40	B	301	CLA	MG-NB	-5.84	1.94	2.05
40	a	818	CLA	MG-ND	-5.83	1.94	2.05
40	X	311	CLA	MG-NB	-5.83	1.94	2.05
40	u	302	CLA	MG-NB	-5.83	1.94	2.05
40	v	310	CLA	C1D-ND	5.83	1.45	1.37
40	p	307	CLA	MG-ND	-5.83	1.94	2.05
40	W	311	CLA	MG-ND	-5.83	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	u	311	CLA	MG-NB	-5.83	1.94	2.05
40	z	308	CLA	C1D-ND	5.83	1.45	1.37
40	b	811	CLA	MG-ND	-5.82	1.94	2.05
40	L	306	CLA	MG-ND	-5.82	1.94	2.05
40	C	307	CLA	MG-NB	-5.82	1.94	2.05
40	k	202	CLA	MG-ND	-5.81	1.94	2.05
40	B	306	CLA	MG-NB	-5.81	1.94	2.05
40	C	309	CLA	MG-NB	-5.80	1.94	2.05
40	y	309	CLA	MG-NB	-5.80	1.94	2.05
40	p	307	CLA	MG-NB	-5.79	1.94	2.05
41	o	302	KC2	C4B-NB	5.79	1.45	1.37
40	x	311	CLA	MG-ND	-5.79	1.94	2.05
40	i	101	CLA	MG-ND	-5.79	1.94	2.05
40	M	304	CLA	MG-ND	-5.79	1.94	2.05
40	o	312	CLA	MG-NB	-5.79	1.94	2.05
40	X	310	CLA	MG-NB	-5.78	1.94	2.05
40	p	314	CLA	MG-NA	-5.78	1.92	2.06
41	T	308	KC2	C4B-NB	5.78	1.45	1.37
40	a	808	CLA	MG-ND	-5.78	1.94	2.05
40	G	204	CLA	MG-ND	-5.78	1.94	2.05
40	O	310	CLA	MG-ND	-5.78	1.94	2.05
40	v	305	CLA	MG-ND	-5.78	1.94	2.05
40	u	306	CLA	MG-ND	-5.78	1.94	2.05
41	M	309	KC2	C4B-NB	5.78	1.45	1.37
41	N	313	KC2	C4B-NB	5.78	1.45	1.37
41	R	311	KC2	C4B-NB	5.78	1.45	1.37
40	R	316	CLA	MG-ND	-5.78	1.94	2.05
40	S	312	CLA	MG-NA	-5.78	1.92	2.06
40	x	311	CLA	C1D-ND	5.77	1.45	1.37
40	u	311	CLA	MG-ND	-5.77	1.94	2.05
40	A	304	CLA	MG-NB	-5.77	1.94	2.05
40	R	310	CLA	MG-ND	-5.77	1.94	2.05
40	Y	312	CLA	MG-ND	-5.77	1.94	2.05
40	q	311	CLA	MG-NB	-5.77	1.94	2.05
40	L	310	CLA	MG-NA	-5.77	1.92	2.06
40	Z	312	CLA	MG-NA	-5.77	1.92	2.06
41	E	319	KC2	C4B-NB	5.76	1.45	1.37
40	x	311	CLA	MG-NB	-5.76	1.94	2.05
40	Z	311	CLA	MG-ND	-5.76	1.94	2.05
40	a	838	CLA	MG-ND	-5.76	1.94	2.05
40	W	308	CLA	MG-NB	-5.76	1.94	2.05
40	b	834	CLA	MG-ND	-5.76	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	v	301	CLA	MG-NB	-5.76	1.94	2.05
40	C	308	CLA	MG-ND	-5.76	1.94	2.05
40	b	828	CLA	MG-ND	-5.76	1.94	2.05
40	q	310	CLA	MG-ND	-5.76	1.94	2.05
41	J	304	KC2	C4B-NB	5.75	1.45	1.37
40	Q	202	CLA	MG-ND	-5.75	1.94	2.05
40	B	307	CLA	MG-NB	-5.75	1.94	2.05
40	K	308	CLA	MG-NB	-5.75	1.94	2.05
40	b	810	CLA	MG-ND	-5.75	1.94	2.05
40	b	840	CLA	MG-NB	-5.74	1.94	2.05
41	w	301	KC2	C4B-NB	5.74	1.45	1.37
40	a	842	CLA	MG-ND	-5.74	1.94	2.05
40	S	305	CLA	MG-ND	-5.74	1.94	2.05
41	z	303	KC2	C4B-NB	5.74	1.45	1.37
40	v	310	CLA	MG-ND	-5.74	1.94	2.05
40	E	314	CLA	C1D-ND	5.73	1.45	1.37
40	b	822	CLA	MG-NA	-5.73	1.92	2.06
40	J	303	CLA	MG-ND	-5.73	1.94	2.05
40	u	314	CLA	MG-NA	-5.73	1.92	2.06
41	O	302	KC2	C4B-NB	5.73	1.45	1.37
40	U	206	CLA	MG-ND	-5.73	1.94	2.05
40	j	102	CLA	MG-NB	-5.73	1.94	2.05
40	z	311	CLA	C1D-ND	5.73	1.45	1.37
40	J	302	CLA	MG-ND	-5.73	1.94	2.05
41	T	311	KC2	C4B-NB	5.72	1.45	1.37
40	v	301	CLA	C1D-ND	5.72	1.45	1.37
40	b	808	CLA	C1D-ND	5.72	1.45	1.37
40	p	313	CLA	MG-ND	-5.72	1.94	2.05
40	b	834	CLA	C1D-ND	5.72	1.45	1.37
41	R	308	KC2	C4B-NB	5.72	1.45	1.37
41	Y	314	KC2	C4B-NB	5.72	1.45	1.37
40	b	817	CLA	MG-ND	-5.72	1.94	2.05
40	a	822	CLA	MG-ND	-5.72	1.94	2.05
40	q	304	CLA	MG-ND	-5.72	1.94	2.05
40	b	838	CLA	MG-NB	-5.71	1.94	2.05
41	N	308	KC2	C4B-NB	5.71	1.45	1.37
40	u	307	CLA	MG-NB	-5.71	1.94	2.05
41	A	310	KC2	C4B-NB	5.71	1.45	1.37
40	b	801	CLA	MG-NA	-5.71	1.92	2.06
40	v	306	CLA	MG-ND	-5.70	1.94	2.05
40	J	310	CLA	MG-ND	-5.70	1.94	2.05
40	E	302	CLA	MG-ND	-5.70	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	q	306	CLA	MG-ND	-5.70	1.94	2.05
40	b	801	CLA	MG-ND	-5.69	1.94	2.05
41	F	302	KC2	C4B-NB	5.69	1.45	1.37
41	H	303	KC2	C4B-NB	5.69	1.45	1.37
41	W	310	KC2	C4B-NB	5.69	1.45	1.37
40	b	821	CLA	MG-ND	-5.69	1.94	2.05
40	X	305	CLA	MG-ND	-5.69	1.94	2.05
41	K	309	KC2	C4B-NB	5.69	1.45	1.37
40	v	304	CLA	MG-ND	-5.69	1.94	2.05
40	W	311	CLA	MG-NA	-5.69	1.92	2.06
40	l	205	CLA	MG-NA	-5.69	1.92	2.06
40	z	305	CLA	C1D-ND	5.69	1.45	1.37
40	a	832	CLA	MG-ND	-5.69	1.94	2.05
40	t	302	CLA	MG-ND	-5.69	1.94	2.05
40	W	308	CLA	MG-ND	-5.69	1.94	2.05
40	Z	310	CLA	MG-NB	-5.69	1.94	2.05
40	O	305	CLA	MG-ND	-5.69	1.94	2.05
40	q	310	CLA	MG-NA	-5.68	1.92	2.06
40	I	204	CLA	MG-ND	-5.68	1.94	2.05
40	C	302	CLA	MG-ND	-5.68	1.94	2.05
40	v	311	CLA	MG-NB	-5.68	1.94	2.05
41	y	301	KC2	C4B-NB	5.68	1.45	1.37
40	a	813	CLA	MG-ND	-5.68	1.94	2.05
40	X	306	CLA	MG-NB	-5.67	1.94	2.05
40	o	306	CLA	MG-ND	-5.67	1.94	2.05
41	t	301	KC2	C4B-NB	5.67	1.45	1.37
40	M	311	CLA	MG-NB	-5.67	1.94	2.05
40	o	313	CLA	MG-NA	-5.67	1.92	2.06
40	I	208	CLA	MG-NB	-5.67	1.94	2.05
41	T	302	KC2	C4B-NB	5.67	1.45	1.37
41	Q	216	KC2	C4B-NB	5.66	1.45	1.37
40	C	307	CLA	MG-NA	-5.66	1.92	2.06
40	Y	313	CLA	MG-NB	-5.66	1.94	2.05
40	b	813	CLA	MG-ND	-5.66	1.94	2.05
40	B	306	CLA	MG-NA	-5.66	1.92	2.06
40	H	302	CLA	MG-NB	-5.66	1.94	2.05
40	w	309	CLA	MG-NB	-5.66	1.94	2.05
41	p	310	KC2	C4B-NB	5.66	1.45	1.37
40	b	826	CLA	MG-NB	-5.66	1.94	2.05
40	L	311	CLA	MG-ND	-5.66	1.94	2.05
40	b	836	CLA	MG-NB	-5.66	1.94	2.05
40	p	314	CLA	MG-ND	-5.65	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	b	832	CLA	MG-ND	-5.65	1.94	2.05
40	q	305	CLA	MG-ND	-5.65	1.94	2.05
40	I	203	CLA	MG-ND	-5.65	1.94	2.05
40	o	304	CLA	MG-ND	-5.65	1.94	2.05
40	U	207	CLA	MG-ND	-5.65	1.94	2.05
41	K	302	KC2	C4B-NB	5.65	1.45	1.37
40	J	306	CLA	MG-ND	-5.65	1.94	2.05
40	O	305	CLA	MG-NB	-5.65	1.94	2.05
40	b	825	CLA	C1D-ND	5.64	1.45	1.37
41	K	305	KC2	C4B-NB	5.64	1.45	1.37
40	u	305	CLA	MG-ND	-5.64	1.94	2.05
40	U	205	CLA	MG-ND	-5.64	1.94	2.05
41	R	302	KC2	C4B-NB	5.64	1.45	1.37
41	u	315	KC2	C4B-NB	5.64	1.45	1.37
40	a	824	CLA	MG-ND	-5.64	1.94	2.05
40	b	829	CLA	MG-ND	-5.64	1.94	2.05
41	G	202	KC2	C4B-NB	5.64	1.45	1.37
40	o	312	CLA	MG-ND	-5.64	1.94	2.05
40	E	303	CLA	MG-ND	-5.64	1.94	2.05
40	X	312	CLA	MG-NB	-5.63	1.94	2.05
40	x	305	CLA	MG-ND	-5.63	1.94	2.05
41	Y	309	KC2	C4B-NB	5.63	1.45	1.37
40	L	305	CLA	MG-ND	-5.63	1.94	2.05
40	Q	208	CLA	MG-ND	-5.63	1.94	2.05
40	q	301	CLA	MG-ND	-5.63	1.94	2.05
40	y	302	CLA	MG-NA	-5.63	1.92	2.06
40	Z	306	CLA	MG-ND	-5.63	1.94	2.05
40	b	822	CLA	MG-ND	-5.63	1.94	2.05
40	b	826	CLA	MG-ND	-5.63	1.94	2.05
40	a	840	CLA	MG-ND	-5.63	1.94	2.05
40	b	825	CLA	MG-ND	-5.63	1.94	2.05
40	J	305	CLA	MG-ND	-5.63	1.94	2.05
40	u	311	CLA	C1D-ND	5.63	1.45	1.37
40	R	305	CLA	MG-ND	-5.63	1.94	2.05
40	p	306	CLA	MG-ND	-5.63	1.94	2.05
41	Z	309	KC2	C4B-NB	5.63	1.45	1.37
40	a	811	CLA	MG-ND	-5.63	1.94	2.05
40	F	321	CLA	MG-ND	-5.62	1.94	2.05
40	U	202	CLA	MG-NB	-5.62	1.94	2.05
41	w	307	KC2	C4B-NB	5.62	1.45	1.37
40	p	305	CLA	MG-ND	-5.62	1.94	2.05
40	B	306	CLA	MG-ND	-5.62	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	S	307	CLA	MG-ND	-5.62	1.94	2.05
40	b	820	CLA	MG-NA	-5.62	1.92	2.06
40	a	807	CLA	MG-ND	-5.62	1.94	2.05
40	o	313	CLA	C1B-NB	5.62	1.45	1.37
40	S	312	CLA	MG-ND	-5.62	1.94	2.05
40	z	313	CLA	MG-ND	-5.61	1.94	2.05
40	p	311	CLA	MG-ND	-5.61	1.94	2.05
40	O	307	CLA	MG-ND	-5.61	1.94	2.05
40	B	304	CLA	MG-NB	-5.61	1.94	2.05
40	l	203	CLA	MG-ND	-5.61	1.94	2.05
40	b	816	CLA	MG-ND	-5.61	1.94	2.05
40	f	205	CLA	MG-ND	-5.61	1.94	2.05
40	C	308	CLA	MG-NA	-5.61	1.92	2.06
40	N	310	CLA	MG-ND	-5.61	1.94	2.05
40	U	208	CLA	MG-ND	-5.61	1.94	2.05
40	Z	313	CLA	MG-ND	-5.60	1.94	2.05
40	a	826	CLA	MG-ND	-5.60	1.94	2.05
40	T	304	CLA	MG-ND	-5.60	1.94	2.05
41	Y	302	KC2	C4B-NB	5.60	1.45	1.37
40	E	304	CLA	MG-ND	-5.60	1.94	2.05
40	H	309	CLA	MG-NB	-5.60	1.94	2.05
40	w	302	CLA	MG-ND	-5.60	1.94	2.05
40	z	314	CLA	MG-NA	-5.60	1.93	2.06
40	a	809	CLA	MG-ND	-5.60	1.94	2.05
40	D	311	CLA	MG-NA	-5.60	1.93	2.06
40	A	303	CLA	MG-ND	-5.60	1.94	2.05
40	b	816	CLA	MG-NB	-5.59	1.94	2.05
40	x	308	CLA	MG-ND	-5.59	1.94	2.05
41	x	315	KC2	C4B-NB	5.59	1.45	1.37
40	U	205	CLA	MG-NB	-5.59	1.94	2.05
40	Y	313	CLA	MG-NA	-5.59	1.93	2.06
40	z	307	CLA	MG-ND	-5.59	1.94	2.05
40	A	307	CLA	MG-NB	-5.59	1.94	2.05
40	Z	304	CLA	MG-NB	-5.59	1.94	2.05
40	a	835	CLA	MG-ND	-5.59	1.94	2.05
41	O	309	KC2	C4B-NB	5.59	1.45	1.37
40	t	303	CLA	MG-ND	-5.58	1.94	2.05
41	S	310	KC2	C4B-NB	5.58	1.45	1.37
40	M	305	CLA	MG-ND	-5.58	1.94	2.05
40	P	307	CLA	MG-ND	-5.58	1.94	2.05
40	E	311	CLA	MG-NB	-5.58	1.94	2.05
40	W	312	CLA	MG-NB	-5.57	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	X	306	CLA	MG-ND	-5.57	1.94	2.05
40	E	312	CLA	MG-ND	-5.57	1.94	2.05
41	y	307	KC2	C4B-NB	5.57	1.45	1.37
40	T	305	CLA	MG-NB	-5.57	1.94	2.05
40	I	203	CLA	MG-NA	-5.57	1.93	2.06
40	N	306	CLA	MG-ND	-5.57	1.94	2.05
40	Z	307	CLA	MG-ND	-5.57	1.94	2.05
40	P	311	CLA	MG-NA	-5.56	1.93	2.06
40	X	304	CLA	MG-NB	-5.56	1.94	2.05
40	b	833	CLA	MG-ND	-5.56	1.94	2.05
40	Z	313	CLA	MG-NA	-5.56	1.93	2.06
40	G	213	CLA	MG-ND	-5.56	1.94	2.05
40	J	312	CLA	MG-ND	-5.56	1.94	2.05
40	K	304	CLA	MG-ND	-5.56	1.94	2.05
40	N	304	CLA	MG-ND	-5.56	1.94	2.05
40	G	213	CLA	MG-NB	-5.56	1.94	2.05
40	I	208	CLA	MG-NA	-5.56	1.93	2.06
40	O	310	CLA	MG-NA	-5.56	1.93	2.06
40	o	311	CLA	MG-ND	-5.56	1.94	2.05
40	q	312	CLA	MG-ND	-5.56	1.94	2.05
40	t	307	CLA	MG-NB	-5.56	1.94	2.05
41	Y	308	KC2	C4B-NB	5.56	1.45	1.37
40	H	307	CLA	MG-NA	-5.56	1.93	2.06
40	N	311	CLA	MG-ND	-5.55	1.94	2.05
40	Z	310	CLA	MG-ND	-5.55	1.94	2.05
40	z	308	CLA	MG-NA	-5.55	1.93	2.06
40	J	310	CLA	MG-NA	-5.55	1.93	2.06
40	b	809	CLA	MG-NB	-5.55	1.94	2.05
40	a	834	CLA	MG-ND	-5.55	1.94	2.05
40	b	830	CLA	MG-ND	-5.55	1.94	2.05
40	P	311	CLA	MG-NB	-5.55	1.94	2.05
40	F	304	CLA	MG-NA	-5.55	1.93	2.06
41	p	304	KC2	C4B-NB	5.55	1.45	1.37
40	G	207	CLA	MG-ND	-5.54	1.94	2.05
40	C	305	CLA	MG-ND	-5.54	1.94	2.05
40	E	305	CLA	MG-ND	-5.54	1.94	2.05
40	z	314	CLA	MG-ND	-5.54	1.94	2.05
41	I	214	KC2	C4B-NB	5.54	1.45	1.37
40	a	816	CLA	MG-ND	-5.54	1.94	2.05
41	o	309	KC2	C4B-NB	5.54	1.45	1.37
40	X	312	CLA	MG-NA	-5.54	1.93	2.06
40	D	303	CLA	MG-ND	-5.54	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	L	302	KC2	C4B-NB	5.54	1.45	1.37
40	S	301	CLA	MG-ND	-5.54	1.94	2.05
40	F	306	CLA	MG-ND	-5.54	1.94	2.05
40	f	201	CLA	MG-ND	-5.53	1.94	2.05
40	S	314	CLA	MG-ND	-5.53	1.94	2.05
40	z	306	CLA	MG-ND	-5.53	1.94	2.05
40	S	311	CLA	MG-ND	-5.53	1.94	2.05
40	Y	310	CLA	MG-ND	-5.53	1.94	2.05
40	C	307	CLA	MG-ND	-5.53	1.94	2.05
40	J	310	CLA	MG-NB	-5.53	1.94	2.05
40	U	204	CLA	MG-ND	-5.53	1.94	2.05
41	L	303	KC2	C4B-NB	5.53	1.45	1.37
40	b	832	CLA	MG-NA	-5.53	1.93	2.06
40	F	306	CLA	MG-NB	-5.53	1.94	2.05
40	v	306	CLA	MG-NB	-5.53	1.94	2.05
40	a	838	CLA	MG-NB	-5.53	1.94	2.05
40	U	202	CLA	MG-ND	-5.53	1.94	2.05
40	C	301	CLA	MG-NB	-5.53	1.94	2.05
40	T	307	CLA	MG-ND	-5.53	1.94	2.05
40	K	301	CLA	MG-ND	-5.53	1.94	2.05
40	v	313	CLA	MG-ND	-5.53	1.94	2.05
40	C	302	CLA	MG-NB	-5.53	1.94	2.05
40	L	301	CLA	MG-NB	-5.52	1.94	2.05
40	L	301	CLA	MG-ND	-5.52	1.94	2.05
40	x	306	CLA	MG-ND	-5.52	1.94	2.05
40	J	311	CLA	C1B-NB	5.52	1.45	1.37
40	F	304	CLA	MG-NB	-5.52	1.94	2.05
40	a	829	CLA	MG-ND	-5.52	1.94	2.05
40	H	304	CLA	MG-ND	-5.52	1.94	2.05
40	Y	301	CLA	MG-NB	-5.52	1.94	2.05
40	D	301	CLA	MG-ND	-5.52	1.94	2.05
41	L	309	KC2	C4B-NB	5.51	1.45	1.37
40	W	311	CLA	MG-NB	-5.51	1.94	2.05
40	v	307	CLA	MG-ND	-5.51	1.94	2.05
40	S	314	CLA	MG-NB	-5.51	1.94	2.05
40	a	818	CLA	MG-NB	-5.51	1.94	2.05
40	a	850	CLA	C1D-ND	5.51	1.45	1.37
40	H	306	CLA	MG-ND	-5.51	1.94	2.05
40	L	312	CLA	MG-NB	-5.51	1.94	2.05
40	M	311	CLA	MG-ND	-5.51	1.94	2.05
40	j	102	CLA	MG-ND	-5.51	1.94	2.05
40	Q	203	CLA	MG-ND	-5.51	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	o	305	CLA	MG-ND	-5.51	1.94	2.05
41	N	312	KC2	C4B-NB	5.51	1.45	1.37
40	q	307	CLA	MG-NA	-5.51	1.93	2.06
40	D	306	CLA	MG-ND	-5.51	1.94	2.05
40	y	305	CLA	MG-ND	-5.50	1.94	2.05
40	b	801	CLA	C1D-ND	5.50	1.45	1.37
41	v	308	KC2	C4B-NB	5.50	1.45	1.37
40	T	305	CLA	MG-ND	-5.50	1.94	2.05
40	J	305	CLA	MG-NB	-5.50	1.94	2.05
40	Y	313	CLA	C1B-NB	5.50	1.45	1.37
40	b	816	CLA	MG-NA	-5.50	1.93	2.06
41	W	303	KC2	C4B-NB	5.50	1.45	1.37
40	q	307	CLA	MG-ND	-5.50	1.94	2.05
40	o	307	CLA	MG-NA	-5.50	1.93	2.06
40	I	201	CLA	MG-ND	-5.50	1.94	2.05
40	X	310	CLA	MG-ND	-5.50	1.94	2.05
40	v	313	CLA	MG-NB	-5.50	1.94	2.05
40	a	820	CLA	MG-ND	-5.50	1.94	2.05
40	R	307	CLA	MG-ND	-5.50	1.94	2.05
40	U	202	CLA	MG-NA	-5.50	1.93	2.06
40	u	314	CLA	MG-NB	-5.50	1.94	2.05
40	b	808	CLA	MG-NA	-5.50	1.93	2.06
40	S	302	CLA	MG-ND	-5.50	1.94	2.05
40	a	828	CLA	MG-ND	-5.50	1.94	2.05
40	a	837	CLA	MG-ND	-5.50	1.94	2.05
41	L	308	KC2	C4B-NB	5.50	1.45	1.37
41	p	309	KC2	C4B-NB	5.50	1.45	1.37
40	C	309	CLA	MG-ND	-5.49	1.94	2.05
40	W	307	CLA	MG-ND	-5.49	1.94	2.05
40	b	818	CLA	MG-ND	-5.49	1.94	2.05
40	D	302	CLA	MG-NB	-5.49	1.94	2.05
40	X	313	CLA	MG-NA	-5.49	1.93	2.06
40	Q	209	CLA	MG-ND	-5.49	1.94	2.05
40	a	830	CLA	MG-ND	-5.49	1.94	2.05
40	v	307	CLA	MG-NA	-5.49	1.93	2.06
41	P	310	KC2	C4B-NB	5.49	1.45	1.37
40	a	831	CLA	MG-ND	-5.49	1.94	2.05
41	T	301	KC2	C4B-NB	5.49	1.45	1.37
40	L	311	CLA	MG-NB	-5.49	1.94	2.05
40	H	309	CLA	MG-NA	-5.49	1.93	2.06
40	J	307	CLA	MG-NB	-5.49	1.94	2.05
40	K	307	CLA	MG-ND	-5.49	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	x	314	CLA	MG-ND	-5.49	1.94	2.05
41	F	309	KC2	C4B-NB	5.49	1.45	1.37
40	I	207	CLA	MG-ND	-5.48	1.94	2.05
40	D	310	CLA	MG-NB	-5.48	1.94	2.05
40	b	815	CLA	MG-ND	-5.48	1.94	2.05
40	w	303	CLA	MG-ND	-5.48	1.94	2.05
40	J	309	CLA	C1B-NB	5.48	1.45	1.37
40	b	834	CLA	MG-NA	-5.48	1.93	2.06
40	A	311	CLA	MG-ND	-5.48	1.94	2.05
40	o	306	CLA	MG-NB	-5.48	1.94	2.05
40	b	841	CLA	MG-ND	-5.48	1.94	2.05
40	J	318	CLA	MG-ND	-5.48	1.94	2.05
40	Z	306	CLA	MG-NB	-5.48	1.94	2.05
40	b	805	CLA	MG-ND	-5.48	1.94	2.05
40	p	302	CLA	MG-NB	-5.48	1.94	2.05
40	H	311	CLA	MG-NB	-5.48	1.94	2.05
40	R	306	CLA	MG-ND	-5.48	1.94	2.05
41	M	301	KC2	C4B-NB	5.48	1.45	1.37
40	I	205	CLA	MG-ND	-5.48	1.94	2.05
40	W	305	CLA	MG-ND	-5.48	1.94	2.05
40	Z	312	CLA	MG-ND	-5.48	1.94	2.05
41	W	309	KC2	C4B-NB	5.47	1.45	1.37
40	a	834	CLA	MG-NA	-5.47	1.93	2.06
40	z	313	CLA	MG-NA	-5.47	1.93	2.06
41	T	309	KC2	C4B-NB	5.47	1.45	1.37
40	M	305	CLA	MG-NB	-5.47	1.94	2.05
40	Z	301	CLA	MG-ND	-5.47	1.94	2.05
40	a	841	CLA	MG-ND	-5.47	1.94	2.05
40	E	302	CLA	MG-NB	-5.47	1.95	2.05
40	b	835	CLA	MG-ND	-5.47	1.95	2.05
40	C	301	CLA	MG-ND	-5.47	1.95	2.05
40	w	305	CLA	MG-ND	-5.47	1.95	2.05
40	S	308	CLA	MG-NB	-5.46	1.95	2.05
40	y	304	CLA	MG-ND	-5.46	1.95	2.05
40	p	311	CLA	C1B-NB	5.46	1.45	1.37
40	X	305	CLA	MG-NB	-5.46	1.95	2.05
40	b	809	CLA	MG-ND	-5.46	1.95	2.05
40	V	201	CLA	MG-ND	-5.46	1.95	2.05
40	z	324	CLA	MG-NB	-5.46	1.95	2.05
41	I	209	KC2	C4B-NB	5.46	1.45	1.37
40	a	850	CLA	MG-NB	-5.46	1.95	2.05
40	b	802	CLA	MG-ND	-5.46	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	S	305	CLA	MG-NB	-5.46	1.95	2.05
40	y	305	CLA	MG-NB	-5.46	1.95	2.05
41	q	308	KC2	C4B-NB	5.46	1.45	1.37
40	D	312	CLA	MG-ND	-5.46	1.95	2.05
40	F	304	CLA	MG-ND	-5.46	1.95	2.05
40	a	808	CLA	MG-NB	-5.46	1.95	2.05
40	S	311	CLA	C1B-NB	5.46	1.45	1.37
40	C	304	CLA	MG-ND	-5.46	1.95	2.05
40	b	812	CLA	MG-NB	-5.46	1.95	2.05
40	x	313	CLA	MG-NB	-5.46	1.95	2.05
40	a	823	CLA	MG-ND	-5.45	1.95	2.05
40	u	314	CLA	MG-ND	-5.45	1.95	2.05
40	P	312	CLA	MG-ND	-5.45	1.95	2.05
40	Q	209	CLA	MG-NB	-5.45	1.95	2.05
40	S	308	CLA	MG-ND	-5.45	1.95	2.05
40	b	837	CLA	MG-ND	-5.45	1.95	2.05
41	P	309	KC2	C4B-NB	5.45	1.45	1.37
40	F	305	CLA	MG-NA	-5.45	1.93	2.06
40	a	821	CLA	MG-ND	-5.45	1.95	2.05
40	H	310	CLA	MG-ND	-5.45	1.95	2.05
40	b	829	CLA	MG-NB	-5.45	1.95	2.05
40	B	303	CLA	MG-ND	-5.45	1.95	2.05
40	A	305	CLA	MG-ND	-5.45	1.95	2.05
40	a	836	CLA	MG-ND	-5.45	1.95	2.05
40	a	837	CLA	MG-NB	-5.45	1.95	2.05
40	Z	313	CLA	MG-NB	-5.45	1.95	2.05
40	a	833	CLA	MG-ND	-5.45	1.95	2.05
40	b	820	CLA	MG-NB	-5.45	1.95	2.05
40	b	839	CLA	MG-NA	-5.45	1.93	2.06
40	v	313	CLA	MG-NA	-5.45	1.93	2.06
40	u	308	CLA	MG-ND	-5.45	1.95	2.05
40	Y	306	CLA	MG-ND	-5.45	1.95	2.05
40	q	306	CLA	MG-NB	-5.45	1.95	2.05
40	p	307	CLA	C1B-NB	5.45	1.45	1.37
40	F	303	CLA	MG-ND	-5.45	1.95	2.05
40	o	301	CLA	MG-ND	-5.45	1.95	2.05
40	b	817	CLA	MG-NB	-5.44	1.95	2.05
40	S	301	CLA	MG-NA	-5.44	1.93	2.06
40	T	317	CLA	MG-ND	-5.44	1.95	2.05
40	b	839	CLA	MG-NB	-5.44	1.95	2.05
40	p	312	CLA	C1B-NB	5.44	1.45	1.37
40	q	301	CLA	MG-NB	-5.44	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	I	207	CLA	C1B-NB	5.44	1.45	1.37
40	F	301	CLA	MG-ND	-5.44	1.95	2.05
40	a	817	CLA	MG-ND	-5.44	1.95	2.05
40	a	820	CLA	MG-NB	-5.44	1.95	2.05
40	o	310	CLA	MG-ND	-5.44	1.95	2.05
40	b	830	CLA	MG-NA	-5.44	1.93	2.06
40	E	310	CLA	MG-ND	-5.44	1.95	2.05
40	Y	304	CLA	MG-NB	-5.44	1.95	2.05
40	E	303	CLA	MG-NB	-5.44	1.95	2.05
40	z	314	CLA	MG-NB	-5.44	1.95	2.05
40	p	302	CLA	MG-ND	-5.43	1.95	2.05
40	b	807	CLA	C1D-ND	5.43	1.45	1.37
40	A	307	CLA	MG-ND	-5.43	1.95	2.05
40	G	201	CLA	MG-ND	-5.43	1.95	2.05
40	i	101	CLA	MG-NA	-5.43	1.93	2.06
40	b	824	CLA	MG-ND	-5.43	1.95	2.05
40	J	303	CLA	MG-NB	-5.43	1.95	2.05
40	K	306	CLA	MG-ND	-5.43	1.95	2.05
40	F	305	CLA	MG-ND	-5.43	1.95	2.05
40	K	312	CLA	MG-ND	-5.43	1.95	2.05
40	x	312	CLA	MG-ND	-5.43	1.95	2.05
40	t	304	CLA	MG-ND	-5.43	1.95	2.05
40	L	304	CLA	MG-NB	-5.43	1.95	2.05
40	Z	307	CLA	MG-NB	-5.43	1.95	2.05
40	b	803	CLA	MG-NB	-5.43	1.95	2.05
40	a	834	CLA	MG-NB	-5.43	1.95	2.05
40	b	839	CLA	MG-ND	-5.42	1.95	2.05
40	a	813	CLA	MG-NA	-5.42	1.93	2.06
40	E	309	CLA	MG-ND	-5.42	1.95	2.05
40	O	316	CLA	MG-ND	-5.42	1.95	2.05
40	b	820	CLA	MG-ND	-5.42	1.95	2.05
40	M	307	CLA	MG-ND	-5.42	1.95	2.05
40	J	306	CLA	C1B-NB	5.42	1.45	1.37
40	o	301	CLA	MG-NB	-5.42	1.95	2.05
40	z	312	CLA	MG-NB	-5.42	1.95	2.05
40	Q	209	CLA	MG-NA	-5.42	1.93	2.06
40	a	811	CLA	MG-NA	-5.42	1.93	2.06
40	E	313	CLA	MG-ND	-5.42	1.95	2.05
40	H	304	CLA	MG-NB	-5.42	1.95	2.05
40	Q	202	CLA	MG-NB	-5.42	1.95	2.05
40	A	304	CLA	MG-NA	-5.42	1.93	2.06
40	l	204	CLA	MG-ND	-5.42	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	x	308	CLA	MG-NB	-5.42	1.95	2.05
40	U	202	CLA	C1B-NB	5.42	1.45	1.37
40	E	308	CLA	MG-ND	-5.42	1.95	2.05
40	L	311	CLA	MG-NA	-5.42	1.93	2.06
40	E	312	CLA	MG-NA	-5.42	1.93	2.06
40	V	202	CLA	MG-ND	-5.42	1.95	2.05
40	b	842	CLA	MG-NB	-5.41	1.95	2.05
40	D	311	CLA	MG-ND	-5.41	1.95	2.05
40	a	839	CLA	MG-ND	-5.41	1.95	2.05
40	L	305	CLA	MG-NB	-5.41	1.95	2.05
40	B	304	CLA	MG-NA	-5.41	1.93	2.06
40	G	213	CLA	MG-NA	-5.41	1.93	2.06
40	M	310	CLA	MG-ND	-5.41	1.95	2.05
40	l	202	CLA	MG-ND	-5.41	1.95	2.05
40	S	308	CLA	MG-NA	-5.41	1.93	2.06
40	D	306	CLA	MG-NB	-5.41	1.95	2.05
40	w	308	CLA	MG-ND	-5.41	1.95	2.05
41	M	308	KC2	C4B-NB	5.41	1.45	1.37
40	S	313	CLA	MG-ND	-5.41	1.95	2.05
40	t	305	CLA	MG-NB	-5.41	1.95	2.05
40	a	805	CLA	MG-ND	-5.41	1.95	2.05
40	Y	301	CLA	MG-ND	-5.41	1.95	2.05
40	P	313	CLA	MG-ND	-5.41	1.95	2.05
40	Y	311	CLA	MG-ND	-5.41	1.95	2.05
40	J	302	CLA	MG-NB	-5.41	1.95	2.05
40	y	308	CLA	MG-ND	-5.41	1.95	2.05
40	G	207	CLA	MG-NB	-5.41	1.95	2.05
40	X	313	CLA	C1B-NB	5.41	1.45	1.37
40	b	814	CLA	MG-ND	-5.41	1.95	2.05
40	A	308	CLA	MG-ND	-5.40	1.95	2.05
41	z	310	KC2	C4B-NB	5.40	1.45	1.37
40	a	803	CLA	MG-NB	-5.40	1.95	2.05
40	t	305	CLA	MG-ND	-5.40	1.95	2.05
40	U	207	CLA	C1B-NB	5.40	1.45	1.37
40	a	813	CLA	MG-NB	-5.40	1.95	2.05
40	J	303	CLA	C1B-NB	5.40	1.45	1.37
40	w	303	CLA	MG-NB	-5.40	1.95	2.05
40	Z	311	CLA	MG-NB	-5.40	1.95	2.05
40	a	812	CLA	MG-ND	-5.40	1.95	2.05
40	b	823	CLA	MG-ND	-5.40	1.95	2.05
40	Y	312	CLA	C1B-NB	5.40	1.45	1.37
40	z	305	CLA	MG-NB	-5.40	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	a	815	CLA	MG-ND	-5.40	1.95	2.05
40	A	306	CLA	MG-ND	-5.40	1.95	2.05
40	t	309	CLA	MG-ND	-5.40	1.95	2.05
40	R	306	CLA	MG-NB	-5.40	1.95	2.05
40	H	310	CLA	MG-NB	-5.40	1.95	2.05
40	X	312	CLA	MG-ND	-5.40	1.95	2.05
40	a	822	CLA	MG-NB	-5.39	1.95	2.05
40	t	305	CLA	C1B-NB	5.39	1.44	1.37
40	H	311	CLA	MG-ND	-5.39	1.95	2.05
40	O	304	CLA	MG-ND	-5.39	1.95	2.05
40	J	308	CLA	MG-ND	-5.39	1.95	2.05
40	Y	313	CLA	MG-ND	-5.39	1.95	2.05
40	a	838	CLA	MG-NA	-5.39	1.93	2.06
40	M	306	CLA	MG-ND	-5.39	1.95	2.05
40	x	313	CLA	MG-ND	-5.39	1.95	2.05
40	A	306	CLA	MG-NB	-5.39	1.95	2.05
40	b	827	CLA	MG-NB	-5.39	1.95	2.05
40	Y	304	CLA	C1B-NB	5.39	1.44	1.37
40	R	305	CLA	MG-NB	-5.39	1.95	2.05
40	L	307	CLA	MG-ND	-5.39	1.95	2.05
41	o	308	KC2	C4B-NB	5.39	1.44	1.37
40	a	825	CLA	MG-NB	-5.39	1.95	2.05
40	z	307	CLA	MG-NB	-5.39	1.95	2.05
40	Z	306	CLA	C1B-NB	5.39	1.44	1.37
40	b	805	CLA	MG-NA	-5.39	1.93	2.06
40	p	308	CLA	MG-ND	-5.38	1.95	2.05
40	a	809	CLA	MG-NA	-5.38	1.93	2.06
40	P	308	CLA	MG-ND	-5.38	1.95	2.05
40	b	831	CLA	MG-ND	-5.38	1.95	2.05
40	u	307	CLA	MG-NA	-5.38	1.93	2.06
40	C	302	CLA	C1B-NB	5.38	1.44	1.37
40	E	312	CLA	MG-NB	-5.38	1.95	2.05
40	H	307	CLA	MG-NB	-5.38	1.95	2.05
40	o	311	CLA	MG-NB	-5.38	1.95	2.05
40	D	305	CLA	MG-ND	-5.38	1.95	2.05
40	N	305	CLA	MG-NB	-5.38	1.95	2.05
40	T	306	CLA	MG-ND	-5.38	1.95	2.05
40	Z	305	CLA	MG-ND	-5.38	1.95	2.05
40	a	811	CLA	MG-NB	-5.38	1.95	2.05
40	p	312	CLA	MG-ND	-5.38	1.95	2.05
40	z	307	CLA	C1B-NB	5.38	1.44	1.37
40	Z	311	CLA	MG-NA	-5.38	1.93	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	b	828	CLA	MG-NB	-5.37	1.95	2.05
40	E	302	CLA	MG-NA	-5.37	1.93	2.06
40	A	304	CLA	MG-ND	-5.37	1.95	2.05
40	H	306	CLA	MG-NB	-5.37	1.95	2.05
40	b	811	CLA	MG-NB	-5.37	1.95	2.05
40	D	304	CLA	MG-NB	-5.37	1.95	2.05
40	F	308	CLA	MG-NB	-5.37	1.95	2.05
40	I	208	CLA	MG-ND	-5.37	1.95	2.05
41	z	304	KC2	C4B-NB	5.37	1.44	1.37
40	z	324	CLA	MG-NA	-5.37	1.93	2.06
40	X	301	CLA	MG-ND	-5.37	1.95	2.05
40	Q	205	CLA	MG-ND	-5.37	1.95	2.05
40	q	311	CLA	C1B-NB	5.37	1.44	1.37
41	P	302	KC2	C4B-NB	5.37	1.44	1.37
40	b	819	CLA	MG-ND	-5.36	1.95	2.05
41	N	301	KC2	C4B-NB	5.36	1.44	1.37
41	O	303	KC2	C4B-NB	5.36	1.44	1.37
40	D	304	CLA	MG-ND	-5.36	1.95	2.05
40	p	314	CLA	MG-NB	-5.36	1.95	2.05
40	b	806	CLA	MG-ND	-5.36	1.95	2.05
40	Q	206	CLA	MG-ND	-5.36	1.95	2.05
40	v	305	CLA	MG-NB	-5.36	1.95	2.05
40	V	201	CLA	MG-NB	-5.36	1.95	2.05
40	u	306	CLA	MG-NB	-5.36	1.95	2.05
40	F	307	CLA	MG-ND	-5.36	1.95	2.05
40	o	305	CLA	MG-NB	-5.36	1.95	2.05
40	S	312	CLA	MG-NB	-5.35	1.95	2.05
40	J	310	CLA	C1B-NB	5.35	1.44	1.37
40	a	803	CLA	C1D-ND	5.35	1.44	1.37
40	D	311	CLA	MG-NB	-5.35	1.95	2.05
40	z	302	CLA	MG-ND	-5.35	1.95	2.05
40	H	302	CLA	MG-ND	-5.35	1.95	2.05
40	W	313	CLA	MG-ND	-5.35	1.95	2.05
40	P	306	CLA	MG-ND	-5.35	1.95	2.05
40	o	307	CLA	MG-ND	-5.35	1.95	2.05
40	A	309	CLA	MG-ND	-5.35	1.95	2.05
40	W	306	CLA	MG-NB	-5.35	1.95	2.05
40	L	310	CLA	MG-ND	-5.35	1.95	2.05
40	z	324	CLA	MG-ND	-5.35	1.95	2.05
40	D	312	CLA	C1B-NB	5.35	1.44	1.37
41	N	302	KC2	C4B-NB	5.34	1.44	1.37
40	J	311	CLA	MG-ND	-5.34	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	k	201	CLA	C1B-NB	5.34	1.44	1.37
40	T	304	CLA	MG-NB	-5.34	1.95	2.05
40	W	306	CLA	MG-ND	-5.34	1.95	2.05
40	E	303	CLA	C1B-NB	5.34	1.44	1.37
40	b	801	CLA	MG-NB	-5.34	1.95	2.05
40	a	841	CLA	MG-NA	-5.34	1.93	2.06
40	a	852	CLA	MG-ND	-5.34	1.95	2.05
40	k	202	CLA	MG-NB	-5.34	1.95	2.05
40	w	304	CLA	MG-ND	-5.34	1.95	2.05
40	Y	307	CLA	C1B-NB	5.34	1.44	1.37
41	w	306	KC2	C4B-NB	5.34	1.44	1.37
40	U	203	CLA	MG-NA	-5.34	1.93	2.06
40	C	305	CLA	C1B-NB	5.33	1.44	1.37
40	o	311	CLA	C1B-NB	5.33	1.44	1.37
40	A	309	CLA	MG-NB	-5.33	1.95	2.05
40	N	311	CLA	MG-NB	-5.33	1.95	2.05
40	R	304	CLA	MG-ND	-5.33	1.95	2.05
40	u	314	CLA	C1B-NB	5.33	1.44	1.37
40	f	204	CLA	MG-ND	-5.33	1.95	2.05
40	y	303	CLA	MG-NB	-5.33	1.95	2.05
40	Q	203	CLA	MG-NA	-5.33	1.93	2.06
40	H	307	CLA	MG-ND	-5.33	1.95	2.05
40	A	302	CLA	MG-ND	-5.33	1.95	2.05
40	b	808	CLA	MG-NB	-5.33	1.95	2.05
40	L	305	CLA	C1B-NB	5.33	1.44	1.37
40	S	301	CLA	MG-NB	-5.33	1.95	2.05
40	F	307	CLA	MG-NB	-5.33	1.95	2.05
40	O	307	CLA	MG-NB	-5.33	1.95	2.05
40	b	821	CLA	MG-NB	-5.33	1.95	2.05
40	B	301	CLA	C1B-NB	5.33	1.44	1.37
40	F	311	CLA	C1B-NB	5.32	1.44	1.37
40	t	309	CLA	C1B-NB	5.32	1.44	1.37
40	a	827	CLA	MG-NB	-5.32	1.95	2.05
40	y	303	CLA	C1B-NB	5.32	1.44	1.37
40	S	306	CLA	MG-ND	-5.32	1.95	2.05
40	u	313	CLA	MG-NB	-5.32	1.95	2.05
40	R	310	CLA	MG-NA	-5.32	1.93	2.06
40	S	319	CLA	MG-ND	-5.32	1.95	2.05
40	L	301	CLA	C1B-NB	5.32	1.44	1.37
40	a	809	CLA	MG-NB	-5.32	1.95	2.05
40	H	311	CLA	C1B-NB	5.32	1.44	1.37
40	l	204	CLA	MG-NB	-5.32	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	q	310	CLA	MG-NB	-5.32	1.95	2.05
40	C	306	CLA	MG-NB	-5.32	1.95	2.05
40	u	312	CLA	MG-ND	-5.32	1.95	2.05
40	x	302	CLA	MG-NA	-5.32	1.93	2.06
40	F	308	CLA	C1B-NB	5.32	1.44	1.37
40	v	311	CLA	C1B-NB	5.32	1.44	1.37
40	P	306	CLA	MG-NB	-5.32	1.95	2.05
40	J	308	CLA	C1B-NB	5.31	1.44	1.37
40	q	313	CLA	C1B-NB	5.31	1.44	1.37
40	o	312	CLA	MG-NA	-5.31	1.93	2.06
40	H	301	CLA	MG-NB	-5.31	1.95	2.05
40	E	302	CLA	C1B-NB	5.31	1.44	1.37
40	B	301	CLA	MG-ND	-5.31	1.95	2.05
40	X	312	CLA	C1B-NB	5.31	1.44	1.37
40	a	815	CLA	C1B-NB	5.31	1.44	1.37
41	v	309	KC2	C4B-NB	5.31	1.44	1.37
40	w	303	CLA	C1B-NB	5.31	1.44	1.37
40	l	203	CLA	MG-NA	-5.31	1.93	2.06
40	a	851	CLA	MG-ND	-5.31	1.95	2.05
40	D	307	CLA	MG-ND	-5.31	1.95	2.05
40	k	201	CLA	MG-ND	-5.31	1.95	2.05
40	b	828	CLA	C1B-NB	5.31	1.44	1.37
40	P	307	CLA	MG-NB	-5.31	1.95	2.05
40	C	309	CLA	MG-NA	-5.31	1.93	2.06
40	J	309	CLA	MG-ND	-5.30	1.95	2.05
40	Y	307	CLA	MG-ND	-5.30	1.95	2.05
40	a	827	CLA	MG-ND	-5.30	1.95	2.05
40	Q	204	CLA	MG-ND	-5.30	1.95	2.05
40	Z	313	CLA	C1B-NB	5.30	1.44	1.37
40	S	312	CLA	C1B-NB	5.30	1.44	1.37
40	X	307	CLA	MG-NA	-5.30	1.93	2.06
40	D	308	CLA	MG-ND	-5.30	1.95	2.05
40	E	313	CLA	C1B-NB	5.30	1.44	1.37
40	a	804	CLA	MG-ND	-5.30	1.95	2.05
40	J	311	CLA	MG-NA	-5.30	1.93	2.06
41	K	303	KC2	C4B-NB	5.30	1.44	1.37
41	x	310	KC2	C4B-NB	5.30	1.44	1.37
41	X	303	KC2	C4B-NB	5.30	1.44	1.37
40	C	302	CLA	MG-NA	-5.30	1.93	2.06
40	G	205	CLA	MG-NB	-5.30	1.95	2.05
40	H	305	CLA	MG-NB	-5.30	1.95	2.05
40	b	805	CLA	MG-NB	-5.30	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	u	310	KC2	C4B-NB	5.30	1.44	1.37
40	L	310	CLA	MG-NB	-5.30	1.95	2.05
41	q	309	KC2	C4B-NB	5.30	1.44	1.37
41	t	306	KC2	C4B-NB	5.30	1.44	1.37
40	E	311	CLA	MG-ND	-5.30	1.95	2.05
40	q	313	CLA	MG-ND	-5.30	1.95	2.05
40	a	824	CLA	MG-NB	-5.29	1.95	2.05
40	u	313	CLA	MG-ND	-5.29	1.95	2.05
40	S	307	CLA	MG-NB	-5.29	1.95	2.05
40	v	310	CLA	MG-NB	-5.29	1.95	2.05
40	q	305	CLA	MG-NB	-5.29	1.95	2.05
40	S	314	CLA	MG-NA	-5.29	1.93	2.06
40	E	306	CLA	MG-NB	-5.29	1.95	2.05
40	a	820	CLA	MG-NA	-5.29	1.93	2.06
40	Y	307	CLA	MG-NA	-5.29	1.93	2.06
40	M	312	CLA	MG-ND	-5.29	1.95	2.05
40	b	807	CLA	MG-NB	-5.29	1.95	2.05
40	z	308	CLA	MG-ND	-5.29	1.95	2.05
40	a	806	CLA	MG-ND	-5.29	1.95	2.05
40	p	307	CLA	MG-NA	-5.29	1.93	2.06
40	v	301	CLA	MG-NA	-5.29	1.93	2.06
40	b	836	CLA	MG-ND	-5.29	1.95	2.05
40	l	202	CLA	MG-NB	-5.29	1.95	2.05
40	Y	306	CLA	C1B-NB	5.29	1.44	1.37
40	p	308	CLA	C1B-NB	5.29	1.44	1.37
40	v	313	CLA	C1B-NB	5.29	1.44	1.37
40	U	205	CLA	MG-NA	-5.29	1.93	2.06
40	U	204	CLA	C1B-NB	5.29	1.44	1.37
40	o	312	CLA	C1B-NB	5.29	1.44	1.37
40	Z	307	CLA	MG-NA	-5.29	1.93	2.06
40	b	827	CLA	MG-NA	-5.29	1.93	2.06
40	z	313	CLA	C1B-NB	5.28	1.44	1.37
40	U	205	CLA	C1B-NB	5.28	1.44	1.37
40	T	310	CLA	MG-NA	-5.28	1.93	2.06
40	N	305	CLA	MG-ND	-5.28	1.95	2.05
40	v	312	CLA	MG-ND	-5.28	1.95	2.05
41	y	306	KC2	C4B-NB	5.28	1.44	1.37
40	C	301	CLA	MG-NA	-5.28	1.93	2.06
40	F	308	CLA	MG-NA	-5.28	1.93	2.06
40	E	307	CLA	MG-ND	-5.28	1.95	2.05
40	L	310	CLA	C1B-NB	5.28	1.44	1.37
40	L	311	CLA	C1B-NB	5.28	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	O	307	CLA	C1B-NB	5.28	1.44	1.37
40	E	311	CLA	MG-NA	-5.28	1.93	2.06
40	O	316	CLA	MG-NB	-5.28	1.95	2.05
40	Y	306	CLA	MG-NB	-5.28	1.95	2.05
40	H	302	CLA	C1B-NB	5.28	1.44	1.37
40	I	208	CLA	C1B-NB	5.28	1.44	1.37
40	G	203	CLA	MG-ND	-5.28	1.95	2.05
40	b	829	CLA	MG-NA	-5.28	1.93	2.06
40	a	841	CLA	MG-NB	-5.27	1.95	2.05
40	b	806	CLA	MG-NB	-5.27	1.95	2.05
40	Y	311	CLA	MG-NB	-5.27	1.95	2.05
40	C	306	CLA	MG-ND	-5.27	1.95	2.05
40	N	310	CLA	MG-NB	-5.27	1.95	2.05
40	b	825	CLA	MG-NA	-5.27	1.93	2.06
40	X	301	CLA	MG-NB	-5.27	1.95	2.05
40	M	312	CLA	C1B-NB	5.27	1.44	1.37
41	Z	308	KC2	C4B-NB	5.27	1.44	1.37
40	T	307	CLA	MG-NB	-5.27	1.95	2.05
40	D	312	CLA	MG-NB	-5.27	1.95	2.05
40	Q	205	CLA	MG-NB	-5.27	1.95	2.05
40	a	815	CLA	MG-NB	-5.27	1.95	2.05
40	O	306	CLA	MG-ND	-5.27	1.95	2.05
40	M	304	CLA	MG-NB	-5.27	1.95	2.05
40	a	829	CLA	MG-NB	-5.27	1.95	2.05
40	E	303	CLA	MG-NA	-5.27	1.93	2.06
40	A	305	CLA	MG-NB	-5.27	1.95	2.05
40	G	201	CLA	MG-NB	-5.27	1.95	2.05
40	t	303	CLA	MG-NB	-5.27	1.95	2.05
40	A	302	CLA	MG-NB	-5.27	1.95	2.05
41	o	303	KC2	C4B-NB	5.27	1.44	1.37
40	H	304	CLA	C1B-NB	5.27	1.44	1.37
40	w	305	CLA	C1B-NB	5.27	1.44	1.37
40	N	311	CLA	MG-NA	-5.26	1.93	2.06
40	B	307	CLA	C1D-ND	5.26	1.44	1.37
40	a	814	CLA	MG-NB	-5.26	1.95	2.05
40	b	822	CLA	MG-NB	-5.26	1.95	2.05
40	J	306	CLA	MG-NB	-5.26	1.95	2.05
40	S	302	CLA	MG-NB	-5.26	1.95	2.05
40	a	804	CLA	C1B-NB	5.26	1.44	1.37
40	a	807	CLA	MG-NB	-5.26	1.95	2.05
40	L	301	CLA	MG-NA	-5.26	1.93	2.06
40	R	310	CLA	MG-NB	-5.26	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	I	206	CLA	MG-ND	-5.26	1.95	2.05
40	b	824	CLA	MG-NA	-5.26	1.93	2.06
40	Q	202	CLA	MG-NA	-5.26	1.93	2.06
40	K	307	CLA	MG-NB	-5.25	1.95	2.05
40	b	830	CLA	MG-NB	-5.25	1.95	2.05
40	o	313	CLA	MG-NB	-5.25	1.95	2.05
40	T	307	CLA	C1B-NB	5.25	1.44	1.37
41	Z	303	KC2	C4B-NB	5.25	1.44	1.37
40	y	304	CLA	MG-NB	-5.25	1.95	2.05
40	U	207	CLA	MG-NA	-5.25	1.93	2.06
40	u	305	CLA	MG-NA	-5.25	1.93	2.06
40	G	206	CLA	MG-ND	-5.25	1.95	2.05
41	G	208	KC2	C4B-NB	5.25	1.44	1.37
40	Y	310	CLA	MG-NB	-5.25	1.95	2.05
40	o	301	CLA	C1B-NB	5.25	1.44	1.37
40	a	814	CLA	MG-NA	-5.25	1.93	2.06
40	a	819	CLA	MG-ND	-5.25	1.95	2.05
40	b	818	CLA	C1B-NB	5.25	1.44	1.37
40	D	309	CLA	MG-ND	-5.25	1.95	2.05
40	Z	301	CLA	MG-NB	-5.25	1.95	2.05
41	O	301	KC2	C4B-NB	5.25	1.44	1.37
40	F	305	CLA	C1B-NB	5.25	1.44	1.37
40	y	305	CLA	C1B-NB	5.25	1.44	1.37
40	D	305	CLA	C1B-NB	5.25	1.44	1.37
40	x	314	CLA	MG-NA	-5.25	1.93	2.06
40	q	313	CLA	MG-NB	-5.25	1.95	2.05
40	U	207	CLA	MG-NB	-5.25	1.95	2.05
41	W	302	KC2	C4B-NB	5.25	1.44	1.37
40	E	307	CLA	MG-NB	-5.24	1.95	2.05
40	J	311	CLA	MG-NB	-5.24	1.95	2.05
40	u	308	CLA	MG-NB	-5.24	1.95	2.05
40	a	837	CLA	C1B-NB	5.24	1.44	1.37
40	D	302	CLA	MG-ND	-5.24	1.95	2.05
40	V	202	CLA	MG-NA	-5.24	1.93	2.06
40	x	307	CLA	MG-NA	-5.24	1.93	2.06
40	j	102	CLA	C1B-NB	5.24	1.44	1.37
40	t	309	CLA	MG-NB	-5.24	1.95	2.05
40	k	202	CLA	MG-NA	-5.24	1.93	2.06
40	a	819	CLA	C1B-NB	5.24	1.44	1.37
40	G	204	CLA	MG-NB	-5.24	1.95	2.05
40	S	301	CLA	C1B-NB	5.24	1.44	1.37
40	C	305	CLA	MG-NB	-5.23	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	t	302	CLA	MG-NB	-5.23	1.95	2.05
40	a	831	CLA	MG-NB	-5.23	1.95	2.05
40	T	310	CLA	MG-NB	-5.23	1.95	2.05
40	a	806	CLA	MG-NA	-5.23	1.93	2.06
40	a	804	CLA	MG-NA	-5.23	1.93	2.06
40	E	308	CLA	MG-NB	-5.23	1.95	2.05
40	x	314	CLA	MG-NB	-5.23	1.95	2.05
40	F	308	CLA	MG-ND	-5.23	1.95	2.05
40	C	301	CLA	C1B-NB	5.23	1.44	1.37
40	y	309	CLA	MG-NA	-5.23	1.93	2.06
40	F	310	CLA	MG-NB	-5.23	1.95	2.05
40	w	304	CLA	MG-NB	-5.23	1.95	2.05
40	t	303	CLA	C1B-NB	5.23	1.44	1.37
40	H	310	CLA	C1B-NB	5.22	1.44	1.37
40	y	308	CLA	C1B-NB	5.22	1.44	1.37
40	F	321	CLA	MG-NB	-5.22	1.95	2.05
40	o	305	CLA	MG-NA	-5.22	1.93	2.06
40	C	308	CLA	C1B-NB	5.22	1.44	1.37
40	w	308	CLA	C1B-NB	5.22	1.44	1.37
40	H	304	CLA	MG-NA	-5.22	1.93	2.06
40	F	311	CLA	MG-ND	-5.22	1.95	2.05
40	L	312	CLA	C1B-NB	5.22	1.44	1.37
40	a	810	CLA	C1B-NB	5.22	1.44	1.37
40	a	852	CLA	C1B-NB	5.22	1.44	1.37
40	q	312	CLA	MG-NB	-5.22	1.95	2.05
40	u	305	CLA	MG-NB	-5.22	1.95	2.05
40	J	303	CLA	MG-NA	-5.22	1.93	2.06
40	X	305	CLA	MG-NA	-5.22	1.93	2.06
40	x	307	CLA	C1B-NB	5.22	1.44	1.37
40	a	806	CLA	MG-NB	-5.22	1.95	2.05
40	b	840	CLA	MG-NA	-5.22	1.93	2.06
40	q	301	CLA	MG-NA	-5.22	1.93	2.06
40	i	101	CLA	C1B-NB	5.22	1.44	1.37
40	t	309	CLA	MG-NA	-5.22	1.93	2.06
40	C	309	CLA	C1B-NB	5.22	1.44	1.37
40	N	306	CLA	MG-NB	-5.21	1.95	2.05
40	b	836	CLA	MG-NA	-5.21	1.93	2.06
40	I	201	CLA	MG-NB	-5.21	1.95	2.05
40	b	815	CLA	C1B-NB	5.21	1.44	1.37
40	Z	311	CLA	C1B-NB	5.21	1.44	1.37
40	F	301	CLA	C1B-NB	5.21	1.44	1.37
40	F	301	CLA	MG-NB	-5.21	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	a	829	CLA	MG-NA	-5.21	1.93	2.06
40	J	312	CLA	C1B-NB	5.21	1.44	1.37
40	a	814	CLA	MG-ND	-5.21	1.95	2.05
40	L	304	CLA	MG-NA	-5.21	1.93	2.06
40	w	305	CLA	MG-NB	-5.21	1.95	2.05
40	a	814	CLA	C1B-NB	5.21	1.44	1.37
40	p	314	CLA	C1B-NB	5.20	1.44	1.37
40	U	204	CLA	MG-NB	-5.20	1.95	2.05
40	U	206	CLA	MG-NB	-5.20	1.95	2.05
40	a	851	CLA	MG-NA	-5.20	1.93	2.06
40	X	307	CLA	MG-ND	-5.20	1.95	2.05
40	a	810	CLA	MG-ND	-5.20	1.95	2.05
40	C	304	CLA	MG-NA	-5.20	1.93	2.06
40	R	316	CLA	MG-NB	-5.20	1.95	2.05
40	Q	209	CLA	C1B-NB	5.20	1.44	1.37
40	E	305	CLA	MG-NA	-5.20	1.93	2.06
40	a	823	CLA	C1B-NB	5.20	1.44	1.37
40	b	825	CLA	MG-NB	-5.20	1.95	2.05
40	a	831	CLA	C1B-NB	5.20	1.44	1.37
40	t	304	CLA	MG-NB	-5.20	1.95	2.05
40	N	307	CLA	MG-ND	-5.20	1.95	2.05
40	Y	305	CLA	MG-ND	-5.20	1.95	2.05
40	a	816	CLA	MG-NB	-5.20	1.95	2.05
40	z	306	CLA	MG-NB	-5.19	1.95	2.05
40	I	202	CLA	C1B-NB	5.19	1.44	1.37
40	I	207	CLA	MG-NB	-5.19	1.95	2.05
40	X	310	CLA	C1B-NB	5.19	1.44	1.37
40	W	308	CLA	C1B-NB	5.19	1.44	1.37
40	D	301	CLA	MG-NB	-5.19	1.95	2.05
40	u	312	CLA	C1B-NB	5.19	1.44	1.37
40	b	828	CLA	MG-NA	-5.19	1.93	2.06
40	I	205	CLA	MG-NB	-5.19	1.95	2.05
40	A	309	CLA	C1B-NB	5.19	1.44	1.37
40	X	313	CLA	MG-ND	-5.19	1.95	2.05
40	I	202	CLA	MG-ND	-5.19	1.95	2.05
40	D	304	CLA	C1B-NB	5.19	1.44	1.37
40	D	309	CLA	C1B-NB	5.19	1.44	1.37
40	a	833	CLA	C1B-NB	5.19	1.44	1.37
40	t	302	CLA	MG-NA	-5.19	1.93	2.06
40	H	308	CLA	MG-ND	-5.19	1.95	2.05
40	J	302	CLA	C1B-NB	5.19	1.44	1.37
41	X	309	KC2	C4B-NB	5.19	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	R	307	CLA	MG-NB	-5.18	1.95	2.05
40	X	301	CLA	C1B-NB	5.18	1.44	1.37
40	I	207	CLA	MG-NA	-5.18	1.94	2.06
41	u	309	KC2	C4B-NB	5.18	1.44	1.37
41	X	308	KC2	C4B-NB	5.18	1.44	1.37
40	I	201	CLA	C1B-NB	5.18	1.44	1.37
40	a	817	CLA	C1B-NB	5.18	1.44	1.37
40	B	303	CLA	C1B-NB	5.18	1.44	1.37
40	o	313	CLA	MG-ND	-5.18	1.95	2.05
40	x	314	CLA	C1B-NB	5.18	1.44	1.37
40	b	837	CLA	MG-NA	-5.18	1.94	2.06
40	O	306	CLA	MG-NB	-5.18	1.95	2.05
40	P	305	CLA	MG-NB	-5.18	1.95	2.05
40	W	305	CLA	MG-NA	-5.18	1.94	2.06
40	z	312	CLA	C1B-NB	5.18	1.44	1.37
40	G	205	CLA	MG-ND	-5.17	1.95	2.05
40	U	206	CLA	C1B-NB	5.17	1.44	1.37
40	X	311	CLA	MG-NA	-5.17	1.94	2.06
40	Q	207	CLA	C1B-NB	5.17	1.44	1.37
40	u	305	CLA	C1B-NB	5.17	1.44	1.37
40	O	306	CLA	MG-NA	-5.17	1.94	2.06
40	X	307	CLA	MG-NB	-5.17	1.95	2.05
40	a	830	CLA	C1B-NB	5.17	1.44	1.37
40	v	312	CLA	MG-NB	-5.17	1.95	2.05
40	a	823	CLA	MG-NB	-5.17	1.95	2.05
40	W	313	CLA	MG-NB	-5.17	1.95	2.05
40	T	304	CLA	C1B-NB	5.17	1.44	1.37
40	l	202	CLA	C1B-NB	5.17	1.44	1.37
40	p	306	CLA	MG-NB	-5.16	1.95	2.05
40	Y	304	CLA	MG-NA	-5.16	1.94	2.06
40	V	202	CLA	MG-NB	-5.16	1.95	2.05
40	p	302	CLA	C1B-NB	5.16	1.44	1.37
40	y	302	CLA	C1B-NB	5.16	1.44	1.37
40	J	305	CLA	MG-NA	-5.16	1.94	2.06
40	a	815	CLA	MG-NA	-5.16	1.94	2.06
40	E	312	CLA	C1B-NB	5.16	1.44	1.37
40	U	203	CLA	C1B-NB	5.16	1.44	1.37
40	H	308	CLA	C1B-NB	5.16	1.44	1.37
40	t	307	CLA	MG-NA	-5.16	1.94	2.06
40	v	307	CLA	MG-NB	-5.16	1.95	2.05
40	A	303	CLA	MG-NB	-5.16	1.95	2.05
40	D	308	CLA	MG-NB	-5.16	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	P	313	CLA	MG-NB	-5.16	1.95	2.05
40	A	308	CLA	MG-NB	-5.16	1.95	2.05
40	X	306	CLA	MG-NA	-5.16	1.94	2.06
40	a	850	CLA	MG-NA	-5.15	1.94	2.06
40	T	306	CLA	MG-NB	-5.15	1.95	2.05
40	u	311	CLA	C1B-NB	5.15	1.44	1.37
40	D	302	CLA	MG-NA	-5.15	1.94	2.06
40	A	302	CLA	C1B-NB	5.15	1.44	1.37
41	N	309	KC2	C4B-NB	5.15	1.44	1.37
40	W	307	CLA	MG-NB	-5.15	1.95	2.05
40	W	313	CLA	C1B-NB	5.15	1.44	1.37
40	D	309	CLA	MG-NA	-5.15	1.94	2.06
40	b	840	CLA	C1B-NB	5.15	1.44	1.37
40	o	306	CLA	C1B-NB	5.15	1.44	1.37
40	A	307	CLA	C1B-NB	5.15	1.44	1.37
40	z	302	CLA	MG-NB	-5.15	1.95	2.05
40	D	308	CLA	C1B-NB	5.15	1.44	1.37
40	w	302	CLA	C1B-NB	5.15	1.44	1.37
40	J	305	CLA	C1B-NB	5.15	1.44	1.37
40	a	820	CLA	C1B-NB	5.15	1.44	1.37
40	b	838	CLA	MG-NA	-5.14	1.94	2.06
40	o	307	CLA	C1B-NB	5.14	1.44	1.37
40	b	815	CLA	MG-NB	-5.14	1.95	2.05
40	f	202	CLA	MG-NB	-5.14	1.95	2.05
40	E	310	CLA	C1B-NB	5.14	1.44	1.37
40	S	313	CLA	C1B-NB	5.14	1.44	1.37
40	p	306	CLA	C1B-NB	5.14	1.44	1.37
40	W	305	CLA	MG-NB	-5.14	1.95	2.05
40	Z	301	CLA	C1B-NB	5.14	1.44	1.37
40	M	307	CLA	MG-NB	-5.14	1.95	2.05
40	u	312	CLA	MG-NB	-5.14	1.95	2.05
40	b	802	CLA	MG-NA	-5.13	1.94	2.06
40	J	318	CLA	C1B-NB	5.13	1.44	1.37
40	b	810	CLA	MG-NB	-5.13	1.95	2.05
40	G	203	CLA	MG-NA	-5.13	1.94	2.06
40	T	304	CLA	MG-NA	-5.13	1.94	2.06
40	b	819	CLA	MG-NB	-5.13	1.95	2.05
40	W	306	CLA	C1B-NB	5.13	1.44	1.37
40	q	305	CLA	MG-NA	-5.13	1.94	2.06
40	D	309	CLA	MG-NB	-5.13	1.95	2.05
40	R	304	CLA	C1B-NB	5.13	1.44	1.37
40	T	317	CLA	C1B-NB	5.13	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	P	306	CLA	C1B-NB	5.13	1.44	1.37
40	q	307	CLA	C1B-NB	5.13	1.44	1.37
40	N	304	CLA	C1B-NB	5.13	1.44	1.37
40	B	306	CLA	C1B-NB	5.13	1.44	1.37
40	E	311	CLA	C1B-NB	5.13	1.44	1.37
40	O	304	CLA	C1B-NB	5.13	1.44	1.37
40	a	809	CLA	C1B-NB	5.13	1.44	1.37
40	A	307	CLA	MG-NA	-5.12	1.94	2.06
40	L	312	CLA	MG-NA	-5.12	1.94	2.06
40	o	304	CLA	MG-NB	-5.12	1.95	2.05
40	b	801	CLA	C1B-NB	5.12	1.44	1.37
40	x	312	CLA	C1B-NB	5.12	1.44	1.37
40	G	203	CLA	MG-NB	-5.12	1.95	2.05
40	a	807	CLA	C1B-NB	5.12	1.44	1.37
40	u	308	CLA	C1B-NB	5.12	1.44	1.37
40	H	311	CLA	MG-NA	-5.12	1.94	2.06
40	H	301	CLA	C1B-NB	5.12	1.44	1.37
40	K	304	CLA	MG-NA	-5.12	1.94	2.06
40	C	304	CLA	C1B-NB	5.12	1.44	1.37
40	G	205	CLA	C1B-NB	5.12	1.44	1.37
40	t	307	CLA	C1B-NB	5.12	1.44	1.37
40	z	311	CLA	C1B-NB	5.12	1.44	1.37
40	y	304	CLA	C1B-NB	5.12	1.44	1.37
40	p	312	CLA	MG-NB	-5.11	1.95	2.05
40	F	304	CLA	C1B-NB	5.11	1.44	1.37
40	b	832	CLA	C1B-NB	5.11	1.44	1.37
40	B	304	CLA	C1B-NB	5.11	1.44	1.37
40	E	310	CLA	MG-NB	-5.11	1.95	2.05
40	a	821	CLA	MG-NB	-5.11	1.95	2.05
40	I	206	CLA	C1B-NB	5.11	1.44	1.37
40	P	312	CLA	C1B-NB	5.11	1.44	1.37
40	v	305	CLA	MG-NA	-5.11	1.94	2.06
40	o	311	CLA	MG-NA	-5.11	1.94	2.06
40	b	818	CLA	MG-NB	-5.11	1.95	2.05
40	z	314	CLA	C1B-NB	5.11	1.44	1.37
40	X	304	CLA	MG-NA	-5.11	1.94	2.06
40	a	819	CLA	MG-NB	-5.11	1.95	2.05
40	E	308	CLA	MG-NA	-5.11	1.94	2.06
40	S	319	CLA	C1B-NB	5.11	1.44	1.37
40	Q	203	CLA	C1B-NB	5.11	1.44	1.37
40	b	819	CLA	C1B-NB	5.11	1.44	1.37
40	q	301	CLA	C1B-NB	5.11	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	P	308	CLA	C1B-NB	5.10	1.44	1.37
40	a	838	CLA	C1B-NB	5.10	1.44	1.37
40	f	201	CLA	C1B-NB	5.10	1.44	1.37
41	z	309	KC2	C4B-NB	5.10	1.44	1.37
40	u	306	CLA	C1B-NB	5.10	1.44	1.37
40	R	304	CLA	MG-NA	-5.10	1.94	2.06
40	Y	305	CLA	C1B-NB	5.10	1.44	1.37
40	a	852	CLA	MG-NB	-5.10	1.95	2.05
40	b	829	CLA	C1B-NB	5.10	1.44	1.37
40	V	201	CLA	C1B-NB	5.10	1.44	1.37
40	Y	311	CLA	C1B-NB	5.10	1.44	1.37
41	x	304	KC2	C4B-NB	5.10	1.44	1.37
40	b	823	CLA	MG-NB	-5.10	1.95	2.05
40	p	308	CLA	MG-NB	-5.10	1.95	2.05
40	a	839	CLA	C1B-NB	5.10	1.44	1.37
40	E	309	CLA	MG-NB	-5.10	1.95	2.05
40	Q	204	CLA	MG-NA	-5.10	1.94	2.06
40	v	307	CLA	C1B-NB	5.10	1.44	1.37
40	A	301	CLA	MG-NA	-5.10	1.94	2.06
40	w	309	CLA	MG-NA	-5.10	1.94	2.06
40	A	308	CLA	C1B-NB	5.10	1.44	1.37
40	X	307	CLA	C1B-NB	5.10	1.44	1.37
40	F	311	CLA	MG-NB	-5.10	1.95	2.05
40	v	304	CLA	MG-NB	-5.09	1.95	2.05
40	K	301	CLA	MG-NB	-5.09	1.95	2.05
40	S	305	CLA	C1B-NB	5.09	1.44	1.37
40	S	308	CLA	C1B-NB	5.09	1.44	1.37
40	I	204	CLA	MG-NB	-5.09	1.95	2.05
40	f	204	CLA	C1B-NB	5.09	1.44	1.37
40	L	307	CLA	C1B-NB	5.09	1.44	1.37
40	x	306	CLA	MG-NA	-5.09	1.94	2.06
40	b	836	CLA	C1B-NB	5.09	1.44	1.37
40	w	304	CLA	C1B-NB	5.09	1.44	1.37
40	A	305	CLA	C1B-NB	5.09	1.44	1.37
40	W	313	CLA	MG-NA	-5.09	1.94	2.06
40	H	309	CLA	C1B-NB	5.09	1.44	1.37
40	X	313	CLA	MG-NB	-5.09	1.95	2.05
40	q	311	CLA	MG-NA	-5.09	1.94	2.06
40	M	306	CLA	MG-NB	-5.09	1.95	2.05
40	K	301	CLA	C1B-NB	5.09	1.44	1.37
40	W	311	CLA	C1B-NB	5.08	1.44	1.37
40	o	310	CLA	C1B-NB	5.08	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	Q	202	CLA	C1B-NB	5.08	1.44	1.37
40	a	834	CLA	C1B-NB	5.08	1.44	1.37
40	z	306	CLA	MG-NA	-5.08	1.94	2.06
40	N	305	CLA	MG-NA	-5.08	1.94	2.06
40	C	304	CLA	MG-NB	-5.08	1.95	2.05
40	F	301	CLA	MG-NA	-5.08	1.94	2.06
41	u	304	KC2	C4B-NB	5.08	1.44	1.37
40	z	305	CLA	MG-NA	-5.08	1.94	2.06
40	v	306	CLA	C1B-NB	5.08	1.44	1.37
40	a	840	CLA	MG-NB	-5.08	1.95	2.05
40	N	307	CLA	C1B-NB	5.08	1.44	1.37
40	W	305	CLA	C1B-NB	5.08	1.44	1.37
40	D	307	CLA	MG-NB	-5.08	1.95	2.05
40	F	321	CLA	MG-NA	-5.08	1.94	2.06
40	P	312	CLA	MG-NB	-5.08	1.95	2.05
40	B	303	CLA	MG-NB	-5.08	1.95	2.05
41	H	316	KC2	C4B-NB	5.08	1.44	1.37
40	F	307	CLA	MG-NA	-5.08	1.94	2.06
40	J	309	CLA	MG-NB	-5.07	1.95	2.05
40	q	307	CLA	MG-NB	-5.07	1.95	2.05
40	w	302	CLA	MG-NB	-5.07	1.95	2.05
48	P	320	A1EB4	C32-C31	-5.07	1.46	1.54
40	A	306	CLA	C1B-NB	5.07	1.44	1.37
40	D	304	CLA	MG-NA	-5.07	1.94	2.06
40	a	807	CLA	MG-NA	-5.07	1.94	2.06
40	F	305	CLA	MG-NB	-5.07	1.95	2.05
40	K	306	CLA	MG-NB	-5.07	1.95	2.05
40	R	307	CLA	MG-NA	-5.07	1.94	2.06
40	Z	304	CLA	MG-NA	-5.07	1.94	2.06
40	a	833	CLA	MG-NA	-5.07	1.94	2.06
40	Y	307	CLA	MG-NB	-5.07	1.95	2.05
40	K	312	CLA	C1B-NB	5.07	1.44	1.37
40	b	806	CLA	C1B-NB	5.07	1.44	1.37
40	u	307	CLA	C1B-NB	5.07	1.44	1.37
40	b	822	CLA	C1B-NB	5.07	1.44	1.37
40	q	312	CLA	C1B-NB	5.07	1.44	1.37
40	b	820	CLA	C1B-NB	5.07	1.44	1.37
40	x	311	CLA	C1B-NB	5.07	1.44	1.37
40	R	310	CLA	C1B-NB	5.07	1.44	1.37
41	N	303	KC2	C4B-NB	5.07	1.44	1.37
40	E	310	CLA	MG-NA	-5.07	1.94	2.06
40	A	305	CLA	MG-NA	-5.06	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	p	308	CLA	MG-NA	-5.06	1.94	2.06
40	v	312	CLA	C1B-NB	5.06	1.44	1.37
40	N	304	CLA	MG-NA	-5.06	1.94	2.06
40	P	307	CLA	C1B-NB	5.06	1.44	1.37
40	o	307	CLA	MG-NB	-5.06	1.95	2.05
40	S	314	CLA	C1B-NB	5.06	1.44	1.37
40	x	306	CLA	MG-NB	-5.06	1.95	2.05
40	p	302	CLA	MG-NA	-5.06	1.94	2.06
40	D	307	CLA	C1B-NB	5.06	1.44	1.37
40	X	306	CLA	C1B-NB	5.06	1.44	1.37
40	q	304	CLA	MG-NB	-5.06	1.95	2.05
40	G	204	CLA	C1B-NB	5.06	1.44	1.37
40	D	303	CLA	C1B-NB	5.06	1.44	1.37
40	q	306	CLA	C1B-NB	5.06	1.44	1.37
40	X	311	CLA	C1B-NB	5.05	1.44	1.37
40	Y	310	CLA	C1B-NB	5.05	1.44	1.37
40	p	305	CLA	C1B-NB	5.05	1.44	1.37
40	U	208	CLA	MG-NB	-5.05	1.95	2.05
40	M	311	CLA	C1B-NB	5.05	1.44	1.37
40	Z	312	CLA	C1B-NB	5.05	1.44	1.37
40	a	812	CLA	C1B-NB	5.05	1.44	1.37
40	C	305	CLA	MG-NA	-5.05	1.94	2.06
40	I	203	CLA	C1B-NB	5.05	1.44	1.37
40	Q	205	CLA	C1B-NB	5.05	1.44	1.37
40	x	308	CLA	MG-NA	-5.05	1.94	2.06
40	a	832	CLA	C1B-NB	5.05	1.44	1.37
40	w	302	CLA	MG-NA	-5.05	1.94	2.06
40	u	308	CLA	MG-NA	-5.05	1.94	2.06
40	t	304	CLA	C1B-NB	5.05	1.44	1.37
40	f	201	CLA	MG-NB	-5.05	1.95	2.05
40	E	304	CLA	C1B-NB	5.05	1.44	1.37
40	R	307	CLA	C1B-NB	5.05	1.44	1.37
40	Y	301	CLA	C1B-NB	5.05	1.44	1.37
40	a	836	CLA	MG-NB	-5.05	1.95	2.05
40	v	305	CLA	C1B-NB	5.05	1.44	1.37
40	o	304	CLA	C1B-NB	5.05	1.44	1.37
41	R	301	KC2	C4B-NB	5.05	1.44	1.37
40	E	304	CLA	MG-NB	-5.04	1.95	2.05
40	b	837	CLA	MG-NB	-5.04	1.95	2.05
40	O	310	CLA	C1B-NB	5.04	1.44	1.37
40	a	841	CLA	C1B-NB	5.04	1.44	1.37
40	A	309	CLA	MG-NA	-5.04	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	Z	305	CLA	MG-NB	-5.04	1.95	2.05
40	a	816	CLA	MG-NA	-5.04	1.94	2.06
40	a	821	CLA	MG-NA	-5.04	1.94	2.06
40	b	802	CLA	MG-NB	-5.04	1.95	2.05
40	a	819	CLA	MG-NA	-5.04	1.94	2.06
40	a	839	CLA	MG-NA	-5.04	1.94	2.06
40	Q	205	CLA	MG-NA	-5.04	1.94	2.06
40	R	316	CLA	C1B-NB	5.04	1.44	1.37
40	W	307	CLA	C1B-NB	5.04	1.44	1.37
40	b	831	CLA	MG-NB	-5.04	1.95	2.05
40	x	308	CLA	C1B-NB	5.04	1.44	1.37
40	S	306	CLA	C1B-NB	5.04	1.44	1.37
40	L	307	CLA	MG-NB	-5.03	1.95	2.05
44	X	321	A86	C32-C31	-5.03	1.46	1.54
40	a	828	CLA	MG-NB	-5.03	1.95	2.05
40	S	302	CLA	C1B-NB	5.03	1.44	1.37
40	a	829	CLA	C1B-NB	5.03	1.44	1.37
40	Q	208	CLA	MG-NB	-5.03	1.95	2.05
40	P	308	CLA	MG-NB	-5.03	1.95	2.05
40	a	836	CLA	C1B-NB	5.03	1.44	1.37
40	a	833	CLA	MG-NB	-5.03	1.95	2.05
40	M	307	CLA	C1B-NB	5.03	1.44	1.37
40	z	324	CLA	C1B-NB	5.03	1.44	1.37
40	H	302	CLA	MG-NA	-5.03	1.94	2.06
40	R	306	CLA	C1B-NB	5.03	1.44	1.37
40	w	309	CLA	C1B-NB	5.02	1.44	1.37
40	q	306	CLA	MG-NA	-5.02	1.94	2.06
40	p	306	CLA	MG-NA	-5.02	1.94	2.06
40	Y	310	CLA	MG-NA	-5.02	1.94	2.06
40	S	307	CLA	C1B-NB	5.02	1.44	1.37
40	a	842	CLA	MG-NB	-5.02	1.95	2.05
40	x	302	CLA	C1B-NB	5.02	1.44	1.37
41	S	304	KC2	C4B-NB	5.02	1.44	1.37
40	C	306	CLA	C1B-NB	5.01	1.44	1.37
40	E	308	CLA	C1B-NB	5.01	1.44	1.37
40	Z	307	CLA	C1B-NB	5.01	1.44	1.37
41	S	309	KC2	C4B-NB	5.01	1.44	1.37
40	L	306	CLA	C1B-NB	5.01	1.44	1.37
40	l	203	CLA	MG-NB	-5.01	1.95	2.05
40	J	312	CLA	MG-NB	-5.01	1.95	2.05
40	K	304	CLA	MG-NB	-5.01	1.95	2.05
40	L	304	CLA	C1B-NB	5.01	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	I	201	CLA	MG-NA	-5.01	1.94	2.06
40	F	311	CLA	MG-NA	-5.01	1.94	2.06
40	X	305	CLA	C1B-NB	5.01	1.44	1.37
40	K	308	CLA	C1B-NB	5.01	1.44	1.37
40	J	306	CLA	MG-NA	-5.01	1.94	2.06
40	N	304	CLA	MG-NB	-5.01	1.95	2.05
40	I	205	CLA	C1B-NB	5.01	1.44	1.37
40	q	313	CLA	MG-NA	-5.01	1.94	2.06
40	N	306	CLA	C1B-NB	5.01	1.44	1.37
40	G	207	CLA	C1B-NB	5.00	1.44	1.37
40	S	306	CLA	MG-NB	-5.00	1.95	2.05
40	b	826	CLA	MG-NA	-5.00	1.94	2.06
40	Y	305	CLA	MG-NB	-5.00	1.95	2.05
40	b	814	CLA	MG-NB	-5.00	1.95	2.05
40	D	301	CLA	C1B-NB	5.00	1.44	1.37
40	b	842	CLA	C1B-NB	5.00	1.44	1.37
40	a	830	CLA	MG-NB	-5.00	1.95	2.05
40	b	815	CLA	MG-NA	-5.00	1.94	2.06
40	I	204	CLA	MG-NA	-5.00	1.94	2.06
40	D	302	CLA	C1B-NB	5.00	1.44	1.37
40	b	816	CLA	C1B-NB	5.00	1.44	1.37
40	L	305	CLA	MG-NA	-5.00	1.94	2.06
40	I	206	CLA	MG-NB	-5.00	1.95	2.05
40	F	321	CLA	C1B-NB	4.99	1.44	1.37
40	M	304	CLA	C1B-NB	4.99	1.44	1.37
40	Z	310	CLA	C1B-NB	4.99	1.44	1.37
40	a	803	CLA	MG-NA	-4.99	1.94	2.06
40	a	805	CLA	MG-NA	-4.99	1.94	2.06
40	v	311	CLA	MG-NA	-4.99	1.94	2.06
40	U	204	CLA	MG-NA	-4.99	1.94	2.06
40	y	309	CLA	C1B-NB	4.99	1.44	1.37
40	I	204	CLA	C1B-NB	4.99	1.44	1.37
40	Z	306	CLA	MG-NA	-4.99	1.94	2.06
40	B	302	CLA	MG-ND	-4.99	1.95	2.05
40	b	833	CLA	MG-NB	-4.98	1.95	2.05
40	z	307	CLA	MG-NA	-4.98	1.94	2.06
40	E	306	CLA	C1B-NB	4.98	1.44	1.37
40	a	813	CLA	C1B-NB	4.98	1.44	1.37
41	x	309	KC2	C4B-NB	4.98	1.44	1.37
40	o	306	CLA	MG-NA	-4.98	1.94	2.06
40	b	809	CLA	C1B-NB	4.98	1.44	1.37
40	z	302	CLA	C1B-NB	4.98	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	a	851	CLA	MG-NB	-4.98	1.95	2.05
40	O	305	CLA	C1B-NB	4.98	1.44	1.37
41	W	304	KC2	C4B-NB	4.98	1.44	1.37
40	b	839	CLA	C1B-NB	4.98	1.44	1.37
40	a	832	CLA	MG-NB	-4.97	1.95	2.05
40	x	312	CLA	MG-NB	-4.97	1.95	2.05
40	D	308	CLA	MG-NA	-4.97	1.94	2.06
40	t	302	CLA	C1B-NB	4.97	1.44	1.37
40	a	817	CLA	MG-NB	-4.97	1.95	2.05
40	K	307	CLA	C1B-NB	4.97	1.44	1.37
40	P	308	CLA	MG-NA	-4.97	1.94	2.06
40	E	314	CLA	C1B-NB	4.97	1.44	1.37
40	a	826	CLA	MG-NA	-4.97	1.94	2.06
40	P	313	CLA	MG-NA	-4.97	1.94	2.06
40	y	308	CLA	MG-NB	-4.96	1.95	2.05
40	H	305	CLA	MG-NA	-4.96	1.94	2.06
40	F	303	CLA	MG-NB	-4.96	1.96	2.05
40	G	201	CLA	C1B-NB	4.96	1.44	1.37
40	O	306	CLA	C1B-NB	4.96	1.44	1.37
40	z	308	CLA	MG-NB	-4.96	1.96	2.05
40	M	306	CLA	C1B-NB	4.96	1.44	1.37
40	T	306	CLA	C1B-NB	4.96	1.44	1.37
40	Y	305	CLA	MG-NA	-4.96	1.94	2.06
40	N	311	CLA	C1B-NB	4.96	1.44	1.37
40	a	806	CLA	C1B-NB	4.96	1.44	1.37
40	a	828	CLA	C1B-NB	4.96	1.44	1.37
40	M	307	CLA	MG-NA	-4.95	1.94	2.06
40	E	309	CLA	C1B-NB	4.95	1.44	1.37
40	D	312	CLA	MG-NA	-4.95	1.94	2.06
40	T	317	CLA	MG-NB	-4.95	1.96	2.05
40	A	311	CLA	MG-NB	-4.95	1.96	2.05
40	Y	306	CLA	MG-NA	-4.95	1.94	2.06
40	G	206	CLA	C1B-NB	4.95	1.44	1.37
40	A	303	CLA	C1B-NB	4.95	1.44	1.37
40	b	823	CLA	MG-NA	-4.95	1.94	2.06
40	N	307	CLA	MG-NB	-4.95	1.96	2.05
40	D	306	CLA	C1B-NB	4.94	1.44	1.37
40	A	301	CLA	C1B-NB	4.94	1.44	1.37
40	F	306	CLA	C1B-NB	4.94	1.44	1.37
40	b	813	CLA	MG-NB	-4.94	1.96	2.05
40	q	305	CLA	C1B-NB	4.94	1.44	1.37
40	u	306	CLA	MG-NA	-4.94	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	f	205	CLA	MG-NB	-4.94	1.96	2.05
40	M	310	CLA	MG-NB	-4.94	1.96	2.05
40	b	807	CLA	MG-NA	-4.94	1.94	2.06
40	b	817	CLA	MG-NA	-4.94	1.94	2.06
41	R	303	KC2	C4B-NB	4.94	1.44	1.37
40	b	842	CLA	MG-NA	-4.94	1.94	2.06
40	Q	204	CLA	MG-NB	-4.93	1.96	2.05
40	A	308	CLA	MG-NA	-4.93	1.94	2.06
40	a	827	CLA	MG-NA	-4.93	1.94	2.06
40	J	308	CLA	MG-NB	-4.93	1.96	2.05
40	b	805	CLA	C1B-NB	4.93	1.44	1.37
40	b	833	CLA	C1B-NB	4.93	1.44	1.37
40	O	316	CLA	C1B-NB	4.93	1.44	1.37
40	P	305	CLA	C1B-NB	4.92	1.44	1.37
40	v	310	CLA	C1B-NB	4.92	1.44	1.37
41	q	303	KC2	C4B-NB	4.92	1.44	1.37
40	B	303	CLA	MG-NA	-4.92	1.94	2.06
40	A	311	CLA	C1B-NB	4.92	1.44	1.37
40	q	310	CLA	C1B-NB	4.92	1.44	1.37
40	A	304	CLA	C1B-NB	4.92	1.44	1.37
40	a	837	CLA	MG-NA	-4.92	1.94	2.06
40	a	835	CLA	C1B-NB	4.92	1.44	1.37
40	b	823	CLA	C1B-NB	4.92	1.44	1.37
40	H	306	CLA	C1B-NB	4.92	1.44	1.37
40	D	303	CLA	MG-NB	-4.91	1.96	2.05
40	b	824	CLA	C1B-NB	4.91	1.44	1.37
40	Q	206	CLA	MG-NB	-4.91	1.96	2.05
40	b	832	CLA	MG-NB	-4.91	1.96	2.05
40	y	304	CLA	MG-NA	-4.91	1.94	2.06
40	V	201	CLA	MG-NA	-4.91	1.94	2.06
40	E	307	CLA	MG-NA	-4.91	1.94	2.06
40	H	301	CLA	MG-NA	-4.91	1.94	2.06
40	b	835	CLA	MG-NA	-4.91	1.94	2.06
40	a	835	CLA	MG-NB	-4.91	1.96	2.05
40	v	306	CLA	MG-NA	-4.91	1.94	2.06
40	M	312	CLA	MG-NB	-4.91	1.96	2.05
40	H	307	CLA	C1B-NB	4.91	1.44	1.37
40	v	301	CLA	C1B-NB	4.91	1.44	1.37
40	J	318	CLA	MG-NA	-4.91	1.94	2.06
40	D	305	CLA	MG-NA	-4.91	1.94	2.06
40	I	205	CLA	MG-NA	-4.91	1.94	2.06
40	a	839	CLA	MG-NB	-4.91	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	x	305	CLA	MG-NB	-4.91	1.96	2.05
40	a	810	CLA	MG-NA	-4.91	1.94	2.06
40	C	307	CLA	C1B-NB	4.90	1.44	1.37
40	J	302	CLA	MG-NA	-4.90	1.94	2.06
40	o	305	CLA	C1B-NB	4.90	1.44	1.37
40	a	808	CLA	C1B-NB	4.90	1.44	1.37
40	Q	203	CLA	MG-NB	-4.90	1.96	2.05
40	Y	311	CLA	MG-NA	-4.90	1.94	2.06
40	b	824	CLA	MG-NB	-4.89	1.96	2.05
40	S	313	CLA	MG-NA	-4.89	1.94	2.06
40	W	306	CLA	MG-NA	-4.89	1.94	2.06
40	w	304	CLA	MG-NA	-4.89	1.94	2.06
40	M	305	CLA	C1B-NB	4.89	1.44	1.37
40	J	318	CLA	MG-NB	-4.89	1.96	2.05
40	a	822	CLA	C1B-NB	4.89	1.44	1.37
40	a	804	CLA	MG-NB	-4.89	1.96	2.05
40	T	307	CLA	MG-NA	-4.89	1.94	2.06
40	N	307	CLA	MG-NA	-4.88	1.94	2.06
40	E	309	CLA	MG-NA	-4.88	1.94	2.06
40	a	835	CLA	MG-NA	-4.88	1.94	2.06
40	Q	208	CLA	C1B-NB	4.88	1.44	1.37
40	o	301	CLA	MG-NA	-4.88	1.94	2.06
40	P	313	CLA	C1B-NB	4.88	1.44	1.37
40	w	308	CLA	MG-NB	-4.88	1.96	2.05
40	L	307	CLA	MG-NA	-4.88	1.94	2.06
40	z	312	CLA	MG-NA	-4.88	1.94	2.06
40	f	204	CLA	MG-NB	-4.88	1.96	2.05
40	b	803	CLA	MG-NA	-4.88	1.94	2.06
40	b	827	CLA	C1B-NB	4.87	1.44	1.37
40	E	306	CLA	MG-NA	-4.87	1.94	2.06
40	b	819	CLA	MG-NA	-4.87	1.94	2.06
40	f	201	CLA	MG-NA	-4.87	1.94	2.06
40	Q	204	CLA	C1B-NB	4.87	1.44	1.37
40	K	312	CLA	MG-NB	-4.87	1.96	2.05
40	Z	304	CLA	C1B-NB	4.87	1.44	1.37
40	x	313	CLA	C1B-NB	4.87	1.44	1.37
40	a	826	CLA	C1B-NB	4.87	1.44	1.37
40	b	833	CLA	MG-NA	-4.87	1.94	2.06
40	w	305	CLA	MG-NA	-4.86	1.94	2.06
40	A	311	CLA	MG-NA	-4.86	1.94	2.06
40	R	305	CLA	MG-NA	-4.86	1.94	2.06
40	G	207	CLA	MG-NA	-4.86	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	b	802	CLA	C1B-NB	4.86	1.44	1.37
40	Z	305	CLA	C1B-NB	4.86	1.44	1.37
40	u	313	CLA	C1B-NB	4.86	1.44	1.37
40	x	305	CLA	MG-NA	-4.86	1.94	2.06
40	a	812	CLA	MG-NB	-4.86	1.96	2.05
40	t	305	CLA	MG-NA	-4.86	1.94	2.06
40	U	206	CLA	MG-NA	-4.86	1.94	2.06
40	b	808	CLA	C1B-NB	4.85	1.44	1.37
40	q	304	CLA	C1B-NB	4.85	1.44	1.37
40	S	319	CLA	MG-NB	-4.85	1.96	2.05
40	l	204	CLA	C1B-NB	4.85	1.44	1.37
40	R	304	CLA	MG-NB	-4.85	1.96	2.05
40	b	841	CLA	C1B-NB	4.85	1.44	1.37
40	a	816	CLA	C1B-NB	4.85	1.44	1.37
40	t	304	CLA	MG-NA	-4.85	1.94	2.06
40	E	313	CLA	MG-NB	-4.85	1.96	2.05
40	E	305	CLA	C1B-NB	4.85	1.44	1.37
40	b	813	CLA	MG-NA	-4.85	1.94	2.06
40	K	306	CLA	MG-NA	-4.84	1.94	2.06
40	k	201	CLA	MG-NA	-4.84	1.94	2.06
40	F	303	CLA	C1B-NB	4.84	1.44	1.37
40	N	310	CLA	C1B-NB	4.84	1.44	1.37
40	K	308	CLA	MG-NA	-4.84	1.94	2.06
40	k	202	CLA	C1B-NB	4.84	1.44	1.37
40	y	305	CLA	MG-NA	-4.84	1.94	2.06
40	b	831	CLA	C1B-NB	4.84	1.44	1.37
40	z	305	CLA	C1B-NB	4.83	1.44	1.37
40	b	835	CLA	MG-NB	-4.83	1.96	2.05
40	v	304	CLA	C1B-NB	4.83	1.44	1.37
40	O	304	CLA	MG-NA	-4.83	1.94	2.06
40	H	310	CLA	MG-NA	-4.83	1.94	2.06
40	T	305	CLA	MG-NA	-4.83	1.94	2.06
40	u	302	CLA	MG-NA	-4.83	1.94	2.06
40	a	851	CLA	C1B-NB	4.83	1.44	1.37
40	G	206	CLA	MG-NB	-4.83	1.96	2.05
40	o	304	CLA	MG-NA	-4.83	1.94	2.06
40	a	830	CLA	MG-NA	-4.82	1.94	2.06
40	X	301	CLA	MG-NA	-4.82	1.94	2.06
40	R	305	CLA	C1B-NB	4.82	1.44	1.37
40	b	830	CLA	C1B-NB	4.82	1.44	1.37
40	K	304	CLA	C1B-NB	4.82	1.44	1.37
40	T	305	CLA	C1B-NB	4.82	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	S	313	CLA	MG-NB	-4.81	1.96	2.05
40	a	831	CLA	MG-NA	-4.81	1.94	2.06
40	U	208	CLA	C1B-NB	4.81	1.44	1.37
40	Y	301	CLA	MG-NA	-4.81	1.94	2.06
40	b	831	CLA	MG-NA	-4.81	1.94	2.06
40	p	312	CLA	MG-NA	-4.81	1.94	2.06
40	D	305	CLA	MG-NB	-4.81	1.96	2.05
40	R	306	CLA	MG-NA	-4.81	1.94	2.06
40	G	204	CLA	MG-NA	-4.81	1.94	2.06
40	M	311	CLA	MG-NA	-4.80	1.94	2.06
40	b	810	CLA	MG-NA	-4.80	1.94	2.06
40	D	311	CLA	C1B-NB	4.80	1.44	1.37
40	D	307	CLA	MG-NA	-4.80	1.94	2.06
40	a	827	CLA	C1B-NB	4.80	1.44	1.37
40	y	303	CLA	MG-NA	-4.80	1.94	2.06
40	b	812	CLA	MG-NA	-4.80	1.94	2.06
40	K	312	CLA	MG-NA	-4.80	1.94	2.06
40	G	205	CLA	MG-NA	-4.80	1.94	2.06
40	w	303	CLA	MG-NA	-4.79	1.94	2.06
40	F	306	CLA	MG-NA	-4.79	1.94	2.06
40	C	306	CLA	MG-NA	-4.79	1.94	2.06
40	N	305	CLA	C1B-NB	4.79	1.44	1.37
40	u	313	CLA	MG-NA	-4.79	1.94	2.06
40	M	304	CLA	MG-NA	-4.79	1.94	2.06
40	D	306	CLA	MG-NA	-4.79	1.94	2.06
40	S	306	CLA	MG-NA	-4.78	1.94	2.06
40	a	840	CLA	C1B-NB	4.78	1.44	1.37
40	Z	301	CLA	MG-NA	-4.78	1.94	2.06
40	N	306	CLA	MG-NA	-4.78	1.94	2.06
40	J	307	CLA	MG-NA	-4.78	1.94	2.06
40	u	302	CLA	C1B-NB	4.78	1.44	1.37
40	b	811	CLA	MG-NA	-4.78	1.94	2.06
40	O	304	CLA	MG-NB	-4.77	1.96	2.05
40	a	805	CLA	MG-NB	-4.77	1.96	2.05
40	a	821	CLA	C1B-NB	4.77	1.44	1.37
40	P	311	CLA	C1B-NB	4.76	1.44	1.37
40	K	306	CLA	C1B-NB	4.76	1.44	1.37
40	z	306	CLA	C1B-NB	4.76	1.44	1.37
40	P	312	CLA	MG-NA	-4.75	1.95	2.06
40	z	302	CLA	MG-NA	-4.75	1.95	2.06
40	D	310	CLA	MG-NA	-4.75	1.95	2.06
40	a	842	CLA	MG-NA	-4.75	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	b	841	CLA	MG-NB	-4.75	1.96	2.05
40	a	825	CLA	MG-NA	-4.75	1.95	2.06
40	a	811	CLA	C1B-NB	4.74	1.44	1.37
40	a	805	CLA	C1B-NB	4.74	1.44	1.37
40	a	842	CLA	C1B-NB	4.74	1.44	1.37
40	J	309	CLA	MG-NA	-4.74	1.95	2.06
40	a	818	CLA	MG-NA	-4.74	1.95	2.06
40	a	828	CLA	MG-NA	-4.74	1.95	2.06
40	y	308	CLA	MG-NA	-4.73	1.95	2.06
41	T	303	KC2	C4B-NB	4.73	1.44	1.37
40	M	310	CLA	MG-NA	-4.73	1.95	2.06
40	M	306	CLA	MG-NA	-4.73	1.95	2.06
40	H	308	CLA	MG-NB	-4.73	1.96	2.05
40	a	832	CLA	MG-NA	-4.73	1.95	2.06
40	T	310	CLA	C1B-NB	4.73	1.44	1.37
41	v	303	KC2	C4B-NB	4.73	1.44	1.37
40	k	201	CLA	MG-NB	-4.72	1.96	2.05
40	p	305	CLA	MG-NB	-4.72	1.96	2.05
40	M	312	CLA	MG-NA	-4.72	1.95	2.06
40	H	306	CLA	MG-NA	-4.72	1.95	2.06
40	P	306	CLA	MG-NA	-4.72	1.95	2.06
40	b	806	CLA	MG-NA	-4.72	1.95	2.06
40	t	303	CLA	MG-NA	-4.72	1.95	2.06
40	M	310	CLA	C1B-NB	4.71	1.44	1.37
40	q	304	CLA	MG-NA	-4.71	1.95	2.06
40	x	305	CLA	C1B-NB	4.71	1.44	1.37
40	I	202	CLA	MG-NA	-4.71	1.95	2.06
40	f	205	CLA	C1B-NB	4.71	1.44	1.37
40	O	307	CLA	MG-NA	-4.71	1.95	2.06
40	P	305	CLA	MG-NA	-4.71	1.95	2.06
40	E	307	CLA	C1B-NB	4.70	1.44	1.37
40	a	810	CLA	MG-NB	-4.69	1.96	2.05
40	b	818	CLA	MG-NA	-4.69	1.95	2.06
41	Y	303	KC2	C4B-NB	4.69	1.44	1.37
40	p	313	CLA	MG-NA	-4.69	1.95	2.06
40	T	306	CLA	MG-NA	-4.68	1.95	2.06
40	D	301	CLA	MG-NA	-4.68	1.95	2.06
40	a	836	CLA	MG-NA	-4.67	1.95	2.06
40	l	205	CLA	C1B-NB	4.67	1.44	1.37
40	a	826	CLA	MG-NB	-4.67	1.96	2.05
40	a	824	CLA	C1B-NB	4.67	1.44	1.37
40	v	304	CLA	MG-NA	-4.67	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	b	803	CLA	C1B-NB	4.67	1.44	1.37
40	I	206	CLA	MG-NA	-4.67	1.95	2.06
40	l	202	CLA	MG-NA	-4.67	1.95	2.06
40	W	312	CLA	C1B-NB	4.66	1.44	1.37
40	S	307	CLA	MG-NA	-4.66	1.95	2.06
40	v	312	CLA	MG-NA	-4.66	1.95	2.06
40	a	803	CLA	C1B-NB	4.66	1.44	1.37
40	b	826	CLA	C1B-NB	4.65	1.44	1.37
40	a	840	CLA	MG-NA	-4.65	1.95	2.06
40	p	305	CLA	MG-NA	-4.65	1.95	2.06
40	H	308	CLA	MG-NA	-4.65	1.95	2.06
40	X	304	CLA	C1B-NB	4.65	1.44	1.37
40	b	814	CLA	MG-NA	-4.64	1.95	2.06
40	A	302	CLA	MG-NA	-4.64	1.95	2.06
40	G	213	CLA	C1B-NB	4.64	1.44	1.37
40	b	814	CLA	C1B-NB	4.64	1.44	1.37
40	Z	305	CLA	MG-NA	-4.63	1.95	2.06
40	a	825	CLA	C1B-NB	4.63	1.43	1.37
40	p	313	CLA	C1B-NB	4.63	1.43	1.37
40	z	308	CLA	C1B-NB	4.62	1.43	1.37
40	O	305	CLA	MG-NA	-4.62	1.95	2.06
40	W	307	CLA	MG-NA	-4.62	1.95	2.06
40	a	823	CLA	MG-NA	-4.61	1.95	2.06
40	a	817	CLA	MG-NA	-4.61	1.95	2.06
40	a	852	CLA	MG-NA	-4.61	1.95	2.06
40	P	307	CLA	MG-NA	-4.61	1.95	2.06
40	a	822	CLA	MG-NA	-4.60	1.95	2.06
40	b	810	CLA	C1B-NB	4.59	1.43	1.37
40	I	202	CLA	MG-NB	-4.59	1.96	2.05
40	b	817	CLA	C1B-NB	4.59	1.43	1.37
41	P	304	KC2	C4B-NB	4.57	1.43	1.37
40	x	313	CLA	MG-NA	-4.57	1.95	2.06
41	M	303	KC2	C4B-NB	4.57	1.43	1.37
40	H	305	CLA	C1B-NB	4.56	1.43	1.37
40	a	812	CLA	MG-NA	-4.56	1.95	2.06
40	l	203	CLA	C1B-NB	4.56	1.43	1.37
40	b	821	CLA	C1B-NB	4.55	1.43	1.37
40	l	204	CLA	MG-NA	-4.55	1.95	2.06
40	q	312	CLA	MG-NA	-4.55	1.95	2.06
40	B	307	CLA	C1B-NB	4.55	1.43	1.37
40	V	202	CLA	C1B-NB	4.54	1.43	1.37
40	F	303	CLA	MG-NA	-4.54	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	b	834	CLA	C1B-NB	4.54	1.43	1.37
40	b	812	CLA	C1B-NB	4.54	1.43	1.37
40	A	306	CLA	MG-NA	-4.53	1.95	2.06
44	R	312	A86	C32-C31	-4.53	1.47	1.54
40	w	308	CLA	MG-NA	-4.53	1.95	2.06
40	G	201	CLA	MG-NA	-4.52	1.95	2.06
41	P	304	KC2	C4C-NC	4.52	1.45	1.37
40	S	302	CLA	MG-NA	-4.51	1.95	2.06
40	Q	206	CLA	MG-NA	-4.51	1.95	2.06
40	K	301	CLA	MG-NA	-4.51	1.95	2.06
40	E	313	CLA	MG-NA	-4.50	1.95	2.06
40	a	818	CLA	C1B-NB	4.49	1.43	1.37
40	O	316	CLA	MG-NA	-4.49	1.95	2.06
40	u	312	CLA	MG-NA	-4.49	1.95	2.06
40	b	813	CLA	C1B-NB	4.48	1.43	1.37
40	F	310	CLA	C1B-NB	4.48	1.43	1.37
40	b	825	CLA	C1B-NB	4.48	1.43	1.37
40	R	316	CLA	MG-NA	-4.47	1.95	2.06
40	J	307	CLA	C1B-NB	4.46	1.43	1.37
40	J	308	CLA	MG-NA	-4.46	1.95	2.06
40	Z	310	CLA	MG-NC	-4.45	1.95	2.06
46	I	215	SQD	O8-S	4.45	1.64	1.47
40	M	305	CLA	MG-NA	-4.45	1.95	2.06
46	P	319	SQD	O8-S	4.45	1.63	1.47
40	B	302	CLA	C1B-NB	4.45	1.43	1.37
40	b	838	CLA	C1B-NB	4.44	1.43	1.37
46	W	318	SQD	O8-S	4.44	1.63	1.47
46	k	205	SQD	O8-S	4.44	1.63	1.47
40	S	319	CLA	MG-NA	-4.44	1.95	2.06
40	b	841	CLA	MG-NA	-4.43	1.95	2.06
46	F	320	SQD	O8-S	4.43	1.63	1.47
40	Q	208	CLA	MG-NA	-4.42	1.95	2.06
46	M	318	SQD	O8-S	4.40	1.63	1.47
40	U	208	CLA	MG-NA	-4.40	1.95	2.06
40	p	311	CLA	MG-NC	-4.38	1.95	2.06
46	k	205	SQD	O48-C23	4.37	1.46	1.33
40	b	837	CLA	C1B-NB	4.37	1.43	1.37
40	G	206	CLA	MG-NA	-4.37	1.95	2.06
44	L	314	A86	C32-C31	-4.37	1.47	1.54
40	J	312	CLA	MG-NA	-4.36	1.95	2.06
40	f	202	CLA	MG-NA	-4.33	1.96	2.06
40	W	312	CLA	MG-NA	-4.33	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	I	215	SQD	O48-C23	4.32	1.45	1.33
46	I	215	SQD	O47-C7	4.31	1.46	1.34
40	f	202	CLA	C1B-NB	4.31	1.43	1.37
40	x	306	CLA	C1B-NB	4.31	1.43	1.37
40	T	317	CLA	MG-NA	-4.30	1.96	2.06
40	b	811	CLA	C1B-NB	4.30	1.43	1.37
41	Y	302	KC2	C1B-NB	4.30	1.43	1.37
40	x	311	CLA	MG-NC	-4.30	1.96	2.06
40	a	850	CLA	C1B-NB	4.30	1.43	1.37
40	D	310	CLA	C1B-NB	4.29	1.43	1.37
40	b	807	CLA	C1B-NB	4.29	1.43	1.37
40	u	311	CLA	MG-NC	-4.28	1.96	2.06
40	Y	312	CLA	MG-NC	-4.28	1.96	2.06
40	x	312	CLA	MG-NA	-4.28	1.96	2.06
40	f	204	CLA	MG-NA	-4.28	1.96	2.06
40	E	304	CLA	MG-NA	-4.27	1.96	2.06
40	b	821	CLA	MG-NA	-4.26	1.96	2.06
46	F	320	SQD	O48-C23	4.26	1.45	1.33
46	W	318	SQD	O48-C23	4.25	1.45	1.33
40	f	205	CLA	MG-NA	-4.25	1.96	2.06
46	P	319	SQD	O48-C23	4.23	1.45	1.33
40	A	303	CLA	MG-NA	-4.23	1.96	2.06
40	a	824	CLA	MG-NA	-4.22	1.96	2.06
40	K	307	CLA	MG-NA	-4.21	1.96	2.06
40	Q	207	CLA	MG-NC	-4.18	1.96	2.06
40	o	313	CLA	C4B-NB	4.18	1.43	1.37
46	M	318	SQD	O47-C7	4.15	1.46	1.34
44	C	311	A86	C32-C31	-4.15	1.47	1.54
41	R	302	KC2	C1B-NB	4.14	1.43	1.37
40	X	310	CLA	MG-NC	-4.14	1.96	2.06
41	L	302	KC2	C1B-NB	4.14	1.43	1.37
40	U	207	CLA	C4B-NB	4.13	1.43	1.37
40	F	310	CLA	MG-NA	-4.13	1.96	2.06
40	S	311	CLA	MG-NC	-4.13	1.96	2.06
46	W	318	SQD	O47-C7	4.13	1.45	1.34
40	F	304	CLA	MG-NC	-4.12	1.96	2.06
48	W	319	A1EB4	C32-C31	-4.12	1.47	1.54
46	k	205	SQD	O47-C7	4.12	1.45	1.34
40	z	311	CLA	MG-NC	-4.12	1.96	2.06
40	H	308	CLA	C4B-NB	4.10	1.43	1.37
40	J	309	CLA	C4B-NB	4.10	1.43	1.37
46	M	318	SQD	O48-C23	4.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	J	318	CLA	C4B-NB	4.09	1.43	1.37
44	N	318	A86	C32-C31	-4.08	1.47	1.54
46	P	319	SQD	O47-C7	4.08	1.45	1.34
40	p	306	CLA	C4B-NB	4.06	1.43	1.37
41	R	303	KC2	C4C-NC	4.05	1.44	1.37
46	F	320	SQD	O47-C7	4.04	1.45	1.34
41	w	306	KC2	C1B-NB	4.04	1.43	1.37
41	X	303	KC2	C1B-NB	4.03	1.43	1.37
41	Y	302	KC2	C4C-NC	4.02	1.44	1.37
40	D	303	CLA	MG-NA	-4.02	1.96	2.06
40	E	314	CLA	MG-NC	-4.01	1.96	2.06
40	a	808	CLA	MG-NC	-4.01	1.96	2.06
47	v	324	A1EB1	C32-C31	-4.01	1.47	1.54
41	S	309	KC2	C1B-NB	4.00	1.43	1.37
41	M	309	KC2	C1B-NB	4.00	1.43	1.37
40	D	305	CLA	C4B-NB	3.99	1.43	1.37
40	k	201	CLA	C4B-NB	3.99	1.43	1.37
40	B	307	CLA	MG-NC	-3.99	1.96	2.06
40	a	826	CLA	C4B-NB	3.99	1.43	1.37
44	w	315	A86	C32-C31	-3.98	1.47	1.54
44	N	315	A86	C32-C31	-3.98	1.47	1.54
41	p	303	KC2	C1B-NB	3.97	1.43	1.37
44	Y	318	A86	C32-C31	-3.97	1.47	1.54
44	W	314	A86	C32-C31	-3.97	1.47	1.54
40	Q	206	CLA	C4B-NB	3.97	1.43	1.37
40	J	312	CLA	C4B-NB	3.96	1.43	1.37
40	W	308	CLA	MG-NC	-3.96	1.96	2.06
40	p	312	CLA	C4B-NB	3.96	1.43	1.37
41	N	302	KC2	C1B-NB	3.95	1.43	1.37
44	Y	321	A86	C32-C31	-3.95	1.47	1.54
40	u	312	CLA	C4B-NB	3.94	1.43	1.37
41	z	304	KC2	C1B-NB	3.94	1.43	1.37
40	G	213	CLA	MG-NC	-3.94	1.96	2.06
40	o	313	CLA	MG-NC	-3.93	1.96	2.06
40	W	311	CLA	MG-NC	-3.93	1.96	2.06
41	y	306	KC2	C1B-NB	3.93	1.43	1.37
41	u	303	KC2	C1B-NB	3.93	1.43	1.37
41	o	303	KC2	C1B-NB	3.93	1.43	1.37
40	S	306	CLA	C4B-NB	3.93	1.43	1.37
44	T	315	A86	C32-C31	-3.92	1.48	1.54
41	v	303	KC2	C1B-NB	3.92	1.43	1.37
41	O	303	KC2	C1B-NB	3.91	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	a	810	CLA	C4B-NB	3.91	1.43	1.37
40	o	310	CLA	MG-NC	-3.91	1.97	2.06
41	W	303	KC2	C1B-NB	3.91	1.43	1.37
40	z	324	CLA	MG-NC	-3.90	1.97	2.06
41	T	303	KC2	C4C-NC	3.90	1.44	1.37
41	L	309	KC2	C1B-NB	3.90	1.43	1.37
41	S	304	KC2	C1B-NB	3.89	1.43	1.37
41	M	303	KC2	C4C-NC	3.89	1.44	1.37
40	Q	203	CLA	C4B-NB	3.89	1.43	1.37
40	X	313	CLA	C4B-NB	3.89	1.43	1.37
41	Y	308	KC2	C1B-NB	3.89	1.43	1.37
40	V	202	CLA	MG-NC	-3.89	1.97	2.06
40	y	303	CLA	C4B-NB	3.88	1.43	1.37
40	T	317	CLA	C4B-NB	3.88	1.43	1.37
40	b	808	CLA	MG-NC	-3.88	1.97	2.06
40	a	827	CLA	C4B-NB	3.88	1.43	1.37
40	U	206	CLA	C4B-NB	3.88	1.43	1.37
40	f	201	CLA	C4B-NB	3.88	1.43	1.37
40	j	102	CLA	MG-NC	-3.88	1.97	2.06
40	G	201	CLA	C4B-NB	3.88	1.43	1.37
40	S	319	CLA	C4B-NB	3.87	1.43	1.37
41	p	310	KC2	C1B-NB	3.87	1.43	1.37
40	N	310	CLA	MG-NC	-3.87	1.97	2.06
40	F	303	CLA	C4B-NB	3.87	1.42	1.37
40	J	306	CLA	C4B-NB	3.86	1.42	1.37
40	N	307	CLA	C4B-NB	3.86	1.42	1.37
40	C	305	CLA	C4B-NB	3.86	1.42	1.37
41	o	302	KC2	C1B-NB	3.86	1.42	1.37
40	v	310	CLA	MG-NC	-3.86	1.97	2.06
44	R	313	A86	C32-C31	-3.86	1.48	1.54
40	I	202	CLA	C4B-NB	3.85	1.42	1.37
40	w	308	CLA	C4B-NB	3.85	1.42	1.37
40	a	832	CLA	C4B-NB	3.85	1.42	1.37
40	C	307	CLA	MG-NC	-3.85	1.97	2.06
40	l	204	CLA	C4B-NB	3.85	1.42	1.37
40	I	207	CLA	C4B-NB	3.85	1.42	1.37
40	I	206	CLA	C4B-NB	3.85	1.42	1.37
40	Q	205	CLA	C4B-NB	3.85	1.42	1.37
40	w	303	CLA	C4B-NB	3.85	1.42	1.37
40	J	308	CLA	C4B-NB	3.84	1.42	1.37
41	I	214	KC2	C1B-NB	3.84	1.42	1.37
41	v	302	KC2	C1B-NB	3.84	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	A	308	CLA	C4B-NB	3.84	1.42	1.37
47	G	212	A1EB1	C32-C31	-3.84	1.48	1.54
41	L	308	KC2	C4C-NC	3.84	1.44	1.37
41	L	308	KC2	C1B-NB	3.84	1.42	1.37
47	x	322	A1EB1	C32-C31	-3.84	1.48	1.54
40	F	301	CLA	C4B-NB	3.84	1.42	1.37
40	K	301	CLA	C4B-NB	3.84	1.42	1.37
40	a	852	CLA	C4B-NB	3.84	1.42	1.37
40	L	312	CLA	C4B-NB	3.84	1.42	1.37
41	J	304	KC2	C1B-NB	3.84	1.42	1.37
41	Z	302	KC2	C1B-NB	3.84	1.42	1.37
40	D	312	CLA	C4B-NB	3.84	1.42	1.37
40	J	310	CLA	C4B-NB	3.83	1.42	1.37
41	x	310	KC2	C1B-NB	3.83	1.42	1.37
41	T	303	KC2	C1B-NB	3.83	1.42	1.37
41	I	214	KC2	C4C-NC	3.83	1.44	1.37
40	J	310	CLA	MG-NC	-3.83	1.97	2.06
40	a	812	CLA	C4B-NB	3.83	1.42	1.37
40	S	305	CLA	MG-NC	-3.83	1.97	2.06
40	O	304	CLA	C4B-NB	3.83	1.42	1.37
40	A	302	CLA	C4B-NB	3.82	1.42	1.37
40	S	312	CLA	C4B-NB	3.82	1.42	1.37
41	Y	314	KC2	C1B-NB	3.82	1.42	1.37
40	U	204	CLA	C4B-NB	3.82	1.42	1.37
40	L	306	CLA	MG-NC	-3.82	1.97	2.06
41	G	208	KC2	C1B-NB	3.81	1.42	1.37
41	L	303	KC2	C4C-NC	3.81	1.44	1.37
40	N	304	CLA	C4B-NB	3.81	1.42	1.37
41	P	303	KC2	C4C-NC	3.81	1.44	1.37
40	D	303	CLA	C4B-NB	3.81	1.42	1.37
40	O	316	CLA	C4B-NB	3.81	1.42	1.37
40	Y	313	CLA	C4B-NB	3.81	1.42	1.37
40	f	204	CLA	C4B-NB	3.81	1.42	1.37
40	W	313	CLA	C4B-NB	3.80	1.42	1.37
40	L	307	CLA	C4B-NB	3.80	1.42	1.37
40	H	311	CLA	C4B-NB	3.80	1.42	1.37
40	S	312	CLA	MG-NC	-3.80	1.97	2.06
40	D	307	CLA	C4B-NB	3.80	1.42	1.37
40	b	809	CLA	MG-NC	-3.80	1.97	2.06
40	y	308	CLA	C4B-NB	3.80	1.42	1.37
40	M	312	CLA	C4B-NB	3.80	1.42	1.37
47	y	314	A1EB1	C32-C31	-3.80	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	F	311	CLA	C4B-NB	3.80	1.42	1.37
40	b	841	CLA	C4B-NB	3.80	1.42	1.37
40	a	837	CLA	C4B-NB	3.80	1.42	1.37
40	B	306	CLA	MG-NC	-3.79	1.97	2.06
40	D	308	CLA	C4B-NB	3.79	1.42	1.37
41	R	303	KC2	C1B-NB	3.79	1.42	1.37
40	J	303	CLA	MG-NC	-3.79	1.97	2.06
40	L	305	CLA	C4B-NB	3.79	1.42	1.37
40	x	312	CLA	C4B-NB	3.79	1.42	1.37
40	F	308	CLA	C4B-NB	3.79	1.42	1.37
40	z	314	CLA	MG-NC	-3.79	1.97	2.06
40	o	301	CLA	C4B-NB	3.79	1.42	1.37
41	I	209	KC2	C1B-NB	3.79	1.42	1.37
40	y	302	CLA	MG-NC	-3.79	1.97	2.06
44	X	318	A86	C32-C31	-3.79	1.48	1.54
40	a	833	CLA	C4B-NB	3.79	1.42	1.37
40	J	311	CLA	C4B-NB	3.78	1.42	1.37
40	z	308	CLA	MG-NC	-3.78	1.97	2.06
40	p	308	CLA	C4B-NB	3.78	1.42	1.37
40	a	809	CLA	MG-NC	-3.78	1.97	2.06
41	W	304	KC2	C1B-NB	3.78	1.42	1.37
40	Z	312	CLA	MG-NC	-3.78	1.97	2.06
40	L	311	CLA	C4B-NB	3.78	1.42	1.37
41	F	309	KC2	C1B-NB	3.78	1.42	1.37
41	R	311	KC2	C1B-NB	3.78	1.42	1.37
40	L	301	CLA	C4B-NB	3.78	1.42	1.37
40	P	306	CLA	C4B-NB	3.78	1.42	1.37
41	P	303	KC2	C1B-NB	3.78	1.42	1.37
40	Y	304	CLA	C4B-NB	3.78	1.42	1.37
41	T	311	KC2	C1B-NB	3.78	1.42	1.37
40	H	302	CLA	C4B-NB	3.77	1.42	1.37
47	t	314	A1EB1	C32-C31	-3.77	1.48	1.54
40	F	304	CLA	C4B-NB	3.77	1.42	1.37
40	l	205	CLA	MG-NC	-3.77	1.97	2.06
40	a	819	CLA	C4B-NB	3.77	1.42	1.37
41	q	302	KC2	C1B-NB	3.77	1.42	1.37
40	a	804	CLA	C4B-NB	3.76	1.42	1.37
40	H	307	CLA	MG-NC	-3.76	1.97	2.06
40	a	831	CLA	C4B-NB	3.76	1.42	1.37
41	z	303	KC2	C1B-NB	3.76	1.42	1.37
41	p	303	KC2	C4C-NC	3.76	1.43	1.37
40	E	310	CLA	C4B-NB	3.76	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	L	310	CLA	C4B-NB	3.76	1.42	1.37
48	M	319	A1EB4	C32-C31	-3.76	1.48	1.54
40	t	302	CLA	C4B-NB	3.76	1.42	1.37
40	Y	305	CLA	C4B-NB	3.75	1.42	1.37
40	O	307	CLA	C4B-NB	3.75	1.42	1.37
41	J	304	KC2	C4C-NC	3.75	1.43	1.37
40	t	305	CLA	C4B-NB	3.75	1.42	1.37
41	q	309	KC2	C1B-NB	3.75	1.42	1.37
41	W	309	KC2	C1B-NB	3.75	1.42	1.37
41	t	308	KC2	C1B-NB	3.75	1.42	1.37
40	X	301	CLA	C4B-NB	3.74	1.42	1.37
40	a	820	CLA	C4B-NB	3.74	1.42	1.37
40	q	313	CLA	C4B-NB	3.74	1.42	1.37
41	M	303	KC2	C1B-NB	3.74	1.42	1.37
40	a	811	CLA	MG-NC	-3.74	1.97	2.06
40	q	310	CLA	MG-NC	-3.74	1.97	2.06
40	E	304	CLA	C4B-NB	3.74	1.42	1.37
41	T	302	KC2	C1B-NB	3.74	1.42	1.37
40	D	311	CLA	MG-NC	-3.74	1.97	2.06
41	Z	308	KC2	C1B-NB	3.74	1.42	1.37
44	o	318	A86	C32-C31	-3.74	1.48	1.54
47	o	322	A1EB1	C32-C31	-3.74	1.48	1.54
40	v	312	CLA	C4B-NB	3.73	1.42	1.37
40	q	312	CLA	C4B-NB	3.73	1.42	1.37
40	C	308	CLA	C4B-NB	3.73	1.42	1.37
41	M	308	KC2	C1B-NB	3.73	1.42	1.37
40	X	313	CLA	MG-NC	-3.73	1.97	2.06
40	R	316	CLA	C4B-NB	3.73	1.42	1.37
40	V	201	CLA	C4B-NB	3.73	1.42	1.37
41	o	308	KC2	C1B-NB	3.73	1.42	1.37
40	B	303	CLA	C4B-NB	3.73	1.42	1.37
41	N	308	KC2	C1B-NB	3.73	1.42	1.37
40	Z	305	CLA	C4B-NB	3.73	1.42	1.37
40	B	301	CLA	MG-NC	-3.73	1.97	2.06
41	S	310	KC2	C1B-NB	3.72	1.42	1.37
40	A	309	CLA	C4B-NB	3.72	1.42	1.37
40	R	304	CLA	C4B-NB	3.72	1.42	1.37
40	F	310	CLA	C4B-NB	3.72	1.42	1.37
41	N	312	KC2	C1B-NB	3.72	1.42	1.37
44	T	319	A86	C32-C31	-3.72	1.48	1.54
41	y	307	KC2	C1B-NB	3.71	1.42	1.37
40	a	809	CLA	C4B-NB	3.71	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	Z	302	KC2	C4C-NC	3.71	1.43	1.37
40	D	309	CLA	C4B-NB	3.71	1.42	1.37
40	Q	209	CLA	C4B-NB	3.71	1.42	1.37
40	a	815	CLA	C4B-NB	3.71	1.42	1.37
40	p	314	CLA	C4B-NB	3.71	1.42	1.37
40	I	208	CLA	C4B-NB	3.70	1.42	1.37
40	a	811	CLA	C4B-NB	3.70	1.42	1.37
47	q	323	A1EB1	C32-C31	-3.70	1.48	1.54
41	P	304	KC2	C1B-NB	3.70	1.42	1.37
41	w	307	KC2	C1B-NB	3.70	1.42	1.37
40	E	313	CLA	C4B-NB	3.70	1.42	1.37
40	E	306	CLA	C4B-NB	3.70	1.42	1.37
40	a	817	CLA	C4B-NB	3.70	1.42	1.37
40	P	311	CLA	MG-NC	-3.70	1.97	2.06
40	H	309	CLA	MG-NC	-3.70	1.97	2.06
40	R	310	CLA	C4B-NB	3.70	1.42	1.37
40	Q	204	CLA	C4B-NB	3.70	1.42	1.37
40	I	203	CLA	MG-NC	-3.69	1.97	2.06
40	A	306	CLA	C4B-NB	3.69	1.42	1.37
40	K	307	CLA	C4B-NB	3.69	1.42	1.37
40	E	307	CLA	C4B-NB	3.69	1.42	1.37
40	S	302	CLA	C4B-NB	3.69	1.42	1.37
40	D	302	CLA	C4B-NB	3.69	1.42	1.37
41	P	309	KC2	C1B-NB	3.69	1.42	1.37
41	W	302	KC2	C4C-NC	3.69	1.43	1.37
40	a	814	CLA	C4B-NB	3.69	1.42	1.37
44	t	316	A86	C32-C31	-3.69	1.48	1.54
40	P	312	CLA	C4B-NB	3.69	1.42	1.37
41	Q	201	KC2	C4C-NC	3.69	1.43	1.37
40	Z	301	CLA	C4B-NB	3.68	1.42	1.37
41	x	303	KC2	C1B-NB	3.68	1.42	1.37
41	H	303	KC2	C4C-NC	3.68	1.43	1.37
41	p	309	KC2	C1B-NB	3.68	1.42	1.37
41	O	311	KC2	C1B-NB	3.68	1.42	1.37
40	f	205	CLA	C4B-NB	3.68	1.42	1.37
40	b	832	CLA	MG-NC	-3.68	1.97	2.06
41	F	302	KC2	C1B-NB	3.68	1.42	1.37
40	b	836	CLA	MG-NC	-3.68	1.97	2.06
40	b	832	CLA	C4B-NB	3.68	1.42	1.37
40	t	304	CLA	C4B-NB	3.68	1.42	1.37
40	L	310	CLA	MG-NC	-3.68	1.97	2.06
40	Y	311	CLA	C4B-NB	3.67	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	T	307	CLA	C4B-NB	3.67	1.42	1.37
40	t	309	CLA	C4B-NB	3.67	1.42	1.37
40	o	307	CLA	MG-NC	-3.67	1.97	2.06
40	E	303	CLA	C4B-NB	3.67	1.42	1.37
41	K	302	KC2	C1B-NB	3.67	1.42	1.37
40	u	314	CLA	MG-NC	-3.67	1.97	2.06
41	F	309	KC2	C4C-NC	3.67	1.43	1.37
40	P	307	CLA	C4B-NB	3.67	1.42	1.37
41	W	302	KC2	C1B-NB	3.67	1.42	1.37
40	I	205	CLA	C4B-NB	3.66	1.42	1.37
40	S	313	CLA	C4B-NB	3.66	1.42	1.37
40	Q	204	CLA	MG-NC	-3.66	1.97	2.06
40	b	820	CLA	MG-NC	-3.66	1.97	2.06
40	W	307	CLA	C4B-NB	3.66	1.42	1.37
40	I	204	CLA	C4B-NB	3.66	1.42	1.37
41	S	304	KC2	C4C-NC	3.66	1.43	1.37
40	b	821	CLA	C4B-NB	3.66	1.42	1.37
41	L	302	KC2	C4C-NC	3.66	1.43	1.37
44	z	320	A86	C32-C31	-3.66	1.48	1.54
41	O	308	KC2	C4C-NC	3.66	1.43	1.37
40	C	301	CLA	C4B-NB	3.66	1.42	1.37
40	L	304	CLA	C4B-NB	3.65	1.42	1.37
40	v	307	CLA	MG-NC	-3.65	1.97	2.06
40	b	819	CLA	C4B-NB	3.65	1.42	1.37
41	t	306	KC2	C1B-NB	3.65	1.42	1.37
40	W	306	CLA	C4B-NB	3.65	1.42	1.37
40	b	806	CLA	C4B-NB	3.65	1.42	1.37
41	U	201	KC2	C1B-NB	3.65	1.42	1.37
40	R	306	CLA	C4B-NB	3.65	1.42	1.37
40	X	307	CLA	C4B-NB	3.65	1.42	1.37
40	z	302	CLA	C4B-NB	3.65	1.42	1.37
40	O	305	CLA	C4B-NB	3.65	1.42	1.37
40	o	305	CLA	C4B-NB	3.65	1.42	1.37
41	T	308	KC2	C1B-NB	3.65	1.42	1.37
40	C	309	CLA	MG-NC	-3.65	1.97	2.06
41	G	208	KC2	C4C-NC	3.65	1.43	1.37
41	N	303	KC2	C4C-NC	3.65	1.43	1.37
40	A	303	CLA	C4B-NB	3.65	1.42	1.37
40	y	305	CLA	C4B-NB	3.65	1.42	1.37
40	C	306	CLA	C4B-NB	3.65	1.42	1.37
40	G	205	CLA	C4B-NB	3.64	1.42	1.37
40	w	305	CLA	C4B-NB	3.64	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	X	308	KC2	C1B-NB	3.64	1.42	1.37
40	U	202	CLA	MG-NC	-3.64	1.97	2.06
40	q	307	CLA	MG-NC	-3.64	1.97	2.06
40	u	314	CLA	C4B-NB	3.64	1.42	1.37
40	C	304	CLA	MG-NC	-3.64	1.97	2.06
41	X	309	KC2	C4C-NC	3.64	1.43	1.37
40	G	207	CLA	C4B-NB	3.64	1.42	1.37
40	C	308	CLA	MG-NC	-3.64	1.97	2.06
40	b	839	CLA	MG-NC	-3.64	1.97	2.06
40	J	303	CLA	C4B-NB	3.64	1.42	1.37
40	N	306	CLA	C4B-NB	3.64	1.42	1.37
40	z	313	CLA	MG-NC	-3.64	1.97	2.06
41	M	301	KC2	C1B-NB	3.64	1.42	1.37
40	X	312	CLA	C4B-NB	3.64	1.42	1.37
41	z	310	KC2	C1B-NB	3.63	1.42	1.37
40	X	312	CLA	MG-NC	-3.63	1.97	2.06
47	L	318	A1EB1	C32-C31	-3.63	1.48	1.54
40	Q	202	CLA	C4B-NB	3.63	1.42	1.37
40	a	828	CLA	C4B-NB	3.63	1.42	1.37
40	X	305	CLA	C4B-NB	3.63	1.42	1.37
40	G	206	CLA	C4B-NB	3.63	1.42	1.37
41	R	301	KC2	C1B-NB	3.63	1.42	1.37
40	E	305	CLA	MG-NC	-3.63	1.97	2.06
41	T	301	KC2	C1B-NB	3.63	1.42	1.37
40	E	309	CLA	C4B-NB	3.63	1.42	1.37
40	b	815	CLA	C4B-NB	3.63	1.42	1.37
40	W	305	CLA	C4B-NB	3.63	1.42	1.37
40	l	203	CLA	MG-NC	-3.63	1.97	2.06
41	H	303	KC2	C1B-NB	3.63	1.42	1.37
40	b	801	CLA	MG-NC	-3.62	1.97	2.06
40	X	305	CLA	MG-NC	-3.62	1.97	2.06
40	Q	203	CLA	MG-NC	-3.62	1.97	2.06
40	H	307	CLA	C4B-NB	3.62	1.42	1.37
41	A	310	KC2	C1B-NB	3.62	1.42	1.37
40	E	311	CLA	MG-NC	-3.62	1.97	2.06
40	b	834	CLA	MG-NC	-3.62	1.97	2.06
40	a	816	CLA	C4B-NB	3.62	1.42	1.37
41	t	301	KC2	C1B-NB	3.62	1.42	1.37
40	C	309	CLA	C4B-NB	3.62	1.42	1.37
40	a	850	CLA	MG-NC	-3.62	1.97	2.06
41	O	303	KC2	C4C-NC	3.62	1.43	1.37
40	y	304	CLA	C4B-NB	3.61	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	X	302	KC2	C4C-NC	3.61	1.43	1.37
40	Y	313	CLA	MG-NC	-3.61	1.97	2.06
40	K	304	CLA	C4B-NB	3.61	1.42	1.37
40	Q	208	CLA	C4B-NB	3.61	1.42	1.37
41	R	302	KC2	C4C-NC	3.61	1.43	1.37
40	B	301	CLA	C4B-NB	3.61	1.42	1.37
41	W	310	KC2	C1B-NB	3.61	1.42	1.37
40	E	311	CLA	C4B-NB	3.61	1.42	1.37
40	a	823	CLA	C4B-NB	3.61	1.42	1.37
41	O	302	KC2	C4C-NC	3.61	1.43	1.37
40	Z	313	CLA	C4B-NB	3.61	1.42	1.37
40	A	311	CLA	C4B-NB	3.61	1.42	1.37
40	J	307	CLA	C4B-NB	3.60	1.42	1.37
40	o	312	CLA	C4B-NB	3.60	1.42	1.37
41	z	303	KC2	C4C-NC	3.60	1.43	1.37
41	w	307	KC2	C4C-NC	3.60	1.43	1.37
40	a	838	CLA	C4B-NB	3.60	1.42	1.37
44	Y	320	A86	C32-C31	-3.60	1.48	1.54
47	K	315	A1EB1	C32-C31	-3.60	1.48	1.54
40	b	813	CLA	C4B-NB	3.60	1.42	1.37
47	R	317	A1EB1	C32-C31	-3.60	1.48	1.54
40	J	305	CLA	C4B-NB	3.60	1.42	1.37
40	p	314	CLA	MG-NC	-3.60	1.97	2.06
40	Q	209	CLA	MG-NC	-3.59	1.97	2.06
40	b	814	CLA	C4B-NB	3.59	1.42	1.37
40	H	306	CLA	C4B-NB	3.59	1.42	1.37
40	v	313	CLA	C4B-NB	3.59	1.42	1.37
41	u	310	KC2	C1B-NB	3.59	1.42	1.37
41	O	308	KC2	C1B-NB	3.59	1.42	1.37
40	Y	301	CLA	C4B-NB	3.59	1.42	1.37
40	i	101	CLA	MG-NC	-3.59	1.97	2.06
40	H	304	CLA	C4B-NB	3.59	1.42	1.37
40	u	313	CLA	C4B-NB	3.59	1.42	1.37
40	v	304	CLA	C4B-NB	3.59	1.42	1.37
41	Z	308	KC2	C4C-NC	3.59	1.43	1.37
41	p	310	KC2	C4C-NC	3.59	1.43	1.37
40	C	302	CLA	C4B-NB	3.59	1.42	1.37
40	F	306	CLA	C4B-NB	3.58	1.42	1.37
40	S	301	CLA	C4B-NB	3.58	1.42	1.37
40	z	324	CLA	C4B-NB	3.58	1.42	1.37
41	C	303	KC2	C1B-NB	3.58	1.42	1.37
40	a	804	CLA	MG-NC	-3.58	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	u	304	KC2	C1B-NB	3.58	1.42	1.37
41	O	311	KC2	C4C-NC	3.58	1.43	1.37
41	W	304	KC2	C4C-NC	3.58	1.43	1.37
40	x	306	CLA	MG-NC	-3.58	1.97	2.06
41	u	310	KC2	C4C-NC	3.58	1.43	1.37
40	M	305	CLA	C4B-NB	3.58	1.42	1.37
40	b	842	CLA	C4B-NB	3.58	1.42	1.37
40	M	306	CLA	C4B-NB	3.58	1.42	1.37
40	O	310	CLA	C4B-NB	3.58	1.42	1.37
41	Y	303	KC2	C1B-NB	3.58	1.42	1.37
40	F	305	CLA	C4B-NB	3.58	1.42	1.37
41	x	304	KC2	C4C-NC	3.58	1.43	1.37
40	Q	207	CLA	C4B-NB	3.58	1.42	1.37
41	v	309	KC2	C1B-NB	3.58	1.42	1.37
40	q	304	CLA	C4B-NB	3.58	1.42	1.37
40	a	822	CLA	C4B-NB	3.58	1.42	1.37
41	N	308	KC2	C4C-NC	3.57	1.43	1.37
40	b	822	CLA	MG-NC	-3.57	1.97	2.06
41	y	301	KC2	C1B-NB	3.57	1.42	1.37
40	Z	311	CLA	MG-NC	-3.57	1.97	2.06
40	D	304	CLA	C4B-NB	3.57	1.42	1.37
40	W	308	CLA	C4B-NB	3.57	1.42	1.37
41	K	303	KC2	C1B-NB	3.57	1.42	1.37
40	a	841	CLA	MG-NC	-3.57	1.97	2.06
41	M	302	KC2	C1B-NB	3.57	1.42	1.37
40	H	310	CLA	C4B-NB	3.57	1.42	1.37
40	t	307	CLA	C4B-NB	3.57	1.42	1.37
41	x	303	KC2	C4C-NC	3.57	1.43	1.37
41	Z	303	KC2	C1B-NB	3.57	1.42	1.37
47	Z	321	A1EB1	C32-C31	-3.57	1.48	1.54
40	M	310	CLA	C4B-NB	3.57	1.42	1.37
41	C	303	KC2	C4C-NC	3.56	1.43	1.37
41	q	303	KC2	C4C-NC	3.56	1.43	1.37
40	G	213	CLA	C4B-NB	3.56	1.42	1.37
40	R	307	CLA	C4B-NB	3.56	1.42	1.37
40	b	823	CLA	C4B-NB	3.56	1.42	1.37
41	S	303	KC2	C4C-NC	3.56	1.43	1.37
44	Z	317	A86	C32-C31	-3.56	1.48	1.54
40	a	824	CLA	C4B-NB	3.56	1.42	1.37
40	x	314	CLA	C4B-NB	3.56	1.42	1.37
41	P	309	KC2	C4C-NC	3.56	1.43	1.37
40	S	314	CLA	MG-NC	-3.56	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	x	309	KC2	C4C-NC	3.56	1.43	1.37
40	a	820	CLA	MG-NC	-3.56	1.97	2.06
41	M	302	KC2	C4C-NC	3.56	1.43	1.37
40	E	312	CLA	C4B-NB	3.56	1.42	1.37
40	T	306	CLA	C4B-NB	3.56	1.42	1.37
40	Q	205	CLA	MG-NC	-3.55	1.97	2.06
40	Z	306	CLA	C4B-NB	3.55	1.42	1.37
40	t	303	CLA	C4B-NB	3.55	1.42	1.37
41	L	313	KC2	C1B-NB	3.55	1.42	1.37
41	O	301	KC2	C1B-NB	3.55	1.42	1.37
41	K	309	KC2	C1B-NB	3.55	1.42	1.37
41	v	302	KC2	C4C-NC	3.55	1.43	1.37
41	Q	216	KC2	C1B-NB	3.55	1.42	1.37
41	p	309	KC2	C4C-NC	3.54	1.43	1.37
40	D	306	CLA	C4B-NB	3.54	1.42	1.37
40	z	313	CLA	C4B-NB	3.54	1.42	1.37
41	O	302	KC2	C1B-NB	3.54	1.42	1.37
40	a	806	CLA	MG-NC	-3.54	1.97	2.06
40	O	310	CLA	MG-NC	-3.54	1.97	2.06
40	Z	313	CLA	MG-NC	-3.54	1.97	2.06
40	a	838	CLA	MG-NC	-3.54	1.97	2.06
40	a	851	CLA	C4B-NB	3.54	1.42	1.37
41	R	309	KC2	C4C-NC	3.54	1.43	1.37
41	Q	201	KC2	C1B-NB	3.54	1.42	1.37
40	H	302	CLA	MG-NC	-3.54	1.97	2.06
41	T	301	KC2	C4C-NC	3.54	1.43	1.37
40	S	305	CLA	C4B-NB	3.54	1.42	1.37
41	K	302	KC2	C4C-NC	3.54	1.43	1.37
41	T	311	KC2	C4C-NC	3.54	1.43	1.37
41	M	309	KC2	C4C-NC	3.54	1.43	1.37
40	U	207	CLA	MG-NC	-3.54	1.97	2.06
40	Y	305	CLA	MG-NC	-3.54	1.97	2.06
40	w	304	CLA	C4B-NB	3.53	1.42	1.37
40	a	840	CLA	C4B-NB	3.53	1.42	1.37
40	u	305	CLA	C4B-NB	3.53	1.42	1.37
41	S	310	KC2	C4C-NC	3.53	1.43	1.37
41	U	201	KC2	C4C-NC	3.53	1.43	1.37
40	L	301	CLA	MG-NC	-3.53	1.97	2.06
40	b	827	CLA	MG-NC	-3.53	1.97	2.06
40	T	310	CLA	MG-NC	-3.53	1.97	2.06
40	Y	306	CLA	C4B-NB	3.53	1.42	1.37
40	D	301	CLA	C4B-NB	3.53	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	J	302	CLA	C4B-NB	3.53	1.42	1.37
40	a	829	CLA	C4B-NB	3.52	1.42	1.37
41	q	309	KC2	C4C-NC	3.52	1.43	1.37
40	z	306	CLA	MG-NC	-3.52	1.97	2.06
40	G	204	CLA	C4B-NB	3.52	1.42	1.37
41	X	302	KC2	C1B-NB	3.52	1.42	1.37
40	H	309	CLA	C4B-NB	3.52	1.42	1.37
40	b	831	CLA	C4B-NB	3.52	1.42	1.37
41	Q	216	KC2	C4C-NC	3.52	1.43	1.37
41	O	301	KC2	C4C-NC	3.52	1.43	1.37
40	a	836	CLA	C4B-NB	3.52	1.42	1.37
40	P	308	CLA	C4B-NB	3.52	1.42	1.37
40	z	307	CLA	C4B-NB	3.52	1.42	1.37
41	M	301	KC2	C4C-NC	3.52	1.43	1.37
40	w	302	CLA	C4B-NB	3.52	1.42	1.37
41	R	301	KC2	C4C-NC	3.52	1.43	1.37
40	b	805	CLA	MG-NC	-3.52	1.97	2.06
40	M	307	CLA	C4B-NB	3.52	1.42	1.37
40	w	309	CLA	C4B-NB	3.52	1.42	1.37
40	l	202	CLA	C4B-NB	3.51	1.42	1.37
40	b	829	CLA	MG-NC	-3.51	1.97	2.06
40	a	839	CLA	C4B-NB	3.51	1.42	1.37
40	I	208	CLA	MG-NC	-3.51	1.97	2.06
40	a	834	CLA	MG-NC	-3.51	1.97	2.06
40	a	851	CLA	MG-NC	-3.51	1.97	2.06
40	U	205	CLA	C4B-NB	3.51	1.42	1.37
41	Z	303	KC2	C4C-NC	3.51	1.43	1.37
40	b	830	CLA	MG-NC	-3.51	1.97	2.06
40	o	312	CLA	MG-NC	-3.51	1.97	2.06
40	o	304	CLA	C4B-NB	3.51	1.42	1.37
40	M	304	CLA	C4B-NB	3.51	1.42	1.37
41	A	310	KC2	C4C-NC	3.51	1.43	1.37
40	Y	310	CLA	C4B-NB	3.51	1.42	1.37
40	K	312	CLA	C4B-NB	3.50	1.42	1.37
40	H	305	CLA	C4B-NB	3.50	1.42	1.37
41	P	310	KC2	C4C-NC	3.50	1.43	1.37
40	f	202	CLA	C4B-NB	3.50	1.42	1.37
41	T	302	KC2	C4C-NC	3.50	1.43	1.37
41	S	309	KC2	C4C-NC	3.50	1.43	1.37
41	T	309	KC2	C4C-NC	3.50	1.43	1.37
40	B	304	CLA	MG-NC	-3.50	1.98	2.06
41	X	303	KC2	C4C-NC	3.50	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	y	302	CLA	C4B-NB	3.50	1.42	1.37
41	N	313	KC2	C1B-NB	3.50	1.42	1.37
40	S	307	CLA	C4B-NB	3.50	1.42	1.37
41	P	302	KC2	C4C-NC	3.50	1.43	1.37
40	P	305	CLA	C4B-NB	3.50	1.42	1.37
40	b	835	CLA	C4B-NB	3.50	1.42	1.37
40	j	102	CLA	C4B-NB	3.50	1.42	1.37
41	z	310	KC2	C4C-NC	3.49	1.43	1.37
41	L	303	KC2	C1B-NB	3.49	1.42	1.37
41	W	303	KC2	C4C-NC	3.49	1.43	1.37
41	q	303	KC2	C1B-NB	3.49	1.42	1.37
41	y	306	KC2	C4C-NC	3.49	1.43	1.37
41	L	309	KC2	C4C-NC	3.49	1.43	1.37
41	q	308	KC2	C4C-NC	3.49	1.43	1.37
47	O	317	A1EB1	C32-C31	-3.49	1.48	1.54
41	t	308	KC2	C4C-NC	3.49	1.43	1.37
41	M	308	KC2	C4C-NC	3.49	1.43	1.37
40	P	311	CLA	C4B-NB	3.49	1.42	1.37
40	L	311	CLA	MG-NC	-3.49	1.98	2.06
40	E	305	CLA	C4B-NB	3.49	1.42	1.37
40	T	305	CLA	C4B-NB	3.49	1.42	1.37
40	a	813	CLA	C4B-NB	3.48	1.42	1.37
40	L	304	CLA	MG-NC	-3.48	1.98	2.06
40	a	825	CLA	C4B-NB	3.48	1.42	1.37
41	o	308	KC2	C4C-NC	3.48	1.43	1.37
40	b	805	CLA	C4B-NB	3.48	1.42	1.37
41	u	309	KC2	C1B-NB	3.48	1.42	1.37
41	K	305	KC2	C4C-NC	3.48	1.43	1.37
41	v	308	KC2	C1B-NB	3.48	1.42	1.37
40	a	806	CLA	C4B-NB	3.48	1.42	1.37
40	B	304	CLA	C4B-NB	3.48	1.42	1.37
40	I	207	CLA	MG-NC	-3.48	1.98	2.06
41	u	303	KC2	C4C-NC	3.48	1.43	1.37
40	S	301	CLA	MG-NC	-3.48	1.98	2.06
41	G	202	KC2	C1B-NB	3.48	1.42	1.37
40	D	311	CLA	C4B-NB	3.48	1.42	1.37
41	I	209	KC2	C4C-NC	3.48	1.43	1.37
40	A	304	CLA	MG-NC	-3.47	1.98	2.06
40	b	801	CLA	C4B-NB	3.47	1.42	1.37
41	Y	314	KC2	C4C-NC	3.47	1.43	1.37
40	p	306	CLA	MG-NC	-3.47	1.98	2.06
41	o	302	KC2	C4C-NC	3.47	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	b	836	CLA	C4B-NB	3.47	1.42	1.37
40	x	313	CLA	C4B-NB	3.47	1.42	1.37
41	y	301	KC2	C4C-NC	3.47	1.43	1.37
40	p	302	CLA	C4B-NB	3.47	1.42	1.37
40	U	205	CLA	MG-NC	-3.47	1.98	2.06
41	E	319	KC2	C1B-NB	3.47	1.42	1.37
40	O	306	CLA	MG-NC	-3.47	1.98	2.06
40	a	807	CLA	C4B-NB	3.47	1.42	1.37
40	R	305	CLA	C4B-NB	3.47	1.42	1.37
41	N	301	KC2	C4C-NC	3.46	1.43	1.37
40	T	304	CLA	C4B-NB	3.46	1.42	1.37
40	v	307	CLA	C4B-NB	3.46	1.42	1.37
40	S	311	CLA	C4B-NB	3.46	1.42	1.37
41	q	308	KC2	C1B-NB	3.46	1.42	1.37
40	A	307	CLA	C4B-NB	3.46	1.42	1.37
41	p	315	KC2	C4C-NC	3.46	1.43	1.37
40	x	307	CLA	MG-NC	-3.46	1.98	2.06
41	x	309	KC2	C1B-NB	3.46	1.42	1.37
40	b	837	CLA	MG-NC	-3.46	1.98	2.06
41	R	308	KC2	C1B-NB	3.46	1.42	1.37
40	J	307	CLA	MG-NC	-3.46	1.98	2.06
47	F	322	A1EB1	C32-C31	-3.46	1.48	1.54
40	N	305	CLA	C4B-NB	3.46	1.42	1.37
41	Y	309	KC2	C1B-NB	3.46	1.42	1.37
41	S	303	KC2	C1B-NB	3.46	1.42	1.37
41	Z	309	KC2	C4C-NC	3.46	1.43	1.37
40	u	308	CLA	C4B-NB	3.46	1.42	1.37
41	X	308	KC2	C4C-NC	3.45	1.43	1.37
41	P	310	KC2	C1B-NB	3.45	1.42	1.37
40	N	310	CLA	C4B-NB	3.45	1.42	1.37
40	O	306	CLA	C4B-NB	3.45	1.42	1.37
40	a	805	CLA	C4B-NB	3.45	1.42	1.37
41	R	308	KC2	C4C-NC	3.45	1.43	1.37
41	K	309	KC2	C4C-NC	3.45	1.43	1.37
40	a	814	CLA	MG-NC	-3.45	1.98	2.06
40	a	830	CLA	C4B-NB	3.45	1.42	1.37
41	N	309	KC2	C1B-NB	3.45	1.42	1.37
40	Y	307	CLA	MG-NC	-3.45	1.98	2.06
40	u	306	CLA	C4B-NB	3.45	1.42	1.37
41	T	308	KC2	C4C-NC	3.45	1.43	1.37
40	S	314	CLA	C4B-NB	3.45	1.42	1.37
41	N	302	KC2	C4C-NC	3.45	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	J	318	CLA	MG-NC	-3.45	1.98	2.06
40	B	307	CLA	C4B-NB	3.44	1.42	1.37
40	b	820	CLA	C4B-NB	3.44	1.42	1.37
40	E	302	CLA	C4B-NB	3.44	1.42	1.37
40	b	826	CLA	C4B-NB	3.44	1.42	1.37
40	X	306	CLA	MG-NC	-3.44	1.98	2.06
40	k	202	CLA	MG-NC	-3.44	1.98	2.06
40	S	308	CLA	MG-NC	-3.44	1.98	2.06
40	C	306	CLA	MG-NC	-3.44	1.98	2.06
44	Z	316	A86	C32-C31	-3.44	1.48	1.54
41	O	309	KC2	C4C-NC	3.44	1.43	1.37
41	R	311	KC2	C4C-NC	3.44	1.43	1.37
40	a	829	CLA	MG-NC	-3.44	1.98	2.06
41	u	309	KC2	C4C-NC	3.44	1.43	1.37
41	N	312	KC2	C4C-NC	3.43	1.43	1.37
40	I	201	CLA	C4B-NB	3.43	1.42	1.37
41	W	310	KC2	C4C-NC	3.43	1.43	1.37
40	t	302	CLA	MG-NC	-3.43	1.98	2.06
41	y	307	KC2	C4C-NC	3.43	1.43	1.37
41	p	315	KC2	C1B-NB	3.43	1.42	1.37
40	H	305	CLA	MG-NC	-3.43	1.98	2.06
40	q	305	CLA	MG-NC	-3.43	1.98	2.06
41	v	308	KC2	C4C-NC	3.43	1.43	1.37
40	N	305	CLA	MG-NC	-3.43	1.98	2.06
40	H	311	CLA	MG-NC	-3.43	1.98	2.06
40	U	204	CLA	MG-NC	-3.43	1.98	2.06
40	p	313	CLA	C4B-NB	3.43	1.42	1.37
40	L	312	CLA	MG-NC	-3.43	1.98	2.06
40	W	305	CLA	MG-NC	-3.43	1.98	2.06
41	E	319	KC2	C4C-NC	3.43	1.43	1.37
40	y	309	CLA	MG-NC	-3.43	1.98	2.06
40	K	306	CLA	C4B-NB	3.43	1.42	1.37
41	u	304	KC2	C4C-NC	3.42	1.43	1.37
40	Y	307	CLA	C4B-NB	3.42	1.42	1.37
40	p	307	CLA	C4B-NB	3.42	1.42	1.37
41	N	301	KC2	C1B-NB	3.42	1.42	1.37
41	x	304	KC2	C1B-NB	3.42	1.42	1.37
41	w	306	KC2	C4C-NC	3.42	1.43	1.37
40	a	821	CLA	C4B-NB	3.42	1.42	1.37
40	x	302	CLA	MG-NC	-3.42	1.98	2.06
40	v	301	CLA	MG-NC	-3.42	1.98	2.06
41	G	202	KC2	C4C-NC	3.42	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	Z	307	CLA	C4B-NB	3.41	1.42	1.37
40	X	311	CLA	MG-NC	-3.41	1.98	2.06
41	Y	308	KC2	C4C-NC	3.41	1.43	1.37
41	F	302	KC2	C4C-NC	3.41	1.43	1.37
40	U	202	CLA	C4B-NB	3.41	1.42	1.37
40	C	301	CLA	MG-NC	-3.41	1.98	2.06
40	D	302	CLA	MG-NC	-3.41	1.98	2.06
40	a	808	CLA	C4B-NB	3.41	1.42	1.37
40	Y	312	CLA	C4B-NB	3.41	1.42	1.37
40	u	307	CLA	MG-NC	-3.41	1.98	2.06
41	x	310	KC2	C4C-NC	3.41	1.43	1.37
40	C	304	CLA	C4B-NB	3.41	1.42	1.37
40	b	827	CLA	C4B-NB	3.40	1.42	1.37
40	R	310	CLA	MG-NC	-3.40	1.98	2.06
40	E	308	CLA	C4B-NB	3.40	1.42	1.37
40	F	308	CLA	MG-NC	-3.40	1.98	2.06
40	p	305	CLA	C4B-NB	3.40	1.42	1.37
40	b	829	CLA	C4B-NB	3.40	1.42	1.37
40	E	303	CLA	MG-NC	-3.40	1.98	2.06
40	b	816	CLA	MG-NC	-3.40	1.98	2.06
41	w	301	KC2	C1B-NB	3.40	1.42	1.37
40	U	203	CLA	MG-NC	-3.40	1.98	2.06
40	F	305	CLA	MG-NC	-3.40	1.98	2.06
41	w	301	KC2	C4C-NC	3.40	1.43	1.37
40	b	825	CLA	C4B-NB	3.40	1.42	1.37
40	A	305	CLA	C4B-NB	3.39	1.42	1.37
40	a	842	CLA	C4B-NB	3.39	1.42	1.37
40	a	803	CLA	MG-NC	-3.39	1.98	2.06
41	L	313	KC2	C4C-NC	3.39	1.43	1.37
41	Y	309	KC2	C4C-NC	3.39	1.43	1.37
40	o	306	CLA	C4B-NB	3.39	1.42	1.37
41	v	309	KC2	C4C-NC	3.39	1.43	1.37
40	o	307	CLA	C4B-NB	3.39	1.42	1.37
40	F	307	CLA	C4B-NB	3.39	1.42	1.37
40	a	835	CLA	C4B-NB	3.39	1.42	1.37
41	o	303	KC2	C4C-NC	3.39	1.43	1.37
40	v	313	CLA	MG-NC	-3.39	1.98	2.06
40	Z	307	CLA	MG-NC	-3.39	1.98	2.06
40	u	305	CLA	MG-NC	-3.39	1.98	2.06
41	K	303	KC2	C4C-NC	3.39	1.43	1.37
40	F	301	CLA	MG-NC	-3.39	1.98	2.06
40	N	311	CLA	C4B-NB	3.38	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	P	302	KC2	C1B-NB	3.38	1.42	1.37
41	p	304	KC2	C4C-NC	3.38	1.43	1.37
40	X	306	CLA	C4B-NB	3.38	1.42	1.37
40	x	305	CLA	C4B-NB	3.38	1.42	1.37
40	a	827	CLA	MG-NC	-3.38	1.98	2.06
40	t	307	CLA	MG-NC	-3.38	1.98	2.06
40	k	202	CLA	C4B-NB	3.38	1.42	1.37
47	P	301	A1EB1	C32-C31	-3.38	1.48	1.54
40	X	307	CLA	MG-NC	-3.38	1.98	2.06
40	E	312	CLA	MG-NC	-3.38	1.98	2.06
40	X	304	CLA	MG-NC	-3.38	1.98	2.06
40	a	815	CLA	MG-NC	-3.38	1.98	2.06
40	D	309	CLA	MG-NC	-3.38	1.98	2.06
40	b	818	CLA	C4B-NB	3.37	1.42	1.37
40	I	203	CLA	C4B-NB	3.37	1.42	1.37
40	U	208	CLA	C4B-NB	3.37	1.42	1.37
44	u	317	A86	C32-C31	-3.37	1.48	1.54
41	R	309	KC2	C1B-NB	3.37	1.42	1.37
40	W	306	CLA	MG-NC	-3.37	1.98	2.06
40	X	304	CLA	C4B-NB	3.37	1.42	1.37
40	Z	312	CLA	C4B-NB	3.37	1.42	1.37
40	x	308	CLA	C4B-NB	3.37	1.42	1.37
40	H	301	CLA	C4B-NB	3.37	1.42	1.37
40	b	809	CLA	C4B-NB	3.37	1.42	1.37
40	a	816	CLA	MG-NC	-3.37	1.98	2.06
41	z	309	KC2	C1B-NB	3.37	1.42	1.37
41	T	309	KC2	C1B-NB	3.37	1.42	1.37
40	J	311	CLA	MG-NC	-3.37	1.98	2.06
40	q	310	CLA	C4B-NB	3.37	1.42	1.37
40	v	301	CLA	C4B-NB	3.37	1.42	1.37
40	Y	301	CLA	MG-NC	-3.37	1.98	2.06
40	v	305	CLA	MG-NC	-3.37	1.98	2.06
41	u	315	KC2	C4C-NC	3.36	1.43	1.37
40	D	310	CLA	C4B-NB	3.36	1.42	1.37
41	t	306	KC2	C4C-NC	3.36	1.43	1.37
41	N	313	KC2	C4C-NC	3.36	1.43	1.37
40	q	307	CLA	C4B-NB	3.36	1.42	1.37
40	o	310	CLA	C4B-NB	3.36	1.42	1.37
40	u	308	CLA	MG-NC	-3.36	1.98	2.06
40	M	311	CLA	C4B-NB	3.36	1.42	1.37
41	H	316	KC2	C1B-NB	3.36	1.42	1.37
47	x	321	A1EB1	C32-C31	-3.36	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	o	309	KC2	C1B-NB	3.36	1.42	1.37
44	X	314	A86	C32-C31	-3.36	1.48	1.54
44	v	315	A86	C32-C31	-3.36	1.48	1.54
40	b	839	CLA	C4B-NB	3.35	1.42	1.37
47	v	323	A1EB1	C32-C31	-3.35	1.48	1.54
41	o	309	KC2	C4C-NC	3.35	1.43	1.37
40	R	305	CLA	MG-NC	-3.35	1.98	2.06
40	T	310	CLA	C4B-NB	3.35	1.42	1.37
40	Y	311	CLA	MG-NC	-3.35	1.98	2.06
40	Z	304	CLA	MG-NC	-3.35	1.98	2.06
40	q	301	CLA	C4B-NB	3.35	1.42	1.37
44	z	318	A86	C32-C31	-3.34	1.48	1.54
40	a	813	CLA	MG-NC	-3.34	1.98	2.06
40	A	309	CLA	MG-NC	-3.34	1.98	2.06
40	U	206	CLA	MG-NC	-3.34	1.98	2.06
40	a	821	CLA	MG-NC	-3.34	1.98	2.06
40	K	304	CLA	MG-NC	-3.34	1.98	2.06
40	b	825	CLA	MG-NC	-3.34	1.98	2.06
40	D	306	CLA	MG-NC	-3.34	1.98	2.06
40	b	824	CLA	MG-NC	-3.34	1.98	2.06
40	H	304	CLA	MG-NC	-3.34	1.98	2.06
40	q	306	CLA	C4B-NB	3.33	1.42	1.37
40	F	321	CLA	C4B-NB	3.33	1.42	1.37
40	b	838	CLA	MG-NC	-3.33	1.98	2.06
40	b	837	CLA	C4B-NB	3.33	1.42	1.37
40	N	304	CLA	MG-NC	-3.33	1.98	2.06
40	y	309	CLA	C4B-NB	3.33	1.42	1.37
40	L	305	CLA	MG-NC	-3.33	1.98	2.06
44	S	316	A86	C32-C31	-3.33	1.49	1.54
40	N	311	CLA	MG-NC	-3.33	1.98	2.06
41	W	309	KC2	C4C-NC	3.33	1.43	1.37
40	x	306	CLA	C4B-NB	3.33	1.42	1.37
40	B	306	CLA	C4B-NB	3.33	1.42	1.37
41	x	315	KC2	C4C-NC	3.32	1.43	1.37
40	Y	304	CLA	MG-NC	-3.32	1.98	2.06
40	L	306	CLA	C4B-NB	3.32	1.42	1.37
40	b	808	CLA	C4B-NB	3.32	1.42	1.37
40	F	307	CLA	MG-NC	-3.32	1.98	2.06
40	T	304	CLA	MG-NC	-3.32	1.98	2.06
40	x	314	CLA	MG-NC	-3.32	1.98	2.06
40	G	207	CLA	MG-NC	-3.32	1.98	2.06
40	A	305	CLA	MG-NC	-3.32	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	a	810	CLA	MG-NC	-3.32	1.98	2.06
40	V	202	CLA	C4B-NB	3.32	1.42	1.37
40	q	301	CLA	MG-NC	-3.32	1.98	2.06
41	v	303	KC2	C4C-NC	3.31	1.43	1.37
41	p	304	KC2	C1B-NB	3.31	1.42	1.37
40	F	303	CLA	MG-NC	-3.31	1.98	2.06
44	v	316	A86	C32-C31	-3.31	1.49	1.54
40	b	840	CLA	MG-NC	-3.31	1.98	2.06
40	o	305	CLA	MG-NC	-3.31	1.98	2.06
40	C	302	CLA	MG-NC	-3.31	1.98	2.06
44	x	317	A86	C32-C31	-3.31	1.49	1.54
40	C	305	CLA	MG-NC	-3.31	1.98	2.06
40	q	313	CLA	MG-NC	-3.31	1.98	2.06
40	I	205	CLA	MG-NC	-3.31	1.98	2.06
40	R	307	CLA	MG-NC	-3.31	1.98	2.06
40	B	302	CLA	C4B-NB	3.31	1.42	1.37
40	b	822	CLA	C4B-NB	3.31	1.42	1.37
40	J	305	CLA	MG-NC	-3.30	1.98	2.06
40	Z	304	CLA	C4B-NB	3.30	1.42	1.37
40	v	305	CLA	C4B-NB	3.30	1.42	1.37
40	G	203	CLA	MG-NC	-3.30	1.98	2.06
40	D	308	CLA	MG-NC	-3.30	1.98	2.06
40	p	308	CLA	MG-NC	-3.30	1.98	2.06
41	z	309	KC2	C4C-NC	3.30	1.43	1.37
40	E	309	CLA	MG-NC	-3.30	1.98	2.06
40	I	204	CLA	MG-NC	-3.30	1.98	2.06
44	z	317	A86	C32-C31	-3.30	1.49	1.54
40	p	307	CLA	MG-NC	-3.30	1.98	2.06
40	H	306	CLA	MG-NC	-3.30	1.98	2.06
47	p	324	A1EB1	C32-C31	-3.30	1.49	1.54
41	x	315	KC2	C1B-NB	3.30	1.42	1.37
40	b	828	CLA	MG-NC	-3.30	1.98	2.06
40	w	309	CLA	MG-NC	-3.30	1.98	2.06
40	b	802	CLA	C4B-NB	3.29	1.42	1.37
40	W	313	CLA	MG-NC	-3.29	1.98	2.06
40	O	304	CLA	MG-NC	-3.29	1.98	2.06
40	o	311	CLA	C4B-NB	3.29	1.42	1.37
40	b	833	CLA	C4B-NB	3.29	1.42	1.37
40	R	304	CLA	MG-NC	-3.29	1.98	2.06
40	u	313	CLA	MG-NC	-3.29	1.98	2.06
40	D	310	CLA	MG-NC	-3.29	1.98	2.06
40	M	307	CLA	MG-NC	-3.28	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	E	302	CLA	MG-NC	-3.28	1.98	2.06
40	S	308	CLA	C4B-NB	3.28	1.42	1.37
41	N	303	KC2	C1B-NB	3.28	1.42	1.37
40	F	311	CLA	MG-NC	-3.28	1.98	2.06
40	v	310	CLA	C4B-NB	3.28	1.42	1.37
40	a	818	CLA	C4B-NB	3.28	1.42	1.37
41	Y	303	KC2	C4C-NC	3.28	1.43	1.37
44	o	316	A86	C32-C31	-3.28	1.49	1.54
40	Z	311	CLA	C4B-NB	3.27	1.42	1.37
40	p	311	CLA	C4B-NB	3.27	1.42	1.37
40	J	306	CLA	MG-NC	-3.27	1.98	2.06
40	z	314	CLA	C4B-NB	3.27	1.42	1.37
40	B	303	CLA	MG-NC	-3.27	1.98	2.06
40	b	835	CLA	MG-NC	-3.27	1.98	2.06
40	S	306	CLA	MG-NC	-3.27	1.98	2.06
40	u	306	CLA	MG-NC	-3.26	1.98	2.06
44	q	316	A86	C32-C31	-3.26	1.49	1.54
40	x	305	CLA	MG-NC	-3.26	1.98	2.06
40	b	816	CLA	C4B-NB	3.26	1.42	1.37
40	A	308	CLA	MG-NC	-3.26	1.98	2.06
40	W	311	CLA	C4B-NB	3.26	1.42	1.37
40	M	311	CLA	MG-NC	-3.26	1.98	2.06
41	X	309	KC2	C1B-NB	3.26	1.42	1.37
40	Q	202	CLA	MG-NC	-3.26	1.98	2.06
44	p	317	A86	C32-C31	-3.26	1.49	1.54
44	o	315	A86	C32-C31	-3.26	1.49	1.54
40	b	828	CLA	C4B-NB	3.26	1.42	1.37
40	V	201	CLA	MG-NC	-3.26	1.98	2.06
40	y	303	CLA	MG-NC	-3.26	1.98	2.06
40	b	815	CLA	MG-NC	-3.26	1.98	2.06
40	z	305	CLA	C4B-NB	3.26	1.42	1.37
40	G	205	CLA	MG-NC	-3.25	1.98	2.06
40	x	302	CLA	C4B-NB	3.25	1.42	1.37
40	Z	306	CLA	MG-NC	-3.25	1.98	2.06
47	u	323	A1EB1	C32-C31	-3.25	1.49	1.54
47	L	316	A1EB1	C32-C31	-3.25	1.49	1.54
40	z	307	CLA	MG-NC	-3.25	1.98	2.06
40	l	205	CLA	C4B-NB	3.25	1.42	1.37
40	a	805	CLA	MG-NC	-3.24	1.98	2.06
40	w	303	CLA	MG-NC	-3.24	1.98	2.06
40	p	302	CLA	MG-NC	-3.24	1.98	2.06
40	b	810	CLA	C4B-NB	3.24	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	J	309	CLA	MG-NC	-3.24	1.98	2.06
40	b	802	CLA	MG-NC	-3.24	1.98	2.06
40	w	302	CLA	MG-NC	-3.24	1.98	2.06
41	N	309	KC2	C4C-NC	3.24	1.43	1.37
40	x	308	CLA	MG-NC	-3.24	1.98	2.06
40	a	803	CLA	C4B-NB	3.24	1.42	1.37
47	K	313	A1EB1	C32-C31	-3.24	1.49	1.54
40	f	201	CLA	MG-NC	-3.23	1.98	2.06
40	z	305	CLA	MG-NC	-3.23	1.98	2.06
40	C	307	CLA	C4B-NB	3.23	1.42	1.37
41	H	316	KC2	C4C-NC	3.23	1.43	1.37
40	P	313	CLA	MG-NC	-3.22	1.98	2.06
40	R	306	CLA	MG-NC	-3.22	1.98	2.06
40	y	305	CLA	MG-NC	-3.22	1.98	2.06
40	b	807	CLA	MG-NC	-3.22	1.98	2.06
40	D	307	CLA	MG-NC	-3.22	1.98	2.06
40	b	831	CLA	MG-NC	-3.22	1.98	2.06
40	A	307	CLA	MG-NC	-3.22	1.98	2.06
40	b	817	CLA	MG-NC	-3.22	1.98	2.06
40	o	306	CLA	MG-NC	-3.22	1.98	2.06
40	L	307	CLA	MG-NC	-3.22	1.98	2.06
40	S	313	CLA	MG-NC	-3.22	1.98	2.06
40	T	307	CLA	MG-NC	-3.21	1.98	2.06
40	b	823	CLA	MG-NC	-3.21	1.98	2.06
40	a	834	CLA	C4B-NB	3.21	1.42	1.37
40	A	301	CLA	C4B-NB	3.21	1.42	1.37
40	a	831	CLA	MG-NC	-3.21	1.98	2.06
40	D	312	CLA	MG-NC	-3.21	1.98	2.06
40	A	301	CLA	MG-NC	-3.20	1.98	2.06
40	a	833	CLA	MG-NC	-3.20	1.98	2.06
41	u	315	KC2	C1B-NB	3.20	1.42	1.37
40	v	306	CLA	C4B-NB	3.20	1.42	1.37
40	t	305	CLA	MG-NC	-3.20	1.98	2.06
40	O	305	CLA	MG-NC	-3.20	1.98	2.06
40	b	834	CLA	C4B-NB	3.20	1.42	1.37
40	X	310	CLA	C4B-NB	3.20	1.42	1.37
40	D	304	CLA	MG-NC	-3.20	1.98	2.06
40	Y	306	CLA	MG-NC	-3.20	1.98	2.06
40	z	306	CLA	C4B-NB	3.20	1.42	1.37
40	I	201	CLA	MG-NC	-3.20	1.98	2.06
41	O	309	KC2	C1B-NB	3.19	1.42	1.37
44	z	316	A86	C32-C31	-3.19	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	i	101	CLA	C4B-NB	3.19	1.42	1.37
40	F	321	CLA	MG-NC	-3.19	1.98	2.06
40	N	307	CLA	MG-NC	-3.19	1.98	2.06
40	b	830	CLA	C4B-NB	3.19	1.42	1.37
40	a	841	CLA	C4B-NB	3.19	1.42	1.37
40	X	311	CLA	C4B-NB	3.19	1.42	1.37
40	o	301	CLA	MG-NC	-3.19	1.98	2.06
44	X	320	A86	C32-C31	-3.18	1.49	1.54
40	a	819	CLA	MG-NC	-3.18	1.98	2.06
40	a	837	CLA	MG-NC	-3.18	1.98	2.06
40	w	304	CLA	MG-NC	-3.18	1.98	2.06
40	u	307	CLA	C4B-NB	3.18	1.42	1.37
40	D	305	CLA	MG-NC	-3.17	1.98	2.06
40	E	310	CLA	MG-NC	-3.17	1.98	2.06
40	P	306	CLA	MG-NC	-3.17	1.98	2.06
40	G	203	CLA	C4B-NB	3.17	1.42	1.37
40	a	826	CLA	MG-NC	-3.17	1.98	2.06
40	u	311	CLA	C4B-NB	3.17	1.42	1.37
40	q	304	CLA	MG-NC	-3.17	1.98	2.06
40	u	302	CLA	C4B-NB	3.16	1.42	1.37
40	b	812	CLA	C4B-NB	3.16	1.42	1.37
40	H	310	CLA	MG-NC	-3.16	1.98	2.06
40	P	308	CLA	MG-NC	-3.16	1.98	2.06
40	P	313	CLA	C4B-NB	3.15	1.42	1.37
40	b	826	CLA	MG-NC	-3.15	1.98	2.06
40	Q	206	CLA	MG-NC	-3.15	1.98	2.06
40	H	308	CLA	MG-NC	-3.15	1.98	2.06
40	o	311	CLA	MG-NC	-3.15	1.98	2.06
44	z	319	A86	C32-C31	-3.15	1.49	1.54
40	b	819	CLA	MG-NC	-3.15	1.98	2.06
40	x	311	CLA	C4B-NB	3.15	1.42	1.37
40	b	810	CLA	MG-NC	-3.15	1.98	2.06
40	a	839	CLA	MG-NC	-3.15	1.98	2.06
40	u	302	CLA	MG-NC	-3.15	1.98	2.06
40	a	832	CLA	MG-NC	-3.15	1.98	2.06
40	F	306	CLA	MG-NC	-3.15	1.98	2.06
44	q	314	A86	C32-C31	-3.15	1.49	1.54
40	G	204	CLA	MG-NC	-3.14	1.98	2.06
40	v	304	CLA	MG-NC	-3.14	1.98	2.06
40	l	203	CLA	C4B-NB	3.14	1.42	1.37
41	t	301	KC2	C4C-NC	3.14	1.43	1.37
40	a	830	CLA	MG-NC	-3.14	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	b	813	CLA	MG-NC	-3.14	1.98	2.06
40	b	842	CLA	MG-NC	-3.14	1.98	2.06
40	M	310	CLA	MG-NC	-3.14	1.98	2.06
41	Z	309	KC2	C1B-NB	3.14	1.42	1.37
40	Z	305	CLA	MG-NC	-3.13	1.98	2.06
40	E	306	CLA	MG-NC	-3.13	1.98	2.06
40	G	201	CLA	MG-NC	-3.13	1.98	2.06
40	Y	310	CLA	MG-NC	-3.13	1.98	2.06
40	X	301	CLA	MG-NC	-3.13	1.98	2.06
40	y	304	CLA	MG-NC	-3.13	1.98	2.06
40	b	807	CLA	C4B-NB	3.13	1.42	1.37
40	w	305	CLA	MG-NC	-3.12	1.98	2.06
40	q	305	CLA	C4B-NB	3.12	1.42	1.37
40	p	312	CLA	MG-NC	-3.12	1.98	2.06
44	y	310	A86	C32-C31	-3.12	1.49	1.54
40	b	811	CLA	MG-NC	-3.12	1.98	2.06
40	E	308	CLA	MG-NC	-3.12	1.98	2.06
40	a	807	CLA	MG-NC	-3.12	1.98	2.06
40	x	307	CLA	C4B-NB	3.12	1.42	1.37
40	a	840	CLA	MG-NC	-3.12	1.98	2.06
40	J	302	CLA	MG-NC	-3.11	1.98	2.06
40	o	304	CLA	MG-NC	-3.11	1.98	2.06
40	z	312	CLA	MG-NC	-3.11	1.98	2.06
40	T	305	CLA	MG-NC	-3.11	1.98	2.06
40	P	312	CLA	MG-NC	-3.10	1.98	2.06
40	t	309	CLA	MG-NC	-3.10	1.98	2.06
47	z	323	A1EB1	C32-C31	-3.10	1.49	1.54
40	x	313	CLA	MG-NC	-3.09	1.98	2.06
47	S	320	A1EB1	C32-C31	-3.09	1.49	1.54
40	a	835	CLA	MG-NC	-3.09	1.98	2.06
40	D	305	CLA	C4D-CHA	3.08	1.44	1.39
40	l	204	CLA	MG-NC	-3.08	1.98	2.06
41	z	304	KC2	C4C-NC	3.08	1.42	1.37
40	b	812	CLA	MG-NC	-3.08	1.99	2.06
40	t	303	CLA	MG-NC	-3.08	1.99	2.06
40	K	312	CLA	MG-NC	-3.08	1.99	2.06
40	Z	301	CLA	MG-NC	-3.08	1.99	2.06
40	Z	310	CLA	C4B-NB	3.08	1.41	1.37
44	Y	315	A86	C32-C31	-3.08	1.49	1.54
40	O	307	CLA	MG-NC	-3.08	1.99	2.06
40	b	814	CLA	MG-NC	-3.08	1.99	2.06
40	k	201	CLA	MG-NC	-3.08	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	G	211	A86	C32-C31	-3.07	1.49	1.54
44	M	315	A86	C32-C31	-3.07	1.49	1.54
52	b	850	DGD	O1G-C1G	-3.07	1.38	1.45
47	o	321	A1EB1	C32-C31	-3.07	1.49	1.54
40	N	306	CLA	MG-NC	-3.07	1.99	2.06
40	b	824	CLA	C4B-NB	3.07	1.41	1.37
40	E	307	CLA	MG-NC	-3.06	1.99	2.06
40	A	304	CLA	C4B-NB	3.06	1.41	1.37
40	b	817	CLA	C4B-NB	3.06	1.41	1.37
40	B	302	CLA	MG-NC	-3.06	1.99	2.06
40	q	306	CLA	MG-NC	-3.06	1.99	2.06
40	a	852	CLA	MG-NC	-3.06	1.99	2.06
40	A	302	CLA	MG-NC	-3.06	1.99	2.06
44	w	316	A86	C32-C31	-3.06	1.49	1.54
40	b	803	CLA	MG-NC	-3.06	1.99	2.06
40	K	306	CLA	MG-NC	-3.06	1.99	2.06
44	t	311	A86	C32-C31	-3.06	1.49	1.54
41	K	305	KC2	C1B-NB	3.05	1.41	1.37
40	H	301	CLA	MG-NC	-3.05	1.99	2.06
40	t	304	CLA	MG-NC	-3.05	1.99	2.06
44	Y	317	A86	C32-C31	-3.05	1.49	1.54
40	a	842	CLA	MG-NC	-3.04	1.99	2.06
40	M	312	CLA	MG-NC	-3.04	1.99	2.06
40	v	311	CLA	C4B-NB	3.04	1.41	1.37
40	q	311	CLA	C4B-NB	3.04	1.41	1.37
40	S	307	CLA	MG-NC	-3.03	1.99	2.06
40	z	308	CLA	C4B-NB	3.03	1.41	1.37
40	v	306	CLA	MG-NC	-3.02	1.99	2.06
40	O	316	CLA	MG-NC	-3.02	1.99	2.06
40	S	302	CLA	MG-NC	-3.02	1.99	2.06
40	a	825	CLA	MG-NC	-3.02	1.99	2.06
44	N	314	A86	C32-C31	-3.02	1.49	1.54
40	a	836	CLA	MG-NC	-3.01	1.99	2.06
40	z	311	CLA	C4B-NB	3.01	1.41	1.37
40	A	311	CLA	MG-NC	-3.01	1.99	2.06
44	G	209	A86	C32-C31	-3.01	1.49	1.54
40	E	314	CLA	C4B-NB	3.01	1.41	1.37
40	K	308	CLA	C4B-NB	3.01	1.41	1.37
40	a	822	CLA	MG-NC	-3.01	1.99	2.06
40	z	302	CLA	MG-NC	-3.01	1.99	2.06
40	v	312	CLA	MG-NC	-3.01	1.99	2.06
40	b	833	CLA	MG-NC	-3.00	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	b	838	CLA	C4B-NB	3.00	1.41	1.37
40	P	307	CLA	MG-NC	-3.00	1.99	2.06
40	M	306	CLA	MG-NC	-3.00	1.99	2.06
40	l	202	CLA	MG-NC	-2.99	1.99	2.06
40	q	311	CLA	MG-NC	-2.99	1.99	2.06
47	Z	319	A1EB1	C32-C31	-2.98	1.49	1.54
40	a	812	CLA	MG-NC	-2.98	1.99	2.06
40	v	311	CLA	MG-NC	-2.98	1.99	2.06
40	D	305	CLA	C3D-C2D	2.98	1.42	1.35
40	q	312	CLA	MG-NC	-2.98	1.99	2.06
40	A	306	CLA	MG-NC	-2.98	1.99	2.06
40	E	313	CLA	MG-NC	-2.98	1.99	2.06
47	q	321	A1EB1	C32-C31	-2.97	1.49	1.54
40	a	818	CLA	MG-NC	-2.97	1.99	2.06
40	S	319	CLA	MG-NC	-2.97	1.99	2.06
40	I	206	CLA	MG-NC	-2.97	1.99	2.06
40	a	817	CLA	MG-NC	-2.97	1.99	2.06
44	X	316	A86	C32-C31	-2.97	1.49	1.54
44	t	310	A86	C32-C31	-2.96	1.49	1.54
40	a	828	CLA	MG-NC	-2.96	1.99	2.06
40	I	202	CLA	MG-NC	-2.96	1.99	2.06
40	K	301	CLA	MG-NC	-2.95	1.99	2.06
40	Q	208	CLA	MG-NC	-2.95	1.99	2.06
40	W	307	CLA	MG-NC	-2.95	1.99	2.06
40	b	841	CLA	MG-NC	-2.95	1.99	2.06
40	R	316	CLA	MG-NC	-2.94	1.99	2.06
40	a	824	CLA	MG-NC	-2.94	1.99	2.06
40	z	312	CLA	C4B-NB	2.94	1.41	1.37
40	W	312	CLA	C4B-NB	2.94	1.41	1.37
40	D	301	CLA	MG-NC	-2.93	1.99	2.06
44	P	321	A86	C32-C31	-2.93	1.49	1.54
40	b	806	CLA	MG-NC	-2.92	1.99	2.06
40	M	305	CLA	MG-NC	-2.92	1.99	2.06
40	K	307	CLA	MG-NC	-2.91	1.99	2.06
47	T	316	A1EB1	C32-C31	-2.91	1.49	1.54
44	v	314	A86	C32-C31	-2.91	1.49	1.54
40	K	308	CLA	MG-NC	-2.91	1.99	2.06
40	b	811	CLA	C4B-NB	2.91	1.41	1.37
40	a	823	CLA	MG-NC	-2.91	1.99	2.06
40	p	305	CLA	MG-NC	-2.90	1.99	2.06
47	w	314	A1EB1	C32-C31	-2.89	1.49	1.54
40	y	308	CLA	MG-NC	-2.89	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	w	308	CLA	MG-NC	-2.89	1.99	2.06
40	G	206	CLA	MG-NC	-2.89	1.99	2.06
41	q	302	KC2	C4C-NC	2.88	1.42	1.37
44	T	312	A86	C32-C31	-2.88	1.49	1.54
40	M	304	CLA	MG-NC	-2.87	1.99	2.06
40	F	310	CLA	MG-NC	-2.86	1.99	2.06
44	q	315	A86	C32-C31	-2.86	1.49	1.54
40	T	306	CLA	MG-NC	-2.85	1.99	2.06
40	x	312	CLA	MG-NC	-2.85	1.99	2.06
40	U	203	CLA	C4B-NB	2.85	1.41	1.37
40	f	205	CLA	MG-NC	-2.84	1.99	2.06
44	F	312	A86	C32-C31	-2.84	1.49	1.54
40	b	840	CLA	C4B-NB	2.83	1.41	1.37
40	J	308	CLA	MG-NC	-2.83	1.99	2.06
44	M	316	A86	C32-C31	-2.83	1.49	1.54
40	b	821	CLA	MG-NC	-2.82	1.99	2.06
47	v	321	A1EB1	C32-C31	-2.82	1.49	1.54
44	Z	315	A86	C32-C31	-2.81	1.49	1.54
40	T	317	CLA	MG-NC	-2.81	1.99	2.06
40	P	305	CLA	MG-NC	-2.80	1.99	2.06
43	S	322	LMG	C7-C8	2.79	1.59	1.50
40	b	818	CLA	MG-NC	-2.78	1.99	2.06
40	f	202	CLA	MG-NC	-2.78	1.99	2.06
40	J	312	CLA	MG-NC	-2.77	1.99	2.06
40	p	313	CLA	MG-NC	-2.77	1.99	2.06
40	b	803	CLA	C4B-NB	2.76	1.41	1.37
40	U	208	CLA	MG-NC	-2.76	1.99	2.06
40	A	303	CLA	MG-NC	-2.75	1.99	2.06
40	E	304	CLA	MG-NC	-2.75	1.99	2.06
40	D	303	CLA	MG-NC	-2.75	1.99	2.06
44	z	301	A86	C32-C31	-2.74	1.50	1.54
44	O	312	A86	C32-C31	-2.73	1.50	1.54
44	N	321	A86	C32-C31	-2.72	1.50	1.54
44	Q	215	A86	C32-C31	-2.72	1.50	1.54
40	f	204	CLA	MG-NC	-2.71	1.99	2.06
43	P	318	LMG	C4-C5	2.71	1.58	1.53
44	R	315	A86	C32-C31	-2.68	1.50	1.54
47	y	313	A1EB1	C32-C31	-2.67	1.50	1.54
40	a	850	CLA	C4B-NB	2.67	1.41	1.37
47	S	321	A1EB1	C32-C31	-2.66	1.50	1.54
44	K	314	A86	C32-C31	-2.64	1.50	1.54
40	u	312	CLA	MG-NC	-2.64	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	S	317	A86	C32-C31	-2.64	1.50	1.54
44	D	320	A86	C32-C31	-2.63	1.50	1.54
44	H	315	A86	C32-C31	-2.62	1.50	1.54
44	W	301	A86	C32-C31	-2.62	1.50	1.54
44	x	318	A86	C32-C31	-2.60	1.50	1.54
44	q	317	A86	C32-C31	-2.58	1.50	1.54
40	D	305	CLA	C3D-C4D	-2.58	1.39	1.44
47	w	313	A1EB1	C32-C31	-2.57	1.50	1.54
47	t	315	A1EB1	C32-C31	-2.57	1.50	1.54
40	v	301	CLA	C1D-C2D	-2.56	1.40	1.45
44	D	319	A86	C32-C31	-2.56	1.50	1.54
43	E	321	LMG	C4-C5	2.53	1.58	1.53
44	X	317	A86	C32-C31	-2.53	1.50	1.54
44	v	317	A86	C32-C31	-2.52	1.50	1.54
40	a	825	CLA	C1D-C2D	-2.52	1.40	1.45
40	W	312	CLA	MG-NC	-2.52	2.00	2.06
47	y	312	A1EB1	C32-C31	-2.50	1.50	1.54
44	Z	314	A86	C32-C31	-2.50	1.50	1.54
40	B	307	CLA	C1D-C2D	-2.49	1.40	1.45
40	b	821	CLA	C1D-C2D	-2.49	1.40	1.45
44	Y	316	A86	C32-C31	-2.49	1.50	1.54
40	a	850	CLA	C3D-C4D	-2.46	1.38	1.44
45	F	319	LHG	P-O6	2.46	1.69	1.59
40	b	807	CLA	C1D-C2D	-2.44	1.40	1.45
40	p	313	CLA	C1D-C2D	-2.44	1.40	1.45
40	b	808	CLA	C1D-C2D	-2.44	1.40	1.45
44	o	314	A86	C32-C31	-2.44	1.50	1.54
40	a	824	CLA	C1D-C2D	-2.44	1.40	1.45
40	b	825	CLA	C1D-C2D	-2.43	1.40	1.45
47	t	313	A1EB1	C32-C31	-2.42	1.50	1.54
44	o	317	A86	C32-C31	-2.42	1.50	1.54
40	J	307	CLA	C1D-C2D	-2.41	1.40	1.45
44	P	317	A86	C32-C31	-2.40	1.50	1.54
44	p	318	A86	C32-C31	-2.40	1.50	1.54
44	w	310	A86	C32-C31	-2.40	1.50	1.54
40	f	201	CLA	C1D-C2D	-2.39	1.40	1.45
40	f	205	CLA	C1D-C2D	-2.38	1.40	1.45
40	y	303	CLA	C3D-C4D	-2.38	1.38	1.44
40	Q	206	CLA	C1D-C2D	-2.38	1.40	1.45
40	x	313	CLA	C1D-C2D	-2.38	1.40	1.45
44	u	318	A86	C32-C31	-2.37	1.50	1.54
40	Q	208	CLA	C1D-C2D	-2.37	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	a	832	CLA	C1D-C2D	-2.37	1.40	1.45
40	b	838	CLA	C3D-C4D	-2.37	1.38	1.44
40	b	834	CLA	C1D-C2D	-2.37	1.40	1.45
40	W	312	CLA	C1D-C2D	-2.37	1.40	1.45
40	x	302	CLA	C3D-C4D	-2.36	1.38	1.44
44	S	318	A86	C32-C31	-2.36	1.50	1.54
40	X	304	CLA	C1D-C2D	-2.36	1.40	1.45
40	b	835	CLA	C1D-C2D	-2.36	1.40	1.45
40	a	837	CLA	C1D-C2D	-2.35	1.40	1.45
40	b	841	CLA	C1D-C2D	-2.35	1.40	1.45
40	b	834	CLA	C3D-C4D	-2.35	1.38	1.44
43	x	301	LMG	C4-C5	2.35	1.58	1.53
40	b	815	CLA	C3D-C4D	-2.34	1.38	1.44
40	z	305	CLA	C1D-C2D	-2.34	1.40	1.45
40	a	842	CLA	C1D-C2D	-2.34	1.40	1.45
44	Y	319	A86	C32-C31	-2.34	1.50	1.54
40	a	827	CLA	C1D-C2D	-2.34	1.40	1.45
40	x	308	CLA	C1D-C2D	-2.34	1.40	1.45
40	J	312	CLA	C1D-C2D	-2.34	1.40	1.45
40	B	306	CLA	C1D-C2D	-2.33	1.40	1.45
40	S	307	CLA	C3D-C4D	-2.33	1.38	1.44
40	a	803	CLA	C1D-C2D	-2.33	1.40	1.45
40	W	311	CLA	C3D-C4D	-2.33	1.38	1.44
40	t	302	CLA	C3D-C4D	-2.33	1.38	1.44
40	S	302	CLA	C1D-C2D	-2.33	1.40	1.45
40	b	806	CLA	C1D-C2D	-2.33	1.40	1.45
40	A	302	CLA	C1D-C2D	-2.33	1.40	1.45
40	Z	304	CLA	C1D-C2D	-2.33	1.40	1.45
40	H	305	CLA	C1D-C2D	-2.33	1.40	1.45
40	q	312	CLA	C1D-C2D	-2.33	1.40	1.45
40	J	305	CLA	C1D-C2D	-2.33	1.40	1.45
40	A	303	CLA	C1D-C2D	-2.33	1.40	1.45
40	l	205	CLA	C1D-C2D	-2.33	1.40	1.45
40	f	202	CLA	C1D-C2D	-2.33	1.40	1.45
40	v	311	CLA	C1D-C2D	-2.33	1.40	1.45
40	z	302	CLA	C1D-C2D	-2.33	1.40	1.45
40	A	311	CLA	C1D-C2D	-2.33	1.40	1.45
40	z	311	CLA	C3D-C4D	-2.32	1.39	1.44
40	P	305	CLA	C1D-C2D	-2.32	1.40	1.45
40	H	304	CLA	C1D-C2D	-2.32	1.40	1.45
40	F	304	CLA	C1D-C2D	-2.32	1.40	1.45
40	C	308	CLA	C1D-C2D	-2.32	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	T	320	A1EB1	C32-C31	-2.32	1.50	1.54
40	u	311	CLA	C3D-C4D	-2.32	1.39	1.44
40	a	806	CLA	C3D-C4D	-2.32	1.39	1.44
40	T	305	CLA	C1D-C2D	-2.32	1.40	1.45
40	X	310	CLA	C3D-C4D	-2.32	1.39	1.44
40	z	305	CLA	C3D-C4D	-2.32	1.39	1.44
40	l	204	CLA	C1D-C2D	-2.32	1.40	1.45
40	u	313	CLA	C1D-C2D	-2.31	1.40	1.45
44	X	319	A86	C32-C31	-2.31	1.50	1.54
40	o	307	CLA	C3D-C4D	-2.31	1.39	1.44
40	L	305	CLA	C1D-C2D	-2.31	1.40	1.45
40	Z	305	CLA	C1D-C2D	-2.31	1.40	1.45
40	O	305	CLA	C3D-C4D	-2.31	1.39	1.44
40	u	302	CLA	C3D-C4D	-2.31	1.39	1.44
40	P	306	CLA	C1D-C2D	-2.31	1.40	1.45
40	b	826	CLA	C1D-C2D	-2.31	1.40	1.45
40	S	319	CLA	C1D-C2D	-2.31	1.40	1.45
40	D	306	CLA	C1D-C2D	-2.31	1.40	1.45
40	F	303	CLA	C1D-C2D	-2.31	1.40	1.45
40	p	314	CLA	C1D-C2D	-2.31	1.40	1.45
40	X	311	CLA	C3D-C4D	-2.30	1.39	1.44
40	a	812	CLA	C1D-C2D	-2.30	1.40	1.45
40	Y	305	CLA	C1D-C2D	-2.30	1.40	1.45
40	a	826	CLA	C1D-C2D	-2.30	1.40	1.45
44	p	319	A86	C32-C31	-2.30	1.50	1.54
40	b	822	CLA	C3D-C4D	-2.30	1.39	1.44
40	v	305	CLA	C3D-C4D	-2.30	1.39	1.44
40	b	842	CLA	C1D-C2D	-2.30	1.40	1.45
40	Z	307	CLA	C3D-C4D	-2.30	1.39	1.44
40	z	308	CLA	C3D-C4D	-2.30	1.39	1.44
40	u	305	CLA	C3D-C4D	-2.30	1.39	1.44
40	w	309	CLA	C3D-C4D	-2.30	1.39	1.44
40	R	305	CLA	C3D-C4D	-2.30	1.39	1.44
40	p	305	CLA	C3D-C4D	-2.30	1.39	1.44
40	b	831	CLA	C1D-C2D	-2.30	1.40	1.45
40	q	307	CLA	C3D-C4D	-2.30	1.39	1.44
40	E	304	CLA	C1D-C2D	-2.30	1.40	1.45
40	O	307	CLA	C1D-C2D	-2.30	1.40	1.45
40	E	307	CLA	C1D-C2D	-2.30	1.40	1.45
40	A	304	CLA	C3D-C4D	-2.30	1.39	1.44
40	b	813	CLA	C1D-C2D	-2.30	1.40	1.45
40	z	307	CLA	C1D-C2D	-2.29	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	D	310	CLA	C3D-C4D	-2.29	1.39	1.44
40	l	203	CLA	C3D-C4D	-2.29	1.39	1.44
40	x	312	CLA	C1D-C2D	-2.29	1.40	1.45
40	E	306	CLA	C3D-C4D	-2.29	1.39	1.44
40	T	317	CLA	C1D-C2D	-2.29	1.40	1.45
40	L	304	CLA	C3D-C4D	-2.29	1.39	1.44
40	o	304	CLA	C3D-C4D	-2.29	1.39	1.44
40	N	306	CLA	C1D-C2D	-2.29	1.40	1.45
44	F	317	A86	C32-C31	-2.29	1.50	1.54
40	G	201	CLA	C1D-C2D	-2.29	1.40	1.45
40	K	308	CLA	C1D-C2D	-2.29	1.40	1.45
40	F	306	CLA	C1D-C2D	-2.29	1.40	1.45
40	J	309	CLA	C1D-C2D	-2.29	1.40	1.45
40	v	307	CLA	C3D-C4D	-2.29	1.39	1.44
40	P	311	CLA	C1D-C2D	-2.29	1.40	1.45
40	B	302	CLA	C1D-C2D	-2.29	1.40	1.45
40	b	810	CLA	C1D-C2D	-2.29	1.40	1.45
40	U	207	CLA	C1D-C2D	-2.29	1.40	1.45
40	C	307	CLA	C3D-C4D	-2.29	1.39	1.44
40	W	307	CLA	C1D-C2D	-2.29	1.40	1.45
40	b	828	CLA	C1D-C2D	-2.29	1.40	1.45
44	F	313	A86	C32-C31	-2.29	1.50	1.54
40	X	311	CLA	C1D-C2D	-2.28	1.40	1.45
40	a	823	CLA	C1D-C2D	-2.28	1.40	1.45
40	b	812	CLA	C1D-C2D	-2.28	1.40	1.45
40	a	835	CLA	C3D-C4D	-2.28	1.39	1.44
40	H	308	CLA	C1D-C2D	-2.28	1.40	1.45
40	x	311	CLA	C3D-C4D	-2.28	1.39	1.44
40	T	307	CLA	C3D-C4D	-2.28	1.39	1.44
40	x	305	CLA	C3D-C4D	-2.28	1.39	1.44
40	I	206	CLA	C1D-C2D	-2.28	1.40	1.45
40	R	316	CLA	C1D-C2D	-2.28	1.40	1.45
40	t	307	CLA	C3D-C4D	-2.28	1.39	1.44
40	x	307	CLA	C3D-C4D	-2.28	1.39	1.44
40	k	202	CLA	C1D-C2D	-2.28	1.40	1.45
40	Z	310	CLA	C3D-C4D	-2.28	1.39	1.44
40	Q	202	CLA	C1D-C2D	-2.28	1.40	1.45
40	b	824	CLA	C1D-C2D	-2.28	1.40	1.45
40	O	316	CLA	C1D-C2D	-2.28	1.40	1.45
40	q	301	CLA	C1D-C2D	-2.28	1.40	1.45
40	b	840	CLA	C1D-C2D	-2.28	1.40	1.45
40	K	307	CLA	C1D-C2D	-2.28	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	K	308	CLA	C3D-C4D	-2.27	1.39	1.44
40	R	306	CLA	C1D-C2D	-2.27	1.40	1.45
40	G	204	CLA	C3D-C4D	-2.27	1.39	1.44
40	a	818	CLA	C3D-C4D	-2.27	1.39	1.44
40	b	835	CLA	C3D-C4D	-2.27	1.39	1.44
40	f	202	CLA	C3D-C4D	-2.27	1.39	1.44
40	a	834	CLA	C3D-C4D	-2.27	1.39	1.44
40	C	306	CLA	C1D-C2D	-2.27	1.40	1.45
40	H	309	CLA	C1D-C2D	-2.27	1.40	1.45
40	G	207	CLA	C1D-C2D	-2.27	1.40	1.45
40	a	852	CLA	C1D-C2D	-2.27	1.40	1.45
40	b	803	CLA	C3D-C4D	-2.27	1.39	1.44
40	A	309	CLA	C1D-C2D	-2.27	1.40	1.45
40	b	842	CLA	C3D-C4D	-2.27	1.39	1.44
40	q	305	CLA	C3D-C4D	-2.27	1.39	1.44
40	b	837	CLA	C3D-C4D	-2.27	1.39	1.44
40	b	805	CLA	C3D-C4D	-2.27	1.39	1.44
40	E	313	CLA	C1D-C2D	-2.27	1.40	1.45
40	b	833	CLA	C3D-C4D	-2.27	1.39	1.44
43	M	317	LMG	C7-C8	2.27	1.57	1.50
40	b	828	CLA	C3D-C4D	-2.27	1.39	1.44
40	b	838	CLA	C1D-C2D	-2.27	1.40	1.45
40	z	307	CLA	C3D-C4D	-2.27	1.39	1.44
40	C	305	CLA	C3D-C4D	-2.27	1.39	1.44
40	M	304	CLA	C1D-C2D	-2.26	1.40	1.45
40	a	851	CLA	C1D-C2D	-2.26	1.40	1.45
40	E	309	CLA	C1D-C2D	-2.26	1.40	1.45
43	P	318	LMG	C7-C8	2.26	1.57	1.50
40	A	306	CLA	C1D-C2D	-2.26	1.40	1.45
40	D	302	CLA	C1D-C2D	-2.26	1.40	1.45
40	E	306	CLA	C1D-C2D	-2.26	1.40	1.45
40	P	307	CLA	C1D-C2D	-2.26	1.40	1.45
40	b	830	CLA	C3D-C4D	-2.26	1.39	1.44
40	y	309	CLA	C3D-C4D	-2.26	1.39	1.44
40	b	839	CLA	C3D-C4D	-2.26	1.39	1.44
43	T	318	LMG	O7-C8	-2.26	1.41	1.46
40	b	832	CLA	C1D-C2D	-2.26	1.40	1.45
40	Q	207	CLA	C1D-C2D	-2.26	1.40	1.45
40	a	840	CLA	C3D-C4D	-2.26	1.39	1.44
40	F	310	CLA	C1D-C2D	-2.26	1.40	1.45
40	S	305	CLA	C1D-C2D	-2.26	1.40	1.45
40	a	835	CLA	C1D-C2D	-2.26	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	K	304	CLA	C3D-C4D	-2.26	1.39	1.44
40	b	827	CLA	C1D-C2D	-2.26	1.40	1.45
40	F	321	CLA	C1D-C2D	-2.26	1.40	1.45
40	b	840	CLA	C3D-C4D	-2.26	1.39	1.44
40	b	832	CLA	C3D-C4D	-2.26	1.39	1.44
40	v	310	CLA	C3D-C4D	-2.26	1.39	1.44
40	b	801	CLA	C1D-C2D	-2.26	1.40	1.45
40	w	302	CLA	C3D-C4D	-2.26	1.39	1.44
40	Y	313	CLA	C3D-C4D	-2.26	1.39	1.44
40	E	308	CLA	C1D-C2D	-2.26	1.40	1.45
40	O	310	CLA	C1D-C2D	-2.26	1.40	1.45
40	S	313	CLA	C1D-C2D	-2.26	1.40	1.45
40	b	819	CLA	C1D-C2D	-2.25	1.40	1.45
40	E	304	CLA	C3D-C4D	-2.25	1.39	1.44
40	P	307	CLA	C3D-C4D	-2.25	1.39	1.44
40	b	816	CLA	C1D-C2D	-2.25	1.40	1.45
44	x	316	A86	C32-C31	-2.25	1.50	1.54
40	U	208	CLA	C1D-C2D	-2.25	1.40	1.45
40	o	306	CLA	C3D-C4D	-2.25	1.39	1.44
40	u	312	CLA	C3D-C4D	-2.25	1.39	1.44
40	a	826	CLA	C3D-C4D	-2.25	1.39	1.44
40	b	811	CLA	C3D-C4D	-2.25	1.39	1.44
47	Y	323	A1EB1	C32-C31	-2.25	1.50	1.54
40	G	206	CLA	C1D-C2D	-2.25	1.40	1.45
40	W	308	CLA	C3D-C4D	-2.25	1.39	1.44
40	a	808	CLA	C3D-C4D	-2.25	1.39	1.44
40	b	817	CLA	C3D-C4D	-2.25	1.39	1.44
40	V	202	CLA	C1D-C2D	-2.25	1.40	1.45
40	b	805	CLA	C1D-C2D	-2.25	1.40	1.45
40	N	305	CLA	C3D-C4D	-2.25	1.39	1.44
40	Y	306	CLA	C1C-C2C	2.25	1.49	1.44
40	o	301	CLA	C1D-C2D	-2.25	1.40	1.45
40	W	306	CLA	C3D-C4D	-2.25	1.39	1.44
40	u	312	CLA	C1D-C2D	-2.25	1.40	1.45
40	R	304	CLA	C3D-C4D	-2.25	1.39	1.44
40	H	310	CLA	C3D-C4D	-2.25	1.39	1.44
40	K	301	CLA	C1D-C2D	-2.25	1.40	1.45
40	K	312	CLA	C1D-C2D	-2.25	1.40	1.45
40	U	205	CLA	C1D-C2D	-2.25	1.40	1.45
40	a	819	CLA	C1D-C2D	-2.25	1.40	1.45
40	y	302	CLA	C3D-C4D	-2.25	1.39	1.44
40	y	302	CLA	C1D-C2D	-2.25	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	b	817	CLA	C1D-C2D	-2.24	1.40	1.45
40	k	202	CLA	C3D-C4D	-2.24	1.39	1.44
40	F	306	CLA	C3D-C4D	-2.24	1.39	1.44
40	U	204	CLA	C1D-C2D	-2.24	1.40	1.45
40	b	836	CLA	C3D-C4D	-2.24	1.39	1.44
40	u	306	CLA	C1D-C2D	-2.24	1.40	1.45
40	S	306	CLA	C1D-C2D	-2.24	1.40	1.45
40	J	303	CLA	C1D-C2D	-2.24	1.40	1.45
40	b	833	CLA	C1D-C2D	-2.24	1.40	1.45
40	N	310	CLA	C3D-C4D	-2.24	1.39	1.44
40	Y	304	CLA	C1D-C2D	-2.24	1.40	1.45
43	a	802	LMG	C4-C5	2.24	1.57	1.53
40	b	813	CLA	C3D-C4D	-2.24	1.39	1.44
40	J	308	CLA	C1D-C2D	-2.24	1.40	1.45
40	M	310	CLA	C1D-C2D	-2.24	1.40	1.45
40	U	206	CLA	C1D-C2D	-2.24	1.40	1.45
40	y	308	CLA	C1D-C2D	-2.24	1.40	1.45
40	N	304	CLA	C3D-C4D	-2.24	1.39	1.44
40	M	305	CLA	C1D-C2D	-2.24	1.40	1.45
40	E	305	CLA	C3D-C4D	-2.24	1.39	1.44
40	T	304	CLA	C3D-C4D	-2.24	1.39	1.44
40	b	826	CLA	C3D-C4D	-2.24	1.39	1.44
40	z	313	CLA	C3D-C4D	-2.24	1.39	1.44
40	b	820	CLA	C1D-C2D	-2.24	1.40	1.45
40	f	204	CLA	C1D-C2D	-2.24	1.40	1.45
40	B	304	CLA	C1D-C2D	-2.24	1.40	1.45
40	H	306	CLA	C1D-C2D	-2.24	1.40	1.45
40	O	306	CLA	C1D-C2D	-2.24	1.40	1.45
40	T	310	CLA	C1D-C2D	-2.23	1.40	1.45
40	b	829	CLA	C1D-C2D	-2.23	1.40	1.45
40	k	201	CLA	C1D-C2D	-2.23	1.40	1.45
40	R	305	CLA	C1D-C2D	-2.23	1.40	1.45
40	I	205	CLA	C1D-C2D	-2.23	1.40	1.45
40	b	811	CLA	C1D-C2D	-2.23	1.40	1.45
40	x	306	CLA	C1D-C2D	-2.23	1.40	1.45
40	I	207	CLA	C3D-C4D	-2.23	1.39	1.44
40	D	302	CLA	C3D-C4D	-2.23	1.39	1.44
40	z	312	CLA	C3D-C4D	-2.23	1.39	1.44
40	b	822	CLA	C1D-C2D	-2.23	1.40	1.45
40	q	311	CLA	C1D-C2D	-2.23	1.40	1.45
40	R	310	CLA	C1D-C2D	-2.23	1.40	1.45
40	a	813	CLA	C1D-C2D	-2.23	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	a	822	CLA	C1D-C2D	-2.23	1.40	1.45
40	a	831	CLA	C1D-C2D	-2.23	1.40	1.45
40	F	307	CLA	C1D-C2D	-2.23	1.40	1.45
40	i	101	CLA	C3D-C4D	-2.23	1.39	1.44
40	v	306	CLA	C3D-C4D	-2.23	1.39	1.44
40	A	301	CLA	C1D-C2D	-2.23	1.40	1.45
40	a	817	CLA	C1D-C2D	-2.23	1.40	1.45
40	Q	207	CLA	C3D-C4D	-2.23	1.39	1.44
40	u	307	CLA	C3D-C4D	-2.23	1.39	1.44
40	a	836	CLA	C1D-C2D	-2.23	1.40	1.45
40	y	304	CLA	C1D-C2D	-2.23	1.40	1.45
40	q	306	CLA	C3D-C4D	-2.23	1.39	1.44
40	x	308	CLA	C3D-C4D	-2.23	1.39	1.44
40	Z	301	CLA	C1D-C2D	-2.23	1.40	1.45
40	u	311	CLA	C1D-C2D	-2.23	1.40	1.45
40	I	201	CLA	C1D-C2D	-2.23	1.40	1.45
40	p	311	CLA	C3D-C4D	-2.23	1.39	1.44
40	v	306	CLA	C1D-C2D	-2.23	1.40	1.45
40	z	308	CLA	C1D-C2D	-2.23	1.40	1.45
40	z	312	CLA	C1D-C2D	-2.23	1.40	1.45
40	G	203	CLA	C3D-C4D	-2.23	1.39	1.44
40	M	306	CLA	C1D-C2D	-2.23	1.40	1.45
40	a	821	CLA	C1D-C2D	-2.23	1.40	1.45
40	A	303	CLA	C3D-C4D	-2.22	1.39	1.44
40	v	312	CLA	C1D-C2D	-2.22	1.40	1.45
40	z	306	CLA	C1D-C2D	-2.22	1.40	1.45
40	b	814	CLA	C3D-C4D	-2.22	1.39	1.44
43	T	318	LMG	O1-C1	2.22	1.43	1.40
40	D	312	CLA	C1D-C2D	-2.22	1.40	1.45
40	N	305	CLA	C1D-C2D	-2.22	1.40	1.45
40	b	823	CLA	C3D-C4D	-2.22	1.39	1.44
40	L	304	CLA	C1D-C2D	-2.22	1.40	1.45
40	T	306	CLA	C1D-C2D	-2.22	1.40	1.45
40	a	825	CLA	C3D-C4D	-2.22	1.39	1.44
40	o	311	CLA	C3D-C4D	-2.22	1.39	1.44
40	L	311	CLA	C1D-C2D	-2.22	1.40	1.45
40	a	841	CLA	C3D-C4D	-2.22	1.39	1.44
40	V	201	CLA	C1D-C2D	-2.22	1.40	1.45
40	Y	301	CLA	C1D-C2D	-2.22	1.40	1.45
40	p	302	CLA	C3D-C4D	-2.22	1.39	1.44
40	S	311	CLA	C3D-C4D	-2.22	1.39	1.44
40	O	305	CLA	C1D-C2D	-2.22	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	D	303	CLA	C1D-C2D	-2.22	1.40	1.45
40	b	818	CLA	C1D-C2D	-2.22	1.40	1.45
40	E	303	CLA	C1D-C2D	-2.22	1.40	1.45
40	H	311	CLA	C1D-C2D	-2.22	1.40	1.45
43	P	318	LMG	O1-C1	2.22	1.43	1.40
40	q	304	CLA	C3D-C4D	-2.22	1.39	1.44
40	A	308	CLA	C1D-C2D	-2.22	1.40	1.45
40	b	815	CLA	C1D-C2D	-2.22	1.40	1.45
40	A	309	CLA	C3D-C4D	-2.22	1.39	1.44
40	J	306	CLA	C3D-C4D	-2.22	1.39	1.44
40	Z	304	CLA	C3D-C4D	-2.22	1.39	1.44
40	q	310	CLA	C3D-C4D	-2.22	1.39	1.44
40	D	304	CLA	C1D-C2D	-2.22	1.40	1.45
40	b	823	CLA	C1D-C2D	-2.22	1.40	1.45
40	O	304	CLA	C3D-C4D	-2.22	1.39	1.44
40	a	807	CLA	C3D-C4D	-2.22	1.39	1.44
40	a	811	CLA	C1D-C2D	-2.22	1.40	1.45
40	F	310	CLA	CBD-CAD	-2.22	1.46	1.56
40	Q	205	CLA	C1D-C2D	-2.22	1.41	1.45
40	o	305	CLA	C1D-C2D	-2.22	1.41	1.45
40	b	809	CLA	C3D-C4D	-2.22	1.39	1.44
40	K	306	CLA	C1D-C2D	-2.22	1.41	1.45
40	D	304	CLA	C3D-C4D	-2.21	1.39	1.44
40	a	816	CLA	C3D-C4D	-2.21	1.39	1.44
44	Q	210	A86	C32-C31	-2.21	1.50	1.54
40	Q	204	CLA	C1D-C2D	-2.21	1.41	1.45
40	X	305	CLA	C3D-C4D	-2.21	1.39	1.44
40	G	205	CLA	C3D-C4D	-2.21	1.39	1.44
40	b	827	CLA	C3D-C4D	-2.21	1.39	1.44
40	a	841	CLA	C1D-C2D	-2.21	1.41	1.45
40	l	202	CLA	C1D-C2D	-2.21	1.41	1.45
40	o	306	CLA	C1D-C2D	-2.21	1.41	1.45
40	Y	310	CLA	C3D-C4D	-2.21	1.39	1.44
40	o	310	CLA	C3D-C4D	-2.21	1.39	1.44
40	z	306	CLA	C3D-C4D	-2.21	1.39	1.44
40	O	307	CLA	C3D-C4D	-2.21	1.39	1.44
40	o	304	CLA	C1D-C2D	-2.21	1.41	1.45
40	R	304	CLA	C1D-C2D	-2.21	1.41	1.45
40	X	307	CLA	C1D-C2D	-2.21	1.41	1.45
40	a	834	CLA	C1D-C2D	-2.21	1.41	1.45
40	t	304	CLA	C1D-C2D	-2.21	1.41	1.45
40	D	303	CLA	C3D-C4D	-2.21	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	H	309	CLA	C3D-C4D	-2.21	1.39	1.44
40	a	838	CLA	C3D-C4D	-2.21	1.39	1.44
40	b	818	CLA	C3D-C4D	-2.21	1.39	1.44
40	o	311	CLA	C1D-C2D	-2.21	1.41	1.45
40	C	306	CLA	C3D-C4D	-2.21	1.39	1.44
40	F	304	CLA	C3D-C4D	-2.21	1.39	1.44
40	l	205	CLA	C3D-C4D	-2.21	1.39	1.44
40	E	303	CLA	C3D-C4D	-2.21	1.39	1.44
40	L	312	CLA	C1D-C2D	-2.21	1.41	1.45
40	L	311	CLA	C3D-C4D	-2.21	1.39	1.44
40	S	312	CLA	C3D-C4D	-2.21	1.39	1.44
40	C	304	CLA	C1D-C2D	-2.21	1.41	1.45
40	U	203	CLA	C1D-C2D	-2.21	1.41	1.45
40	U	207	CLA	C3D-C4D	-2.21	1.39	1.44
40	p	312	CLA	C1D-C2D	-2.21	1.41	1.45
40	I	202	CLA	C1D-C2D	-2.21	1.41	1.45
40	b	802	CLA	C1D-C2D	-2.21	1.41	1.45
40	w	303	CLA	C1D-C2D	-2.21	1.41	1.45
40	Y	304	CLA	C3D-C4D	-2.21	1.39	1.44
40	b	820	CLA	C3D-C4D	-2.21	1.39	1.44
40	y	309	CLA	C1D-C2D	-2.21	1.41	1.45
40	b	836	CLA	C1D-C2D	-2.21	1.41	1.45
40	p	306	CLA	C1D-C2D	-2.21	1.41	1.45
40	y	303	CLA	C1D-C2D	-2.21	1.41	1.45
40	a	810	CLA	C3D-C4D	-2.21	1.39	1.44
40	X	307	CLA	C3D-C4D	-2.20	1.39	1.44
40	Z	311	CLA	C3D-C4D	-2.20	1.39	1.44
40	t	307	CLA	C1D-C2D	-2.20	1.41	1.45
40	C	302	CLA	C3D-C4D	-2.20	1.39	1.44
40	R	306	CLA	C3D-C4D	-2.20	1.39	1.44
40	H	307	CLA	C1D-C2D	-2.20	1.41	1.45
40	q	305	CLA	C1D-C2D	-2.20	1.41	1.45
40	Y	312	CLA	C3D-C4D	-2.20	1.39	1.44
40	v	312	CLA	C3D-C4D	-2.20	1.39	1.44
40	N	307	CLA	C1D-C2D	-2.20	1.41	1.45
40	D	311	CLA	C1D-C2D	-2.20	1.41	1.45
40	Q	209	CLA	C1D-C2D	-2.20	1.41	1.45
40	o	310	CLA	C1D-C2D	-2.20	1.41	1.45
40	v	304	CLA	C1D-C2D	-2.20	1.41	1.45
40	I	208	CLA	C3D-C4D	-2.20	1.39	1.44
40	b	837	CLA	C1D-C2D	-2.20	1.41	1.45
40	Z	307	CLA	C1D-C2D	-2.20	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	S	314	CLA	C3D-C4D	-2.20	1.39	1.44
40	E	310	CLA	C1D-C2D	-2.20	1.41	1.45
40	L	305	CLA	C3D-C4D	-2.20	1.39	1.44
40	b	810	CLA	C3D-C4D	-2.20	1.39	1.44
40	b	819	CLA	C3D-C4D	-2.20	1.39	1.44
41	z	304	KC2	C1B-C2B	2.20	1.49	1.45
40	v	313	CLA	C3D-C4D	-2.20	1.39	1.44
40	P	305	CLA	C3D-C4D	-2.20	1.39	1.44
40	x	314	CLA	C3D-C4D	-2.20	1.39	1.44
40	x	314	CLA	C1D-C2D	-2.20	1.41	1.45
40	F	307	CLA	C3D-C4D	-2.20	1.39	1.44
40	G	213	CLA	C3D-C4D	-2.20	1.39	1.44
40	t	305	CLA	C3D-C4D	-2.20	1.39	1.44
40	M	304	CLA	C3D-C4D	-2.20	1.39	1.44
40	a	822	CLA	C3D-C4D	-2.20	1.39	1.44
40	D	306	CLA	C3D-C4D	-2.20	1.39	1.44
40	a	811	CLA	C3D-C4D	-2.20	1.39	1.44
40	S	301	CLA	C1D-C2D	-2.20	1.41	1.45
40	W	306	CLA	C1D-C2D	-2.20	1.41	1.45
40	H	306	CLA	C3D-C4D	-2.20	1.39	1.44
40	M	311	CLA	C1D-C2D	-2.20	1.41	1.45
40	t	309	CLA	C3D-C4D	-2.20	1.39	1.44
40	a	851	CLA	C3D-C4D	-2.20	1.39	1.44
40	S	308	CLA	C3D-C4D	-2.20	1.39	1.44
40	U	202	CLA	C3D-C4D	-2.20	1.39	1.44
40	q	306	CLA	C1D-C2D	-2.20	1.41	1.45
40	o	312	CLA	C3D-C4D	-2.20	1.39	1.44
40	w	308	CLA	C1D-C2D	-2.20	1.41	1.45
40	W	305	CLA	C3D-C4D	-2.19	1.39	1.44
40	D	301	CLA	C1D-C2D	-2.19	1.41	1.45
40	Q	205	CLA	C3D-C4D	-2.19	1.39	1.44
40	E	305	CLA	C1D-C2D	-2.19	1.41	1.45
40	Z	312	CLA	C1D-C2D	-2.19	1.41	1.45
40	E	314	CLA	C3D-C4D	-2.19	1.39	1.44
40	I	204	CLA	C3D-C4D	-2.19	1.39	1.44
40	U	203	CLA	C3D-C4D	-2.19	1.39	1.44
40	E	308	CLA	C3D-C4D	-2.19	1.39	1.44
40	A	305	CLA	C3D-C4D	-2.19	1.39	1.44
40	D	308	CLA	C1D-C2D	-2.19	1.41	1.45
40	D	309	CLA	C1D-C2D	-2.19	1.41	1.45
40	o	312	CLA	C1D-C2D	-2.19	1.41	1.45
40	x	302	CLA	C1D-C2D	-2.19	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	a	814	CLA	C3D-C4D	-2.19	1.39	1.44
44	W	316	A86	C32-C31	-2.19	1.50	1.54
40	A	308	CLA	C3D-C4D	-2.19	1.39	1.44
40	T	304	CLA	C1D-C2D	-2.19	1.41	1.45
40	L	310	CLA	C3D-C4D	-2.19	1.39	1.44
40	M	312	CLA	C3D-C4D	-2.19	1.39	1.44
40	q	311	CLA	C3D-C4D	-2.19	1.39	1.44
40	F	301	CLA	C1D-C2D	-2.19	1.41	1.45
43	E	320	LMG	O7-C8	-2.19	1.41	1.46
40	C	309	CLA	C3D-C4D	-2.19	1.39	1.44
40	b	806	CLA	C3D-C4D	-2.19	1.39	1.44
40	F	307	CLA	C1C-C2C	2.19	1.49	1.44
40	A	304	CLA	C1D-C2D	-2.19	1.41	1.45
40	K	304	CLA	C1D-C2D	-2.19	1.41	1.45
40	a	820	CLA	C1D-C2D	-2.19	1.41	1.45
40	w	304	CLA	C1D-C2D	-2.19	1.41	1.45
40	a	842	CLA	C3D-C4D	-2.19	1.39	1.44
40	o	305	CLA	C3D-C4D	-2.19	1.39	1.44
40	b	839	CLA	C1D-C2D	-2.19	1.41	1.45
40	N	311	CLA	C3D-C4D	-2.19	1.39	1.44
40	A	307	CLA	C1D-C2D	-2.19	1.41	1.45
40	a	828	CLA	C1D-C2D	-2.19	1.41	1.45
40	X	305	CLA	C1D-C2D	-2.19	1.41	1.45
40	Z	306	CLA	C1D-C2D	-2.19	1.41	1.45
40	u	306	CLA	C3D-C4D	-2.19	1.39	1.44
40	G	203	CLA	C1D-C2D	-2.19	1.41	1.45
40	b	809	CLA	C1D-C2D	-2.19	1.41	1.45
40	O	310	CLA	C3D-C4D	-2.19	1.39	1.44
40	I	208	CLA	C1D-C2D	-2.19	1.41	1.45
40	W	305	CLA	C1D-C2D	-2.19	1.41	1.45
40	Y	311	CLA	C1D-C2D	-2.19	1.41	1.45
40	E	312	CLA	C3D-C4D	-2.19	1.39	1.44
40	a	831	CLA	C3D-C4D	-2.19	1.39	1.44
40	i	101	CLA	C1D-C2D	-2.19	1.41	1.45
40	o	307	CLA	C1D-C2D	-2.19	1.41	1.45
40	N	307	CLA	C3D-C4D	-2.19	1.39	1.44
40	P	311	CLA	C3D-C4D	-2.19	1.39	1.44
40	G	213	CLA	C1D-C2D	-2.19	1.41	1.45
40	Q	203	CLA	C3D-C4D	-2.19	1.39	1.44
40	X	304	CLA	C3D-C4D	-2.19	1.39	1.44
40	a	817	CLA	C3D-C4D	-2.19	1.39	1.44
40	A	307	CLA	C3D-C4D	-2.18	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	C	301	CLA	C3D-C4D	-2.18	1.39	1.44
40	P	308	CLA	C3D-C4D	-2.18	1.39	1.44
40	a	828	CLA	C3D-C4D	-2.18	1.39	1.44
40	B	307	CLA	C3D-C4D	-2.18	1.39	1.44
40	D	309	CLA	C3D-C4D	-2.18	1.39	1.44
40	a	839	CLA	C1D-C2D	-2.18	1.41	1.45
40	N	304	CLA	C1D-C2D	-2.18	1.41	1.45
40	a	804	CLA	C2C-C1C	2.18	1.44	1.40
40	F	305	CLA	C3D-C4D	-2.18	1.39	1.44
40	M	306	CLA	C3D-C4D	-2.18	1.39	1.44
40	W	313	CLA	C1D-C2D	-2.18	1.41	1.45
40	Y	310	CLA	C1D-C2D	-2.18	1.41	1.45
40	w	309	CLA	C1D-C2D	-2.18	1.41	1.45
40	o	301	CLA	C3D-C4D	-2.18	1.39	1.44
40	z	314	CLA	C3D-C4D	-2.18	1.39	1.44
40	H	310	CLA	C1D-C2D	-2.18	1.41	1.45
40	M	312	CLA	C1D-C2D	-2.18	1.41	1.45
40	z	324	CLA	C3D-C4D	-2.18	1.39	1.44
40	K	312	CLA	C3D-C4D	-2.18	1.39	1.44
40	S	305	CLA	C3D-C4D	-2.18	1.39	1.44
40	a	829	CLA	C3D-C4D	-2.18	1.39	1.44
40	I	203	CLA	C3D-C4D	-2.18	1.39	1.44
40	N	311	CLA	C1D-C2D	-2.18	1.41	1.45
40	R	310	CLA	C3D-C4D	-2.18	1.39	1.44
40	w	303	CLA	C3D-C4D	-2.18	1.39	1.44
40	L	307	CLA	C1D-C2D	-2.18	1.41	1.45
40	O	306	CLA	C3D-C4D	-2.18	1.39	1.44
40	J	306	CLA	C1D-C2D	-2.18	1.41	1.45
40	j	102	CLA	C1D-C2D	-2.18	1.41	1.45
44	w	311	A86	C32-C31	-2.18	1.50	1.54
40	l	203	CLA	C3A-C2A	-2.18	1.48	1.54
40	G	204	CLA	C1D-C2D	-2.18	1.41	1.45
40	q	304	CLA	C1D-C2D	-2.18	1.41	1.45
40	t	309	CLA	C1D-C2D	-2.18	1.41	1.45
40	w	305	CLA	C1D-C2D	-2.18	1.41	1.45
40	a	837	CLA	C3D-C4D	-2.18	1.39	1.44
40	a	840	CLA	C1D-C2D	-2.18	1.41	1.45
40	x	312	CLA	C3D-C4D	-2.18	1.39	1.44
40	S	312	CLA	C1D-C2D	-2.18	1.41	1.45
40	A	306	CLA	C3D-C4D	-2.18	1.39	1.44
40	I	205	CLA	C3D-C4D	-2.18	1.39	1.44
40	b	824	CLA	C3D-C4D	-2.18	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	I	201	CLA	C3D-C4D	-2.18	1.39	1.44
40	t	303	CLA	C3D-C4D	-2.18	1.39	1.44
40	u	314	CLA	C3D-C4D	-2.18	1.39	1.44
40	A	305	CLA	C1D-C2D	-2.18	1.41	1.45
40	H	307	CLA	C3D-C4D	-2.18	1.39	1.44
40	a	807	CLA	C1D-C2D	-2.18	1.41	1.45
40	u	308	CLA	C1D-C2D	-2.18	1.41	1.45
40	G	207	CLA	C3D-C4D	-2.18	1.39	1.44
40	O	304	CLA	C1D-C2D	-2.18	1.41	1.45
40	Z	313	CLA	C3D-C4D	-2.18	1.39	1.44
40	a	819	CLA	C3D-C4D	-2.18	1.39	1.44
40	S	308	CLA	C1D-C2D	-2.17	1.41	1.45
40	a	833	CLA	C1D-C2D	-2.17	1.41	1.45
40	E	302	CLA	C3D-C4D	-2.17	1.39	1.44
43	T	318	LMG	C4-C5	2.17	1.57	1.53
40	Z	312	CLA	C3D-C4D	-2.17	1.39	1.44
40	b	816	CLA	C3D-C4D	-2.17	1.39	1.44
40	R	307	CLA	C1D-C2D	-2.17	1.41	1.45
40	T	310	CLA	C3D-C4D	-2.17	1.39	1.44
40	t	302	CLA	C1D-C2D	-2.17	1.41	1.45
40	b	801	CLA	C3D-C4D	-2.17	1.39	1.44
40	E	312	CLA	C1D-C2D	-2.17	1.41	1.45
40	b	814	CLA	C1D-C2D	-2.17	1.41	1.45
40	q	313	CLA	C1D-C2D	-2.17	1.41	1.45
40	A	301	CLA	C3D-C4D	-2.17	1.39	1.44
40	E	310	CLA	C3D-C4D	-2.17	1.39	1.44
40	b	807	CLA	C3D-C4D	-2.17	1.39	1.44
40	D	307	CLA	C1D-C2D	-2.17	1.41	1.45
40	a	830	CLA	C3D-C4D	-2.17	1.39	1.44
40	a	815	CLA	C1D-C2D	-2.17	1.41	1.45
40	a	838	CLA	C1D-C2D	-2.17	1.41	1.45
40	D	311	CLA	C3D-C4D	-2.17	1.39	1.44
40	E	314	CLA	C1D-C2D	-2.17	1.41	1.45
40	a	830	CLA	C1D-C2D	-2.17	1.41	1.45
40	G	205	CLA	C1D-C2D	-2.17	1.41	1.45
40	y	305	CLA	C1D-C2D	-2.17	1.41	1.45
40	k	201	CLA	C3D-C4D	-2.17	1.39	1.44
40	H	311	CLA	C3D-C4D	-2.17	1.39	1.44
40	W	313	CLA	C3D-C4D	-2.17	1.39	1.44
40	P	312	CLA	C3D-C4D	-2.17	1.39	1.44
40	P	313	CLA	C3D-C4D	-2.17	1.39	1.44
40	v	311	CLA	C3D-C4D	-2.17	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	Z	311	CLA	C1D-C2D	-2.17	1.41	1.45
40	a	829	CLA	C1D-C2D	-2.17	1.41	1.45
44	w	311	A86	C10-C11	2.17	1.40	1.34
40	a	821	CLA	C3D-C4D	-2.17	1.39	1.44
40	P	308	CLA	C1D-C2D	-2.17	1.41	1.45
46	W	318	SQD	O6-C1	2.17	1.43	1.40
40	C	301	CLA	C1D-C2D	-2.17	1.41	1.45
40	T	307	CLA	C1D-C2D	-2.17	1.41	1.45
40	a	808	CLA	C1D-C2D	-2.17	1.41	1.45
40	I	204	CLA	C1D-C2D	-2.17	1.41	1.45
40	H	301	CLA	C3D-C4D	-2.17	1.39	1.44
40	A	302	CLA	C3D-C4D	-2.17	1.39	1.44
40	a	833	CLA	C3D-C4D	-2.17	1.39	1.44
40	B	303	CLA	C1D-C2D	-2.17	1.41	1.45
40	J	318	CLA	C1D-C2D	-2.17	1.41	1.45
40	P	312	CLA	C1D-C2D	-2.17	1.41	1.45
40	x	306	CLA	C3D-C4D	-2.16	1.39	1.44
40	M	307	CLA	C1D-C2D	-2.16	1.41	1.45
40	E	311	CLA	C3D-C4D	-2.16	1.39	1.44
40	a	839	CLA	C3D-C4D	-2.16	1.39	1.44
40	x	311	CLA	C1D-C2D	-2.16	1.41	1.45
40	a	805	CLA	C3D-C4D	-2.16	1.39	1.44
40	I	203	CLA	C1D-C2D	-2.16	1.41	1.45
40	X	301	CLA	C1D-C2D	-2.16	1.41	1.45
40	a	809	CLA	C3D-C4D	-2.16	1.39	1.44
40	t	303	CLA	C1D-C2D	-2.16	1.41	1.45
40	t	305	CLA	C1D-C2D	-2.16	1.41	1.45
40	p	312	CLA	C3D-C4D	-2.16	1.39	1.44
40	u	314	CLA	C1D-C2D	-2.16	1.41	1.45
40	F	308	CLA	C3D-C4D	-2.16	1.39	1.44
40	Z	306	CLA	C3D-C4D	-2.16	1.39	1.44
40	a	823	CLA	C3D-C4D	-2.16	1.39	1.44
40	a	804	CLA	C1D-C2D	-2.16	1.41	1.45
40	a	809	CLA	C1D-C2D	-2.16	1.41	1.45
40	D	307	CLA	C3D-C4D	-2.16	1.39	1.44
40	F	311	CLA	C3D-C4D	-2.16	1.39	1.44
40	u	308	CLA	C3D-C4D	-2.16	1.39	1.44
40	J	310	CLA	C1D-C2D	-2.16	1.41	1.45
40	u	307	CLA	C1D-C2D	-2.16	1.41	1.45
40	R	307	CLA	C3D-C4D	-2.16	1.39	1.44
40	w	308	CLA	C3D-C4D	-2.16	1.39	1.44
40	B	303	CLA	C3D-C4D	-2.16	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	p	308	CLA	C3D-C4D	-2.16	1.39	1.44
40	y	305	CLA	C3D-C4D	-2.16	1.39	1.44
40	E	307	CLA	C3D-C4D	-2.16	1.39	1.44
40	X	306	CLA	C3D-C4D	-2.16	1.39	1.44
44	T	313	A86	C32-C31	-2.16	1.50	1.54
40	K	306	CLA	C3D-C4D	-2.16	1.39	1.44
40	a	827	CLA	C3D-C4D	-2.16	1.39	1.44
40	p	306	CLA	C3D-C4D	-2.16	1.39	1.44
40	H	305	CLA	C3D-C4D	-2.16	1.39	1.44
40	N	306	CLA	C3D-C4D	-2.16	1.39	1.44
40	z	302	CLA	C3D-C4D	-2.16	1.39	1.44
40	X	312	CLA	C1D-C2D	-2.16	1.41	1.45
40	H	308	CLA	C3D-C4D	-2.16	1.39	1.44
40	B	306	CLA	C3D-C4D	-2.16	1.39	1.44
40	T	305	CLA	C3D-C4D	-2.16	1.39	1.44
40	D	305	CLA	CBD-CHA	2.16	1.54	1.51
40	b	830	CLA	C1D-C2D	-2.16	1.41	1.45
40	D	308	CLA	C3D-C4D	-2.16	1.39	1.44
40	v	304	CLA	C3D-C4D	-2.16	1.39	1.44
40	w	305	CLA	C3D-C4D	-2.16	1.39	1.44
40	L	306	CLA	C1D-C2D	-2.16	1.41	1.45
40	p	307	CLA	C1D-C2D	-2.16	1.41	1.45
40	Z	301	CLA	C3D-C4D	-2.15	1.39	1.44
40	H	302	CLA	C1D-C2D	-2.15	1.41	1.45
40	E	309	CLA	C3D-C4D	-2.15	1.39	1.44
40	J	302	CLA	C1D-C2D	-2.15	1.41	1.45
40	W	308	CLA	C1D-C2D	-2.15	1.41	1.45
40	V	201	CLA	C3D-C4D	-2.15	1.39	1.44
40	Y	307	CLA	C3D-C4D	-2.15	1.39	1.44
40	W	311	CLA	C1D-C2D	-2.15	1.41	1.45
40	B	301	CLA	C3D-C4D	-2.15	1.39	1.44
40	v	305	CLA	C1D-C2D	-2.15	1.41	1.45
43	l	201	LMG	C4-C5	2.15	1.57	1.53
40	I	207	CLA	C1D-C2D	-2.15	1.41	1.45
40	C	307	CLA	C1D-C2D	-2.15	1.41	1.45
40	X	313	CLA	C1D-C2D	-2.15	1.41	1.45
40	F	301	CLA	C3D-C4D	-2.15	1.39	1.44
40	a	814	CLA	C1D-C2D	-2.15	1.41	1.45
40	M	305	CLA	C3D-C4D	-2.15	1.39	1.44
40	v	307	CLA	C1D-C2D	-2.15	1.41	1.45
40	F	311	CLA	C1D-C2D	-2.15	1.41	1.45
40	L	301	CLA	C1D-C2D	-2.15	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	a	805	CLA	C1D-C2D	-2.15	1.41	1.45
40	x	305	CLA	C1D-C2D	-2.15	1.41	1.45
40	a	815	CLA	C3D-C4D	-2.15	1.39	1.44
40	J	312	CLA	C3D-C4D	-2.15	1.39	1.44
40	V	202	CLA	C3D-C4D	-2.15	1.39	1.44
40	o	313	CLA	C3D-C4D	-2.15	1.39	1.44
40	S	314	CLA	C1D-C2D	-2.15	1.41	1.45
40	C	304	CLA	C3D-C4D	-2.15	1.39	1.44
40	N	310	CLA	C1D-C2D	-2.15	1.41	1.45
40	Q	209	CLA	C3D-C4D	-2.15	1.39	1.44
40	Y	306	CLA	C3D-C4D	-2.15	1.39	1.44
40	a	824	CLA	C3D-C4D	-2.15	1.39	1.44
40	p	314	CLA	C3D-C4D	-2.15	1.39	1.44
40	q	313	CLA	C3D-C4D	-2.15	1.39	1.44
40	a	820	CLA	C3D-C4D	-2.15	1.39	1.44
40	q	301	CLA	C3D-C4D	-2.15	1.39	1.44
40	Z	313	CLA	C1D-C2D	-2.15	1.41	1.45
40	b	825	CLA	C3D-C4D	-2.14	1.39	1.44
40	I	202	CLA	C3D-C4D	-2.14	1.39	1.44
40	L	307	CLA	C3D-C4D	-2.14	1.39	1.44
43	S	322	LMG	C9-C8	2.14	1.57	1.50
40	a	813	CLA	C3D-C4D	-2.14	1.39	1.44
40	b	812	CLA	C3D-C4D	-2.14	1.39	1.44
40	y	308	CLA	C3D-C4D	-2.14	1.39	1.44
40	F	308	CLA	C1D-C2D	-2.14	1.41	1.45
40	x	307	CLA	C1D-C2D	-2.14	1.41	1.45
40	S	306	CLA	C3D-C4D	-2.14	1.39	1.44
40	a	804	CLA	C3D-C4D	-2.14	1.39	1.44
40	a	816	CLA	C1D-C2D	-2.14	1.41	1.45
40	z	314	CLA	C1D-C2D	-2.14	1.41	1.45
40	l	202	CLA	C3D-C4D	-2.14	1.39	1.44
40	J	311	CLA	C1D-C2D	-2.14	1.41	1.45
40	Y	306	CLA	C1D-C2D	-2.14	1.41	1.45
40	D	312	CLA	C3D-C4D	-2.14	1.39	1.44
40	H	301	CLA	C1D-C2D	-2.14	1.41	1.45
40	q	310	CLA	C1D-C2D	-2.14	1.41	1.45
43	j	101	LMG	O7-C8	-2.14	1.41	1.46
40	Y	311	CLA	C3D-C4D	-2.14	1.39	1.44
40	p	307	CLA	C3D-C4D	-2.14	1.39	1.44
40	F	305	CLA	C1D-C2D	-2.14	1.41	1.45
40	X	306	CLA	C1D-C2D	-2.14	1.41	1.45
40	u	302	CLA	C1D-C2D	-2.14	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	b	829	CLA	C3D-C4D	-2.14	1.39	1.44
40	f	204	CLA	C3D-C4D	-2.14	1.39	1.44
40	J	318	CLA	C3D-C4D	-2.14	1.39	1.44
40	w	302	CLA	C1D-C2D	-2.13	1.41	1.45
40	D	301	CLA	C3D-C4D	-2.13	1.39	1.44
40	T	306	CLA	C3D-C4D	-2.13	1.39	1.44
40	X	301	CLA	C3D-C4D	-2.13	1.39	1.44
40	v	301	CLA	C3D-C4D	-2.13	1.39	1.44
40	W	307	CLA	C3D-C4D	-2.13	1.39	1.44
40	Q	203	CLA	C1D-C2D	-2.13	1.41	1.45
40	z	324	CLA	C1D-C2D	-2.13	1.41	1.45
41	t	301	KC2	C1B-C2B	2.13	1.49	1.45
40	M	307	CLA	C3D-C4D	-2.13	1.39	1.44
40	b	802	CLA	C3D-C4D	-2.13	1.39	1.44
40	C	305	CLA	C1D-C2D	-2.13	1.41	1.45
44	S	315	A86	C32-C31	-2.13	1.51	1.54
40	W	312	CLA	C3D-C4D	-2.13	1.39	1.44
40	p	308	CLA	C1D-C2D	-2.13	1.41	1.45
40	L	310	CLA	C1D-C2D	-2.13	1.41	1.45
40	b	831	CLA	C3D-C4D	-2.13	1.39	1.44
44	O	315	A86	C32-C31	-2.13	1.51	1.54
40	b	821	CLA	C3D-C4D	-2.13	1.39	1.44
40	E	302	CLA	C1D-C2D	-2.13	1.41	1.45
40	a	832	CLA	C3D-C4D	-2.13	1.39	1.44
40	H	304	CLA	C1C-C2C	2.13	1.48	1.44
40	j	102	CLA	C3D-C4D	-2.12	1.39	1.44
43	l	201	LMG	O7-C8	-2.12	1.41	1.46
40	I	206	CLA	C3D-C4D	-2.12	1.39	1.44
40	B	302	CLA	C3D-C4D	-2.12	1.39	1.44
40	J	311	CLA	C3D-C4D	-2.12	1.39	1.44
40	E	311	CLA	C1D-C2D	-2.12	1.41	1.45
40	J	310	CLA	C3D-C4D	-2.12	1.39	1.44
40	p	313	CLA	C3D-C4D	-2.12	1.39	1.44
40	t	304	CLA	C3D-C4D	-2.12	1.39	1.44
40	X	312	CLA	C3D-C4D	-2.12	1.39	1.44
40	D	310	CLA	C1D-C2D	-2.12	1.41	1.45
40	K	301	CLA	C3D-C4D	-2.12	1.39	1.44
40	L	306	CLA	C3D-C4D	-2.12	1.39	1.44
40	a	806	CLA	C1D-C2D	-2.12	1.41	1.45
40	o	313	CLA	C1C-C2C	2.12	1.48	1.44
40	v	313	CLA	C1D-C2D	-2.12	1.41	1.45
40	a	852	CLA	C3D-C4D	-2.12	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	p	311	CLA	C1D-C2D	-2.12	1.41	1.45
40	J	308	CLA	C3D-C4D	-2.12	1.39	1.44
40	Q	204	CLA	C3D-C4D	-2.12	1.39	1.44
40	S	301	CLA	C3D-C4D	-2.12	1.39	1.44
40	q	307	CLA	C1D-C2D	-2.12	1.41	1.45
40	Q	202	CLA	C3D-C4D	-2.12	1.39	1.44
40	U	204	CLA	C3D-C4D	-2.12	1.39	1.44
40	w	304	CLA	C3D-C4D	-2.12	1.39	1.44
40	W	306	CLA	CBD-CAD	-2.11	1.47	1.56
40	z	311	CLA	C1D-C2D	-2.11	1.41	1.45
40	A	311	CLA	C3D-C4D	-2.11	1.39	1.44
40	X	313	CLA	C3D-C4D	-2.11	1.39	1.44
44	u	320	A86	C32-C31	-2.11	1.51	1.54
40	q	312	CLA	C3D-C4D	-2.11	1.39	1.44
41	T	302	KC2	C1B-C2B	2.11	1.49	1.45
40	H	302	CLA	C3D-C4D	-2.11	1.39	1.44
40	b	803	CLA	C1D-C2D	-2.11	1.41	1.45
40	y	304	CLA	C3D-C4D	-2.11	1.39	1.44
44	M	313	A86	C32-C31	-2.11	1.51	1.54
40	H	304	CLA	C3D-C4D	-2.11	1.39	1.44
40	C	302	CLA	C1D-C2D	-2.11	1.41	1.45
40	z	313	CLA	C1D-C2D	-2.11	1.41	1.45
40	F	321	CLA	C3D-C4D	-2.10	1.39	1.44
40	Z	310	CLA	C1D-C2D	-2.10	1.41	1.45
40	S	313	CLA	C3D-C4D	-2.10	1.39	1.44
40	x	313	CLA	C3D-C4D	-2.10	1.39	1.44
40	Z	305	CLA	C3D-C4D	-2.10	1.39	1.44
40	C	309	CLA	C1D-C2D	-2.10	1.41	1.45
40	P	306	CLA	C3D-C4D	-2.10	1.39	1.44
40	J	308	CLA	C1C-C2C	2.10	1.48	1.44
40	M	311	CLA	C3D-C4D	-2.10	1.39	1.44
40	U	205	CLA	C3D-C4D	-2.10	1.39	1.44
40	Y	301	CLA	C3D-C4D	-2.10	1.39	1.44
44	u	316	A86	C32-C31	-2.10	1.51	1.54
44	M	320	A86	C32-C31	-2.10	1.51	1.54
40	F	303	CLA	C3D-C4D	-2.09	1.39	1.44
40	Q	206	CLA	C3D-C4D	-2.09	1.39	1.44
40	G	201	CLA	C3D-C4D	-2.09	1.39	1.44
40	P	313	CLA	C1D-C2D	-2.09	1.41	1.45
40	a	850	CLA	C1D-C2D	-2.09	1.41	1.45
40	f	205	CLA	C3D-C4D	-2.09	1.39	1.44
40	a	810	CLA	C1D-C2D	-2.09	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	S	319	CLA	C3D-C4D	-2.09	1.39	1.44
40	M	310	CLA	C3D-C4D	-2.09	1.39	1.44
40	S	307	CLA	C1D-C2D	-2.09	1.41	1.45
40	J	305	CLA	C3D-C4D	-2.09	1.39	1.44
40	U	202	CLA	C1D-C2D	-2.09	1.41	1.45
40	v	310	CLA	C1D-C2D	-2.09	1.41	1.45
40	F	310	CLA	C3D-C4D	-2.09	1.39	1.44
40	a	803	CLA	C3D-C4D	-2.09	1.39	1.44
44	u	319	A86	C32-C31	-2.09	1.51	1.54
40	a	812	CLA	C3D-C4D	-2.09	1.39	1.44
40	u	305	CLA	C1D-C2D	-2.09	1.41	1.45
40	D	303	CLA	CBD-CAD	-2.09	1.47	1.56
40	E	304	CLA	CBD-CAD	-2.09	1.47	1.56
40	Y	305	CLA	C3D-C4D	-2.09	1.39	1.44
40	E	313	CLA	C3D-C4D	-2.08	1.39	1.44
40	u	313	CLA	C3D-C4D	-2.08	1.39	1.44
40	b	841	CLA	C3D-C4D	-2.08	1.39	1.44
40	l	203	CLA	C1D-C2D	-2.08	1.41	1.45
40	G	206	CLA	C3D-C4D	-2.08	1.39	1.44
40	a	836	CLA	C3D-C4D	-2.08	1.39	1.44
40	b	808	CLA	C3D-C4D	-2.08	1.39	1.44
41	O	302	KC2	C1B-C2B	2.08	1.49	1.45
40	Y	313	CLA	C1D-C2D	-2.08	1.41	1.45
41	o	303	KC2	C1B-C2B	2.08	1.49	1.45
40	l	204	CLA	C3D-C4D	-2.08	1.39	1.44
40	y	304	CLA	C1C-C2C	2.07	1.48	1.44
41	R	302	KC2	C1B-C2B	2.07	1.49	1.45
40	o	313	CLA	C1D-C2D	-2.07	1.41	1.45
40	T	306	CLA	C1C-C2C	2.07	1.48	1.44
40	B	304	CLA	C3D-C4D	-2.07	1.39	1.44
40	S	302	CLA	C3D-C4D	-2.07	1.39	1.44
40	S	311	CLA	C1D-C2D	-2.07	1.41	1.45
40	L	312	CLA	C3D-C4D	-2.06	1.39	1.44
40	p	302	CLA	C1D-C2D	-2.06	1.41	1.45
40	U	206	CLA	C3D-C4D	-2.06	1.39	1.44
40	f	201	CLA	C3D-C4D	-2.05	1.39	1.44
40	J	309	CLA	C3D-C4D	-2.05	1.39	1.44
40	K	307	CLA	C3D-C4D	-2.05	1.39	1.44
44	P	316	A86	C32-C31	-2.05	1.51	1.54
46	k	205	SQD	O6-C1	2.05	1.43	1.40
40	b	801	CLA	C1C-C2C	2.05	1.48	1.44
40	a	818	CLA	C1D-C2D	-2.04	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	Y	307	CLA	C1D-C2D	-2.04	1.41	1.45
44	U	210	A86	C32-C31	-2.04	1.51	1.54
43	u	301	LMG	O7-C8	-2.04	1.41	1.46
40	C	308	CLA	C3D-C4D	-2.03	1.39	1.44
40	Y	312	CLA	C1D-C2D	-2.03	1.41	1.45
52	b	850	DGD	O6D-C5D	-2.03	1.39	1.44
40	A	307	CLA	C1C-C2C	2.03	1.48	1.44
40	J	307	CLA	C3D-C4D	-2.03	1.39	1.44
40	Q	206	CLA	C2C-C1C	2.03	1.44	1.40
40	J	305	CLA	C1C-C2C	2.03	1.48	1.44
40	p	305	CLA	C1D-C2D	-2.02	1.41	1.45
40	J	302	CLA	C3D-C4D	-2.02	1.39	1.44
40	O	316	CLA	C3D-C4D	-2.02	1.39	1.44
40	C	304	CLA	C1C-C2C	2.02	1.48	1.44
43	a	801	LMG	O7-C8	-2.02	1.41	1.46
40	a	806	CLA	C3A-C2A	-2.02	1.49	1.54
45	S	323	LHG	O7-C5	-2.02	1.41	1.46
40	O	306	CLA	C1C-C2C	2.02	1.48	1.44
45	S	323	LHG	P-O6	2.02	1.67	1.59
43	M	317	LMG	C9-C8	2.01	1.57	1.50
40	B	301	CLA	C1D-C2D	-2.01	1.41	1.45
40	U	208	CLA	C3D-C4D	-2.01	1.39	1.44
40	o	306	CLA	C1C-C2C	2.01	1.48	1.44
40	D	304	CLA	C1C-C2C	2.01	1.48	1.44
40	S	307	CLA	CBD-CAD	-2.00	1.47	1.56

All (4057) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	M	313	A86	O1-C20-C19	-11.55	102.66	113.49
40	F	303	CLA	C1C-NC-C4C	-9.80	102.21	106.68
40	Q	206	CLA	C1C-NC-C4C	-9.59	102.31	106.68
44	X	318	A86	O1-C20-C19	9.46	122.36	113.49
40	D	305	CLA	CBD-CHA-C1A	9.36	131.24	118.85
40	Q	204	CLA	C1C-NC-C4C	-9.17	102.50	106.68
40	D	305	CLA	CHA-C4D-ND	9.10	133.01	125.22
40	Q	205	CLA	C1C-NC-C4C	-9.04	102.56	106.68
40	E	314	CLA	C4A-NA-C1A	-8.99	102.58	106.68
44	z	317	A86	O1-C20-C19	-8.85	105.20	113.49
40	x	307	CLA	C4A-NA-C1A	-8.83	102.65	106.68
40	z	311	CLA	C4A-NA-C1A	-8.80	102.66	106.68
44	z	316	A86	O1-C20-C19	8.58	121.53	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	u	307	CLA	C4A-NA-C1A	-8.58	102.77	106.68
40	p	307	CLA	C4A-NA-C1A	-8.54	102.78	106.68
40	x	311	CLA	C4A-NA-C1A	-8.54	102.78	106.68
40	a	804	CLA	C1C-NC-C4C	-8.30	102.89	106.68
40	Q	203	CLA	C1C-NC-C4C	-8.29	102.90	106.68
40	o	313	CLA	C4A-NA-C1A	-8.29	102.90	106.68
40	y	309	CLA	C4A-NA-C1A	-8.27	102.91	106.68
40	u	311	CLA	C4A-NA-C1A	-8.14	102.97	106.68
47	K	313	A1EB1	C33-C32-C31	-8.11	101.33	109.21
40	E	302	CLA	C4A-NA-C1A	-8.07	103.00	106.68
40	a	808	CLA	C4A-NA-C1A	-8.03	103.02	106.68
40	a	811	CLA	C1C-NC-C4C	-8.00	103.03	106.68
44	q	316	A86	O1-C20-C19	-7.99	106.00	113.49
40	Z	310	CLA	C4A-NA-C1A	-7.99	103.03	106.68
40	H	309	CLA	C4A-NA-C1A	-7.99	103.04	106.68
40	w	309	CLA	C4A-NA-C1A	-7.97	103.04	106.68
44	Y	320	A86	O1-C20-C19	-7.94	106.05	113.49
40	X	310	CLA	C4A-NA-C1A	-7.84	103.10	106.68
40	t	307	CLA	C4A-NA-C1A	-7.84	103.10	106.68
40	S	311	CLA	C4A-NA-C1A	-7.83	103.11	106.68
40	i	101	CLA	C4A-NA-C1A	-7.82	103.11	106.68
40	Q	207	CLA	C4A-NA-C1A	-7.76	103.14	106.68
40	Z	313	CLA	C4A-NA-C1A	-7.76	103.14	106.68
40	z	314	CLA	C4A-NA-C1A	-7.74	103.15	106.68
44	v	316	A86	O1-C20-C19	-7.73	106.25	113.49
44	p	319	A86	O1-C20-C19	-7.72	106.26	113.49
40	b	827	CLA	C4A-NA-C1A	-7.71	103.16	106.68
40	O	310	CLA	C4A-NA-C1A	-7.68	103.17	106.68
40	C	302	CLA	C4A-NA-C1A	-7.68	103.18	106.68
40	p	311	CLA	C4A-NA-C1A	-7.67	103.18	106.68
40	a	816	CLA	C4A-NA-C1A	-7.66	103.18	106.68
48	P	320	A1EB4	C33-C32-C31	7.64	116.64	109.21
40	b	809	CLA	C4A-NA-C1A	-7.63	103.20	106.68
40	a	838	CLA	C4A-NA-C1A	-7.62	103.20	106.68
40	Y	313	CLA	C4A-NA-C1A	-7.61	103.21	106.68
44	u	317	A86	O1-C20-C19	-7.61	106.36	113.49
40	l	203	CLA	C4A-NA-C1A	-7.60	103.21	106.68
40	y	303	CLA	C4A-NA-C1A	-7.58	103.22	106.68
40	B	307	CLA	C4A-NA-C1A	-7.56	103.23	106.68
40	L	306	CLA	C4A-NA-C1A	-7.47	103.27	106.68
40	S	314	CLA	C4A-NA-C1A	-7.46	103.28	106.68
40	u	314	CLA	C4A-NA-C1A	-7.43	103.29	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	X	313	CLA	C4A-NA-C1A	-7.42	103.30	106.68
40	x	302	CLA	C4A-NA-C1A	-7.42	103.30	106.68
40	B	301	CLA	C4A-NA-C1A	-7.40	103.30	106.68
40	J	310	CLA	C4A-NA-C1A	-7.40	103.30	106.68
40	C	307	CLA	C4A-NA-C1A	-7.36	103.32	106.68
40	o	312	CLA	C4A-NA-C1A	-7.34	103.33	106.68
44	u	318	A86	O1-C20-C19	-7.33	106.62	113.49
40	E	303	CLA	C4A-NA-C1A	-7.33	103.34	106.68
40	b	839	CLA	C4A-NA-C1A	-7.33	103.34	106.68
40	b	838	CLA	C4A-NA-C1A	-7.29	103.35	106.68
44	Q	215	A86	O1-C20-C19	-7.27	106.68	113.49
40	p	308	CLA	C4A-NA-C1A	-7.26	103.37	106.68
40	Q	202	CLA	C4A-NA-C1A	-7.25	103.37	106.68
40	X	311	CLA	C4A-NA-C1A	-7.25	103.37	106.68
40	u	305	CLA	C4A-NA-C1A	-7.24	103.38	106.68
40	q	311	CLA	C4A-NA-C1A	-7.23	103.38	106.68
40	b	832	CLA	C4A-NA-C1A	-7.23	103.38	106.68
40	z	313	CLA	C4A-NA-C1A	-7.22	103.38	106.68
40	a	806	CLA	C4A-NA-C1A	-7.19	103.40	106.68
40	D	305	CLA	C3D-C4D-ND	7.19	114.43	109.68
40	Y	312	CLA	C4A-NA-C1A	-7.19	103.40	106.68
40	U	202	CLA	C4A-NA-C1A	-7.18	103.41	106.68
40	E	312	CLA	C4A-NA-C1A	-7.13	103.42	106.68
40	v	313	CLA	C4A-NA-C1A	-7.12	103.43	106.68
40	v	307	CLA	C4A-NA-C1A	-7.12	103.43	106.68
40	N	311	CLA	C4A-NA-C1A	-7.10	103.44	106.68
44	R	312	A86	C33-C32-C31	-7.07	102.34	109.21
40	q	307	CLA	C4A-NA-C1A	-7.06	103.46	106.68
40	a	820	CLA	C4A-NA-C1A	-7.03	103.47	106.68
40	a	829	CLA	C4A-NA-C1A	-7.00	103.48	106.68
40	Z	306	CLA	C4A-NA-C1A	-7.00	103.49	106.68
40	b	840	CLA	C4A-NA-C1A	-6.99	103.49	106.68
40	b	830	CLA	C4A-NA-C1A	-6.98	103.49	106.68
44	p	317	A86	O1-C20-C19	-6.98	106.95	113.49
40	S	305	CLA	C4A-NA-C1A	-6.92	103.52	106.68
40	I	207	CLA	C4A-NA-C1A	-6.91	103.53	106.68
40	U	207	CLA	C4A-NA-C1A	-6.86	103.55	106.68
40	S	312	CLA	C4A-NA-C1A	-6.85	103.56	106.68
44	x	319	A86	O1-C20-C19	-6.84	107.08	113.49
40	I	208	CLA	C4A-NA-C1A	-6.84	103.56	106.68
40	l	205	CLA	C4A-NA-C1A	-6.84	103.56	106.68
40	u	302	CLA	C4A-NA-C1A	-6.83	103.56	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	v	311	CLA	C4A-NA-C1A	-6.82	103.57	106.68
40	W	308	CLA	C4A-NA-C1A	-6.81	103.57	106.68
40	G	213	CLA	C4A-NA-C1A	-6.81	103.57	106.68
40	J	311	CLA	C4A-NA-C1A	-6.80	103.58	106.68
40	q	301	CLA	C4A-NA-C1A	-6.79	103.58	106.68
40	I	203	CLA	C4A-NA-C1A	-6.79	103.58	106.68
40	P	311	CLA	C4A-NA-C1A	-6.77	103.59	106.68
40	X	306	CLA	C4A-NA-C1A	-6.77	103.59	106.68
40	u	308	CLA	C4A-NA-C1A	-6.77	103.59	106.68
40	q	310	CLA	C4A-NA-C1A	-6.76	103.60	106.68
40	a	807	CLA	C4A-NA-C1A	-6.74	103.60	106.68
40	o	310	CLA	C4A-NA-C1A	-6.74	103.60	106.68
40	a	850	CLA	C4A-NA-C1A	-6.74	103.61	106.68
40	Y	306	CLA	C4A-NA-C1A	-6.71	103.62	106.68
40	L	304	CLA	C4A-NA-C1A	-6.70	103.62	106.68
40	p	314	CLA	C4A-NA-C1A	-6.69	103.63	106.68
40	a	818	CLA	C4A-NA-C1A	-6.68	103.63	106.68
40	x	308	CLA	C4A-NA-C1A	-6.68	103.63	106.68
40	b	828	CLA	C4A-NA-C1A	-6.67	103.64	106.68
40	C	308	CLA	C4A-NA-C1A	-6.66	103.64	106.68
40	J	306	CLA	C4A-NA-C1A	-6.65	103.64	106.68
40	a	834	CLA	C4A-NA-C1A	-6.65	103.64	106.68
40	v	301	CLA	C4A-NA-C1A	-6.65	103.64	106.68
44	X	319	A86	O1-C20-C19	-6.64	107.27	113.49
40	Z	311	CLA	C4A-NA-C1A	-6.63	103.66	106.68
44	X	315	A86	C33-C32-C31	6.63	115.65	109.21
40	a	815	CLA	C4A-NA-C1A	-6.61	103.66	106.68
40	v	310	CLA	C4A-NA-C1A	-6.61	103.66	106.68
40	L	310	CLA	C4A-NA-C1A	-6.60	103.67	106.68
40	z	312	CLA	C4A-NA-C1A	-6.60	103.67	106.68
40	J	303	CLA	C4A-NA-C1A	-6.58	103.68	106.68
40	y	302	CLA	C4A-NA-C1A	-6.58	103.68	106.68
40	Y	307	CLA	C4A-NA-C1A	-6.58	103.68	106.68
40	a	813	CLA	C4A-NA-C1A	-6.55	103.69	106.68
40	R	307	CLA	C4A-NA-C1A	-6.55	103.69	106.68
40	A	307	CLA	C4A-NA-C1A	-6.54	103.70	106.68
40	b	822	CLA	C4A-NA-C1A	-6.53	103.70	106.68
40	D	304	CLA	C4A-NA-C1A	-6.49	103.72	106.68
40	z	307	CLA	C4A-NA-C1A	-6.49	103.72	106.68
40	X	310	CLA	C1D-ND-C4D	-6.49	101.76	106.31
40	C	301	CLA	C4A-NA-C1A	-6.48	103.72	106.68
40	R	310	CLA	C4A-NA-C1A	-6.46	103.73	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	B	304	CLA	C4A-NA-C1A	-6.46	103.73	106.68
40	U	205	CLA	C4A-NA-C1A	-6.46	103.73	106.68
40	E	308	CLA	C4A-NA-C1A	-6.45	103.74	106.68
40	L	311	CLA	C4A-NA-C1A	-6.44	103.74	106.68
40	Q	209	CLA	C4A-NA-C1A	-6.44	103.74	106.68
40	W	311	CLA	C4A-NA-C1A	-6.43	103.75	106.68
40	U	203	CLA	C4A-NA-C1A	-6.42	103.75	106.68
40	o	307	CLA	C4A-NA-C1A	-6.40	103.76	106.68
44	x	316	A86	C33-C32-C31	6.40	115.43	109.21
40	C	309	CLA	C1D-ND-C4D	-6.40	101.82	106.31
40	v	312	CLA	C1D-ND-C4D	-6.39	101.83	106.31
40	A	304	CLA	C1D-ND-C4D	-6.38	101.83	106.31
40	a	804	CLA	C1D-ND-C4D	-6.38	101.84	106.31
40	a	810	CLA	C1D-ND-C4D	-6.37	101.84	106.31
40	P	307	CLA	C4A-NA-C1A	-6.37	103.77	106.68
40	z	305	CLA	C4A-NA-C1A	-6.37	103.77	106.68
40	C	305	CLA	C4A-NA-C1A	-6.37	103.77	106.68
40	S	307	CLA	C1D-ND-C4D	-6.37	101.85	106.31
40	o	311	CLA	C4A-NA-C1A	-6.36	103.78	106.68
40	X	312	CLA	C4A-NA-C1A	-6.34	103.78	106.68
40	F	308	CLA	C1D-ND-C4D	-6.34	101.86	106.31
40	t	305	CLA	C1D-ND-C4D	-6.34	101.86	106.31
40	b	816	CLA	C4A-NA-C1A	-6.33	103.79	106.68
40	A	309	CLA	C1D-ND-C4D	-6.33	101.87	106.31
40	I	202	CLA	C1D-ND-C4D	-6.33	101.87	106.31
40	D	305	CLA	C4A-NA-C1A	-6.32	103.80	106.68
47	R	317	A1EB1	C33-C32-C31	-6.32	103.07	109.21
40	U	202	CLA	C1D-ND-C4D	-6.32	101.88	106.31
40	a	839	CLA	C4A-NA-C1A	-6.31	103.80	106.68
40	b	803	CLA	C4A-NA-C1A	-6.31	103.80	106.68
44	v	314	A86	C34-O4-C38	6.31	128.99	117.85
40	Y	313	CLA	C1D-ND-C4D	-6.31	101.89	106.31
40	o	307	CLA	C1D-ND-C4D	-6.30	101.89	106.31
40	a	814	CLA	C1D-ND-C4D	-6.30	101.89	106.31
40	M	312	CLA	C1D-ND-C4D	-6.29	101.90	106.31
40	N	310	CLA	C4A-NA-C1A	-6.29	103.81	106.68
40	v	305	CLA	C4A-NA-C1A	-6.29	103.81	106.68
40	F	305	CLA	C1D-ND-C4D	-6.27	101.91	106.31
40	F	307	CLA	C1D-ND-C4D	-6.27	101.91	106.31
44	u	319	A86	O1-C20-C19	-6.27	107.61	113.49
40	b	842	CLA	C4A-NA-C1A	-6.27	103.82	106.68
40	A	307	CLA	C1D-ND-C4D	-6.27	101.91	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	R	305	CLA	C1D-ND-C4D	-6.27	101.92	106.31
40	p	302	CLA	C1D-ND-C4D	-6.27	101.92	106.31
40	S	311	CLA	C1D-ND-C4D	-6.26	101.92	106.31
40	o	306	CLA	C1D-ND-C4D	-6.26	101.92	106.31
40	v	305	CLA	C1D-ND-C4D	-6.26	101.92	106.31
40	H	308	CLA	C1D-ND-C4D	-6.26	101.92	106.31
40	v	307	CLA	C1D-ND-C4D	-6.26	101.92	106.31
40	W	306	CLA	C1D-ND-C4D	-6.25	101.92	106.31
40	E	309	CLA	C1D-ND-C4D	-6.25	101.92	106.31
40	W	313	CLA	C1D-ND-C4D	-6.25	101.92	106.31
40	N	307	CLA	C1D-ND-C4D	-6.25	101.93	106.31
40	a	851	CLA	C1D-ND-C4D	-6.25	101.93	106.31
40	Y	306	CLA	C1D-ND-C4D	-6.25	101.93	106.31
40	M	311	CLA	C1D-ND-C4D	-6.25	101.93	106.31
40	H	311	CLA	C1D-ND-C4D	-6.24	101.93	106.31
40	K	304	CLA	C4A-NA-C1A	-6.24	103.83	106.68
40	Q	205	CLA	C1D-ND-C4D	-6.24	101.94	106.31
40	F	311	CLA	C1D-ND-C4D	-6.24	101.94	106.31
40	O	306	CLA	C1D-ND-C4D	-6.23	101.94	106.31
40	Y	307	CLA	C1D-ND-C4D	-6.23	101.94	106.31
40	D	309	CLA	C1D-ND-C4D	-6.23	101.94	106.31
44	q	314	A86	C34-O4-C38	6.22	128.84	117.85
40	D	304	CLA	C1D-ND-C4D	-6.22	101.94	106.31
40	y	305	CLA	C1D-ND-C4D	-6.22	101.95	106.31
40	a	806	CLA	C1D-ND-C4D	-6.22	101.95	106.31
40	J	305	CLA	C4A-NA-C1A	-6.22	103.84	106.68
40	F	306	CLA	C1D-ND-C4D	-6.22	101.95	106.31
40	H	302	CLA	C1D-ND-C4D	-6.22	101.95	106.31
40	R	304	CLA	C1D-ND-C4D	-6.22	101.95	106.31
40	E	311	CLA	C1D-ND-C4D	-6.21	101.95	106.31
40	a	827	CLA	C1D-ND-C4D	-6.21	101.95	106.31
40	a	841	CLA	C1D-ND-C4D	-6.21	101.95	106.31
40	o	313	CLA	C1D-ND-C4D	-6.21	101.95	106.31
40	T	310	CLA	C4A-NA-C1A	-6.21	103.84	106.68
40	u	305	CLA	C1D-ND-C4D	-6.21	101.96	106.31
40	z	308	CLA	C1D-ND-C4D	-6.21	101.96	106.31
44	z	315	A86	C34-O4-C38	6.20	128.81	117.85
40	Y	311	CLA	C1D-ND-C4D	-6.20	101.96	106.31
40	x	314	CLA	C4A-NA-C1A	-6.20	103.85	106.68
40	K	304	CLA	C1D-ND-C4D	-6.20	101.96	106.31
40	K	308	CLA	C1D-ND-C4D	-6.20	101.96	106.31
40	O	305	CLA	C1D-ND-C4D	-6.20	101.96	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	l	203	CLA	C1D-ND-C4D	-6.20	101.96	106.31
40	u	314	CLA	C1D-ND-C4D	-6.20	101.96	106.31
40	M	306	CLA	C1D-ND-C4D	-6.20	101.96	106.31
40	T	304	CLA	C4A-NA-C1A	-6.20	103.85	106.68
40	T	307	CLA	C1D-ND-C4D	-6.20	101.96	106.31
40	q	307	CLA	C1D-ND-C4D	-6.19	101.97	106.31
40	F	304	CLA	C1D-ND-C4D	-6.19	101.97	106.31
40	F	321	CLA	C4A-NA-C1A	-6.19	103.86	106.68
40	A	306	CLA	C1D-ND-C4D	-6.19	101.97	106.31
40	b	814	CLA	C1D-ND-C4D	-6.19	101.97	106.31
40	b	836	CLA	C1D-ND-C4D	-6.19	101.97	106.31
40	G	203	CLA	C1D-ND-C4D	-6.18	101.98	106.31
40	X	306	CLA	C1D-ND-C4D	-6.18	101.98	106.31
40	Y	301	CLA	C1D-ND-C4D	-6.18	101.98	106.31
40	D	307	CLA	C1D-ND-C4D	-6.18	101.98	106.31
40	D	305	CLA	C3D-C4D-CHA	-6.18	112.53	124.84
40	u	312	CLA	C1D-ND-C4D	-6.17	101.98	106.31
40	P	308	CLA	C1D-ND-C4D	-6.17	101.98	106.31
40	j	102	CLA	C4A-NA-C1A	-6.17	103.86	106.68
40	a	819	CLA	C1D-ND-C4D	-6.17	101.98	106.31
40	P	312	CLA	C1D-ND-C4D	-6.16	101.99	106.31
40	J	311	CLA	C1D-ND-C4D	-6.16	101.99	106.31
40	R	306	CLA	C1D-ND-C4D	-6.16	101.99	106.31
40	F	303	CLA	C1D-ND-C4D	-6.16	101.99	106.31
40	N	305	CLA	C1D-ND-C4D	-6.16	101.99	106.31
40	S	308	CLA	C1D-ND-C4D	-6.16	101.99	106.31
40	w	305	CLA	C1D-ND-C4D	-6.16	101.99	106.31
40	k	201	CLA	C1D-ND-C4D	-6.16	101.99	106.31
40	b	811	CLA	C4A-NA-C1A	-6.15	103.87	106.68
40	a	817	CLA	C1D-ND-C4D	-6.15	101.99	106.31
40	w	302	CLA	C1D-ND-C4D	-6.15	101.99	106.31
44	S	315	A86	O1-C20-C19	-6.15	107.73	113.49
40	z	324	CLA	C1D-ND-C4D	-6.15	102.00	106.31
40	E	305	CLA	C1D-ND-C4D	-6.15	102.00	106.31
40	z	307	CLA	C1D-ND-C4D	-6.15	102.00	106.31
40	S	301	CLA	C4A-NA-C1A	-6.15	103.88	106.68
40	a	852	CLA	C1D-ND-C4D	-6.15	102.00	106.31
40	D	308	CLA	C1D-ND-C4D	-6.14	102.00	106.31
40	Z	312	CLA	C4A-NA-C1A	-6.14	103.88	106.68
40	L	307	CLA	C1D-ND-C4D	-6.14	102.00	106.31
40	q	305	CLA	C1D-ND-C4D	-6.14	102.00	106.31
40	q	313	CLA	C1D-ND-C4D	-6.14	102.00	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	t	302	CLA	C1D-ND-C4D	-6.14	102.00	106.31
40	F	307	CLA	C4A-NA-C1A	-6.14	103.88	106.68
40	o	306	CLA	C4A-NA-C1A	-6.13	103.88	106.68
40	C	302	CLA	C1D-ND-C4D	-6.13	102.01	106.31
40	D	302	CLA	C1D-ND-C4D	-6.13	102.01	106.31
40	D	312	CLA	C1D-ND-C4D	-6.13	102.01	106.31
40	H	307	CLA	C1D-ND-C4D	-6.13	102.01	106.31
40	T	306	CLA	C1D-ND-C4D	-6.13	102.01	106.31
40	w	303	CLA	C1D-ND-C4D	-6.13	102.01	106.31
40	A	303	CLA	C1D-ND-C4D	-6.12	102.02	106.31
40	E	304	CLA	C1D-ND-C4D	-6.12	102.02	106.31
40	Y	305	CLA	C1D-ND-C4D	-6.12	102.02	106.31
40	a	831	CLA	C1D-ND-C4D	-6.12	102.02	106.31
40	q	306	CLA	C1D-ND-C4D	-6.12	102.02	106.31
40	G	204	CLA	C4A-NA-C1A	-6.12	103.89	106.68
40	X	307	CLA	C1D-ND-C4D	-6.12	102.02	106.31
40	a	834	CLA	C1D-ND-C4D	-6.12	102.02	106.31
40	p	305	CLA	C1D-ND-C4D	-6.12	102.02	106.31
40	H	310	CLA	C1D-ND-C4D	-6.11	102.02	106.31
40	a	823	CLA	C1D-ND-C4D	-6.11	102.02	106.31
40	t	309	CLA	C1D-ND-C4D	-6.11	102.02	106.31
40	Z	306	CLA	C1D-ND-C4D	-6.11	102.02	106.31
40	a	833	CLA	C1D-ND-C4D	-6.11	102.02	106.31
40	A	305	CLA	C4A-NA-C1A	-6.11	103.89	106.68
40	p	302	CLA	C4A-NA-C1A	-6.11	103.89	106.68
40	o	301	CLA	C1D-ND-C4D	-6.11	102.03	106.31
40	b	834	CLA	C4A-NA-C1A	-6.11	103.89	106.68
40	b	826	CLA	C1D-ND-C4D	-6.11	102.03	106.31
40	I	203	CLA	C1D-ND-C4D	-6.10	102.03	106.31
40	b	837	CLA	C1D-ND-C4D	-6.10	102.03	106.31
40	G	213	CLA	C1D-ND-C4D	-6.10	102.03	106.31
40	b	815	CLA	C1D-ND-C4D	-6.10	102.03	106.31
40	p	313	CLA	C1D-ND-C4D	-6.10	102.03	106.31
40	a	804	CLA	C4A-NA-C1A	-6.10	103.90	106.68
40	b	831	CLA	C1D-ND-C4D	-6.10	102.03	106.31
40	z	302	CLA	C1D-ND-C4D	-6.10	102.03	106.31
40	b	809	CLA	C1D-ND-C4D	-6.09	102.04	106.31
40	C	306	CLA	C1D-ND-C4D	-6.09	102.04	106.31
40	X	301	CLA	C1D-ND-C4D	-6.09	102.04	106.31
40	I	208	CLA	C1D-ND-C4D	-6.09	102.04	106.31
40	E	313	CLA	C1D-ND-C4D	-6.09	102.04	106.31
40	I	207	CLA	C1D-ND-C4D	-6.09	102.04	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	t	305	CLA	C4A-NA-C1A	-6.09	103.90	106.68
40	J	309	CLA	C1D-ND-C4D	-6.09	102.04	106.31
40	u	313	CLA	C1D-ND-C4D	-6.09	102.04	106.31
40	O	307	CLA	C1D-ND-C4D	-6.08	102.04	106.31
40	Y	310	CLA	C1D-ND-C4D	-6.08	102.04	106.31
40	D	311	CLA	C4A-NA-C1A	-6.08	103.90	106.68
40	y	305	CLA	C4A-NA-C1A	-6.08	103.91	106.68
40	F	301	CLA	C1D-ND-C4D	-6.08	102.05	106.31
40	P	307	CLA	C1D-ND-C4D	-6.08	102.05	106.31
40	I	206	CLA	C1D-ND-C4D	-6.08	102.05	106.31
40	P	313	CLA	C1D-ND-C4D	-6.07	102.05	106.31
40	v	306	CLA	C4A-NA-C1A	-6.07	103.91	106.68
40	D	303	CLA	C1D-ND-C4D	-6.07	102.05	106.31
40	J	308	CLA	C1D-ND-C4D	-6.07	102.05	106.31
40	V	202	CLA	C1D-ND-C4D	-6.07	102.05	106.31
40	a	820	CLA	C1D-ND-C4D	-6.07	102.05	106.31
40	f	204	CLA	C1D-ND-C4D	-6.07	102.05	106.31
40	Z	310	CLA	C1D-ND-C4D	-6.07	102.05	106.31
40	b	819	CLA	C1D-ND-C4D	-6.07	102.06	106.31
40	A	305	CLA	C1D-ND-C4D	-6.07	102.06	106.31
40	k	202	CLA	C4A-NA-C1A	-6.06	103.91	106.68
40	B	301	CLA	C1D-ND-C4D	-6.06	102.06	106.31
40	b	818	CLA	C1D-ND-C4D	-6.06	102.06	106.31
40	o	311	CLA	C1D-ND-C4D	-6.06	102.06	106.31
40	R	307	CLA	C1D-ND-C4D	-6.06	102.06	106.31
40	A	308	CLA	C1D-ND-C4D	-6.06	102.06	106.31
40	K	306	CLA	C1D-ND-C4D	-6.06	102.06	106.31
40	O	304	CLA	C1D-ND-C4D	-6.06	102.06	106.31
40	y	304	CLA	C1D-ND-C4D	-6.06	102.06	106.31
44	u	320	A86	O1-C20-C19	-6.06	107.81	113.49
40	p	311	CLA	C1D-ND-C4D	-6.06	102.06	106.31
40	a	815	CLA	C1D-ND-C4D	-6.05	102.06	106.31
40	p	312	CLA	C1D-ND-C4D	-6.05	102.06	106.31
40	Q	203	CLA	C1D-ND-C4D	-6.05	102.07	106.31
40	a	812	CLA	C1D-ND-C4D	-6.05	102.07	106.31
40	V	201	CLA	C1D-ND-C4D	-6.05	102.07	106.31
40	a	835	CLA	C1D-ND-C4D	-6.05	102.07	106.31
40	F	308	CLA	C4A-NA-C1A	-6.05	103.92	106.68
40	a	840	CLA	C1D-ND-C4D	-6.04	102.07	106.31
40	a	830	CLA	C1D-ND-C4D	-6.04	102.07	106.31
40	q	306	CLA	C4A-NA-C1A	-6.04	103.92	106.68
40	G	201	CLA	C1D-ND-C4D	-6.04	102.08	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	B	306	CLA	C1D-ND-C4D	-6.04	102.08	106.31
40	w	304	CLA	C1D-ND-C4D	-6.04	102.08	106.31
40	p	306	CLA	C4A-NA-C1A	-6.04	103.92	106.68
40	H	310	CLA	C4A-NA-C1A	-6.03	103.93	106.68
40	b	823	CLA	C1D-ND-C4D	-6.03	102.08	106.31
40	C	305	CLA	C1D-ND-C4D	-6.03	102.08	106.31
40	D	301	CLA	C1D-ND-C4D	-6.03	102.08	106.31
40	b	820	CLA	C1D-ND-C4D	-6.03	102.08	106.31
40	o	310	CLA	C1D-ND-C4D	-6.03	102.08	106.31
40	C	307	CLA	C1D-ND-C4D	-6.02	102.08	106.31
40	a	816	CLA	C1D-ND-C4D	-6.02	102.08	106.31
40	t	303	CLA	C1D-ND-C4D	-6.02	102.08	106.31
40	E	308	CLA	C1D-ND-C4D	-6.02	102.09	106.31
40	a	839	CLA	C1D-ND-C4D	-6.02	102.09	106.31
40	w	305	CLA	C4A-NA-C1A	-6.02	103.93	106.68
40	a	821	CLA	C1D-ND-C4D	-6.02	102.09	106.31
40	a	822	CLA	C1D-ND-C4D	-6.02	102.09	106.31
40	b	825	CLA	C4A-NA-C1A	-6.02	103.93	106.68
40	z	314	CLA	C1D-ND-C4D	-6.02	102.09	106.31
40	y	303	CLA	C1D-ND-C4D	-6.02	102.09	106.31
40	z	313	CLA	C1D-ND-C4D	-6.02	102.09	106.31
40	b	828	CLA	C1D-ND-C4D	-6.01	102.09	106.31
40	x	313	CLA	C1D-ND-C4D	-6.01	102.09	106.31
40	z	308	CLA	C4A-NA-C1A	-6.01	103.94	106.68
40	M	307	CLA	C1D-ND-C4D	-6.01	102.10	106.31
40	Z	307	CLA	C1D-ND-C4D	-6.01	102.10	106.31
40	l	202	CLA	C1D-ND-C4D	-6.01	102.10	106.31
40	w	308	CLA	C1D-ND-C4D	-6.01	102.10	106.31
40	z	311	CLA	C1D-ND-C4D	-6.01	102.10	106.31
40	U	207	CLA	C1D-ND-C4D	-6.00	102.10	106.31
40	a	829	CLA	C1D-ND-C4D	-6.00	102.10	106.31
40	t	303	CLA	C4A-NA-C1A	-6.00	103.94	106.68
40	S	319	CLA	C1D-ND-C4D	-6.00	102.10	106.31
40	x	312	CLA	C1D-ND-C4D	-6.00	102.10	106.31
40	b	822	CLA	C1D-ND-C4D	-6.00	102.10	106.31
40	y	308	CLA	C1D-ND-C4D	-6.00	102.10	106.31
40	Q	203	CLA	C4A-NA-C1A	-6.00	103.94	106.68
40	E	310	CLA	C1D-ND-C4D	-6.00	102.10	106.31
40	w	302	CLA	C4A-NA-C1A	-6.00	103.94	106.68
40	E	307	CLA	C1D-ND-C4D	-6.00	102.10	106.31
40	b	830	CLA	C1D-ND-C4D	-6.00	102.11	106.31
40	E	310	CLA	C4A-NA-C1A	-5.99	103.94	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	T	307	CLA	C4A-NA-C1A	-5.99	103.94	106.68
40	E	306	CLA	C1D-ND-C4D	-5.99	102.11	106.31
40	L	310	CLA	C1D-ND-C4D	-5.99	102.11	106.31
40	K	308	CLA	C4A-NA-C1A	-5.99	103.94	106.68
40	a	837	CLA	C4A-NA-C1A	-5.99	103.94	106.68
40	q	312	CLA	C1D-ND-C4D	-5.99	102.11	106.31
40	q	305	CLA	C4A-NA-C1A	-5.99	103.95	106.68
40	x	305	CLA	C1D-ND-C4D	-5.99	102.11	106.31
40	L	305	CLA	C4A-NA-C1A	-5.99	103.95	106.68
40	I	201	CLA	C1D-ND-C4D	-5.99	102.11	106.31
40	M	304	CLA	C1D-ND-C4D	-5.99	102.11	106.31
40	E	302	CLA	C1D-ND-C4D	-5.99	102.11	106.31
40	D	306	CLA	C1D-ND-C4D	-5.98	102.11	106.31
40	b	813	CLA	C1D-ND-C4D	-5.98	102.11	106.31
40	Q	204	CLA	C1D-ND-C4D	-5.98	102.11	106.31
40	b	801	CLA	C4A-NA-C1A	-5.98	103.95	106.68
40	E	312	CLA	C1D-ND-C4D	-5.98	102.12	106.31
40	b	820	CLA	C4A-NA-C1A	-5.98	103.95	106.68
40	D	311	CLA	C1D-ND-C4D	-5.98	102.12	106.31
40	J	306	CLA	C1D-ND-C4D	-5.98	102.12	106.31
40	M	305	CLA	C1D-ND-C4D	-5.98	102.12	106.31
40	a	805	CLA	C1D-ND-C4D	-5.98	102.12	106.31
40	x	302	CLA	C1D-ND-C4D	-5.98	102.12	106.31
40	B	303	CLA	C1D-ND-C4D	-5.97	102.12	106.31
40	E	303	CLA	C1D-ND-C4D	-5.97	102.12	106.31
40	G	206	CLA	C1D-ND-C4D	-5.97	102.12	106.31
40	S	306	CLA	C1D-ND-C4D	-5.97	102.12	106.31
40	U	204	CLA	C1D-ND-C4D	-5.97	102.12	106.31
40	Y	310	CLA	C4A-NA-C1A	-5.97	103.96	106.68
40	A	302	CLA	C1D-ND-C4D	-5.96	102.13	106.31
40	X	313	CLA	C1D-ND-C4D	-5.96	102.13	106.31
40	t	304	CLA	C1D-ND-C4D	-5.96	102.13	106.31
40	C	309	CLA	C4A-NA-C1A	-5.96	103.96	106.68
40	I	201	CLA	C4A-NA-C1A	-5.96	103.96	106.68
40	u	306	CLA	C4A-NA-C1A	-5.96	103.96	106.68
40	G	207	CLA	C1D-ND-C4D	-5.96	102.13	106.31
40	Z	301	CLA	C1D-ND-C4D	-5.96	102.13	106.31
40	b	839	CLA	C1D-ND-C4D	-5.96	102.13	106.31
44	v	314	A86	O1-C20-C19	5.96	119.08	113.49
40	b	823	CLA	C4A-NA-C1A	-5.96	103.96	106.68
40	p	305	CLA	C4A-NA-C1A	-5.96	103.96	106.68
40	X	312	CLA	C1D-ND-C4D	-5.96	102.13	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	U	203	CLA	C1D-ND-C4D	-5.96	102.13	106.31
40	a	807	CLA	C1D-ND-C4D	-5.95	102.13	106.31
44	u	316	A86	C33-C32-C31	5.95	115.00	109.21
40	b	806	CLA	C1D-ND-C4D	-5.95	102.14	106.31
40	z	306	CLA	C1D-ND-C4D	-5.95	102.14	106.31
44	o	314	A86	C34-O4-C38	5.95	128.35	117.85
40	a	818	CLA	C1D-ND-C4D	-5.95	102.14	106.31
40	S	307	CLA	C4A-NA-C1A	-5.95	103.97	106.68
40	C	301	CLA	C1D-ND-C4D	-5.95	102.14	106.31
40	W	308	CLA	C1D-ND-C4D	-5.95	102.14	106.31
40	Z	307	CLA	C4A-NA-C1A	-5.95	103.97	106.68
40	v	313	CLA	C1D-ND-C4D	-5.95	102.14	106.31
40	b	818	CLA	C4A-NA-C1A	-5.94	103.97	106.68
40	Q	206	CLA	C1D-ND-C4D	-5.94	102.14	106.31
40	H	306	CLA	C1D-ND-C4D	-5.94	102.14	106.31
44	X	315	A86	C34-O4-C38	5.94	128.34	117.85
40	N	306	CLA	C1D-ND-C4D	-5.94	102.15	106.31
40	o	312	CLA	C1D-ND-C4D	-5.94	102.15	106.31
44	Z	314	A86	C34-O4-C38	5.94	128.33	117.85
40	L	311	CLA	C1D-ND-C4D	-5.93	102.15	106.31
40	b	805	CLA	C1D-ND-C4D	-5.93	102.15	106.31
40	a	850	CLA	C1D-ND-C4D	-5.93	102.15	106.31
40	u	311	CLA	C1D-ND-C4D	-5.93	102.15	106.31
40	N	311	CLA	C1D-ND-C4D	-5.93	102.15	106.31
40	a	837	CLA	C1D-ND-C4D	-5.93	102.15	106.31
40	H	301	CLA	C1D-ND-C4D	-5.93	102.15	106.31
40	N	304	CLA	C1D-ND-C4D	-5.93	102.15	106.31
40	x	311	CLA	C1D-ND-C4D	-5.93	102.15	106.31
40	W	305	CLA	C1D-ND-C4D	-5.92	102.16	106.31
40	b	811	CLA	C1D-ND-C4D	-5.92	102.16	106.31
40	i	101	CLA	C1D-ND-C4D	-5.92	102.16	106.31
40	F	304	CLA	C4A-NA-C1A	-5.92	103.98	106.68
44	R	315	A86	C34-O4-C38	5.92	128.30	117.85
40	S	301	CLA	C1D-ND-C4D	-5.92	102.16	106.31
40	M	304	CLA	C4A-NA-C1A	-5.91	103.98	106.68
40	Z	312	CLA	C1D-ND-C4D	-5.91	102.17	106.31
40	a	832	CLA	C1D-ND-C4D	-5.91	102.17	106.31
40	S	302	CLA	C1D-ND-C4D	-5.91	102.17	106.31
44	X	316	A86	O1-C20-C19	-5.91	107.95	113.49
40	b	833	CLA	C1D-ND-C4D	-5.90	102.17	106.31
40	b	840	CLA	C1D-ND-C4D	-5.90	102.17	106.31
40	Y	312	CLA	C1D-ND-C4D	-5.90	102.17	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	a	838	CLA	C1D-ND-C4D	-5.90	102.17	106.31
40	J	312	CLA	C1D-ND-C4D	-5.90	102.17	106.31
40	J	318	CLA	C1D-ND-C4D	-5.90	102.17	106.31
40	a	828	CLA	C1D-ND-C4D	-5.90	102.17	106.31
40	u	302	CLA	C1D-ND-C4D	-5.89	102.18	106.31
40	M	307	CLA	C4A-NA-C1A	-5.89	103.99	106.68
40	p	308	CLA	C1D-ND-C4D	-5.89	102.18	106.31
40	x	314	CLA	C1D-ND-C4D	-5.89	102.18	106.31
40	b	835	CLA	C1D-ND-C4D	-5.89	102.18	106.31
40	w	303	CLA	C4A-NA-C1A	-5.89	103.99	106.68
40	G	205	CLA	C1D-ND-C4D	-5.88	102.18	106.31
40	S	314	CLA	C1D-ND-C4D	-5.88	102.18	106.31
40	T	304	CLA	C1D-ND-C4D	-5.88	102.18	106.31
40	Q	209	CLA	C1D-ND-C4D	-5.88	102.18	106.31
40	K	301	CLA	C1D-ND-C4D	-5.88	102.19	106.31
40	l	204	CLA	C1D-ND-C4D	-5.88	102.19	106.31
40	v	306	CLA	C1D-ND-C4D	-5.88	102.19	106.31
40	b	821	CLA	C1D-ND-C4D	-5.88	102.19	106.31
40	O	305	CLA	C4A-NA-C1A	-5.88	104.00	106.68
40	o	304	CLA	C1D-ND-C4D	-5.87	102.19	106.31
40	X	305	CLA	C1D-ND-C4D	-5.87	102.19	106.31
40	L	305	CLA	C1D-ND-C4D	-5.87	102.19	106.31
40	b	819	CLA	C4A-NA-C1A	-5.87	104.00	106.68
40	b	802	CLA	C1D-ND-C4D	-5.86	102.20	106.31
40	a	810	CLA	C4A-NA-C1A	-5.86	104.00	106.68
40	b	837	CLA	C4A-NA-C1A	-5.86	104.00	106.68
40	p	312	CLA	C4A-NA-C1A	-5.86	104.01	106.68
40	p	307	CLA	C1D-ND-C4D	-5.86	102.20	106.31
40	b	815	CLA	C4A-NA-C1A	-5.85	104.01	106.68
40	b	817	CLA	C1D-ND-C4D	-5.85	102.20	106.31
40	A	311	CLA	C4A-NA-C1A	-5.85	104.01	106.68
40	u	308	CLA	C1D-ND-C4D	-5.85	102.21	106.31
40	B	306	CLA	C4A-NA-C1A	-5.85	104.01	106.68
40	Y	304	CLA	C4A-NA-C1A	-5.85	104.01	106.68
40	L	301	CLA	C1D-ND-C4D	-5.84	102.21	106.31
40	b	842	CLA	C1D-ND-C4D	-5.84	102.22	106.31
40	Z	311	CLA	C1D-ND-C4D	-5.83	102.22	106.31
40	a	833	CLA	C4A-NA-C1A	-5.83	104.02	106.68
40	q	301	CLA	C1D-ND-C4D	-5.83	102.22	106.31
40	x	308	CLA	C1D-ND-C4D	-5.83	102.22	106.31
40	q	311	CLA	C1D-ND-C4D	-5.83	102.22	106.31
40	o	305	CLA	C1D-ND-C4D	-5.83	102.22	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	j	102	CLA	C1D-ND-C4D	-5.82	102.22	106.31
44	Y	315	A86	C34-O4-C38	5.82	128.13	117.85
40	t	307	CLA	C1D-ND-C4D	-5.82	102.23	106.31
40	a	811	CLA	C1D-ND-C4D	-5.82	102.23	106.31
40	L	312	CLA	C4A-NA-C1A	-5.82	104.03	106.68
40	k	201	CLA	C4A-NA-C1A	-5.82	104.03	106.68
40	P	305	CLA	C1D-ND-C4D	-5.81	102.23	106.31
40	a	825	CLA	C4A-NA-C1A	-5.81	104.03	106.68
40	a	824	CLA	C1D-ND-C4D	-5.81	102.23	106.31
40	a	835	CLA	C4A-NA-C1A	-5.81	104.03	106.68
40	S	313	CLA	C1D-ND-C4D	-5.81	102.24	106.31
40	b	838	CLA	C1D-ND-C4D	-5.80	102.24	106.31
40	H	307	CLA	C4A-NA-C1A	-5.80	104.03	106.68
40	Q	207	CLA	C1D-ND-C4D	-5.80	102.24	106.31
44	v	319	A86	C34-O4-C38	5.80	128.09	117.85
40	I	205	CLA	C1D-ND-C4D	-5.79	102.25	106.31
40	R	310	CLA	C1D-ND-C4D	-5.79	102.25	106.31
40	T	305	CLA	C1D-ND-C4D	-5.79	102.25	106.31
40	b	824	CLA	C1D-ND-C4D	-5.79	102.25	106.31
40	b	834	CLA	C1D-ND-C4D	-5.79	102.25	106.31
40	G	204	CLA	C1D-ND-C4D	-5.79	102.25	106.31
40	J	305	CLA	C1D-ND-C4D	-5.79	102.25	106.31
40	Z	313	CLA	C1D-ND-C4D	-5.79	102.25	106.31
40	L	307	CLA	C4A-NA-C1A	-5.79	104.04	106.68
40	H	304	CLA	C1D-ND-C4D	-5.79	102.25	106.31
44	q	319	A86	C34-O4-C38	5.79	128.06	117.85
40	U	205	CLA	C1D-ND-C4D	-5.79	102.25	106.31
40	a	808	CLA	C1D-ND-C4D	-5.78	102.25	106.31
40	b	841	CLA	C1D-ND-C4D	-5.78	102.26	106.31
40	H	304	CLA	C4A-NA-C1A	-5.78	104.04	106.68
40	W	307	CLA	C1D-ND-C4D	-5.78	102.26	106.31
40	N	304	CLA	C4A-NA-C1A	-5.78	104.04	106.68
40	v	311	CLA	C1D-ND-C4D	-5.78	102.26	106.31
40	v	310	CLA	C1D-ND-C4D	-5.77	102.26	106.31
40	K	312	CLA	C1D-ND-C4D	-5.77	102.26	106.31
40	M	310	CLA	C1D-ND-C4D	-5.77	102.26	106.31
40	R	305	CLA	C4A-NA-C1A	-5.77	104.05	106.68
40	x	306	CLA	C1D-ND-C4D	-5.77	102.27	106.31
40	y	302	CLA	C1D-ND-C4D	-5.77	102.27	106.31
40	J	310	CLA	C1D-ND-C4D	-5.76	102.27	106.31
40	R	306	CLA	C4A-NA-C1A	-5.76	104.05	106.68
40	O	306	CLA	C4A-NA-C1A	-5.76	104.05	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	N	305	CLA	C4A-NA-C1A	-5.75	104.05	106.68
40	a	842	CLA	C1D-ND-C4D	-5.75	102.28	106.31
44	T	315	A86	O1-C20-C19	5.75	118.88	113.49
40	O	310	CLA	C1D-ND-C4D	-5.75	102.28	106.31
40	q	310	CLA	C1D-ND-C4D	-5.75	102.28	106.31
40	W	306	CLA	C4A-NA-C1A	-5.75	104.06	106.68
40	o	304	CLA	C4A-NA-C1A	-5.75	104.06	106.68
40	K	307	CLA	C1D-ND-C4D	-5.75	102.28	106.31
40	A	304	CLA	C4A-NA-C1A	-5.75	104.06	106.68
40	J	303	CLA	C1D-ND-C4D	-5.75	102.28	106.31
40	A	311	CLA	C1D-ND-C4D	-5.75	102.28	106.31
47	N	320	A1EB1	C34-O4-C38	5.74	127.99	117.85
40	S	312	CLA	C1D-ND-C4D	-5.74	102.28	106.31
40	Z	305	CLA	C1D-ND-C4D	-5.74	102.28	106.31
40	w	309	CLA	C1D-ND-C4D	-5.74	102.28	106.31
40	a	836	CLA	C1D-ND-C4D	-5.73	102.29	106.31
40	z	324	CLA	C4A-NA-C1A	-5.73	104.06	106.68
40	D	305	CLA	C4D-ND-C1D	-5.73	102.29	106.31
40	u	306	CLA	C1D-ND-C4D	-5.73	102.29	106.31
40	L	304	CLA	C1D-ND-C4D	-5.73	102.30	106.31
47	p	323	A1EB1	C34-O4-C38	5.72	127.95	117.85
40	I	204	CLA	C1D-ND-C4D	-5.72	102.30	106.31
40	a	822	CLA	C4A-NA-C1A	-5.72	104.07	106.68
40	N	310	CLA	C1D-ND-C4D	-5.72	102.30	106.31
40	J	302	CLA	C1D-ND-C4D	-5.72	102.30	106.31
40	L	306	CLA	C1D-ND-C4D	-5.71	102.30	106.31
40	x	307	CLA	C1D-ND-C4D	-5.71	102.31	106.31
40	A	301	CLA	C4A-NA-C1A	-5.71	104.08	106.68
40	f	202	CLA	C1D-ND-C4D	-5.70	102.31	106.31
40	T	317	CLA	C1D-ND-C4D	-5.70	102.31	106.31
44	x	318	A86	O1-C20-C19	-5.70	108.15	113.49
40	Y	304	CLA	C1D-ND-C4D	-5.70	102.31	106.31
40	C	304	CLA	C4A-NA-C1A	-5.69	104.08	106.68
40	D	312	CLA	C4A-NA-C1A	-5.69	104.08	106.68
40	z	305	CLA	C1D-ND-C4D	-5.69	102.32	106.31
40	x	305	CLA	C4A-NA-C1A	-5.69	104.08	106.68
44	H	315	A86	C21-C20-C19	-5.69	107.85	114.24
44	P	321	A86	O1-C20-C19	5.69	118.82	113.49
40	F	321	CLA	C1D-ND-C4D	-5.69	102.32	106.31
40	A	303	CLA	C4A-NA-C1A	-5.68	104.09	106.68
40	G	205	CLA	C4A-NA-C1A	-5.68	104.09	106.68
40	a	809	CLA	C1D-ND-C4D	-5.68	102.33	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	u	307	CLA	C1D-ND-C4D	-5.68	102.33	106.31
40	G	207	CLA	C4A-NA-C1A	-5.68	104.09	106.68
40	O	307	CLA	C4A-NA-C1A	-5.68	104.09	106.68
40	p	306	CLA	C1D-ND-C4D	-5.68	102.33	106.31
40	E	304	CLA	C4A-NA-C1A	-5.67	104.09	106.68
40	P	305	CLA	C4A-NA-C1A	-5.67	104.09	106.68
40	b	832	CLA	C1D-ND-C4D	-5.67	102.33	106.31
40	a	840	CLA	C4A-NA-C1A	-5.67	104.09	106.68
40	y	309	CLA	C1D-ND-C4D	-5.66	102.34	106.31
40	b	827	CLA	C1D-ND-C4D	-5.66	102.34	106.31
40	f	205	CLA	C1D-ND-C4D	-5.65	102.34	106.31
40	E	313	CLA	C4A-NA-C1A	-5.65	104.10	106.68
40	p	314	CLA	C1D-ND-C4D	-5.65	102.35	106.31
40	b	836	CLA	C4A-NA-C1A	-5.65	104.10	106.68
40	L	301	CLA	C4A-NA-C1A	-5.65	104.10	106.68
40	F	310	CLA	C1D-ND-C4D	-5.64	102.35	106.31
40	U	206	CLA	C1D-ND-C4D	-5.64	102.36	106.31
40	A	301	CLA	C1D-ND-C4D	-5.64	102.36	106.31
40	C	304	CLA	C1D-ND-C4D	-5.64	102.36	106.31
40	q	313	CLA	C4A-NA-C1A	-5.64	104.11	106.68
40	b	829	CLA	C1D-ND-C4D	-5.64	102.36	106.31
40	b	810	CLA	C1D-ND-C4D	-5.63	102.36	106.31
40	P	306	CLA	C1D-ND-C4D	-5.63	102.36	106.31
40	W	311	CLA	C1D-ND-C4D	-5.63	102.36	106.31
40	Z	304	CLA	C4A-NA-C1A	-5.63	104.11	106.68
40	b	816	CLA	C1D-ND-C4D	-5.62	102.37	106.31
40	b	803	CLA	C1D-ND-C4D	-5.62	102.37	106.31
40	X	307	CLA	C4A-NA-C1A	-5.62	104.12	106.68
40	a	814	CLA	C4A-NA-C1A	-5.62	104.12	106.68
40	O	316	CLA	C1D-ND-C4D	-5.62	102.37	106.31
40	a	811	CLA	C4A-NA-C1A	-5.62	104.12	106.68
40	Q	208	CLA	C1D-ND-C4D	-5.61	102.37	106.31
40	F	305	CLA	C4A-NA-C1A	-5.61	104.12	106.68
40	a	813	CLA	C1D-ND-C4D	-5.61	102.38	106.31
40	E	306	CLA	C4A-NA-C1A	-5.60	104.12	106.68
40	a	826	CLA	C1D-ND-C4D	-5.60	102.39	106.31
40	D	302	CLA	C4A-NA-C1A	-5.59	104.13	106.68
40	R	304	CLA	C4A-NA-C1A	-5.58	104.13	106.68
42	N	317	DD6	C14-C13-C11	5.58	134.19	125.53
47	u	322	A1EB1	C34-O4-C38	5.58	127.71	117.85
40	U	208	CLA	C1D-ND-C4D	-5.58	102.40	106.31
40	z	312	CLA	C1D-ND-C4D	-5.58	102.40	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	M	312	CLA	C4A-NA-C1A	-5.57	104.14	106.68
40	q	304	CLA	C1D-ND-C4D	-5.57	102.41	106.31
40	X	304	CLA	C4A-NA-C1A	-5.57	104.14	106.68
40	a	830	CLA	C4A-NA-C1A	-5.57	104.14	106.68
40	S	305	CLA	C1D-ND-C4D	-5.57	102.41	106.31
40	X	311	CLA	C1D-ND-C4D	-5.56	102.41	106.31
40	D	301	CLA	C4A-NA-C1A	-5.56	104.14	106.68
40	F	301	CLA	C4A-NA-C1A	-5.56	104.14	106.68
40	O	304	CLA	C4A-NA-C1A	-5.56	104.14	106.68
40	a	828	CLA	C4A-NA-C1A	-5.56	104.14	106.68
40	W	313	CLA	C4A-NA-C1A	-5.55	104.15	106.68
44	w	310	A86	O1-C20-C19	-5.55	108.29	113.49
40	k	202	CLA	C1D-ND-C4D	-5.54	102.42	106.31
40	l	205	CLA	C1D-ND-C4D	-5.53	102.43	106.31
40	K	312	CLA	C4A-NA-C1A	-5.53	104.16	106.68
40	X	304	CLA	C1D-ND-C4D	-5.53	102.43	106.31
40	D	307	CLA	C4A-NA-C1A	-5.52	104.16	106.68
40	H	309	CLA	C1D-ND-C4D	-5.52	102.44	106.31
40	D	310	CLA	C1D-ND-C4D	-5.52	102.44	106.31
40	W	312	CLA	C1D-ND-C4D	-5.51	102.44	106.31
44	M	315	A86	O1-C20-C19	-5.51	108.33	113.49
40	f	201	CLA	C1D-ND-C4D	-5.51	102.45	106.31
40	b	825	CLA	C1D-ND-C4D	-5.50	102.45	106.31
40	o	305	CLA	C4A-NA-C1A	-5.50	104.17	106.68
40	l	202	CLA	C4A-NA-C1A	-5.50	104.17	106.68
40	P	311	CLA	C1D-ND-C4D	-5.50	102.46	106.31
40	v	304	CLA	C1D-ND-C4D	-5.50	102.46	106.31
40	U	204	CLA	C4A-NA-C1A	-5.50	104.17	106.68
40	b	805	CLA	C4A-NA-C1A	-5.50	104.17	106.68
40	V	201	CLA	C4A-NA-C1A	-5.49	104.17	106.68
40	o	301	CLA	C4A-NA-C1A	-5.49	104.17	106.68
40	X	301	CLA	C4A-NA-C1A	-5.49	104.17	106.68
40	a	819	CLA	C4A-NA-C1A	-5.49	104.17	106.68
40	B	302	CLA	C1D-ND-C4D	-5.48	102.46	106.31
44	p	318	A86	O1-C20-C19	-5.48	108.36	113.49
40	b	812	CLA	C1D-ND-C4D	-5.48	102.47	106.31
40	t	309	CLA	C4A-NA-C1A	-5.48	104.18	106.68
40	E	305	CLA	C4A-NA-C1A	-5.48	104.18	106.68
40	Q	202	CLA	C1D-ND-C4D	-5.47	102.47	106.31
40	F	311	CLA	C4A-NA-C1A	-5.47	104.19	106.68
40	a	852	CLA	C4A-NA-C1A	-5.47	104.19	106.68
40	t	304	CLA	C4A-NA-C1A	-5.46	104.19	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	T	305	CLA	C4A-NA-C1A	-5.46	104.19	106.68
44	p	316	A86	C33-C32-C31	5.46	114.52	109.21
40	C	308	CLA	C1D-ND-C4D	-5.46	102.48	106.31
40	S	308	CLA	C4A-NA-C1A	-5.46	104.19	106.68
44	q	317	A86	O1-C20-C19	-5.46	108.38	113.49
40	H	305	CLA	C4A-NA-C1A	-5.45	104.19	106.68
40	a	841	CLA	C4A-NA-C1A	-5.45	104.19	106.68
40	a	825	CLA	C1D-ND-C4D	-5.44	102.49	106.31
40	Z	301	CLA	C4A-NA-C1A	-5.43	104.20	106.68
44	S	318	A86	O1-C20-C19	5.41	118.56	113.49
40	Z	304	CLA	C1D-ND-C4D	-5.41	102.52	106.31
40	W	305	CLA	C4A-NA-C1A	-5.41	104.21	106.68
40	T	310	CLA	C1D-ND-C4D	-5.40	102.52	106.31
40	a	826	CLA	C4A-NA-C1A	-5.40	104.21	106.68
40	D	308	CLA	C4A-NA-C1A	-5.40	104.22	106.68
40	a	821	CLA	C4A-NA-C1A	-5.40	104.22	106.68
40	H	306	CLA	C4A-NA-C1A	-5.40	104.22	106.68
40	a	805	CLA	C4A-NA-C1A	-5.39	104.22	106.68
47	v	324	A1EB1	C33-C32-C31	5.38	114.44	109.21
40	D	309	CLA	C4A-NA-C1A	-5.38	104.22	106.68
40	H	311	CLA	C4A-NA-C1A	-5.37	104.23	106.68
40	I	205	CLA	C4A-NA-C1A	-5.36	104.23	106.68
40	M	306	CLA	C4A-NA-C1A	-5.36	104.23	106.68
40	b	810	CLA	C4A-NA-C1A	-5.36	104.23	106.68
44	X	318	A86	C21-C20-C19	-5.35	108.23	114.24
40	M	305	CLA	C4A-NA-C1A	-5.35	104.24	106.68
40	f	204	CLA	C4A-NA-C1A	-5.35	104.24	106.68
40	B	303	CLA	C4A-NA-C1A	-5.34	104.24	106.68
40	b	817	CLA	C4A-NA-C1A	-5.33	104.25	106.68
44	N	315	A86	O1-C20-C19	-5.33	108.49	113.49
40	f	202	CLA	C4A-NA-C1A	-5.32	104.25	106.68
40	b	829	CLA	C4A-NA-C1A	-5.32	104.25	106.68
40	b	806	CLA	C4A-NA-C1A	-5.30	104.26	106.68
40	E	311	CLA	C4A-NA-C1A	-5.30	104.26	106.68
40	b	801	CLA	C1D-ND-C4D	-5.30	102.60	106.31
40	v	301	CLA	C1D-ND-C4D	-5.29	102.60	106.31
40	a	827	CLA	C4A-NA-C1A	-5.29	104.27	106.68
40	b	826	CLA	C4A-NA-C1A	-5.29	104.27	106.68
40	H	302	CLA	C4A-NA-C1A	-5.28	104.27	106.68
40	W	307	CLA	C4A-NA-C1A	-5.28	104.27	106.68
40	y	304	CLA	C4A-NA-C1A	-5.26	104.28	106.68
44	z	319	A86	O1-C20-C19	-5.26	108.56	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	a	817	CLA	C4A-NA-C1A	-5.26	104.28	106.68
40	a	831	CLA	C4A-NA-C1A	-5.26	104.28	106.68
40	N	307	CLA	C4A-NA-C1A	-5.25	104.28	106.68
44	P	321	A86	C21-C20-C19	-5.25	108.35	114.24
40	a	842	CLA	C4A-NA-C1A	-5.24	104.29	106.68
40	z	306	CLA	C4A-NA-C1A	-5.24	104.29	106.68
40	P	308	CLA	C4A-NA-C1A	-5.23	104.29	106.68
40	E	314	CLA	C1D-ND-C4D	-5.23	102.64	106.31
40	a	832	CLA	C4A-NA-C1A	-5.22	104.30	106.68
40	K	301	CLA	C4A-NA-C1A	-5.21	104.30	106.68
40	S	306	CLA	C4A-NA-C1A	-5.19	104.31	106.68
40	A	309	CLA	C4A-NA-C1A	-5.18	104.31	106.68
40	B	307	CLA	C1D-ND-C4D	-5.18	102.68	106.31
40	T	306	CLA	C4A-NA-C1A	-5.16	104.32	106.68
40	D	306	CLA	C4A-NA-C1A	-5.16	104.33	106.68
44	L	314	A86	O1-C20-C19	5.16	118.32	113.49
40	H	305	CLA	C1D-ND-C4D	-5.16	102.69	106.31
42	C	312	DD6	C14-C13-C11	5.15	133.51	125.53
40	R	316	CLA	C1D-ND-C4D	-5.15	102.70	106.31
40	Y	301	CLA	C4A-NA-C1A	-5.14	104.33	106.68
40	P	312	CLA	C4A-NA-C1A	-5.14	104.33	106.68
40	b	831	CLA	C4A-NA-C1A	-5.13	104.34	106.68
40	N	306	CLA	C4A-NA-C1A	-5.12	104.34	106.68
40	P	313	CLA	C4A-NA-C1A	-5.11	104.35	106.68
40	I	206	CLA	C4A-NA-C1A	-5.11	104.35	106.68
44	Z	316	A86	C21-C20-C19	-5.11	108.50	114.24
40	L	312	CLA	C1D-ND-C4D	-5.11	102.73	106.31
40	G	203	CLA	C4A-NA-C1A	-5.10	104.35	106.68
40	M	311	CLA	C4A-NA-C1A	-5.10	104.35	106.68
40	A	308	CLA	C4A-NA-C1A	-5.10	104.35	106.68
40	a	851	CLA	C4A-NA-C1A	-5.10	104.35	106.68
42	N	319	DD6	C14-C13-C11	5.08	133.41	125.53
40	t	302	CLA	C4A-NA-C1A	-5.08	104.36	106.68
40	b	812	CLA	C4A-NA-C1A	-5.07	104.36	106.68
40	D	303	CLA	C4A-NA-C1A	-5.07	104.37	106.68
40	b	833	CLA	C4A-NA-C1A	-5.06	104.37	106.68
40	P	306	CLA	C4A-NA-C1A	-5.06	104.37	106.68
40	w	304	CLA	C4A-NA-C1A	-5.06	104.37	106.68
40	a	823	CLA	C4A-NA-C1A	-5.05	104.37	106.68
40	B	304	CLA	C1D-ND-C4D	-5.04	102.77	106.31
40	J	307	CLA	C1D-ND-C4D	-5.03	102.78	106.31
40	F	306	CLA	C4A-NA-C1A	-5.03	104.38	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	H	301	CLA	C4A-NA-C1A	-5.03	104.38	106.68
40	J	307	CLA	C4A-NA-C1A	-5.03	104.38	106.68
40	a	803	CLA	C4A-NA-C1A	-5.02	104.39	106.68
40	A	306	CLA	C4A-NA-C1A	-5.02	104.39	106.68
40	J	302	CLA	C4A-NA-C1A	-5.02	104.39	106.68
40	b	807	CLA	C4A-NA-C1A	-5.01	104.39	106.68
40	b	814	CLA	C4A-NA-C1A	-5.01	104.39	106.68
42	F	315	DD6	C14-C13-C11	5.01	133.30	125.53
40	x	306	CLA	C4A-NA-C1A	-5.00	104.40	106.68
44	y	310	A86	O1-C20-C19	-4.98	108.82	113.49
40	Y	305	CLA	C4A-NA-C1A	-4.97	104.41	106.68
40	x	312	CLA	C4A-NA-C1A	-4.97	104.41	106.68
40	J	312	CLA	C4A-NA-C1A	-4.96	104.41	106.68
44	v	325	A86	C33-C32-C31	4.96	114.04	109.21
40	J	308	CLA	C4A-NA-C1A	-4.96	104.42	106.68
40	a	812	CLA	C4A-NA-C1A	-4.95	104.42	106.68
44	X	321	A86	C21-C20-C19	-4.94	108.69	114.24
40	b	802	CLA	C4A-NA-C1A	-4.94	104.42	106.68
40	D	310	CLA	C4A-NA-C1A	-4.93	104.43	106.68
40	a	836	CLA	C4A-NA-C1A	-4.93	104.43	106.68
40	J	318	CLA	C4A-NA-C1A	-4.93	104.43	106.68
40	y	308	CLA	C4A-NA-C1A	-4.93	104.43	106.68
40	w	308	CLA	C4A-NA-C1A	-4.93	104.43	106.68
40	b	808	CLA	C1D-ND-C4D	-4.93	102.86	106.31
44	Z	315	A86	O1-C20-C19	-4.92	108.88	113.49
40	a	809	CLA	C4A-NA-C1A	-4.92	104.43	106.68
40	X	305	CLA	C4A-NA-C1A	-4.91	104.44	106.68
40	I	202	CLA	C4A-NA-C1A	-4.89	104.45	106.68
40	Q	205	CLA	C4A-NA-C1A	-4.89	104.45	106.68
40	q	312	CLA	C4A-NA-C1A	-4.89	104.45	106.68
40	S	302	CLA	C4A-NA-C1A	-4.89	104.45	106.68
40	v	312	CLA	C4A-NA-C1A	-4.89	104.45	106.68
40	K	306	CLA	C4A-NA-C1A	-4.88	104.45	106.68
42	t	312	DD6	C14-C13-C11	4.85	133.06	125.53
40	G	206	CLA	C4A-NA-C1A	-4.85	104.47	106.68
40	Q	204	CLA	C4A-NA-C1A	-4.84	104.47	106.68
40	u	312	CLA	C4A-NA-C1A	-4.84	104.47	106.68
40	b	824	CLA	C4A-NA-C1A	-4.81	104.48	106.68
44	t	311	A86	C34-O4-C38	4.81	126.34	117.85
40	a	803	CLA	C1D-ND-C4D	-4.81	102.94	106.31
52	b	850	DGD	O3G-C3G-C2G	-4.80	99.15	110.82
40	G	201	CLA	C4A-NA-C1A	-4.79	104.49	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	f	201	CLA	C4A-NA-C1A	-4.79	104.49	106.68
44	T	312	A86	O1-C20-C19	-4.78	109.01	113.49
47	z	323	A1EB1	C28-O6-C42	4.77	125.64	115.64
42	y	311	DD6	C14-C13-C11	4.77	132.93	125.53
44	z	315	A86	O4-C34-C33	4.76	119.82	107.64
44	X	320	A86	O1-C20-C19	-4.76	109.03	113.49
42	D	315	DD6	C14-C13-C11	4.75	132.90	125.53
40	v	304	CLA	C4A-NA-C1A	-4.75	104.51	106.68
40	b	835	CLA	C4A-NA-C1A	-4.71	104.53	106.68
40	F	310	CLA	C4A-NA-C1A	-4.71	104.53	106.68
40	W	312	CLA	C4A-NA-C1A	-4.70	104.54	106.68
40	z	302	CLA	C4A-NA-C1A	-4.69	104.54	106.68
40	S	313	CLA	C4A-NA-C1A	-4.68	104.54	106.68
44	t	311	A86	O1-C20-C19	-4.66	109.12	113.49
40	a	824	CLA	C4A-NA-C1A	-4.66	104.56	106.68
40	q	304	CLA	C4A-NA-C1A	-4.64	104.56	106.68
44	Z	314	A86	O4-C34-C33	4.63	119.50	107.64
44	q	314	A86	O1-C20-C19	4.62	117.82	113.49
40	J	309	CLA	C4A-NA-C1A	-4.61	104.58	106.68
41	R	303	KC2	C1D-ND-C4D	4.60	109.54	106.31
44	Z	317	A86	O1-C20-C19	-4.59	109.19	113.49
40	b	813	CLA	C4A-NA-C1A	-4.59	104.58	106.68
47	u	322	A1EB1	O4-C34-C35	4.59	119.38	107.64
44	z	301	A86	O1-C20-C19	-4.58	109.20	113.49
44	z	316	A86	C21-C20-C19	-4.56	109.11	114.24
40	H	308	CLA	C4A-NA-C1A	-4.54	104.61	106.68
40	C	306	CLA	C4A-NA-C1A	-4.50	104.62	106.68
40	b	808	CLA	C4A-NA-C1A	-4.50	104.63	106.68
42	D	314	DD6	C14-C13-C11	4.49	132.49	125.53
40	E	307	CLA	C4A-NA-C1A	-4.47	104.64	106.68
41	x	315	KC2	C1D-ND-C4D	4.47	109.45	106.31
42	I	211	DD6	C14-C13-C11	4.46	132.45	125.53
44	K	314	A86	O1-C20-C19	4.45	117.67	113.49
49	l	207	BCR	C7-C8-C9	4.45	132.82	126.23
40	I	204	CLA	C4A-NA-C1A	-4.45	104.65	106.68
45	S	323	LHG	O4-P-O5	4.43	133.07	112.44
41	T	303	KC2	C1D-ND-C4D	4.43	109.42	106.31
44	o	316	A86	C21-C20-C19	-4.42	109.27	114.24
47	p	323	A1EB1	O4-C34-C35	4.42	118.94	107.64
46	P	319	SQD	O47-C7-C8	4.41	121.02	111.48
44	q	324	A86	C33-C32-C31	4.41	113.50	109.21
45	a	848	LHG	O4-P-O5	4.40	132.91	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	a	849	LHG	O4-P-O5	4.39	132.89	112.44
40	f	205	CLA	C4A-NA-C1A	-4.39	104.68	106.68
41	H	316	KC2	C1D-ND-C4D	4.38	109.39	106.31
40	b	821	CLA	C4A-NA-C1A	-4.38	104.68	106.68
46	k	205	SQD	O47-C7-C8	4.36	120.90	111.48
44	v	317	A86	O1-C20-C19	-4.35	109.42	113.49
40	U	206	CLA	C4A-NA-C1A	-4.35	104.70	106.68
42	P	315	DD6	O1-C20-C19	-4.34	109.42	113.49
40	Y	311	CLA	C4A-NA-C1A	-4.33	104.70	106.68
40	T	317	CLA	C4A-NA-C1A	-4.32	104.71	106.68
42	z	322	DD6	O1-C20-C19	-4.31	109.45	113.49
44	t	310	A86	C21-C20-C19	-4.31	109.40	114.24
42	I	210	DD6	C14-C13-C11	4.30	132.21	125.53
44	p	320	A86	C36-C31-C32	4.30	123.96	119.70
40	M	310	CLA	C4A-NA-C1A	-4.30	104.72	106.68
41	u	315	KC2	C1D-ND-C4D	4.29	109.33	106.31
40	Q	208	CLA	C4A-NA-C1A	-4.29	104.72	106.68
45	F	319	LHG	O4-P-O5	4.28	132.37	112.44
41	X	309	KC2	C1D-ND-C4D	4.28	109.32	106.31
44	w	311	A86	C33-C32-C31	4.28	113.37	109.21
40	D	305	CLA	CBD-CHA-C4D	-4.27	109.75	117.29
46	F	320	SQD	O47-C7-C8	4.25	120.68	111.48
44	v	314	A86	O4-C34-C33	4.25	118.50	107.64
44	G	209	A86	O1-C20-C19	-4.24	109.52	113.49
40	b	830	CLA	C1-C2-C3	4.23	133.13	126.20
40	U	208	CLA	C4A-NA-C1A	-4.23	104.75	106.68
40	b	807	CLA	C1D-ND-C4D	-4.22	103.35	106.31
42	N	316	DD6	O1-C20-C19	-4.22	109.54	113.49
40	R	316	CLA	C4A-NA-C1A	-4.22	104.75	106.68
44	R	315	A86	O4-C34-C33	4.19	118.37	107.64
44	q	314	A86	O4-C34-C33	4.19	118.37	107.64
40	O	316	CLA	C4A-NA-C1A	-4.19	104.77	106.68
47	N	320	A1EB1	O4-C34-C35	4.17	118.31	107.64
40	E	314	CLA	C2A-C3A-C4A	-4.17	95.13	101.87
40	b	841	CLA	C4A-NA-C1A	-4.17	104.78	106.68
40	E	314	CLA	C3A-C2A-C1A	-4.17	95.10	101.34
44	O	312	A86	O1-C20-C19	4.16	117.39	113.49
41	z	309	KC2	C1D-ND-C4D	4.16	109.23	106.31
40	Z	305	CLA	C4A-NA-C1A	-4.15	104.78	106.68
44	o	314	A86	O4-C34-C33	4.14	118.24	107.64
46	I	215	SQD	O47-C7-C8	4.13	120.42	111.48
41	O	301	KC2	C1D-ND-C4D	4.13	109.21	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	F	303	CLA	C4A-NA-C1A	-4.13	104.79	106.68
44	C	311	A86	C21-C20-C19	-4.13	109.60	114.24
44	Q	210	A86	C21-C20-C19	-4.13	109.61	114.24
41	N	301	KC2	C1D-ND-C4D	4.12	109.20	106.31
40	E	309	CLA	C4A-NA-C1A	-4.12	104.80	106.68
41	Y	314	KC2	C1D-ND-C4D	4.12	109.20	106.31
41	q	308	KC2	C1D-ND-C4D	4.11	109.20	106.31
44	o	315	A86	C21-C20-C19	-4.11	109.62	114.24
47	o	322	A1EB1	C33-C32-C31	-4.11	105.22	109.21
47	Y	323	A1EB1	C33-C32-C31	-4.08	105.24	109.21
41	R	301	KC2	C1D-ND-C4D	4.07	109.17	106.31
41	E	319	KC2	C1D-ND-C4D	4.07	109.17	106.31
42	A	312	DD6	C14-C13-C11	4.07	131.85	125.53
44	Z	314	A86	O1-C20-C19	4.07	117.30	113.49
42	D	313	DD6	C14-C13-C11	4.05	131.81	125.53
41	N	308	KC2	C1D-ND-C4D	4.05	109.15	106.31
44	T	312	A86	C33-C32-C31	4.05	113.14	109.21
40	V	202	CLA	C4A-NA-C1A	-4.04	104.83	106.68
44	S	317	A86	C36-C31-C32	4.04	123.71	119.70
42	Q	214	DD6	C14-C13-C11	4.04	131.80	125.53
42	Z	318	DD6	C14-C13-C11	4.04	131.80	125.53
44	v	319	A86	O4-C34-C33	4.03	117.95	107.64
44	q	319	A86	O4-C34-C33	4.03	117.95	107.64
41	p	309	KC2	C1D-ND-C4D	4.03	109.14	106.31
41	u	309	KC2	C1D-ND-C4D	4.02	109.13	106.31
44	U	210	A86	C33-C32-C31	4.02	113.12	109.21
40	A	302	CLA	C4A-NA-C1A	-4.02	104.85	106.68
41	K	303	KC2	C1D-ND-C4D	4.02	109.13	106.31
40	B	302	CLA	C4A-NA-C1A	-4.01	104.85	106.68
44	o	315	A86	O1-C20-C19	4.00	117.24	113.49
40	X	310	CLA	CHD-C1D-ND	-4.00	119.17	124.80
40	K	307	CLA	C4A-NA-C1A	-3.99	104.86	106.68
44	p	319	A86	C34-O4-C38	3.99	124.89	117.85
41	P	310	KC2	C1D-ND-C4D	3.97	109.10	106.31
44	u	319	A86	C34-O4-C38	3.97	124.86	117.85
41	W	302	KC2	C1D-ND-C4D	3.97	109.10	106.31
41	P	302	KC2	C1D-ND-C4D	3.97	109.09	106.31
42	R	314	DD6	C14-C13-C11	3.96	131.68	125.53
41	O	309	KC2	C1D-ND-C4D	3.96	109.09	106.31
41	K	309	KC2	C1D-ND-C4D	3.96	109.09	106.31
41	v	308	KC2	C1D-ND-C4D	3.96	109.09	106.31
41	X	308	KC2	C1D-ND-C4D	3.96	109.09	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	N	315	A86	C34-O4-C38	3.96	124.83	117.85
44	p	320	A86	C33-C32-C31	3.95	113.05	109.21
41	K	305	KC2	C1D-ND-C4D	3.95	109.08	106.31
41	x	304	KC2	C1D-ND-C4D	3.95	109.08	106.31
47	t	314	A1EB1	C28-O6-C42	3.94	123.91	115.64
41	M	303	KC2	C1D-ND-C4D	3.94	109.08	106.31
41	T	308	KC2	C1D-ND-C4D	3.94	109.08	106.31
40	J	307	CLA	C2A-C1A-CHA	3.94	130.70	123.87
44	w	316	A86	C34-O4-C38	3.94	124.80	117.85
41	T	309	KC2	C1D-ND-C4D	3.94	109.07	106.31
41	v	309	KC2	C1D-ND-C4D	3.93	109.07	106.31
41	P	304	KC2	C1D-ND-C4D	3.93	109.07	106.31
41	x	309	KC2	C1D-ND-C4D	3.92	109.06	106.31
41	W	304	KC2	C1D-ND-C4D	3.92	109.06	106.31
44	D	319	A86	C34-O4-C38	3.92	124.77	117.85
44	x	319	A86	C34-O4-C38	3.91	124.76	117.85
41	p	315	KC2	C1D-ND-C4D	3.91	109.06	106.31
44	S	316	A86	C34-O4-C38	3.91	124.75	117.85
41	v	303	KC2	C1D-ND-C4D	3.91	109.05	106.31
41	H	303	KC2	C1D-ND-C4D	3.90	109.05	106.31
41	T	311	KC2	C1D-ND-C4D	3.90	109.05	106.31
41	u	304	KC2	C1D-ND-C4D	3.89	109.04	106.31
47	q	321	A1EB1	C28-O6-C42	3.88	123.77	115.64
47	v	321	A1EB1	C28-O6-C42	3.87	123.76	115.64
41	w	301	KC2	C1D-ND-C4D	3.87	109.03	106.31
41	T	301	KC2	C1D-ND-C4D	3.87	109.03	106.31
47	T	320	A1EB1	C34-O4-C38	3.87	124.67	117.85
44	Y	319	A86	O1-C20-C19	-3.86	109.87	113.49
41	F	309	KC2	C1D-ND-C4D	3.86	109.02	106.31
41	N	309	KC2	C1D-ND-C4D	3.86	109.02	106.31
44	q	324	A86	C21-C20-C19	-3.85	109.91	114.24
44	P	316	A86	C34-O4-C38	3.85	124.64	117.85
41	L	313	KC2	C1D-ND-C4D	3.85	109.01	106.31
41	R	311	KC2	C1D-ND-C4D	3.85	109.01	106.31
47	L	316	A1EB1	C34-O4-C38	3.85	124.64	117.85
41	W	310	KC2	C1D-ND-C4D	3.85	109.01	106.31
41	O	303	KC2	C1D-ND-C4D	3.84	109.01	106.31
44	U	210	A86	C34-O4-C38	3.84	124.63	117.85
46	W	318	SQD	O47-C7-C8	3.84	119.78	111.48
41	N	303	KC2	C1D-ND-C4D	3.84	109.00	106.31
41	G	208	KC2	C1D-ND-C4D	3.83	109.00	106.31
41	q	309	KC2	C1D-ND-C4D	3.83	109.00	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	M	313	A86	C34-O4-C38	3.83	124.60	117.85
41	t	306	KC2	C1D-ND-C4D	3.82	109.00	106.31
41	p	304	KC2	C1D-ND-C4D	3.82	108.99	106.31
41	o	303	KC2	C1D-ND-C4D	3.82	108.99	106.31
41	R	309	KC2	C1D-ND-C4D	3.82	108.99	106.31
44	z	301	A86	C21-C20-C19	-3.81	109.96	114.24
41	O	311	KC2	C1D-ND-C4D	3.81	108.99	106.31
52	b	850	DGD	O6D-C1D-O3G	-3.81	101.03	110.04
44	p	318	A86	C34-O4-C38	3.81	124.58	117.85
41	P	309	KC2	C1D-ND-C4D	3.81	108.98	106.31
41	I	209	KC2	C1D-ND-C4D	3.81	108.98	106.31
41	M	302	KC2	C1D-ND-C4D	3.81	108.98	106.31
41	Q	216	KC2	C1D-ND-C4D	3.81	108.98	106.31
41	z	310	KC2	C1D-ND-C4D	3.81	108.98	106.31
44	N	314	A86	C34-O4-C38	3.81	124.57	117.85
41	M	301	KC2	C1D-ND-C4D	3.80	108.98	106.31
44	u	318	A86	C34-O4-C38	3.80	124.56	117.85
40	p	313	CLA	C4A-NA-C1A	-3.80	104.94	106.68
47	T	316	A1EB1	C34-O4-C38	3.80	124.56	117.85
41	q	303	KC2	C1D-ND-C4D	3.80	108.97	106.31
41	t	301	KC2	C1D-ND-C4D	3.79	108.97	106.31
44	T	319	A86	C21-C20-C19	-3.79	109.99	114.24
44	X	315	A86	C21-C20-C19	-3.79	109.99	114.24
41	A	310	KC2	C1D-ND-C4D	3.78	108.97	106.31
44	D	320	A86	C34-O4-C38	3.78	124.53	117.85
44	x	316	A86	C34-O4-C38	3.78	124.53	117.85
41	Z	308	KC2	C1D-ND-C4D	3.78	108.96	106.31
41	y	306	KC2	C1D-ND-C4D	3.78	108.96	106.31
41	R	308	KC2	C1D-ND-C4D	3.77	108.96	106.31
43	P	318	LMG	O6-C1-C2	-3.77	102.62	110.37
44	o	317	A86	C34-O4-C38	3.77	124.51	117.85
44	Z	316	A86	O1-C20-C19	3.77	117.03	113.49
44	u	316	A86	C34-O4-C38	3.77	124.50	117.85
41	N	302	KC2	C1D-ND-C4D	3.77	108.96	106.31
47	O	317	A1EB1	C33-C32-C31	-3.76	105.55	109.21
41	U	201	KC2	C1D-ND-C4D	3.76	108.95	106.31
41	y	301	KC2	C1D-ND-C4D	3.76	108.95	106.31
40	b	801	CLA	CHD-C1D-ND	-3.75	119.52	124.80
44	Y	317	A86	C34-O4-C38	3.75	124.47	117.85
47	t	313	A1EB1	C34-O4-C38	3.75	124.47	117.85
44	H	315	A86	C34-O4-C38	3.75	124.47	117.85
40	x	302	CLA	CHD-C1D-ND	-3.75	119.53	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	Y	315	A86	O4-C34-C33	3.74	117.22	107.64
41	z	303	KC2	C1D-ND-C4D	3.74	108.94	106.31
41	p	310	KC2	C1D-ND-C4D	3.74	108.94	106.31
41	o	309	KC2	C1D-ND-C4D	3.74	108.93	106.31
41	S	303	KC2	C1D-ND-C4D	3.73	108.93	106.31
40	E	311	CLA	CHD-C1D-ND	-3.73	119.55	124.80
44	M	315	A86	C34-O4-C38	3.73	124.43	117.85
44	x	317	A86	C34-O4-C38	3.73	124.43	117.85
41	F	302	KC2	C1D-ND-C4D	3.73	108.93	106.31
41	W	303	KC2	C1D-ND-C4D	3.72	108.92	106.31
41	w	307	KC2	C1D-ND-C4D	3.72	108.92	106.31
41	x	310	KC2	C1D-ND-C4D	3.72	108.92	106.31
44	Z	316	A86	C34-O4-C38	3.72	124.42	117.85
44	C	311	A86	C34-O4-C38	3.72	124.41	117.85
44	Y	320	A86	C34-O4-C38	3.72	124.41	117.85
44	R	312	A86	C34-O4-C38	3.72	124.41	117.85
47	t	315	A1EB1	C34-O4-C38	3.72	124.41	117.85
44	Y	319	A86	C34-O4-C38	3.71	124.41	117.85
41	O	308	KC2	C1D-ND-C4D	3.71	108.92	106.31
40	D	310	CLA	CHD-C1D-ND	-3.71	119.58	124.80
44	T	313	A86	C34-O4-C38	3.71	124.40	117.85
41	T	302	KC2	C1D-ND-C4D	3.71	108.92	106.31
44	p	316	A86	C34-O4-C38	3.71	124.40	117.85
41	M	308	KC2	C1D-ND-C4D	3.71	108.91	106.31
41	N	312	KC2	C1D-ND-C4D	3.71	108.91	106.31
44	w	316	A86	O1-C20-C19	-3.71	110.02	113.49
41	K	302	KC2	C1D-ND-C4D	3.71	108.91	106.31
43	M	317	LMG	O1-C1-C2	-3.71	102.64	108.27
44	N	314	A86	C21-C20-C19	-3.71	110.08	114.24
44	z	317	A86	C34-O4-C38	3.70	124.39	117.85
44	w	311	A86	C34-O4-C38	3.70	124.38	117.85
44	x	318	A86	C34-O4-C38	3.70	124.38	117.85
47	L	318	A1EB1	C34-O4-C38	3.70	124.38	117.85
41	L	302	KC2	C1D-ND-C4D	3.69	108.90	106.31
40	X	301	CLA	CHD-C1D-ND	-3.69	119.61	124.80
41	O	302	KC2	C1D-ND-C4D	3.69	108.90	106.31
41	L	303	KC2	C1D-ND-C4D	3.69	108.90	106.31
41	N	313	KC2	C1D-ND-C4D	3.69	108.90	106.31
41	J	304	KC2	C1D-ND-C4D	3.68	108.90	106.31
44	Y	318	A86	C34-O4-C38	3.68	124.35	117.85
47	G	212	A1EB1	C34-O4-C38	3.68	124.35	117.85
44	H	315	A86	O1-C20-C19	3.68	116.94	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	v	324	A1EB1	C28-O6-C42	3.68	123.36	115.64
44	X	316	A86	C34-O4-C38	3.68	124.34	117.85
44	w	310	A86	C34-O4-C38	3.68	124.34	117.85
47	R	317	A1EB1	C34-O4-C38	3.68	124.34	117.85
47	S	320	A1EB1	C34-O4-C38	3.68	124.34	117.85
44	o	316	A86	C34-O4-C38	3.67	124.33	117.85
41	Y	309	KC2	C1D-ND-C4D	3.67	108.89	106.31
40	S	319	CLA	C4A-NA-C1A	-3.67	105.00	106.68
47	S	321	A1EB1	C34-O4-C38	3.67	124.32	117.85
41	y	307	KC2	C1D-ND-C4D	3.67	108.89	106.31
41	C	303	KC2	C1D-ND-C4D	3.66	108.88	106.31
44	X	315	A86	O1-C20-C19	-3.66	110.06	113.49
40	G	203	CLA	C4B-NB-C1B	-3.66	103.74	106.31
44	F	312	A86	C34-O4-C38	3.66	124.31	117.85
40	Y	313	CLA	CHD-C1D-ND	-3.66	119.65	124.80
44	P	314	A86	C34-O4-C38	3.66	124.31	117.85
47	w	314	A1EB1	C34-O4-C38	3.66	124.30	117.85
44	z	318	A86	C34-O4-C38	3.65	124.30	117.85
47	v	322	A1EB1	C34-O4-C38	3.65	124.30	117.85
41	R	302	KC2	C1D-ND-C4D	3.65	108.88	106.31
40	W	311	CLA	CHD-C1D-ND	-3.65	119.66	124.80
44	G	211	A86	C34-O4-C38	3.65	124.30	117.85
44	v	315	A86	C34-O4-C38	3.65	124.30	117.85
41	P	303	KC2	C1D-ND-C4D	3.65	108.87	106.31
40	H	310	CLA	CHD-C1D-ND	-3.65	119.67	124.80
40	z	324	CLA	CHD-C1D-ND	-3.65	119.67	124.80
40	Y	307	CLA	CHD-C1D-ND	-3.64	119.67	124.80
40	a	850	CLA	CHD-C1D-ND	-3.64	119.67	124.80
40	O	306	CLA	CHD-C1D-ND	-3.64	119.68	124.80
40	a	806	CLA	CHD-C1D-ND	-3.64	119.68	124.80
44	S	316	A86	O1-C20-C19	3.64	116.90	113.49
47	q	322	A1EB1	C34-O4-C38	3.64	124.27	117.85
40	l	204	CLA	C4A-NA-C1A	-3.64	105.02	106.68
42	F	316	DD6	C14-C13-C11	3.64	131.17	125.53
44	Z	315	A86	C34-O4-C38	3.63	124.27	117.85
44	D	319	A86	O1-C20-C19	3.63	116.90	113.49
41	S	304	KC2	C1D-ND-C4D	3.63	108.86	106.31
40	Y	312	CLA	CHD-C1D-ND	-3.63	119.69	124.80
40	Z	310	CLA	CHD-C1D-ND	-3.63	119.69	124.80
40	H	309	CLA	C3A-C2A-C1A	-3.63	95.91	101.34
41	S	309	KC2	C1D-ND-C4D	3.63	108.86	106.31
44	W	314	A86	C34-O4-C38	3.63	124.25	117.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	b	803	CLA	CHD-C1D-ND	-3.62	119.71	124.80
40	z	311	CLA	CHD-C1D-ND	-3.62	119.71	124.80
44	L	314	A86	C34-O4-C38	3.62	124.24	117.85
41	Y	308	KC2	C1D-ND-C4D	3.62	108.85	106.31
44	q	315	A86	C34-O4-C38	3.62	124.23	117.85
44	X	319	A86	C34-O4-C38	3.61	124.23	117.85
42	H	312	DD6	O1-C20-C19	-3.61	110.10	113.49
42	q	318	DD6	O1-C20-C19	-3.61	110.11	113.49
41	I	214	KC2	C1D-ND-C4D	3.61	108.84	106.31
41	Y	303	KC2	C1D-ND-C4D	3.61	108.84	106.31
40	C	309	CLA	CHD-C1D-ND	-3.61	119.73	124.80
44	X	321	A86	C34-O4-C38	3.61	124.21	117.85
44	X	314	A86	C34-O4-C38	3.60	124.21	117.85
44	X	318	A86	C34-O4-C38	3.60	124.21	117.85
44	O	315	A86	C21-C20-C19	-3.60	110.19	114.24
44	N	321	A86	C34-O4-C38	3.60	124.21	117.85
40	G	213	CLA	CHD-C1D-ND	-3.60	119.74	124.80
44	X	315	A86	O4-C34-C35	3.60	116.85	107.64
44	p	321	A86	C33-C32-C31	3.59	112.70	109.21
40	Q	206	CLA	C4B-NB-C1B	-3.59	103.79	106.31
40	V	202	CLA	CHD-C1D-ND	-3.59	119.75	124.80
40	i	101	CLA	CHD-C1D-ND	-3.59	119.75	124.80
40	D	311	CLA	CHD-C1D-ND	-3.59	119.76	124.80
41	o	308	KC2	C1D-ND-C4D	3.58	108.83	106.31
44	F	317	A86	C21-C20-C19	-3.58	110.22	114.24
40	F	307	CLA	C4B-NB-C1B	-3.58	103.80	106.31
41	M	309	KC2	C1D-ND-C4D	3.58	108.82	106.31
47	z	323	A1EB1	C34-O4-C38	3.58	124.17	117.85
41	o	302	KC2	C1D-ND-C4D	3.58	108.82	106.31
44	p	320	A86	C21-C20-C19	-3.58	110.22	114.24
41	S	310	KC2	C1D-ND-C4D	3.57	108.82	106.31
40	x	307	CLA	CHD-C1D-ND	-3.57	119.78	124.80
40	J	318	CLA	CHD-C1D-ND	-3.57	119.78	124.80
40	o	313	CLA	CHD-C1D-ND	-3.57	119.78	124.80
40	p	311	CLA	CHD-C1D-ND	-3.57	119.78	124.80
40	a	818	CLA	CHD-C1D-ND	-3.57	119.78	124.80
42	J	313	DD6	C14-C13-C11	3.56	131.06	125.53
40	C	307	CLA	CHD-C1D-ND	-3.56	119.79	124.80
40	a	811	CLA	CHD-C1D-ND	-3.56	119.79	124.80
40	F	304	CLA	CHD-C1D-ND	-3.56	119.80	124.80
40	b	835	CLA	C4B-NB-C1B	-3.56	103.82	106.31
40	S	311	CLA	CHD-C1D-ND	-3.56	119.80	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	U	202	CLA	CHD-C1D-ND	-3.56	119.80	124.80
40	u	302	CLA	CHD-C1D-ND	-3.55	119.80	124.80
40	D	303	CLA	CHD-C1D-ND	-3.55	119.80	124.80
44	G	209	A86	C34-O4-C38	3.55	124.12	117.85
40	p	302	CLA	CHD-C1D-ND	-3.55	119.80	124.80
40	E	305	CLA	CHD-C1D-ND	-3.55	119.81	124.80
46	M	318	SQD	O47-C7-C8	3.55	119.16	111.48
44	X	317	A86	O1-C20-C19	-3.55	110.17	113.49
42	N	316	DD6	O1-C15-C14	-3.54	106.72	116.88
40	b	835	CLA	C1-C2-C3	-3.54	120.40	126.20
40	q	307	CLA	CHD-C1D-ND	-3.54	119.83	124.80
40	x	313	CLA	C4A-NA-C1A	-3.53	105.07	106.68
40	a	809	CLA	CHD-C1D-ND	-3.53	119.83	124.80
47	S	320	A1EB1	C33-C32-C31	-3.53	105.78	109.21
42	H	314	DD6	C14-C13-C11	3.53	131.01	125.53
40	D	307	CLA	CHD-C1D-ND	-3.53	119.84	124.80
41	w	306	KC2	C1D-ND-C4D	3.53	108.79	106.31
44	W	316	A86	C21-C20-C19	-3.52	110.28	114.24
40	p	308	CLA	CHD-C1D-ND	-3.52	119.84	124.80
41	t	308	KC2	C1D-ND-C4D	3.52	108.78	106.31
40	a	819	CLA	CAA-C2A-C1A	-3.52	100.43	111.97
40	l	203	CLA	CHD-C1D-ND	-3.52	119.85	124.80
40	x	305	CLA	CHD-C1D-ND	-3.52	119.85	124.80
40	N	310	CLA	CHD-C1D-ND	-3.52	119.85	124.80
40	a	841	CLA	CHD-C1D-ND	-3.52	119.85	124.80
40	W	308	CLA	CHD-C1D-ND	-3.52	119.85	124.80
40	S	307	CLA	CHD-C1D-ND	-3.52	119.86	124.80
40	v	307	CLA	CHD-C1D-ND	-3.51	119.86	124.80
41	L	308	KC2	C1D-ND-C4D	3.51	108.78	106.31
41	Z	309	KC2	C1D-ND-C4D	3.51	108.77	106.31
42	C	310	DD6	C14-C13-C11	3.51	130.97	125.53
44	W	314	A86	O1-C20-C19	-3.50	110.21	113.49
41	z	304	KC2	C1D-ND-C4D	3.50	108.77	106.31
40	B	302	CLA	CHD-C1D-ND	-3.50	119.88	124.80
40	H	302	CLA	CHD-C1D-ND	-3.50	119.88	124.80
40	E	314	CLA	CHD-C1D-ND	-3.50	119.88	124.80
40	a	808	CLA	CHD-C1D-ND	-3.49	119.88	124.80
40	o	307	CLA	CHD-C1D-ND	-3.49	119.89	124.80
40	a	803	CLA	CHD-C1D-ND	-3.49	119.89	124.80
40	b	808	CLA	CHD-C1D-ND	-3.49	119.89	124.80
40	u	311	CLA	CHD-C1D-ND	-3.49	119.89	124.80
41	X	303	KC2	C1D-ND-C4D	3.49	108.76	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	Z	303	KC2	C1D-ND-C4D	3.49	108.76	106.31
40	A	305	CLA	CHD-C1D-ND	-3.49	119.89	124.80
47	Z	319	A1EB1	C34-O4-C38	3.49	124.00	117.85
41	G	202	KC2	C1D-ND-C4D	3.48	108.76	106.31
40	S	312	CLA	CHD-C1D-ND	-3.48	119.90	124.80
40	z	314	CLA	CHD-C1D-ND	-3.48	119.90	124.80
40	J	311	CLA	CHD-C1D-ND	-3.48	119.91	124.80
40	b	809	CLA	CHD-C1D-ND	-3.48	119.91	124.80
41	X	302	KC2	C1D-ND-C4D	3.48	108.75	106.31
40	P	313	CLA	CHD-C1D-ND	-3.48	119.91	124.80
40	X	306	CLA	CHD-C1D-ND	-3.47	119.91	124.80
40	B	301	CLA	C4D-CHA-C1A	-3.47	117.10	121.24
40	a	840	CLA	CHD-C1D-ND	-3.47	119.92	124.80
40	J	303	CLA	CHD-C1D-ND	-3.47	119.92	124.80
40	W	306	CLA	CHD-C1D-ND	-3.47	119.92	124.80
40	x	311	CLA	CHD-C1D-ND	-3.47	119.92	124.80
40	x	311	CLA	C2A-C3A-C4A	-3.47	96.27	101.87
40	p	305	CLA	CHD-C1D-ND	-3.47	119.92	124.80
40	G	206	CLA	CHD-C1D-ND	-3.47	119.92	124.80
40	b	830	CLA	CHD-C1D-ND	-3.47	119.92	124.80
47	y	313	A1EB1	C34-O4-C38	3.47	123.97	117.85
40	Y	312	CLA	C3A-C2A-C1A	-3.47	96.15	101.34
41	Y	302	KC2	C1D-ND-C4D	3.46	108.74	106.31
40	u	314	CLA	CHD-C1D-ND	-3.46	119.93	124.80
40	X	313	CLA	CHD-C1D-ND	-3.46	119.93	124.80
40	b	834	CLA	CHD-C1D-ND	-3.46	119.93	124.80
40	b	839	CLA	CHD-C1D-ND	-3.46	119.93	124.80
41	Z	302	KC2	C1D-ND-C4D	3.46	108.74	106.31
40	u	305	CLA	CHD-C1D-ND	-3.46	119.93	124.80
40	u	308	CLA	CHD-C1D-ND	-3.46	119.93	124.80
44	u	316	A86	O1-C20-C19	3.46	116.73	113.49
41	u	310	KC2	C1D-ND-C4D	3.46	108.74	106.31
40	a	810	CLA	CHD-C1D-ND	-3.46	119.94	124.80
47	v	324	A1EB1	C34-O4-C38	3.45	123.95	117.85
40	z	311	CLA	C3A-C2A-C1A	-3.45	96.17	101.34
40	H	307	CLA	CHD-C1D-ND	-3.45	119.94	124.80
40	X	305	CLA	CHD-C1D-ND	-3.45	119.94	124.80
47	q	321	A1EB1	C34-O4-C38	3.45	123.94	117.85
47	t	314	A1EB1	C34-O4-C38	3.45	123.94	117.85
40	v	310	CLA	CHD-C1D-ND	-3.45	119.95	124.80
40	q	305	CLA	CHD-C1D-ND	-3.45	119.95	124.80
40	Z	312	CLA	CHD-C1D-ND	-3.44	119.96	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	p	307	CLA	CHD-C1D-ND	-3.44	119.96	124.80
40	b	838	CLA	CHD-C1D-ND	-3.44	119.96	124.80
44	Q	215	A86	C33-C32-C31	3.44	112.56	109.21
40	a	805	CLA	CHD-C1D-ND	-3.44	119.96	124.80
47	y	312	A1EB1	C34-O4-C38	3.44	123.92	117.85
44	z	315	A86	C36-C31-C32	3.44	123.11	119.70
40	b	823	CLA	C1-C2-C3	-3.43	120.57	126.20
40	b	820	CLA	CHD-C1D-ND	-3.43	119.97	124.80
40	v	305	CLA	CHD-C1D-ND	-3.43	119.97	124.80
41	W	309	KC2	C1D-ND-C4D	3.43	108.72	106.31
42	E	315	DD6	C14-C13-C11	3.43	130.85	125.53
47	w	313	A1EB1	C34-O4-C38	3.43	123.90	117.85
42	E	315	DD6	O1-C20-C19	-3.43	110.28	113.49
40	Q	203	CLA	CHD-C1D-ND	-3.43	119.98	124.80
40	o	310	CLA	CHD-C1D-ND	-3.42	119.98	124.80
40	a	850	CLA	C3D-C4D-ND	3.42	115.55	109.99
40	v	304	CLA	CHD-C1D-ND	-3.42	119.98	124.80
40	t	302	CLA	CHD-C1D-ND	-3.42	119.99	124.80
40	C	304	CLA	CHD-C1D-ND	-3.42	119.99	124.80
40	S	305	CLA	CHD-C1D-ND	-3.42	119.99	124.80
40	u	311	CLA	C2A-C3A-C4A	-3.42	96.35	101.87
40	Z	311	CLA	CHD-C1D-ND	-3.42	119.99	124.80
42	I	211	DD6	O1-C20-C19	-3.42	110.29	113.49
41	x	303	KC2	C1D-ND-C4D	3.41	108.71	106.31
40	C	302	CLA	CHD-C1D-ND	-3.41	120.00	124.80
40	b	822	CLA	CHD-C1D-ND	-3.41	120.00	124.80
41	L	309	KC2	C1D-ND-C4D	3.41	108.71	106.31
40	a	834	CLA	CHD-C1D-ND	-3.41	120.00	124.80
40	a	804	CLA	CHD-C1D-ND	-3.41	120.01	124.80
40	A	304	CLA	CHD-C1D-ND	-3.41	120.01	124.80
40	o	305	CLA	CHD-C1D-ND	-3.41	120.01	124.80
40	G	203	CLA	CHD-C1D-ND	-3.40	120.01	124.80
40	J	310	CLA	CHD-C1D-ND	-3.40	120.01	124.80
42	w	312	DD6	C14-C13-C11	3.40	130.81	125.53
40	F	310	CLA	C2A-C1A-CHA	3.40	129.77	123.87
40	q	313	CLA	CHD-C1D-ND	-3.40	120.02	124.80
40	Q	205	CLA	CHD-C1D-ND	-3.39	120.03	124.80
40	Z	313	CLA	CHD-C1D-ND	-3.39	120.03	124.80
40	q	310	CLA	CHD-C1D-ND	-3.39	120.03	124.80
40	b	829	CLA	CHD-C1D-ND	-3.39	120.03	124.80
40	a	830	CLA	CHD-C1D-ND	-3.39	120.03	124.80
40	y	302	CLA	CHD-C1D-ND	-3.39	120.03	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	y	309	CLA	CHD-C1D-ND	-3.39	120.03	124.80
40	z	306	CLA	CHD-C1D-ND	-3.39	120.03	124.80
40	R	306	CLA	CHD-C1D-ND	-3.39	120.04	124.80
40	E	310	CLA	C1-C2-C3	-3.39	120.65	126.20
40	z	308	CLA	CHD-C1D-ND	-3.39	120.04	124.80
40	I	206	CLA	CHD-C1D-ND	-3.38	120.04	124.80
40	B	301	CLA	CHD-C1D-ND	-3.38	120.04	124.80
47	v	321	A1EB1	C34-O4-C38	3.38	123.82	117.85
40	L	306	CLA	C3A-C2A-C1A	-3.38	96.28	101.34
40	b	836	CLA	CHD-C1D-ND	-3.38	120.05	124.80
40	X	310	CLA	C3D-C4D-ND	3.38	115.48	109.99
40	L	306	CLA	CHD-C1D-ND	-3.38	120.05	124.80
41	v	302	KC2	C1D-ND-C4D	3.38	108.68	106.31
40	Q	207	CLA	CHD-C1D-ND	-3.38	120.05	124.80
40	a	838	CLA	CHD-C1D-ND	-3.38	120.05	124.80
40	I	207	CLA	CHD-C1D-ND	-3.37	120.05	124.80
40	A	307	CLA	CHD-C1D-ND	-3.37	120.06	124.80
40	F	305	CLA	CHD-C1D-ND	-3.37	120.06	124.80
40	a	820	CLA	CHD-C1D-ND	-3.37	120.06	124.80
40	L	301	CLA	CHD-C1D-ND	-3.37	120.06	124.80
40	b	811	CLA	CHD-C1D-ND	-3.37	120.06	124.80
40	b	813	CLA	C1-C2-C3	-3.37	121.31	126.76
44	o	314	A86	C33-C32-C31	3.37	112.48	109.21
40	b	837	CLA	CHD-C1D-ND	-3.37	120.06	124.80
40	z	313	CLA	CHD-C1D-ND	-3.37	120.06	124.80
40	u	307	CLA	CHD-C1D-ND	-3.37	120.06	124.80
40	Y	306	CLA	CHD-C1D-ND	-3.37	120.06	124.80
44	p	321	A86	C21-C20-C19	-3.37	110.46	114.24
40	T	307	CLA	CHD-C1D-ND	-3.36	120.07	124.80
40	t	307	CLA	CHD-C1D-ND	-3.36	120.07	124.80
42	A	315	DD6	C14-C13-C11	3.36	130.75	125.53
40	W	313	CLA	CHD-C1D-ND	-3.36	120.07	124.80
48	W	319	A1EB4	C33-C32-C31	3.36	112.48	109.21
40	b	805	CLA	CHD-C1D-ND	-3.36	120.08	124.80
40	B	304	CLA	CHD-C1D-ND	-3.36	120.08	124.80
40	Q	206	CLA	C4A-NA-C1A	-3.36	105.15	106.68
40	b	817	CLA	CHD-C1D-ND	-3.35	120.08	124.80
40	a	814	CLA	CHD-C1D-ND	-3.35	120.09	124.80
40	z	311	CLA	C2A-C3A-C4A	-3.35	96.46	101.87
40	P	308	CLA	CHD-C1D-ND	-3.35	120.09	124.80
40	l	205	CLA	CHD-C1D-ND	-3.35	120.09	124.80
42	o	319	DD6	C14-C13-C11	3.35	130.72	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	W	305	CLA	CHD-C1D-ND	-3.35	120.09	124.80
40	F	311	CLA	CHD-C1D-ND	-3.35	120.09	124.80
40	F	307	CLA	CHD-C1D-ND	-3.35	120.09	124.80
40	x	306	CLA	CHD-C1D-ND	-3.35	120.09	124.80
47	u	322	A1EB1	C33-C32-C31	3.35	112.46	109.21
40	a	826	CLA	CHD-C1D-ND	-3.34	120.10	124.80
40	R	307	CLA	CHD-C1D-ND	-3.34	120.10	124.80
40	q	304	CLA	CHD-C1D-ND	-3.34	120.10	124.80
40	q	306	CLA	CHD-C1D-ND	-3.34	120.10	124.80
40	Z	306	CLA	CHD-C1D-ND	-3.34	120.10	124.80
40	o	304	CLA	CHD-C1D-ND	-3.34	120.10	124.80
46	F	320	SQD	C45-O47-C7	-3.34	109.80	117.80
42	z	321	DD6	C14-C13-C11	3.34	130.71	125.53
40	a	829	CLA	CHD-C1D-ND	-3.34	120.10	124.80
40	o	311	CLA	CHD-C1D-ND	-3.34	120.10	124.80
40	F	308	CLA	CHD-C1D-ND	-3.34	120.10	124.80
44	w	311	A86	O1-C20-C19	-3.33	110.37	113.49
40	j	102	CLA	CHD-C1D-ND	-3.33	120.11	124.80
44	v	325	A86	C21-C20-C19	-3.33	110.50	114.24
41	p	303	KC2	C1D-ND-C4D	3.33	108.65	106.31
40	q	301	CLA	CHD-C1D-ND	-3.33	120.11	124.80
40	S	314	CLA	CHD-C1D-ND	-3.33	120.11	124.80
40	C	305	CLA	CHD-C1D-ND	-3.33	120.11	124.80
40	Q	204	CLA	CHD-C1D-ND	-3.33	120.12	124.80
40	w	309	CLA	CHD-C1D-ND	-3.33	120.12	124.80
42	Q	212	DD6	C14-C13-C11	3.33	130.69	125.53
40	E	302	CLA	CHD-C1D-ND	-3.33	120.12	124.80
40	S	308	CLA	CHD-C1D-ND	-3.33	120.12	124.80
40	T	306	CLA	CHD-C1D-ND	-3.33	120.12	124.80
40	a	816	CLA	CHD-C1D-ND	-3.33	120.12	124.80
40	D	308	CLA	CHD-C1D-ND	-3.32	120.12	124.80
44	X	317	A86	C21-C20-C19	-3.32	110.51	114.24
40	b	815	CLA	CHD-C1D-ND	-3.32	120.13	124.80
41	u	303	KC2	C1D-ND-C4D	3.32	108.64	106.31
40	z	308	CLA	C3D-C4D-ND	3.32	115.39	109.99
40	M	312	CLA	CHD-C1D-ND	-3.32	120.13	124.80
40	y	303	CLA	CHD-C1D-ND	-3.32	120.13	124.80
40	L	307	CLA	CHD-C1D-ND	-3.32	120.13	124.80
40	a	821	CLA	CHD-C1D-ND	-3.32	120.13	124.80
40	o	312	CLA	CHD-C1D-ND	-3.32	120.13	124.80
40	H	311	CLA	CHD-C1D-ND	-3.32	120.14	124.80
40	X	307	CLA	CHD-C1D-ND	-3.32	120.14	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	z	320	A86	O1-C20-C19	-3.32	110.38	113.49
40	L	310	CLA	CHD-C1D-ND	-3.32	120.14	124.80
40	U	204	CLA	CHD-C1D-ND	-3.32	120.14	124.80
40	G	205	CLA	CHD-C1D-ND	-3.31	120.14	124.80
40	f	204	CLA	CHD-C1D-ND	-3.31	120.14	124.80
40	w	303	CLA	CHD-C1D-ND	-3.31	120.14	124.80
40	N	304	CLA	CHD-C1D-ND	-3.31	120.14	124.80
40	T	310	CLA	CHD-C1D-ND	-3.31	120.14	124.80
40	C	301	CLA	CHD-C1D-ND	-3.31	120.14	124.80
40	R	304	CLA	CAA-C2A-C1A	-3.31	101.13	111.97
40	T	304	CLA	CHD-C1D-ND	-3.31	120.15	124.80
40	b	819	CLA	CHD-C1D-ND	-3.31	120.15	124.80
40	x	314	CLA	CHD-C1D-ND	-3.31	120.15	124.80
40	M	311	CLA	CHD-C1D-ND	-3.30	120.15	124.80
40	E	303	CLA	CHD-C1D-ND	-3.30	120.15	124.80
40	O	304	CLA	CHD-C1D-ND	-3.30	120.15	124.80
40	u	313	CLA	C4A-NA-C1A	-3.30	105.17	106.68
40	w	302	CLA	CHD-C1D-ND	-3.30	120.16	124.80
44	z	315	A86	C33-C32-C31	3.30	112.42	109.21
40	O	305	CLA	CHD-C1D-ND	-3.30	120.16	124.80
40	b	827	CLA	CHD-C1D-ND	-3.30	120.16	124.80
40	G	204	CLA	CHD-C1D-ND	-3.30	120.16	124.80
40	D	309	CLA	CHD-C1D-ND	-3.29	120.17	124.80
40	Z	307	CLA	CHD-C1D-ND	-3.29	120.17	124.80
40	L	311	CLA	CHD-C1D-ND	-3.29	120.17	124.80
40	t	305	CLA	CHD-C1D-ND	-3.29	120.17	124.80
40	a	836	CLA	CHD-C1D-ND	-3.29	120.17	124.80
44	v	319	A86	O4-C34-C35	3.29	116.05	107.64
40	I	201	CLA	CHD-C1D-ND	-3.29	120.17	124.80
40	K	304	CLA	CHD-C1D-ND	-3.29	120.17	124.80
40	b	823	CLA	CHD-C1D-ND	-3.29	120.17	124.80
40	v	313	CLA	CHD-C1D-ND	-3.29	120.18	124.80
40	A	309	CLA	CHD-C1D-ND	-3.29	120.18	124.80
40	C	306	CLA	CHD-C1D-ND	-3.29	120.18	124.80
40	L	304	CLA	CHD-C1D-ND	-3.29	120.18	124.80
40	b	824	CLA	CHD-C1D-ND	-3.29	120.18	124.80
40	p	302	CLA	C3D-C4D-ND	3.28	115.33	109.99
40	x	308	CLA	CHD-C1D-ND	-3.28	120.18	124.80
40	z	307	CLA	CHD-C1D-ND	-3.28	120.18	124.80
40	U	206	CLA	CHD-C1D-ND	-3.28	120.18	124.80
42	Q	213	DD6	C14-C13-C11	3.28	130.62	125.53
40	M	307	CLA	CHD-C1D-ND	-3.28	120.18	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	S	313	CLA	CHD-C1D-ND	-3.28	120.18	124.80
40	E	308	CLA	CHD-C1D-ND	-3.28	120.19	124.80
40	H	305	CLA	CHD-C1D-ND	-3.28	120.19	124.80
40	I	203	CLA	CHD-C1D-ND	-3.28	120.19	124.80
40	G	201	CLA	CHD-C1D-ND	-3.28	120.19	124.80
40	Y	301	CLA	CHD-C1D-ND	-3.28	120.19	124.80
40	a	851	CLA	CHD-C1D-ND	-3.28	120.19	124.80
40	F	321	CLA	CHD-C1D-ND	-3.28	120.19	124.80
40	R	304	CLA	CHD-C1D-ND	-3.28	120.19	124.80
40	a	813	CLA	CHD-C1D-ND	-3.28	120.19	124.80
40	X	311	CLA	CHD-C1D-ND	-3.28	120.19	124.80
40	P	311	CLA	CHD-C1D-ND	-3.27	120.19	124.80
40	Q	209	CLA	CHD-C1D-ND	-3.27	120.20	124.80
40	U	202	CLA	C3D-C4D-ND	3.27	115.31	109.99
40	z	311	CLA	C3D-C4D-ND	3.27	115.31	109.99
40	F	301	CLA	CHD-C1D-ND	-3.27	120.20	124.80
40	Q	202	CLA	CHD-C1D-ND	-3.27	120.20	124.80
40	a	839	CLA	CHD-C1D-ND	-3.27	120.20	124.80
44	X	314	A86	O1-C20-C19	3.27	116.56	113.49
40	L	312	CLA	CHD-C1D-ND	-3.27	120.20	124.80
40	b	816	CLA	CHD-C1D-ND	-3.27	120.20	124.80
40	N	305	CLA	CHD-C1D-ND	-3.27	120.21	124.80
40	V	202	CLA	C2C-C1C-NC	3.27	113.41	109.98
40	S	301	CLA	CHD-C1D-ND	-3.27	120.21	124.80
40	S	311	CLA	C3D-C4D-ND	3.26	115.29	109.99
40	a	815	CLA	CHD-C1D-ND	-3.26	120.21	124.80
40	Y	310	CLA	CHD-C1D-ND	-3.26	120.21	124.80
40	a	817	CLA	CHD-C1D-ND	-3.26	120.21	124.80
52	b	850	DGD	C3G-C2G-C1G	-3.26	104.18	111.78
40	b	840	CLA	CHD-C1D-ND	-3.26	120.21	124.80
40	I	205	CLA	CHD-C1D-ND	-3.26	120.22	124.80
40	Y	311	CLA	CHD-C1D-ND	-3.26	120.22	124.80
40	b	835	CLA	CHD-C1D-ND	-3.26	120.22	124.80
40	D	304	CLA	CHD-C1D-ND	-3.26	120.22	124.80
40	b	842	CLA	CHD-C1D-ND	-3.26	120.22	124.80
40	K	306	CLA	CHD-C1D-ND	-3.26	120.22	124.80
40	U	205	CLA	CHD-C1D-ND	-3.26	120.22	124.80
40	Y	304	CLA	CHD-C1D-ND	-3.26	120.22	124.80
40	y	305	CLA	CHD-C1D-ND	-3.26	120.22	124.80
40	b	806	CLA	CHD-C1D-ND	-3.26	120.22	124.80
40	B	303	CLA	CHD-C1D-ND	-3.25	120.22	124.80
40	D	305	CLA	CHD-C1D-ND	-3.25	120.25	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	a	833	CLA	CHD-C1D-ND	-3.25	120.23	124.80
40	b	828	CLA	CHD-C1D-ND	-3.25	120.23	124.80
40	b	832	CLA	CHD-C1D-ND	-3.25	120.23	124.80
40	I	208	CLA	CHD-C1D-ND	-3.25	120.23	124.80
40	H	304	CLA	CHD-C1D-ND	-3.25	120.23	124.80
40	p	306	CLA	CHD-C1D-ND	-3.25	120.23	124.80
40	R	310	CLA	CHD-C1D-ND	-3.25	120.23	124.80
40	Y	305	CLA	CHD-C1D-ND	-3.25	120.23	124.80
44	y	310	A86	C21-C20-C19	-3.25	110.59	114.24
40	K	308	CLA	C3D-C4D-ND	3.25	115.27	109.99
40	M	310	CLA	CHD-C1D-ND	-3.25	120.23	124.80
40	t	303	CLA	CHD-C1D-ND	-3.24	120.24	124.80
42	E	316	DD6	C14-C13-C11	3.24	130.56	125.53
40	p	311	CLA	C3D-C4D-ND	3.24	115.26	109.99
40	b	813	CLA	CHD-C1D-ND	-3.24	120.24	124.80
40	o	306	CLA	CHD-C1D-ND	-3.24	120.24	124.80
40	N	306	CLA	CHD-C1D-ND	-3.24	120.24	124.80
40	a	819	CLA	CHD-C1D-ND	-3.24	120.24	124.80
40	b	833	CLA	CHD-C1D-ND	-3.24	120.24	124.80
40	L	305	CLA	CHD-C1D-ND	-3.24	120.24	124.80
40	F	308	CLA	C3D-C4D-ND	3.24	115.25	109.99
40	Z	310	CLA	C3D-C4D-ND	3.24	115.25	109.99
40	J	306	CLA	CHD-C1D-ND	-3.24	120.24	124.80
40	b	802	CLA	CHD-C1D-ND	-3.24	120.24	124.80
40	F	306	CLA	C3D-C4D-ND	3.24	115.25	109.99
41	Q	201	KC2	C1D-ND-C4D	3.24	108.58	106.31
40	N	311	CLA	CHD-C1D-ND	-3.24	120.25	124.80
40	D	302	CLA	CHD-C1D-ND	-3.24	120.25	124.80
44	q	319	A86	O4-C34-C35	3.24	115.92	107.64
40	M	306	CLA	CHD-C1D-ND	-3.23	120.25	124.80
40	v	306	CLA	CHD-C1D-ND	-3.23	120.25	124.80
40	S	308	CLA	C1-C2-C3	-3.23	121.53	126.76
40	a	804	CLA	C3D-C4D-ND	3.23	115.24	109.99
40	E	309	CLA	CHD-C1D-ND	-3.23	120.25	124.80
40	k	201	CLA	CHD-C1D-ND	-3.23	120.25	124.80
40	H	301	CLA	CHD-C1D-ND	-3.23	120.26	124.80
40	a	831	CLA	CHD-C1D-ND	-3.23	120.26	124.80
40	X	312	CLA	CHD-C1D-ND	-3.23	120.26	124.80
40	t	309	CLA	CHD-C1D-ND	-3.23	120.26	124.80
40	E	306	CLA	CHD-C1D-ND	-3.23	120.26	124.80
40	v	307	CLA	C3D-C4D-ND	3.22	115.23	109.99
40	G	207	CLA	CHD-C1D-ND	-3.22	120.27	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	o	307	CLA	C3D-C4D-ND	3.22	115.22	109.99
40	x	311	CLA	C3D-C4D-ND	3.22	115.22	109.99
44	O	313	A86	C33-C32-C31	3.22	112.34	109.21
40	o	301	CLA	CHD-C1D-ND	-3.22	120.27	124.80
40	A	304	CLA	C3D-C4D-ND	3.22	115.22	109.99
40	b	812	CLA	CHD-C1D-ND	-3.22	120.27	124.80
40	l	202	CLA	CHD-C1D-ND	-3.22	120.27	124.80
40	z	302	CLA	CHD-C1D-ND	-3.22	120.27	124.80
40	N	307	CLA	CHD-C1D-ND	-3.22	120.27	124.80
40	A	306	CLA	CHD-C1D-ND	-3.22	120.27	124.80
40	O	310	CLA	CHD-C1D-ND	-3.22	120.28	124.80
40	P	312	CLA	CHD-C1D-ND	-3.22	120.28	124.80
40	k	202	CLA	CHD-C1D-ND	-3.22	120.28	124.80
40	z	305	CLA	CHD-C1D-ND	-3.21	120.28	124.80
40	v	305	CLA	C3D-C4D-ND	3.21	115.21	109.99
40	R	316	CLA	CHD-C1D-ND	-3.21	120.28	124.80
40	y	304	CLA	CHD-C1D-ND	-3.21	120.28	124.80
43	l	201	LMG	C1-C2-C3	-3.21	103.26	110.01
40	H	309	CLA	CHD-C1D-ND	-3.21	120.28	124.80
44	M	316	A86	C33-C32-C31	3.21	112.33	109.21
40	E	305	CLA	C3D-C4D-ND	3.21	115.20	109.99
42	H	312	DD6	C21-C20-C19	3.20	117.84	114.24
40	K	301	CLA	CHD-C1D-ND	-3.20	120.29	124.80
40	A	308	CLA	CHD-C1D-ND	-3.20	120.30	124.80
40	B	307	CLA	C3A-C2A-C1A	-3.20	96.55	101.34
40	a	816	CLA	C3D-C4D-ND	3.20	115.18	109.99
40	U	203	CLA	CHD-C1D-ND	-3.20	120.31	124.80
40	R	305	CLA	CHD-C1D-ND	-3.19	120.31	124.80
40	S	306	CLA	CHD-C1D-ND	-3.19	120.31	124.80
40	W	307	CLA	CHD-C1D-ND	-3.19	120.31	124.80
40	a	808	CLA	C2A-C3A-C4A	-3.19	96.71	101.87
40	u	305	CLA	C3D-C4D-ND	3.19	115.17	109.99
40	U	207	CLA	CHD-C1D-ND	-3.19	120.31	124.80
40	K	312	CLA	CHD-C1D-ND	-3.19	120.31	124.80
40	a	814	CLA	C3D-C4D-ND	3.19	115.17	109.99
40	H	306	CLA	CHD-C1D-ND	-3.19	120.32	124.80
40	G	203	CLA	C3D-C4D-ND	3.19	115.17	109.99
40	Y	312	CLA	C3D-C4D-ND	3.18	115.16	109.99
40	o	313	CLA	C3D-C4D-ND	3.18	115.16	109.99
40	p	311	CLA	C2A-C3A-C4A	-3.18	96.73	101.87
40	b	810	CLA	CHD-C1D-ND	-3.18	120.33	124.80
40	Z	301	CLA	CHD-C1D-ND	-3.18	120.33	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	v	312	CLA	CHD-C1D-ND	-3.18	120.33	124.80
40	w	302	CLA	C3D-C4D-ND	3.18	115.16	109.99
40	b	826	CLA	CHD-C1D-ND	-3.18	120.33	124.80
44	p	321	A86	O1-C20-C19	3.18	116.47	113.49
40	I	202	CLA	CHD-C1D-ND	-3.18	120.33	124.80
40	Z	304	CLA	CHD-C1D-ND	-3.18	120.33	124.80
44	P	317	A86	C21-C20-C19	-3.18	110.67	114.24
40	X	306	CLA	C3D-C4D-ND	3.17	115.15	109.99
40	I	208	CLA	C3D-C4D-ND	3.17	115.15	109.99
40	a	835	CLA	CHD-C1D-ND	-3.17	120.34	124.80
40	Y	306	CLA	C3D-C4D-ND	3.17	115.14	109.99
40	A	307	CLA	C3D-C4D-ND	3.17	115.14	109.99
40	l	203	CLA	C3D-C4D-ND	3.17	115.14	109.99
40	Y	313	CLA	C3D-C4D-ND	3.17	115.14	109.99
40	p	314	CLA	CHD-C1D-ND	-3.17	120.34	124.80
40	b	814	CLA	CHD-C1D-ND	-3.17	120.34	124.80
40	x	312	CLA	CHD-C1D-ND	-3.17	120.35	124.80
40	B	307	CLA	CHD-C1D-ND	-3.17	120.35	124.80
40	D	304	CLA	C3D-C4D-ND	3.17	115.13	109.99
40	a	806	CLA	C3D-C4D-ND	3.17	115.13	109.99
40	C	302	CLA	C3D-C4D-ND	3.16	115.13	109.99
40	b	835	CLA	CGD-CBD-CAD	-3.16	100.61	110.85
40	D	312	CLA	CHD-C1D-ND	-3.16	120.36	124.80
40	E	310	CLA	CHD-C1D-ND	-3.16	120.36	124.80
40	t	304	CLA	CHD-C1D-ND	-3.16	120.36	124.80
40	J	308	CLA	CHD-C1D-ND	-3.16	120.36	124.80
40	w	308	CLA	CHD-C1D-ND	-3.16	120.36	124.80
40	a	810	CLA	C3D-C4D-ND	3.16	115.12	109.99
40	V	201	CLA	CHD-C1D-ND	-3.16	120.36	124.80
40	P	307	CLA	CHD-C1D-ND	-3.16	120.36	124.80
40	w	304	CLA	CHD-C1D-ND	-3.16	120.36	124.80
40	F	307	CLA	C3D-C4D-ND	3.16	115.12	109.99
40	q	305	CLA	C3D-C4D-ND	3.16	115.12	109.99
40	F	303	CLA	CHD-C1D-ND	-3.16	120.36	124.80
42	K	311	DD6	C14-C13-C11	3.15	130.43	125.53
40	z	305	CLA	C3D-C4D-ND	3.15	115.11	109.99
40	C	309	CLA	C3D-C4D-ND	3.15	115.11	109.99
40	t	305	CLA	C3D-C4D-ND	3.15	115.11	109.99
40	w	305	CLA	CHD-C1D-ND	-3.15	120.36	124.80
40	K	304	CLA	C3D-C4D-ND	3.15	115.11	109.99
40	T	307	CLA	C3D-C4D-ND	3.15	115.11	109.99
40	u	311	CLA	C3D-C4D-ND	3.15	115.11	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	q	307	CLA	C3D-C4D-ND	3.15	115.11	109.99
40	x	311	CLA	C3A-C2A-C1A	-3.15	96.62	101.34
40	b	809	CLA	C3D-C4D-ND	3.15	115.11	109.99
40	z	324	CLA	C3D-C4D-ND	3.15	115.11	109.99
40	D	306	CLA	CHD-C1D-ND	-3.15	120.38	124.80
40	z	312	CLA	CHD-C1D-ND	-3.15	120.38	124.80
40	H	307	CLA	C3D-C4D-ND	3.14	115.10	109.99
44	t	310	A86	C36-C31-C32	-3.14	116.58	119.70
40	o	306	CLA	C3D-C4D-ND	3.14	115.09	109.99
40	b	807	CLA	C4D-CHA-C1A	-3.14	117.50	121.24
40	P	306	CLA	CHD-C1D-ND	-3.14	120.38	124.80
40	F	306	CLA	CHD-C1D-ND	-3.14	120.38	124.80
40	O	316	CLA	CHD-C1D-ND	-3.14	120.38	124.80
40	t	302	CLA	C3D-C4D-ND	3.14	115.09	109.99
40	z	314	CLA	C3D-C4D-ND	3.14	115.09	109.99
40	C	308	CLA	CBA-CAA-C2A	3.14	123.13	113.79
40	E	307	CLA	CHD-C1D-ND	-3.14	120.39	124.80
40	B	306	CLA	CHD-C1D-ND	-3.14	120.39	124.80
40	E	313	CLA	CHD-C1D-ND	-3.14	120.39	124.80
43	j	101	LMG	C1-C2-C3	-3.13	103.42	110.01
40	I	204	CLA	CHD-C1D-ND	-3.13	120.39	124.80
40	K	307	CLA	CHD-C1D-ND	-3.13	120.39	124.80
40	S	319	CLA	CHD-C1D-ND	-3.13	120.39	124.80
40	a	852	CLA	CHD-C1D-ND	-3.13	120.39	124.80
41	W	309	KC2	C2A-C3A-C4A	3.13	108.76	106.41
40	X	307	CLA	C3D-C4D-ND	3.13	115.08	109.99
40	p	312	CLA	CHD-C1D-ND	-3.13	120.39	124.80
40	v	301	CLA	CHD-C1D-ND	-3.13	120.39	124.80
40	W	306	CLA	C3D-C4D-ND	3.13	115.08	109.99
40	b	831	CLA	CHD-C1D-ND	-3.13	120.40	124.80
40	T	305	CLA	CHD-C1D-ND	-3.13	120.40	124.80
40	p	311	CLA	C3A-C2A-C1A	-3.13	96.65	101.34
40	E	312	CLA	CHD-C1D-ND	-3.13	120.40	124.80
40	u	314	CLA	C3D-C4D-ND	3.13	115.07	109.99
40	E	314	CLA	C2A-C1A-CHA	3.13	129.29	123.87
40	z	313	CLA	C3D-C4D-ND	3.13	115.07	109.99
42	B	305	DD6	C21-C20-C19	3.12	117.75	114.24
40	a	841	CLA	C3D-C4D-ND	3.12	115.07	109.99
40	a	822	CLA	CBA-CAA-C2A	3.12	123.09	113.79
44	S	315	A86	C36-C31-C32	-3.12	116.60	119.70
40	W	313	CLA	C3D-C4D-ND	3.12	115.06	109.99
44	p	319	A86	C33-C32-C31	3.12	112.24	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	Q	203	CLA	C3D-C4D-ND	3.12	115.06	109.99
40	a	822	CLA	C3D-C4D-ND	3.12	115.06	109.99
40	Q	208	CLA	CHD-C1D-ND	-3.12	120.41	124.80
40	l	204	CLA	CHD-C1D-ND	-3.12	120.41	124.80
40	a	828	CLA	CHD-C1D-ND	-3.12	120.42	124.80
40	O	307	CLA	CHD-C1D-ND	-3.12	120.42	124.80
40	b	815	CLA	C3D-C4D-ND	3.12	115.05	109.99
40	a	812	CLA	CHD-C1D-ND	-3.11	120.42	124.80
40	f	201	CLA	CHD-C1D-ND	-3.11	120.42	124.80
40	A	302	CLA	CHD-C1D-ND	-3.11	120.42	124.80
40	C	305	CLA	C3D-C4D-ND	3.11	115.04	109.99
40	C	307	CLA	C3D-C4D-ND	3.11	115.04	109.99
40	U	203	CLA	C3D-C4D-ND	3.11	115.04	109.99
40	A	311	CLA	CHD-C1D-ND	-3.11	120.43	124.80
40	u	312	CLA	CHD-C1D-ND	-3.11	120.43	124.80
44	X	319	A86	C33-C32-C31	3.10	112.23	109.21
40	q	311	CLA	CHD-C1D-ND	-3.10	120.43	124.80
42	H	312	DD6	C14-C13-C11	3.10	130.34	125.53
40	E	304	CLA	CHD-C1D-ND	-3.10	120.44	124.80
40	N	305	CLA	C3D-C4D-ND	3.10	115.03	109.99
40	a	823	CLA	CHD-C1D-ND	-3.10	120.44	124.80
40	a	834	CLA	C3D-C4D-ND	3.10	115.03	109.99
40	X	304	CLA	CHD-C1D-ND	-3.10	120.44	124.80
40	v	311	CLA	CHD-C1D-ND	-3.10	120.44	124.80
40	H	308	CLA	CHD-C1D-ND	-3.10	120.44	124.80
40	a	827	CLA	CHD-C1D-ND	-3.10	120.44	124.80
40	Y	307	CLA	C3D-C4D-ND	3.10	115.03	109.99
40	C	308	CLA	CHD-C1D-ND	-3.10	120.44	124.80
40	u	306	CLA	CHD-C1D-ND	-3.10	120.44	124.80
42	M	314	DD6	C14-C13-C11	3.10	130.34	125.53
40	J	309	CLA	CHD-C1D-ND	-3.10	120.44	124.80
40	Z	310	CLA	C2A-C3A-C4A	-3.10	96.87	101.87
40	M	312	CLA	C3D-C4D-ND	3.10	115.02	109.99
40	T	317	CLA	CHD-C1D-ND	-3.10	120.44	124.80
40	G	213	CLA	C3D-C4D-ND	3.10	115.02	109.99
40	D	309	CLA	C3D-C4D-ND	3.09	115.02	109.99
40	H	302	CLA	C3D-C4D-ND	3.09	115.02	109.99
40	E	302	CLA	C3D-C4D-ND	3.09	115.02	109.99
40	Z	306	CLA	C3D-C4D-ND	3.09	115.01	109.99
40	Z	313	CLA	C3A-C2A-C1A	-3.09	96.71	101.34
40	b	818	CLA	CHD-C1D-ND	-3.09	120.45	124.80
40	y	308	CLA	CHD-C1D-ND	-3.09	120.45	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	o	314	A86	O1-C20-C19	-3.09	110.59	113.49
40	H	311	CLA	C3D-C4D-ND	3.09	115.01	109.99
40	o	313	CLA	C3A-C2A-C1A	-3.09	96.71	101.34
40	T	304	CLA	C3D-C4D-ND	3.09	115.01	109.99
44	X	317	A86	C33-C32-C31	3.09	112.21	109.21
40	J	305	CLA	CHD-C1D-ND	-3.09	120.46	124.80
40	y	305	CLA	C3D-C4D-ND	3.09	115.00	109.99
44	w	316	A86	C21-C20-C19	-3.08	110.78	114.24
40	b	822	CLA	C3D-C4D-ND	3.08	115.00	109.99
40	a	830	CLA	C3D-C4D-ND	3.08	114.99	109.99
40	E	311	CLA	C3D-C4D-ND	3.08	114.99	109.99
40	a	827	CLA	C3D-C4D-ND	3.08	114.99	109.99
40	M	311	CLA	C3D-C4D-ND	3.08	114.99	109.99
44	F	317	A86	C33-C32-C31	3.08	112.20	109.21
44	q	315	A86	C33-C32-C31	3.08	112.20	109.21
40	J	311	CLA	C3D-C4D-ND	3.08	114.99	109.99
44	z	318	A86	O1-C20-C19	3.08	116.37	113.49
40	I	203	CLA	C3D-C4D-ND	3.07	114.98	109.99
40	R	304	CLA	C3D-C4D-ND	3.07	114.98	109.99
40	R	307	CLA	C3D-C4D-ND	3.07	114.98	109.99
40	D	301	CLA	CHD-C1D-ND	-3.07	120.48	124.80
40	I	206	CLA	C1-C2-C3	-3.07	121.16	126.20
40	F	310	CLA	CHD-C1D-ND	-3.07	120.48	124.80
40	Z	311	CLA	C3D-C4D-ND	3.07	114.98	109.99
40	S	307	CLA	C3D-C4D-ND	3.07	114.98	109.99
40	b	836	CLA	C3D-C4D-ND	3.07	114.98	109.99
40	F	305	CLA	C3D-C4D-ND	3.07	114.97	109.99
40	b	837	CLA	C3D-C4D-ND	3.07	114.97	109.99
40	a	815	CLA	C3D-C4D-ND	3.07	114.97	109.99
42	F	316	DD6	C30-C29-C27	-3.07	165.81	176.23
40	F	311	CLA	C3D-C4D-ND	3.07	114.97	109.99
40	I	207	CLA	C3D-C4D-ND	3.07	114.97	109.99
40	D	307	CLA	C3D-C4D-ND	3.06	114.97	109.99
40	a	807	CLA	CHD-C1D-ND	-3.06	120.49	124.80
40	E	308	CLA	C3D-C4D-ND	3.06	114.97	109.99
40	F	304	CLA	C3D-C4D-ND	3.06	114.97	109.99
40	b	839	CLA	C3D-C4D-ND	3.06	114.97	109.99
40	J	302	CLA	CHD-C1D-ND	-3.06	120.49	124.80
40	A	303	CLA	CHD-C1D-ND	-3.06	120.49	124.80
40	v	312	CLA	C3D-C4D-ND	3.06	114.97	109.99
40	f	202	CLA	CHD-C1D-ND	-3.06	120.49	124.80
40	A	309	CLA	C3D-C4D-ND	3.06	114.96	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	M	304	CLA	C3D-C4D-ND	3.06	114.96	109.99
40	q	306	CLA	C3D-C4D-ND	3.06	114.96	109.99
45	F	319	LHG	O8-C23-C24	3.06	121.16	111.83
40	N	307	CLA	C3D-C4D-ND	3.06	114.96	109.99
40	a	817	CLA	C3D-C4D-ND	3.06	114.96	109.99
40	a	839	CLA	C3D-C4D-ND	3.06	114.96	109.99
40	a	822	CLA	CHD-C1D-ND	-3.06	120.50	124.80
40	O	307	CLA	C3D-C4D-ND	3.06	114.96	109.99
40	O	306	CLA	C3D-C4D-ND	3.05	114.95	109.99
40	p	305	CLA	C3D-C4D-ND	3.05	114.95	109.99
47	p	323	A1EB1	O4-C34-C33	3.05	115.45	107.64
43	W	317	LMG	O1-C1-C2	-3.05	103.64	108.27
40	u	302	CLA	C3D-C4D-ND	3.05	114.95	109.99
40	a	808	CLA	C3D-C4D-ND	3.05	114.95	109.99
40	M	305	CLA	CHD-C1D-ND	-3.05	120.51	124.80
40	A	301	CLA	CHD-C1D-ND	-3.05	120.51	124.80
40	u	311	CLA	C3A-C2A-C1A	-3.05	96.77	101.34
40	a	835	CLA	C3D-C4D-ND	3.05	114.94	109.99
47	x	322	A1EB1	C36-C31-C32	-3.05	116.67	119.70
40	Q	205	CLA	C3D-C4D-ND	3.05	114.94	109.99
40	D	302	CLA	C3D-C4D-ND	3.05	114.94	109.99
40	b	830	CLA	C3D-C4D-ND	3.05	114.94	109.99
40	v	313	CLA	C3D-C4D-ND	3.05	114.94	109.99
40	a	820	CLA	C3D-C4D-ND	3.05	114.94	109.99
40	w	303	CLA	C3D-C4D-ND	3.05	114.94	109.99
40	E	310	CLA	C3D-C4D-ND	3.04	114.94	109.99
40	a	837	CLA	CHD-C1D-ND	-3.04	120.52	124.80
40	b	841	CLA	CHD-C1D-ND	-3.04	120.52	124.80
40	b	828	CLA	C3D-C4D-ND	3.04	114.93	109.99
40	A	305	CLA	C3D-C4D-ND	3.04	114.93	109.99
40	a	842	CLA	CHD-C1D-ND	-3.04	120.52	124.80
40	L	310	CLA	C3D-C4D-ND	3.04	114.93	109.99
40	b	817	CLA	C3D-C4D-ND	3.04	114.93	109.99
44	S	317	A86	C33-C32-C31	3.04	112.16	109.21
40	Y	310	CLA	C3D-C4D-ND	3.04	114.92	109.99
40	b	823	CLA	C3D-C4D-ND	3.04	114.92	109.99
46	I	215	SQD	O48-C23-C24	3.04	121.09	111.83
40	N	304	CLA	C3D-C4D-ND	3.04	114.92	109.99
40	x	305	CLA	C3D-C4D-ND	3.03	114.92	109.99
40	I	202	CLA	C3D-C4D-ND	3.03	114.92	109.99
40	a	819	CLA	C3D-C4D-ND	3.03	114.91	109.99
40	u	313	CLA	CHD-C1D-ND	-3.03	120.54	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	a	838	CLA	C3D-C4D-ND	3.03	114.91	109.99
40	J	312	CLA	CHD-C1D-ND	-3.03	120.54	124.80
40	N	311	CLA	C3D-C4D-ND	3.03	114.91	109.99
40	K	308	CLA	CAC-C3C-C4C	3.03	128.73	124.79
40	J	306	CLA	C3D-C4D-ND	3.03	114.91	109.99
40	B	301	CLA	C3D-C4D-ND	3.03	114.91	109.99
40	E	309	CLA	C3D-C4D-ND	3.03	114.91	109.99
40	W	305	CLA	C3D-C4D-ND	3.03	114.91	109.99
40	a	818	CLA	C3D-C4D-ND	3.03	114.91	109.99
40	L	307	CLA	C3D-C4D-ND	3.03	114.91	109.99
40	O	304	CLA	C3D-C4D-ND	3.03	114.91	109.99
40	a	851	CLA	C3D-C4D-ND	3.03	114.90	109.99
40	K	306	CLA	C3D-C4D-ND	3.02	114.90	109.99
40	B	307	CLA	CHB-C1B-NB	-3.02	119.51	124.05
44	X	319	A86	C21-C20-C19	-3.02	110.84	114.24
40	V	202	CLA	C3D-C4D-ND	3.02	114.90	109.99
40	J	307	CLA	CHA-C1A-NA	-3.02	119.55	126.39
42	w	312	DD6	O1-C20-C19	-3.02	110.66	113.49
40	A	306	CLA	C3D-C4D-ND	3.02	114.90	109.99
40	S	302	CLA	CHD-C1D-ND	-3.02	120.55	124.80
40	Z	305	CLA	CHD-C1D-ND	-3.02	120.55	124.80
40	o	310	CLA	C3D-C4D-ND	3.02	114.90	109.99
40	K	308	CLA	CHD-C1D-ND	-3.02	120.56	124.80
40	I	201	CLA	C3D-C4D-ND	3.02	114.89	109.99
40	F	301	CLA	C3D-C4D-ND	3.02	114.89	109.99
40	M	307	CLA	C3D-C4D-ND	3.02	114.89	109.99
40	b	820	CLA	C3D-C4D-ND	3.02	114.89	109.99
40	q	313	CLA	C3D-C4D-ND	3.02	114.89	109.99
40	J	307	CLA	CHD-C1D-ND	-3.02	120.56	124.80
40	w	305	CLA	C3D-C4D-ND	3.02	114.89	109.99
40	a	807	CLA	C3D-C4D-ND	3.01	114.89	109.99
40	b	805	CLA	C3D-C4D-ND	3.01	114.89	109.99
40	M	306	CLA	C3D-C4D-ND	3.01	114.89	109.99
40	U	207	CLA	C3D-C4D-ND	3.01	114.89	109.99
47	q	321	A1EB1	C33-C32-C31	-3.01	106.28	109.21
40	O	305	CLA	C3D-C4D-ND	3.01	114.88	109.99
40	x	302	CLA	C3D-C4D-ND	3.01	114.88	109.99
40	z	307	CLA	C3D-C4D-ND	3.01	114.88	109.99
40	R	306	CLA	C3D-C4D-ND	3.01	114.88	109.99
40	R	305	CLA	C3D-C4D-ND	3.01	114.88	109.99
40	a	837	CLA	C3D-C4D-ND	3.01	114.88	109.99
40	X	313	CLA	C3D-C4D-ND	3.01	114.88	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	k	201	CLA	C3D-C4D-ND	3.01	114.88	109.99
40	b	834	CLA	C3D-C4D-ND	3.01	114.87	109.99
40	b	807	CLA	CHB-C1B-NB	-3.01	119.54	124.05
40	x	313	CLA	CHD-C1D-ND	-3.01	120.57	124.80
40	i	101	CLA	C3D-C4D-ND	3.01	114.87	109.99
40	b	807	CLA	CHD-C1D-ND	-3.01	120.57	124.80
40	B	303	CLA	C3D-C4D-ND	3.00	114.87	109.99
40	W	308	CLA	C3D-C4D-ND	3.00	114.87	109.99
44	q	319	A86	C33-C32-C31	3.00	112.13	109.21
40	b	816	CLA	CAA-C2A-C1A	-3.00	102.14	111.97
40	Q	206	CLA	CHD-C1D-ND	-3.00	120.58	124.80
40	E	312	CLA	C3D-C4D-ND	3.00	114.87	109.99
40	a	833	CLA	C3D-C4D-ND	3.00	114.86	109.99
40	y	302	CLA	C3D-C4D-ND	3.00	114.86	109.99
42	C	310	DD6	O1-C20-C19	-3.00	110.68	113.49
40	p	308	CLA	C3D-C4D-ND	3.00	114.86	109.99
40	P	308	CLA	C3D-C4D-ND	3.00	114.86	109.99
40	b	818	CLA	C3D-C4D-ND	2.99	114.86	109.99
40	V	201	CLA	C3D-C4D-ND	2.99	114.85	109.99
40	E	303	CLA	C3D-C4D-ND	2.99	114.85	109.99
40	D	308	CLA	C3D-C4D-ND	2.99	114.85	109.99
40	D	311	CLA	C3D-C4D-ND	2.99	114.85	109.99
40	P	307	CLA	C3D-C4D-ND	2.99	114.85	109.99
40	t	309	CLA	C3D-C4D-ND	2.99	114.85	109.99
40	q	312	CLA	CHD-C1D-ND	-2.99	120.59	124.80
40	v	306	CLA	C3D-C4D-ND	2.99	114.85	109.99
40	a	852	CLA	C3D-C4D-ND	2.99	114.84	109.99
40	b	814	CLA	C3D-C4D-ND	2.99	114.84	109.99
40	T	306	CLA	C3D-C4D-ND	2.99	114.84	109.99
40	x	314	CLA	C3D-C4D-ND	2.99	114.84	109.99
44	o	316	A86	C33-C32-C31	2.99	112.11	109.21
40	M	304	CLA	CHD-C1D-ND	-2.99	120.60	124.80
40	Y	301	CLA	C3D-C4D-ND	2.99	114.84	109.99
40	a	829	CLA	C3D-C4D-ND	2.99	114.84	109.99
40	b	803	CLA	C3D-C4D-ND	2.98	114.84	109.99
40	S	308	CLA	C3D-C4D-ND	2.98	114.83	109.99
40	a	831	CLA	C3D-C4D-ND	2.98	114.83	109.99
40	o	311	CLA	C3D-C4D-ND	2.98	114.83	109.99
44	u	319	A86	C36-C31-C32	-2.98	116.74	119.70
40	o	304	CLA	C3D-C4D-ND	2.98	114.83	109.99
40	U	208	CLA	CHD-C1D-ND	-2.98	120.61	124.80
40	f	205	CLA	CHD-C1D-ND	-2.98	120.61	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	a	805	CLA	C3D-C4D-ND	2.97	114.82	109.99
40	A	308	CLA	C3D-C4D-ND	2.97	114.82	109.99
40	z	302	CLA	C3D-C4D-ND	2.97	114.81	109.99
40	D	301	CLA	C3D-C4D-ND	2.97	114.81	109.99
47	v	323	A1EB1	C33-C32-C31	-2.97	106.33	109.21
40	J	318	CLA	C3D-C4D-ND	2.97	114.81	109.99
44	P	314	A86	O1-C20-C19	-2.97	110.71	113.49
44	t	311	A86	C21-C20-C19	-2.96	110.91	114.24
40	P	312	CLA	C3D-C4D-ND	2.96	114.80	109.99
40	M	305	CLA	C3D-C4D-ND	2.96	114.80	109.99
40	I	206	CLA	C3D-C4D-ND	2.96	114.80	109.99
40	b	826	CLA	C3D-C4D-ND	2.96	114.80	109.99
40	u	307	CLA	C3A-C2A-C1A	-2.96	96.90	101.34
44	O	313	A86	C21-C20-C19	-2.96	110.92	114.24
40	b	802	CLA	C3D-C4D-ND	2.96	114.80	109.99
40	a	824	CLA	CHD-C1D-ND	-2.95	120.64	124.80
40	b	819	CLA	C3D-C4D-ND	2.95	114.79	109.99
40	q	304	CLA	C3D-C4D-ND	2.95	114.79	109.99
40	J	310	CLA	C3D-C4D-ND	2.95	114.78	109.99
40	x	312	CLA	C1-C2-C3	-2.95	121.36	126.20
40	Z	307	CLA	C3D-C4D-ND	2.95	114.78	109.99
40	b	811	CLA	C3D-C4D-ND	2.95	114.78	109.99
40	x	307	CLA	C3D-C4D-ND	2.95	114.78	109.99
40	B	307	CLA	C3D-C4D-ND	2.95	114.78	109.99
40	B	301	CLA	C3A-C2A-C1A	-2.95	96.93	101.34
44	N	321	A86	O1-C20-C19	2.95	116.25	113.49
40	Z	301	CLA	C3D-C4D-ND	2.95	114.78	109.99
40	Q	207	CLA	C3D-C4D-ND	2.94	114.77	109.99
40	b	814	CLA	CHB-C1B-NB	-2.94	119.63	124.05
40	t	303	CLA	C3D-C4D-ND	2.94	114.77	109.99
44	v	319	A86	C33-C32-C31	2.94	112.07	109.21
42	I	212	DD6	C14-C13-C11	2.94	130.10	125.53
40	N	310	CLA	C3D-C4D-ND	2.94	114.77	109.99
40	z	306	CLA	C3D-C4D-ND	2.94	114.77	109.99
40	Y	311	CLA	C3D-C4D-ND	2.94	114.77	109.99
40	P	313	CLA	C3D-C4D-ND	2.94	114.77	109.99
40	w	304	CLA	C3D-C4D-ND	2.94	114.77	109.99
44	Y	318	A86	C21-C20-C19	-2.94	110.94	114.24
40	E	306	CLA	C3D-C4D-ND	2.94	114.77	109.99
40	x	308	CLA	C3D-C4D-ND	2.94	114.77	109.99
42	J	314	DD6	C14-C13-C11	2.94	130.09	125.53
40	A	303	CLA	C3D-C4D-ND	2.94	114.76	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	u	307	CLA	C3D-C4D-ND	2.94	114.76	109.99
40	X	305	CLA	C3D-C4D-ND	2.94	114.76	109.99
40	H	301	CLA	C3D-C4D-ND	2.94	114.76	109.99
40	y	304	CLA	C3D-C4D-ND	2.94	114.76	109.99
44	Y	319	A86	C21-C20-C19	-2.93	110.94	114.24
40	a	828	CLA	C3D-C4D-ND	2.93	114.76	109.99
40	S	314	CLA	C3D-C4D-ND	2.93	114.75	109.99
40	t	307	CLA	C3D-C4D-ND	2.93	114.75	109.99
40	C	301	CLA	C3D-C4D-ND	2.93	114.75	109.99
40	a	821	CLA	C3D-C4D-ND	2.93	114.75	109.99
40	a	808	CLA	C3A-C2A-C1A	-2.93	96.95	101.34
40	X	312	CLA	C3D-C4D-ND	2.93	114.75	109.99
40	P	305	CLA	C3D-C4D-ND	2.93	114.75	109.99
40	H	310	CLA	C3D-C4D-ND	2.93	114.75	109.99
40	b	838	CLA	C3D-C4D-ND	2.93	114.75	109.99
42	U	209	DD6	O1-C20-C19	-2.93	110.75	113.49
42	A	313	DD6	C14-C13-C11	2.93	130.07	125.53
40	Q	207	CLA	C3A-C2A-C1A	-2.93	96.96	101.34
40	Q	209	CLA	C3D-C4D-ND	2.93	114.74	109.99
40	D	312	CLA	C3D-C4D-ND	2.93	114.74	109.99
40	l	202	CLA	C3D-C4D-ND	2.93	114.74	109.99
40	b	840	CLA	C3D-C4D-ND	2.92	114.74	109.99
40	L	301	CLA	C3D-C4D-ND	2.92	114.74	109.99
40	G	207	CLA	C3D-C4D-ND	2.92	114.74	109.99
40	v	310	CLA	C3D-C4D-ND	2.92	114.74	109.99
42	y	311	DD6	O1-C20-C19	-2.92	110.75	113.49
44	P	316	A86	O1-C20-C19	2.92	116.23	113.49
40	O	306	CLA	CAA-C2A-C1A	-2.92	102.41	111.97
40	J	307	CLA	C3A-C2A-C1A	-2.92	96.97	101.34
40	w	309	CLA	C3D-C4D-ND	2.92	114.73	109.99
40	G	204	CLA	C3D-C4D-ND	2.92	114.73	109.99
40	Z	313	CLA	C3D-C4D-ND	2.92	114.73	109.99
40	u	308	CLA	C3D-C4D-ND	2.92	114.73	109.99
40	b	824	CLA	C3D-C4D-ND	2.92	114.73	109.99
40	b	803	CLA	CHB-C1B-NB	-2.92	119.67	124.05
42	I	213	DD6	C14-C13-C11	2.92	130.05	125.53
40	C	306	CLA	C3D-C4D-ND	2.92	114.73	109.99
40	t	304	CLA	C3D-C4D-ND	2.92	114.73	109.99
40	b	821	CLA	CHD-C1D-ND	-2.92	120.70	124.80
40	y	303	CLA	C3D-C4D-ND	2.91	114.72	109.99
40	y	308	CLA	C3D-C4D-ND	2.91	114.72	109.99
41	q	302	KC2	CHD-C4C-NC	2.91	128.70	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	W	311	CLA	C3D-C4D-ND	2.91	114.72	109.99
40	q	301	CLA	C3D-C4D-ND	2.91	114.72	109.99
40	V	202	CLA	CHB-C1B-NB	-2.91	119.68	124.05
40	Z	312	CLA	C3D-C4D-ND	2.91	114.72	109.99
40	C	308	CLA	C2A-C1A-CHA	2.91	128.92	123.87
40	f	204	CLA	C3D-C4D-ND	2.91	114.72	109.99
40	q	312	CLA	C3D-C4D-ND	2.91	114.72	109.99
40	b	842	CLA	C3D-C4D-ND	2.91	114.71	109.99
40	R	310	CLA	C3D-C4D-ND	2.91	114.71	109.99
40	U	205	CLA	C3D-C4D-ND	2.91	114.71	109.99
40	F	305	CLA	CHB-C1B-NB	-2.91	119.69	124.05
40	o	312	CLA	C3D-C4D-ND	2.91	114.71	109.99
40	H	308	CLA	C3D-C4D-ND	2.90	114.71	109.99
40	S	306	CLA	C3D-C4D-ND	2.90	114.71	109.99
40	Y	305	CLA	C3D-C4D-ND	2.90	114.71	109.99
40	j	102	CLA	C3D-C4D-ND	2.90	114.71	109.99
40	o	301	CLA	C3D-C4D-ND	2.90	114.71	109.99
40	v	304	CLA	C3D-C4D-ND	2.90	114.71	109.99
40	S	301	CLA	C3D-C4D-ND	2.90	114.70	109.99
44	u	318	A86	C21-C20-C19	-2.90	110.98	114.24
41	q	302	KC2	C1D-ND-C4D	2.90	108.35	106.31
40	b	833	CLA	C3D-C4D-ND	2.90	114.70	109.99
40	A	302	CLA	C1-C2-C3	2.90	130.95	126.20
40	b	831	CLA	C3D-C4D-ND	2.90	114.70	109.99
40	a	820	CLA	C1-C2-C3	-2.90	121.45	126.20
40	a	832	CLA	CHD-C1D-ND	-2.90	120.73	124.80
40	U	204	CLA	C3D-C4D-ND	2.90	114.69	109.99
40	H	304	CLA	C3D-C4D-ND	2.90	114.69	109.99
40	q	310	CLA	C3D-C4D-ND	2.90	114.69	109.99
40	p	307	CLA	C3D-C4D-ND	2.89	114.69	109.99
40	B	306	CLA	C3D-C4D-ND	2.89	114.69	109.99
40	N	306	CLA	C3D-C4D-ND	2.89	114.69	109.99
40	y	309	CLA	C3D-C4D-ND	2.89	114.69	109.99
40	L	311	CLA	C3D-C4D-ND	2.89	114.69	109.99
40	X	301	CLA	C3D-C4D-ND	2.89	114.69	109.99
40	a	825	CLA	CHD-C1D-ND	-2.89	120.74	124.80
40	q	311	CLA	C3D-C4D-ND	2.89	114.68	109.99
40	O	310	CLA	C3D-C4D-ND	2.89	114.68	109.99
40	F	303	CLA	C2C-C1C-CHC	-2.89	119.64	127.21
40	P	305	CLA	CHD-C1D-ND	-2.88	120.74	124.80
42	D	317	DD6	C30-C29-C27	-2.88	166.43	176.23
42	v	318	DD6	C14-C13-C11	2.88	130.00	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	E	304	CLA	C3D-C4D-ND	2.88	114.67	109.99
44	p	316	A86	O1-C20-C19	2.88	116.19	113.49
40	J	305	CLA	C3D-C4D-ND	2.88	114.67	109.99
40	J	308	CLA	C3D-C4D-ND	2.88	114.67	109.99
40	b	825	CLA	C3D-C4D-ND	2.88	114.67	109.99
40	D	310	CLA	C3D-C4D-ND	2.88	114.67	109.99
40	L	304	CLA	C3D-C4D-ND	2.88	114.66	109.99
40	L	305	CLA	C3D-C4D-ND	2.88	114.66	109.99
40	b	827	CLA	C3D-C4D-ND	2.88	114.66	109.99
40	a	803	CLA	CHB-C1B-NB	-2.88	119.73	124.05
40	o	310	CLA	C4D-CHA-C1A	-2.88	117.81	121.24
40	K	312	CLA	C3D-C4D-ND	2.87	114.66	109.99
40	J	309	CLA	C3D-C4D-ND	2.87	114.66	109.99
42	N	317	DD6	O1-C15-C14	-2.87	108.65	116.88
40	L	306	CLA	C3D-C4D-ND	2.87	114.65	109.99
40	G	205	CLA	C3D-C4D-ND	2.87	114.65	109.99
40	a	823	CLA	C3D-C4D-ND	2.87	114.65	109.99
43	F	318	LMG	O6-C1-O1	-2.87	103.26	110.04
44	y	310	A86	C36-C31-C32	-2.87	116.85	119.70
40	K	301	CLA	C3D-C4D-ND	2.87	114.65	109.99
40	H	306	CLA	C3D-C4D-ND	2.87	114.65	109.99
40	a	840	CLA	C3D-C4D-ND	2.87	114.65	109.99
40	b	801	CLA	C3D-C4D-ND	2.86	114.64	109.99
40	Q	204	CLA	C2C-C1C-CHC	-2.86	119.70	127.21
40	u	306	CLA	C3D-C4D-ND	2.86	114.64	109.99
40	A	301	CLA	C3D-C4D-ND	2.86	114.63	109.99
40	E	313	CLA	C3D-C4D-ND	2.86	114.63	109.99
40	o	305	CLA	C3D-C4D-ND	2.86	114.63	109.99
44	o	317	A86	O1-C20-C19	2.86	116.17	113.49
40	Q	204	CLA	C3D-C4D-ND	2.85	114.63	109.99
40	Z	310	CLA	C3A-C2A-C1A	-2.85	97.06	101.34
40	b	822	CLA	CHB-C1B-NB	-2.85	119.77	124.05
44	P	316	A86	C36-C31-C32	-2.85	116.86	119.70
40	a	832	CLA	C3D-C4D-ND	2.85	114.62	109.99
40	b	806	CLA	C3D-C4D-ND	2.85	114.62	109.99
40	b	833	CLA	CHB-C1B-NB	-2.85	119.77	124.05
40	v	311	CLA	C3D-C4D-ND	2.85	114.61	109.99
45	a	848	LHG	O8-C23-C24	2.85	120.52	111.83
40	H	309	CLA	C3D-C4D-ND	2.85	114.61	109.99
40	a	812	CLA	C3D-C4D-ND	2.85	114.61	109.99
40	p	313	CLA	CHD-C1D-ND	-2.85	120.80	124.80
40	S	312	CLA	C3D-C4D-ND	2.85	114.61	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	a	836	CLA	C3D-C4D-ND	2.84	114.61	109.99
43	M	317	LMG	O6-C1-O1	-2.84	103.32	110.04
40	F	303	CLA	C3D-C4D-ND	2.84	114.61	109.99
40	Q	203	CLA	C2C-C1C-CHC	-2.84	119.75	127.21
40	u	312	CLA	C3D-C4D-ND	2.84	114.61	109.99
40	w	308	CLA	C3D-C4D-ND	2.84	114.61	109.99
47	y	313	A1EB1	C36-C31-C32	-2.84	116.88	119.70
40	D	303	CLA	C3D-C4D-ND	2.84	114.61	109.99
40	x	306	CLA	C3D-C4D-ND	2.84	114.61	109.99
44	X	321	A86	O1-C20-C19	-2.84	110.83	113.49
40	I	204	CLA	C3D-C4D-ND	2.84	114.60	109.99
42	A	314	DD6	C14-C13-C11	2.84	129.93	125.53
40	C	308	CLA	CHA-C1A-NA	-2.84	119.97	126.39
40	b	813	CLA	CHB-C1B-NB	-2.84	119.80	124.05
44	w	315	A86	O1-C20-C19	2.83	116.15	113.49
40	H	307	CLA	C6-C7-C8	2.83	125.39	115.97
40	E	314	CLA	C3D-C4D-ND	2.83	114.59	109.99
40	X	304	CLA	C3D-C4D-ND	2.83	114.59	109.99
40	I	205	CLA	C3D-C4D-ND	2.83	114.59	109.99
40	G	201	CLA	C3D-C4D-ND	2.83	114.59	109.99
40	b	825	CLA	CHD-C1D-ND	-2.83	120.82	124.80
40	E	307	CLA	C3D-C4D-ND	2.83	114.59	109.99
44	F	313	A86	C36-C31-C32	-2.83	116.89	119.70
40	Q	205	CLA	C2C-C1C-CHC	-2.83	119.79	127.21
40	p	302	CLA	C1-C2-C3	-2.83	121.56	126.20
43	u	301	LMG	C1-C2-C3	-2.83	104.06	110.01
40	p	312	CLA	C3D-C4D-ND	2.83	114.58	109.99
40	b	832	CLA	C3D-C4D-ND	2.83	114.58	109.99
40	a	842	CLA	C3D-C4D-ND	2.83	114.58	109.99
41	T	303	KC2	C4B-C3B-C2B	2.82	109.26	106.81
40	p	306	CLA	C3D-C4D-ND	2.82	114.58	109.99
40	o	310	CLA	CAA-C2A-C1A	-2.82	102.73	111.97
48	P	320	A1EB4	C36-C31-C32	2.82	122.49	119.70
40	H	309	CLA	CHA-C1A-NA	-2.81	120.02	126.39
42	k	204	DD6	C14-C13-C11	2.81	129.89	125.53
40	J	302	CLA	C3D-C4D-ND	2.81	114.56	109.99
42	F	314	DD6	O1-C20-C19	-2.81	110.86	113.49
46	P	319	SQD	C45-O47-C7	-2.81	111.07	117.80
40	b	813	CLA	C3D-C4D-ND	2.81	114.55	109.99
40	S	305	CLA	C3D-C4D-ND	2.81	114.55	109.99
40	V	202	CLA	CHC-C1C-C2C	-2.81	118.97	126.95
40	P	307	CLA	CMC-C2C-C1C	2.81	129.42	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	F	310	CLA	CHA-C1A-NA	-2.81	120.04	126.39
40	K	306	CLA	CAA-C2A-C3A	2.81	120.58	113.00
40	x	307	CLA	C3A-C2A-C1A	-2.80	97.14	101.34
46	M	318	SQD	O48-C23-C24	2.80	120.38	111.83
40	S	305	CLA	CAA-C2A-C1A	-2.80	102.80	111.97
46	P	319	SQD	O48-C23-C24	2.80	120.37	111.83
40	a	826	CLA	CHB-C1B-NB	-2.80	119.85	124.05
42	J	315	DD6	O1-C20-C19	-2.80	110.87	113.49
40	C	304	CLA	C3D-C4D-ND	2.80	114.53	109.99
40	a	826	CLA	C3D-C4D-ND	2.80	114.53	109.99
40	T	305	CLA	C3D-C4D-ND	2.80	114.53	109.99
40	S	313	CLA	C3D-C4D-ND	2.79	114.52	109.99
40	S	302	CLA	C3D-C4D-ND	2.79	114.52	109.99
40	b	816	CLA	C3D-C4D-ND	2.79	114.52	109.99
42	H	313	DD6	O1-C20-C19	-2.78	110.88	113.49
42	T	314	DD6	C14-C13-C11	2.78	129.85	125.53
40	S	312	CLA	C3A-C2A-C1A	-2.78	97.17	101.34
40	Z	304	CLA	C3D-C4D-ND	2.78	114.51	109.99
46	k	205	SQD	O48-C23-C24	2.78	120.31	111.83
40	P	311	CLA	C3D-C4D-ND	2.78	114.51	109.99
40	l	205	CLA	C3D-C4D-ND	2.78	114.51	109.99
40	a	811	CLA	C3D-C4D-ND	2.78	114.50	109.99
40	k	202	CLA	C3D-C4D-ND	2.77	114.50	109.99
40	W	307	CLA	C3D-C4D-ND	2.77	114.50	109.99
40	b	812	CLA	C3D-C4D-ND	2.77	114.50	109.99
40	p	313	CLA	C3D-C4D-ND	2.77	114.49	109.99
40	M	310	CLA	C3D-C4D-ND	2.77	114.49	109.99
40	Y	304	CLA	C3D-C4D-ND	2.77	114.48	109.99
44	S	316	A86	O4-C34-C33	-2.76	100.56	107.64
43	M	317	LMG	O2-C2-C1	-2.76	103.49	110.08
40	A	311	CLA	CHB-C1B-NB	-2.76	119.91	124.05
40	v	301	CLA	C3D-C4D-ND	2.76	114.48	109.99
45	S	323	LHG	O8-C23-C24	2.76	120.25	111.83
40	D	306	CLA	C3D-C4D-ND	2.76	114.47	109.99
40	f	202	CLA	C3D-C4D-ND	2.76	114.47	109.99
40	F	321	CLA	C3D-C4D-ND	2.76	114.47	109.99
40	P	306	CLA	C3D-C4D-ND	2.75	114.46	109.99
40	Y	312	CLA	C2A-C3A-C4A	-2.75	97.42	101.87
40	a	842	CLA	CHB-C1B-NB	-2.75	119.92	124.05
43	T	318	LMG	C7-O1-C1	2.75	119.69	113.80
42	W	315	DD6	C14-C13-C11	2.75	129.79	125.53
40	a	825	CLA	CHB-C1B-NB	-2.75	119.93	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	E	316	DD6	O1-C20-C19	-2.75	110.92	113.49
40	R	304	CLA	CAA-C2A-C3A	2.75	120.42	113.00
46	F	320	SQD	O48-C23-C24	2.75	120.21	111.83
40	f	201	CLA	C3D-C4D-ND	2.75	114.45	109.99
40	b	835	CLA	C3D-C4D-ND	2.75	114.45	109.99
41	Y	308	KC2	CHD-C1D-ND	-2.75	119.93	124.05
42	O	314	DD6	C14-C13-C11	2.74	129.79	125.53
40	U	206	CLA	C3D-C4D-ND	2.74	114.45	109.99
49	b	844	BCR	C7-C8-C9	2.74	130.29	126.23
40	z	312	CLA	C3D-C4D-ND	2.74	114.45	109.99
40	a	826	CLA	C1-C2-C3	-2.74	121.70	126.20
40	z	314	CLA	C3A-C2A-C1A	-2.74	97.23	101.34
42	z	322	DD6	C21-C20-C19	2.74	117.32	114.24
42	J	315	DD6	C14-C13-C11	2.74	129.78	125.53
40	p	314	CLA	C3A-C2A-C1A	-2.74	97.23	101.34
40	X	311	CLA	C3D-C4D-ND	2.74	114.44	109.99
40	b	829	CLA	C3D-C4D-ND	2.74	114.44	109.99
40	Q	206	CLA	C2C-C1C-CHC	-2.74	120.03	127.21
42	W	315	DD6	O1-C20-C15	-2.73	56.76	58.93
40	D	302	CLA	C1-C2-C3	2.73	130.67	126.20
40	B	302	CLA	CHB-C1B-NB	-2.73	119.95	124.05
40	S	301	CLA	CHB-C1B-NB	-2.73	119.95	124.05
47	Y	323	A1EB1	C29-C30-C31	-2.73	174.44	177.66
41	Y	303	KC2	CHD-C1D-ND	-2.73	119.95	124.05
40	J	312	CLA	C3D-C4D-ND	2.73	114.42	109.99
40	I	203	CLA	CHB-C1B-NB	-2.73	119.95	124.05
42	E	315	DD6	C21-C20-C19	2.73	117.30	114.24
44	Y	321	A86	O1-C20-C19	-2.73	110.94	113.49
40	x	312	CLA	C3D-C4D-ND	2.72	114.42	109.99
40	X	310	CLA	C3A-C2A-C1A	-2.72	97.26	101.34
40	a	813	CLA	C3D-C4D-ND	2.72	114.41	109.99
40	G	206	CLA	C3D-C4D-ND	2.72	114.41	109.99
40	t	309	CLA	CHB-C1B-NB	-2.72	119.97	124.05
40	S	305	CLA	C3A-C2A-C1A	-2.72	97.26	101.34
42	j	104	DD6	C14-C13-C11	2.72	129.75	125.53
42	G	210	DD6	O1-C20-C15	-2.72	56.78	58.93
40	D	311	CLA	CAA-C2A-C1A	-2.71	103.08	111.97
40	p	307	CLA	C3A-C2A-C1A	-2.71	97.27	101.34
43	E	320	LMG	O6-C1-O1	-2.71	103.63	110.04
44	o	317	A86	C36-C31-C32	-2.71	117.01	119.70
42	G	210	DD6	C14-C13-C11	2.71	129.74	125.53
40	a	803	CLA	C4D-CHA-C1A	-2.71	118.01	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	W	312	CLA	CHD-C1D-ND	-2.71	120.99	124.80
44	x	316	A86	C21-C20-C19	-2.71	111.20	114.24
40	a	839	CLA	CHB-C1B-NB	-2.70	119.99	124.05
40	T	310	CLA	C3D-C4D-ND	2.70	114.38	109.99
40	a	825	CLA	C3D-C4D-ND	2.70	114.38	109.99
40	a	836	CLA	C6-C7-C8	2.70	124.94	115.97
40	p	314	CLA	C3D-C4D-ND	2.70	114.37	109.99
40	C	304	CLA	CHC-C4B-NB	-2.70	120.00	124.05
44	R	315	A86	O1-C20-C19	-2.70	110.96	113.49
40	u	313	CLA	C3D-C4D-ND	2.70	114.37	109.99
40	K	312	CLA	CHB-C1B-NB	-2.70	120.00	124.05
40	o	313	CLA	CHC-C4B-NB	-2.70	120.00	124.05
40	A	302	CLA	C3D-C4D-ND	2.69	114.37	109.99
40	a	804	CLA	C1-C2-C3	-2.69	121.78	126.20
47	u	322	A1EB1	C36-C31-C32	2.69	122.37	119.70
47	t	315	A1EB1	C33-C32-C31	-2.69	106.60	109.21
41	O	302	KC2	C2A-C3A-C4A	2.69	108.43	106.41
40	b	837	CLA	CHB-C1B-NB	-2.69	120.02	124.05
47	t	313	A1EB1	C33-C32-C31	-2.69	106.60	109.21
40	z	307	CLA	CMC-C2C-C1C	2.69	129.23	125.03
40	p	307	CLA	CHA-C1A-NA	-2.69	120.31	126.39
42	t	312	DD6	O1-C20-C19	-2.69	110.97	113.49
44	X	314	A86	C33-C32-C31	-2.68	106.60	109.21
40	a	850	CLA	CHC-C4B-NB	-2.68	120.03	124.05
52	b	850	DGD	CAB-C9B-C8B	-2.68	100.83	114.37
42	Z	318	DD6	O1-C20-C19	-2.68	110.98	113.49
40	b	821	CLA	C3D-C4D-ND	2.67	114.33	109.99
40	A	301	CLA	CHB-C1B-NB	-2.67	120.04	124.05
40	y	308	CLA	CHB-C1B-NB	-2.67	120.04	124.05
40	O	306	CLA	CMC-C2C-C1C	2.67	129.21	125.03
40	b	810	CLA	C3D-C4D-ND	2.67	114.33	109.99
41	Q	201	KC2	CHD-C4C-NC	2.67	128.33	124.31
40	b	824	CLA	CHB-C1B-NB	-2.67	120.05	124.05
40	b	828	CLA	CHB-C1B-NB	-2.67	120.05	124.05
40	J	303	CLA	C3D-C4D-ND	2.67	114.32	109.99
40	j	102	CLA	CAA-C2A-C1A	-2.67	103.23	111.97
40	D	306	CLA	C1-C2-C3	2.67	130.57	126.20
40	x	307	CLA	CHA-C1A-NA	-2.67	120.35	126.39
40	a	804	CLA	C2C-C1C-CHC	-2.67	120.22	127.21
44	Y	316	A86	C21-C20-C19	-2.66	111.25	114.24
40	H	307	CLA	CBA-CAA-C2A	2.66	121.72	113.79
42	K	310	DD6	C14-C13-C11	2.66	129.65	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	P	311	CLA	CHB-C1B-NB	-2.65	120.07	124.05
40	x	313	CLA	C3D-C4D-ND	2.65	114.30	109.99
40	z	302	CLA	CHB-C1B-NB	-2.65	120.07	124.05
40	Z	305	CLA	C3D-C4D-ND	2.65	114.29	109.99
44	M	316	A86	C36-C31-C32	2.65	122.32	119.70
44	U	210	A86	O1-C20-C19	2.65	115.97	113.49
41	S	309	KC2	CHD-C1D-ND	-2.65	120.08	124.05
40	a	811	CLA	C2C-C1C-CHC	-2.65	120.27	127.21
40	U	203	CLA	CHB-C1B-NB	-2.65	120.08	124.05
40	Q	202	CLA	C3D-C4D-ND	2.65	114.29	109.99
40	v	311	CLA	CHB-C1B-NB	-2.65	120.08	124.05
47	u	322	A1EB1	O1-C20-C19	-2.65	111.01	113.49
40	F	307	CLA	CMC-C2C-C1C	2.64	129.17	125.03
41	x	315	KC2	CHB-C4A-NA	2.64	128.33	124.23
40	o	306	CLA	CMC-C2C-C1C	2.64	129.16	125.03
42	F	314	DD6	C14-C13-C11	2.64	129.63	125.53
43	j	101	LMG	O6-C1-O1	-2.64	103.80	110.04
40	R	310	CLA	CHB-C1B-NB	-2.64	120.09	124.05
40	T	317	CLA	C3D-C4D-ND	2.64	114.28	109.99
44	M	315	A86	C36-C31-C32	-2.64	117.08	119.70
46	k	205	SQD	C45-O47-C7	-2.64	111.48	117.80
40	S	305	CLA	C2A-C3A-C4A	-2.64	97.61	101.87
40	S	319	CLA	C3D-C4D-ND	2.64	114.27	109.99
42	C	312	DD6	O1-C15-C14	-2.64	109.32	116.88
44	Y	317	A86	C33-C32-C31	2.64	111.77	109.21
40	b	801	CLA	CAA-C2A-C1A	-2.63	103.35	111.97
40	l	204	CLA	C3D-C4D-ND	2.63	114.27	109.99
40	a	809	CLA	C3D-C4D-ND	2.63	114.26	109.99
40	b	808	CLA	CHB-C1B-NB	-2.62	120.11	124.05
40	T	306	CLA	CMC-C2C-C1C	2.62	129.13	125.03
41	x	309	KC2	CHB-C4A-NA	2.62	128.30	124.23
44	N	314	A86	O1-C20-C19	2.62	115.95	113.49
40	u	311	CLA	C4D-CHA-C1A	-2.62	118.12	121.24
40	A	311	CLA	C3D-C4D-ND	2.62	114.25	109.99
41	z	304	KC2	CHD-C1D-ND	-2.62	120.12	124.05
40	J	318	CLA	CHB-C1B-NB	-2.62	120.12	124.05
44	Y	318	A86	O1-C20-C19	-2.62	111.04	113.49
40	Q	207	CLA	CHC-C4B-NB	-2.62	120.13	124.05
40	a	850	CLA	CHB-C1B-NB	-2.61	120.13	124.05
48	M	319	A1EB4	C33-C32-C31	2.61	111.75	109.21
41	v	302	KC2	CHD-C4C-NC	2.61	128.24	124.31
40	b	821	CLA	CMA-C3A-C4A	2.61	118.78	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	G	213	CLA	CHB-C1B-NB	-2.61	120.14	124.05
40	b	808	CLA	C3D-C4D-ND	2.61	114.22	109.99
40	w	304	CLA	CBA-CAA-C2A	2.61	121.54	113.79
40	b	841	CLA	C3D-C4D-ND	2.60	114.22	109.99
43	S	322	LMG	O1-C1-C2	-2.60	104.32	108.27
40	W	311	CLA	CHB-C1B-NB	-2.60	120.15	124.05
40	u	313	CLA	CHB-C1B-NB	-2.60	120.15	124.05
40	p	311	CLA	C4D-CHA-C1A	-2.60	118.14	121.24
40	o	307	CLA	CHC-C4B-NB	-2.60	120.15	124.05
40	P	313	CLA	CHB-C1B-NB	-2.60	120.15	124.05
41	p	315	KC2	C2A-C3A-C4A	2.60	108.36	106.41
41	q	302	KC2	CHD-C1D-ND	-2.60	120.15	124.05
40	y	304	CLA	CBA-CAA-C2A	2.60	121.52	113.79
41	H	316	KC2	CHB-C4A-NA	2.60	128.26	124.23
40	Q	203	CLA	CHB-C1B-NB	-2.60	120.15	124.05
40	b	831	CLA	CHB-C1B-NB	-2.60	120.16	124.05
47	p	323	A1EB1	O1-C20-C19	-2.59	111.06	113.49
40	Y	313	CLA	C3A-C2A-C1A	-2.59	97.45	101.34
42	H	314	DD6	C21-C20-C19	2.59	117.15	114.24
43	A	317	LMG	O6-C1-O1	-2.59	103.92	110.04
40	E	314	CLA	CHA-C1A-NA	-2.59	120.53	126.39
40	J	308	CLA	CBA-CAA-C2A	2.59	121.49	113.79
40	Z	312	CLA	CBA-CAA-C2A	2.59	121.49	113.79
40	b	809	CLA	C4D-CHA-C1A	-2.59	118.16	121.24
44	T	313	A86	O1-C20-C19	2.59	115.91	113.49
44	Y	320	A86	C33-C32-C31	2.58	111.72	109.21
41	Y	308	KC2	CHD-C4C-NC	2.58	128.20	124.31
40	u	307	CLA	CHA-C1A-NA	-2.58	120.54	126.39
40	z	307	CLA	C1-C2-C3	2.58	130.43	126.20
42	K	311	DD6	O1-C20-C15	-2.58	56.88	58.93
47	v	321	A1EB1	C33-C32-C31	-2.58	106.70	109.21
40	K	307	CLA	CHA-C1A-NA	-2.58	120.55	126.39
40	X	311	CLA	CHA-C1A-NA	-2.58	120.55	126.39
43	a	801	LMG	O6-C1-O1	-2.58	103.95	110.04
44	y	310	A86	C33-C32-C31	2.58	111.72	109.21
41	Y	314	KC2	CHD-C1D-ND	-2.58	120.18	124.05
40	C	308	CLA	C3A-C2A-C1A	-2.58	97.48	101.34
40	J	309	CLA	CHB-C1B-NB	-2.58	120.18	124.05
50	b	849	PQN	C11-C3-C4	-2.58	115.87	118.58
40	a	830	CLA	CHB-C1B-NB	-2.58	120.19	124.05
42	E	316	DD6	C21-C20-C19	2.57	117.13	114.24
40	f	205	CLA	CHA-C1A-NA	-2.57	120.56	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	p	313	CLA	CHB-C1B-NB	-2.57	120.19	124.05
41	Z	303	KC2	CHD-C1D-ND	-2.57	120.19	124.05
41	z	304	KC2	CHD-C4C-NC	2.57	128.19	124.31
40	D	304	CLA	CMC-C2C-C1C	2.57	129.06	125.03
42	D	317	DD6	C14-C13-C11	2.57	129.52	125.53
40	B	302	CLA	C3D-C4D-ND	2.57	114.17	109.99
42	H	313	DD6	C15-C14-C13	2.57	131.43	125.99
47	u	322	A1EB1	O4-C34-C33	2.57	114.21	107.64
41	Q	201	KC2	CHD-C1D-ND	-2.57	120.20	124.05
41	R	309	KC2	C2A-C3A-C4A	2.57	108.34	106.41
40	a	809	CLA	CHB-C1B-NB	-2.57	120.20	124.05
43	W	317	LMG	O2-C2-C1	-2.57	103.96	110.08
40	y	309	CLA	CHA-C1A-NA	-2.57	120.58	126.39
40	a	803	CLA	C3D-C4D-ND	2.57	114.16	109.99
40	W	308	CLA	C1-C2-C3	-2.57	121.99	126.20
40	D	311	CLA	CHB-C1B-NB	-2.57	120.20	124.05
42	H	314	DD6	O1-C20-C19	-2.57	111.09	113.49
40	a	811	CLA	CHB-C1B-NB	-2.56	120.20	124.05
41	o	308	KC2	CHD-C1D-ND	-2.56	120.20	124.05
40	O	316	CLA	C3D-C4D-ND	2.56	114.15	109.99
40	q	310	CLA	C3A-C2A-C1A	-2.56	97.50	101.34
42	k	204	DD6	C23-C16-C15	2.56	116.97	110.05
40	A	304	CLA	CAA-C2A-C1A	-2.56	103.58	111.97
40	N	311	CLA	CAA-C2A-C1A	-2.56	103.58	111.97
40	X	310	CLA	CHD-C1D-C2D	2.56	130.82	125.49
44	K	314	A86	C33-C32-C31	2.56	111.70	109.21
40	I	204	CLA	CHB-C1B-NB	-2.56	120.21	124.05
41	G	202	KC2	C2A-C3A-C4A	2.56	108.33	106.41
40	C	308	CLA	CHB-C1B-NB	-2.56	120.21	124.05
40	b	832	CLA	CHB-C1B-NB	-2.56	120.21	124.05
40	J	311	CLA	CHB-C1B-NB	-2.56	120.21	124.05
43	F	318	LMG	O1-C1-C2	-2.56	104.39	108.27
40	a	805	CLA	CHB-C1B-NB	-2.56	120.22	124.05
40	y	303	CLA	CHA-C1A-NA	-2.55	120.61	126.39
40	U	208	CLA	C3D-C4D-ND	2.55	114.13	109.99
40	O	304	CLA	CBA-CAA-C2A	2.55	121.38	113.79
40	A	302	CLA	CHB-C1B-NB	-2.55	120.22	124.05
42	J	317	DD6	C14-C13-C11	2.55	129.49	125.53
44	X	320	A86	C33-C32-C31	2.55	111.69	109.21
40	O	310	CLA	C4D-CHA-C1A	-2.55	118.20	121.24
41	p	309	KC2	CHB-C4A-NA	2.55	128.18	124.23
41	X	302	KC2	CHD-C1D-ND	-2.55	120.23	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	H	315	A86	C33-C32-C31	2.55	111.69	109.21
40	L	312	CLA	C3D-C4D-ND	2.55	114.12	109.99
40	v	312	CLA	CHB-C1B-NB	-2.54	120.23	124.05
41	I	209	KC2	CHD-C1D-ND	-2.54	120.23	124.05
41	p	303	KC2	CHD-C4C-NC	2.54	128.14	124.31
40	b	810	CLA	CHB-C1B-NB	-2.54	120.24	124.05
40	K	307	CLA	C3D-C4D-ND	2.54	114.11	109.99
40	W	312	CLA	CAC-C3C-C4C	2.54	128.09	124.79
44	D	320	A86	O1-C20-C19	2.54	115.87	113.49
41	N	303	KC2	CHD-C1D-ND	-2.54	120.24	124.05
40	R	305	CLA	CHB-C1B-NB	-2.54	120.24	124.05
40	N	310	CLA	CHB-C1B-NB	-2.54	120.25	124.05
41	J	304	KC2	CHD-C1D-ND	-2.54	120.25	124.05
41	W	304	KC2	CHD-C1D-ND	-2.54	120.25	124.05
40	b	825	CLA	CHB-C1B-NB	-2.54	120.25	124.05
40	l	203	CLA	CHB-C1B-NB	-2.54	120.25	124.05
40	p	314	CLA	CHB-C1B-NB	-2.53	120.25	124.05
40	Q	208	CLA	CHB-C1B-NB	-2.53	120.25	124.05
40	Z	310	CLA	C4D-CHA-C1A	-2.53	118.22	121.24
44	F	313	A86	C21-C20-C19	-2.53	111.40	114.24
40	a	808	CLA	CHB-C1B-NB	-2.53	120.25	124.05
41	u	315	KC2	CHB-C4A-NA	2.53	128.15	124.23
40	z	308	CLA	CHC-C4B-NB	-2.53	120.26	124.05
40	E	313	CLA	CHB-C1B-NB	-2.53	120.26	124.05
40	u	312	CLA	CHB-C1B-NB	-2.53	120.26	124.05
40	a	824	CLA	C3D-C4D-ND	2.53	114.09	109.99
40	G	203	CLA	CHB-C1B-NB	-2.53	120.43	124.08
40	G	203	CLA	CAA-C2A-C1A	-2.53	103.70	111.97
44	M	313	A86	C36-C31-C32	-2.53	117.19	119.70
40	u	314	CLA	CHB-C1B-NB	-2.53	120.26	124.05
40	H	301	CLA	CHB-C1B-NB	-2.52	120.27	124.05
40	I	205	CLA	CHB-C1B-NB	-2.52	120.27	124.05
41	v	308	KC2	CHB-C4A-NA	2.52	128.14	124.23
41	Y	314	KC2	CHD-C4C-NC	2.52	128.11	124.31
40	S	313	CLA	CHB-C1B-NB	-2.52	120.27	124.05
41	P	302	KC2	CHD-C1D-ND	-2.52	120.27	124.05
40	t	302	CLA	CHB-C1B-NB	-2.52	120.27	124.05
49	l	207	BCR	C8-C9-C10	2.52	122.97	119.01
40	H	305	CLA	C3D-C4D-ND	2.52	114.08	109.99
40	W	312	CLA	C3D-C4D-ND	2.52	114.08	109.99
40	a	804	CLA	CHB-C1B-NB	-2.52	120.27	124.05
40	Q	206	CLA	C3D-C4D-ND	2.52	114.08	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	j	102	CLA	C3A-C2A-C1A	-2.51	97.57	101.34
42	I	210	DD6	O1-C15-C14	-2.51	109.67	116.88
46	W	318	SQD	O48-C23-C24	2.51	119.50	111.83
40	H	305	CLA	CHB-C1B-NB	-2.51	120.28	124.05
40	Y	305	CLA	CHB-C1B-NB	-2.51	120.28	124.05
43	P	318	LMG	C1-C2-C3	-2.51	104.72	110.01
40	B	304	CLA	C3D-C4D-ND	2.51	114.07	109.99
40	b	835	CLA	CHB-C1B-NB	-2.51	120.45	124.08
40	q	304	CLA	CHB-C1B-NB	-2.51	120.28	124.05
40	q	313	CLA	CHB-C1B-NB	-2.51	120.28	124.05
41	M	308	KC2	CHD-C1D-ND	-2.51	120.28	124.05
40	W	308	CLA	C3A-C2A-C1A	-2.51	97.58	101.34
43	W	317	LMG	O3-C3-C2	-2.51	104.46	110.38
40	S	305	CLA	C4D-CHA-C1A	-2.51	118.25	121.24
40	J	308	CLA	CHB-C1B-NB	-2.51	120.28	124.05
40	M	304	CLA	CHB-C1B-NB	-2.51	120.28	124.05
40	x	314	CLA	CHB-C1B-NB	-2.51	120.29	124.05
40	a	821	CLA	CHB-C1B-NB	-2.51	120.29	124.05
41	z	309	KC2	CHD-C1D-ND	-2.51	120.29	124.05
40	L	312	CLA	CHB-C1B-NB	-2.50	120.29	124.05
40	q	305	CLA	CHB-C1B-NB	-2.50	120.29	124.05
41	Y	302	KC2	CHD-C1D-ND	-2.50	120.29	124.05
41	Z	308	KC2	CHD-C1D-ND	-2.50	120.29	124.05
40	Q	205	CLA	CHB-C1B-NB	-2.50	120.29	124.05
40	T	310	CLA	CHB-C1B-NB	-2.50	120.29	124.05
40	q	306	CLA	CHB-C1B-NB	-2.50	120.29	124.05
41	G	202	KC2	CHD-C1D-ND	-2.50	120.29	124.05
40	a	819	CLA	CAA-C2A-C3A	2.50	119.76	113.00
43	M	317	LMG	O3-C3-C2	-2.50	104.48	110.38
40	p	311	CLA	CHB-C1B-NB	-2.50	120.30	124.05
41	t	301	KC2	CHD-C1D-ND	-2.50	120.30	124.05
40	a	813	CLA	CHB-C1B-NB	-2.50	120.30	124.05
40	F	306	CLA	CHB-C1B-NB	-2.50	120.31	124.05
40	U	205	CLA	CHB-C1B-NB	-2.49	120.31	124.05
40	A	307	CLA	CMC-C2C-C1C	2.49	128.93	125.03
40	b	830	CLA	CHB-C1B-NB	-2.49	120.31	124.05
41	z	310	KC2	CHD-C1D-ND	-2.49	120.31	124.05
43	L	319	LMG	O6-C1-O1	-2.49	104.15	110.04
41	P	303	KC2	CHD-C1D-ND	-2.49	120.31	124.05
40	b	824	CLA	CAA-C2A-C1A	-2.49	103.81	111.97
40	b	801	CLA	CHB-C1B-NB	-2.49	120.31	124.05
40	x	305	CLA	CHB-C1B-NB	-2.49	120.31	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	b	807	CLA	CHA-C1A-NA	-2.49	120.75	126.39
40	H	304	CLA	CHB-C1B-NB	-2.49	120.31	124.05
41	p	310	KC2	CHD-C1D-ND	-2.49	120.31	124.05
40	b	801	CLA	CMC-C2C-C1C	2.49	128.93	125.03
40	T	305	CLA	CHB-C1B-NB	-2.49	120.31	124.05
43	T	318	LMG	C1-C2-C3	-2.49	104.77	110.01
41	w	306	KC2	CHD-C1D-ND	-2.49	120.31	124.05
44	t	310	A86	C33-C32-C31	2.49	111.63	109.21
41	S	310	KC2	CHD-C1D-ND	-2.49	120.32	124.05
41	u	303	KC2	CHD-C4C-NC	2.49	128.06	124.31
40	w	309	CLA	CHA-C1A-NA	-2.49	120.76	126.39
40	J	310	CLA	CHA-C1A-NA	-2.49	120.76	126.39
40	Q	208	CLA	CHA-C1A-NA	-2.49	120.76	126.39
40	W	312	CLA	CHB-C1B-NB	-2.49	120.32	124.05
40	L	306	CLA	CHA-C1A-NA	-2.49	120.76	126.39
40	p	314	CLA	C4D-CHA-C1A	-2.49	118.28	121.24
41	X	303	KC2	CHD-C1D-ND	-2.49	120.32	124.05
41	p	303	KC2	CHD-C1D-ND	-2.49	120.32	124.05
41	F	309	KC2	CHD-C1D-ND	-2.48	120.32	124.05
40	M	311	CLA	CHB-C1B-NB	-2.48	120.32	124.05
40	v	304	CLA	CHB-C1B-NB	-2.48	120.33	124.05
40	C	307	CLA	CAA-C2A-C1A	-2.48	103.84	111.97
40	L	301	CLA	CHB-C1B-NB	-2.48	120.33	124.05
44	Y	317	A86	C21-C20-C19	-2.48	111.45	114.24
41	O	308	KC2	C2A-C3A-C4A	2.48	108.27	106.41
40	N	307	CLA	C1-C2-C3	-2.48	122.14	126.20
40	j	102	CLA	CHB-C1B-NB	-2.48	120.33	124.05
40	F	321	CLA	CHB-C1B-NB	-2.48	120.33	124.05
41	U	201	KC2	CHD-C1D-ND	-2.48	120.33	124.05
42	Y	322	DD6	O1-C20-C19	-2.48	111.17	113.49
40	v	305	CLA	CHB-C1B-NB	-2.48	120.33	124.05
40	T	306	CLA	CHB-C1B-NB	-2.48	120.33	124.05
40	p	308	CLA	CHB-C1B-NB	-2.48	120.34	124.05
41	W	303	KC2	CHD-C1D-ND	-2.48	120.34	124.05
40	C	308	CLA	C3D-C4D-ND	2.47	114.01	109.99
40	f	205	CLA	C3D-C4D-ND	2.47	114.01	109.99
40	L	310	CLA	C4D-CHA-C1A	-2.47	118.30	121.24
40	a	824	CLA	CHB-C1B-NB	-2.47	120.34	124.05
40	P	306	CLA	CHB-C1B-NB	-2.47	120.34	124.05
41	R	302	KC2	CHD-C1D-ND	-2.47	120.34	124.05
41	X	302	KC2	CHD-C4C-NC	2.47	128.03	124.31
40	p	305	CLA	CHB-C1B-NB	-2.47	120.34	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	H	316	KC2	CHD-C1D-ND	-2.47	120.34	124.05
40	b	836	CLA	CHB-C1B-NB	-2.47	120.35	124.05
41	y	301	KC2	CHD-C1D-ND	-2.47	120.35	124.05
40	t	304	CLA	CBA-CAA-C2A	2.47	121.14	113.79
40	b	811	CLA	CHB-C1B-NB	-2.47	120.35	124.05
41	F	302	KC2	CHD-C1D-ND	-2.47	120.35	124.05
40	Q	208	CLA	C3D-C4D-ND	2.47	114.00	109.99
40	H	307	CLA	CHB-C1B-NB	-2.47	120.35	124.05
40	X	312	CLA	CHB-C1B-NB	-2.47	120.35	124.05
43	S	322	LMG	O2-C2-C1	-2.46	104.20	110.08
40	Z	312	CLA	C4D-CHA-C1A	-2.46	118.31	121.24
40	R	316	CLA	CHB-C1B-NB	-2.46	120.35	124.05
41	M	301	KC2	CHD-C1D-ND	-2.46	120.35	124.05
41	u	310	KC2	CHD-C1D-ND	-2.46	120.35	124.05
40	R	304	CLA	CHB-C1B-NB	-2.46	120.36	124.05
40	S	302	CLA	CHB-C1B-NB	-2.46	120.36	124.05
44	v	314	A86	C33-C32-C31	2.46	111.60	109.21
41	L	303	KC2	CHD-C1D-ND	-2.46	120.36	124.05
40	a	841	CLA	C1-C2-C3	-2.46	122.17	126.20
40	t	307	CLA	CHA-C1A-NA	-2.46	120.82	126.39
40	E	302	CLA	CHB-C1B-NB	-2.46	120.36	124.05
40	R	304	CLA	CBA-CAA-C2A	2.46	121.11	113.79
41	L	302	KC2	CHD-C1D-ND	-2.46	120.36	124.05
42	X	322	DD6	O1-C20-C19	-2.46	111.19	113.49
40	t	304	CLA	CHB-C1B-NB	-2.46	120.36	124.05
41	P	309	KC2	CHD-C1D-ND	-2.46	120.36	124.05
40	F	306	CLA	C1-C2-C3	-2.46	122.17	126.20
40	a	827	CLA	CHB-C1B-NB	-2.46	120.36	124.05
40	J	307	CLA	C2A-C3A-C4A	-2.45	97.90	101.87
41	K	302	KC2	CHD-C1D-ND	-2.45	120.37	124.05
41	v	302	KC2	CHD-C1D-ND	-2.45	120.37	124.05
41	y	306	KC2	CHD-C1D-ND	-2.45	120.37	124.05
41	z	304	KC2	C4C-C3C-C2C	2.45	109.53	107.28
41	t	308	KC2	CHD-C1D-ND	-2.45	120.37	124.05
40	J	305	CLA	CHB-C1B-NB	-2.45	120.37	124.05
41	t	308	KC2	CHD-C4C-NC	2.45	128.00	124.31
40	a	812	CLA	CHB-C1B-NB	-2.45	120.37	124.05
40	S	312	CLA	C4D-CHA-C1A	-2.45	118.32	121.24
41	N	308	KC2	CHD-C1D-ND	-2.45	120.37	124.05
40	U	203	CLA	CHA-C1A-NA	-2.45	120.84	126.39
40	b	827	CLA	CHA-C1A-NA	-2.45	120.84	126.39
41	u	309	KC2	CHB-C4A-NA	2.45	128.03	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	J	307	CLA	CHB-C1B-NB	-2.45	120.37	124.05
40	K	306	CLA	CHB-C1B-NB	-2.45	120.38	124.05
41	M	302	KC2	CHD-C1D-ND	-2.45	120.38	124.05
41	W	309	KC2	C3A-C4A-NA	-2.45	107.42	110.45
40	B	301	CLA	CHB-C1B-NB	-2.45	120.38	124.05
40	U	206	CLA	CHB-C1B-NB	-2.45	120.38	124.05
40	x	306	CLA	CHB-C1B-NB	-2.45	120.38	124.05
40	Q	206	CLA	CHB-C1B-NB	-2.45	120.54	124.08
40	D	310	CLA	CHD-C1D-C2D	2.45	130.58	125.49
40	A	307	CLA	CHB-C1B-NB	-2.45	120.38	124.05
41	u	303	KC2	CHD-C1D-ND	-2.45	120.38	124.05
47	Y	323	A1EB1	C36-C31-C32	-2.45	117.27	119.70
40	P	312	CLA	CHB-C1B-NB	-2.45	120.38	124.05
40	o	304	CLA	CHB-C1B-NB	-2.45	120.38	124.05
40	b	841	CLA	C1-C2-C3	-2.45	122.19	126.20
41	S	310	KC2	CHD-C4C-NC	2.44	127.99	124.31
40	E	304	CLA	CHB-C1B-NB	-2.44	120.38	124.05
40	o	305	CLA	CHB-C1B-NB	-2.44	120.38	124.05
41	Z	302	KC2	CHD-C1D-ND	-2.44	120.38	124.05
40	B	304	CLA	CHB-C1B-NB	-2.44	120.38	124.05
40	L	311	CLA	CHB-C1B-NB	-2.44	120.39	124.05
40	v	313	CLA	CHB-C1B-NB	-2.44	120.39	124.05
40	v	311	CLA	C2C-C1C-NC	2.44	112.55	109.98
40	W	305	CLA	CHB-C1B-NB	-2.44	120.39	124.05
40	b	827	CLA	CHB-C1B-NB	-2.44	120.39	124.05
41	R	308	KC2	CHD-C1D-ND	-2.44	120.39	124.05
41	S	304	KC2	CHD-C1D-ND	-2.44	120.39	124.05
40	M	310	CLA	CHB-C1B-NB	-2.44	120.39	124.05
40	b	802	CLA	CHB-C1B-NB	-2.44	120.39	124.05
41	T	302	KC2	CHD-C1D-ND	-2.44	120.39	124.05
44	F	312	A86	O1-C20-C19	2.44	115.78	113.49
41	S	303	KC2	CHD-C4C-NC	2.44	127.99	124.31
40	z	311	CLA	C2A-C1A-CHA	2.44	128.10	123.87
40	N	306	CLA	CHB-C1B-NB	-2.44	120.39	124.05
40	q	307	CLA	CHC-C4B-NB	-2.44	120.39	124.05
40	b	816	CLA	CHB-C1B-NB	-2.44	120.40	124.05
40	J	303	CLA	CHA-C1A-NA	-2.43	120.88	126.39
44	W	301	A86	C33-C32-C31	2.43	111.58	109.21
40	U	204	CLA	CHB-C1B-NB	-2.43	120.40	124.05
41	O	308	KC2	CHD-C1D-ND	-2.43	120.40	124.05
41	q	309	KC2	CHD-C1D-ND	-2.43	120.40	124.05
41	t	306	KC2	CHD-C1D-ND	-2.43	120.40	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	w	307	KC2	CHD-C1D-ND	-2.43	120.40	124.05
41	S	309	KC2	CHD-C4C-NC	2.43	127.97	124.31
40	J	302	CLA	CHB-C1B-NB	-2.43	120.40	124.05
40	S	311	CLA	C3A-C2A-C1A	-2.43	97.70	101.34
41	N	303	KC2	C4C-C3C-C2C	2.43	109.52	107.28
43	p	301	LMG	O6-C1-O1	-2.43	104.30	110.04
40	D	306	CLA	CHB-C1B-NB	-2.43	120.40	124.05
40	R	316	CLA	C3D-C4D-ND	2.43	113.94	109.99
40	Q	204	CLA	CHB-C1B-NB	-2.43	120.40	124.05
40	Y	304	CLA	CHB-C1B-NB	-2.43	120.40	124.05
40	b	823	CLA	CHB-C1B-NB	-2.43	120.40	124.05
40	v	307	CLA	CHC-C4B-NB	-2.43	120.40	124.05
40	P	305	CLA	C1-C2-C3	-2.43	122.22	126.20
40	a	851	CLA	CHB-C1B-NB	-2.43	120.41	124.05
40	F	310	CLA	C3D-C4D-ND	2.43	113.94	109.99
40	Z	311	CLA	CHB-C1B-NB	-2.43	120.41	124.05
41	Y	309	KC2	CHD-C1D-ND	-2.43	120.41	124.05
41	N	302	KC2	C4B-C3B-C2B	2.43	108.92	106.81
40	S	312	CLA	CHB-C1B-NB	-2.43	120.41	124.05
40	l	204	CLA	CHB-C1B-NB	-2.43	120.41	124.05
40	F	311	CLA	CHB-C1B-NB	-2.42	120.41	124.05
40	f	202	CLA	CHB-C1B-NB	-2.42	120.41	124.05
41	W	302	KC2	CHD-C1D-ND	-2.42	120.41	124.05
44	N	314	A86	C33-C32-C31	-2.42	106.86	109.21
42	C	310	DD6	O1-C15-C14	-2.42	109.94	116.88
41	Q	216	KC2	CHD-C1D-ND	-2.42	120.42	124.05
40	a	814	CLA	CHB-C1B-NB	-2.42	120.42	124.05
43	x	301	LMG	O6-C1-O1	-2.42	104.32	110.04
40	Q	209	CLA	CHB-C1B-NB	-2.42	120.42	124.05
41	v	309	KC2	CHD-C1D-ND	-2.42	120.42	124.05
40	D	312	CLA	CHB-C1B-NB	-2.42	120.42	124.05
40	f	201	CLA	CHB-C1B-NB	-2.42	120.42	124.05
41	H	303	KC2	CHD-C1D-ND	-2.42	120.42	124.05
41	Z	302	KC2	CHD-C4C-NC	2.42	127.96	124.31
43	D	318	LMG	O1-C1-C2	-2.42	104.60	108.27
40	Y	312	CLA	CHC-C4B-NB	-2.42	120.42	124.05
43	a	802	LMG	O6-C1-O1	-2.42	104.33	110.04
42	k	204	DD6	O1-C20-C15	-2.42	57.01	58.93
41	o	302	KC2	CHB-C4A-NA	2.42	127.98	124.23
40	x	311	CLA	C4D-CHA-C1A	-2.42	118.36	121.24
40	q	311	CLA	CHB-C1B-NB	-2.42	120.42	124.05
40	x	313	CLA	CHB-C1B-NB	-2.42	120.42	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	O	316	CLA	CHB-C1B-NB	-2.42	120.42	124.05
40	E	306	CLA	CHB-C1B-NB	-2.42	120.42	124.05
40	E	312	CLA	CHB-C1B-NB	-2.42	120.43	124.05
40	F	301	CLA	CHB-C1B-NB	-2.42	120.43	124.05
41	p	304	KC2	CHD-C1D-ND	-2.42	120.43	124.05
41	q	308	KC2	CHB-C4A-NA	2.42	127.98	124.23
42	o	320	DD6	O1-C20-C19	-2.41	111.23	113.49
40	w	308	CLA	CHB-C1B-NB	-2.41	120.43	124.05
40	Z	307	CLA	CHB-C1B-NB	-2.41	120.43	124.05
41	K	303	KC2	CHD-C1D-ND	-2.41	120.43	124.05
44	P	317	A86	C36-C31-C32	-2.41	117.30	119.70
41	y	307	KC2	CHD-C1D-ND	-2.41	120.43	124.05
40	E	311	CLA	CHB-C1B-NB	-2.41	120.43	124.05
40	a	828	CLA	CHB-C1B-NB	-2.41	120.43	124.05
40	b	841	CLA	CHB-C1B-NB	-2.41	120.43	124.05
40	S	306	CLA	CHB-C1B-NB	-2.41	120.43	124.05
40	L	306	CLA	C2A-C1A-CHA	2.41	128.05	123.87
40	W	312	CLA	C2C-C1C-NC	2.41	112.51	109.98
41	o	308	KC2	CHD-C4C-NC	2.41	127.94	124.31
40	J	310	CLA	C3A-C2A-C1A	-2.41	97.73	101.34
41	O	309	KC2	CHB-C4A-NA	2.41	127.97	124.23
40	A	301	CLA	C2C-C1C-NC	2.41	112.51	109.98
40	E	303	CLA	CHB-C1B-NB	-2.41	120.44	124.05
40	b	822	CLA	CAA-C2A-C1A	-2.41	104.09	111.97
40	E	309	CLA	CHB-C1B-NB	-2.41	120.44	124.05
40	Z	304	CLA	CHB-C1B-NB	-2.41	120.44	124.05
40	A	304	CLA	CAA-C2A-C3A	2.41	119.50	113.00
40	b	808	CLA	CHB-C4A-NA	2.41	127.87	124.40
40	F	303	CLA	CHB-C1B-NB	-2.41	120.44	124.05
41	N	303	KC2	CHD-C4C-NC	2.41	127.94	124.31
44	C	311	A86	O1-C20-C19	-2.41	111.24	113.49
41	C	303	KC2	CHB-C4A-NA	2.41	127.96	124.23
40	B	306	CLA	CHB-C1B-NB	-2.41	120.44	124.05
40	G	204	CLA	CHB-C1B-NB	-2.41	120.44	124.05
40	J	310	CLA	CHC-C4B-NB	-2.41	120.44	124.05
40	L	305	CLA	CHB-C1B-NB	-2.41	120.44	124.05
42	q	318	DD6	C14-C13-C11	2.40	129.26	125.53
40	q	306	CLA	CMC-C2C-C1C	2.40	128.79	125.03
40	E	308	CLA	CHB-C1B-NB	-2.40	120.44	124.05
40	z	305	CLA	CHB-C1B-NB	-2.40	120.44	124.05
42	C	313	DD6	C21-C20-C19	2.40	116.94	114.24
40	a	833	CLA	CHB-C1B-NB	-2.40	120.45	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	S	314	CLA	CHA-C1A-NA	-2.40	120.95	126.39
40	X	313	CLA	CHB-C1B-NB	-2.40	120.45	124.05
41	O	311	KC2	CHD-C1D-ND	-2.40	120.45	124.05
41	R	311	KC2	CHD-C1D-ND	-2.40	120.45	124.05
40	K	307	CLA	CHB-C1B-NB	-2.40	120.45	124.05
40	a	835	CLA	CHB-C1B-NB	-2.40	120.45	124.05
41	M	309	KC2	CHD-C1D-ND	-2.40	120.45	124.05
40	I	206	CLA	CHB-C1B-NB	-2.40	120.45	124.05
40	q	310	CLA	CHB-C1B-NB	-2.40	120.45	124.05
42	v	318	DD6	C30-C29-C27	-2.40	168.08	176.23
40	Y	313	CLA	CHB-C1B-NB	-2.40	120.45	124.05
40	J	318	CLA	CHC-C1C-C2C	-2.40	120.13	126.95
40	z	312	CLA	C1-C2-C3	-2.40	122.27	126.20
41	R	301	KC2	CHD-C1D-ND	-2.40	120.45	124.05
40	X	306	CLA	CBA-CAA-C2A	2.40	120.93	113.79
40	b	803	CLA	CHA-C1A-NA	-2.40	120.96	126.39
40	L	306	CLA	CHB-C1B-NB	-2.40	120.45	124.05
40	Z	305	CLA	CHB-C1B-NB	-2.40	120.45	124.05
41	x	310	KC2	CHD-C1D-ND	-2.40	120.45	124.05
41	u	310	KC2	CHD-C4C-NC	2.40	127.92	124.31
40	o	301	CLA	CHB-C1B-NB	-2.40	120.45	124.05
43	D	318	LMG	O6-C1-O1	-2.40	104.38	110.04
40	p	311	CLA	CAA-C2A-C1A	-2.39	104.13	111.97
40	y	302	CLA	CHB-C1B-NB	-2.39	120.46	124.05
40	b	826	CLA	CHB-C1B-NB	-2.39	120.46	124.05
40	t	307	CLA	CHB-C1B-NB	-2.39	120.46	124.05
42	J	301	DD6	C21-C20-C19	2.39	116.93	114.24
45	S	323	LHG	C11-C10-C9	-2.39	102.27	114.37
40	v	310	CLA	CHB-C1B-NB	-2.39	120.46	124.05
40	w	304	CLA	CHB-C1B-NB	-2.39	120.46	124.05
41	S	304	KC2	C4B-C3B-C2B	2.39	108.89	106.81
40	A	304	CLA	CBA-CAA-C2A	2.39	120.91	113.79
43	S	322	LMG	O3-C3-C2	-2.39	104.74	110.38
40	u	314	CLA	C3A-C2A-C1A	-2.39	97.76	101.34
40	x	311	CLA	C2A-C1A-CHA	2.39	128.01	123.87
40	C	306	CLA	CHB-C1B-NB	-2.39	120.46	124.05
40	b	812	CLA	CHB-C1B-NB	-2.39	120.46	124.05
47	x	321	A1EB1	C33-C32-C31	2.39	111.53	109.21
40	N	304	CLA	CHB-C1B-NB	-2.39	120.47	124.05
41	Q	216	KC2	CHB-C4A-NA	2.39	127.93	124.23
40	a	809	CLA	CHB-C4A-NA	2.39	127.84	124.40
40	a	815	CLA	CHB-C1B-NB	-2.39	120.47	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	a	836	CLA	CHB-C1B-NB	-2.39	120.47	124.05
41	S	309	KC2	C4B-C3B-C2B	2.39	108.88	106.81
40	W	311	CLA	CAA-C2A-C1A	-2.39	104.16	111.97
40	X	304	CLA	CHB-C1B-NB	-2.39	120.47	124.05
40	x	308	CLA	CHB-C1B-NB	-2.39	120.47	124.05
40	k	201	CLA	CHB-C1B-NB	-2.39	120.47	124.05
41	x	303	KC2	CHD-C4C-NC	2.38	127.90	124.31
41	y	307	KC2	CHD-C4C-NC	2.38	127.90	124.31
40	H	310	CLA	CHB-C1B-NB	-2.38	120.47	124.05
40	a	817	CLA	CHB-C1B-NB	-2.38	120.47	124.05
43	F	318	LMG	O2-C2-C1	-2.38	104.40	110.08
40	L	310	CLA	CHB-C1B-NB	-2.38	120.48	124.05
41	N	312	KC2	CHD-C1D-ND	-2.38	120.48	124.05
41	O	303	KC2	CHD-C1D-ND	-2.38	120.48	124.05
40	R	306	CLA	C1-C2-C3	-2.38	122.30	126.20
42	I	211	DD6	C21-C20-C19	2.38	116.92	114.24
40	G	205	CLA	CHB-C1B-NB	-2.38	120.48	124.05
40	b	820	CLA	CHB-C1B-NB	-2.38	120.48	124.05
41	w	301	KC2	CHD-C1D-ND	-2.38	120.48	124.05
40	B	306	CLA	C4D-CHA-C1A	-2.38	118.41	121.24
41	N	302	KC2	CHD-C1D-ND	-2.38	120.48	124.05
41	O	302	KC2	CHD-C1D-ND	-2.38	120.48	124.05
41	x	303	KC2	CHD-C1D-ND	-2.38	120.48	124.05
42	o	319	DD6	O1-C20-C19	-2.38	111.26	113.49
40	D	308	CLA	C1-C2-C3	-2.38	122.30	126.20
40	b	829	CLA	CHB-C1B-NB	-2.38	120.48	124.05
43	W	317	LMG	O7-C10-O9	-2.38	118.15	123.70
40	u	311	CLA	C2A-C1A-CHA	2.38	127.99	123.87
41	C	303	KC2	CHD-C1D-ND	-2.38	120.48	124.05
40	D	308	CLA	CHB-C1B-NB	-2.38	120.48	124.05
40	P	308	CLA	CHB-C1B-NB	-2.38	120.48	124.05
43	S	322	LMG	O6-C1-O1	-2.38	104.43	110.04
40	Q	205	CLA	CBA-CAA-C2A	2.38	120.86	113.79
40	H	304	CLA	CMC-C2C-C1C	2.37	128.74	125.03
41	v	308	KC2	CHD-C1D-ND	-2.37	120.49	124.05
40	K	308	CLA	CHB-C1B-NB	-2.37	120.49	124.05
40	z	324	CLA	CHB-C1B-NB	-2.37	120.49	124.05
44	q	324	A86	O1-C20-C19	2.37	115.72	113.49
40	S	308	CLA	CMC-C2C-C1C	2.37	128.74	125.03
40	b	841	CLA	CHA-C1A-NA	-2.37	121.02	126.39
40	F	304	CLA	CHB-C1B-NB	-2.37	120.49	124.05
40	M	312	CLA	CHB-C1B-NB	-2.37	120.49	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	a	834	CLA	CHB-C1B-NB	-2.37	120.49	124.05
41	L	308	KC2	CHD-C1D-ND	-2.37	120.49	124.05
41	T	311	KC2	CHD-C1D-ND	-2.37	120.49	124.05
40	C	309	CLA	CHB-C1B-NB	-2.37	120.49	124.05
41	w	306	KC2	CHD-C4C-NC	2.37	127.88	124.31
40	y	304	CLA	CMC-C2C-C1C	2.37	128.74	125.03
40	D	310	CLA	CHB-C1B-NB	-2.37	120.49	124.05
40	y	304	CLA	CHB-C1B-NB	-2.37	120.49	124.05
43	E	301	LMG	O6-C1-O1	-2.37	104.44	110.04
41	o	302	KC2	CHD-C1D-ND	-2.37	120.50	124.05
40	Q	205	CLA	CAA-C2A-C3A	2.37	119.40	113.00
40	b	819	CLA	CHB-C1B-NB	-2.37	120.50	124.05
40	z	307	CLA	CHB-C1B-NB	-2.37	120.50	124.05
41	p	309	KC2	CHD-C1D-ND	-2.37	120.50	124.05
40	b	816	CLA	C3A-C2A-C1A	-2.37	97.79	101.34
52	b	850	DGD	O5D-C6D-C5D	-2.37	104.08	109.42
40	X	305	CLA	CHB-C1B-NB	-2.37	120.50	124.05
40	q	312	CLA	CHB-C1B-NB	-2.37	120.50	124.05
40	X	310	CLA	C2A-C3A-C4A	-2.37	98.05	101.87
40	A	308	CLA	CHB-C1B-NB	-2.37	120.50	124.05
40	H	306	CLA	CHB-C1B-NB	-2.37	120.50	124.05
40	D	309	CLA	CHB-C1B-NB	-2.37	120.50	124.05
40	f	204	CLA	CHB-C1B-NB	-2.37	120.50	124.05
40	J	308	CLA	CMC-C2C-C1C	2.36	128.73	125.03
40	v	307	CLA	CMC-C2C-C1C	2.36	128.73	125.03
41	u	304	KC2	CHD-C1D-ND	-2.36	120.50	124.05
40	K	306	CLA	CMC-C2C-C1C	2.36	128.73	125.03
40	A	303	CLA	CHB-C1B-NB	-2.36	120.50	124.05
41	N	301	KC2	CHD-C1D-ND	-2.36	120.50	124.05
41	t	308	KC2	C2A-C3A-C4A	2.36	108.19	106.41
40	Z	312	CLA	CHB-C1B-NB	-2.36	120.50	124.05
43	a	802	LMG	O6-C5-C4	2.36	113.95	109.70
41	q	308	KC2	CHD-C1D-ND	-2.36	120.51	124.05
40	i	101	CLA	CHA-C1A-NA	-2.36	121.04	126.39
40	D	305	CLA	CHB-C1B-NB	-2.36	120.51	124.05
40	F	308	CLA	CHB-C1B-NB	-2.36	120.51	124.05
40	q	311	CLA	CHA-C1A-NA	-2.36	121.05	126.39
43	P	318	LMG	O6-C5-C4	2.36	113.95	109.70
40	S	314	CLA	CHB-C1B-NB	-2.36	120.51	124.05
40	F	321	CLA	CHA-C1A-NA	-2.36	121.05	126.39
41	S	303	KC2	CHD-C1D-ND	-2.36	120.51	124.05
41	X	308	KC2	CHD-C1D-ND	-2.36	120.51	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	G	206	CLA	CBA-CAA-C2A	2.36	120.81	113.79
44	p	317	A86	C21-C20-C19	-2.36	111.59	114.24
40	H	311	CLA	CHB-C1B-NB	-2.36	120.51	124.05
42	Y	322	DD6	O1-C20-C15	-2.36	57.06	58.93
40	f	205	CLA	CHB-C1B-NB	-2.36	120.51	124.05
40	a	819	CLA	CHB-C1B-NB	-2.36	120.51	124.05
40	a	824	CLA	CHA-C1A-NA	-2.36	121.06	126.39
40	v	310	CLA	C3A-C2A-C1A	-2.36	97.81	101.34
43	F	318	LMG	O1-C7-C8	-2.36	105.09	110.82
40	C	301	CLA	CHB-C1B-NB	-2.36	120.52	124.05
40	K	304	CLA	CHB-C1B-NB	-2.36	120.52	124.05
41	x	309	KC2	CHD-C4C-NC	2.36	127.86	124.31
40	Z	304	CLA	CHA-C1A-NA	-2.36	121.06	126.39
41	W	309	KC2	CHD-C1D-ND	-2.36	120.52	124.05
40	A	306	CLA	CHB-C1B-NB	-2.35	120.52	124.05
40	a	820	CLA	CHB-C1B-NB	-2.35	120.52	124.05
43	F	318	LMG	O7-C10-O9	-2.35	118.20	123.70
41	p	304	KC2	CHB-C4A-NA	2.35	127.88	124.23
40	T	307	CLA	CHB-C1B-NB	-2.35	120.52	124.05
40	v	306	CLA	CHB-C1B-NB	-2.35	120.52	124.05
42	J	316	DD6	O1-C20-C19	-2.35	111.29	113.49
40	a	810	CLA	CHB-C1B-NB	-2.35	120.52	124.05
40	o	307	CLA	CMC-C2C-C1C	2.35	128.71	125.03
41	K	303	KC2	C4B-C3B-C2B	2.35	108.85	106.81
40	Q	203	CLA	CHC-C1C-NC	2.35	127.79	124.33
40	a	823	CLA	CHB-C1B-NB	-2.35	120.52	124.05
40	p	306	CLA	CHB-C1B-NB	-2.35	120.52	124.05
40	F	304	CLA	CHC-C4B-NB	-2.35	120.52	124.05
42	L	317	DD6	O1-C20-C15	-2.35	57.07	58.93
40	K	308	CLA	C1-C2-C3	-2.35	122.35	126.20
40	a	820	CLA	CHA-C1A-NA	-2.35	121.07	126.39
41	z	303	KC2	CHD-C4C-NC	2.35	127.85	124.31
42	J	316	DD6	C14-C13-C11	2.35	129.18	125.53
40	D	303	CLA	CHB-C1B-NB	-2.35	120.53	124.05
40	S	307	CLA	CHB-C1B-NB	-2.35	120.53	124.05
41	K	305	KC2	CHD-C1D-ND	-2.35	120.53	124.05
40	G	213	CLA	C2C-C1C-NC	2.35	112.45	109.98
40	o	310	CLA	CHB-C1B-NB	-2.35	120.53	124.05
41	R	303	KC2	CHB-C4A-NA	2.35	127.87	124.23
42	E	318	DD6	C21-C20-C19	2.35	116.88	114.24
42	N	317	DD6	C30-C29-C27	-2.35	168.26	176.23
41	P	309	KC2	CHB-C4A-NA	2.35	127.87	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	Z	303	KC2	CHD-C4C-NC	2.35	127.84	124.31
41	q	309	KC2	CHD-C4C-NC	2.35	127.84	124.31
41	R	311	KC2	CHB-C4A-NA	2.35	127.87	124.23
40	b	815	CLA	CHB-C1B-NB	-2.35	120.53	124.05
41	E	319	KC2	CHB-C4A-NA	2.34	127.87	124.23
40	L	307	CLA	CHB-C1B-NB	-2.34	120.53	124.05
40	O	306	CLA	CHB-C1B-NB	-2.34	120.53	124.05
41	T	301	KC2	CHD-C1D-ND	-2.34	120.53	124.05
40	Z	312	CLA	CHA-C1A-NA	-2.34	121.08	126.39
40	p	311	CLA	C2A-C1A-CHA	2.34	127.93	123.87
40	E	310	CLA	CHB-C1B-NB	-2.34	120.53	124.05
40	b	801	CLA	CHB-C4A-NA	2.34	127.78	124.40
40	A	304	CLA	CHB-C1B-NB	-2.34	120.54	124.05
40	I	202	CLA	CHB-C1B-NB	-2.34	120.54	124.05
40	V	201	CLA	CHB-C1B-NB	-2.34	120.54	124.05
41	A	310	KC2	CHD-C1D-ND	-2.34	120.54	124.05
42	w	312	DD6	O1-C20-C15	-2.34	57.07	58.93
40	L	301	CLA	CHA-C1A-NA	-2.34	121.09	126.39
41	K	309	KC2	CHB-C4A-NA	2.34	127.86	124.23
40	O	310	CLA	C2A-C3A-C4A	-2.34	98.09	101.87
40	a	806	CLA	CHB-C1B-NB	-2.34	120.54	124.05
41	U	201	KC2	CHD-C4C-NC	2.34	127.84	124.31
41	T	308	KC2	CHD-C1D-ND	-2.34	120.54	124.05
40	a	832	CLA	C11-C12-C13	2.34	123.74	115.97
41	O	308	KC2	CHD-C4C-NC	2.34	127.83	124.31
40	G	213	CLA	CHC-C1C-C2C	-2.34	120.30	126.95
40	F	307	CLA	CHB-C1B-NB	-2.34	120.70	124.08
40	H	308	CLA	CHB-C1B-NB	-2.34	120.54	124.05
40	R	316	CLA	CHA-C1A-NA	-2.34	121.10	126.39
40	b	818	CLA	CHB-C1B-NB	-2.34	120.55	124.05
40	b	832	CLA	CHC-C4B-NB	-2.34	120.55	124.05
41	M	308	KC2	CHD-C4C-NC	2.34	127.83	124.31
40	W	311	CLA	CHD-C1D-C2D	2.34	130.34	125.49
40	C	302	CLA	CHA-C1A-NA	-2.34	121.10	126.39
40	H	302	CLA	CHB-C1B-NB	-2.34	120.55	124.05
41	o	303	KC2	CHD-C1D-ND	-2.33	120.55	124.05
43	x	301	LMG	O2-C2-C1	-2.33	104.51	110.08
40	L	312	CLA	CHA-C1A-NA	-2.33	121.11	126.39
42	t	312	DD6	O1-C15-C14	-2.33	110.19	116.88
41	I	214	KC2	CHB-C4A-NA	2.33	127.85	124.23
41	U	201	KC2	CHB-C4A-NA	2.33	127.85	124.23
40	I	208	CLA	CHB-C1B-NB	-2.33	120.55	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	S	319	CLA	CHB-C1B-NB	-2.33	120.55	124.05
40	u	308	CLA	CHB-C1B-NB	-2.33	120.55	124.05
40	D	307	CLA	C1-C2-C3	-2.33	122.38	126.20
40	P	311	CLA	CHA-C1A-NA	-2.33	121.11	126.39
40	Y	310	CLA	CHB-C1B-NB	-2.33	120.55	124.05
40	a	816	CLA	CBA-CAA-C2A	2.33	120.73	113.79
40	B	303	CLA	CHB-C1B-NB	-2.33	120.55	124.05
44	T	312	A86	C21-C20-C19	-2.33	111.62	114.24
40	N	305	CLA	CHB-C1B-NB	-2.33	120.55	124.05
40	Y	312	CLA	CHB-C1B-NB	-2.33	120.55	124.05
40	p	313	CLA	C2C-C1C-NC	2.33	112.43	109.98
40	o	306	CLA	CHB-C1B-NB	-2.33	120.56	124.05
42	N	319	DD6	O1-C15-C14	-2.33	110.21	116.88
42	q	318	DD6	C21-C20-C19	2.33	116.86	114.24
40	D	301	CLA	CHB-C1B-NB	-2.33	120.56	124.05
40	S	308	CLA	CHB-C1B-NB	-2.33	120.56	124.05
40	b	817	CLA	CHB-C1B-NB	-2.33	120.56	124.05
40	b	812	CLA	CHA-C1A-NA	-2.33	121.12	126.39
43	D	318	LMG	O1-C7-C8	-2.33	105.16	110.82
40	E	307	CLA	CHB-C1B-NB	-2.33	120.56	124.05
40	b	842	CLA	CHB-C1B-NB	-2.33	120.56	124.05
40	S	305	CLA	C2A-C1A-CHA	2.33	127.90	123.87
40	A	309	CLA	CHB-C1B-NB	-2.33	120.56	124.05
40	N	307	CLA	CHB-C1B-NB	-2.33	120.56	124.05
41	O	311	KC2	CHB-C4A-NA	2.32	127.84	124.23
41	P	309	KC2	CHD-C4C-NC	2.32	127.81	124.31
41	v	309	KC2	CHD-C4C-NC	2.32	127.81	124.31
40	a	840	CLA	CHB-C1B-NB	-2.32	120.56	124.05
40	O	305	CLA	CHB-C1B-NB	-2.32	120.56	124.05
40	a	850	CLA	CHD-C1D-C2D	2.32	130.32	125.49
40	S	305	CLA	CHB-C1B-NB	-2.32	120.56	124.05
46	M	318	SQD	O48-C23-O10	-2.32	117.82	123.63
41	F	309	KC2	CHB-C4A-NA	2.32	127.83	124.23
40	W	307	CLA	CHB-C1B-NB	-2.32	120.57	124.05
40	b	806	CLA	CHB-C1B-NB	-2.32	120.57	124.05
40	U	208	CLA	CHA-C1A-NA	-2.32	121.13	126.39
40	X	301	CLA	CHB-C1B-NB	-2.32	120.57	124.05
44	P	314	A86	C33-C32-C31	2.32	111.47	109.21
40	l	205	CLA	C3A-C2A-C1A	-2.32	97.86	101.34
40	T	306	CLA	C1-C2-C3	-2.32	122.40	126.20
44	u	317	A86	C21-C20-C19	-2.32	111.64	114.24
40	v	301	CLA	CHB-C1B-NB	-2.32	120.57	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	u	304	KC2	CHB-C4A-NA	2.32	127.83	124.23
40	Z	311	CLA	CHA-C1A-NA	-2.32	121.14	126.39
40	i	101	CLA	CAA-C2A-C1A	-2.32	104.38	111.97
40	D	302	CLA	CHB-C1B-NB	-2.32	120.57	124.05
40	P	305	CLA	CHB-C1B-NB	-2.32	120.57	124.05
40	Q	202	CLA	CHB-C1B-NB	-2.32	120.57	124.05
40	a	841	CLA	CHB-C1B-NB	-2.32	120.57	124.05
40	u	311	CLA	CHB-C1B-NB	-2.32	120.57	124.05
41	z	303	KC2	CHD-C1D-ND	-2.32	120.57	124.05
40	D	303	CLA	CHA-C1A-NA	-2.32	121.14	126.39
40	b	824	CLA	CHB-C4A-NA	2.32	127.75	124.40
41	I	214	KC2	CHD-C1D-ND	-2.32	120.57	124.05
40	u	307	CLA	CHB-C1B-NB	-2.32	120.57	124.05
40	I	203	CLA	CHA-C1A-NA	-2.32	121.14	126.39
43	E	321	LMG	O2-C2-C1	-2.32	104.55	110.08
40	J	307	CLA	CGD-CBD-CAD	-2.32	103.35	110.85
40	y	302	CLA	CHA-C1A-NA	-2.32	121.14	126.39
42	t	312	DD6	O1-C20-C15	-2.32	57.09	58.93
40	Y	312	CLA	C2A-C1A-CHA	2.32	127.89	123.87
40	p	307	CLA	CHB-C1B-NB	-2.32	120.58	124.05
40	p	312	CLA	CHB-C1B-NB	-2.32	120.58	124.05
40	B	304	CLA	CHA-C1A-NA	-2.31	121.15	126.39
41	L	302	KC2	C4B-C3B-C2B	2.31	108.82	106.81
40	L	306	CLA	C4D-CHA-C1A	-2.31	118.48	121.24
40	k	201	CLA	O2A-C1-C2	-2.31	99.20	108.11
40	q	307	CLA	CMC-C2C-C1C	2.31	128.65	125.03
40	a	831	CLA	CHB-C1B-NB	-2.31	120.58	124.05
41	x	309	KC2	CHD-C1D-ND	-2.31	120.58	124.05
40	W	306	CLA	CGD-CBD-CAD	-2.31	103.36	110.85
40	a	837	CLA	CHB-C1B-NB	-2.31	120.58	124.05
41	K	309	KC2	CHD-C1D-ND	-2.31	120.58	124.05
40	a	803	CLA	CHA-C1A-NA	-2.31	121.16	126.39
40	a	826	CLA	CHC-C4B-NB	-2.31	120.58	124.05
40	N	310	CLA	C3A-C2A-C1A	-2.31	97.88	101.34
40	a	829	CLA	CHB-C1B-NB	-2.31	120.58	124.05
41	P	310	KC2	CHD-C1D-ND	-2.31	120.58	124.05
40	L	310	CLA	C3A-C2A-C1A	-2.31	97.88	101.34
40	b	805	CLA	CHB-C1B-NB	-2.31	120.58	124.05
40	Y	311	CLA	CHB-C1B-NB	-2.31	120.59	124.05
40	x	311	CLA	CHB-C1B-NB	-2.31	120.59	124.05
41	u	309	KC2	CHD-C1D-ND	-2.31	120.59	124.05
40	b	825	CLA	CBA-CAA-C2A	2.31	120.66	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	O	309	KC2	CHD-C1D-ND	-2.31	120.59	124.05
40	Z	310	CLA	CHD-C1D-C2D	2.31	130.29	125.49
40	x	312	CLA	CMA-C3A-C4A	2.31	117.97	111.77
50	a	847	PQN	C12-C11-C3	-2.31	106.40	112.08
40	J	318	CLA	C2C-C1C-NC	2.31	112.40	109.98
40	M	305	CLA	CHB-C1B-NB	-2.30	120.59	124.05
40	O	307	CLA	CHB-C1B-NB	-2.30	120.59	124.05
40	E	314	CLA	CHB-C1B-NB	-2.30	120.59	124.05
40	Q	207	CLA	C4D-CHA-C1A	-2.30	118.50	121.24
40	z	311	CLA	CHD-C1D-C2D	2.30	130.27	125.49
40	x	313	CLA	CGD-CBD-CAD	-2.30	103.40	110.85
40	a	806	CLA	CHD-C1D-C2D	2.30	130.27	125.49
40	G	206	CLA	CHB-C1B-NB	-2.30	120.60	124.05
40	W	308	CLA	CHB-C1B-NB	-2.30	120.60	124.05
43	E	321	LMG	O7-C10-O9	-2.30	118.33	123.70
40	w	303	CLA	CHB-C1B-NB	-2.30	120.60	124.05
41	R	303	KC2	C4B-C3B-C2B	2.30	108.81	106.81
40	H	304	CLA	CBA-CAA-C2A	2.30	120.63	113.79
40	z	324	CLA	CHD-C1D-C2D	2.30	130.27	125.49
41	F	309	KC2	CHD-C4C-NC	2.30	127.77	124.31
41	O	301	KC2	CHB-C4A-NA	2.30	127.79	124.23
41	T	311	KC2	CHB-C4A-NA	2.30	127.79	124.23
40	Y	313	CLA	CHD-C1D-C2D	2.30	130.26	125.49
41	F	302	KC2	CHD-C4C-NC	2.30	127.77	124.31
41	K	302	KC2	CHD-C4C-NC	2.30	127.77	124.31
42	I	213	DD6	O1-C20-C19	2.30	115.64	113.49
41	o	302	KC2	CHD-C4C-NC	2.30	127.77	124.31
40	x	302	CLA	CHB-C1B-NB	-2.30	120.61	124.05
41	R	302	KC2	CHD-C4C-NC	2.29	127.77	124.31
40	W	306	CLA	CHB-C1B-NB	-2.29	120.61	124.05
41	P	303	KC2	CHD-C4C-NC	2.29	127.77	124.31
40	a	852	CLA	CHB-C1B-NB	-2.29	120.61	124.05
52	b	850	DGD	O3G-C1D-C2D	-2.29	104.79	108.27
41	N	313	KC2	CHD-C1D-ND	-2.29	120.61	124.05
45	a	849	LHG	O8-C23-C24	2.29	118.83	111.83
40	T	304	CLA	CHB-C1B-NB	-2.29	120.61	124.05
40	a	830	CLA	CAA-C2A-C3A	2.29	119.19	113.00
40	W	313	CLA	CHB-C1B-NB	-2.29	120.61	124.05
40	C	305	CLA	CHB-C1B-NB	-2.29	120.61	124.05
42	J	314	DD6	O1-C20-C15	-2.29	57.11	58.93
40	w	302	CLA	CHB-C1B-NB	-2.29	120.61	124.05
42	Q	213	DD6	O1-C20-C19	-2.29	111.35	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	W	312	CLA	CHA-C1A-NA	-2.29	121.21	126.39
41	O	309	KC2	CHD-C4C-NC	2.29	127.76	124.31
40	q	311	CLA	C2C-C1C-NC	2.29	112.39	109.98
41	p	315	KC2	CHD-C1D-ND	-2.29	120.62	124.05
41	x	310	KC2	CHD-C4C-NC	2.29	127.76	124.31
40	Z	310	CLA	CHB-C1B-NB	-2.29	120.62	124.05
40	A	303	CLA	CHA-C1A-NA	-2.29	121.21	126.39
40	M	306	CLA	CHB-C1B-NB	-2.29	120.62	124.05
40	D	307	CLA	CBA-CAA-C2A	2.29	120.60	113.79
40	G	201	CLA	CHB-C1B-NB	-2.29	120.62	124.05
40	A	304	CLA	C6-C7-C8	2.29	123.56	115.97
40	Y	312	CLA	CHD-C1D-C2D	2.29	130.24	125.49
42	N	317	DD6	O1-C20-C19	-2.28	111.35	113.49
40	Q	202	CLA	CHA-C1A-NA	-2.28	121.22	126.39
40	f	202	CLA	CHA-C1A-NA	-2.28	121.22	126.39
40	o	312	CLA	CHB-C1B-NB	-2.28	120.62	124.05
40	z	313	CLA	CHB-C1B-NB	-2.28	120.62	124.05
40	b	808	CLA	CHA-C1A-NA	-2.28	121.22	126.39
42	F	314	DD6	C21-C20-C19	2.28	116.81	114.24
41	G	202	KC2	CHD-C4C-NC	2.28	127.75	124.31
41	L	302	KC2	CHD-C4C-NC	2.28	127.75	124.31
40	H	305	CLA	CHA-C1A-NA	-2.28	121.22	126.39
40	Y	307	CLA	CHD-C1D-C2D	2.28	130.23	125.49
40	b	842	CLA	CHA-C1A-NA	-2.28	121.23	126.39
40	a	832	CLA	CHB-C1B-NB	-2.28	120.63	124.05
41	x	304	KC2	CHD-C1D-ND	-2.28	120.63	124.05
41	y	301	KC2	CHB-C4A-NA	2.28	127.77	124.23
40	b	803	CLA	CHD-C1D-C2D	2.28	130.23	125.49
40	I	207	CLA	CHB-C1B-NB	-2.28	120.63	124.05
40	v	311	CLA	CHA-C1A-NA	-2.28	121.23	126.39
40	z	311	CLA	C1-C2-C3	-2.28	122.47	126.20
40	Z	313	CLA	CHB-C1B-NB	-2.28	120.63	124.05
40	U	203	CLA	CAC-C3C-C4C	2.28	127.75	124.79
40	y	309	CLA	C3A-C2A-C1A	-2.28	97.93	101.34
40	z	313	CLA	C3A-C2A-C1A	-2.28	97.93	101.34
42	Q	211	DD6	C14-C13-C11	2.28	129.06	125.53
40	H	310	CLA	CHD-C1D-C2D	2.28	130.22	125.49
49	l	208	BCR	C16-C15-C14	-2.28	118.86	123.52
40	x	312	CLA	CHB-C1B-NB	-2.28	120.64	124.05
41	X	302	KC2	CHB-C4A-NA	2.28	127.76	124.23
40	D	307	CLA	CHB-C1B-NB	-2.28	120.64	124.05
41	Q	201	KC2	C3C-C2C-C1C	2.27	108.12	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	R	302	KC2	C4B-C3B-C2B	2.27	108.79	106.81
40	C	302	CLA	CHB-C1B-NB	-2.27	120.64	124.05
40	Z	307	CLA	CGD-CBD-CAD	-2.27	103.49	110.85
40	T	317	CLA	CHB-C1B-NB	-2.27	120.64	124.05
40	q	307	CLA	CHB-C1B-NB	-2.27	120.64	124.05
40	P	311	CLA	C3A-C2A-C1A	-2.27	97.94	101.34
40	a	811	CLA	CHD-C1D-C2D	2.27	130.21	125.49
41	O	302	KC2	CHD-C4C-NC	2.27	127.73	124.31
40	Y	304	CLA	CHA-C1A-NA	-2.27	121.25	126.39
40	v	310	CLA	CHB-C4A-NA	2.27	127.68	124.40
41	w	307	KC2	CHD-C4C-NC	2.27	127.73	124.31
40	C	309	CLA	CHD-C1D-C2D	2.27	130.21	125.49
40	G	213	CLA	CHD-C1D-C2D	2.27	130.21	125.49
47	t	314	A1EB1	C33-C32-C31	-2.27	107.00	109.21
40	K	306	CLA	CBA-CAA-C2A	2.27	120.55	113.79
40	l	205	CLA	CHB-C1B-NB	-2.27	120.64	124.05
40	p	302	CLA	CHB-C1B-NB	-2.27	120.64	124.05
43	a	802	LMG	O2-C2-C1	-2.27	104.67	110.08
40	z	306	CLA	CHB-C1B-NB	-2.27	120.65	124.05
40	X	305	CLA	CHC-C4B-NB	-2.27	120.65	124.05
41	x	304	KC2	CHB-C4A-NA	2.27	127.75	124.23
40	U	208	CLA	CHB-C1B-NB	-2.27	120.65	124.05
40	u	305	CLA	CHB-C1B-NB	-2.27	120.65	124.05
40	y	309	CLA	CHB-C1B-NB	-2.27	120.65	124.05
40	S	311	CLA	C2A-C3A-C4A	-2.27	98.21	101.87
40	E	311	CLA	CHD-C1D-C2D	2.27	130.20	125.49
40	U	205	CLA	CHA-C1A-NA	-2.27	121.26	126.39
40	A	305	CLA	CHB-C1B-NB	-2.27	120.65	124.05
41	G	208	KC2	CHD-C1D-ND	-2.27	120.65	124.05
40	a	818	CLA	CHD-C1D-C2D	2.26	130.20	125.49
40	a	834	CLA	C1-C2-C3	-2.26	122.49	126.20
41	Q	216	KC2	CHD-C4C-NC	2.26	127.72	124.31
41	S	303	KC2	CHB-C4A-NA	2.26	127.74	124.23
40	H	307	CLA	O2A-C1-C2	2.26	116.81	108.11
40	Y	301	CLA	CHB-C1B-NB	-2.26	120.66	124.05
41	L	313	KC2	CHD-C4C-NC	2.26	127.72	124.31
40	D	307	CLA	CAA-C2A-C3A	2.26	119.11	113.00
41	G	208	KC2	CHB-C4A-NA	2.26	127.74	124.23
41	Z	308	KC2	CHD-C4C-NC	2.26	127.72	124.31
44	u	319	A86	C33-C32-C31	2.26	111.41	109.21
40	p	311	CLA	CHD-C1D-C2D	2.26	130.19	125.49
40	z	311	CLA	CHA-C1A-NA	-2.26	121.27	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	W	303	KC2	CHB-C4A-NA	2.26	127.73	124.23
41	v	303	KC2	C4B-C3B-C2B	2.26	108.77	106.81
41	N	312	KC2	CHD-C4C-NC	2.26	127.71	124.31
40	a	838	CLA	CHA-C1A-NA	-2.26	121.28	126.39
40	a	819	CLA	CBA-CAA-C2A	2.26	120.51	113.79
41	t	306	KC2	CHD-C4C-NC	2.26	127.71	124.31
40	G	204	CLA	C1-C2-C3	-2.26	122.50	126.20
40	S	311	CLA	CHB-C1B-NB	-2.26	120.66	124.05
40	a	807	CLA	CHB-C1B-NB	-2.26	120.66	124.05
40	i	101	CLA	CHD-C1D-C2D	2.26	130.18	125.49
43	a	801	LMG	O3-C3-C2	-2.26	105.06	110.38
44	o	314	A86	O4-C34-C35	2.26	113.41	107.64
41	R	309	KC2	CHD-C1D-ND	-2.26	120.67	124.05
41	T	308	KC2	CHB-C4A-NA	2.26	127.73	124.23
40	a	816	CLA	CHA-C1A-NA	-2.26	121.28	126.39
41	Y	309	KC2	CHD-C4C-NC	2.25	127.71	124.31
41	o	309	KC2	CHD-C4C-NC	2.25	127.71	124.31
40	z	314	CLA	CHB-C1B-NB	-2.25	120.67	124.05
42	E	317	DD6	C14-C13-C11	2.25	129.03	125.53
46	P	319	SQD	O7-S-C6	2.25	110.12	106.76
41	S	304	KC2	CHD-C4C-NC	2.25	127.71	124.31
41	p	310	KC2	CHD-C4C-NC	2.25	127.71	124.31
42	x	320	DD6	O1-C15-C14	2.25	123.33	116.88
40	X	310	CLA	CHB-C1B-NB	-2.25	120.67	124.05
41	H	303	KC2	CHB-C4A-NA	2.25	127.73	124.23
41	S	309	KC2	CHB-C4A-NA	2.25	127.73	124.23
42	y	311	DD6	O1-C20-C15	-2.25	57.14	58.93
49	l	207	BCR	C11-C10-C9	2.25	130.44	127.28
41	L	313	KC2	CHB-C4A-NA	2.25	127.72	124.23
40	N	310	CLA	CAA-C2A-C1A	-2.25	104.59	111.97
40	W	308	CLA	CHA-C1A-NA	-2.25	121.29	126.39
40	z	313	CLA	CHA-C1A-NA	-2.25	121.29	126.39
40	Y	313	CLA	C4D-CHA-C1A	-2.25	118.56	121.24
40	F	310	CLA	C2A-C3A-C4A	-2.25	98.23	101.87
41	q	303	KC2	CHD-C1D-ND	-2.25	120.67	124.05
40	U	202	CLA	CHA-C1A-NA	-2.25	121.30	126.39
41	w	301	KC2	CHB-C4A-NA	2.25	127.72	124.23
40	C	304	CLA	CHB-C1B-NB	-2.25	120.67	124.05
42	z	322	DD6	O1-C15-C14	-2.25	110.43	116.88
41	M	309	KC2	CHD-C4C-NC	2.25	127.70	124.31
40	K	308	CLA	CBA-CAA-C2A	2.25	120.48	113.79
46	W	318	SQD	C45-O47-C7	-2.25	112.41	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	P	318	LMG	C7-O1-C1	2.25	118.62	113.80
40	Q	202	CLA	CBA-CAA-C2A	2.25	120.48	113.79
40	b	840	CLA	CMC-C2C-C1C	2.25	128.55	125.03
44	G	209	A86	C21-C20-C19	-2.25	111.72	114.24
40	w	309	CLA	CHB-C1B-NB	-2.25	120.68	124.05
40	Q	209	CLA	CAA-C2A-C1A	-2.25	104.61	111.97
41	w	307	KC2	C2A-C3A-C4A	2.25	108.10	106.41
40	V	202	CLA	CHD-C1D-C2D	2.25	130.16	125.49
40	Z	301	CLA	CHB-C1B-NB	-2.25	120.68	124.05
41	o	309	KC2	CHD-C1D-ND	-2.25	120.68	124.05
40	H	309	CLA	CHB-C1B-NB	-2.25	120.68	124.05
41	C	303	KC2	CHD-C4C-NC	2.25	127.69	124.31
41	R	309	KC2	CHD-C4C-NC	2.24	127.69	124.31
40	x	308	CLA	CHA-C1A-NA	-2.24	121.31	126.39
40	D	304	CLA	CHB-C1B-NB	-2.24	120.68	124.05
44	R	312	A86	C21-C20-C19	-2.24	111.72	114.24
40	x	307	CLA	CHD-C1D-C2D	2.24	130.15	125.49
40	y	303	CLA	CHB-C1B-NB	-2.24	120.68	124.05
41	M	303	KC2	C4B-C3B-C2B	2.24	108.76	106.81
40	O	307	CLA	CMC-C2C-C1C	2.24	128.54	125.03
40	O	304	CLA	CHB-C1B-NB	-2.24	120.69	124.05
40	O	310	CLA	CHB-C1B-NB	-2.24	120.69	124.05
41	W	303	KC2	CHD-C4C-NC	2.24	127.69	124.31
40	Y	312	CLA	CHA-C1A-NA	-2.24	121.31	126.39
43	E	321	LMG	O1-C1-C2	-2.24	104.87	108.27
41	q	308	KC2	CHD-C4C-NC	2.24	127.69	124.31
40	O	310	CLA	C2A-C1A-CHA	2.24	127.75	123.87
41	O	311	KC2	CHD-C4C-NC	2.24	127.69	124.31
40	z	314	CLA	CHC-C4B-NB	-2.24	120.69	124.05
40	J	312	CLA	CHB-C1B-NB	-2.24	120.69	124.05
40	I	201	CLA	CHB-C1B-NB	-2.24	120.69	124.05
40	J	303	CLA	CHB-C1B-NB	-2.24	120.69	124.05
40	P	307	CLA	CHB-C1B-NB	-2.24	120.69	124.05
41	E	319	KC2	CHD-C1D-ND	-2.24	120.69	124.05
41	N	308	KC2	CHD-C4C-NC	2.24	127.68	124.31
40	C	304	CLA	CBA-CAA-C2A	2.24	120.45	113.79
40	H	301	CLA	CHC-C1C-C2C	-2.24	120.59	126.95
40	M	305	CLA	CHA-C1A-NA	-2.24	121.33	126.39
40	X	304	CLA	CHA-C1A-NA	-2.24	121.33	126.39
42	J	316	DD6	O1-C20-C15	-2.24	57.16	58.93
40	S	307	CLA	CHD-C1D-C2D	2.23	130.13	125.49
41	W	310	KC2	CHD-C1D-ND	-2.23	120.70	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	W	308	CLA	CHD-C1D-C2D	2.23	130.13	125.49
40	M	311	CLA	C2C-C1C-NC	2.23	112.33	109.98
43	u	301	LMG	O2-C2-C1	-2.23	104.75	110.08
40	E	309	CLA	CBA-CAA-C2A	2.23	120.44	113.79
40	x	305	CLA	CHD-C1D-C2D	2.23	130.13	125.49
40	A	301	CLA	CHA-C1A-NA	-2.23	121.34	126.39
40	v	304	CLA	CHA-C1A-NA	-2.23	121.34	126.39
41	S	304	KC2	CHB-C4A-NA	2.23	127.69	124.23
40	A	301	CLA	CHC-C1C-C2C	-2.23	120.61	126.95
41	K	309	KC2	CHD-C4C-NC	2.23	127.67	124.31
41	Y	302	KC2	C4B-C3B-C2B	2.23	108.75	106.81
40	J	306	CLA	C1-C2-C3	-2.23	122.54	126.20
40	T	317	CLA	CHA-C1A-NA	-2.23	121.34	126.39
40	D	303	CLA	CHD-C1D-C2D	2.23	130.13	125.49
40	o	307	CLA	CHB-C1B-NB	-2.23	120.70	124.05
41	W	309	KC2	CHD-C4C-NC	2.23	127.67	124.31
40	E	314	CLA	CHD-C1D-C2D	2.23	130.12	125.49
40	J	318	CLA	CHD-C1D-C2D	2.23	130.12	125.49
40	l	202	CLA	CHB-C1B-NB	-2.23	120.70	124.05
40	K	301	CLA	CHB-C1B-NB	-2.23	120.70	124.05
42	A	316	DD6	O1-C20-C15	-2.23	57.16	58.93
40	F	310	CLA	CHB-C1B-NB	-2.23	120.71	124.05
41	W	304	KC2	CHD-C4C-NC	2.23	127.67	124.31
42	P	315	DD6	O1-C20-C15	-2.23	57.16	58.93
40	F	303	CLA	CHA-C1A-NA	-2.23	121.35	126.39
40	v	307	CLA	CHB-C1B-NB	-2.23	120.71	124.05
40	R	306	CLA	CHB-C1B-NB	-2.23	120.71	124.05
40	q	301	CLA	CHB-C1B-NB	-2.23	120.71	124.05
41	E	319	KC2	CHD-C4C-NC	2.23	127.67	124.31
41	R	308	KC2	CHB-C4A-NA	2.23	127.68	124.23
47	p	323	A1EB1	C33-C32-C31	2.23	111.38	109.21
40	O	306	CLA	CHD-C1D-C2D	2.23	130.12	125.49
40	H	305	CLA	CBA-CAA-C2A	2.22	120.41	113.79
40	J	306	CLA	CHB-C1B-NB	-2.22	120.71	124.05
40	B	307	CLA	CHA-C1A-NA	-2.22	121.35	126.39
40	S	311	CLA	CHD-C1D-C2D	2.22	130.11	125.49
41	O	303	KC2	CHB-C4A-NA	2.22	127.68	124.23
40	t	303	CLA	CHB-C1B-NB	-2.22	120.71	124.05
40	o	312	CLA	CHA-C1A-NA	-2.22	121.36	126.39
40	p	308	CLA	CHA-C1A-NA	-2.22	121.36	126.39
40	Z	306	CLA	CHA-C1A-NA	-2.22	121.36	126.39
40	a	825	CLA	CHA-C1A-NA	-2.22	121.36	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	p	303	KC2	CHB-C4A-NA	2.22	127.68	124.23
43	P	318	LMG	C6-C5-C4	-2.22	107.56	113.02
47	v	324	A1EB1	C36-C31-C32	-2.22	117.49	119.70
41	M	303	KC2	CHD-C1D-ND	-2.22	120.72	124.05
40	o	313	CLA	CHA-C1A-NA	-2.22	121.36	126.39
42	U	211	DD6	C14-C13-C11	2.22	128.98	125.53
40	q	304	CLA	CHA-C1A-NA	-2.22	121.36	126.39
40	q	307	CLA	CHB-C4A-NA	2.22	127.60	124.40
41	z	303	KC2	CHB-C4A-NA	2.22	127.67	124.23
40	v	305	CLA	CMC-C2C-C1C	2.22	128.50	125.03
40	u	306	CLA	CHB-C1B-NB	-2.22	120.72	124.05
41	K	305	KC2	CHD-C4C-NC	2.22	127.65	124.31
40	b	838	CLA	CHD-C1D-C2D	2.22	130.10	125.49
40	M	307	CLA	CHB-C1B-NB	-2.22	120.72	124.05
43	P	318	LMG	O3-C3-C2	-2.22	105.15	110.38
40	p	308	CLA	CHD-C1D-C2D	2.22	130.10	125.49
42	v	318	DD6	O1-C20-C15	-2.22	57.17	58.93
40	b	801	CLA	C3A-C2A-C1A	-2.22	98.02	101.34
40	P	313	CLA	CHD-C1D-C2D	2.21	130.09	125.49
40	Y	305	CLA	CHC-C4B-NB	-2.21	120.73	124.05
41	L	313	KC2	CHD-C1D-ND	-2.21	120.73	124.05
41	P	304	KC2	CAC-C3C-C2C	-2.21	121.23	128.43
40	a	808	CLA	CHD-C1D-C2D	2.21	130.09	125.49
40	w	305	CLA	CHB-C1B-NB	-2.21	120.73	124.05
40	z	308	CLA	CHB-C1B-NB	-2.21	120.73	124.05
40	Z	313	CLA	CBA-CAA-C2A	2.21	120.38	113.79
43	x	301	LMG	O8-C28-O10	-2.21	118.09	123.63
41	K	303	KC2	CHB-C4A-NA	2.21	127.66	124.23
41	N	302	KC2	CHD-C4C-NC	2.21	127.64	124.31
40	u	302	CLA	C1-C2-C3	-2.21	122.57	126.20
40	N	310	CLA	CHD-C1D-C2D	2.21	130.09	125.49
41	y	306	KC2	CHD-C4C-NC	2.21	127.64	124.31
40	Q	207	CLA	C2A-C3A-C4A	-2.21	98.30	101.87
40	G	213	CLA	CHA-C1A-NA	-2.21	121.39	126.39
40	p	305	CLA	CHD-C1D-C2D	2.21	130.08	125.49
40	N	310	CLA	CHB-C4A-NA	2.21	127.59	124.40
42	U	209	DD6	C21-C20-C19	2.21	116.72	114.24
41	L	308	KC2	CHB-C4A-NA	2.21	127.66	124.23
40	F	303	CLA	C2C-C1C-NC	2.21	112.80	109.48
40	Z	313	CLA	CHA-C1A-NA	-2.21	121.39	126.39
40	G	203	CLA	CAA-C2A-C3A	2.21	118.97	113.00
40	o	311	CLA	CHB-C1B-NB	-2.21	120.74	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	l	205	CLA	CHA-C1A-NA	-2.21	121.40	126.39
40	G	207	CLA	CHB-C1B-NB	-2.21	120.74	124.05
41	N	309	KC2	CHD-C1D-ND	-2.21	120.74	124.05
41	M	303	KC2	CAC-C3C-C2C	-2.21	121.26	128.43
40	H	309	CLA	O2A-C1-C2	2.21	116.59	108.11
40	H	305	CLA	C1-C2-C3	-2.20	122.59	126.20
40	u	308	CLA	CHD-C1D-C2D	2.20	130.07	125.49
40	u	311	CLA	CHD-C1D-C2D	2.20	130.07	125.49
43	D	318	LMG	O3-C3-C2	-2.20	105.18	110.38
41	H	303	KC2	CHD-C4C-NC	2.20	127.63	124.31
40	E	302	CLA	CHA-C1A-NA	-2.20	121.40	126.39
40	o	310	CLA	C3A-C2A-C1A	-2.20	98.04	101.34
40	a	809	CLA	CHD-C1D-C2D	2.20	130.07	125.49
40	x	311	CLA	CHD-C1D-C2D	2.20	130.07	125.49
40	J	306	CLA	CHA-C1A-NA	-2.20	121.40	126.39
40	p	302	CLA	CHD-C1D-C2D	2.20	130.07	125.49
40	z	307	CLA	CBA-CAA-C2A	2.20	120.35	113.79
41	K	303	KC2	CHD-C4C-NC	2.20	127.63	124.31
43	T	318	LMG	O3-C3-C2	-2.20	105.19	110.38
41	N	313	KC2	CHD-C4C-NC	2.20	127.63	124.31
40	C	307	CLA	CHD-C1D-C2D	2.20	130.07	125.49
41	Y	308	KC2	CHB-C4A-NA	2.20	127.64	124.23
40	y	302	CLA	C3A-C2A-C1A	-2.20	98.04	101.34
43	A	317	LMG	O3-C3-C2	-2.20	105.19	110.38
40	J	311	CLA	CHD-C1D-C2D	2.20	130.06	125.49
41	p	315	KC2	CHD-C4C-NC	2.20	127.63	124.31
40	S	308	CLA	CHB-C4A-NA	2.20	127.58	124.40
40	a	803	CLA	CHD-C1D-C2D	2.20	130.06	125.49
40	v	310	CLA	CHD-C1D-C2D	2.20	130.06	125.49
40	p	312	CLA	CGD-CBD-CAD	-2.20	103.72	110.85
41	R	303	KC2	CHD-C1D-ND	-2.20	120.75	124.05
40	X	311	CLA	CHB-C1B-NB	-2.20	120.75	124.05
40	D	310	CLA	CHA-C1A-NA	-2.20	121.41	126.39
40	q	307	CLA	CHD-C1D-C2D	2.20	130.06	125.49
40	O	305	CLA	CHA-C1A-NA	-2.20	121.41	126.39
40	a	822	CLA	CAA-C2A-C3A	2.20	118.94	113.00
40	o	313	CLA	CHD-C1D-C2D	2.20	130.06	125.49
40	Z	306	CLA	CHB-C1B-NB	-2.20	120.75	124.05
41	I	209	KC2	CHD-C4C-NC	2.20	127.62	124.31
41	v	308	KC2	CHD-C4C-NC	2.20	127.62	124.31
40	E	313	CLA	CHA-C1A-NA	-2.20	121.42	126.39
41	z	304	KC2	CHB-C4A-NA	2.20	127.64	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	M	310	CLA	CHB-C4A-NA	2.20	127.57	124.40
40	a	822	CLA	CHB-C1B-NB	-2.20	120.75	124.05
40	a	812	CLA	CHA-C1A-NA	-2.20	121.42	126.39
40	W	312	CLA	CHC-C1C-C2C	-2.20	120.71	126.95
41	M	301	KC2	CHD-C4C-NC	2.20	127.62	124.31
40	U	202	CLA	CHD-C1D-C2D	2.19	130.05	125.49
40	E	304	CLA	CHA-C1A-NA	-2.19	121.42	126.39
41	M	302	KC2	CHD-C4C-NC	2.19	127.62	124.31
40	v	307	CLA	CHD-C1D-C2D	2.19	130.05	125.49
40	t	304	CLA	CHA-C1A-NA	-2.19	121.42	126.39
41	T	301	KC2	CHB-C4A-NA	2.19	127.63	124.23
40	u	305	CLA	CHD-C1D-C2D	2.19	130.05	125.49
44	X	314	A86	C4-C3-C2	2.19	128.00	123.52
41	L	309	KC2	CHD-C1D-ND	-2.19	120.76	124.05
41	T	303	KC2	CHD-C1D-ND	-2.19	120.76	124.05
40	X	301	CLA	CHD-C1D-C2D	2.19	130.04	125.49
41	A	310	KC2	CHB-C4A-NA	2.19	127.63	124.23
41	T	309	KC2	CHD-C1D-ND	-2.19	120.76	124.05
44	X	318	A86	C36-C31-C32	-2.19	117.52	119.70
40	H	301	CLA	C2C-C1C-NC	2.19	112.28	109.98
40	S	302	CLA	CHA-C1A-NA	-2.19	121.43	126.39
40	a	837	CLA	CHA-C1A-NA	-2.19	121.43	126.39
40	F	321	CLA	CHB-C4A-NA	2.19	127.56	124.40
41	O	301	KC2	CHD-C4C-NC	2.19	127.61	124.31
43	A	317	LMG	O8-C28-O10	-2.19	118.15	123.63
40	Z	311	CLA	CHB-C4A-NA	2.19	127.56	124.40
40	D	306	CLA	CHA-C1A-NA	-2.19	121.43	126.39
40	Y	311	CLA	CGD-CBD-CAD	-2.19	103.76	110.85
41	F	302	KC2	CHB-C4A-NA	2.19	127.62	124.23
40	V	202	CLA	CHC-C1C-NC	2.19	127.61	124.31
42	L	315	DD6	O1-C20-C15	-2.19	57.20	58.93
46	P	319	SQD	O47-C7-O49	-2.19	118.59	123.70
40	X	306	CLA	CMC-C2C-C1C	2.19	128.45	125.03
41	T	308	KC2	CHD-C4C-NC	2.19	127.61	124.31
40	S	311	CLA	CHA-C1A-NA	-2.19	121.44	126.39
41	W	304	KC2	C4C-C3C-C2C	2.19	109.29	107.28
41	u	315	KC2	CHD-C1D-ND	-2.19	120.77	124.05
40	u	314	CLA	CHA-C1A-NA	-2.19	121.44	126.39
40	X	306	CLA	CHD-C1D-C2D	2.19	130.03	125.49
40	z	324	CLA	CHC-C1C-C2C	-2.19	120.74	126.95
43	E	321	LMG	O6-C1-O1	-2.18	104.88	110.04
40	C	308	CLA	C4D-CHA-C1A	-2.18	118.64	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	M	318	SQD	O7-S-C6	2.18	110.02	106.76
40	X	307	CLA	CHB-C1B-NB	-2.18	120.77	124.05
41	P	310	KC2	CHD-C4C-NC	2.18	127.60	124.31
40	U	207	CLA	CHB-C1B-NB	-2.18	120.77	124.05
40	u	308	CLA	CHA-C1A-NA	-2.18	121.45	126.39
41	N	312	KC2	CHB-C4A-NA	2.18	127.62	124.23
40	Y	306	CLA	CMC-C2C-C1C	2.18	128.45	125.03
44	v	314	A86	O4-C34-C35	2.18	113.22	107.64
40	G	203	CLA	CMC-C2C-C1C	2.18	128.44	125.03
42	J	314	DD6	O1-C15-C14	-2.18	110.62	116.88
43	L	319	LMG	O3-C3-C2	-2.18	105.23	110.38
40	o	307	CLA	CBA-CAA-C2A	2.18	120.28	113.79
41	R	301	KC2	CHB-C4A-NA	2.18	127.61	124.23
40	A	301	CLA	CAC-C3C-C4C	2.18	127.63	124.79
40	W	306	CLA	CHA-C1A-NA	-2.18	121.45	126.39
40	a	822	CLA	CHA-C1A-NA	-2.18	121.45	126.39
41	P	304	KC2	C4B-C3B-C2B	2.18	108.70	106.81
40	A	305	CLA	CHD-C1D-C2D	2.18	130.02	125.49
40	I	205	CLA	CHA-C1A-NA	-2.18	121.45	126.39
40	q	307	CLA	CHA-C1A-NA	-2.18	121.45	126.39
41	P	302	KC2	CHB-C4A-NA	2.18	127.61	124.23
43	l	201	LMG	O6-C1-O1	-2.18	104.89	110.04
40	b	840	CLA	CHA-C1A-NA	-2.18	121.46	126.39
41	L	309	KC2	CHD-C4C-NC	2.18	127.59	124.31
40	a	840	CLA	CHD-C1D-C2D	2.18	130.02	125.49
41	W	304	KC2	C4B-C3B-C2B	2.18	108.70	106.81
41	x	310	KC2	C4B-C3B-C2B	2.18	108.70	106.81
40	X	306	CLA	CHA-C1A-NA	-2.18	121.46	126.39
41	T	302	KC2	CHD-C4C-NC	2.18	127.59	124.31
40	J	310	CLA	CHB-C1B-NB	-2.18	120.78	124.05
40	o	313	CLA	CHB-C1B-NB	-2.18	120.78	124.05
41	z	309	KC2	CHD-C4C-NC	2.18	127.59	124.31
40	H	302	CLA	CHD-C1D-C2D	2.18	130.01	125.49
40	J	310	CLA	CHD-C1D-C2D	2.18	130.01	125.49
43	E	301	LMG	C1-C2-C3	-2.18	105.43	110.01
40	W	306	CLA	CHD-C1D-C2D	2.18	130.01	125.49
40	z	305	CLA	CAC-C3C-C4C	2.18	127.62	124.79
40	b	809	CLA	CHD-C1D-C2D	2.18	130.01	125.49
40	v	304	CLA	CHD-C1D-C2D	2.17	130.01	125.49
40	Q	204	CLA	C2C-C1C-NC	2.17	112.75	109.48
40	z	314	CLA	CHA-C1A-NA	-2.17	121.47	126.39
40	x	302	CLA	CHD-C1D-C2D	2.17	130.01	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	D	310	CLA	CHC-C1C-C2C	-2.17	120.77	126.95
41	X	303	KC2	CHD-C4C-NC	2.17	127.58	124.31
43	A	317	LMG	O2-C2-C1	-2.17	104.90	110.08
40	a	808	CLA	C1-C2-C3	-2.17	122.64	126.20
40	a	810	CLA	CHD-C1D-C2D	2.17	130.01	125.49
40	b	830	CLA	CHD-C1D-C2D	2.17	130.01	125.49
40	u	314	CLA	CHD-C1D-C2D	2.17	130.01	125.49
40	Z	312	CLA	CAA-C2A-C3A	2.17	118.87	113.00
49	k	203	BCR	C24-C23-C22	2.17	129.45	126.23
41	p	309	KC2	CHD-C4C-NC	2.17	127.58	124.31
40	y	304	CLA	CHA-C1A-NA	-2.17	121.47	126.39
40	U	208	CLA	CAC-C3C-C4C	2.17	127.62	124.79
40	Z	311	CLA	CHD-C1D-C2D	2.17	130.00	125.49
41	O	301	KC2	C4B-C3B-C2B	2.17	108.70	106.81
42	E	318	DD6	O1-C20-C19	-2.17	111.46	113.49
43	T	318	LMG	O1-C7-C8	-2.17	105.54	110.82
43	W	317	LMG	O8-C28-O10	-2.17	118.20	123.63
41	Y	314	KC2	CHB-C4A-NA	2.17	127.60	124.23
41	o	303	KC2	C4B-C3B-C2B	2.17	108.70	106.81
43	E	321	LMG	O3-C3-C2	-2.17	105.26	110.38
40	z	314	CLA	CHD-C1D-C2D	2.17	130.00	125.49
40	o	305	CLA	CHA-C1A-NA	-2.17	121.48	126.39
40	t	307	CLA	C3A-C2A-C1A	-2.17	98.09	101.34
40	a	807	CLA	CAC-C3C-C4C	2.17	127.61	124.79
40	E	314	CLA	CHC-C4B-NB	-2.17	120.80	124.05
40	b	840	CLA	CHB-C1B-NB	-2.17	120.80	124.05
40	D	311	CLA	CHD-C1D-C2D	2.17	130.00	125.49
40	E	305	CLA	CHB-C1B-NB	-2.17	120.80	124.05
42	D	315	DD6	O1-C20-C15	-2.17	57.21	58.93
43	E	321	LMG	O6-C5-C4	2.17	113.61	109.70
40	b	821	CLA	CHB-C1B-NB	-2.17	120.80	124.05
40	b	822	CLA	CHD-C1D-C2D	2.17	130.00	125.49
40	a	834	CLA	CAA-C2A-C1A	-2.17	104.87	111.97
41	A	310	KC2	CHD-C4C-NC	2.17	127.57	124.31
40	Z	306	CLA	CMC-C2C-C1C	2.17	128.42	125.03
40	Y	313	CLA	CHA-C1A-NA	-2.17	121.49	126.39
40	u	302	CLA	CHD-C1D-C2D	2.17	129.99	125.49
41	R	311	KC2	CHD-C4C-NC	2.17	127.57	124.31
43	x	301	LMG	C1-C2-C3	-2.17	105.45	110.01
40	S	305	CLA	CHD-C1D-C2D	2.17	129.99	125.49
41	o	308	KC2	CHB-C4A-NA	2.17	127.59	124.23
40	t	305	CLA	CHB-C1B-NB	-2.17	120.80	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	v	318	DD6	O1-C20-C19	-2.16	111.46	113.49
40	I	208	CLA	C3A-C2A-C1A	-2.16	98.10	101.34
41	M	308	KC2	C4C-C3C-C2C	2.16	109.27	107.28
43	a	801	LMG	O2-C2-C1	-2.16	104.92	110.08
40	a	816	CLA	CHC-C4B-NB	-2.16	120.80	124.05
40	b	801	CLA	CHD-C1D-C2D	2.16	129.99	125.49
40	b	838	CLA	CHA-C1A-NA	-2.16	121.49	126.39
41	L	303	KC2	C4C-C3C-C2C	2.16	109.27	107.28
46	I	215	SQD	O7-S-C6	2.16	109.98	106.76
40	a	842	CLA	CHA-C1A-NA	-2.16	121.50	126.39
40	z	312	CLA	CHB-C1B-NB	-2.16	120.81	124.05
40	X	305	CLA	CHD-C1D-C2D	2.16	129.98	125.49
40	b	833	CLA	C1-C2-C3	-2.16	122.66	126.20
40	F	310	CLA	CGD-CBD-CAD	-2.16	103.85	110.85
40	M	311	CLA	CHA-C1A-NA	-2.16	121.50	126.39
40	b	821	CLA	CHA-C1A-NA	-2.16	121.50	126.39
41	K	305	KC2	CHB-C4A-NA	2.16	127.58	124.23
40	a	838	CLA	CHB-C1B-NB	-2.16	120.81	124.05
40	y	309	CLA	CHD-C1D-C2D	2.16	129.98	125.49
41	o	303	KC2	CHB-C4A-NA	2.16	127.58	124.23
40	Y	305	CLA	C1-C2-C3	2.16	129.74	126.20
42	Q	213	DD6	O1-C15-C14	-2.16	110.69	116.88
40	X	313	CLA	CHD-C1D-C2D	2.16	129.98	125.49
40	E	312	CLA	CHA-C1A-NA	-2.16	121.50	126.39
40	v	310	CLA	C4D-CHA-C1A	-2.16	118.67	121.24
40	q	305	CLA	CHD-C1D-C2D	2.16	129.98	125.49
40	C	302	CLA	CHD-C1D-C2D	2.16	129.97	125.49
40	o	310	CLA	C2A-C1A-CHA	2.16	127.61	123.87
40	C	309	CLA	CHA-C1A-NA	-2.16	121.51	126.39
40	O	310	CLA	CHA-C1A-NA	-2.16	121.51	126.39
41	q	303	KC2	CHB-C4A-NA	2.16	127.58	124.23
44	S	316	A86	C21-C20-C19	-2.16	111.82	114.24
40	X	310	CLA	CHA-C1A-NA	-2.15	121.51	126.39
40	J	305	CLA	CHA-C1A-NA	-2.15	121.51	126.39
40	b	824	CLA	CAA-C2A-C3A	2.15	118.82	113.00
40	b	839	CLA	CHD-C1D-C2D	2.15	129.97	125.49
40	k	202	CLA	CHB-C1B-NB	-2.15	120.82	124.05
40	Q	204	CLA	CHB-C4A-NA	2.15	127.51	124.40
40	Z	310	CLA	C2A-C1A-CHA	2.15	127.60	123.87
41	J	304	KC2	CHB-C4A-NA	2.15	127.57	124.23
40	a	818	CLA	CHB-C1B-NB	-2.15	120.82	124.05
40	y	305	CLA	CHB-C1B-NB	-2.15	120.82	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	X	303	KC2	C4B-C3B-C2B	2.15	108.68	106.81
43	a	802	LMG	O3-C3-C2	-2.15	105.30	110.38
40	S	302	CLA	O2A-C1-C2	2.15	116.39	108.11
40	q	310	CLA	CHD-C1D-C2D	2.15	129.96	125.49
40	Q	209	CLA	CHA-C1A-NA	-2.15	121.52	126.39
40	P	305	CLA	CMC-C2C-C1C	2.15	128.40	125.03
41	y	307	KC2	C4C-C3C-C2C	2.15	109.26	107.28
47	K	313	A1EB1	C40-C32-C33	2.15	119.25	109.06
41	v	303	KC2	CHB-C4A-NA	2.15	127.57	124.23
41	w	306	KC2	C4B-C3B-C2B	2.15	108.68	106.81
40	J	302	CLA	CHA-C1A-NA	-2.15	121.52	126.39
40	I	207	CLA	CHD-C1D-C2D	2.15	129.96	125.49
40	Q	203	CLA	CHD-C1D-C2D	2.15	129.96	125.49
41	W	310	KC2	CHD-C4C-NC	2.15	127.55	124.31
40	b	831	CLA	CHA-C1A-NA	-2.15	121.52	126.39
40	a	805	CLA	CHD-C1D-C2D	2.15	129.96	125.49
40	t	302	CLA	CHD-C1D-C2D	2.15	129.96	125.49
40	D	307	CLA	CHD-C1D-C2D	2.15	129.96	125.49
40	Q	207	CLA	CHD-C1D-C2D	2.15	129.96	125.49
40	y	302	CLA	CHD-C1D-C2D	2.15	129.96	125.49
41	X	303	KC2	CHB-C4A-NA	2.15	127.56	124.23
43	F	318	LMG	O3-C3-C2	-2.15	105.32	110.38
40	C	304	CLA	CMC-C2C-C1C	2.15	128.39	125.03
40	v	313	CLA	CHA-C1A-NA	-2.15	121.53	126.39
40	Z	313	CLA	CHD-C1D-C2D	2.15	129.95	125.49
40	x	302	CLA	CHA-C1A-NA	-2.15	121.53	126.39
40	Z	310	CLA	CAA-C2A-C1A	-2.15	104.94	111.97
40	u	302	CLA	CHA-C1A-NA	-2.15	121.53	126.39
44	q	314	A86	O4-C34-C35	2.14	113.13	107.64
40	N	311	CLA	CHB-C1B-NB	-2.14	120.83	124.05
40	X	313	CLA	CHA-C1A-NA	-2.14	121.53	126.39
40	z	313	CLA	CHD-C1D-C2D	2.14	129.95	125.49
40	b	829	CLA	CHA-C1A-NA	-2.14	121.54	126.39
43	p	301	LMG	O3-C3-C2	-2.14	105.32	110.38
44	T	319	A86	O1-C20-C19	2.14	115.50	113.49
40	U	207	CLA	CHA-C1A-NA	-2.14	121.54	126.39
40	b	808	CLA	CHD-C1D-C2D	2.14	129.94	125.49
40	a	815	CLA	CHA-C1A-NA	-2.14	121.54	126.39
40	q	313	CLA	CHD-C1D-C2D	2.14	129.94	125.49
40	C	304	CLA	CHB-C4A-NA	2.14	127.49	124.40
44	u	320	A86	C36-C31-C32	-2.14	117.57	119.70
40	b	829	CLA	CHD-C1D-C2D	2.14	129.94	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	N	303	KC2	CHB-C4A-NA	2.14	127.55	124.23
40	P	307	CLA	CHA-C1A-NA	-2.14	121.54	126.39
40	l	204	CLA	CHA-C1A-NA	-2.14	121.54	126.39
40	E	305	CLA	CHD-C1D-C2D	2.14	129.94	125.49
40	W	307	CLA	CBA-CAA-C2A	2.14	120.16	113.79
40	C	307	CLA	CHA-C1A-NA	-2.14	121.54	126.39
43	W	317	LMG	O6-C1-O1	-2.14	104.98	110.04
49	b	846	BCR	C24-C23-C22	2.14	129.40	126.23
40	b	816	CLA	CHA-C1A-NA	-2.14	121.54	126.39
40	y	303	CLA	C4D-CHA-C1A	-2.14	118.69	121.24
40	o	310	CLA	CHD-C1D-C2D	2.14	129.94	125.49
40	v	313	CLA	C3A-C2A-C1A	-2.14	98.14	101.34
40	b	801	CLA	CHA-C1A-NA	-2.14	121.55	126.39
40	Z	312	CLA	CHD-C1D-C2D	2.14	129.93	125.49
40	b	811	CLA	CHA-C1A-NA	-2.14	121.55	126.39
40	b	820	CLA	CHA-C1A-NA	-2.14	121.55	126.39
40	j	102	CLA	CHA-C1A-NA	-2.14	121.55	126.39
40	U	202	CLA	CHB-C1B-NB	-2.14	120.84	124.05
41	I	209	KC2	CHB-C4A-NA	2.14	127.55	124.23
40	Z	312	CLA	C3A-C2A-C1A	-2.14	98.14	101.34
40	p	306	CLA	CHA-C1A-NA	-2.14	121.55	126.39
40	a	838	CLA	CHD-C1D-C2D	2.14	129.93	125.49
40	u	305	CLA	CHC-C4B-NB	-2.14	120.84	124.05
40	G	207	CLA	CHA-C1A-NA	-2.14	121.55	126.39
49	l	208	BCR	C15-C16-C17	2.13	127.89	123.52
40	v	305	CLA	CHD-C1D-C2D	2.13	129.93	125.49
40	Q	207	CLA	CHA-C1A-NA	-2.13	121.56	126.39
41	z	310	KC2	CHD-C4C-NC	2.13	127.52	124.31
40	L	304	CLA	CHB-C1B-NB	-2.13	120.85	124.05
40	Y	306	CLA	CHB-C1B-NB	-2.13	120.85	124.05
40	E	303	CLA	CHA-C1A-NA	-2.13	121.56	126.39
40	Y	307	CLA	CHB-C1B-NB	-2.13	120.85	124.05
45	a	848	LHG	C11-C10-C9	-2.13	103.59	114.37
40	A	311	CLA	CHA-C1A-NA	-2.13	121.56	126.39
40	B	301	CLA	CHD-C1D-C2D	2.13	129.92	125.49
40	b	811	CLA	CHD-C1D-C2D	2.13	129.92	125.49
40	H	302	CLA	CHA-C1A-NA	-2.13	121.56	126.39
40	Z	312	CLA	CMC-C2C-C1C	2.13	128.37	125.03
40	E	302	CLA	C3A-C2A-C1A	-2.13	98.15	101.34
47	t	313	A1EB1	C36-C31-C32	-2.13	117.58	119.70
40	S	313	CLA	CHB-C4A-NA	2.13	127.47	124.40
41	Y	303	KC2	CHD-C4C-NC	2.13	127.52	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	w	301	KC2	CHD-C4C-NC	2.13	127.52	124.31
41	q	302	KC2	C1A-NA-C4A	2.13	107.65	106.68
40	U	207	CLA	CHC-C4B-NB	-2.13	120.85	124.05
40	l	203	CLA	CHD-C1D-C2D	2.13	129.92	125.49
40	w	309	CLA	CHD-C1D-C2D	2.13	129.92	125.49
41	I	209	KC2	C4B-C3B-C2B	2.13	108.66	106.81
41	W	303	KC2	C4B-C3B-C2B	2.13	108.66	106.81
40	w	304	CLA	CHA-C1A-NA	-2.13	121.57	126.39
40	a	833	CLA	C6-C7-C8	2.13	123.04	115.97
40	E	305	CLA	CMC-C2C-C1C	2.13	128.36	125.03
42	Q	212	DD6	O1-C20-C15	-2.13	57.24	58.93
40	a	816	CLA	CAA-C2A-C3A	2.13	118.75	113.00
40	Q	205	CLA	CHD-C1D-C2D	2.13	129.91	125.49
40	b	828	CLA	CHA-C1A-NA	-2.13	121.57	126.39
40	a	850	CLA	CHA-C1A-NA	-2.13	121.57	126.39
40	C	307	CLA	CHB-C1B-NB	-2.13	120.86	124.05
40	t	307	CLA	CHD-C1D-C2D	2.13	129.91	125.49
40	z	324	CLA	C2C-C1C-NC	2.13	112.22	109.98
40	u	306	CLA	CHB-C4A-NA	2.13	127.47	124.40
45	S	323	LHG	C27-C26-C25	-2.13	103.62	114.37
41	G	202	KC2	C3A-C4A-NA	-2.13	107.82	110.45
40	a	813	CLA	CHA-C1A-NA	-2.13	121.58	126.39
46	F	320	SQD	O47-C7-O49	-2.13	118.73	123.70
40	q	304	CLA	CHD-C1D-C2D	2.13	129.91	125.49
40	a	840	CLA	CHA-C1A-NA	-2.13	121.58	126.39
40	b	838	CLA	CHB-C1B-NB	-2.13	120.86	124.05
40	S	312	CLA	CHD-C1D-C2D	2.13	129.91	125.49
40	o	307	CLA	CHD-C1D-C2D	2.13	129.91	125.49
40	a	829	CLA	CHA-C1A-NA	-2.13	121.58	126.39
41	M	308	KC2	CHB-C4A-NA	2.13	127.53	124.23
41	t	301	KC2	CHB-C4A-NA	2.13	127.53	124.23
42	N	319	DD6	O1-C20-C15	-2.12	57.25	58.93
40	X	312	CLA	C4D-CHA-C1A	-2.12	118.71	121.24
41	O	301	KC2	CHD-C1D-ND	-2.12	120.86	124.05
40	S	314	CLA	CHD-C1D-C2D	2.12	129.90	125.49
46	F	320	SQD	O6-C1-C2	2.12	111.50	108.27
40	M	312	CLA	CBA-CAA-C2A	2.12	120.11	113.79
41	L	303	KC2	CHD-C4C-NC	2.12	127.51	124.31
40	q	306	CLA	CHD-C1D-C2D	2.12	129.90	125.49
40	a	851	CLA	CHB-C4A-NA	2.12	127.46	124.40
40	b	835	CLA	CHB-C4A-NA	2.12	127.46	124.40
40	b	834	CLA	CHB-C1B-NB	-2.12	120.86	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	A	303	CLA	C2C-C1C-NC	2.12	112.21	109.98
40	A	307	CLA	CHA-C1A-NA	-2.12	121.59	126.39
40	C	304	CLA	CHD-C1D-C2D	2.12	129.90	125.49
40	G	206	CLA	CHD-C1D-C2D	2.12	129.90	125.49
40	J	303	CLA	CHD-C1D-C2D	2.12	129.90	125.49
44	q	314	A86	C33-C32-C31	2.12	111.27	109.21
40	v	307	CLA	CHA-C1A-NA	-2.12	121.59	126.39
40	M	305	CLA	C6-C7-C8	2.12	123.01	115.97
40	t	304	CLA	CMC-C2C-C1C	2.12	128.35	125.03
40	B	301	CLA	C2A-C1A-CHA	2.12	127.55	123.87
40	D	307	CLA	CHA-C1A-NA	-2.12	121.59	126.39
40	X	312	CLA	CHA-C1A-NA	-2.12	121.59	126.39
40	a	830	CLA	CBA-CAA-C2A	2.12	120.10	113.79
40	z	306	CLA	CHD-C1D-C2D	2.12	129.89	125.49
41	N	302	KC2	CHB-C4A-NA	2.12	127.52	124.23
43	a	801	LMG	C1-O6-C5	-2.12	109.58	113.72
40	B	304	CLA	CHD-C1D-C2D	2.12	129.89	125.49
40	o	310	CLA	C2A-C3A-C4A	-2.12	98.45	101.87
40	G	201	CLA	CHA-C1A-NA	-2.12	121.60	126.39
44	x	317	A86	C33-C32-C31	2.12	111.27	109.21
40	X	306	CLA	CHB-C1B-NB	-2.12	120.87	124.05
40	Q	205	CLA	CHC-C1C-NC	2.12	127.44	124.33
40	a	830	CLA	CHD-C1D-C2D	2.12	129.89	125.49
40	Y	306	CLA	CBA-CAA-C2A	2.12	120.09	113.79
40	B	306	CLA	CHB-C4A-NA	2.12	127.45	124.40
40	F	304	CLA	CHD-C1D-C2D	2.12	129.89	125.49
40	F	305	CLA	CHD-C1D-C2D	2.12	129.89	125.49
40	b	808	CLA	C4D-CHA-C1A	-2.12	118.72	121.24
41	O	303	KC2	C4B-C3B-C2B	2.12	108.65	106.81
40	Q	205	CLA	C2C-C1C-NC	2.11	112.66	109.48
40	a	841	CLA	CHD-C1D-C2D	2.11	129.88	125.49
40	T	307	CLA	C1-C2-C3	-2.11	122.73	126.20
40	Q	204	CLA	CHC-C1C-NC	2.11	127.44	124.33
40	a	834	CLA	CHD-C1D-C2D	2.11	129.88	125.49
41	Z	303	KC2	CHB-C4A-NA	2.11	127.51	124.23
40	T	304	CLA	CHD-C1D-C2D	2.11	129.88	125.49
40	T	307	CLA	CHD-C1D-C2D	2.11	129.88	125.49
40	R	310	CLA	CHA-C1A-NA	-2.11	121.61	126.39
40	u	311	CLA	CAA-C2A-C1A	-2.11	105.05	111.97
40	x	314	CLA	CHA-C1A-NA	-2.11	121.61	126.39
40	M	310	CLA	CHA-C1A-NA	-2.11	121.61	126.39
40	Z	312	CLA	CAA-C2A-C1A	-2.11	105.06	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	b	803	CLA	C1-C2-C3	2.11	129.66	126.20
40	a	806	CLA	C11-C12-C13	2.11	122.98	115.97
40	a	823	CLA	CHA-C1A-NA	-2.11	121.61	126.39
40	a	804	CLA	CHC-C1C-NC	2.11	127.43	124.33
40	v	307	CLA	CHB-C4A-NA	2.11	127.45	124.40
47	N	320	A1EB1	O4-C34-C33	2.11	113.04	107.64
40	C	305	CLA	C1-C2-C3	2.11	129.66	126.20
40	B	302	CLA	CHA-C1A-NA	-2.11	121.61	126.39
40	z	308	CLA	CBA-CAA-C2A	2.11	120.07	113.79
40	S	306	CLA	CHC-C4B-NB	-2.11	120.88	124.05
40	b	820	CLA	CHD-C1D-C2D	2.11	129.88	125.49
40	o	305	CLA	CHD-C1D-C2D	2.11	129.87	125.49
40	x	311	CLA	CAA-C2A-C1A	-2.11	105.06	111.97
40	G	206	CLA	CHA-C1A-NA	-2.11	121.62	126.39
41	R	303	KC2	CAC-C3C-C2C	-2.11	121.58	128.43
40	x	306	CLA	CHC-C1C-C2C	-2.11	120.96	126.95
41	T	303	KC2	CAC-C3C-C2C	-2.11	121.58	128.43
40	u	306	CLA	CHA-C1A-NA	-2.11	121.62	126.39
40	F	308	CLA	CHD-C1D-C2D	2.11	129.87	125.49
52	b	850	DGD	CCB-CBB-CAB	-2.11	103.72	114.37
44	K	314	A86	C21-C20-C19	-2.11	111.87	114.24
40	R	307	CLA	CHB-C1B-NB	-2.11	120.89	124.05
41	R	308	KC2	CHD-C4C-NC	2.11	127.48	124.31
41	v	303	KC2	CHD-C1D-ND	-2.11	120.89	124.05
40	W	305	CLA	CHD-C1D-C2D	2.11	129.87	125.49
40	a	804	CLA	CHD-C1D-C2D	2.11	129.87	125.49
40	J	312	CLA	CBA-CAA-C2A	2.11	120.06	113.79
40	b	810	CLA	CHA-C1A-NA	-2.11	121.62	126.39
40	b	809	CLA	CAA-C2A-C1A	-2.11	105.08	111.97
44	Z	315	A86	C33-C32-C31	2.11	111.26	109.21
44	w	315	A86	C36-C31-C32	-2.11	117.61	119.70
40	F	311	CLA	CHD-C1D-C2D	2.10	129.87	125.49
40	o	304	CLA	CHD-C1D-C2D	2.10	129.86	125.49
40	p	307	CLA	CHD-C1D-C2D	2.10	129.86	125.49
40	H	307	CLA	CHD-C1D-C2D	2.10	129.86	125.49
40	a	820	CLA	CHD-C1D-C2D	2.10	129.86	125.49
41	x	315	KC2	CHD-C1D-ND	-2.10	120.89	124.05
40	Y	306	CLA	CHD-C1D-C2D	2.10	129.86	125.49
40	x	306	CLA	CHD-C1D-C2D	2.10	129.86	125.49
40	a	830	CLA	CHA-C1A-NA	-2.10	121.63	126.39
40	R	307	CLA	CHD-C1D-C2D	2.10	129.86	125.49
40	L	311	CLA	CHA-C1A-NA	-2.10	121.63	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	W	318	SQD	O9-S-C6	2.10	109.89	106.76
44	o	315	A86	C36-C31-C32	-2.10	117.61	119.70
40	P	306	CLA	CHA-C1A-NA	-2.10	121.63	126.39
40	v	301	CLA	CHA-C1A-NA	-2.10	121.64	126.39
40	N	310	CLA	C4D-CHA-C1A	-2.10	118.74	121.24
40	p	305	CLA	CAC-C3C-C4C	2.10	127.52	124.79
41	L	302	KC2	CHB-C4A-NA	2.10	127.49	124.23
40	x	306	CLA	CHA-C1A-NA	-2.10	121.64	126.39
40	L	304	CLA	CHA-C1A-NA	-2.10	121.64	126.39
40	b	817	CLA	C2C-C1C-NC	2.10	112.19	109.98
40	b	805	CLA	CHD-C1D-C2D	2.10	129.85	125.49
41	P	310	KC2	CHB-C4A-NA	2.10	127.48	124.23
43	E	301	LMG	O2-C2-C1	-2.10	105.08	110.08
40	a	833	CLA	CHB-C4A-NA	2.10	127.43	124.40
40	T	310	CLA	CHD-C1D-C2D	2.10	129.85	125.49
40	W	313	CLA	CHD-C1D-C2D	2.10	129.85	125.49
40	y	303	CLA	CHD-C1D-C2D	2.10	129.85	125.49
41	R	302	KC2	CHB-C4A-NA	2.10	127.48	124.23
41	u	303	KC2	CHB-C4A-NA	2.10	127.48	124.23
41	x	303	KC2	CHB-C4A-NA	2.10	127.48	124.23
40	a	809	CLA	CHA-C1A-NA	-2.10	121.65	126.39
40	G	204	CLA	CHD-C1D-C2D	2.10	129.84	125.49
40	X	311	CLA	CHD-C1D-C2D	2.10	129.84	125.49
43	u	301	LMG	O3-C3-C2	-2.10	105.44	110.38
42	u	321	DD6	O1-C15-C14	2.10	122.88	116.88
41	Y	303	KC2	CHB-C4A-NA	2.10	127.48	124.23
40	O	310	CLA	C3A-C2A-C1A	-2.09	98.20	101.34
40	W	307	CLA	CHA-C1A-NA	-2.09	121.65	126.39
40	v	313	CLA	CHD-C1D-C2D	2.09	129.84	125.49
40	Y	307	CLA	C6-C7-C8	2.09	122.93	115.97
43	L	319	LMG	O2-C2-C1	-2.09	105.09	110.08
40	T	305	CLA	CHA-C1A-NA	-2.09	121.65	126.39
40	b	813	CLA	CHD-C1D-C2D	2.09	129.84	125.49
42	N	319	DD6	C30-C29-C27	-2.09	169.12	176.23
40	a	829	CLA	CHD-C1D-C2D	2.09	129.84	125.49
40	H	304	CLA	CHA-C1A-NA	-2.09	121.65	126.39
40	o	312	CLA	CHD-C1D-C2D	2.09	129.84	125.49
40	u	307	CLA	CHD-C1D-C2D	2.09	129.84	125.49
40	Z	307	CLA	CHA-C1A-NA	-2.09	121.66	126.39
40	v	305	CLA	CHA-C1A-NA	-2.09	121.66	126.39
44	z	316	A86	C36-C31-C32	-2.09	117.62	119.70
47	t	313	A1EB1	C29-C30-C31	-2.09	175.19	177.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	S	312	CLA	C2A-C3A-C4A	-2.09	98.49	101.87
41	P	304	KC2	CHD-C1D-ND	-2.09	120.91	124.05
40	O	316	CLA	CHA-C1A-NA	-2.09	121.66	126.39
40	a	810	CLA	CHC-C4B-NB	-2.09	120.92	124.05
40	N	304	CLA	CHD-C1D-C2D	2.09	129.83	125.49
43	L	319	LMG	O7-C10-O9	-2.09	118.82	123.70
40	L	301	CLA	CHD-C1D-C2D	2.09	129.83	125.49
40	Z	306	CLA	CHD-C1D-C2D	2.09	129.83	125.49
40	Z	312	CLA	C2A-C1A-CHA	2.09	127.49	123.87
40	o	307	CLA	CGD-CBD-CAD	-2.09	104.09	110.85
40	u	313	CLA	CGD-CBD-CAD	-2.09	104.09	110.85
40	L	304	CLA	CHD-C1D-C2D	2.09	129.83	125.49
40	i	101	CLA	CHB-C1B-NB	-2.09	120.92	124.05
40	a	814	CLA	CHD-C1D-C2D	2.09	129.83	125.49
41	N	303	KC2	CAC-C3C-C2C	-2.09	121.64	128.43
42	A	313	DD6	O1-C20-C15	-2.09	57.28	58.93
40	U	208	CLA	CMA-C3A-C4A	2.09	117.38	111.77
40	b	829	CLA	CHB-C4A-NA	2.09	127.41	124.40
41	T	303	KC2	C3C-C2C-C1C	2.09	107.98	106.41
40	L	306	CLA	CHD-C1D-C2D	2.09	129.83	125.49
40	j	102	CLA	CHD-C1D-C2D	2.09	129.83	125.49
40	a	842	CLA	CHB-C4A-NA	2.09	127.41	124.40
41	O	303	KC2	CHD-C4C-NC	2.09	127.45	124.31
40	b	815	CLA	CHD-C1D-C2D	2.09	129.82	125.49
40	B	307	CLA	CHC-C1C-C2C	-2.09	121.02	126.95
40	b	837	CLA	CHD-C1D-C2D	2.09	129.82	125.49
40	l	205	CLA	CHD-C1D-C2D	2.09	129.82	125.49
40	S	308	CLA	CHD-C1D-C2D	2.08	129.82	125.49
40	b	836	CLA	CHD-C1D-C2D	2.08	129.82	125.49
41	H	316	KC2	CHC-C1C-C2C	-2.08	121.74	125.03
40	b	822	CLA	C4D-CHA-C1A	-2.08	118.76	121.24
40	O	304	CLA	CHD-C1D-C2D	2.08	129.82	125.49
41	T	311	KC2	CHD-C4C-NC	2.08	127.45	124.31
43	p	301	LMG	O2-C2-C1	-2.08	105.11	110.08
40	E	302	CLA	CHD-C1D-C2D	2.08	129.82	125.49
40	q	304	CLA	CHB-C4A-NA	2.08	127.41	124.40
50	a	847	PQN	C11-C3-C4	-2.08	116.39	118.58
40	P	308	CLA	CHD-C1D-C2D	2.08	129.82	125.49
40	b	807	CLA	C3D-C4D-ND	2.08	113.37	109.99
40	X	310	CLA	C2A-C1A-CHA	2.08	127.48	123.87
40	I	204	CLA	CHC-C1C-C2C	-2.08	121.03	126.95
40	v	311	CLA	CHC-C1C-C2C	-2.08	121.03	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	Q	206	CLA	CHC-C1C-NC	2.08	127.39	124.33
40	I	207	CLA	CHA-C1A-NA	-2.08	121.68	126.39
40	o	311	CLA	CHD-C1D-C2D	2.08	129.81	125.49
40	H	305	CLA	CHD-C1D-C2D	2.08	129.81	125.49
40	a	816	CLA	CHD-C1D-C2D	2.08	129.81	125.49
40	R	304	CLA	CHB-C4A-NA	2.08	127.40	124.40
40	b	802	CLA	C1-C2-C3	-2.08	122.79	126.20
40	a	826	CLA	CHD-C1D-C2D	2.08	129.81	125.49
40	Y	307	CLA	CHB-C4A-NA	2.08	127.40	124.40
40	E	314	CLA	C4D-CHA-C1A	-2.08	118.76	121.24
40	q	310	CLA	CHB-C4A-NA	2.08	127.40	124.40
40	q	313	CLA	CAA-C2A-C1A	-2.08	105.16	111.97
42	k	204	DD6	O1-C15-C14	-2.08	110.92	116.88
41	M	301	KC2	CHB-C4A-NA	2.08	127.45	124.23
43	j	101	LMG	C6-C5-C4	-2.08	107.92	113.02
40	W	305	CLA	CHB-C4A-NA	2.08	127.40	124.40
40	a	835	CLA	CHC-C4B-NB	-2.08	120.93	124.05
40	U	206	CLA	CHC-C1C-C2C	-2.08	121.04	126.95
44	N	315	A86	C21-C20-C19	2.08	116.57	114.24
41	R	301	KC2	C4B-C3B-C2B	2.08	108.61	106.81
41	N	313	KC2	CHB-C4A-NA	2.08	127.45	124.23
40	z	305	CLA	O2A-C1-C2	2.08	116.10	108.11
40	b	828	CLA	CHB-C4A-NA	2.08	127.40	124.40
40	E	306	CLA	CHD-C1D-C2D	2.08	129.81	125.49
43	a	802	LMG	O7-C10-O9	-2.08	118.85	123.70
40	L	310	CLA	CHD-C1D-C2D	2.08	129.80	125.49
40	M	312	CLA	CHD-C1D-C2D	2.08	129.80	125.49
40	Q	204	CLA	CHD-C1D-C2D	2.08	129.80	125.49
40	D	312	CLA	CHA-C1A-NA	-2.08	121.69	126.39
40	M	307	CLA	C1-C2-C3	-2.08	122.80	126.20
40	b	817	CLA	CHD-C1D-C2D	2.08	129.80	125.49
40	b	827	CLA	CHD-C1D-C2D	2.08	129.80	125.49
41	y	307	KC2	CHB-C4A-NA	2.08	127.45	124.23
41	Z	309	KC2	CHD-C4C-NC	2.07	127.44	124.31
44	O	312	A86	C21-C20-C19	-2.07	111.91	114.24
40	C	301	CLA	CHD-C1D-C2D	2.07	129.80	125.49
40	b	836	CLA	CAA-C2A-C1A	-2.07	105.18	111.97
40	C	305	CLA	CHD-C1D-C2D	2.07	129.80	125.49
40	a	821	CLA	CHD-C1D-C2D	2.07	129.80	125.49
40	x	314	CLA	CHD-C1D-C2D	2.07	129.80	125.49
41	T	302	KC2	CHB-C4A-NA	2.07	127.45	124.23
40	F	321	CLA	CHD-C1D-C2D	2.07	129.80	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	D	318	LMG	O2-C2-C1	-2.07	105.14	110.08
40	Q	208	CLA	CAC-C3C-C4C	2.07	127.49	124.79
40	z	312	CLA	CHA-C1A-NA	-2.07	121.70	126.39
40	G	203	CLA	CHD-C1D-C2D	2.07	129.80	125.49
40	b	816	CLA	C4D-CHA-C1A	-2.07	118.77	121.24
40	p	312	CLA	CHA-C1A-NA	-2.07	121.70	126.39
44	p	319	A86	C36-C31-C32	-2.07	117.64	119.70
41	H	316	KC2	CHD-C4C-NC	2.07	127.43	124.31
40	O	305	CLA	CHD-C1D-C2D	2.07	129.79	125.49
40	q	305	CLA	CHB-C4A-NA	2.07	127.39	124.40
40	x	306	CLA	CHB-C4A-NA	2.07	127.39	124.40
40	L	311	CLA	CHD-C1D-C2D	2.07	129.79	125.49
40	F	306	CLA	CHA-C1A-NA	-2.07	121.70	126.39
40	o	306	CLA	CHA-C1A-NA	-2.07	121.70	126.39
40	H	309	CLA	CHD-C1D-C2D	2.07	129.79	125.49
46	P	319	SQD	O48-C23-O10	-2.07	118.45	123.63
40	b	824	CLA	CHD-C1D-C2D	2.07	129.79	125.49
40	a	813	CLA	CHD-C1D-C2D	2.07	129.79	125.49
40	T	310	CLA	CHA-C1A-NA	-2.07	121.71	126.39
40	w	302	CLA	CHD-C1D-C2D	2.07	129.79	125.49
40	L	312	CLA	CHD-C1D-C2D	2.07	129.79	125.49
41	N	309	KC2	CHB-C4A-NA	2.07	127.44	124.23
40	O	304	CLA	CHB-C4A-NA	2.07	127.38	124.40
40	z	306	CLA	CHB-C4A-NA	2.07	127.38	124.40
40	a	808	CLA	C4D-CHA-C1A	-2.07	118.78	121.24
40	b	830	CLA	CHB-C4A-NA	2.07	127.38	124.40
40	E	303	CLA	CHD-C1D-C2D	2.07	129.78	125.49
43	E	301	LMG	O3-C3-C2	-2.07	105.50	110.38
40	J	308	CLA	CHA-C1A-NA	-2.07	121.71	126.39
41	L	303	KC2	CHB-C4A-NA	2.07	127.44	124.23
40	A	307	CLA	CHD-C1D-C2D	2.07	129.78	125.49
40	H	302	CLA	CBA-CAA-C2A	2.07	119.94	113.79
40	E	309	CLA	CHC-C1C-C2C	-2.07	121.08	126.95
43	u	301	LMG	C1-O6-C5	-2.06	109.69	113.72
41	Y	302	KC2	CHD-C4C-NC	2.06	127.42	124.31
40	P	311	CLA	CHD-C1D-C2D	2.06	129.78	125.49
41	R	301	KC2	CHD-C4C-NC	2.06	127.42	124.31
40	Z	310	CLA	CHC-C4B-NB	-2.06	120.95	124.05
40	f	204	CLA	CHD-C1D-C2D	2.06	129.78	125.49
40	z	308	CLA	O2A-C1-C2	2.06	116.04	108.11
40	H	301	CLA	CHD-C1D-C2D	2.06	129.78	125.49
40	Y	304	CLA	CHD-C1D-C2D	2.06	129.78	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	M	311	CLA	CHD-C1D-C2D	2.06	129.77	125.49
40	b	809	CLA	CHB-C1B-NB	-2.06	120.96	124.05
40	S	306	CLA	CHA-C1A-NA	-2.06	121.72	126.39
41	N	309	KC2	CHD-C4C-NC	2.06	127.42	124.31
43	l	201	LMG	O3-C3-C2	-2.06	105.52	110.38
40	j	102	CLA	C4D-CHA-C1A	-2.06	118.79	121.24
41	N	309	KC2	C4B-C3B-C2B	2.06	108.60	106.81
40	F	307	CLA	CHD-C1D-C2D	2.06	129.77	125.49
40	H	311	CLA	CHD-C1D-C2D	2.06	129.77	125.49
40	X	313	CLA	C4D-CHA-C1A	-2.06	118.79	121.24
40	z	308	CLA	CHD-C1D-C2D	2.06	129.77	125.49
41	P	302	KC2	CHD-C4C-NC	2.06	127.41	124.31
42	J	315	DD6	O1-C15-C14	-2.06	110.98	116.88
40	P	311	CLA	CHB-C4A-NA	2.06	127.37	124.40
40	X	305	CLA	CMC-C2C-C1C	2.06	128.25	125.03
40	F	303	CLA	CHC-C1C-NC	2.06	127.35	124.33
40	J	309	CLA	CHC-C1C-C2C	-2.06	121.10	126.95
41	u	309	KC2	CHD-C4C-NC	2.06	127.41	124.31
40	b	820	CLA	CHB-C4A-NA	2.06	127.37	124.40
41	t	301	KC2	CHD-C4C-NC	2.06	127.41	124.31
40	S	311	CLA	C2A-C1A-CHA	2.06	127.43	123.87
40	D	301	CLA	CHC-C1C-C2C	-2.06	121.11	126.95
41	O	309	KC2	C2A-C3A-C4A	2.05	107.95	106.41
40	a	839	CLA	CHD-C1D-C2D	2.05	129.76	125.49
40	F	304	CLA	CHA-C1A-NA	-2.05	121.74	126.39
40	O	304	CLA	CHC-C4B-NB	-2.05	120.97	124.05
41	M	303	KC2	CHB-C4A-NA	2.05	127.42	124.23
41	o	309	KC2	CHB-C4A-NA	2.05	127.42	124.23
41	q	309	KC2	CHB-C4A-NA	2.05	127.42	124.23
40	B	303	CLA	CHD-C1D-C2D	2.05	129.76	125.49
40	C	305	CLA	CHA-C1A-NA	-2.05	121.74	126.39
40	q	305	CLA	CHA-C1A-NA	-2.05	121.74	126.39
41	q	302	KC2	C4C-C3C-C2C	2.05	109.17	107.28
40	a	829	CLA	CBA-CAA-C2A	2.05	119.90	113.79
40	o	306	CLA	CBA-CAA-C2A	2.05	119.90	113.79
40	Q	209	CLA	CHD-C1D-C2D	2.05	129.76	125.49
40	w	303	CLA	CHD-C1D-C2D	2.05	129.76	125.49
40	E	308	CLA	CMC-C2C-C1C	2.05	128.24	125.03
43	a	802	LMG	C1-O6-C5	2.05	117.73	113.72
40	A	306	CLA	CHA-C1A-NA	-2.05	121.74	126.39
40	C	306	CLA	CHA-C1A-NA	-2.05	121.74	126.39
41	Z	302	KC2	CHB-C4A-NA	2.05	127.41	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	D	308	CLA	CHD-C1D-C2D	2.05	129.76	125.49
40	I	203	CLA	CHD-C1D-C2D	2.05	129.76	125.49
40	U	206	CLA	CHD-C1D-C2D	2.05	129.75	125.49
40	t	305	CLA	CHD-C1D-C2D	2.05	129.75	125.49
40	F	310	CLA	CBA-CAA-C2A	2.05	119.90	113.79
41	w	306	KC2	CHB-C4A-NA	2.05	127.41	124.23
42	E	317	DD6	C21-C20-C19	2.05	116.55	114.24
40	x	308	CLA	CHD-C1D-C2D	2.05	129.75	125.49
46	M	318	SQD	C45-O47-C7	-2.05	112.89	117.80
40	a	829	CLA	C1-C2-C3	-2.05	122.84	126.20
40	F	305	CLA	CHB-C4A-NA	2.05	127.36	124.40
41	S	303	KC2	CGD-CBD-CAD	-2.05	104.21	110.85
52	b	850	DGD	C5B-C4B-C3B	-2.05	104.01	114.37
40	B	307	CLA	C2A-C3A-C4A	-2.05	98.56	101.87
40	P	312	CLA	CHC-C1C-C2C	-2.05	121.12	126.95
41	J	304	KC2	CHD-C4C-NC	2.05	127.40	124.31
40	a	811	CLA	CHC-C1C-NC	2.05	127.34	124.33
40	x	311	CLA	CHA-C1A-NA	-2.05	121.75	126.39
42	o	319	DD6	C21-C20-C19	2.05	116.54	114.24
40	W	307	CLA	CMC-C2C-C1C	2.05	128.24	125.03
40	J	307	CLA	C3D-C4D-ND	2.05	113.32	109.99
40	U	204	CLA	CHD-C1D-C2D	2.05	129.75	125.49
41	X	309	KC2	C4B-C3B-C2B	2.05	108.59	106.81
40	S	308	CLA	CHA-C1A-NA	-2.05	121.75	126.39
40	G	205	CLA	CHD-C1D-C2D	2.05	129.74	125.49
40	R	310	CLA	CHD-C1D-C2D	2.05	129.74	125.49
40	K	312	CLA	CHB-C4A-NA	2.05	127.35	124.40
43	E	321	LMG	O1-C7-C8	-2.05	105.84	110.82
41	P	304	KC2	CHB-C4A-NA	2.05	127.40	124.23
40	b	810	CLA	C2C-C1C-NC	2.05	112.13	109.98
40	b	818	CLA	C1-C2-C3	-2.05	122.84	126.20
40	D	305	CLA	CHB-C4A-NA	2.05	127.35	124.40
40	a	815	CLA	CAA-C2A-C1A	-2.05	105.27	111.97
46	M	318	SQD	O9-S-C6	2.05	109.81	106.76
40	X	307	CLA	CHC-C4B-NB	-2.05	120.98	124.05
40	C	306	CLA	CHB-C4A-NA	2.04	127.35	124.40
40	L	307	CLA	CHD-C1D-C2D	2.04	129.74	125.49
40	a	815	CLA	CHD-C1D-C2D	2.04	129.74	125.49
44	p	318	A86	C36-C31-C32	-2.04	117.67	119.70
40	Z	304	CLA	CHD-C1D-C2D	2.04	129.74	125.49
40	Q	206	CLA	C2C-C1C-NC	2.04	112.55	109.48
41	Y	302	KC2	CHB-C4A-NA	2.04	127.40	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	b	823	CLA	CHD-C1D-C2D	2.04	129.74	125.49
40	b	801	CLA	C4D-CHA-C1A	-2.04	118.81	121.24
40	K	306	CLA	CHA-C1A-NA	-2.04	121.77	126.39
40	b	811	CLA	CHC-C1C-C2C	-2.04	121.14	126.95
40	C	304	CLA	CHA-C1A-NA	-2.04	121.77	126.39
40	Y	306	CLA	CHA-C1A-NA	-2.04	121.77	126.39
40	f	201	CLA	CHA-C1A-NA	-2.04	121.77	126.39
43	l	201	LMG	O7-C10-O9	-2.04	118.93	123.70
40	T	317	CLA	C2C-C1C-NC	2.04	112.13	109.98
40	G	203	CLA	CHB-C4A-NA	2.04	127.35	124.40
40	x	313	CLA	CHA-C1A-NA	-2.04	121.77	126.39
40	b	840	CLA	CHD-C1D-C2D	2.04	129.73	125.49
40	k	202	CLA	CBA-CAA-C2A	2.04	119.87	113.79
41	Y	314	KC2	CGD-CBD-CAD	-2.04	104.24	110.85
40	I	205	CLA	CHD-C1D-C2D	2.04	129.73	125.49
40	R	304	CLA	CHD-C1D-C2D	2.04	129.73	125.49
40	v	306	CLA	CHD-C1D-C2D	2.04	129.73	125.49
40	S	301	CLA	CHD-C1D-C2D	2.04	129.73	125.49
40	o	305	CLA	CHB-C4A-NA	2.04	127.34	124.40
40	u	305	CLA	CHA-C1A-NA	-2.04	121.77	126.39
40	P	312	CLA	CHA-C1A-NA	-2.04	121.77	126.39
40	W	305	CLA	CHC-C1C-C2C	-2.04	121.15	126.95
40	q	311	CLA	CHC-C1C-C2C	-2.04	121.15	126.95
42	D	313	DD6	O1-C20-C19	-2.04	111.58	113.49
42	Q	211	DD6	O1-C20-C15	-2.04	57.31	58.93
41	v	302	KC2	CHB-C4A-NA	2.04	127.39	124.23
40	y	305	CLA	CHD-C1D-C2D	2.04	129.73	125.49
40	J	306	CLA	CHD-C1D-C2D	2.04	129.73	125.49
41	R	309	KC2	CGD-CBD-CAD	-2.04	104.25	110.85
40	K	308	CLA	CHA-C1A-NA	-2.04	121.78	126.39
40	N	306	CLA	CHA-C1A-NA	-2.04	121.78	126.39
42	z	322	DD6	C14-C13-C11	2.04	128.69	125.53
40	u	311	CLA	CHC-C4B-NB	-2.04	120.99	124.05
40	I	201	CLA	CHD-C1D-C2D	2.04	129.72	125.49
40	Y	311	CLA	CHD-C1D-C2D	2.04	129.72	125.49
40	b	828	CLA	CHD-C1D-C2D	2.04	129.72	125.49
40	f	205	CLA	CMA-C3A-C4A	2.04	117.25	111.77
40	X	310	CLA	C1-C2-C3	-2.04	122.86	126.20
40	K	304	CLA	CHD-C1D-C2D	2.04	129.72	125.49
40	l	202	CLA	CHD-C1D-C2D	2.04	129.72	125.49
40	a	807	CLA	CHA-C1A-NA	-2.04	121.78	126.39
41	q	302	KC2	CHB-C4A-NA	2.04	127.39	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	F	301	CLA	CHD-C1D-C2D	2.04	129.72	125.49
41	T	309	KC2	CHD-C4C-NC	2.04	127.38	124.31
41	I	209	KC2	C4C-C3C-C2C	2.04	109.15	107.28
42	I	210	DD6	O1-C20-C15	-2.04	57.32	58.93
40	E	308	CLA	CHD-C1D-C2D	2.04	129.72	125.49
40	I	206	CLA	CHD-C1D-C2D	2.04	129.72	125.49
40	O	310	CLA	CHD-C1D-C2D	2.04	129.72	125.49
40	U	202	CLA	CMC-C2C-C1C	2.03	128.21	125.03
40	a	812	CLA	CHC-C1C-C2C	-2.03	121.17	126.95
40	C	301	CLA	CHA-C1A-NA	-2.03	121.78	126.39
40	H	306	CLA	CHA-C1A-NA	-2.03	121.78	126.39
40	y	305	CLA	CHA-C1A-NA	-2.03	121.78	126.39
41	T	301	KC2	CHD-C4C-NC	2.03	127.38	124.31
40	Y	310	CLA	CHD-C1D-C2D	2.03	129.72	125.49
40	z	308	CLA	CHB-C4A-NA	2.03	127.33	124.40
40	b	842	CLA	CHD-C1D-C2D	2.03	129.72	125.49
40	L	310	CLA	CHB-C4A-NA	2.03	127.33	124.40
41	W	304	KC2	CHB-C4A-NA	2.03	127.38	124.23
40	z	311	CLA	CHB-C1B-NB	-2.03	121.00	124.05
40	Q	208	CLA	CHC-C1C-C2C	-2.03	121.17	126.95
40	a	818	CLA	CHC-C1C-C2C	-2.03	121.17	126.95
40	M	307	CLA	CHD-C1D-C2D	2.03	129.72	125.49
40	a	817	CLA	CHD-C1D-C2D	2.03	129.72	125.49
40	K	301	CLA	CHA-C1A-NA	-2.03	121.79	126.39
40	D	309	CLA	CHD-C1D-C2D	2.03	129.71	125.49
40	B	306	CLA	CHA-C1A-NA	-2.03	121.79	126.39
40	S	313	CLA	CHD-C1D-C2D	2.03	129.71	125.49
40	Z	307	CLA	CHD-C1D-C2D	2.03	129.71	125.49
40	p	306	CLA	CHD-C1D-C2D	2.03	129.71	125.49
40	u	302	CLA	CHB-C1B-NB	-2.03	121.00	124.05
40	D	304	CLA	C6-C7-C8	2.03	122.72	115.97
41	P	302	KC2	C4C-C3C-C2C	2.03	109.15	107.28
46	F	320	SQD	O9-S-C6	2.03	109.79	106.76
41	T	303	KC2	CHB-C4A-NA	2.03	127.38	124.23
40	N	311	CLA	CHD-C1D-C2D	2.03	129.71	125.49
40	P	306	CLA	C2C-C1C-NC	2.03	112.11	109.98
40	b	818	CLA	CHA-C1A-NA	-2.03	121.80	126.39
40	z	324	CLA	CHA-C1A-NA	-2.03	121.80	126.39
43	a	802	LMG	O1-C7-C8	-2.03	105.88	110.82
40	R	306	CLA	CHD-C1D-C2D	2.03	129.71	125.49
40	b	833	CLA	CHD-C1D-C2D	2.03	129.71	125.49
40	b	813	CLA	CHC-C1C-C2C	-2.03	121.18	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	U	203	CLA	CHC-C1C-C2C	-2.03	121.18	126.95
40	a	812	CLA	CHB-C4A-NA	2.03	127.33	124.40
40	b	830	CLA	CHA-C1A-NA	-2.03	121.80	126.39
42	B	305	DD6	C14-C13-C11	2.03	128.68	125.53
40	v	306	CLA	CBA-CAA-C2A	2.03	119.83	113.79
40	l	202	CLA	C1-O2A-CGA	-2.03	111.74	116.65
40	l	203	CLA	CHA-C1A-NA	-2.03	121.80	126.39
40	b	809	CLA	C2A-C3A-C4A	-2.03	98.59	101.87
40	J	303	CLA	CHC-C1C-C2C	-2.03	121.19	126.95
47	p	324	A1EB1	C36-C31-C32	-2.03	117.69	119.70
40	a	828	CLA	CHA-C1A-NA	-2.03	121.80	126.39
40	X	312	CLA	CHD-C1D-C2D	2.03	129.70	125.49
41	t	308	KC2	C4C-C3C-C2C	2.03	109.14	107.28
41	W	302	KC2	CHD-C4C-NC	2.03	127.36	124.31
40	b	810	CLA	CHC-C1C-C2C	-2.03	121.19	126.95
40	a	832	CLA	CHC-C1C-C2C	-2.02	121.19	126.95
40	G	207	CLA	CHD-C1D-C2D	2.02	129.70	125.49
43	T	318	LMG	O2-C2-C1	-2.02	105.25	110.08
40	l	202	CLA	CHA-C1A-NA	-2.02	121.81	126.39
40	v	305	CLA	CHB-C4A-NA	2.02	127.32	124.40
40	a	836	CLA	CHD-C1D-C2D	2.02	129.70	125.49
43	x	301	LMG	O7-C10-O9	-2.02	118.97	123.70
40	o	313	CLA	C4D-CHA-C1A	-2.02	118.83	121.24
40	o	307	CLA	CHB-C4A-NA	2.02	127.32	124.40
41	x	309	KC2	CGD-CBD-CAD	-2.02	104.30	110.85
41	X	308	KC2	CHB-C4A-NA	2.02	127.37	124.23
40	a	851	CLA	CHD-C1D-C2D	2.02	129.69	125.49
40	P	308	CLA	CHA-C1A-NA	-2.02	121.81	126.39
40	t	309	CLA	CHD-C1D-C2D	2.02	129.69	125.49
41	Y	308	KC2	C4C-C3C-C2C	2.02	109.14	107.28
41	u	315	KC2	CHD-C4C-NC	2.02	127.36	124.31
40	I	206	CLA	CMC-C2C-C1C	2.02	128.19	125.03
40	b	802	CLA	CHB-C4A-NA	2.02	127.32	124.40
40	b	807	CLA	CHB-C4A-NA	2.02	127.32	124.40
40	Q	207	CLA	CHB-C1B-NB	-2.02	121.02	124.05
40	K	306	CLA	CHD-C1D-C2D	2.02	129.69	125.49
40	b	832	CLA	CHD-C1D-C2D	2.02	129.69	125.49
40	T	317	CLA	CHC-C1C-C2C	-2.02	121.21	126.95
44	M	316	A86	O1-C20-C19	2.02	115.38	113.49
41	H	316	KC2	CHC-C1C-NC	2.02	127.36	124.23
42	N	317	DD6	O1-C20-C15	-2.02	57.33	58.93
40	M	311	CLA	CHC-C1C-C2C	-2.02	121.21	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	f	204	CLA	CHA-C1A-NA	-2.02	121.82	126.39
40	k	202	CLA	CHD-C1D-C2D	2.02	129.69	125.49
40	Q	204	CLA	CHA-C1A-NA	-2.02	121.82	126.39
41	W	310	KC2	CHB-C4A-NA	2.02	127.36	124.23
40	U	203	CLA	CHD-C1D-C2D	2.02	129.68	125.49
40	a	835	CLA	CHD-C1D-C2D	2.02	129.68	125.49
41	z	309	KC2	CHB-C4A-NA	2.02	127.36	124.23
40	Y	301	CLA	CHD-C1D-C2D	2.02	129.68	125.49
40	T	306	CLA	CBA-CAA-C2A	2.02	119.79	113.79
40	A	304	CLA	CHD-C1D-C2D	2.02	129.68	125.49
40	M	310	CLA	CHD-C1D-C2D	2.02	129.68	125.49
43	u	301	LMG	O6-C1-O1	-2.02	105.28	110.04
40	X	307	CLA	CHD-C1D-C2D	2.02	129.68	125.49
44	X	315	A86	O4-C38-C39	2.02	114.68	111.09
40	N	305	CLA	CHD-C1D-C2D	2.02	129.68	125.49
40	l	203	CLA	C11-C10-C8	2.02	122.66	115.97
41	x	315	KC2	CHD-C4C-NC	2.02	127.35	124.31
40	M	307	CLA	CHA-C1A-NA	-2.02	121.83	126.39
40	k	201	CLA	CHD-C1D-C2D	2.01	129.68	125.49
42	A	316	DD6	O1-C20-C19	-2.01	111.60	113.49
40	X	313	CLA	CHC-C4B-NB	-2.01	121.03	124.05
42	H	314	DD6	C30-C29-C27	-2.01	169.39	176.23
40	q	301	CLA	CHD-C1D-C2D	2.01	129.68	125.49
40	b	839	CLA	CHB-C1B-NB	-2.01	121.03	124.05
40	R	316	CLA	CHC-C1C-C2C	-2.01	121.22	126.95
40	t	303	CLA	CHD-C1D-C2D	2.01	129.67	125.49
42	x	320	DD6	O1-C20-C15	-2.01	57.33	58.93
40	L	305	CLA	CHA-C1A-NA	-2.01	121.83	126.39
40	x	312	CLA	CHA-C1A-NA	-2.01	121.83	126.39
40	F	304	CLA	CHD-C4C-C3C	-2.01	121.84	124.77
40	U	205	CLA	CBA-CAA-C2A	2.01	119.78	113.79
40	b	812	CLA	CHD-C1D-C2D	2.01	129.67	125.49
40	P	311	CLA	CHC-C1C-C2C	-2.01	121.23	126.95
44	T	313	A86	C33-C32-C31	2.01	111.17	109.21
40	F	304	CLA	CBA-CAA-C2A	2.01	119.78	113.79
43	E	320	LMG	O7-C10-O9	-2.01	119.00	123.70
41	Z	308	KC2	CHB-C4A-NA	2.01	127.35	124.23
40	H	305	CLA	CHC-C1C-C2C	-2.01	121.23	126.95
41	K	309	KC2	C4C-C3C-C2C	2.01	109.13	107.28
40	I	205	CLA	CHC-C1C-C2C	-2.01	121.23	126.95
40	a	810	CLA	CHC-C1C-C2C	-2.01	121.24	126.95
40	J	307	CLA	CBA-CAA-C2A	2.01	119.77	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	E	318	DD6	C14-C13-C11	2.01	128.65	125.53
43	E	301	LMG	C6-C5-C4	-2.01	108.08	113.02
40	N	306	CLA	CHD-C1D-C2D	2.01	129.67	125.49
40	T	306	CLA	CHD-C1D-C2D	2.01	129.67	125.49
40	U	207	CLA	CHD-C1D-C2D	2.01	129.66	125.49
40	a	821	CLA	CHA-C1A-NA	-2.01	121.84	126.39
40	Z	307	CLA	C4D-CHA-C1A	-2.01	118.85	121.24
40	U	203	CLA	C2C-C1C-NC	2.01	112.09	109.98
40	v	304	CLA	CHB-C4A-NA	2.01	127.30	124.40
41	M	302	KC2	CHB-C4A-NA	2.01	127.34	124.23
40	y	304	CLA	CHD-C1D-C2D	2.01	129.66	125.49
40	J	311	CLA	CAA-C2A-C1A	-2.01	105.40	111.97
40	A	309	CLA	CHD-C1D-C2D	2.01	129.66	125.49
40	a	836	CLA	CHA-C1A-NA	-2.01	121.85	126.39
43	P	318	LMG	O8-C28-O10	-2.01	118.61	123.63
41	z	310	KC2	CHB-C4A-NA	2.01	127.34	124.23
40	b	802	CLA	CHD-C1D-C2D	2.01	129.66	125.49
40	b	833	CLA	CHC-C1C-C2C	-2.01	121.25	126.95
40	l	203	CLA	CAC-C3C-C4C	2.01	127.40	124.79
41	v	309	KC2	CHB-C4A-NA	2.01	127.34	124.23
40	D	304	CLA	CHD-C1D-C2D	2.01	129.66	125.49
40	X	306	CLA	CAA-C2A-C3A	2.01	118.42	113.00
40	Z	305	CLA	CHA-C1A-NA	-2.01	121.85	126.39
40	D	310	CLA	C2C-C1C-NC	2.01	112.09	109.98
40	B	306	CLA	CHC-C1C-C2C	-2.00	121.25	126.95
40	b	835	CLA	CHD-C1D-C2D	2.00	129.66	125.49
40	z	307	CLA	CHA-C1A-NA	-2.00	121.85	126.39
40	b	833	CLA	CHB-C4A-NA	2.00	127.29	124.40
41	N	308	KC2	CHB-C4A-NA	2.00	127.34	124.23
40	S	306	CLA	CHD-C1D-C2D	2.00	129.65	125.49
40	o	306	CLA	CHD-C1D-C2D	2.00	129.65	125.49
40	x	305	CLA	CHC-C4B-NB	-2.00	121.04	124.05
40	x	307	CLA	CHB-C1B-NB	-2.00	121.04	124.05
40	z	307	CLA	CHD-C1D-C2D	2.00	129.65	125.49
40	U	208	CLA	CHC-C1C-C2C	-2.00	121.26	126.95
40	H	304	CLA	CHB-C4A-NA	2.00	127.29	124.40
40	z	305	CLA	CHA-C1A-NA	-2.00	121.86	126.39
52	b	850	DGD	C7A-C6A-C5A	-2.00	104.25	114.37
40	b	819	CLA	CHD-C1D-C2D	2.00	129.65	125.49
40	t	303	CLA	CHA-C1A-NA	-2.00	121.86	126.39
40	b	832	CLA	C3A-C2A-C1A	-2.00	98.34	101.34
40	y	304	CLA	CHB-C4A-NA	2.00	127.29	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	C	306	CLA	CHD-C1D-C2D	2.00	129.65	125.49
41	p	303	KC2	C3C-C2C-C1C	2.00	107.91	106.41
40	K	301	CLA	CHD-C1D-C2D	2.00	129.65	125.49
40	K	312	CLA	CHD-C1D-C2D	2.00	129.65	125.49
40	p	302	CLA	CAA-C2A-C1A	-2.00	105.42	111.97
40	E	305	CLA	CHA-C1A-NA	-2.00	121.86	126.39
40	a	818	CLA	CHA-C1A-NA	-2.00	121.86	126.39
40	I	208	CLA	CHD-C1D-C2D	2.00	129.65	125.49
40	E	311	CLA	C1-C2-C3	-2.00	123.53	126.76
40	A	305	CLA	C1-C2-C3	-2.00	122.92	126.20
40	S	319	CLA	CBA-CAA-C2A	2.00	119.75	113.79
40	U	205	CLA	CHD-C1D-C2D	2.00	129.65	125.49

All (388) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	A	301	CLA	ND
40	A	302	CLA	ND
40	A	303	CLA	ND
40	A	304	CLA	ND
40	A	305	CLA	ND
40	A	306	CLA	ND
40	A	307	CLA	ND
40	A	308	CLA	ND
40	A	309	CLA	ND
40	A	311	CLA	ND
40	B	301	CLA	ND
40	B	302	CLA	ND
40	B	303	CLA	ND
40	B	304	CLA	ND
40	B	306	CLA	ND
40	B	307	CLA	ND
40	C	301	CLA	ND
40	C	302	CLA	ND
40	C	304	CLA	ND
40	C	305	CLA	ND
40	C	306	CLA	ND
40	C	307	CLA	ND
40	C	308	CLA	ND
40	C	309	CLA	ND
40	D	301	CLA	ND
40	D	302	CLA	ND

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Mol	Chain	Res	Type	Atom
40	D	303	CLA	ND
40	D	304	CLA	ND
40	D	305	CLA	ND
40	D	306	CLA	ND
40	D	307	CLA	ND
40	D	308	CLA	ND
40	D	309	CLA	ND
40	D	310	CLA	ND
40	D	311	CLA	ND
40	D	312	CLA	ND
40	E	302	CLA	ND
40	E	303	CLA	ND
40	E	304	CLA	ND
40	E	305	CLA	ND
40	E	306	CLA	ND
40	E	307	CLA	ND
40	E	308	CLA	ND
40	E	309	CLA	ND
40	E	310	CLA	ND
40	E	311	CLA	ND
40	E	312	CLA	ND
40	E	313	CLA	ND
40	E	314	CLA	ND
40	F	301	CLA	ND
40	F	303	CLA	ND
40	F	304	CLA	ND
40	F	305	CLA	ND
40	F	306	CLA	ND
40	F	307	CLA	ND
40	F	308	CLA	ND
40	F	310	CLA	ND
40	F	311	CLA	ND
40	F	321	CLA	ND
40	G	201	CLA	ND
40	G	203	CLA	ND
40	G	204	CLA	ND
40	G	205	CLA	ND
40	G	206	CLA	ND
40	G	207	CLA	ND
40	G	213	CLA	ND
40	H	301	CLA	ND
40	H	302	CLA	ND

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Mol	Chain	Res	Type	Atom
40	H	304	CLA	ND
40	H	305	CLA	ND
40	H	306	CLA	ND
40	H	307	CLA	ND
40	H	308	CLA	ND
40	H	309	CLA	ND
40	H	310	CLA	ND
40	H	311	CLA	ND
40	I	201	CLA	ND
40	I	202	CLA	ND
40	I	203	CLA	ND
40	I	204	CLA	ND
40	I	205	CLA	ND
40	I	206	CLA	ND
40	I	207	CLA	ND
40	I	208	CLA	ND
40	J	302	CLA	ND
40	J	303	CLA	ND
40	J	305	CLA	ND
40	J	306	CLA	ND
40	J	307	CLA	ND
40	J	308	CLA	ND
40	J	309	CLA	ND
40	J	310	CLA	ND
40	J	311	CLA	ND
40	J	312	CLA	ND
40	J	318	CLA	ND
40	K	301	CLA	ND
40	K	304	CLA	ND
40	K	306	CLA	ND
40	K	307	CLA	ND
40	K	308	CLA	ND
40	K	312	CLA	ND
40	L	301	CLA	ND
40	L	304	CLA	ND
40	L	305	CLA	ND
40	L	306	CLA	ND
40	L	307	CLA	ND
40	L	310	CLA	ND
40	L	311	CLA	ND
40	L	312	CLA	ND
40	M	304	CLA	ND

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Mol	Chain	Res	Type	Atom
40	M	305	CLA	ND
40	M	306	CLA	ND
40	M	307	CLA	ND
40	M	310	CLA	ND
40	M	311	CLA	ND
40	M	312	CLA	ND
40	N	304	CLA	ND
40	N	305	CLA	ND
40	N	306	CLA	ND
40	N	307	CLA	ND
40	N	310	CLA	ND
40	N	311	CLA	ND
40	O	304	CLA	ND
40	O	305	CLA	ND
40	O	306	CLA	ND
40	O	307	CLA	ND
40	O	310	CLA	ND
40	O	316	CLA	ND
40	P	305	CLA	ND
40	P	306	CLA	ND
40	P	307	CLA	ND
40	P	308	CLA	ND
40	P	311	CLA	ND
40	P	312	CLA	ND
40	P	313	CLA	ND
40	Q	202	CLA	ND
40	Q	203	CLA	ND
40	Q	204	CLA	ND
40	Q	205	CLA	ND
40	Q	206	CLA	ND
40	Q	207	CLA	ND
40	Q	208	CLA	ND
40	Q	209	CLA	ND
40	R	304	CLA	ND
40	R	305	CLA	ND
40	R	306	CLA	ND
40	R	307	CLA	ND
40	R	310	CLA	ND
40	R	316	CLA	ND
40	S	301	CLA	ND
40	S	302	CLA	ND
40	S	305	CLA	ND

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Mol	Chain	Res	Type	Atom
40	S	306	CLA	ND
40	S	307	CLA	ND
40	S	308	CLA	ND
40	S	311	CLA	ND
40	S	312	CLA	ND
40	S	313	CLA	ND
40	S	314	CLA	ND
40	S	319	CLA	ND
40	T	304	CLA	ND
40	T	305	CLA	ND
40	T	306	CLA	ND
40	T	307	CLA	ND
40	T	310	CLA	ND
40	T	317	CLA	ND
40	U	202	CLA	ND
40	U	203	CLA	ND
40	U	204	CLA	ND
40	U	205	CLA	ND
40	U	206	CLA	ND
40	U	207	CLA	ND
40	U	208	CLA	ND
40	V	201	CLA	ND
40	V	202	CLA	ND
40	W	305	CLA	ND
40	W	306	CLA	ND
40	W	307	CLA	ND
40	W	308	CLA	ND
40	W	311	CLA	ND
40	W	312	CLA	ND
40	W	313	CLA	ND
40	X	301	CLA	ND
40	X	304	CLA	ND
40	X	305	CLA	ND
40	X	306	CLA	ND
40	X	307	CLA	ND
40	X	310	CLA	ND
40	X	311	CLA	ND
40	X	312	CLA	ND
40	X	313	CLA	ND
40	Y	301	CLA	ND
40	Y	304	CLA	ND
40	Y	305	CLA	ND

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Mol	Chain	Res	Type	Atom
40	Y	306	CLA	ND
40	Y	307	CLA	ND
40	Y	310	CLA	ND
40	Y	311	CLA	ND
40	Y	312	CLA	ND
40	Y	313	CLA	ND
40	Z	301	CLA	ND
40	Z	304	CLA	ND
40	Z	305	CLA	ND
40	Z	306	CLA	ND
40	Z	307	CLA	ND
40	Z	310	CLA	ND
40	Z	311	CLA	ND
40	Z	312	CLA	ND
40	Z	313	CLA	ND
40	a	803	CLA	ND
40	a	804	CLA	ND
40	a	805	CLA	ND
40	a	806	CLA	ND
40	a	807	CLA	ND
40	a	808	CLA	ND
40	a	809	CLA	ND
40	a	810	CLA	ND
40	a	811	CLA	ND
40	a	812	CLA	ND
40	a	813	CLA	ND
40	a	814	CLA	ND
40	a	815	CLA	ND
40	a	816	CLA	ND
40	a	817	CLA	ND
40	a	818	CLA	ND
40	a	819	CLA	ND
40	a	820	CLA	ND
40	a	821	CLA	ND
40	a	822	CLA	ND
40	a	823	CLA	ND
40	a	824	CLA	ND
40	a	825	CLA	ND
40	a	826	CLA	ND
40	a	827	CLA	ND
40	a	828	CLA	ND
40	a	829	CLA	ND

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Mol	Chain	Res	Type	Atom
40	a	830	CLA	ND
40	a	831	CLA	ND
40	a	832	CLA	ND
40	a	833	CLA	ND
40	a	834	CLA	ND
40	a	835	CLA	ND
40	a	836	CLA	ND
40	a	837	CLA	ND
40	a	838	CLA	ND
40	a	839	CLA	ND
40	a	840	CLA	ND
40	a	841	CLA	ND
40	a	842	CLA	ND
40	a	850	CLA	ND
40	a	851	CLA	ND
40	a	852	CLA	ND
40	b	801	CLA	ND
40	b	802	CLA	ND
40	b	803	CLA	ND
40	b	805	CLA	ND
40	b	806	CLA	ND
40	b	807	CLA	ND
40	b	808	CLA	ND
40	b	809	CLA	ND
40	b	810	CLA	ND
40	b	811	CLA	ND
40	b	812	CLA	ND
40	b	813	CLA	ND
40	b	814	CLA	ND
40	b	815	CLA	ND
40	b	816	CLA	ND
40	b	817	CLA	ND
40	b	818	CLA	ND
40	b	819	CLA	ND
40	b	820	CLA	ND
40	b	821	CLA	ND
40	b	822	CLA	ND
40	b	823	CLA	ND
40	b	824	CLA	ND
40	b	825	CLA	ND
40	b	826	CLA	ND
40	b	827	CLA	ND

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Mol	Chain	Res	Type	Atom
40	b	828	CLA	ND
40	b	829	CLA	ND
40	b	830	CLA	ND
40	b	831	CLA	ND
40	b	832	CLA	ND
40	b	833	CLA	ND
40	b	834	CLA	ND
40	b	835	CLA	ND
40	b	836	CLA	ND
40	b	837	CLA	ND
40	b	838	CLA	ND
40	b	839	CLA	ND
40	b	840	CLA	ND
40	b	841	CLA	ND
40	b	842	CLA	ND
40	f	201	CLA	ND
40	f	202	CLA	ND
40	f	204	CLA	ND
40	f	205	CLA	ND
40	i	101	CLA	ND
40	j	102	CLA	ND
40	k	201	CLA	ND
40	k	202	CLA	ND
40	l	202	CLA	ND
40	l	203	CLA	ND
40	l	204	CLA	ND
40	l	205	CLA	ND
40	o	301	CLA	ND
40	o	304	CLA	ND
40	o	305	CLA	ND
40	o	306	CLA	ND
40	o	307	CLA	ND
40	o	310	CLA	ND
40	o	311	CLA	ND
40	o	312	CLA	ND
40	o	313	CLA	ND
40	p	302	CLA	ND
40	p	305	CLA	ND
40	p	306	CLA	ND
40	p	307	CLA	ND
40	p	308	CLA	ND
40	p	311	CLA	ND

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Mol	Chain	Res	Type	Atom
40	p	312	CLA	ND
40	p	313	CLA	ND
40	p	314	CLA	ND
40	q	301	CLA	ND
40	q	304	CLA	ND
40	q	305	CLA	ND
40	q	306	CLA	ND
40	q	307	CLA	ND
40	q	310	CLA	ND
40	q	311	CLA	ND
40	q	312	CLA	ND
40	q	313	CLA	ND
40	t	302	CLA	ND
40	t	303	CLA	ND
40	t	304	CLA	ND
40	t	305	CLA	ND
40	t	307	CLA	ND
40	t	309	CLA	ND
40	u	302	CLA	ND
40	u	305	CLA	ND
40	u	306	CLA	ND
40	u	307	CLA	ND
40	u	308	CLA	ND
40	u	311	CLA	ND
40	u	312	CLA	ND
40	u	313	CLA	ND
40	u	314	CLA	ND
40	v	301	CLA	ND
40	v	304	CLA	ND
40	v	305	CLA	ND
40	v	306	CLA	ND
40	v	307	CLA	ND
40	v	310	CLA	ND
40	v	311	CLA	ND
40	v	312	CLA	ND
40	v	313	CLA	ND
40	w	302	CLA	ND
40	w	303	CLA	ND
40	w	304	CLA	ND
40	w	305	CLA	ND
40	w	308	CLA	ND
40	w	309	CLA	ND

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Mol	Chain	Res	Type	Atom
40	x	302	CLA	ND
40	x	305	CLA	ND
40	x	306	CLA	ND
40	x	307	CLA	ND
40	x	308	CLA	ND
40	x	311	CLA	ND
40	x	312	CLA	ND
40	x	313	CLA	ND
40	x	314	CLA	ND
40	y	302	CLA	ND
40	y	303	CLA	ND
40	y	304	CLA	ND
40	y	305	CLA	ND
40	y	308	CLA	ND
40	y	309	CLA	ND
40	z	302	CLA	ND
40	z	305	CLA	ND
40	z	306	CLA	ND
40	z	307	CLA	ND
40	z	308	CLA	ND
40	z	311	CLA	ND
40	z	312	CLA	ND
40	z	313	CLA	ND
40	z	314	CLA	ND
40	z	324	CLA	ND
42	P	315	DD6	C20

All (4962) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	A	303	CLA	C1A-C2A-CAA-CBA
40	A	303	CLA	C3A-C2A-CAA-CBA
40	A	304	CLA	C1A-C2A-CAA-CBA
40	A	304	CLA	C3A-C2A-CAA-CBA
40	A	305	CLA	C2B-C3B-CAB-CBB
40	A	305	CLA	C4B-C3B-CAB-CBB
40	A	306	CLA	C2B-C3B-CAB-CBB
40	A	306	CLA	C4B-C3B-CAB-CBB
40	A	307	CLA	C2B-C3B-CAB-CBB
40	A	307	CLA	C4B-C3B-CAB-CBB
40	A	309	CLA	CHA-CBD-CGD-O1D
40	A	309	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
40	B	301	CLA	C1A-C2A-CAA-CBA
40	B	302	CLA	C1A-C2A-CAA-CBA
40	B	304	CLA	C1A-C2A-CAA-CBA
40	B	306	CLA	CHA-CBD-CGD-O2D
40	B	307	CLA	CHA-CBD-CGD-O1D
40	B	307	CLA	CHA-CBD-CGD-O2D
40	C	301	CLA	C1A-C2A-CAA-CBA
40	C	301	CLA	C3A-C2A-CAA-CBA
40	C	301	CLA	CHA-CBD-CGD-O1D
40	C	301	CLA	CHA-CBD-CGD-O2D
40	C	304	CLA	C4B-C3B-CAB-CBB
40	C	306	CLA	CHA-CBD-CGD-O2D
40	C	307	CLA	C2B-C3B-CAB-CBB
40	C	307	CLA	C4B-C3B-CAB-CBB
40	D	302	CLA	C1A-C2A-CAA-CBA
40	D	302	CLA	C2-C3-C5-C6
40	D	302	CLA	C4-C3-C5-C6
40	D	307	CLA	C1A-C2A-CAA-CBA
40	D	307	CLA	C3A-C2A-CAA-CBA
40	D	309	CLA	CAD-CBD-CGD-O2D
40	D	310	CLA	C1A-C2A-CAA-CBA
40	D	310	CLA	C3A-C2A-CAA-CBA
40	D	310	CLA	C2B-C3B-CAB-CBB
40	D	310	CLA	C4B-C3B-CAB-CBB
40	D	311	CLA	C1A-C2A-CAA-CBA
40	D	311	CLA	CHA-CBD-CGD-O1D
40	D	311	CLA	CHA-CBD-CGD-O2D
40	D	312	CLA	CHA-CBD-CGD-O1D
40	D	312	CLA	CHA-CBD-CGD-O2D
40	E	302	CLA	C1A-C2A-CAA-CBA
40	E	305	CLA	C2B-C3B-CAB-CBB
40	E	305	CLA	C4B-C3B-CAB-CBB
40	E	307	CLA	C1A-C2A-CAA-CBA
40	E	308	CLA	C2B-C3B-CAB-CBB
40	E	308	CLA	C4B-C3B-CAB-CBB
40	E	314	CLA	C1A-C2A-CAA-CBA
40	E	314	CLA	CAD-CBD-CGD-O1D
40	E	314	CLA	CAD-CBD-CGD-O2D
40	F	303	CLA	C2-C3-C5-C6
40	F	304	CLA	C4B-C3B-CAB-CBB
40	F	305	CLA	C1A-C2A-CAA-CBA
40	F	307	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
40	F	310	CLA	CHA-CBD-CGD-O1D
40	F	310	CLA	CHA-CBD-CGD-O2D
40	F	311	CLA	C1A-C2A-CAA-CBA
40	F	311	CLA	C3A-C2A-CAA-CBA
40	F	311	CLA	CAD-CBD-CGD-O2D
40	F	321	CLA	C1A-C2A-CAA-CBA
40	G	203	CLA	C1A-C2A-CAA-CBA
40	G	203	CLA	C3A-C2A-CAA-CBA
40	G	206	CLA	C1A-C2A-CAA-CBA
40	G	206	CLA	C3A-C2A-CAA-CBA
40	G	206	CLA	C2B-C3B-CAB-CBB
40	G	206	CLA	C4B-C3B-CAB-CBB
40	G	206	CLA	CAD-CBD-CGD-O1D
40	G	206	CLA	CAD-CBD-CGD-O2D
40	G	213	CLA	C1A-C2A-CAA-CBA
40	G	213	CLA	C2B-C3B-CAB-CBB
40	G	213	CLA	C4B-C3B-CAB-CBB
40	H	304	CLA	C2B-C3B-CAB-CBB
40	H	304	CLA	C4B-C3B-CAB-CBB
40	H	307	CLA	C2-C3-C5-C6
40	H	307	CLA	C4-C3-C5-C6
40	H	307	CLA	C6-C7-C8-C9
40	I	202	CLA	C1A-C2A-CAA-CBA
40	I	202	CLA	C3A-C2A-CAA-CBA
40	I	203	CLA	CHA-CBD-CGD-O2D
40	I	205	CLA	C3A-C2A-CAA-CBA
40	I	206	CLA	C4B-C3B-CAB-CBB
40	I	207	CLA	C3A-C2A-CAA-CBA
40	I	208	CLA	C3A-C2A-CAA-CBA
40	I	208	CLA	CAD-CBD-CGD-O1D
40	I	208	CLA	CAD-CBD-CGD-O2D
40	J	303	CLA	C1A-C2A-CAA-CBA
40	J	305	CLA	C2B-C3B-CAB-CBB
40	J	305	CLA	C4B-C3B-CAB-CBB
40	J	306	CLA	C3-C5-C6-C7
40	J	308	CLA	C2B-C3B-CAB-CBB
40	J	308	CLA	C4B-C3B-CAB-CBB
40	J	310	CLA	C1A-C2A-CAA-CBA
40	J	311	CLA	CHA-CBD-CGD-O1D
40	J	311	CLA	CHA-CBD-CGD-O2D
40	K	306	CLA	C3A-C2A-CAA-CBA
40	K	308	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
40	L	305	CLA	C1A-C2A-CAA-CBA
40	L	306	CLA	C2B-C3B-CAB-CBB
40	L	306	CLA	C4B-C3B-CAB-CBB
40	L	310	CLA	C1A-C2A-CAA-CBA
40	L	311	CLA	CAD-CBD-CGD-O2D
40	L	312	CLA	C1A-C2A-CAA-CBA
40	M	304	CLA	C2B-C3B-CAB-CBB
40	M	304	CLA	C4B-C3B-CAB-CBB
40	M	305	CLA	C1A-C2A-CAA-CBA
40	M	310	CLA	C4B-C3B-CAB-CBB
40	M	312	CLA	C6-C7-C8-C9
40	N	310	CLA	C3A-C2A-CAA-CBA
40	O	304	CLA	C1A-C2A-CAA-CBA
40	O	307	CLA	CAD-CBD-CGD-O2D
40	P	311	CLA	C1A-C2A-CAA-CBA
40	Q	204	CLA	C3A-C2A-CAA-CBA
40	Q	205	CLA	C1A-C2A-CAA-CBA
40	Q	205	CLA	C3A-C2A-CAA-CBA
40	Q	205	CLA	C4B-C3B-CAB-CBB
40	Q	206	CLA	C4B-C3B-CAB-CBB
40	Q	207	CLA	C1A-C2A-CAA-CBA
40	R	304	CLA	C1A-C2A-CAA-CBA
40	R	304	CLA	C3A-C2A-CAA-CBA
40	S	305	CLA	C1A-C2A-CAA-CBA
40	S	307	CLA	C2B-C3B-CAB-CBB
40	S	307	CLA	C4B-C3B-CAB-CBB
40	S	311	CLA	C1A-C2A-CAA-CBA
40	S	312	CLA	C1A-C2A-CAA-CBA
40	S	313	CLA	CAD-CBD-CGD-O1D
40	S	313	CLA	CAD-CBD-CGD-O2D
40	S	314	CLA	C2B-C3B-CAB-CBB
40	S	314	CLA	C4B-C3B-CAB-CBB
40	S	314	CLA	C4-C3-C5-C6
40	T	305	CLA	C2B-C3B-CAB-CBB
40	T	305	CLA	C4B-C3B-CAB-CBB
40	T	310	CLA	C1A-C2A-CAA-CBA
40	U	202	CLA	CHA-CBD-CGD-O1D
40	U	202	CLA	CHA-CBD-CGD-O2D
40	U	204	CLA	C1A-C2A-CAA-CBA
40	U	205	CLA	C2B-C3B-CAB-CBB
40	U	205	CLA	C4B-C3B-CAB-CBB
40	V	201	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
40	V	202	CLA	C1A-C2A-CAA-CBA
40	V	202	CLA	C3A-C2A-CAA-CBA
40	V	202	CLA	C2B-C3B-CAB-CBB
40	V	202	CLA	C4B-C3B-CAB-CBB
40	W	307	CLA	CAD-CBD-CGD-O1D
40	W	307	CLA	CAD-CBD-CGD-O2D
40	W	312	CLA	CHA-CBD-CGD-O1D
40	W	312	CLA	CHA-CBD-CGD-O2D
40	X	301	CLA	C2B-C3B-CAB-CBB
40	X	301	CLA	C4B-C3B-CAB-CBB
40	X	305	CLA	C1A-C2A-CAA-CBA
40	X	305	CLA	C3A-C2A-CAA-CBA
40	X	306	CLA	C1A-C2A-CAA-CBA
40	X	306	CLA	C3A-C2A-CAA-CBA
40	X	306	CLA	C2B-C3B-CAB-CBB
40	X	306	CLA	C4B-C3B-CAB-CBB
40	X	310	CLA	C1A-C2A-CAA-CBA
40	X	312	CLA	CAD-CBD-CGD-O1D
40	X	312	CLA	CAD-CBD-CGD-O2D
40	X	313	CLA	C1A-C2A-CAA-CBA
40	Y	306	CLA	C4B-C3B-CAB-CBB
40	Y	312	CLA	C1A-C2A-CAA-CBA
40	Y	313	CLA	C4B-C3B-CAB-CBB
40	Y	313	CLA	CAD-CBD-CGD-O1D
40	Y	313	CLA	CAD-CBD-CGD-O2D
40	Z	301	CLA	C2B-C3B-CAB-CBB
40	Z	301	CLA	C4B-C3B-CAB-CBB
40	Z	306	CLA	C2B-C3B-CAB-CBB
40	Z	306	CLA	C4B-C3B-CAB-CBB
40	Z	306	CLA	CHA-CBD-CGD-O1D
40	Z	306	CLA	CHA-CBD-CGD-O2D
40	Z	307	CLA	C2B-C3B-CAB-CBB
40	Z	307	CLA	C4B-C3B-CAB-CBB
40	Z	307	CLA	CAD-CBD-CGD-O1D
40	Z	307	CLA	CAD-CBD-CGD-O2D
40	Z	310	CLA	C1A-C2A-CAA-CBA
40	Z	310	CLA	C4B-C3B-CAB-CBB
40	Z	312	CLA	C1A-C2A-CAA-CBA
40	Z	312	CLA	C3A-C2A-CAA-CBA
40	Z	313	CLA	C1A-C2A-CAA-CBA
40	Z	313	CLA	C3A-C2A-CAA-CBA
40	a	806	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
40	a	807	CLA	C3A-C2A-CAA-CBA
40	a	809	CLA	C1A-C2A-CAA-CBA
40	a	811	CLA	C1A-C2A-CAA-CBA
40	a	811	CLA	C3A-C2A-CAA-CBA
40	a	813	CLA	C1A-C2A-CAA-CBA
40	a	816	CLA	C1A-C2A-CAA-CBA
40	a	816	CLA	C3A-C2A-CAA-CBA
40	a	819	CLA	C1A-C2A-CAA-CBA
40	a	819	CLA	C3A-C2A-CAA-CBA
40	a	822	CLA	C1A-C2A-CAA-CBA
40	a	822	CLA	C3A-C2A-CAA-CBA
40	a	824	CLA	C1A-C2A-CAA-CBA
40	a	826	CLA	C6-C7-C8-C9
40	a	828	CLA	C2B-C3B-CAB-CBB
40	a	828	CLA	C4B-C3B-CAB-CBB
40	a	830	CLA	C3A-C2A-CAA-CBA
40	a	833	CLA	CHA-CBD-CGD-O2D
40	a	836	CLA	C6-C7-C8-C9
40	a	837	CLA	CHA-CBD-CGD-O1D
40	a	837	CLA	CHA-CBD-CGD-O2D
40	a	838	CLA	C1A-C2A-CAA-CBA
40	a	841	CLA	CHA-CBD-CGD-O1D
40	a	841	CLA	CHA-CBD-CGD-O2D
40	a	842	CLA	C2B-C3B-CAB-CBB
40	a	842	CLA	C4B-C3B-CAB-CBB
40	b	802	CLA	C2B-C3B-CAB-CBB
40	b	802	CLA	C4B-C3B-CAB-CBB
40	b	803	CLA	C2B-C3B-CAB-CBB
40	b	803	CLA	C4B-C3B-CAB-CBB
40	b	807	CLA	C1A-C2A-CAA-CBA
40	b	808	CLA	C11-C12-C13-C14
40	b	809	CLA	C1A-C2A-CAA-CBA
40	b	812	CLA	C1A-C2A-CAA-CBA
40	b	812	CLA	C3A-C2A-CAA-CBA
40	b	815	CLA	CHA-CBD-CGD-O1D
40	b	815	CLA	CHA-CBD-CGD-O2D
40	b	816	CLA	CHA-CBD-CGD-O1D
40	b	816	CLA	CHA-CBD-CGD-O2D
40	b	822	CLA	CHA-CBD-CGD-O1D
40	b	822	CLA	CHA-CBD-CGD-O2D
40	b	824	CLA	C1A-C2A-CAA-CBA
40	b	824	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
40	b	824	CLA	C2B-C3B-CAB-CBB
40	b	824	CLA	C4B-C3B-CAB-CBB
40	b	825	CLA	CHA-CBD-CGD-O1D
40	b	825	CLA	CHA-CBD-CGD-O2D
40	b	831	CLA	C2-C3-C5-C6
40	b	833	CLA	CAD-CBD-CGD-O1D
40	b	833	CLA	CAD-CBD-CGD-O2D
40	b	835	CLA	CHA-CBD-CGD-O1D
40	b	835	CLA	CHA-CBD-CGD-O2D
40	b	836	CLA	CHA-CBD-CGD-O1D
40	b	836	CLA	CHA-CBD-CGD-O2D
40	b	837	CLA	C4-C3-C5-C6
40	b	839	CLA	C1A-C2A-CAA-CBA
40	b	840	CLA	C3A-C2A-CAA-CBA
40	b	842	CLA	C1A-C2A-CAA-CBA
40	i	101	CLA	C3A-C2A-CAA-CBA
40	l	205	CLA	C1A-C2A-CAA-CBA
40	o	301	CLA	C4B-C3B-CAB-CBB
40	o	306	CLA	C2B-C3B-CAB-CBB
40	o	306	CLA	C4B-C3B-CAB-CBB
40	o	307	CLA	CAD-CBD-CGD-O1D
40	o	307	CLA	CAD-CBD-CGD-O2D
40	o	311	CLA	CHA-CBD-CGD-O1D
40	o	311	CLA	CHA-CBD-CGD-O2D
40	o	313	CLA	CAD-CBD-CGD-O2D
40	p	302	CLA	C1A-C2A-CAA-CBA
40	p	306	CLA	C1A-C2A-CAA-CBA
40	p	306	CLA	C3A-C2A-CAA-CBA
40	p	314	CLA	C1A-C2A-CAA-CBA
40	p	314	CLA	CAD-CBD-CGD-O1D
40	p	314	CLA	CAD-CBD-CGD-O2D
40	q	304	CLA	C1A-C2A-CAA-CBA
40	q	304	CLA	C3A-C2A-CAA-CBA
40	q	306	CLA	C4B-C3B-CAB-CBB
40	q	310	CLA	C2B-C3B-CAB-CBB
40	q	310	CLA	C4B-C3B-CAB-CBB
40	q	311	CLA	CHA-CBD-CGD-O1D
40	q	311	CLA	CHA-CBD-CGD-O2D
40	q	313	CLA	C3A-C2A-CAA-CBA
40	q	313	CLA	CHA-CBD-CGD-O1D
40	q	313	CLA	CHA-CBD-CGD-O2D
40	t	304	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
40	t	304	CLA	C4B-C3B-CAB-CBB
40	t	307	CLA	O2A-C1-C2-C3
40	t	309	CLA	C2B-C3B-CAB-CBB
40	t	309	CLA	C4B-C3B-CAB-CBB
40	u	302	CLA	C1A-C2A-CAA-CBA
40	u	302	CLA	C2B-C3B-CAB-CBB
40	u	302	CLA	C4B-C3B-CAB-CBB
40	u	311	CLA	C1A-C2A-CAA-CBA
40	u	314	CLA	C1A-C2A-CAA-CBA
40	u	314	CLA	CAD-CBD-CGD-O1D
40	u	314	CLA	CAD-CBD-CGD-O2D
40	v	304	CLA	C1A-C2A-CAA-CBA
40	v	306	CLA	C4B-C3B-CAB-CBB
40	v	310	CLA	C2B-C3B-CAB-CBB
40	v	310	CLA	C4B-C3B-CAB-CBB
40	v	311	CLA	CHA-CBD-CGD-O1D
40	v	311	CLA	CHA-CBD-CGD-O2D
40	w	304	CLA	C1A-C2A-CAA-CBA
40	w	309	CLA	O2A-C1-C2-C3
40	x	311	CLA	C1A-C2A-CAA-CBA
40	x	314	CLA	C2B-C3B-CAB-CBB
40	x	314	CLA	C4B-C3B-CAB-CBB
40	y	303	CLA	C1A-C2A-CAA-CBA
40	y	304	CLA	C1A-C2A-CAA-CBA
40	y	309	CLA	O2A-C1-C2-C3
40	z	305	CLA	C6-C7-C8-C9
40	z	307	CLA	C1A-C2A-CAA-CBA
40	z	311	CLA	C1A-C2A-CAA-CBA
40	z	312	CLA	C1A-C2A-CAA-CBA
40	z	324	CLA	C2B-C3B-CAB-CBB
40	z	324	CLA	C4B-C3B-CAB-CBB
41	A	310	KC2	C2B-C3B-CAB-CBB
41	A	310	KC2	C2C-C3C-CAC-CBC
41	C	303	KC2	C3A-C2A-CAA-CBA
41	E	319	KC2	C1A-C2A-CAA-CBA
41	E	319	KC2	CHA-CBD-CGD-O1D
41	E	319	KC2	CHA-CBD-CGD-O2D
41	F	302	KC2	C1A-C2A-CAA-CBA
41	F	302	KC2	C3A-C2A-CAA-CBA
41	F	302	KC2	C2B-C3B-CAB-CBB
41	F	309	KC2	C1A-C2A-CAA-CBA
41	F	309	KC2	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
41	F	309	KC2	C4B-C3B-CAB-CBB
41	G	202	KC2	C3A-C2A-CAA-CBA
41	G	202	KC2	C2B-C3B-CAB-CBB
41	G	202	KC2	C2C-C3C-CAC-CBC
41	G	202	KC2	CHA-CBD-CGD-O1D
41	G	202	KC2	CHA-CBD-CGD-O2D
41	G	208	KC2	C3A-C2A-CAA-CBA
41	G	208	KC2	C2B-C3B-CAB-CBB
41	H	316	KC2	C2B-C3B-CAB-CBB
41	H	316	KC2	C4B-C3B-CAB-CBB
41	I	209	KC2	C1A-C2A-CAA-CBA
41	I	209	KC2	C2B-C3B-CAB-CBB
41	I	209	KC2	C2C-C3C-CAC-CBC
41	I	214	KC2	C3A-C2A-CAA-CBA
41	J	304	KC2	C1A-C2A-CAA-CBA
41	K	303	KC2	CHA-CBD-CGD-O1D
41	K	303	KC2	CHA-CBD-CGD-O2D
41	K	309	KC2	C1A-C2A-CAA-CBA
41	K	309	KC2	C2C-C3C-CAC-CBC
41	K	309	KC2	C4C-C3C-CAC-CBC
41	L	302	KC2	C1A-C2A-CAA-CBA
41	L	302	KC2	CHA-CBD-CGD-O1D
41	L	302	KC2	CHA-CBD-CGD-O2D
41	L	303	KC2	C2B-C3B-CAB-CBB
41	L	303	KC2	C4B-C3B-CAB-CBB
41	L	303	KC2	CHA-CBD-CGD-O1D
41	L	303	KC2	CHA-CBD-CGD-O2D
41	L	308	KC2	C1A-C2A-CAA-CBA
41	L	309	KC2	C2B-C3B-CAB-CBB
41	L	313	KC2	C3A-C2A-CAA-CBA
41	L	313	KC2	CHA-CBD-CGD-O1D
41	L	313	KC2	CHA-CBD-CGD-O2D
41	M	301	KC2	C1A-C2A-CAA-CBA
41	M	301	KC2	C2C-C3C-CAC-CBC
41	M	303	KC2	CHA-CBD-CGD-O1D
41	M	303	KC2	CHA-CBD-CGD-O2D
41	M	308	KC2	C2C-C3C-CAC-CBC
41	M	308	KC2	C4C-C3C-CAC-CBC
41	M	308	KC2	CAA-CBA-CGA-O2A
41	M	309	KC2	C1A-C2A-CAA-CBA
41	N	301	KC2	C2B-C3B-CAB-CBB
41	N	301	KC2	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
41	N	302	KC2	C3A-C2A-CAA-CBA
41	N	303	KC2	C2B-C3B-CAB-CBB
41	N	303	KC2	C4B-C3B-CAB-CBB
41	N	303	KC2	C2C-C3C-CAC-CBC
41	N	308	KC2	C1A-C2A-CAA-CBA
41	N	308	KC2	C2B-C3B-CAB-CBB
41	N	308	KC2	C2C-C3C-CAC-CBC
41	N	308	KC2	C4C-C3C-CAC-CBC
41	N	312	KC2	C2B-C3B-CAB-CBB
41	O	301	KC2	C2B-C3B-CAB-CBB
41	O	301	KC2	C4B-C3B-CAB-CBB
41	O	301	KC2	C2C-C3C-CAC-CBC
41	O	301	KC2	C4C-C3C-CAC-CBC
41	O	302	KC2	C3A-C2A-CAA-CBA
41	O	302	KC2	CHA-CBD-CGD-O1D
41	O	302	KC2	CHA-CBD-CGD-O2D
41	O	303	KC2	C1A-C2A-CAA-CBA
41	O	303	KC2	C3A-C2A-CAA-CBA
41	O	303	KC2	C2B-C3B-CAB-CBB
41	O	303	KC2	C4B-C3B-CAB-CBB
41	O	308	KC2	C3A-C2A-CAA-CBA
41	O	308	KC2	C2C-C3C-CAC-CBC
41	O	309	KC2	C3A-C2A-CAA-CBA
41	O	309	KC2	C2C-C3C-CAC-CBC
41	O	311	KC2	C2C-C3C-CAC-CBC
41	P	302	KC2	C2B-C3B-CAB-CBB
41	P	304	KC2	CHA-CBD-CGD-O1D
41	P	304	KC2	CHA-CBD-CGD-O2D
41	Q	201	KC2	C2C-C3C-CAC-CBC
41	Q	201	KC2	C4C-C3C-CAC-CBC
41	Q	216	KC2	C3A-C2A-CAA-CBA
41	Q	216	KC2	C2C-C3C-CAC-CBC
41	R	301	KC2	C2B-C3B-CAB-CBB
41	R	301	KC2	C4B-C3B-CAB-CBB
41	R	302	KC2	C1A-C2A-CAA-CBA
41	R	303	KC2	C1A-C2A-CAA-CBA
41	R	303	KC2	C2B-C3B-CAB-CBB
41	R	303	KC2	CHA-CBD-CGD-O2D
41	R	309	KC2	C2B-C3B-CAB-CBB
41	R	309	KC2	C2C-C3C-CAC-CBC
41	R	311	KC2	CHA-CBD-CGD-O1D
41	R	311	KC2	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
41	S	303	KC2	C3A-C2A-CAA-CBA
41	S	309	KC2	C2B-C3B-CAB-CBB
41	S	309	KC2	C2C-C3C-CAC-CBC
41	S	309	KC2	C4C-C3C-CAC-CBC
41	S	309	KC2	CHA-CBD-CGD-O1D
41	S	309	KC2	CHA-CBD-CGD-O2D
41	S	310	KC2	C2B-C3B-CAB-CBB
41	S	310	KC2	C4B-C3B-CAB-CBB
41	S	310	KC2	C2C-C3C-CAC-CBC
41	T	301	KC2	C2B-C3B-CAB-CBB
41	T	301	KC2	C4B-C3B-CAB-CBB
41	T	301	KC2	C2C-C3C-CAC-CBC
41	T	301	KC2	C4C-C3C-CAC-CBC
41	T	311	KC2	C1A-C2A-CAA-CBA
41	U	201	KC2	CHA-CBD-CGD-O1D
41	U	201	KC2	CHA-CBD-CGD-O2D
41	W	302	KC2	C2C-C3C-CAC-CBC
41	W	303	KC2	C3A-C2A-CAA-CBA
41	W	304	KC2	C1A-C2A-CAA-CBA
41	W	304	KC2	C2B-C3B-CAB-CBB
41	W	304	KC2	C4B-C3B-CAB-CBB
41	W	310	KC2	C1A-C2A-CAA-CBA
41	W	310	KC2	C2B-C3B-CAB-CBB
41	X	302	KC2	C3A-C2A-CAA-CBA
41	X	302	KC2	C2C-C3C-CAC-CBC
41	X	309	KC2	C1A-C2A-CAA-CBA
41	Y	302	KC2	C3A-C2A-CAA-CBA
41	Y	303	KC2	C2B-C3B-CAB-CBB
41	Y	303	KC2	CHA-CBD-CGD-O1D
41	Y	303	KC2	CHA-CBD-CGD-O2D
41	Y	309	KC2	C2C-C3C-CAC-CBC
41	Y	309	KC2	CHA-CBD-CGD-O1D
41	Y	309	KC2	CHA-CBD-CGD-O2D
41	Y	314	KC2	C2C-C3C-CAC-CBC
41	Y	314	KC2	CBD-CGD-O2D-CED
41	Z	302	KC2	C3A-C2A-CAA-CBA
41	o	302	KC2	C3A-C2A-CAA-CBA
41	o	303	KC2	CHA-CBD-CGD-O1D
41	o	303	KC2	CHA-CBD-CGD-O2D
41	o	308	KC2	C1A-C2A-CAA-CBA
41	o	308	KC2	C2B-C3B-CAB-CBB
41	o	309	KC2	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
41	o	309	KC2	C2B-C3B-CAB-CBB
41	o	309	KC2	C4B-C3B-CAB-CBB
41	o	309	KC2	CHA-CBD-CGD-O2D
41	p	303	KC2	C3A-C2A-CAA-CBA
41	p	304	KC2	C1A-C2A-CAA-CBA
41	p	304	KC2	C2B-C3B-CAB-CBB
41	p	304	KC2	C4B-C3B-CAB-CBB
41	p	304	KC2	CHA-CBD-CGD-O2D
41	p	309	KC2	C1A-C2A-CAA-CBA
41	p	309	KC2	C3A-C2A-CAA-CBA
41	p	310	KC2	C2B-C3B-CAB-CBB
41	p	315	KC2	C2B-C3B-CAB-CBB
41	p	315	KC2	C4B-C3B-CAB-CBB
41	p	315	KC2	C2C-C3C-CAC-CBC
41	p	315	KC2	C4C-C3C-CAC-CBC
41	p	315	KC2	CHA-CBD-CGD-O1D
41	p	315	KC2	CHA-CBD-CGD-O2D
41	q	302	KC2	C1A-C2A-CAA-CBA
41	q	303	KC2	C2B-C3B-CAB-CBB
41	q	303	KC2	C4B-C3B-CAB-CBB
41	q	303	KC2	CHA-CBD-CGD-O1D
41	q	303	KC2	CHA-CBD-CGD-O2D
41	q	308	KC2	C3A-C2A-CAA-CBA
41	q	308	KC2	C2B-C3B-CAB-CBB
41	q	308	KC2	C2C-C3C-CAC-CBC
41	q	308	KC2	CHA-CBD-CGD-O1D
41	q	308	KC2	CHA-CBD-CGD-O2D
41	q	309	KC2	C2B-C3B-CAB-CBB
41	q	309	KC2	C2C-C3C-CAC-CBC
41	t	301	KC2	C1A-C2A-CAA-CBA
41	t	301	KC2	C3A-C2A-CAA-CBA
41	t	301	KC2	CHA-CBD-CGD-O2D
41	t	306	KC2	C2B-C3B-CAB-CBB
41	t	308	KC2	C2C-C3C-CAC-CBC
41	t	308	KC2	C4C-C3C-CAC-CBC
41	u	303	KC2	C3A-C2A-CAA-CBA
41	u	303	KC2	C2C-C3C-CAC-CBC
41	u	304	KC2	C1A-C2A-CAA-CBA
41	u	304	KC2	C2B-C3B-CAB-CBB
41	u	304	KC2	C4B-C3B-CAB-CBB
41	u	304	KC2	CHA-CBD-CGD-O1D
41	u	304	KC2	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
41	u	309	KC2	C3A-C2A-CAA-CBA
41	u	310	KC2	C2B-C3B-CAB-CBB
41	u	315	KC2	C2B-C3B-CAB-CBB
41	u	315	KC2	C4B-C3B-CAB-CBB
41	u	315	KC2	C2C-C3C-CAC-CBC
41	u	315	KC2	C4C-C3C-CAC-CBC
41	v	302	KC2	C1A-C2A-CAA-CBA
41	v	303	KC2	C2B-C3B-CAB-CBB
41	v	303	KC2	CHA-CBD-CGD-O2D
41	v	308	KC2	C3A-C2A-CAA-CBA
41	v	308	KC2	C2B-C3B-CAB-CBB
41	v	308	KC2	C2C-C3C-CAC-CBC
41	v	308	KC2	CHA-CBD-CGD-O1D
41	v	308	KC2	CHA-CBD-CGD-O2D
41	v	309	KC2	C2B-C3B-CAB-CBB
41	v	309	KC2	C2C-C3C-CAC-CBC
41	w	301	KC2	C1A-C2A-CAA-CBA
41	w	301	KC2	C2B-C3B-CAB-CBB
41	w	301	KC2	C4B-C3B-CAB-CBB
41	x	303	KC2	C3A-C2A-CAA-CBA
41	x	303	KC2	C2C-C3C-CAC-CBC
41	x	304	KC2	C1A-C2A-CAA-CBA
41	x	304	KC2	C3A-C2A-CAA-CBA
41	x	304	KC2	C2B-C3B-CAB-CBB
41	x	304	KC2	C4B-C3B-CAB-CBB
41	x	304	KC2	CHA-CBD-CGD-O2D
41	x	309	KC2	C1A-C2A-CAA-CBA
41	x	309	KC2	C3A-C2A-CAA-CBA
41	x	310	KC2	C2B-C3B-CAB-CBB
41	x	315	KC2	C2B-C3B-CAB-CBB
41	x	315	KC2	C4B-C3B-CAB-CBB
41	x	315	KC2	C2C-C3C-CAC-CBC
41	x	315	KC2	C4C-C3C-CAC-CBC
41	y	301	KC2	C1A-C2A-CAA-CBA
41	y	301	KC2	C3A-C2A-CAA-CBA
41	y	306	KC2	C2B-C3B-CAB-CBB
41	z	303	KC2	C3A-C2A-CAA-CBA
41	z	303	KC2	C2C-C3C-CAC-CBC
41	z	303	KC2	C4C-C3C-CAC-CBC
41	z	304	KC2	CHA-CBD-CGD-O1D
41	z	304	KC2	CHA-CBD-CGD-O2D
41	z	310	KC2	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
42	C	312	DD6	C13-C14-C15-O1
42	C	313	DD6	C13-C14-C15-C16
42	D	316	DD6	C13-C14-C15-O1
42	E	318	DD6	C13-C14-C15-C16
42	F	314	DD6	C13-C14-C15-C16
42	F	315	DD6	C13-C14-C15-O1
42	F	316	DD6	C13-C14-C15-C20
42	H	313	DD6	C12-C11-C13-C14
42	H	313	DD6	C13-C14-C15-C16
42	H	313	DD6	C5-C6-C8-C9
42	I	213	DD6	C13-C14-C15-O1
42	J	301	DD6	C13-C14-C15-C20
42	J	313	DD6	C13-C14-C15-O1
42	J	315	DD6	C13-C14-C15-O1
42	K	311	DD6	C13-C14-C15-O1
42	N	317	DD6	C13-C14-C15-O1
42	N	319	DD6	C13-C14-C15-O1
42	Q	211	DD6	C13-C14-C15-O1
42	Q	214	DD6	C13-C14-C15-O1
42	Y	322	DD6	C5-C6-C8-C9
42	Z	318	DD6	C13-C14-C15-O1
42	j	104	DD6	C13-C14-C15-O1
42	o	319	DD6	C13-C14-C15-O1
42	p	322	DD6	C13-C14-C15-O1
42	q	320	DD6	C10-C11-C13-C14
42	q	320	DD6	C5-C6-C8-C9
42	v	320	DD6	C10-C11-C13-C14
42	v	320	DD6	C5-C6-C8-C9
42	z	322	DD6	C13-C14-C15-C16
43	A	317	LMG	O7-C8-C9-O8
43	A	317	LMG	C11-C10-O7-C8
43	E	301	LMG	O6-C1-O1-C7
43	E	320	LMG	O6-C1-O1-C7
43	E	320	LMG	O9-C10-O7-C8
43	E	320	LMG	C11-C10-O7-C8
43	E	321	LMG	O9-C10-O7-C8
43	E	321	LMG	C11-C10-O7-C8
43	F	318	LMG	O9-C10-O7-C8
43	L	319	LMG	C7-C8-O7-C10
43	M	317	LMG	O9-C10-O7-C8
43	P	318	LMG	O9-C10-O7-C8
43	P	318	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
43	T	318	LMG	C11-C10-O7-C8
43	a	802	LMG	C11-C10-O7-C8
43	p	301	LMG	O7-C8-C9-O8
43	x	301	LMG	O7-C8-C9-O8
44	C	311	A86	C9-C10-C11-C13
44	C	311	A86	C10-C11-C13-O
44	C	311	A86	C12-C11-C13-O
44	D	320	A86	C9-C10-C11-C12
44	D	320	A86	C9-C10-C11-C13
44	D	320	A86	C13-C14-C15-O1
44	F	317	A86	C9-C10-C11-C12
44	F	317	A86	C9-C10-C11-C13
44	F	317	A86	C12-C11-C13-C14
44	G	209	A86	C9-C10-C11-C13
44	G	209	A86	C13-C14-C15-O1
44	G	211	A86	C10-C11-C13-O
44	G	211	A86	C12-C11-C13-O
44	H	315	A86	C13-C14-C15-O1
44	K	314	A86	C13-C14-C15-O1
44	K	314	A86	C26-C27-C29-C30
44	K	314	A86	C28-C27-C29-C30
44	M	320	A86	C5-C6-C8-C9
44	N	315	A86	C12-C11-C13-C14
44	N	321	A86	C9-C10-C11-C13
44	N	321	A86	C28-C27-C29-C30
44	O	312	A86	C13-C14-C15-O1
44	O	315	A86	C9-C10-C11-C12
44	O	315	A86	C9-C10-C11-C13
44	O	315	A86	C12-C11-C13-C14
44	O	315	A86	C13-C14-C15-C16
44	O	315	A86	C13-C14-C15-O1
44	P	314	A86	C12-C11-C13-C14
44	P	321	A86	C10-C11-C13-C14
44	P	321	A86	C12-C11-C13-C14
44	P	321	A86	C13-C14-C15-O1
44	Q	210	A86	O-C13-C14-C15
44	R	313	A86	C9-C10-C11-C13
44	R	315	A86	C9-C10-C11-C12
44	R	315	A86	C9-C10-C11-C13
44	S	315	A86	C9-C10-C11-C12
44	S	315	A86	C9-C10-C11-C13
44	S	315	A86	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
44	S	315	A86	C13-C14-C15-O1
44	S	317	A86	C9-C10-C11-C13
44	S	317	A86	O-C13-C14-C15
44	S	317	A86	C13-C14-C15-C16
44	T	315	A86	C9-C10-C11-C12
44	T	315	A86	C9-C10-C11-C13
44	T	315	A86	C13-C14-C15-C16
44	T	315	A86	C5-C6-C8-C9
44	T	319	A86	C12-C11-C13-C14
44	T	319	A86	C13-C14-C15-O1
44	W	314	A86	C26-C27-C29-C30
44	W	314	A86	C28-C27-C29-C30
44	W	316	A86	C13-C14-C15-O1
44	X	317	A86	C28-C27-C29-C30
44	X	319	A86	C13-C14-C15-O1
44	X	320	A86	O-C13-C14-C15
44	X	320	A86	C13-C14-C15-C16
44	X	320	A86	C13-C14-C15-O1
44	X	321	A86	C9-C10-C11-C13
44	Y	316	A86	C5-C6-C8-C9
44	Y	317	A86	C9-C10-C11-C12
44	Y	317	A86	C9-C10-C11-C13
44	Y	318	A86	C2-C1-C24-C25
44	Y	318	A86	C26-C27-C29-C30
44	Y	318	A86	C5-C6-C8-C9
44	Y	318	A86	C7-C6-C8-C9
44	Y	319	A86	C9-C10-C11-C12
44	Y	319	A86	C9-C10-C11-C13
44	Y	320	A86	C9-C10-C11-C12
44	Y	320	A86	C9-C10-C11-C13
44	Y	321	A86	C9-C10-C11-C12
44	Y	321	A86	C9-C10-C11-C13
44	Z	315	A86	C13-C14-C15-C16
44	Z	315	A86	C13-C14-C15-O1
44	Z	315	A86	C5-C6-C8-C9
44	Z	316	A86	C13-C14-C15-O1
44	o	314	A86	C9-C10-C11-C12
44	o	314	A86	C9-C10-C11-C13
44	o	314	A86	C10-C11-C13-C14
44	o	314	A86	C12-C11-C13-C14
44	o	316	A86	C10-C11-C13-C14
44	o	316	A86	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
44	o	316	A86	O-C13-C14-C15
44	o	316	A86	C13-C14-C15-O1
44	o	317	A86	C9-C10-C11-C12
44	o	317	A86	C9-C10-C11-C13
44	o	318	A86	C9-C10-C11-C12
44	o	318	A86	C9-C10-C11-C13
44	p	316	A86	O-C13-C14-C15
44	p	318	A86	C13-C14-C15-C16
44	p	318	A86	C26-C27-C29-C30
44	p	319	A86	C9-C10-C11-C12
44	p	319	A86	C9-C10-C11-C13
44	p	319	A86	C28-C27-C29-C30
44	p	320	A86	C9-C10-C11-C12
44	p	320	A86	C9-C10-C11-C13
44	p	320	A86	C28-C27-C29-C30
44	p	321	A86	C10-C11-C13-C14
44	p	321	A86	C12-C11-C13-O
44	q	316	A86	C9-C10-C11-C12
44	q	316	A86	C9-C10-C11-C13
44	q	319	A86	C13-C14-C15-C16
44	q	319	A86	C13-C14-C15-O1
44	q	319	A86	C26-C27-C29-C30
44	q	324	A86	C10-C11-C13-O
44	t	310	A86	C2-C1-C24-C25
44	t	310	A86	C13-C14-C15-O1
44	t	310	A86	C28-C27-C29-C30
44	t	316	A86	C12-C11-C13-C14
44	u	316	A86	O-C13-C14-C15
44	u	318	A86	C13-C14-C15-O1
44	u	318	A86	C28-C27-C29-C30
44	u	319	A86	C9-C10-C11-C13
44	u	319	A86	C13-C14-C15-C16
44	v	316	A86	C9-C10-C11-C12
44	v	316	A86	C9-C10-C11-C13
44	v	319	A86	C13-C14-C15-C16
44	w	310	A86	C28-C27-C29-C30
44	w	315	A86	C13-C14-C15-C16
44	w	315	A86	C13-C14-C15-O1
44	w	315	A86	C26-C27-C29-C30
44	w	315	A86	C28-C27-C29-C30
44	x	316	A86	O-C13-C14-C15
44	x	316	A86	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
44	x	317	A86	C9-C10-C11-C13
44	x	319	A86	C9-C10-C11-C13
44	x	319	A86	C13-C14-C15-C16
44	x	319	A86	C28-C27-C29-C30
44	y	310	A86	C2-C1-C24-C25
44	y	310	A86	C28-C27-C29-C30
44	z	301	A86	C12-C11-C13-O
44	z	301	A86	C5-C6-C8-C9
44	z	301	A86	C7-C6-C8-C9
44	z	316	A86	C9-C10-C11-C12
44	z	316	A86	C9-C10-C11-C13
44	z	316	A86	C10-C11-C13-O
44	z	316	A86	C12-C11-C13-O
44	z	316	A86	C5-C6-C8-C9
44	z	318	A86	C9-C10-C11-C12
44	z	318	A86	C9-C10-C11-C13
44	z	319	A86	C9-C10-C11-C12
44	z	319	A86	C9-C10-C11-C13
44	z	319	A86	C12-C11-C13-C14
44	z	319	A86	C13-C14-C15-O1
45	F	319	LHG	C3-O3-P-O4
45	F	319	LHG	C3-O3-P-O6
45	F	319	LHG	C4-O6-P-O5
45	S	323	LHG	O2-C2-C3-O3
45	S	323	LHG	C3-O3-P-O5
45	S	323	LHG	C8-C7-O7-C5
45	S	323	LHG	O10-C23-O8-C6
45	a	848	LHG	O1-C1-C2-C3
45	a	848	LHG	C3-O3-P-O6
45	a	849	LHG	O1-C1-C2-O2
45	a	849	LHG	O1-C1-C2-C3
45	a	849	LHG	C3-O3-P-O5
45	a	849	LHG	C3-O3-P-O6
46	I	215	SQD	O5-C1-O6-C44
46	I	215	SQD	C8-C7-O47-C45
46	I	215	SQD	O5-C5-C6-S
46	M	318	SQD	C5-C6-S-O7
46	M	318	SQD	C5-C6-S-O8
46	M	318	SQD	C5-C6-S-O9
46	P	319	SQD	C5-C6-S-O7
46	P	319	SQD	C5-C6-S-O8
46	P	319	SQD	C5-C6-S-O9

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Mol	Chain	Res	Type	Atoms
46	k	205	SQD	C8-C7-O47-C45
47	F	322	A1EB1	C12-C11-C13-C14
47	F	322	A1EB1	C25-C26-C27-C28
47	F	322	A1EB1	C25-C26-C27-C29
47	G	212	A1EB1	C26-C27-C29-C30
47	K	313	A1EB1	C13-C14-C15-O1
47	K	313	A1EB1	C25-C26-C27-C28
47	K	315	A1EB1	C13-C14-C15-C16
47	K	315	A1EB1	C13-C14-C15-C20
47	K	315	A1EB1	C13-C14-C15-O1
47	K	315	A1EB1	C25-C26-C27-C28
47	K	315	A1EB1	C25-C26-C27-C29
47	L	316	A1EB1	C25-C26-C27-C28
47	L	316	A1EB1	C26-C27-C28-O6
47	L	316	A1EB1	C29-C27-C28-O6
47	L	316	A1EB1	C26-C27-C29-C30
47	L	318	A1EB1	C10-C11-C13-C14
47	L	318	A1EB1	C12-C11-C13-C14
47	L	318	A1EB1	C13-C14-C15-O1
47	L	318	A1EB1	C26-C27-C29-C30
47	N	320	A1EB1	C2-C1-C24-C25
47	N	320	A1EB1	C26-C27-C28-O6
47	N	320	A1EB1	C29-C27-C28-O6
47	N	320	A1EB1	C26-C27-C29-C30
47	O	317	A1EB1	C25-C26-C27-C28
47	O	317	A1EB1	C26-C27-C29-C30
47	P	301	A1EB1	C9-C10-C11-C12
47	P	301	A1EB1	C9-C10-C11-C13
47	P	301	A1EB1	C10-C11-C13-O
47	P	301	A1EB1	C13-C14-C15-O1
47	P	301	A1EB1	C26-C27-C29-C30
47	R	317	A1EB1	C25-C26-C27-C28
47	R	317	A1EB1	C25-C26-C27-C29
47	R	317	A1EB1	C26-C27-C29-C30
47	R	317	A1EB1	C5-C6-C8-C9
47	S	320	A1EB1	C10-C11-C13-C14
47	S	320	A1EB1	C12-C11-C13-C14
47	S	321	A1EB1	C9-C10-C11-C12
47	S	321	A1EB1	C9-C10-C11-C13
47	S	321	A1EB1	C25-C26-C27-C28
47	S	321	A1EB1	C25-C26-C27-C29
47	S	321	A1EB1	C26-C27-C28-O6

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Mol	Chain	Res	Type	Atoms
47	S	321	A1EB1	C29-C27-C28-O6
47	T	316	A1EB1	C25-C26-C27-C28
47	T	316	A1EB1	C26-C27-C29-C30
47	T	320	A1EB1	C-C1-C24-C25
47	T	320	A1EB1	C2-C1-C24-C25
47	T	320	A1EB1	C26-C27-C28-O6
47	T	320	A1EB1	C29-C27-C28-O6
47	T	320	A1EB1	C26-C27-C29-C30
47	Y	323	A1EB1	C26-C27-C28-O6
47	Y	323	A1EB1	C29-C27-C28-O6
47	Z	319	A1EB1	C25-C26-C27-C28
47	Z	320	A1EB1	C26-C27-C29-C30
47	Z	321	A1EB1	C26-C27-C29-C30
47	o	321	A1EB1	C2-C1-C24-C25
47	o	321	A1EB1	C26-C27-C28-O6
47	o	321	A1EB1	C29-C27-C28-O6
47	o	321	A1EB1	C26-C27-C29-C30
47	o	322	A1EB1	C12-C11-C13-C14
47	o	322	A1EB1	C13-C14-C15-C16
47	o	322	A1EB1	C26-C27-C28-O6
47	o	322	A1EB1	C29-C27-C28-O6
47	p	323	A1EB1	C25-C26-C27-C28
47	q	321	A1EB1	C2-C1-C24-C25
47	q	321	A1EB1	O-C13-C14-C15
47	q	321	A1EB1	C11-C13-C14-C15
47	q	321	A1EB1	C13-C14-C15-O1
47	q	321	A1EB1	C25-C26-C27-C28
47	q	321	A1EB1	C25-C26-C27-C29
47	q	321	A1EB1	C44-C42-O6-C28
47	q	321	A1EB1	O43-C42-O6-C28
47	q	321	A1EB1	C5-C6-C8-C9
47	q	322	A1EB1	C9-C10-C11-C13
47	q	322	A1EB1	C13-C14-C15-O1
47	q	323	A1EB1	C-C1-C24-C25
47	q	323	A1EB1	C2-C1-C24-C25
47	q	323	A1EB1	C9-C10-C11-C12
47	q	323	A1EB1	C9-C10-C11-C13
47	q	323	A1EB1	C25-C26-C27-C28
47	q	323	A1EB1	C25-C26-C27-C29
47	q	323	A1EB1	C26-C27-C29-C30
47	t	313	A1EB1	C9-C10-C11-C13
47	t	313	A1EB1	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
47	t	313	A1EB1	C25-C26-C27-C29
47	t	313	A1EB1	C26-C27-C28-O6
47	t	313	A1EB1	C29-C27-C28-O6
47	t	314	A1EB1	C12-C11-C13-C14
47	t	314	A1EB1	C25-C26-C27-C28
47	t	314	A1EB1	C25-C26-C27-C29
47	t	314	A1EB1	C26-C27-C29-C30
47	t	314	A1EB1	C44-C42-O6-C28
47	t	314	A1EB1	O43-C42-O6-C28
47	t	315	A1EB1	C9-C10-C11-C12
47	t	315	A1EB1	C9-C10-C11-C13
47	t	315	A1EB1	C13-C14-C15-O1
47	t	315	A1EB1	C25-C26-C27-C28
47	t	315	A1EB1	C26-C27-C29-C30
47	u	322	A1EB1	C25-C26-C27-C28
47	u	323	A1EB1	C26-C27-C28-O6
47	u	323	A1EB1	C29-C27-C28-O6
47	v	321	A1EB1	O-C13-C14-C15
47	v	321	A1EB1	C11-C13-C14-C15
47	v	321	A1EB1	C13-C14-C15-O1
47	v	321	A1EB1	C25-C26-C27-C28
47	v	321	A1EB1	C25-C26-C27-C29
47	v	321	A1EB1	C44-C42-O6-C28
47	v	321	A1EB1	O43-C42-O6-C28
47	v	321	A1EB1	C5-C6-C8-C9
47	v	322	A1EB1	C9-C10-C11-C12
47	v	322	A1EB1	C9-C10-C11-C13
47	v	322	A1EB1	C13-C14-C15-O1
47	v	323	A1EB1	C-C1-C24-C25
47	v	323	A1EB1	C2-C1-C24-C25
47	v	323	A1EB1	C9-C10-C11-C12
47	v	323	A1EB1	C9-C10-C11-C13
47	v	323	A1EB1	C25-C26-C27-C28
47	v	323	A1EB1	C25-C26-C27-C29
47	v	323	A1EB1	C26-C27-C29-C30
47	v	324	A1EB1	C9-C10-C11-C12
47	v	324	A1EB1	C9-C10-C11-C13
47	v	324	A1EB1	C25-C26-C27-C28
47	v	324	A1EB1	C25-C26-C27-C29
47	v	324	A1EB1	C26-C27-C29-C30
47	v	324	A1EB1	C44-C42-O6-C28
47	v	324	A1EB1	O43-C42-O6-C28

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Mol	Chain	Res	Type	Atoms
47	w	313	A1EB1	C25-C26-C27-C28
47	w	313	A1EB1	C5-C6-C8-C9
47	w	314	A1EB1	C9-C10-C11-C13
47	w	314	A1EB1	C25-C26-C27-C28
47	w	314	A1EB1	C26-C27-C29-C30
47	x	322	A1EB1	C26-C27-C28-O6
47	x	322	A1EB1	C29-C27-C28-O6
47	x	322	A1EB1	C26-C27-C29-C30
47	y	312	A1EB1	C25-C26-C27-C28
47	y	312	A1EB1	C25-C26-C27-C29
47	y	312	A1EB1	C5-C6-C8-C9
47	y	313	A1EB1	C2-C1-C24-C25
47	y	313	A1EB1	C9-C10-C11-C12
47	y	313	A1EB1	C9-C10-C11-C13
47	y	313	A1EB1	C26-C27-C29-C30
47	y	313	A1EB1	C5-C6-C8-C9
47	y	314	A1EB1	C9-C10-C11-C13
47	y	314	A1EB1	O-C13-C14-C15
47	y	314	A1EB1	C26-C27-C29-C30
47	z	323	A1EB1	C26-C27-C28-O6
47	z	323	A1EB1	C29-C27-C28-O6
47	z	323	A1EB1	C44-C42-O6-C28
47	z	323	A1EB1	O43-C42-O6-C28
48	M	319	A1EB4	C12-C11-C13-C14
48	P	320	A1EB4	C12-C11-C13-C14
48	P	320	A1EB4	C11-C13-C14-C15
48	W	319	A1EB4	C9-C10-C11-C12
48	W	319	A1EB4	C9-C10-C11-C13
48	W	319	A1EB4	C12-C11-C13-C14
48	W	319	A1EB4	C11-C13-C14-C15
49	a	845	BCR	C23-C24-C25-C26
49	a	845	BCR	C23-C24-C25-C30
49	b	848	BCR	C21-C22-C23-C24
49	b	848	BCR	C37-C22-C23-C24
49	j	103	BCR	C1-C6-C7-C8
49	j	103	BCR	C5-C6-C7-C8
49	j	103	BCR	C23-C24-C25-C26
49	k	203	BCR	C17-C18-C19-C20
49	l	206	BCR	C21-C22-C23-C24
49	l	206	BCR	C37-C22-C23-C24
49	l	206	BCR	C23-C24-C25-C26
49	l	206	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
52	b	850	DGD	O6D-C1D-O3G-C3G
44	Z	314	A86	O5-C38-O4-C34
40	C	308	CLA	CBD-CGD-O2D-CED
40	H	302	CLA	CBD-CGD-O2D-CED
40	S	311	CLA	CBD-CGD-O2D-CED
40	W	306	CLA	CBD-CGD-O2D-CED
40	o	312	CLA	CBD-CGD-O2D-CED
40	u	312	CLA	CBD-CGD-O2D-CED
40	C	302	CLA	C4C-C3C-CAC-CBC
40	C	302	CLA	C2C-C3C-CAC-CBC
44	Z	314	A86	C39-C38-O4-C34
44	q	314	A86	C33-C34-O4-C38
44	v	314	A86	C33-C34-O4-C38
45	S	323	LHG	C24-C23-O8-C6
47	u	322	A1EB1	O5-C38-O4-C34
40	D	306	CLA	CBD-CGD-O2D-CED
41	O	301	KC2	CBD-CGD-O2D-CED
43	E	321	LMG	O10-C28-O8-C9
43	F	318	LMG	O10-C28-O8-C9
43	M	317	LMG	O10-C28-O8-C9
43	P	318	LMG	O10-C28-O8-C9
43	S	322	LMG	O10-C28-O8-C9
43	W	317	LMG	O10-C28-O8-C9
43	a	801	LMG	O10-C28-O8-C9
43	a	802	LMG	O10-C28-O8-C9
43	j	101	LMG	O10-C28-O8-C9
43	u	301	LMG	O10-C28-O8-C9
45	a	849	LHG	O10-C23-O8-C6
43	j	101	LMG	C4-C5-C6-O5
47	u	322	A1EB1	C39-C38-O4-C34
41	I	209	KC2	CAA-CBA-CGA-O1A
41	K	302	KC2	CAA-CBA-CGA-O1A
41	K	302	KC2	CAA-CBA-CGA-O2A
41	K	303	KC2	CAA-CBA-CGA-O1A
41	K	303	KC2	CAA-CBA-CGA-O2A
41	M	308	KC2	CAA-CBA-CGA-O1A
41	X	308	KC2	CAA-CBA-CGA-O1A
41	X	308	KC2	CAA-CBA-CGA-O2A
41	Z	302	KC2	CAA-CBA-CGA-O1A
41	Z	302	KC2	CAA-CBA-CGA-O2A
41	q	309	KC2	CAA-CBA-CGA-O2A
41	t	301	KC2	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
41	t	301	KC2	CAA-CBA-CGA-O2A
41	x	304	KC2	CAA-CBA-CGA-O1A
41	z	309	KC2	CAA-CBA-CGA-O2A
44	G	209	A86	O5-C38-O4-C34
40	J	312	CLA	C2C-C3C-CAC-CBC
43	T	318	LMG	O9-C10-O7-C8
43	a	802	LMG	O9-C10-O7-C8
45	S	323	LHG	O9-C7-O7-C5
46	I	215	SQD	O49-C7-O47-C45
46	k	205	SQD	O49-C7-O47-C45
44	z	315	A86	C39-C38-O4-C34
40	A	306	CLA	C3-C5-C6-C7
40	D	306	CLA	C3-C5-C6-C7
40	E	306	CLA	C3-C5-C6-C7
40	F	304	CLA	C3-C5-C6-C7
40	H	305	CLA	C3-C5-C6-C7
40	M	312	CLA	C3-C5-C6-C7
40	N	311	CLA	C3-C5-C6-C7
40	O	307	CLA	C3-C5-C6-C7
40	P	305	CLA	C3-C5-C6-C7
40	S	302	CLA	C3-C5-C6-C7
40	V	201	CLA	C3-C5-C6-C7
40	W	312	CLA	C3-C5-C6-C7
40	a	820	CLA	C3-C5-C6-C7
40	a	833	CLA	C3-C5-C6-C7
40	a	838	CLA	C3-C5-C6-C7
40	b	807	CLA	C3-C5-C6-C7
40	b	812	CLA	C3-C5-C6-C7
40	o	310	CLA	C3-C5-C6-C7
43	L	319	LMG	C29-C28-O8-C9
43	M	317	LMG	C29-C28-O8-C9
43	S	322	LMG	C29-C28-O8-C9
43	W	317	LMG	C29-C28-O8-C9
43	a	802	LMG	C29-C28-O8-C9
43	j	101	LMG	C29-C28-O8-C9
43	u	301	LMG	C29-C28-O8-C9
44	R	315	A86	O5-C38-O4-C34
43	u	301	LMG	O6-C5-C6-O5
40	G	201	CLA	CBD-CGD-O2D-CED
40	G	207	CLA	CBD-CGD-O2D-CED
40	S	319	CLA	CBD-CGD-O2D-CED
40	Y	311	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
40	b	810	CLA	CBD-CGD-O2D-CED
40	q	307	CLA	CBD-CGD-O2D-CED
40	v	307	CLA	CBD-CGD-O2D-CED
40	v	310	CLA	CBD-CGD-O2D-CED
43	F	318	LMG	C11-C10-O7-C8
43	L	319	LMG	C11-C10-O7-C8
43	M	317	LMG	C11-C10-O7-C8
43	W	317	LMG	C11-C10-O7-C8
41	Y	314	KC2	O1D-CGD-O2D-CED
44	R	315	A86	C39-C38-O4-C34
44	X	315	A86	O5-C38-O4-C34
44	z	315	A86	O5-C38-O4-C34
44	G	209	A86	C39-C38-O4-C34
44	X	315	A86	C39-C38-O4-C34
41	I	209	KC2	CAA-CBA-CGA-O2A
41	I	214	KC2	CAA-CBA-CGA-O1A
41	I	214	KC2	CAA-CBA-CGA-O2A
41	O	311	KC2	CAA-CBA-CGA-O1A
41	O	311	KC2	CAA-CBA-CGA-O2A
41	R	303	KC2	CAA-CBA-CGA-O1A
41	R	303	KC2	CAA-CBA-CGA-O2A
41	R	311	KC2	CAA-CBA-CGA-O1A
41	R	311	KC2	CAA-CBA-CGA-O2A
41	S	309	KC2	CAA-CBA-CGA-O1A
41	S	309	KC2	CAA-CBA-CGA-O2A
41	o	308	KC2	CAA-CBA-CGA-O1A
41	o	308	KC2	CAA-CBA-CGA-O2A
41	p	303	KC2	CAA-CBA-CGA-O1A
41	p	303	KC2	CAA-CBA-CGA-O2A
41	p	304	KC2	CAA-CBA-CGA-O1A
41	p	304	KC2	CAA-CBA-CGA-O2A
41	p	315	KC2	CAA-CBA-CGA-O1A
41	p	315	KC2	CAA-CBA-CGA-O2A
41	q	309	KC2	CAA-CBA-CGA-O1A
41	w	307	KC2	CAA-CBA-CGA-O1A
41	w	307	KC2	CAA-CBA-CGA-O2A
41	x	303	KC2	CAA-CBA-CGA-O1A
41	x	303	KC2	CAA-CBA-CGA-O2A
41	x	304	KC2	CAA-CBA-CGA-O2A
41	x	315	KC2	CAA-CBA-CGA-O1A
41	x	315	KC2	CAA-CBA-CGA-O2A
40	C	305	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
40	C	307	CLA	C4-C3-C5-C6
40	D	310	CLA	C4-C3-C5-C6
40	D	312	CLA	C4-C3-C5-C6
40	E	308	CLA	C4-C3-C5-C6
40	E	309	CLA	C4-C3-C5-C6
40	F	303	CLA	C4-C3-C5-C6
40	S	307	CLA	C4-C3-C5-C6
40	Y	305	CLA	C4-C3-C5-C6
40	Y	310	CLA	C4-C3-C5-C6
40	Z	306	CLA	C4-C3-C5-C6
40	b	834	CLA	C4-C3-C5-C6
40	o	304	CLA	C4-C3-C5-C6
40	z	305	CLA	C4-C3-C5-C6
40	C	305	CLA	C2-C3-C5-C6
40	C	307	CLA	C2-C3-C5-C6
40	D	310	CLA	C2-C3-C5-C6
40	D	312	CLA	C2-C3-C5-C6
40	E	308	CLA	C2-C3-C5-C6
40	E	309	CLA	C2-C3-C5-C6
40	S	314	CLA	C2-C3-C5-C6
40	Y	305	CLA	C2-C3-C5-C6
40	Y	310	CLA	C2-C3-C5-C6
40	Z	306	CLA	C2-C3-C5-C6
40	b	834	CLA	C2-C3-C5-C6
40	b	837	CLA	C2-C3-C5-C6
40	z	305	CLA	C2-C3-C5-C6
40	A	301	CLA	C2A-CAA-CBA-CGA
40	U	204	CLA	C2A-CAA-CBA-CGA
40	b	813	CLA	C2A-CAA-CBA-CGA
40	t	303	CLA	C2A-CAA-CBA-CGA
40	w	303	CLA	C2A-CAA-CBA-CGA
40	F	303	CLA	C3-C5-C6-C7
40	P	307	CLA	C3-C5-C6-C7
40	R	306	CLA	C3-C5-C6-C7
40	W	313	CLA	C3-C5-C6-C7
40	X	307	CLA	C3-C5-C6-C7
40	a	823	CLA	C3-C5-C6-C7
40	b	819	CLA	C3-C5-C6-C7
40	b	825	CLA	C3-C5-C6-C7
40	K	308	CLA	C2C-C3C-CAC-CBC
40	H	307	CLA	CBA-CGA-O2A-C1
40	a	824	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
43	E	321	LMG	C29-C28-O8-C9
43	P	318	LMG	C29-C28-O8-C9
43	a	801	LMG	C29-C28-O8-C9
45	a	849	LHG	C24-C23-O8-C6
40	K	308	CLA	C4C-C3C-CAC-CBC
44	o	314	A86	C39-C38-O4-C34
47	N	320	A1EB1	C39-C38-O4-C34
43	j	101	LMG	O6-C5-C6-O5
47	q	323	A1EB1	C24-C25-C26-C27
47	v	323	A1EB1	C24-C25-C26-C27
43	E	320	LMG	O10-C28-O8-C9
43	L	319	LMG	O10-C28-O8-C9
43	x	301	LMG	O10-C28-O8-C9
43	A	317	LMG	O9-C10-O7-C8
43	L	319	LMG	O9-C10-O7-C8
43	W	317	LMG	O9-C10-O7-C8
43	D	318	LMG	O6-C5-C6-O5
44	C	311	A86	C39-C38-O4-C34
44	D	319	A86	C39-C38-O4-C34
44	D	320	A86	C39-C38-O4-C34
44	F	312	A86	C39-C38-O4-C34
44	G	211	A86	C39-C38-O4-C34
44	H	315	A86	C39-C38-O4-C34
44	L	314	A86	C39-C38-O4-C34
44	M	313	A86	C39-C38-O4-C34
44	M	315	A86	C39-C38-O4-C34
44	N	314	A86	C39-C38-O4-C34
44	N	315	A86	C39-C38-O4-C34
44	P	314	A86	C39-C38-O4-C34
44	P	316	A86	C39-C38-O4-C34
44	R	312	A86	C39-C38-O4-C34
44	S	316	A86	C39-C38-O4-C34
44	T	313	A86	C39-C38-O4-C34
44	T	315	A86	C39-C38-O4-C34
44	U	210	A86	C39-C38-O4-C34
44	X	314	A86	C39-C38-O4-C34
44	X	316	A86	C39-C38-O4-C34
44	X	318	A86	C39-C38-O4-C34
44	X	319	A86	C39-C38-O4-C34
44	Y	315	A86	C39-C38-O4-C34
44	Y	317	A86	C39-C38-O4-C34
44	Y	318	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
44	Y	319	A86	C39-C38-O4-C34
44	Y	320	A86	C39-C38-O4-C34
44	Z	316	A86	C39-C38-O4-C34
44	o	314	A86	O5-C38-O4-C34
44	o	316	A86	C39-C38-O4-C34
44	o	317	A86	C39-C38-O4-C34
44	p	316	A86	C39-C38-O4-C34
44	p	318	A86	C39-C38-O4-C34
44	p	319	A86	C39-C38-O4-C34
44	t	311	A86	C39-C38-O4-C34
44	u	316	A86	C39-C38-O4-C34
44	u	318	A86	C39-C38-O4-C34
44	u	319	A86	C39-C38-O4-C34
44	v	315	A86	C39-C38-O4-C34
44	v	319	A86	C39-C38-O4-C34
44	w	310	A86	C39-C38-O4-C34
44	w	311	A86	C39-C38-O4-C34
44	w	315	A86	C39-C38-O4-C34
44	w	316	A86	C39-C38-O4-C34
44	x	318	A86	C39-C38-O4-C34
44	x	319	A86	C39-C38-O4-C34
44	z	317	A86	C39-C38-O4-C34
44	z	318	A86	C39-C38-O4-C34
47	F	322	A1EB1	C39-C38-O4-C34
47	G	212	A1EB1	C39-C38-O4-C34
47	K	315	A1EB1	C39-C38-O4-C34
47	L	318	A1EB1	C39-C38-O4-C34
47	N	320	A1EB1	O5-C38-O4-C34
47	R	317	A1EB1	C39-C38-O4-C34
47	S	320	A1EB1	C39-C38-O4-C34
47	T	316	A1EB1	C39-C38-O4-C34
47	T	320	A1EB1	C39-C38-O4-C34
47	Z	319	A1EB1	C39-C38-O4-C34
47	Z	321	A1EB1	C39-C38-O4-C34
47	o	322	A1EB1	C39-C38-O4-C34
47	t	313	A1EB1	C39-C38-O4-C34
47	t	314	A1EB1	C39-C38-O4-C34
47	v	321	A1EB1	C39-C38-O4-C34
47	v	324	A1EB1	C39-C38-O4-C34
47	w	313	A1EB1	C39-C38-O4-C34
47	y	312	A1EB1	C39-C38-O4-C34
47	y	313	A1EB1	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
47	y	314	A1EB1	C39-C38-O4-C34
47	z	323	A1EB1	C39-C38-O4-C34
48	M	319	A1EB4	C42-C38-O4-C34
48	P	320	A1EB4	C42-C38-O4-C34
48	W	319	A1EB4	C42-C38-O4-C34
41	Q	201	KC2	CAA-CBA-CGA-O1A
41	Q	201	KC2	CAA-CBA-CGA-O2A
41	u	315	KC2	CAA-CBA-CGA-O1A
41	u	315	KC2	CAA-CBA-CGA-O2A
40	A	305	CLA	C3-C5-C6-C7
40	F	321	CLA	C3-C5-C6-C7
40	J	308	CLA	C3-C5-C6-C7
40	Q	205	CLA	C3-C5-C6-C7
40	R	305	CLA	C3-C5-C6-C7
40	S	306	CLA	C3-C5-C6-C7
40	V	202	CLA	C3-C5-C6-C7
40	a	811	CLA	C3-C5-C6-C7
40	a	825	CLA	C3-C5-C6-C7
40	b	827	CLA	C3-C5-C6-C7
40	o	305	CLA	C3-C5-C6-C7
40	u	312	CLA	C3-C5-C6-C7
40	o	307	CLA	CBD-CGD-O2D-CED
40	M	304	CLA	C2C-C3C-CAC-CBC
40	o	312	CLA	O1D-CGD-O2D-CED
40	a	826	CLA	CBA-CGA-O2A-C1
43	E	320	LMG	C29-C28-O8-C9
44	W	314	A86	C39-C38-O4-C34
44	Z	315	A86	C39-C38-O4-C34
44	q	315	A86	C39-C38-O4-C34
44	q	319	A86	C39-C38-O4-C34
44	x	316	A86	C39-C38-O4-C34
47	S	321	A1EB1	C39-C38-O4-C34
47	q	321	A1EB1	C39-C38-O4-C34
47	t	315	A1EB1	C39-C38-O4-C34
44	C	311	A86	O5-C38-O4-C34
44	D	319	A86	O5-C38-O4-C34
44	D	320	A86	O5-C38-O4-C34
44	F	312	A86	O5-C38-O4-C34
44	G	211	A86	O5-C38-O4-C34
44	H	315	A86	O5-C38-O4-C34
44	L	314	A86	O5-C38-O4-C34
44	M	313	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
44	M	315	A86	O5-C38-O4-C34
44	N	314	A86	O5-C38-O4-C34
44	N	315	A86	O5-C38-O4-C34
44	N	321	A86	C39-C38-O4-C34
44	N	321	A86	O5-C38-O4-C34
44	P	314	A86	O5-C38-O4-C34
44	P	316	A86	O5-C38-O4-C34
44	R	312	A86	O5-C38-O4-C34
44	S	316	A86	O5-C38-O4-C34
44	T	313	A86	O5-C38-O4-C34
44	T	315	A86	O5-C38-O4-C34
44	U	210	A86	O5-C38-O4-C34
44	W	314	A86	O5-C38-O4-C34
44	X	314	A86	O5-C38-O4-C34
44	X	316	A86	O5-C38-O4-C34
44	X	318	A86	O5-C38-O4-C34
44	X	319	A86	O5-C38-O4-C34
44	X	321	A86	C39-C38-O4-C34
44	X	321	A86	O5-C38-O4-C34
44	Y	315	A86	O5-C38-O4-C34
44	Y	317	A86	O5-C38-O4-C34
44	Y	318	A86	O5-C38-O4-C34
44	Y	319	A86	O5-C38-O4-C34
44	Y	320	A86	O5-C38-O4-C34
44	Z	315	A86	O5-C38-O4-C34
44	Z	316	A86	O5-C38-O4-C34
44	o	316	A86	O5-C38-O4-C34
44	o	317	A86	O5-C38-O4-C34
44	p	316	A86	O5-C38-O4-C34
44	p	318	A86	O5-C38-O4-C34
44	p	319	A86	O5-C38-O4-C34
44	q	314	A86	C39-C38-O4-C34
44	q	314	A86	O5-C38-O4-C34
44	q	315	A86	O5-C38-O4-C34
44	q	319	A86	O5-C38-O4-C34
44	t	311	A86	O5-C38-O4-C34
44	u	316	A86	O5-C38-O4-C34
44	u	318	A86	O5-C38-O4-C34
44	u	319	A86	O5-C38-O4-C34
44	v	314	A86	C39-C38-O4-C34
44	v	314	A86	O5-C38-O4-C34
44	v	315	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
44	v	319	A86	O5-C38-O4-C34
44	w	310	A86	O5-C38-O4-C34
44	w	311	A86	O5-C38-O4-C34
44	w	315	A86	O5-C38-O4-C34
44	w	316	A86	O5-C38-O4-C34
44	x	316	A86	O5-C38-O4-C34
44	x	317	A86	C39-C38-O4-C34
44	x	317	A86	O5-C38-O4-C34
44	x	318	A86	O5-C38-O4-C34
44	x	319	A86	O5-C38-O4-C34
44	z	317	A86	O5-C38-O4-C34
44	z	318	A86	O5-C38-O4-C34
47	F	322	A1EB1	O5-C38-O4-C34
47	G	212	A1EB1	O5-C38-O4-C34
47	K	315	A1EB1	O5-C38-O4-C34
47	L	316	A1EB1	C39-C38-O4-C34
47	L	316	A1EB1	O5-C38-O4-C34
47	L	318	A1EB1	O5-C38-O4-C34
47	R	317	A1EB1	O5-C38-O4-C34
47	S	320	A1EB1	O5-C38-O4-C34
47	S	321	A1EB1	O5-C38-O4-C34
47	T	316	A1EB1	O5-C38-O4-C34
47	T	320	A1EB1	O5-C38-O4-C34
47	Z	319	A1EB1	O5-C38-O4-C34
47	Z	321	A1EB1	O5-C38-O4-C34
47	o	322	A1EB1	O5-C38-O4-C34
47	p	323	A1EB1	C39-C38-O4-C34
47	p	323	A1EB1	O5-C38-O4-C34
47	q	321	A1EB1	O5-C38-O4-C34
47	q	322	A1EB1	C39-C38-O4-C34
47	q	322	A1EB1	O5-C38-O4-C34
47	t	313	A1EB1	O5-C38-O4-C34
47	t	314	A1EB1	O5-C38-O4-C34
47	t	315	A1EB1	O5-C38-O4-C34
47	v	321	A1EB1	O5-C38-O4-C34
47	v	322	A1EB1	C39-C38-O4-C34
47	v	322	A1EB1	O5-C38-O4-C34
47	v	324	A1EB1	O5-C38-O4-C34
47	w	313	A1EB1	O5-C38-O4-C34
47	w	314	A1EB1	C39-C38-O4-C34
47	w	314	A1EB1	O5-C38-O4-C34
47	y	312	A1EB1	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
47	y	313	A1EB1	O5-C38-O4-C34
47	y	314	A1EB1	O5-C38-O4-C34
47	z	323	A1EB1	O5-C38-O4-C34
48	M	319	A1EB4	O43-C38-O4-C34
48	P	320	A1EB4	O43-C38-O4-C34
48	W	319	A1EB4	O43-C38-O4-C34
43	l	201	LMG	O6-C5-C6-O5
43	x	301	LMG	O6-C5-C6-O5
43	a	801	LMG	C11-C10-O7-C8
46	F	320	SQD	C8-C7-O47-C45
46	W	318	SQD	C8-C7-O47-C45
44	z	315	A86	C33-C34-O4-C38
43	F	318	LMG	O6-C5-C6-O5
40	C	306	CLA	C3-C5-C6-C7
40	M	304	CLA	C3-C5-C6-C7
40	Q	202	CLA	C3-C5-C6-C7
40	z	312	CLA	C3-C5-C6-C7
40	P	308	CLA	CBD-CGD-O2D-CED
40	p	312	CLA	CBD-CGD-O2D-CED
40	q	310	CLA	CBD-CGD-O2D-CED
43	A	317	LMG	O6-C5-C6-O5
40	W	306	CLA	O1D-CGD-O2D-CED
43	F	318	LMG	C29-C28-O8-C9
41	L	303	KC2	CAA-CBA-CGA-O1A
41	L	303	KC2	CAA-CBA-CGA-O2A
41	O	309	KC2	CAA-CBA-CGA-O1A
41	S	304	KC2	CAA-CBA-CGA-O1A
41	S	304	KC2	CAA-CBA-CGA-O2A
41	W	303	KC2	CAA-CBA-CGA-O1A
41	W	309	KC2	CAA-CBA-CGA-O2A
41	Y	309	KC2	CAA-CBA-CGA-O1A
41	q	308	KC2	CAA-CBA-CGA-O1A
41	v	308	KC2	CAA-CBA-CGA-O1A
41	y	307	KC2	CAA-CBA-CGA-O1A
41	y	307	KC2	CAA-CBA-CGA-O2A
41	z	309	KC2	CAA-CBA-CGA-O1A
40	E	305	CLA	C4-C3-C5-C6
40	I	205	CLA	C4-C3-C5-C6
40	K	308	CLA	C4-C3-C5-C6
40	O	306	CLA	C4-C3-C5-C6
40	a	829	CLA	C4-C3-C5-C6
40	b	803	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
40	E	305	CLA	C2-C3-C5-C6
40	I	205	CLA	C2-C3-C5-C6
40	K	308	CLA	C2-C3-C5-C6
40	O	306	CLA	C2-C3-C5-C6
40	Q	208	CLA	C2-C3-C5-C6
40	a	804	CLA	C2-C3-C5-C6
40	a	819	CLA	C2-C3-C5-C6
40	a	829	CLA	C2-C3-C5-C6
40	b	803	CLA	C2-C3-C5-C6
43	T	318	LMG	O10-C28-O8-C9
43	u	301	LMG	C4-C5-C6-O5
40	U	207	CLA	CBD-CGD-O2D-CED
43	L	319	LMG	C4-C5-C6-O5
40	a	825	CLA	C2A-CAA-CBA-CGA
40	b	809	CLA	C2A-CAA-CBA-CGA
40	f	202	CLA	C2A-CAA-CBA-CGA
40	a	824	CLA	O1A-CGA-O2A-C1
43	A	317	LMG	O6-C1-O1-C7
43	p	301	LMG	O6-C1-O1-C7
43	A	317	LMG	C4-C5-C6-O5
40	J	302	CLA	C2C-C3C-CAC-CBC
40	x	312	CLA	CBA-CGA-O2A-C1
43	T	318	LMG	C29-C28-O8-C9
43	x	301	LMG	C29-C28-O8-C9
40	J	312	CLA	CBD-CGD-O2D-CED
40	b	807	CLA	CBD-CGD-O2D-CED
40	b	833	CLA	CBD-CGD-O2D-CED
40	w	308	CLA	CBD-CGD-O2D-CED
41	W	303	KC2	CAA-CBA-CGA-O2A
41	W	309	KC2	CAA-CBA-CGA-O1A
41	Y	314	KC2	CAA-CBA-CGA-O1A
41	u	304	KC2	CAA-CBA-CGA-O2A
41	v	309	KC2	CAA-CBA-CGA-O1A
41	z	303	KC2	CAA-CBA-CGA-O2A
43	E	301	LMG	O6-C5-C6-O5
40	S	311	CLA	O1D-CGD-O2D-CED
40	Y	307	CLA	CBD-CGD-O2D-CED
40	v	306	CLA	CBD-CGD-O2D-CED
40	y	308	CLA	CBD-CGD-O2D-CED
40	y	309	CLA	CBD-CGD-O2D-CED
40	a	840	CLA	C3-C5-C6-C7
40	b	809	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
40	b	837	CLA	C3-C5-C6-C7
40	H	307	CLA	O1A-CGA-O2A-C1
46	W	318	SQD	O49-C7-O47-C45
45	S	323	LHG	C1-C2-C3-O3
40	C	306	CLA	CBA-CGA-O2A-C1
40	H	305	CLA	CBA-CGA-O2A-C1
40	L	310	CLA	CBA-CGA-O2A-C1
40	S	307	CLA	CBA-CGA-O2A-C1
40	U	202	CLA	CBA-CGA-O2A-C1
40	X	305	CLA	CBA-CGA-O2A-C1
40	a	819	CLA	CBA-CGA-O2A-C1
40	z	302	CLA	CBA-CGA-O2A-C1
40	z	305	CLA	CBA-CGA-O2A-C1
45	a	848	LHG	C24-C23-O8-C6
44	S	318	A86	C35-C34-O4-C38
40	X	305	CLA	CBD-CGD-O2D-CED
40	Y	305	CLA	CBD-CGD-O2D-CED
40	p	314	CLA	CBD-CGD-O2D-CED
40	C	308	CLA	O1D-CGD-O2D-CED
40	H	302	CLA	O1D-CGD-O2D-CED
40	u	312	CLA	O1D-CGD-O2D-CED
43	D	318	LMG	C4-C5-C6-O5
43	F	318	LMG	C4-C5-C6-O5
41	G	202	KC2	CAA-CBA-CGA-O1A
41	N	302	KC2	CAA-CBA-CGA-O1A
41	N	308	KC2	CAA-CBA-CGA-O1A
41	O	309	KC2	CAA-CBA-CGA-O2A
41	Q	216	KC2	CAA-CBA-CGA-O1A
41	T	311	KC2	CAA-CBA-CGA-O1A
41	T	311	KC2	CAA-CBA-CGA-O2A
41	Y	308	KC2	CAA-CBA-CGA-O1A
41	Y	308	KC2	CAA-CBA-CGA-O2A
41	Y	309	KC2	CAA-CBA-CGA-O2A
41	q	308	KC2	CAA-CBA-CGA-O2A
41	u	304	KC2	CAA-CBA-CGA-O1A
41	v	302	KC2	CAA-CBA-CGA-O2A
41	v	308	KC2	CAA-CBA-CGA-O2A
41	v	309	KC2	CAA-CBA-CGA-O2A
41	w	301	KC2	CAA-CBA-CGA-O1A
41	w	301	KC2	CAA-CBA-CGA-O2A
41	y	301	KC2	CAA-CBA-CGA-O1A
41	y	301	KC2	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
41	z	303	KC2	CAA-CBA-CGA-O1A
40	A	304	CLA	C4-C3-C5-C6
40	I	203	CLA	C4-C3-C5-C6
40	N	304	CLA	C4-C3-C5-C6
40	Q	208	CLA	C4-C3-C5-C6
40	a	804	CLA	C4-C3-C5-C6
40	a	819	CLA	C4-C3-C5-C6
40	x	306	CLA	C4-C3-C5-C6
40	A	304	CLA	C2-C3-C5-C6
40	I	203	CLA	C2-C3-C5-C6
40	N	304	CLA	C2-C3-C5-C6
40	S	307	CLA	C2-C3-C5-C6
40	b	806	CLA	C2-C3-C5-C6
40	o	304	CLA	C2-C3-C5-C6
40	x	306	CLA	C2-C3-C5-C6
40	q	312	CLA	C3-C5-C6-C7
40	z	307	CLA	C3-C5-C6-C7
40	A	302	CLA	C11-C10-C8-C9
40	A	304	CLA	C6-C7-C8-C9
40	D	302	CLA	C11-C10-C8-C9
40	D	304	CLA	C6-C7-C8-C9
40	F	321	CLA	C6-C7-C8-C9
40	M	305	CLA	C6-C7-C8-C9
40	N	311	CLA	C6-C7-C8-C9
40	P	313	CLA	C6-C7-C8-C9
40	W	305	CLA	C11-C10-C8-C9
40	Z	304	CLA	C6-C7-C8-C9
40	a	815	CLA	C11-C12-C13-C14
40	a	834	CLA	C6-C7-C8-C9
40	a	842	CLA	C11-C10-C8-C9
40	a	851	CLA	C14-C13-C15-C16
40	b	801	CLA	C6-C7-C8-C9
40	b	819	CLA	C11-C10-C8-C9
40	b	835	CLA	C11-C12-C13-C14
40	l	202	CLA	C14-C13-C15-C16
40	l	203	CLA	C11-C10-C8-C9
40	l	205	CLA	C11-C10-C8-C9
43	E	301	LMG	C4-C5-C6-O5
43	l	201	LMG	C4-C5-C6-O5
43	x	301	LMG	C4-C5-C6-O5
40	D	306	CLA	O1D-CGD-O2D-CED
43	A	317	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
43	E	320	LMG	C2-C1-O1-C7
43	p	301	LMG	C2-C1-O1-C7
40	J	312	CLA	C4C-C3C-CAC-CBC
40	Y	310	CLA	CBD-CGD-O2D-CED
42	D	314	DD6	C12-C11-C13-C14
42	F	315	DD6	C12-C11-C13-C14
42	H	313	DD6	C7-C6-C8-C9
42	I	211	DD6	C12-C11-C13-C14
42	q	320	DD6	C12-C11-C13-C14
42	q	320	DD6	C7-C6-C8-C9
42	v	320	DD6	C12-C11-C13-C14
42	v	320	DD6	C7-C6-C8-C9
44	T	315	A86	C7-C6-C8-C9
44	Y	315	A86	C-C1-C24-C25
44	Y	316	A86	C7-C6-C8-C9
44	Z	315	A86	C7-C6-C8-C9
44	o	317	A86	C7-C6-C8-C9
44	t	311	A86	C7-C6-C8-C9
44	w	311	A86	C7-C6-C8-C9
44	w	316	A86	C7-C6-C8-C9
44	y	310	A86	C-C1-C24-C25
44	z	316	A86	C7-C6-C8-C9
47	R	317	A1EB1	C7-C6-C8-C9
47	o	321	A1EB1	C-C1-C24-C25
47	q	321	A1EB1	C7-C6-C8-C9
47	v	321	A1EB1	C7-C6-C8-C9
47	y	312	A1EB1	C7-C6-C8-C9
47	y	313	A1EB1	C-C1-C24-C25
49	b	844	BCR	C7-C8-C9-C34
43	L	319	LMG	O6-C5-C6-O5
42	D	314	DD6	C10-C11-C13-C14
42	H	313	DD6	C10-C11-C13-C14
42	I	211	DD6	C10-C11-C13-C14
44	t	311	A86	C5-C6-C8-C9
44	w	311	A86	C5-C6-C8-C9
44	w	316	A86	C5-C6-C8-C9
49	b	844	BCR	C7-C8-C9-C10
43	L	319	LMG	C10-C11-C12-C13
43	l	201	LMG	C10-C11-C12-C13
40	a	826	CLA	O1A-CGA-O2A-C1
40	x	312	CLA	O1A-CGA-O2A-C1
40	Y	307	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
41	F	302	KC2	CAA-CBA-CGA-O1A
41	F	302	KC2	CAA-CBA-CGA-O2A
41	G	202	KC2	CAA-CBA-CGA-O2A
41	K	309	KC2	CAA-CBA-CGA-O1A
41	L	309	KC2	CAA-CBA-CGA-O1A
41	N	302	KC2	CAA-CBA-CGA-O2A
41	O	302	KC2	CAA-CBA-CGA-O2A
41	P	309	KC2	CAA-CBA-CGA-O1A
41	P	309	KC2	CAA-CBA-CGA-O2A
41	Q	216	KC2	CAA-CBA-CGA-O2A
41	R	309	KC2	CAA-CBA-CGA-O1A
41	R	309	KC2	CAA-CBA-CGA-O2A
41	Y	302	KC2	CAA-CBA-CGA-O1A
41	Y	314	KC2	CAA-CBA-CGA-O2A
41	Z	308	KC2	CAA-CBA-CGA-O2A
41	q	302	KC2	CAA-CBA-CGA-O1A
41	q	302	KC2	CAA-CBA-CGA-O2A
41	v	302	KC2	CAA-CBA-CGA-O1A
46	P	319	SQD	O47-C45-C46-O48
40	B	301	CLA	CBA-CGA-O2A-C1
40	b	839	CLA	CBA-CGA-O2A-C1
40	z	305	CLA	C2-C1-O2A-CGA
41	O	301	KC2	O1D-CGD-O2D-CED
40	K	301	CLA	CBD-CGD-O2D-CED
40	S	308	CLA	CBD-CGD-O2D-CED
40	a	810	CLA	C8-C10-C11-C12
40	a	816	CLA	C13-C15-C16-C17
40	b	840	CLA	C10-C11-C12-C13
40	l	202	CLA	C5-C6-C7-C8
43	u	301	LMG	C10-C11-C12-C13
40	t	307	CLA	CBD-CGD-O2D-CED
40	U	203	CLA	C2C-C3C-CAC-CBC
40	a	832	CLA	C11-C12-C13-C15
40	a	833	CLA	C6-C7-C8-C10
40	l	202	CLA	CBA-CGA-O2A-C1
40	z	308	CLA	CBA-CGA-O2A-C1
41	K	309	KC2	CAA-CBA-CGA-O2A
41	L	309	KC2	CAA-CBA-CGA-O2A
41	N	308	KC2	CAA-CBA-CGA-O2A
41	Y	302	KC2	CAA-CBA-CGA-O2A
40	b	806	CLA	C4-C3-C5-C6
40	B	301	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
43	A	317	LMG	C10-C11-C12-C13
43	u	301	LMG	C28-C29-C30-C31
40	F	307	CLA	C3-C5-C6-C7
44	q	324	A86	C35-C34-O4-C38
43	E	320	LMG	C10-C11-C12-C13
40	C	306	CLA	O1A-CGA-O2A-C1
40	U	202	CLA	O1A-CGA-O2A-C1
40	X	305	CLA	O1A-CGA-O2A-C1
40	z	305	CLA	O1A-CGA-O2A-C1
40	H	301	CLA	CBD-CGD-O2D-CED
40	K	307	CLA	CBD-CGD-O2D-CED
40	l	203	CLA	CBD-CGD-O2D-CED
43	S	322	LMG	C11-C10-O7-C8
43	l	201	LMG	C11-C10-O7-C8
40	D	302	CLA	C5-C6-C7-C8
40	H	310	CLA	C8-C10-C11-C12
40	M	305	CLA	C8-C10-C11-C12
40	P	313	CLA	C10-C11-C12-C13
40	Q	206	CLA	C8-C10-C11-C12
40	S	302	CLA	C5-C6-C7-C8
40	Y	306	CLA	C8-C10-C11-C12
40	a	828	CLA	C15-C16-C17-C18
40	a	836	CLA	C8-C10-C11-C12
40	b	807	CLA	C13-C15-C16-C17
40	b	834	CLA	C15-C16-C17-C18
40	l	204	CLA	C10-C11-C12-C13
40	C	306	CLA	C2A-CAA-CBA-CGA
40	E	313	CLA	C2A-CAA-CBA-CGA
40	H	308	CLA	C2A-CAA-CBA-CGA
40	J	302	CLA	C2A-CAA-CBA-CGA
40	M	311	CLA	C2A-CAA-CBA-CGA
40	Y	313	CLA	C2A-CAA-CBA-CGA
40	a	820	CLA	C2A-CAA-CBA-CGA
40	a	824	CLA	C2A-CAA-CBA-CGA
40	b	803	CLA	C2A-CAA-CBA-CGA
40	p	314	CLA	C2A-CAA-CBA-CGA
41	Z	308	KC2	CAA-CBA-CGA-O1A
40	D	303	CLA	C8-C10-C11-C12
40	Q	202	CLA	C5-C6-C7-C8
40	Y	310	CLA	C5-C6-C7-C8
40	a	821	CLA	C5-C6-C7-C8
40	b	802	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
40	o	304	CLA	C5-C6-C7-C8
44	p	321	A86	C35-C34-O4-C38
44	v	325	A86	C35-C34-O4-C38
43	E	301	LMG	C10-C11-C12-C13
43	E	301	LMG	C28-C29-C30-C31
43	a	801	LMG	C10-C11-C12-C13
43	l	201	LMG	C28-C29-C30-C31
46	I	215	SQD	C23-C24-C25-C26
46	M	318	SQD	C7-C8-C9-C10
48	P	320	A1EB4	C39-C43-C44-C45
40	a	819	CLA	O1A-CGA-O2A-C1
45	a	848	LHG	O10-C23-O8-C6
40	a	836	CLA	C3-C5-C6-C7
43	u	301	LMG	O6-C1-O1-C7
40	F	306	CLA	C10-C11-C12-C13
40	K	304	CLA	C10-C11-C12-C13
40	S	306	CLA	C5-C6-C7-C8
40	T	306	CLA	C10-C11-C12-C13
40	a	811	CLA	C8-C10-C11-C12
40	a	836	CLA	C5-C6-C7-C8
40	b	805	CLA	C5-C6-C7-C8
40	b	820	CLA	C5-C6-C7-C8
40	b	825	CLA	C5-C6-C7-C8
40	l	204	CLA	C13-C15-C16-C17
40	M	312	CLA	CBA-CGA-O2A-C1
40	a	823	CLA	CBD-CGD-O2D-CED
40	H	305	CLA	O1A-CGA-O2A-C1
43	A	317	LMG	C28-C29-C30-C31
43	a	801	LMG	C28-C29-C30-C31
43	a	802	LMG	C10-C11-C12-C13
47	w	313	A1EB1	C42-C44-C45-C46
40	R	306	CLA	C10-C11-C12-C13
40	a	834	CLA	C10-C11-C12-C13
40	f	202	CLA	C10-C11-C12-C13
40	x	302	CLA	C8-C10-C11-C12
46	F	320	SQD	O49-C7-O47-C45
40	S	319	CLA	O1D-CGD-O2D-CED
40	A	309	CLA	C13-C15-C16-C17
40	E	307	CLA	C15-C16-C17-C18
40	Q	205	CLA	C8-C10-C11-C12
40	a	832	CLA	C8-C10-C11-C12
40	a	851	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
41	O	302	KC2	CAA-CBA-CGA-O1A
41	u	303	KC2	CAA-CBA-CGA-O1A
41	t	306	KC2	CBD-CGD-O2D-CED
40	W	306	CLA	C5-C6-C7-C8
40	a	808	CLA	C8-C10-C11-C12
40	b	802	CLA	C15-C16-C17-C18
40	b	821	CLA	C8-C10-C11-C12
40	b	825	CLA	C10-C11-C12-C13
40	F	301	CLA	CBA-CGA-O2A-C1
40	G	206	CLA	CBA-CGA-O2A-C1
40	M	305	CLA	CBA-CGA-O2A-C1
40	S	302	CLA	CBA-CGA-O2A-C1
40	x	307	CLA	CBA-CGA-O2A-C1
41	y	306	KC2	CBD-CGD-O2D-CED
40	b	842	CLA	C8-C10-C11-C12
40	P	313	CLA	C3-C5-C6-C7
40	A	309	CLA	C15-C16-C17-C18
40	b	821	CLA	C15-C16-C17-C18
40	o	307	CLA	C10-C11-C12-C13
41	H	316	KC2	CAA-CBA-CGA-O1A
43	a	801	LMG	O9-C10-O7-C8
40	H	307	CLA	C2A-CAA-CBA-CGA
40	J	308	CLA	C2A-CAA-CBA-CGA
40	Y	305	CLA	C2A-CAA-CBA-CGA
40	z	314	CLA	C2A-CAA-CBA-CGA
40	G	207	CLA	O1D-CGD-O2D-CED
40	E	306	CLA	CBA-CGA-O2A-C1
40	u	307	CLA	CBA-CGA-O2A-C1
46	I	215	SQD	C24-C23-O48-C46
47	o	321	A1EB1	C33-C34-O4-C38
40	N	304	CLA	C10-C11-C12-C13
40	W	308	CLA	C5-C6-C7-C8
40	X	311	CLA	C13-C15-C16-C17
40	Z	301	CLA	C8-C10-C11-C12
40	a	829	CLA	C5-C6-C7-C8
40	a	832	CLA	C13-C15-C16-C17
40	a	840	CLA	C5-C6-C7-C8
40	a	842	CLA	C10-C11-C12-C13
40	b	802	CLA	C5-C6-C7-C8
40	b	835	CLA	C5-C6-C7-C8
40	b	839	CLA	C13-C15-C16-C17
40	v	311	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
40	x	302	CLA	C15-C16-C17-C18
40	z	312	CLA	C5-C6-C7-C8
40	G	201	CLA	O1D-CGD-O2D-CED
40	Y	311	CLA	O1D-CGD-O2D-CED
40	A	304	CLA	C15-C16-C17-C18
40	A	305	CLA	C10-C11-C12-C13
40	H	307	CLA	C5-C6-C7-C8
40	a	806	CLA	C8-C10-C11-C12
40	a	841	CLA	C15-C16-C17-C18
40	b	825	CLA	C15-C16-C17-C18
40	q	311	CLA	C8-C10-C11-C12
44	C	311	A86	C9-C10-C11-C12
44	u	319	A86	C9-C10-C11-C12
44	x	317	A86	C9-C10-C11-C12
44	x	319	A86	C9-C10-C11-C12
47	q	322	A1EB1	C9-C10-C11-C12
47	y	314	A1EB1	C9-C10-C11-C12
40	E	312	CLA	C2C-C3C-CAC-CBC
40	C	306	CLA	C15-C16-C17-C18
40	E	307	CLA	C5-C6-C7-C8
40	H	307	CLA	C8-C10-C11-C12
40	M	304	CLA	C5-C6-C7-C8
40	O	307	CLA	C8-C10-C11-C12
40	Q	208	CLA	C5-C6-C7-C8
40	a	842	CLA	C13-C15-C16-C17
40	b	830	CLA	C8-C10-C11-C12
40	v	306	CLA	C8-C10-C11-C12
40	b	810	CLA	O1D-CGD-O2D-CED
40	v	307	CLA	O1D-CGD-O2D-CED
40	E	309	CLA	CBA-CGA-O2A-C1
40	K	306	CLA	CBA-CGA-O2A-C1
40	a	820	CLA	CBA-CGA-O2A-C1
40	M	306	CLA	C13-C15-C16-C17
41	H	316	KC2	CAA-CBA-CGA-O2A
41	P	310	KC2	CAA-CBA-CGA-O2A
41	o	309	KC2	CAA-CBA-CGA-O2A
41	u	303	KC2	CAA-CBA-CGA-O2A
41	z	310	KC2	CAA-CBA-CGA-O2A
40	Q	202	CLA	C8-C10-C11-C12
40	b	805	CLA	C8-C10-C11-C12
40	I	201	CLA	C3-C5-C6-C7
40	A	311	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
46	M	318	SQD	C8-C7-O47-C45
52	b	850	DGD	C2B-C1B-O2G-C2G
43	E	301	LMG	C2-C1-O1-C7
43	u	301	LMG	C2-C1-O1-C7
40	R	307	CLA	C5-C6-C7-C8
40	a	806	CLA	C10-C11-C12-C13
40	a	829	CLA	C15-C16-C17-C18
40	a	842	CLA	C5-C6-C7-C8
47	y	312	A1EB1	C42-C44-C45-C46
40	Z	310	CLA	CBA-CGA-O2A-C1
40	p	307	CLA	CBA-CGA-O2A-C1
40	b	820	CLA	C16-C17-C18-C19
40	S	302	CLA	C10-C11-C12-C13
40	S	307	CLA	O1A-CGA-O2A-C1
41	Z	309	KC2	CAA-CBA-CGA-O2A
41	z	310	KC2	CAA-CBA-CGA-O1A
40	b	808	CLA	C15-C16-C17-C18
42	H	314	DD6	C12-C11-C13-C14
42	Y	322	DD6	C7-C6-C8-C9
45	F	319	LHG	C5-C4-O6-P
47	N	320	A1EB1	C-C1-C24-C25
47	y	313	A1EB1	C7-C6-C8-C9
49	k	203	BCR	C36-C18-C19-C20
49	l	207	BCR	C7-C8-C9-C34
42	F	315	DD6	C10-C11-C13-C14
42	H	314	DD6	C10-C11-C13-C14
44	Y	315	A86	C2-C1-C24-C25
40	L	310	CLA	O1A-CGA-O2A-C1
40	z	302	CLA	O1A-CGA-O2A-C1
40	B	304	CLA	C2A-CAA-CBA-CGA
40	M	305	CLA	C2A-CAA-CBA-CGA
40	Q	206	CLA	C2A-CAA-CBA-CGA
40	S	314	CLA	C2A-CAA-CBA-CGA
40	V	202	CLA	C2A-CAA-CBA-CGA
40	X	305	CLA	C2A-CAA-CBA-CGA
40	b	802	CLA	C2A-CAA-CBA-CGA
40	a	825	CLA	C5-C6-C7-C8
40	b	806	CLA	C15-C16-C17-C18
40	b	827	CLA	C8-C10-C11-C12
45	F	319	LHG	O1-C1-C2-C3
46	F	320	SQD	C23-C24-C25-C26
40	b	806	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
40	o	311	CLA	O2A-C1-C2-C3
40	q	310	CLA	O2A-C1-C2-C3
43	A	317	LMG	C7-C8-O7-C10
40	W	312	CLA	C2C-C3C-CAC-CBC
47	K	313	A1EB1	C25-C26-C27-C29
47	L	316	A1EB1	C25-C26-C27-C29
47	O	317	A1EB1	C25-C26-C27-C29
47	T	316	A1EB1	C25-C26-C27-C29
47	Z	319	A1EB1	C25-C26-C27-C29
47	o	322	A1EB1	C25-C26-C27-C29
47	p	323	A1EB1	C25-C26-C27-C29
47	t	315	A1EB1	C25-C26-C27-C29
47	u	322	A1EB1	C25-C26-C27-C29
47	w	313	A1EB1	C25-C26-C27-C29
47	w	314	A1EB1	C25-C26-C27-C29
40	N	304	CLA	C11-C12-C13-C15
40	a	837	CLA	C6-C7-C8-C9
40	b	809	CLA	C11-C12-C13-C14
40	v	310	CLA	O1D-CGD-O2D-CED
40	z	305	CLA	C3-C5-C6-C7
40	u	311	CLA	C5-C6-C7-C8
46	M	318	SQD	O49-C7-O47-C45
47	Z	320	A1EB1	C35-C34-O4-C38
41	P	310	KC2	CAA-CBA-CGA-O1A
41	Z	309	KC2	CAA-CBA-CGA-O1A
40	a	819	CLA	C5-C6-C7-C8
40	o	301	CLA	C5-C6-C7-C8
40	q	307	CLA	O1D-CGD-O2D-CED
40	G	203	CLA	CBA-CGA-O2A-C1
40	b	814	CLA	CBA-CGA-O2A-C1
45	F	319	LHG	C24-C23-O8-C6
40	D	310	CLA	C8-C10-C11-C12
40	E	303	CLA	C10-C11-C12-C13
40	F	321	CLA	C10-C11-C12-C13
40	b	824	CLA	C15-C16-C17-C18
40	x	306	CLA	C8-C10-C11-C12
40	x	313	CLA	CBD-CGD-O2D-CED
44	F	312	A86	C9-C10-C11-C13
44	M	316	A86	C9-C10-C11-C13
44	N	318	A86	C9-C10-C11-C13
44	Q	210	A86	C9-C10-C11-C13
44	X	314	A86	C9-C10-C11-C13

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Mol	Chain	Res	Type	Atoms
44	X	317	A86	C9-C10-C11-C13
44	Y	318	A86	C9-C10-C11-C13
44	o	316	A86	C9-C10-C11-C13
44	q	315	A86	C9-C10-C11-C13
44	t	311	A86	C9-C10-C11-C13
44	v	315	A86	C9-C10-C11-C13
44	v	319	A86	C9-C10-C11-C13
44	y	310	A86	C9-C10-C11-C13
47	O	317	A1EB1	C9-C10-C11-C13
47	o	321	A1EB1	C9-C10-C11-C13
47	t	314	A1EB1	C9-C10-C11-C13
47	u	322	A1EB1	C9-C10-C11-C13
40	H	307	CLA	C2-C1-O2A-CGA
40	b	806	CLA	C2-C1-O2A-CGA
40	D	301	CLA	C6-C7-C8-C9
40	P	312	CLA	C11-C12-C13-C15
40	b	820	CLA	C16-C17-C18-C20
40	o	310	CLA	C6-C7-C8-C9
40	Z	306	CLA	C5-C6-C7-C8
40	q	306	CLA	C8-C10-C11-C12
40	W	311	CLA	CBD-CGD-O2D-CED
43	a	801	LMG	C14-C15-C16-C17
46	F	320	SQD	C9-C10-C11-C12
40	L	304	CLA	C5-C6-C7-C8
40	q	311	CLA	C10-C11-C12-C13
41	R	308	KC2	CAA-CBA-CGA-O1A
41	o	309	KC2	CAA-CBA-CGA-O1A
40	X	307	CLA	CBA-CGA-O2A-C1
43	l	201	LMG	C33-C34-C35-C36
45	S	323	LHG	C28-C29-C30-C31
42	G	210	DD6	C27-C29-C30-C31
40	G	207	CLA	C5-C6-C7-C8
43	D	318	LMG	C30-C31-C32-C33
40	P	312	CLA	C5-C6-C7-C8
40	l	205	CLA	C15-C16-C17-C18
40	A	304	CLA	C4B-C3B-CAB-CBB
40	B	302	CLA	C4B-C3B-CAB-CBB
40	B	307	CLA	C4B-C3B-CAB-CBB
40	C	301	CLA	C4B-C3B-CAB-CBB
40	C	302	CLA	C4B-C3B-CAB-CBB
40	D	301	CLA	C4B-C3B-CAB-CBB
40	D	304	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
40	H	302	CLA	C4B-C3B-CAB-CBB
40	L	311	CLA	C4B-C3B-CAB-CBB
40	N	310	CLA	C4B-C3B-CAB-CBB
40	P	307	CLA	C4B-C3B-CAB-CBB
40	P	313	CLA	C4B-C3B-CAB-CBB
40	Q	209	CLA	C4B-C3B-CAB-CBB
40	S	301	CLA	C4B-C3B-CAB-CBB
40	S	302	CLA	C4B-C3B-CAB-CBB
40	X	310	CLA	C4B-C3B-CAB-CBB
40	a	811	CLA	C4B-C3B-CAB-CBB
40	a	818	CLA	C4B-C3B-CAB-CBB
40	a	819	CLA	C4B-C3B-CAB-CBB
40	a	837	CLA	C4B-C3B-CAB-CBB
40	a	840	CLA	C4B-C3B-CAB-CBB
40	a	841	CLA	C4B-C3B-CAB-CBB
40	a	852	CLA	C4B-C3B-CAB-CBB
40	b	806	CLA	C4B-C3B-CAB-CBB
40	b	825	CLA	C4B-C3B-CAB-CBB
40	b	829	CLA	C4B-C3B-CAB-CBB
40	b	830	CLA	C4B-C3B-CAB-CBB
40	l	202	CLA	C4B-C3B-CAB-CBB
40	p	302	CLA	C4B-C3B-CAB-CBB
40	p	305	CLA	C4B-C3B-CAB-CBB
40	p	314	CLA	C4B-C3B-CAB-CBB
40	q	301	CLA	C4B-C3B-CAB-CBB
40	u	308	CLA	C4B-C3B-CAB-CBB
40	w	308	CLA	C4B-C3B-CAB-CBB
40	x	308	CLA	C4B-C3B-CAB-CBB
40	x	312	CLA	C4B-C3B-CAB-CBB
40	y	302	CLA	C4B-C3B-CAB-CBB
40	y	308	CLA	C4B-C3B-CAB-CBB
47	P	301	A1EB1	C33-C34-O4-C38
40	H	307	CLA	C11-C12-C13-C14
40	N	304	CLA	C11-C12-C13-C14
40	U	202	CLA	C6-C7-C8-C9
40	U	202	CLA	C6-C7-C8-C10
40	b	809	CLA	C11-C12-C13-C15
40	i	101	CLA	C6-C7-C8-C10
40	z	308	CLA	C11-C12-C13-C15
52	b	850	DGD	C4E-C5E-C6E-O5E
40	C	308	CLA	C2A-CAA-CBA-CGA
40	F	321	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
40	Q	208	CLA	C8-C10-C11-C12
40	a	832	CLA	C15-C16-C17-C18
43	j	101	LMG	C11-C10-O7-C8
40	D	307	CLA	C6-C7-C8-C10
40	b	836	CLA	C6-C7-C8-C10
47	L	316	A1EB1	C42-C44-C45-C46
40	Z	301	CLA	CBA-CGA-O2A-C1
40	b	813	CLA	CBA-CGA-O2A-C1
40	b	835	CLA	C15-C16-C17-C18
40	f	202	CLA	C8-C10-C11-C12
40	o	311	CLA	C8-C10-C11-C12
40	b	839	CLA	O1A-CGA-O2A-C1
40	z	308	CLA	O1A-CGA-O2A-C1
46	I	215	SQD	O10-C23-O48-C46
40	b	835	CLA	C3-C5-C6-C7
41	O	303	KC2	CAA-CBA-CGA-O1A
41	O	308	KC2	CAA-CBA-CGA-O1A
41	O	308	KC2	CAA-CBA-CGA-O2A
40	A	306	CLA	C3A-C2A-CAA-CBA
40	B	301	CLA	C3A-C2A-CAA-CBA
40	B	307	CLA	C3A-C2A-CAA-CBA
40	D	302	CLA	C3A-C2A-CAA-CBA
40	D	303	CLA	C3A-C2A-CAA-CBA
40	E	307	CLA	C3A-C2A-CAA-CBA
40	E	312	CLA	C3A-C2A-CAA-CBA
40	F	301	CLA	C3A-C2A-CAA-CBA
40	F	303	CLA	C3A-C2A-CAA-CBA
40	F	305	CLA	C3A-C2A-CAA-CBA
40	F	306	CLA	C3A-C2A-CAA-CBA
40	K	307	CLA	C3A-C2A-CAA-CBA
40	K	308	CLA	C3A-C2A-CAA-CBA
40	L	305	CLA	C3A-C2A-CAA-CBA
40	L	310	CLA	C3A-C2A-CAA-CBA
40	L	312	CLA	C3A-C2A-CAA-CBA
40	M	305	CLA	C3A-C2A-CAA-CBA
40	O	304	CLA	C3A-C2A-CAA-CBA
40	O	310	CLA	C3A-C2A-CAA-CBA
40	Q	207	CLA	C3A-C2A-CAA-CBA
40	S	305	CLA	C3A-C2A-CAA-CBA
40	S	312	CLA	C3A-C2A-CAA-CBA
40	U	204	CLA	C3A-C2A-CAA-CBA
40	W	306	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
40	W	311	CLA	C3A-C2A-CAA-CBA
40	Y	312	CLA	C3A-C2A-CAA-CBA
40	a	804	CLA	C3A-C2A-CAA-CBA
40	a	808	CLA	C3A-C2A-CAA-CBA
40	a	809	CLA	C3A-C2A-CAA-CBA
40	a	824	CLA	C3A-C2A-CAA-CBA
40	a	842	CLA	C3A-C2A-CAA-CBA
40	a	850	CLA	C3A-C2A-CAA-CBA
40	b	807	CLA	C3A-C2A-CAA-CBA
40	b	839	CLA	C3A-C2A-CAA-CBA
40	b	842	CLA	C3A-C2A-CAA-CBA
40	l	205	CLA	C3A-C2A-CAA-CBA
40	o	310	CLA	C3A-C2A-CAA-CBA
40	o	312	CLA	C3A-C2A-CAA-CBA
40	o	313	CLA	C3A-C2A-CAA-CBA
40	p	302	CLA	C3A-C2A-CAA-CBA
40	p	311	CLA	C3A-C2A-CAA-CBA
40	q	301	CLA	C3A-C2A-CAA-CBA
40	q	310	CLA	C3A-C2A-CAA-CBA
40	q	311	CLA	C3A-C2A-CAA-CBA
40	t	304	CLA	C3A-C2A-CAA-CBA
40	u	302	CLA	C3A-C2A-CAA-CBA
40	u	306	CLA	C3A-C2A-CAA-CBA
40	v	301	CLA	C3A-C2A-CAA-CBA
40	v	310	CLA	C3A-C2A-CAA-CBA
40	v	311	CLA	C3A-C2A-CAA-CBA
40	w	304	CLA	C3A-C2A-CAA-CBA
40	x	306	CLA	C3A-C2A-CAA-CBA
40	x	311	CLA	C3A-C2A-CAA-CBA
40	y	303	CLA	C3A-C2A-CAA-CBA
40	y	304	CLA	C3A-C2A-CAA-CBA
40	z	307	CLA	C3A-C2A-CAA-CBA
40	z	313	CLA	C3A-C2A-CAA-CBA
44	Z	314	A86	C33-C34-O4-C38
40	B	304	CLA	CBD-CGD-O2D-CED
46	I	215	SQD	C14-C15-C16-C17
40	E	303	CLA	C5-C6-C7-C8
40	a	825	CLA	C10-C11-C12-C13
40	a	835	CLA	C15-C16-C17-C18
40	b	820	CLA	C15-C16-C17-C18
40	o	307	CLA	O1D-CGD-O2D-CED
43	L	319	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
43	D	318	LMG	C31-C32-C33-C34
40	a	837	CLA	C6-C7-C8-C10
40	i	101	CLA	C6-C7-C8-C9
40	o	310	CLA	C6-C7-C8-C10
40	z	308	CLA	C11-C12-C13-C14
40	B	301	CLA	O1A-CGA-O2A-C1
43	S	322	LMG	O9-C10-O7-C8
46	I	215	SQD	C17-C18-C19-C20
40	E	310	CLA	CBA-CGA-O2A-C1
40	v	305	CLA	CBA-CGA-O2A-C1
40	x	305	CLA	CBA-CGA-O2A-C1
43	l	201	LMG	C29-C28-O8-C9
43	A	317	LMG	C31-C32-C33-C34
40	b	842	CLA	C3-C5-C6-C7
40	v	312	CLA	C3-C5-C6-C7
40	u	307	CLA	C5-C6-C7-C8
43	A	317	LMG	C30-C31-C32-C33
43	D	318	LMG	C11-C12-C13-C14
43	l	201	LMG	C11-C12-C13-C14
45	a	848	LHG	C15-C16-C17-C18
46	k	205	SQD	C9-C10-C11-C12
40	M	305	CLA	O1A-CGA-O2A-C1
40	l	202	CLA	O1A-CGA-O2A-C1
41	O	303	KC2	CAA-CBA-CGA-O2A
40	J	302	CLA	C4C-C3C-CAC-CBC
40	D	303	CLA	C5-C6-C7-C8
40	N	305	CLA	C5-C6-C7-C8
40	O	304	CLA	C8-C10-C11-C12
40	P	312	CLA	C11-C12-C13-C14
40	q	307	CLA	C11-C12-C13-C15
46	F	320	SQD	C7-C8-C9-C10
40	M	312	CLA	O1A-CGA-O2A-C1
40	u	307	CLA	O1A-CGA-O2A-C1
40	A	304	CLA	C2B-C3B-CAB-CBB
40	B	307	CLA	C2B-C3B-CAB-CBB
40	C	301	CLA	C2B-C3B-CAB-CBB
40	C	304	CLA	C2B-C3B-CAB-CBB
40	D	301	CLA	C2B-C3B-CAB-CBB
40	D	304	CLA	C2B-C3B-CAB-CBB
40	F	304	CLA	C2B-C3B-CAB-CBB
40	H	302	CLA	C2B-C3B-CAB-CBB
40	I	205	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
40	I	206	CLA	C2B-C3B-CAB-CBB
40	J	303	CLA	C2B-C3B-CAB-CBB
40	L	301	CLA	C2B-C3B-CAB-CBB
40	L	311	CLA	C2B-C3B-CAB-CBB
40	M	310	CLA	C2B-C3B-CAB-CBB
40	P	307	CLA	C2B-C3B-CAB-CBB
40	Q	205	CLA	C2B-C3B-CAB-CBB
40	Q	209	CLA	C2B-C3B-CAB-CBB
40	S	302	CLA	C2B-C3B-CAB-CBB
40	V	201	CLA	C2B-C3B-CAB-CBB
40	X	310	CLA	C2B-C3B-CAB-CBB
40	Y	306	CLA	C2B-C3B-CAB-CBB
40	Y	313	CLA	C2B-C3B-CAB-CBB
40	a	818	CLA	C2B-C3B-CAB-CBB
40	a	819	CLA	C2B-C3B-CAB-CBB
40	a	837	CLA	C2B-C3B-CAB-CBB
40	a	852	CLA	C2B-C3B-CAB-CBB
40	b	806	CLA	C2B-C3B-CAB-CBB
40	b	830	CLA	C2B-C3B-CAB-CBB
40	l	202	CLA	C2B-C3B-CAB-CBB
40	o	301	CLA	C2B-C3B-CAB-CBB
40	p	302	CLA	C2B-C3B-CAB-CBB
40	p	314	CLA	C2B-C3B-CAB-CBB
40	q	301	CLA	C2B-C3B-CAB-CBB
40	q	306	CLA	C2B-C3B-CAB-CBB
40	t	304	CLA	C2B-C3B-CAB-CBB
40	w	308	CLA	C2B-C3B-CAB-CBB
40	y	308	CLA	C2B-C3B-CAB-CBB
49	a	843	BCR	C1-C6-C7-C8
49	a	843	BCR	C5-C6-C7-C8
49	b	844	BCR	C1-C6-C7-C8
49	b	844	BCR	C5-C6-C7-C8
49	i	102	BCR	C1-C6-C7-C8
49	i	102	BCR	C5-C6-C7-C8
49	j	103	BCR	C23-C24-C25-C30
49	l	208	BCR	C1-C6-C7-C8
49	l	208	BCR	C5-C6-C7-C8
40	X	310	CLA	CBD-CGD-O2D-CED
40	M	304	CLA	C4C-C3C-CAC-CBC
40	p	305	CLA	C2C-C3C-CAC-CBC
40	D	310	CLA	CBA-CGA-O2A-C1
40	D	312	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
40	f	202	CLA	CBA-CGA-O2A-C1
40	k	201	CLA	CBA-CGA-O2A-C1
40	A	303	CLA	C10-C11-C12-C13
40	b	830	CLA	C10-C11-C12-C13
40	U	202	CLA	C3-C5-C6-C7
40	P	312	CLA	C2A-CAA-CBA-CGA
40	l	202	CLA	C2A-CAA-CBA-CGA
40	o	313	CLA	C2A-CAA-CBA-CGA
43	S	322	LMG	C33-C34-C35-C36
40	F	301	CLA	O1A-CGA-O2A-C1
40	G	206	CLA	O1A-CGA-O2A-C1
40	S	302	CLA	O1A-CGA-O2A-C1
40	x	307	CLA	O1A-CGA-O2A-C1
40	b	802	CLA	C4-C3-C5-C6
40	v	301	CLA	C4-C3-C5-C6
40	C	305	CLA	C8-C10-C11-C12
40	b	817	CLA	C8-C10-C11-C12
40	p	302	CLA	C15-C16-C17-C18
40	z	307	CLA	C8-C10-C11-C12
45	S	323	LHG	C24-C25-C26-C27
40	H	309	CLA	CBA-CGA-O2A-C1
40	q	305	CLA	CBA-CGA-O2A-C1
40	v	304	CLA	CBA-CGA-O2A-C1
40	V	201	CLA	C11-C10-C8-C9
43	x	301	LMG	C34-C35-C36-C37
40	a	829	CLA	C13-C15-C16-C17
43	a	801	LMG	O6-C1-O1-C7
45	a	849	LHG	C24-C25-C26-C27
52	b	850	DGD	C4A-C5A-C6A-C7A
40	C	306	CLA	C8-C10-C11-C12
40	T	306	CLA	C8-C10-C11-C12
40	Y	307	CLA	C10-C11-C12-C13
40	p	311	CLA	C5-C6-C7-C8
43	E	321	LMG	C31-C32-C33-C34
43	D	318	LMG	C33-C34-C35-C36
44	p	321	A86	C33-C34-O4-C38
44	q	324	A86	C33-C34-O4-C38
44	v	325	A86	C33-C34-O4-C38
41	R	308	KC2	CAA-CBA-CGA-O2A
43	E	301	LMG	C11-C12-C13-C14
46	I	215	SQD	C13-C14-C15-C16
40	a	826	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
40	o	307	CLA	C3-C5-C6-C7
40	z	308	CLA	C3-C5-C6-C7
40	E	314	CLA	CBA-CGA-O2A-C1
40	Q	208	CLA	C11-C12-C13-C14
40	x	306	CLA	C11-C12-C13-C14
43	x	301	LMG	C10-C11-C12-C13
40	J	312	CLA	O1D-CGD-O2D-CED
45	a	848	LHG	C24-C25-C26-C27
40	b	809	CLA	C8-C10-C11-C12
40	l	202	CLA	C10-C11-C12-C13
40	Z	306	CLA	CBD-CGD-O2D-CED
40	a	811	CLA	C5-C6-C7-C8
44	t	310	A86	C-C1-C24-C25
47	w	313	A1EB1	C7-C6-C8-C9
49	l	207	BCR	C11-C12-C13-C35
43	W	317	LMG	C28-C29-C30-C31
42	E	318	DD6	C10-C11-C13-C14
42	I	211	DD6	C5-C6-C8-C9
44	o	317	A86	C5-C6-C8-C9
49	l	207	BCR	C7-C8-C9-C10
40	O	306	CLA	C2A-CAA-CBA-CGA
40	u	314	CLA	C2A-CAA-CBA-CGA
40	D	301	CLA	C6-C7-C8-C10
40	X	307	CLA	C11-C12-C13-C14
40	a	808	CLA	C16-C17-C18-C19
40	b	841	CLA	C16-C17-C18-C20
40	v	307	CLA	C11-C12-C13-C15
41	o	302	KC2	CBD-CGD-O2D-CED
40	a	805	CLA	C4-C3-C5-C6
40	a	822	CLA	C4-C3-C5-C6
40	b	823	CLA	C4-C3-C5-C6
41	C	303	KC2	C2C-C3C-CAC-CBC
41	E	319	KC2	C2B-C3B-CAB-CBB
41	F	302	KC2	C2C-C3C-CAC-CBC
41	H	303	KC2	C2C-C3C-CAC-CBC
41	J	304	KC2	C2B-C3B-CAB-CBB
41	K	305	KC2	C2C-C3C-CAC-CBC
41	L	302	KC2	C2C-C3C-CAC-CBC
41	L	309	KC2	C2C-C3C-CAC-CBC
41	L	313	KC2	C2C-C3C-CAC-CBC
41	M	301	KC2	C2B-C3B-CAB-CBB
41	M	302	KC2	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
41	M	308	KC2	C2B-C3B-CAB-CBB
41	N	309	KC2	C2B-C3B-CAB-CBB
41	N	309	KC2	C2C-C3C-CAC-CBC
41	N	313	KC2	C2C-C3C-CAC-CBC
41	O	302	KC2	C2B-C3B-CAB-CBB
41	O	308	KC2	C2B-C3B-CAB-CBB
41	O	309	KC2	C2B-C3B-CAB-CBB
41	P	310	KC2	C2C-C3C-CAC-CBC
41	R	301	KC2	C2C-C3C-CAC-CBC
41	R	302	KC2	C2C-C3C-CAC-CBC
41	R	303	KC2	C2C-C3C-CAC-CBC
41	R	311	KC2	C2C-C3C-CAC-CBC
41	S	304	KC2	C2B-C3B-CAB-CBB
41	T	302	KC2	C2C-C3C-CAC-CBC
41	T	308	KC2	C2B-C3B-CAB-CBB
41	T	311	KC2	C2C-C3C-CAC-CBC
41	W	309	KC2	C2B-C3B-CAB-CBB
41	W	310	KC2	C2C-C3C-CAC-CBC
41	X	308	KC2	C2B-C3B-CAB-CBB
41	X	309	KC2	C2C-C3C-CAC-CBC
41	Y	308	KC2	C2C-C3C-CAC-CBC
41	Z	302	KC2	C2C-C3C-CAC-CBC
41	o	302	KC2	C2C-C3C-CAC-CBC
41	o	308	KC2	C2C-C3C-CAC-CBC
41	o	309	KC2	C2C-C3C-CAC-CBC
41	p	310	KC2	C2C-C3C-CAC-CBC
41	u	310	KC2	C2C-C3C-CAC-CBC
41	v	302	KC2	C2C-C3C-CAC-CBC
41	x	310	KC2	C2C-C3C-CAC-CBC
41	z	310	KC2	C2C-C3C-CAC-CBC
43	l	201	LMG	C29-C30-C31-C32
40	p	312	CLA	O1D-CGD-O2D-CED
47	Z	320	A1EB1	C33-C34-O4-C38
40	E	309	CLA	C10-C11-C12-C13
40	K	306	CLA	C10-C11-C12-C13
40	K	308	CLA	C8-C10-C11-C12
40	x	302	CLA	C5-C6-C7-C8
40	x	306	CLA	C5-C6-C7-C8
40	z	302	CLA	C8-C10-C11-C12
43	L	319	LMG	C15-C16-C17-C18
40	E	306	CLA	O1A-CGA-O2A-C1
40	K	306	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
40	a	820	CLA	O1A-CGA-O2A-C1
40	a	803	CLA	C3-C5-C6-C7
40	x	311	CLA	C3-C5-C6-C7
52	b	850	DGD	O6E-C5E-C6E-O5E
40	a	825	CLA	C13-C15-C16-C17
40	b	818	CLA	C10-C11-C12-C13
40	b	824	CLA	C5-C6-C7-C8
40	b	824	CLA	C10-C11-C12-C13
40	W	312	CLA	C10-C11-C12-C13
40	p	308	CLA	C5-C6-C7-C8
41	A	310	KC2	C4B-C3B-CAB-CBB
41	A	310	KC2	C4C-C3C-CAC-CBC
41	F	302	KC2	C4B-C3B-CAB-CBB
41	G	202	KC2	C4B-C3B-CAB-CBB
41	G	202	KC2	C4C-C3C-CAC-CBC
41	I	209	KC2	C4C-C3C-CAC-CBC
41	M	301	KC2	C4B-C3B-CAB-CBB
41	M	301	KC2	C4C-C3C-CAC-CBC
41	M	308	KC2	C4B-C3B-CAB-CBB
41	N	301	KC2	C4C-C3C-CAC-CBC
41	N	303	KC2	C4C-C3C-CAC-CBC
41	N	312	KC2	C4B-C3B-CAB-CBB
41	O	308	KC2	C4C-C3C-CAC-CBC
41	O	309	KC2	C4C-C3C-CAC-CBC
41	R	303	KC2	C4C-C3C-CAC-CBC
41	R	309	KC2	C4B-C3B-CAB-CBB
41	R	309	KC2	C4C-C3C-CAC-CBC
41	S	309	KC2	C4B-C3B-CAB-CBB
41	S	310	KC2	C4C-C3C-CAC-CBC
41	W	302	KC2	C4C-C3C-CAC-CBC
41	Y	303	KC2	C4B-C3B-CAB-CBB
41	Y	308	KC2	C4C-C3C-CAC-CBC
41	q	309	KC2	C4C-C3C-CAC-CBC
41	t	306	KC2	C4B-C3B-CAB-CBB
41	u	303	KC2	C4C-C3C-CAC-CBC
41	x	303	KC2	C4C-C3C-CAC-CBC
41	y	306	KC2	C4B-C3B-CAB-CBB
41	z	310	KC2	C4B-C3B-CAB-CBB
41	C	303	KC2	CAA-CBA-CGA-O1A
40	E	309	CLA	O1A-CGA-O2A-C1
40	G	203	CLA	O1A-CGA-O2A-C1
45	a	849	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
40	M	307	CLA	C10-C11-C12-C13
40	P	308	CLA	O1D-CGD-O2D-CED
40	I	202	CLA	C3-C5-C6-C7
40	N	304	CLA	C3-C5-C6-C7
43	u	301	LMG	O7-C8-C9-O8
46	M	318	SQD	O47-C45-C46-O48
40	q	310	CLA	O1D-CGD-O2D-CED
40	v	312	CLA	CBA-CGA-O2A-C1
40	p	307	CLA	O1A-CGA-O2A-C1
43	T	318	LMG	C11-C12-C13-C14
43	l	201	LMG	C14-C15-C16-C17
40	a	807	CLA	C2C-C3C-CAC-CBC
40	o	307	CLA	C11-C12-C13-C14
50	a	847	PQN	C21-C22-C23-C24
40	a	824	CLA	C10-C11-C12-C13
41	F	309	KC2	CAA-CBA-CGA-O1A
41	F	309	KC2	CAA-CBA-CGA-O2A
40	U	207	CLA	O1D-CGD-O2D-CED
45	a	848	LHG	C7-C8-C9-C10
43	l	201	LMG	O9-C10-O7-C8
40	X	311	CLA	C5-C6-C7-C8
40	a	820	CLA	C5-C6-C7-C8
40	G	203	CLA	C2A-CAA-CBA-CGA
40	I	202	CLA	C2A-CAA-CBA-CGA
40	J	307	CLA	C2A-CAA-CBA-CGA
40	L	306	CLA	C2A-CAA-CBA-CGA
40	a	829	CLA	C2A-CAA-CBA-CGA
40	b	808	CLA	C2A-CAA-CBA-CGA
40	b	832	CLA	CBD-CGD-O2D-CED
40	z	311	CLA	CBD-CGD-O2D-CED
47	p	323	A1EB1	C35-C34-O4-C38
40	w	308	CLA	O1D-CGD-O2D-CED
40	W	305	CLA	C10-C11-C12-C13
40	L	306	CLA	CBD-CGD-O2D-CED
43	p	301	LMG	C33-C34-C35-C36
43	a	801	LMG	O6-C5-C6-O5
40	Z	310	CLA	O1A-CGA-O2A-C1
40	a	826	CLA	C3-C5-C6-C7
40	A	306	CLA	C1A-C2A-CAA-CBA
40	B	307	CLA	C1A-C2A-CAA-CBA
40	C	309	CLA	C1A-C2A-CAA-CBA
40	D	303	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
40	E	311	CLA	C1A-C2A-CAA-CBA
40	E	312	CLA	C1A-C2A-CAA-CBA
40	F	301	CLA	C1A-C2A-CAA-CBA
40	F	303	CLA	C1A-C2A-CAA-CBA
40	F	306	CLA	C1A-C2A-CAA-CBA
40	H	304	CLA	C1A-C2A-CAA-CBA
40	H	305	CLA	C1A-C2A-CAA-CBA
40	H	307	CLA	C1A-C2A-CAA-CBA
40	H	308	CLA	C1A-C2A-CAA-CBA
40	I	205	CLA	C1A-C2A-CAA-CBA
40	I	207	CLA	C1A-C2A-CAA-CBA
40	I	208	CLA	C1A-C2A-CAA-CBA
40	J	308	CLA	C1A-C2A-CAA-CBA
40	K	306	CLA	C1A-C2A-CAA-CBA
40	K	307	CLA	C1A-C2A-CAA-CBA
40	M	312	CLA	C1A-C2A-CAA-CBA
40	N	304	CLA	C1A-C2A-CAA-CBA
40	N	310	CLA	C1A-C2A-CAA-CBA
40	O	310	CLA	C1A-C2A-CAA-CBA
40	Q	204	CLA	C1A-C2A-CAA-CBA
40	S	313	CLA	C1A-C2A-CAA-CBA
40	S	319	CLA	C1A-C2A-CAA-CBA
40	U	207	CLA	C1A-C2A-CAA-CBA
40	W	305	CLA	C1A-C2A-CAA-CBA
40	W	306	CLA	C1A-C2A-CAA-CBA
40	W	311	CLA	C1A-C2A-CAA-CBA
40	X	304	CLA	C1A-C2A-CAA-CBA
40	X	311	CLA	C1A-C2A-CAA-CBA
40	Y	301	CLA	C1A-C2A-CAA-CBA
40	Y	304	CLA	C1A-C2A-CAA-CBA
40	Y	311	CLA	C1A-C2A-CAA-CBA
40	Z	304	CLA	C1A-C2A-CAA-CBA
40	a	804	CLA	C1A-C2A-CAA-CBA
40	a	807	CLA	C1A-C2A-CAA-CBA
40	a	808	CLA	C1A-C2A-CAA-CBA
40	a	829	CLA	C1A-C2A-CAA-CBA
40	a	830	CLA	C1A-C2A-CAA-CBA
40	a	842	CLA	C1A-C2A-CAA-CBA
40	a	850	CLA	C1A-C2A-CAA-CBA
40	b	806	CLA	C1A-C2A-CAA-CBA
40	b	820	CLA	C1A-C2A-CAA-CBA
40	b	834	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
40	b	838	CLA	C1A-C2A-CAA-CBA
40	b	840	CLA	C1A-C2A-CAA-CBA
40	i	101	CLA	C1A-C2A-CAA-CBA
40	o	310	CLA	C1A-C2A-CAA-CBA
40	o	312	CLA	C1A-C2A-CAA-CBA
40	o	313	CLA	C1A-C2A-CAA-CBA
40	p	305	CLA	C1A-C2A-CAA-CBA
40	p	307	CLA	C1A-C2A-CAA-CBA
40	p	311	CLA	C1A-C2A-CAA-CBA
40	q	301	CLA	C1A-C2A-CAA-CBA
40	q	310	CLA	C1A-C2A-CAA-CBA
40	q	313	CLA	C1A-C2A-CAA-CBA
40	u	306	CLA	C1A-C2A-CAA-CBA
40	v	301	CLA	C1A-C2A-CAA-CBA
40	v	310	CLA	C1A-C2A-CAA-CBA
40	x	306	CLA	C1A-C2A-CAA-CBA
40	y	308	CLA	C1A-C2A-CAA-CBA
40	z	305	CLA	C1A-C2A-CAA-CBA
40	z	313	CLA	C1A-C2A-CAA-CBA
47	P	301	A1EB1	C35-C34-O4-C38
40	M	307	CLA	CBD-CGD-O2D-CED
40	C	306	CLA	C10-C11-C12-C13
40	W	312	CLA	C8-C10-C11-C12
40	a	821	CLA	C8-C10-C11-C12
40	b	837	CLA	C8-C10-C11-C12
44	G	209	A86	C9-C10-C11-C12
44	M	316	A86	C9-C10-C11-C12
44	N	321	A86	C9-C10-C11-C12
44	R	313	A86	C9-C10-C11-C12
44	S	317	A86	C9-C10-C11-C12
44	X	317	A86	C9-C10-C11-C12
44	X	321	A86	C9-C10-C11-C12
44	Y	318	A86	C9-C10-C11-C12
44	v	315	A86	C9-C10-C11-C12
44	v	319	A86	C9-C10-C11-C12
47	O	317	A1EB1	C9-C10-C11-C12
47	o	321	A1EB1	C9-C10-C11-C12
47	t	313	A1EB1	C9-C10-C11-C12
47	w	314	A1EB1	C9-C10-C11-C12
43	p	301	LMG	O9-C10-O7-C8
47	S	321	A1EB1	C44-C45-C46-C47
40	H	307	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
40	M	307	CLA	C3-C5-C6-C7
40	A	304	CLA	C6-C7-C8-C10
40	E	309	CLA	C6-C7-C8-C10
40	F	321	CLA	C6-C7-C8-C10
40	H	305	CLA	C11-C10-C8-C7
40	N	311	CLA	C6-C7-C8-C10
40	O	304	CLA	C6-C7-C8-C10
40	S	302	CLA	C6-C7-C8-C10
40	W	312	CLA	C6-C7-C8-C10
40	Z	306	CLA	C11-C10-C8-C7
40	a	806	CLA	C6-C7-C8-C10
40	a	822	CLA	C6-C7-C8-C10
40	a	828	CLA	C12-C13-C15-C16
40	a	839	CLA	C12-C13-C15-C16
40	a	842	CLA	C11-C10-C8-C7
40	a	851	CLA	C12-C13-C15-C16
40	b	814	CLA	C12-C13-C15-C16
40	b	819	CLA	C11-C10-C8-C7
40	b	824	CLA	C6-C7-C8-C10
40	b	826	CLA	C12-C13-C15-C16
40	b	834	CLA	C6-C7-C8-C10
40	b	838	CLA	C6-C7-C8-C10
40	l	202	CLA	C12-C13-C15-C16
40	l	205	CLA	C11-C10-C8-C7
40	z	305	CLA	C6-C7-C8-C10
40	A	302	CLA	C11-C12-C13-C14
40	O	304	CLA	C15-C16-C17-C18
48	M	319	A1EB4	C10-C11-C12-O3
41	C	303	KC2	CAA-CBA-CGA-O2A
41	E	319	KC2	CAA-CBA-CGA-O1A
41	L	308	KC2	CAA-CBA-CGA-O1A
41	v	303	KC2	CAA-CBA-CGA-O1A
40	J	312	CLA	C5-C6-C7-C8
40	N	307	CLA	C2-C3-C5-C6
45	S	323	LHG	C11-C10-C9-C8
40	I	201	CLA	C13-C15-C16-C17
40	b	840	CLA	C5-C6-C7-C8
40	J	312	CLA	C2A-CAA-CBA-CGA
40	R	304	CLA	C2A-CAA-CBA-CGA
40	A	307	CLA	C6-C7-C8-C9
40	C	307	CLA	C6-C7-C8-C9
40	C	307	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
40	H	305	CLA	C11-C10-C8-C9
40	S	302	CLA	C6-C7-C8-C9
40	Z	306	CLA	C11-C10-C8-C9
40	a	831	CLA	C6-C7-C8-C9
40	a	839	CLA	C14-C13-C15-C16
40	b	805	CLA	C6-C7-C8-C9
40	b	810	CLA	C11-C12-C13-C14
40	b	819	CLA	C14-C13-C15-C16
40	b	824	CLA	C6-C7-C8-C9
40	l	205	CLA	C6-C7-C8-C9
43	A	317	LMG	C33-C34-C35-C36
43	M	317	LMG	C29-C30-C31-C32
52	b	850	DGD	C4B-C5B-C6B-C7B
40	q	307	CLA	C11-C12-C13-C14
43	T	318	LMG	C16-C17-C18-C19
43	x	301	LMG	C29-C30-C31-C32
40	C	308	CLA	CBA-CGA-O2A-C1
40	S	306	CLA	CBA-CGA-O2A-C1
40	W	307	CLA	CBA-CGA-O2A-C1
40	X	304	CLA	CBA-CGA-O2A-C1
40	X	311	CLA	CBA-CGA-O2A-C1
40	b	831	CLA	CBA-CGA-O2A-C1
40	q	304	CLA	CBA-CGA-O2A-C1
40	f	201	CLA	C5-C6-C7-C8
40	u	302	CLA	C15-C16-C17-C18
52	b	850	DGD	C2D-C1D-O3G-C3G
40	X	306	CLA	C5-C6-C7-C8
40	a	836	CLA	C13-C15-C16-C17
43	u	301	LMG	C31-C32-C33-C34
43	E	320	LMG	O6-C5-C6-O5
43	T	318	LMG	O6-C5-C6-O5
41	L	308	KC2	CAA-CBA-CGA-O2A
40	b	842	CLA	C14-C13-C15-C16
43	A	317	LMG	C7-C8-C9-O8
43	E	320	LMG	O1-C7-C8-C9
43	p	301	LMG	C7-C8-C9-O8
46	P	319	SQD	C44-C45-C46-O48
40	K	307	CLA	CBA-CGA-O2A-C1
40	M	310	CLA	CBA-CGA-O2A-C1
43	M	317	LMG	C28-C29-C30-C31
43	a	802	LMG	C28-C29-C30-C31
43	a	802	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
40	a	831	CLA	C11-C12-C13-C14
40	a	839	CLA	C16-C17-C18-C19
40	b	841	CLA	C16-C17-C18-C19
40	o	305	CLA	C6-C7-C8-C9
46	I	215	SQD	C10-C11-C12-C13
40	u	306	CLA	C2C-C3C-CAC-CBC
40	b	807	CLA	O1D-CGD-O2D-CED
40	X	307	CLA	O1A-CGA-O2A-C1
40	b	814	CLA	O1A-CGA-O2A-C1
40	N	307	CLA	C4-C3-C5-C6
40	a	805	CLA	C2-C3-C5-C6
40	a	822	CLA	C2-C3-C5-C6
40	a	837	CLA	C2-C3-C5-C6
40	a	842	CLA	C2-C3-C5-C6
40	b	823	CLA	C2-C3-C5-C6
40	E	307	CLA	C8-C10-C11-C12
40	I	206	CLA	C10-C11-C12-C13
40	a	831	CLA	C10-C11-C12-C13
40	b	826	CLA	C10-C11-C12-C13
44	o	315	A86	C7-C6-C8-C9
40	X	307	CLA	C11-C12-C13-C15
40	a	808	CLA	C16-C17-C18-C20
40	k	201	CLA	O1A-CGA-O2A-C1
40	v	305	CLA	O1A-CGA-O2A-C1
40	Z	305	CLA	C5-C6-C7-C8
40	a	820	CLA	C8-C10-C11-C12
40	b	821	CLA	C13-C15-C16-C17
43	T	318	LMG	C13-C14-C15-C16
47	o	322	A1EB1	C42-C44-C45-C46
40	D	312	CLA	O1A-CGA-O2A-C1
40	a	851	CLA	CBA-CGA-O2A-C1
40	b	811	CLA	CBA-CGA-O2A-C1
40	l	203	CLA	CBA-CGA-O2A-C1
40	F	303	CLA	O2A-C1-C2-C3
40	M	311	CLA	O2A-C1-C2-C3
40	Y	310	CLA	O2A-C1-C2-C3
40	a	834	CLA	O2A-C1-C2-C3
40	b	833	CLA	O2A-C1-C2-C3
40	v	310	CLA	O2A-C1-C2-C3
40	x	306	CLA	O2A-C1-C2-C3
40	z	302	CLA	O2A-C1-C2-C3
40	D	304	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
40	b	814	CLA	C5-C6-C7-C8
40	b	819	CLA	C5-C6-C7-C8
47	x	321	A1EB1	C25-C26-C27-C29
40	v	307	CLA	C11-C12-C13-C14
40	x	306	CLA	C11-C12-C13-C15
48	W	319	A1EB4	C44-C45-C46-C47
47	t	314	A1EB1	C42-C44-C45-C46
40	y	308	CLA	O1D-CGD-O2D-CED
40	U	203	CLA	C4C-C3C-CAC-CBC
45	a	848	LHG	C31-C32-C33-C34
40	i	101	CLA	CBA-CGA-O2A-C1
40	v	307	CLA	CBA-CGA-O2A-C1
52	b	850	DGD	C5A-C6A-C7A-C8A
44	R	315	A86	C33-C34-O4-C38
46	W	318	SQD	C11-C10-C9-C8
41	W	304	KC2	CAA-CBA-CGA-O1A
41	q	303	KC2	CAA-CBA-CGA-O1A
40	Y	301	CLA	C4-C3-C5-C6
40	a	806	CLA	C4-C3-C5-C6
40	K	307	CLA	C2-C3-C5-C6
40	a	839	CLA	C2-C3-C5-C6
40	b	802	CLA	C2-C3-C5-C6
40	z	311	CLA	C2-C3-C5-C6
40	D	307	CLA	C3-C5-C6-C7
40	D	303	CLA	C11-C12-C13-C15
40	a	816	CLA	C16-C17-C18-C19
43	E	301	LMG	C12-C13-C14-C15
43	l	201	LMG	O7-C8-C9-O8
47	z	323	A1EB1	C45-C46-C47-C48
45	a	849	LHG	O2-C2-C3-O3
40	b	819	CLA	C16-C17-C18-C19
43	l	201	LMG	C35-C36-C37-C38
43	j	101	LMG	C29-C30-C31-C32
40	b	832	CLA	C3-C5-C6-C7
40	p	311	CLA	C3-C5-C6-C7
40	u	311	CLA	C3-C5-C6-C7
40	x	302	CLA	C3-C5-C6-C7
44	F	313	A86	C9-C10-C11-C13
44	X	319	A86	C9-C10-C11-C13
47	p	323	A1EB1	C9-C10-C11-C13
43	F	318	LMG	C15-C16-C17-C18
41	E	319	KC2	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
41	W	304	KC2	CAA-CBA-CGA-O2A
41	v	303	KC2	CAA-CBA-CGA-O2A
52	b	850	DGD	C6B-C7B-C8B-C9B
40	E	306	CLA	C6-C7-C8-C10
40	Z	301	CLA	O1A-CGA-O2A-C1
40	b	813	CLA	O1A-CGA-O2A-C1
40	b	833	CLA	C5-C6-C7-C8
40	Q	202	CLA	CBA-CGA-O2A-C1
40	a	822	CLA	CBA-CGA-O2A-C1
40	o	310	CLA	CBA-CGA-O2A-C1
40	q	307	CLA	CBA-CGA-O2A-C1
40	q	310	CLA	CBA-CGA-O2A-C1
40	t	309	CLA	CBD-CGD-O2D-CED
48	W	319	A1EB4	C45-C46-C47-C51
40	W	308	CLA	C8-C10-C11-C12
40	x	311	CLA	C5-C6-C7-C8
43	D	318	LMG	C10-C11-C12-C13
40	Z	306	CLA	C10-C11-C12-C13
40	b	822	CLA	C5-C6-C7-C8
44	t	311	A86	C11-C10-C9-C8
44	w	311	A86	C11-C10-C9-C8
44	w	316	A86	C11-C10-C9-C8
44	v	319	A86	C33-C34-O4-C38
40	A	302	CLA	C4-C3-C5-C6
40	C	306	CLA	C4-C3-C5-C6
40	H	310	CLA	C4-C3-C5-C6
40	P	308	CLA	C4-C3-C5-C6
40	a	821	CLA	C4-C3-C5-C6
40	a	832	CLA	C4-C3-C5-C6
40	a	837	CLA	C4-C3-C5-C6
40	a	851	CLA	C4-C3-C5-C6
40	b	801	CLA	C4-C3-C5-C6
40	b	836	CLA	C4-C3-C5-C6
40	p	311	CLA	C4-C3-C5-C6
40	x	311	CLA	C4-C3-C5-C6
40	z	306	CLA	C4-C3-C5-C6
40	Q	206	CLA	CBA-CGA-O2A-C1
40	R	305	CLA	CBA-CGA-O2A-C1
40	Y	307	CLA	CBA-CGA-O2A-C1
40	N	311	CLA	C8-C10-C11-C12
47	v	321	A1EB1	C44-C45-C46-C47
42	A	314	DD6	C27-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
42	C	310	DD6	C27-C29-C30-C31
42	Q	212	DD6	C27-C29-C30-C31
42	T	314	DD6	C27-C29-C30-C31
42	W	315	DD6	C27-C29-C30-C31
45	a	848	LHG	O1-C1-C2-O2
40	Q	206	CLA	CBD-CGD-O2D-CED
40	E	309	CLA	C6-C7-C8-C9
40	I	206	CLA	C11-C10-C8-C9
40	K	304	CLA	C6-C7-C8-C9
40	O	304	CLA	C6-C7-C8-C9
40	W	312	CLA	C6-C7-C8-C9
40	a	822	CLA	C6-C7-C8-C9
40	a	828	CLA	C14-C13-C15-C16
40	b	806	CLA	C6-C7-C8-C9
40	b	826	CLA	C14-C13-C15-C16
40	b	834	CLA	C6-C7-C8-C9
40	b	838	CLA	C6-C7-C8-C9
40	b	833	CLA	O1D-CGD-O2D-CED
40	x	307	CLA	C5-C6-C7-C8
43	P	318	LMG	C35-C36-C37-C38
40	E	310	CLA	O1A-CGA-O2A-C1
40	x	305	CLA	O1A-CGA-O2A-C1
40	A	308	CLA	C4B-C3B-CAB-CBB
40	A	309	CLA	C4B-C3B-CAB-CBB
40	B	301	CLA	C4B-C3B-CAB-CBB
40	D	312	CLA	C4B-C3B-CAB-CBB
40	E	306	CLA	C4B-C3B-CAB-CBB
40	F	301	CLA	C4B-C3B-CAB-CBB
40	F	308	CLA	C4B-C3B-CAB-CBB
40	F	321	CLA	C4B-C3B-CAB-CBB
40	I	205	CLA	C4B-C3B-CAB-CBB
40	J	303	CLA	C4B-C3B-CAB-CBB
40	L	301	CLA	C4B-C3B-CAB-CBB
40	M	306	CLA	C4B-C3B-CAB-CBB
40	N	306	CLA	C4B-C3B-CAB-CBB
40	P	311	CLA	C4B-C3B-CAB-CBB
40	R	316	CLA	C4B-C3B-CAB-CBB
40	S	319	CLA	C4B-C3B-CAB-CBB
40	T	317	CLA	C4B-C3B-CAB-CBB
40	U	202	CLA	C4B-C3B-CAB-CBB
40	W	307	CLA	C4B-C3B-CAB-CBB
40	W	311	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
40	W	313	CLA	C4B-C3B-CAB-CBB
40	Y	301	CLA	C4B-C3B-CAB-CBB
40	Y	311	CLA	C4B-C3B-CAB-CBB
40	a	814	CLA	C4B-C3B-CAB-CBB
40	a	830	CLA	C4B-C3B-CAB-CBB
40	a	834	CLA	C4B-C3B-CAB-CBB
40	b	814	CLA	C4B-C3B-CAB-CBB
40	b	819	CLA	C4B-C3B-CAB-CBB
40	b	833	CLA	C4B-C3B-CAB-CBB
40	b	840	CLA	C4B-C3B-CAB-CBB
40	l	203	CLA	C4B-C3B-CAB-CBB
40	o	304	CLA	C4B-C3B-CAB-CBB
40	o	310	CLA	C4B-C3B-CAB-CBB
40	p	308	CLA	C4B-C3B-CAB-CBB
40	v	312	CLA	C4B-C3B-CAB-CBB
40	w	304	CLA	C4B-C3B-CAB-CBB
40	y	304	CLA	C4B-C3B-CAB-CBB
40	z	313	CLA	C4B-C3B-CAB-CBB
40	A	305	CLA	C8-C10-C11-C12
40	a	807	CLA	C5-C6-C7-C8
40	q	307	CLA	C5-C6-C7-C8
40	w	309	CLA	CBD-CGD-O2D-CED
40	o	307	CLA	C11-C12-C13-C15
41	q	303	KC2	CAA-CBA-CGA-O2A
40	G	213	CLA	C2C-C3C-CAC-CBC
43	l	201	LMG	C15-C16-C17-C18
40	a	840	CLA	C2A-CAA-CBA-CGA
43	T	318	LMG	C2-C1-O1-C7
43	E	320	LMG	C11-C12-C13-C14
45	S	323	LHG	C16-C17-C18-C19
47	o	322	A1EB1	C25-C26-C27-C28
47	x	321	A1EB1	C25-C26-C27-C28
43	E	301	LMG	C29-C30-C31-C32
45	F	319	LHG	C29-C30-C31-C32
40	A	302	CLA	C11-C10-C8-C7
40	A	303	CLA	C11-C12-C13-C15
40	A	307	CLA	C6-C7-C8-C10
40	C	307	CLA	C11-C10-C8-C7
40	D	304	CLA	C6-C7-C8-C10
40	E	308	CLA	C11-C10-C8-C7
40	F	306	CLA	C6-C7-C8-C10
40	H	307	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
40	M	311	CLA	C12-C13-C15-C16
40	P	305	CLA	C6-C7-C8-C10
40	X	311	CLA	C11-C10-C8-C7
40	a	803	CLA	C6-C7-C8-C10
40	a	804	CLA	C12-C13-C15-C16
40	a	824	CLA	C11-C12-C13-C15
40	a	826	CLA	C6-C7-C8-C10
40	a	828	CLA	C11-C10-C8-C7
40	a	836	CLA	C6-C7-C8-C10
40	b	803	CLA	C11-C12-C13-C15
40	b	805	CLA	C6-C7-C8-C10
40	b	808	CLA	C11-C12-C13-C15
40	b	810	CLA	C11-C12-C13-C15
40	b	818	CLA	C11-C10-C8-C7
40	b	819	CLA	C12-C13-C15-C16
43	x	301	LMG	C28-C29-C30-C31
40	f	202	CLA	O1A-CGA-O2A-C1
40	q	305	CLA	O1A-CGA-O2A-C1
40	D	311	CLA	C3A-C2A-CAA-CBA
40	E	314	CLA	C3A-C2A-CAA-CBA
40	J	305	CLA	C4-C3-C5-C6
40	P	305	CLA	C4-C3-C5-C6
40	Y	313	CLA	C3A-C2A-CAA-CBA
40	a	829	CLA	C3A-C2A-CAA-CBA
40	a	839	CLA	C4-C3-C5-C6
40	a	842	CLA	C4-C3-C5-C6
40	b	824	CLA	C4-C3-C5-C6
40	b	835	CLA	C4-C3-C5-C6
40	p	307	CLA	C3A-C2A-CAA-CBA
40	q	311	CLA	C4-C3-C5-C6
40	u	307	CLA	C3A-C2A-CAA-CBA
40	u	311	CLA	C3A-C2A-CAA-CBA
40	u	311	CLA	C4-C3-C5-C6
40	v	304	CLA	C3A-C2A-CAA-CBA
40	v	311	CLA	C4-C3-C5-C6
40	z	311	CLA	C4-C3-C5-C6
40	z	324	CLA	C3A-C2A-CAA-CBA
40	C	307	CLA	C8-C10-C11-C12
40	O	304	CLA	C5-C6-C7-C8
40	a	852	CLA	C5-C6-C7-C8
40	v	307	CLA	C5-C6-C7-C8
40	b	836	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
40	D	303	CLA	C4C-C3C-CAC-CBC
40	D	310	CLA	O1A-CGA-O2A-C1
40	v	304	CLA	O1A-CGA-O2A-C1
43	D	318	LMG	O10-C28-O8-C9
40	y	309	CLA	CBA-CGA-O2A-C1
40	b	839	CLA	C10-C11-C12-C13
42	B	305	DD6	C7-C6-C8-C9
42	E	318	DD6	C12-C11-C13-C14
42	q	320	DD6	C-C1-C24-C25
44	M	320	A86	C7-C6-C8-C9
44	q	319	A86	C-C1-C24-C25
44	v	319	A86	C-C1-C24-C25
49	a	843	BCR	C37-C22-C23-C24
40	b	831	CLA	C4-C3-C5-C6
40	v	312	CLA	O1A-CGA-O2A-C1
40	b	801	CLA	C8-C10-C11-C12
40	y	305	CLA	CBD-CGD-O2D-CED
44	z	317	A86	C5-C6-C8-C9
47	G	212	A1EB1	C2-C1-C24-C25
40	a	806	CLA	C2A-CAA-CBA-CGA
52	b	850	DGD	C3A-C4A-C5A-C6A
43	E	301	LMG	O1-C7-C8-C9
43	E	321	LMG	C7-C8-C9-O8
43	P	318	LMG	C7-C8-C9-O8
43	T	318	LMG	C7-C8-C9-O8
43	a	801	LMG	C7-C8-C9-O8
43	a	802	LMG	C7-C8-C9-O8
43	l	201	LMG	C7-C8-C9-O8
43	u	301	LMG	C7-C8-C9-O8
44	F	317	A86	C12-C11-C13-O
44	G	209	A86	C12-C11-C13-O
44	M	315	A86	C12-C11-C13-O
44	P	314	A86	C12-C11-C13-O
44	P	316	A86	C12-C11-C13-O
44	P	321	A86	C12-C11-C13-O
44	S	316	A86	C12-C11-C13-O
44	X	320	A86	C12-C11-C13-O
44	Z	317	A86	C12-C11-C13-O
44	o	314	A86	C12-C11-C13-O
44	o	315	A86	C12-C11-C13-O
44	o	316	A86	C12-C11-C13-O
44	p	320	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
44	q	324	A86	C12-C11-C13-O
44	t	311	A86	C12-C11-C13-O
44	t	316	A86	C12-C11-C13-O
44	u	319	A86	C12-C11-C13-O
44	u	320	A86	C12-C11-C13-O
44	v	325	A86	C12-C11-C13-O
44	w	311	A86	C12-C11-C13-O
44	w	316	A86	C12-C11-C13-O
44	x	318	A86	C12-C11-C13-O
44	x	319	A86	C12-C11-C13-O
44	z	315	A86	C12-C11-C13-O
45	a	849	LHG	C4-C5-C6-O8
46	M	318	SQD	C44-C45-C46-O48
47	G	212	A1EB1	C12-C11-C13-O
47	L	318	A1EB1	C12-C11-C13-O
47	P	301	A1EB1	C12-C11-C13-O
47	S	320	A1EB1	C12-C11-C13-O
47	T	320	A1EB1	C12-C11-C13-O
47	Z	320	A1EB1	C12-C11-C13-O
47	Z	321	A1EB1	C12-C11-C13-O
47	t	313	A1EB1	C12-C11-C13-O
47	t	314	A1EB1	C12-C11-C13-O
47	y	314	A1EB1	C12-C11-C13-O
40	T	304	CLA	C3-C5-C6-C7
43	E	321	LMG	C32-C33-C34-C35
40	a	816	CLA	C16-C17-C18-C20
40	b	833	CLA	C8-C10-C11-C12
40	x	312	CLA	C5-C6-C7-C8
47	L	318	A1EB1	C45-C46-C47-C48
41	Y	303	KC2	CAA-CBA-CGA-O1A
40	x	302	CLA	C10-C11-C12-C13
43	A	317	LMG	C14-C15-C16-C17
48	M	319	A1EB4	C44-C45-C46-C47
40	K	307	CLA	C4-C3-C5-C6
40	M	307	CLA	C4-C3-C5-C6
40	b	820	CLA	C4-C3-C5-C6
40	b	839	CLA	C4-C3-C5-C6
40	Q	205	CLA	CBA-CGA-O2A-C1
40	H	309	CLA	C2-C3-C5-C6
40	J	305	CLA	C2-C3-C5-C6
40	P	308	CLA	C2-C3-C5-C6
40	a	832	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
40	b	835	CLA	C2-C3-C5-C6
40	b	839	CLA	C2-C3-C5-C6
40	b	840	CLA	C2-C3-C5-C6
40	x	311	CLA	C2-C3-C5-C6
47	o	321	A1EB1	C35-C34-O4-C38
40	H	309	CLA	O1A-CGA-O2A-C1
40	M	311	CLA	C3-C5-C6-C7
40	b	801	CLA	C3-C5-C6-C7
43	j	101	LMG	C30-C31-C32-C33
40	u	312	CLA	C10-C11-C12-C13
44	F	317	A86	C10-C11-C13-O
44	G	209	A86	C10-C11-C13-O
44	M	315	A86	C10-C11-C13-O
44	M	320	A86	C10-C11-C13-O
44	P	314	A86	C10-C11-C13-O
44	P	316	A86	C10-C11-C13-O
44	P	321	A86	C10-C11-C13-O
44	Q	215	A86	C10-C11-C13-O
44	S	316	A86	C10-C11-C13-O
44	X	316	A86	C10-C11-C13-O
44	Y	315	A86	C10-C11-C13-O
44	Z	317	A86	C10-C11-C13-O
44	o	314	A86	C10-C11-C13-O
44	o	315	A86	C10-C11-C13-O
44	p	320	A86	C10-C11-C13-O
44	p	321	A86	C10-C11-C13-O
44	t	311	A86	C10-C11-C13-O
44	t	316	A86	C10-C11-C13-O
44	u	319	A86	C10-C11-C13-O
44	u	320	A86	C10-C11-C13-O
44	v	325	A86	C10-C11-C13-O
44	w	311	A86	C10-C11-C13-O
44	w	316	A86	C10-C11-C13-O
44	x	318	A86	C10-C11-C13-O
44	x	319	A86	C10-C11-C13-O
44	z	301	A86	C10-C11-C13-O
44	z	315	A86	C10-C11-C13-O
47	G	212	A1EB1	C10-C11-C13-O
47	L	318	A1EB1	C10-C11-C13-O
47	S	320	A1EB1	C10-C11-C13-O
47	T	320	A1EB1	C10-C11-C13-O
47	Z	320	A1EB1	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
47	Z	321	A1EB1	C10-C11-C13-O
47	t	313	A1EB1	C10-C11-C13-O
47	t	314	A1EB1	C10-C11-C13-O
40	I	204	CLA	C2C-C3C-CAC-CBC
43	E	320	LMG	C12-C13-C14-C15
40	l	204	CLA	C5-C6-C7-C8
43	E	321	LMG	C12-C13-C14-C15
45	F	319	LHG	C12-C13-C14-C15
40	Y	305	CLA	O1D-CGD-O2D-CED
40	K	308	CLA	C11-C12-C13-C14
40	B	301	CLA	C2B-C3B-CAB-CBB
40	Z	310	CLA	C2B-C3B-CAB-CBB
40	Z	312	CLA	C2B-C3B-CAB-CBB
40	b	819	CLA	C2B-C3B-CAB-CBB
40	b	825	CLA	C2B-C3B-CAB-CBB
40	b	833	CLA	C2B-C3B-CAB-CBB
40	k	202	CLA	C2B-C3B-CAB-CBB
40	p	311	CLA	C2B-C3B-CAB-CBB
49	b	847	BCR	C23-C24-C25-C30
49	i	102	BCR	C23-C24-C25-C30
49	k	203	BCR	C1-C6-C7-C8
49	r	201	BCR	C23-C24-C25-C30
40	o	311	CLA	C10-C11-C12-C13
44	S	318	A86	C33-C34-O4-C38
44	q	319	A86	C33-C34-O4-C38
47	N	320	A1EB1	C35-C34-O4-C38
43	D	318	LMG	C34-C35-C36-C37
43	L	319	LMG	C16-C17-C18-C19
40	U	203	CLA	C3-C5-C6-C7
40	a	810	CLA	C3-C5-C6-C7
44	N	318	A86	C9-C10-C11-C12
44	X	314	A86	C9-C10-C11-C12
44	q	315	A86	C9-C10-C11-C12
44	y	310	A86	C9-C10-C11-C12
45	S	323	LHG	C10-C11-C12-C13
40	T	304	CLA	C8-C10-C11-C12
40	W	307	CLA	C10-C11-C12-C13
40	b	827	CLA	C10-C11-C12-C13
40	b	836	CLA	C10-C11-C12-C13
41	x	310	KC2	CBD-CGD-O2D-CED
40	v	306	CLA	O1D-CGD-O2D-CED
40	H	307	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
40	a	831	CLA	C11-C12-C13-C15
47	t	313	A1EB1	C42-C44-C45-C46
40	O	306	CLA	C8-C10-C11-C12
40	R	305	CLA	C5-C6-C7-C8
40	a	828	CLA	C8-C10-C11-C12
40	u	308	CLA	C5-C6-C7-C8
43	A	317	LMG	O1-C7-C8-O7
43	E	321	LMG	O7-C8-C9-O8
46	I	215	SQD	O47-C45-C46-O48
46	W	318	SQD	O6-C44-C45-O47
40	p	314	CLA	O1D-CGD-O2D-CED
41	Y	303	KC2	CAA-CBA-CGA-O2A
40	a	807	CLA	C11-C10-C8-C7
40	W	307	CLA	O1A-CGA-O2A-C1
40	b	840	CLA	C4-C3-C5-C6
40	A	311	CLA	O1D-CGD-O2D-CED
40	S	308	CLA	O1D-CGD-O2D-CED
40	Q	205	CLA	C5-C6-C7-C8
40	H	310	CLA	C2-C3-C5-C6
40	M	307	CLA	C2-C3-C5-C6
40	a	821	CLA	C2-C3-C5-C6
40	a	851	CLA	C2-C3-C5-C6
40	b	801	CLA	C2-C3-C5-C6
40	p	311	CLA	C2-C3-C5-C6
40	q	311	CLA	C2-C3-C5-C6
40	u	311	CLA	C2-C3-C5-C6
40	v	311	CLA	C2-C3-C5-C6
45	a	848	LHG	C10-C11-C12-C13
47	u	322	A1EB1	C33-C34-O4-C38
40	A	302	CLA	C11-C12-C13-C15
40	Q	208	CLA	C11-C12-C13-C15
40	o	305	CLA	C6-C7-C8-C10
43	u	301	LMG	C32-C33-C34-C35
40	F	306	CLA	C3-C5-C6-C7
40	M	311	CLA	C14-C13-C15-C16
40	a	803	CLA	C6-C7-C8-C9
40	b	803	CLA	C11-C12-C13-C14
40	b	817	CLA	C14-C13-C15-C16
40	i	101	CLA	C5-C6-C7-C8
41	t	308	KC2	CAA-CBA-CGA-O2A
40	a	823	CLA	O1D-CGD-O2D-CED
40	y	309	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
40	a	839	CLA	C16-C17-C18-C20
50	a	847	PQN	C21-C22-C23-C25
40	X	305	CLA	O1D-CGD-O2D-CED
40	D	309	CLA	C5-C6-C7-C8
40	a	804	CLA	C2A-CAA-CBA-CGA
40	G	207	CLA	C6-C7-C8-C9
40	F	306	CLA	C5-C6-C7-C8
40	o	307	CLA	CBA-CGA-O2A-C1
40	T	310	CLA	C4-C3-C5-C6
45	S	323	LHG	C29-C30-C31-C32
40	C	306	CLA	C2-C3-C5-C6
40	v	301	CLA	C2-C3-C5-C6
40	z	306	CLA	C2-C3-C5-C6
40	a	840	CLA	C6-C7-C8-C10
40	l	202	CLA	C16-C17-C18-C19
43	a	801	LMG	C11-C12-C13-C14
40	E	314	CLA	O1A-CGA-O2A-C1
40	X	311	CLA	O1A-CGA-O2A-C1
40	q	304	CLA	O1A-CGA-O2A-C1
40	b	838	CLA	C3-C5-C6-C7
40	a	830	CLA	CAA-CBA-CGA-O2A
40	S	301	CLA	CBA-CGA-O2A-C1
40	Y	301	CLA	CBA-CGA-O2A-C1
40	P	308	CLA	C5-C6-C7-C8
41	t	308	KC2	CAA-CBA-CGA-O1A
45	S	323	LHG	C14-C15-C16-C17
40	E	305	CLA	C8-C10-C11-C12
40	I	201	CLA	C8-C10-C11-C12
40	W	305	CLA	C13-C15-C16-C17
42	I	211	DD6	C7-C6-C8-C9
42	N	317	DD6	C-C1-C24-C25
44	t	316	A86	C-C1-C24-C25
47	q	321	A1EB1	C-C1-C24-C25
40	A	309	CLA	C6-C7-C8-C10
40	C	306	CLA	C11-C10-C8-C7
40	K	304	CLA	C6-C7-C8-C10
40	N	304	CLA	C6-C7-C8-C10
40	N	307	CLA	C6-C7-C8-C10
40	T	310	CLA	C6-C7-C8-C10
40	a	813	CLA	C6-C7-C8-C10
40	a	815	CLA	C11-C12-C13-C15
40	a	829	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
40	a	831	CLA	C6-C7-C8-C10
40	a	834	CLA	C6-C7-C8-C10
40	b	806	CLA	C6-C7-C8-C10
40	b	812	CLA	C11-C10-C8-C7
40	l	203	CLA	C11-C10-C8-C7
40	z	307	CLA	C6-C7-C8-C10
45	S	323	LHG	C11-C12-C13-C14
47	q	323	A1EB1	C44-C45-C46-C47
40	I	202	CLA	C5-C6-C7-C8
45	a	848	LHG	C35-C36-C37-C38
42	C	313	DD6	C5-C6-C8-C9
42	D	314	DD6	C5-C6-C8-C9
42	N	316	DD6	C10-C11-C13-C14
42	q	320	DD6	C2-C1-C24-C25
42	v	320	DD6	C2-C1-C24-C25
42	z	321	DD6	C2-C1-C24-C25
44	q	319	A86	C2-C1-C24-C25
44	v	319	A86	C2-C1-C24-C25
47	K	315	A1EB1	C5-C6-C8-C9
47	v	321	A1EB1	C2-C1-C24-C25
49	b	845	BCR	C7-C8-C9-C10
49	b	845	BCR	C21-C22-C23-C24
49	l	206	BCR	C11-C12-C13-C14
40	v	310	CLA	CBA-CGA-O2A-C1
40	b	831	CLA	O1A-CGA-O2A-C1
45	F	319	LHG	O10-C23-O8-C6
40	B	301	CLA	C4C-C3C-CAC-CBC
44	Y	315	A86	C33-C34-O4-C38
40	Y	310	CLA	O1D-CGD-O2D-CED
40	b	817	CLA	C5-C6-C7-C8
40	M	310	CLA	C2A-CAA-CBA-CGA
40	Y	307	CLA	O1D-CGD-O2D-CED
43	P	318	LMG	C4-C5-C6-O5
43	j	101	LMG	O9-C10-O7-C8
40	H	309	CLA	C4-C3-C5-C6
40	R	307	CLA	C4-C3-C5-C6
40	K	307	CLA	O1A-CGA-O2A-C1
40	a	851	CLA	O1A-CGA-O2A-C1
40	b	820	CLA	C2-C3-C5-C6
41	E	319	KC2	C2C-C3C-CAC-CBC
41	H	303	KC2	C2B-C3B-CAB-CBB
41	K	302	KC2	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
41	K	302	KC2	C2C-C3C-CAC-CBC
41	K	303	KC2	C2B-C3B-CAB-CBB
41	K	303	KC2	C2C-C3C-CAC-CBC
41	K	309	KC2	C2B-C3B-CAB-CBB
41	L	313	KC2	C2B-C3B-CAB-CBB
41	M	303	KC2	C2B-C3B-CAB-CBB
41	M	309	KC2	C2B-C3B-CAB-CBB
41	N	302	KC2	C2C-C3C-CAC-CBC
41	N	312	KC2	C2C-C3C-CAC-CBC
41	O	302	KC2	C2C-C3C-CAC-CBC
41	O	311	KC2	C2B-C3B-CAB-CBB
41	P	303	KC2	C2C-C3C-CAC-CBC
41	P	309	KC2	C2C-C3C-CAC-CBC
41	P	310	KC2	C2B-C3B-CAB-CBB
41	R	308	KC2	C2B-C3B-CAB-CBB
41	S	303	KC2	C2C-C3C-CAC-CBC
41	T	308	KC2	C2C-C3C-CAC-CBC
41	T	309	KC2	C2B-C3B-CAB-CBB
41	T	309	KC2	C2C-C3C-CAC-CBC
41	T	311	KC2	C2B-C3B-CAB-CBB
41	U	201	KC2	C2C-C3C-CAC-CBC
41	W	302	KC2	C2B-C3B-CAB-CBB
41	W	309	KC2	C2C-C3C-CAC-CBC
41	Y	308	KC2	C2B-C3B-CAB-CBB
41	Y	309	KC2	C2B-C3B-CAB-CBB
41	Y	314	KC2	C2B-C3B-CAB-CBB
41	Z	303	KC2	C2B-C3B-CAB-CBB
41	Z	308	KC2	C2B-C3B-CAB-CBB
41	Z	309	KC2	C2B-C3B-CAB-CBB
41	Z	309	KC2	C2C-C3C-CAC-CBC
41	o	303	KC2	C2B-C3B-CAB-CBB
41	p	303	KC2	C2C-C3C-CAC-CBC
41	p	309	KC2	C2B-C3B-CAB-CBB
41	p	309	KC2	C2C-C3C-CAC-CBC
41	q	302	KC2	C2C-C3C-CAC-CBC
41	t	306	KC2	C2C-C3C-CAC-CBC
41	u	309	KC2	C2C-C3C-CAC-CBC
41	w	306	KC2	C2B-C3B-CAB-CBB
41	w	306	KC2	C2C-C3C-CAC-CBC
41	x	309	KC2	C2B-C3B-CAB-CBB
41	y	301	KC2	C2B-C3B-CAB-CBB
41	y	301	KC2	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
41	y	306	KC2	C2C-C3C-CAC-CBC
41	y	307	KC2	C2B-C3B-CAB-CBB
41	y	307	KC2	C2C-C3C-CAC-CBC
41	z	309	KC2	C2C-C3C-CAC-CBC
47	q	321	A1EB1	C44-C45-C46-C47
40	N	310	CLA	CBD-CGD-O2D-CED
40	b	806	CLA	CBD-CGD-O2D-CED
40	P	305	CLA	O2A-C1-C2-C3
40	X	310	CLA	O2A-C1-C2-C3
40	b	810	CLA	O2A-C1-C2-C3
40	b	818	CLA	C2C-C3C-CAC-CBC
40	C	308	CLA	O1A-CGA-O2A-C1
40	S	306	CLA	O1A-CGA-O2A-C1
40	X	304	CLA	O1A-CGA-O2A-C1
40	l	203	CLA	O1A-CGA-O2A-C1
43	A	317	LMG	C15-C16-C17-C18
43	W	317	LMG	C12-C13-C14-C15
45	a	848	LHG	C33-C34-C35-C36
45	F	319	LHG	C24-C25-C26-C27
47	q	322	A1EB1	C44-C45-C46-C47
40	J	305	CLA	C6-C7-C8-C10
40	a	838	CLA	C6-C7-C8-C9
40	W	307	CLA	C3-C5-C6-C7
40	b	819	CLA	C10-C11-C12-C13
43	E	321	LMG	C29-C30-C31-C32
52	b	850	DGD	O1B-C1B-O2G-C2G
40	M	310	CLA	O1A-CGA-O2A-C1
43	j	101	LMG	C7-C8-C9-O8
43	x	301	LMG	C7-C8-C9-O8
40	H	305	CLA	C8-C10-C11-C12
41	C	303	KC2	C4C-C3C-CAC-CBC
41	E	319	KC2	C4B-C3B-CAB-CBB
41	F	302	KC2	C4C-C3C-CAC-CBC
41	G	208	KC2	C4B-C3B-CAB-CBB
41	I	209	KC2	C4B-C3B-CAB-CBB
41	L	309	KC2	C4B-C3B-CAB-CBB
41	L	309	KC2	C4C-C3C-CAC-CBC
41	N	301	KC2	C4B-C3B-CAB-CBB
41	N	308	KC2	C4B-C3B-CAB-CBB
41	N	313	KC2	C4B-C3B-CAB-CBB
41	N	313	KC2	C4C-C3C-CAC-CBC
41	O	302	KC2	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
41	O	308	KC2	C4B-C3B-CAB-CBB
41	O	309	KC2	C4B-C3B-CAB-CBB
41	O	311	KC2	C4B-C3B-CAB-CBB
41	O	311	KC2	C4C-C3C-CAC-CBC
41	P	310	KC2	C4C-C3C-CAC-CBC
41	Q	216	KC2	C4C-C3C-CAC-CBC
41	R	301	KC2	C4C-C3C-CAC-CBC
41	R	311	KC2	C4C-C3C-CAC-CBC
41	S	304	KC2	C4B-C3B-CAB-CBB
41	T	302	KC2	C4C-C3C-CAC-CBC
41	T	309	KC2	C4C-C3C-CAC-CBC
41	T	311	KC2	C4C-C3C-CAC-CBC
41	U	201	KC2	C4C-C3C-CAC-CBC
41	W	302	KC2	C4B-C3B-CAB-CBB
41	W	310	KC2	C4B-C3B-CAB-CBB
41	W	310	KC2	C4C-C3C-CAC-CBC
41	X	302	KC2	C4C-C3C-CAC-CBC
41	Y	309	KC2	C4C-C3C-CAC-CBC
41	Y	314	KC2	C4C-C3C-CAC-CBC
41	Z	302	KC2	C4C-C3C-CAC-CBC
41	Z	309	KC2	C4C-C3C-CAC-CBC
41	o	308	KC2	C4B-C3B-CAB-CBB
41	p	310	KC2	C4B-C3B-CAB-CBB
41	q	308	KC2	C4B-C3B-CAB-CBB
41	q	308	KC2	C4C-C3C-CAC-CBC
41	q	309	KC2	C4B-C3B-CAB-CBB
41	u	310	KC2	C4B-C3B-CAB-CBB
41	v	302	KC2	C4C-C3C-CAC-CBC
41	v	303	KC2	C4B-C3B-CAB-CBB
41	v	308	KC2	C4B-C3B-CAB-CBB
41	v	308	KC2	C4C-C3C-CAC-CBC
41	v	309	KC2	C4B-C3B-CAB-CBB
41	v	309	KC2	C4C-C3C-CAC-CBC
41	x	310	KC2	C4B-C3B-CAB-CBB
41	y	307	KC2	C4C-C3C-CAC-CBC
40	F	307	CLA	C11-C12-C13-C15
40	W	313	CLA	C5-C6-C7-C8
40	W	313	CLA	C4-C3-C5-C6
40	b	831	CLA	C2A-CAA-CBA-CGA
40	A	302	CLA	C2-C3-C5-C6
40	R	305	CLA	C2-C3-C5-C6
40	a	806	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
40	b	824	CLA	C2-C3-C5-C6
44	S	315	A86	C28-C27-C29-C30
44	u	319	A86	C28-C27-C29-C30
40	S	302	CLA	C8-C10-C11-C12
40	x	308	CLA	C10-C11-C12-C13
44	X	315	A86	C33-C34-O4-C38
40	S	314	CLA	C3-C5-C6-C7
40	b	817	CLA	C3-C5-C6-C7
40	a	813	CLA	CBD-CGD-O2D-CED
43	E	301	LMG	O1-C7-C8-O7
43	E	320	LMG	O1-C7-C8-O7
43	P	318	LMG	O7-C8-C9-O8
43	T	318	LMG	O1-C7-C8-O7
43	a	801	LMG	O7-C8-C9-O8
46	P	319	SQD	O6-C44-C45-O47
40	a	828	CLA	C11-C12-C13-C14
40	b	808	CLA	C11-C10-C8-C9
40	b	821	CLA	C14-C13-C15-C16
40	Y	307	CLA	O1A-CGA-O2A-C1
43	P	318	LMG	C15-C16-C17-C18
47	w	314	A1EB1	C45-C46-C47-C48
43	A	317	LMG	C29-C30-C31-C32
40	a	810	CLA	C10-C11-C12-C13
40	v	311	CLA	C8-C10-C11-C12
44	C	311	A86	C13-C14-C15-O1
44	F	313	A86	C13-C14-C15-O1
44	F	317	A86	C13-C14-C15-O1
44	M	313	A86	C13-C14-C15-O1
44	Q	210	A86	C13-C14-C15-O1
44	R	312	A86	C13-C14-C15-O1
44	S	317	A86	C13-C14-C15-O1
44	T	312	A86	C13-C14-C15-O1
44	T	315	A86	C13-C14-C15-O1
44	X	315	A86	C13-C14-C15-O1
44	X	318	A86	C13-C14-C15-O1
44	Y	316	A86	C13-C14-C15-O1
44	Y	317	A86	C13-C14-C15-O1
44	Y	318	A86	C13-C14-C15-O1
44	Y	320	A86	C13-C14-C15-O1
44	p	316	A86	C13-C14-C15-O1
44	p	318	A86	C13-C14-C15-O1
44	p	319	A86	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
44	p	320	A86	C13-C14-C15-O1
44	q	316	A86	C13-C14-C15-O1
44	t	311	A86	C13-C14-C15-O1
44	u	316	A86	C13-C14-C15-O1
44	u	319	A86	C13-C14-C15-O1
44	u	320	A86	C13-C14-C15-O1
44	v	316	A86	C13-C14-C15-O1
44	v	319	A86	C13-C14-C15-O1
44	w	310	A86	C13-C14-C15-O1
44	w	311	A86	C13-C14-C15-O1
44	w	316	A86	C13-C14-C15-O1
44	x	318	A86	C13-C14-C15-O1
44	x	319	A86	C13-C14-C15-O1
44	y	310	A86	C13-C14-C15-O1
44	z	317	A86	C13-C14-C15-O1
47	F	322	A1EB1	C13-C14-C15-O1
47	Z	319	A1EB1	C13-C14-C15-O1
47	o	322	A1EB1	C13-C14-C15-O1
47	p	323	A1EB1	C13-C14-C15-O1
47	t	314	A1EB1	C13-C14-C15-O1
47	u	322	A1EB1	C13-C14-C15-O1
47	v	323	A1EB1	C13-C14-C15-O1
47	v	324	A1EB1	C13-C14-C15-O1
47	w	314	A1EB1	C13-C14-C15-O1
47	y	314	A1EB1	C13-C14-C15-O1
40	a	833	CLA	C8-C10-C11-C12
50	a	847	PQN	C13-C15-C16-C17
44	D	319	A86	C9-C10-C11-C13
44	G	211	A86	C9-C10-C11-C13
44	N	315	A86	C9-C10-C11-C13
44	S	316	A86	C9-C10-C11-C13
44	X	318	A86	C9-C10-C11-C13
44	Z	315	A86	C9-C10-C11-C13
44	o	315	A86	C9-C10-C11-C13
44	p	318	A86	C9-C10-C11-C13
44	q	319	A86	C9-C10-C11-C13
44	t	310	A86	C9-C10-C11-C13
44	u	318	A86	C9-C10-C11-C13
40	Z	312	CLA	CBA-CGA-O2A-C1
40	Z	310	CLA	C6-C7-C8-C10
40	N	311	CLA	C10-C11-C12-C13
47	G	212	A1EB1	C29-C27-C28-O6

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Mol	Chain	Res	Type	Atoms
47	L	318	A1EB1	C29-C27-C28-O6
47	O	317	A1EB1	C29-C27-C28-O6
47	Z	321	A1EB1	C29-C27-C28-O6
47	p	324	A1EB1	C29-C27-C28-O6
47	t	314	A1EB1	C29-C27-C28-O6
47	v	323	A1EB1	C29-C27-C28-O6
40	S	305	CLA	C4-C3-C5-C6
40	F	301	CLA	C3-C5-C6-C7
45	a	849	LHG	C1-C2-C3-O3
40	W	312	CLA	C4C-C3C-CAC-CBC
40	a	807	CLA	C4C-C3C-CAC-CBC
40	D	303	CLA	C11-C12-C13-C14
40	Q	206	CLA	O1A-CGA-O2A-C1
40	a	822	CLA	O1A-CGA-O2A-C1
40	b	811	CLA	O1A-CGA-O2A-C1
43	a	802	LMG	C13-C14-C15-C16
40	z	302	CLA	C3-C5-C6-C7
40	a	807	CLA	C11-C10-C8-C9
40	b	835	CLA	C4B-C3B-CAB-CBB
40	E	306	CLA	C6-C7-C8-C9
42	E	315	DD6	C27-C29-C30-C31
42	E	317	DD6	C27-C29-C30-C31
42	M	314	DD6	C27-C29-C30-C31
40	a	841	CLA	C5-C6-C7-C8
44	z	317	A86	C7-C6-C8-C9
40	E	312	CLA	C4C-C3C-CAC-CBC
40	U	208	CLA	C2C-C3C-CAC-CBC
40	B	303	CLA	C4B-C3B-CAB-CBB
40	B	306	CLA	C4B-C3B-CAB-CBB
40	C	305	CLA	C4B-C3B-CAB-CBB
40	C	306	CLA	C4B-C3B-CAB-CBB
40	E	302	CLA	C4B-C3B-CAB-CBB
40	E	303	CLA	C4B-C3B-CAB-CBB
40	E	311	CLA	C4B-C3B-CAB-CBB
40	F	308	CLA	C1A-C2A-CAA-CBA
40	F	310	CLA	C4B-C3B-CAB-CBB
40	G	207	CLA	C4B-C3B-CAB-CBB
40	H	311	CLA	C4B-C3B-CAB-CBB
40	I	201	CLA	C4B-C3B-CAB-CBB
40	J	302	CLA	C4B-C3B-CAB-CBB
40	J	309	CLA	C4B-C3B-CAB-CBB
40	L	310	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
40	O	307	CLA	C4B-C3B-CAB-CBB
40	P	305	CLA	C4B-C3B-CAB-CBB
40	P	312	CLA	C4B-C3B-CAB-CBB
40	Q	203	CLA	C4B-C3B-CAB-CBB
40	W	306	CLA	C4B-C3B-CAB-CBB
40	X	311	CLA	C4B-C3B-CAB-CBB
40	Y	307	CLA	C4B-C3B-CAB-CBB
40	Y	310	CLA	C4B-C3B-CAB-CBB
40	Y	313	CLA	C1A-C2A-CAA-CBA
40	Z	311	CLA	C4B-C3B-CAB-CBB
40	Z	312	CLA	C4B-C3B-CAB-CBB
40	Z	313	CLA	C4B-C3B-CAB-CBB
40	a	820	CLA	C4B-C3B-CAB-CBB
40	a	827	CLA	C1A-C2A-CAA-CBA
40	a	828	CLA	C1A-C2A-CAA-CBA
40	a	829	CLA	C4B-C3B-CAB-CBB
40	a	833	CLA	C4B-C3B-CAB-CBB
40	a	838	CLA	C4B-C3B-CAB-CBB
40	a	851	CLA	C4B-C3B-CAB-CBB
40	b	813	CLA	C4B-C3B-CAB-CBB
40	b	833	CLA	C1A-C2A-CAA-CBA
40	b	841	CLA	C4B-C3B-CAB-CBB
40	f	204	CLA	C4B-C3B-CAB-CBB
40	i	101	CLA	C4B-C3B-CAB-CBB
40	k	201	CLA	C4B-C3B-CAB-CBB
40	k	202	CLA	C4B-C3B-CAB-CBB
40	o	307	CLA	C1A-C2A-CAA-CBA
40	p	311	CLA	C4B-C3B-CAB-CBB
40	t	307	CLA	C4B-C3B-CAB-CBB
40	u	307	CLA	C1A-C2A-CAA-CBA
40	v	307	CLA	C1A-C2A-CAA-CBA
40	v	311	CLA	C1A-C2A-CAA-CBA
40	w	308	CLA	C1A-C2A-CAA-CBA
40	w	309	CLA	C4B-C3B-CAB-CBB
40	x	302	CLA	C4B-C3B-CAB-CBB
40	y	309	CLA	C4B-C3B-CAB-CBB
40	z	302	CLA	C1A-C2A-CAA-CBA
40	z	308	CLA	C1A-C2A-CAA-CBA
40	z	308	CLA	C4B-C3B-CAB-CBB
40	z	311	CLA	C4B-C3B-CAB-CBB
40	z	312	CLA	C4B-C3B-CAB-CBB
44	F	317	A86	O-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
44	N	315	A86	O-C13-C14-C15
44	Y	321	A86	O-C13-C14-C15
44	Z	315	A86	O-C13-C14-C15
44	Z	316	A86	O-C13-C14-C15
44	o	314	A86	O-C13-C14-C15
44	p	319	A86	O-C13-C14-C15
44	u	319	A86	O-C13-C14-C15
44	x	319	A86	O-C13-C14-C15
44	z	319	A86	O-C13-C14-C15
47	G	212	A1EB1	O-C13-C14-C15
47	G	212	A1EB1	C26-C27-C28-O6
47	K	315	A1EB1	C26-C27-C28-O6
47	L	318	A1EB1	O-C13-C14-C15
47	L	318	A1EB1	C26-C27-C28-O6
47	O	317	A1EB1	C26-C27-C28-O6
47	P	301	A1EB1	C26-C27-C28-O6
47	R	317	A1EB1	O-C13-C14-C15
47	T	320	A1EB1	O-C13-C14-C15
47	Z	321	A1EB1	C26-C27-C28-O6
47	p	324	A1EB1	C26-C27-C28-O6
47	q	323	A1EB1	O-C13-C14-C15
47	q	323	A1EB1	C26-C27-C28-O6
47	t	313	A1EB1	O-C13-C14-C15
47	t	314	A1EB1	C26-C27-C28-O6
47	t	315	A1EB1	C26-C27-C28-O6
47	v	323	A1EB1	C26-C27-C28-O6
47	v	324	A1EB1	O-C13-C14-C15
47	w	313	A1EB1	C26-C27-C28-O6
47	y	312	A1EB1	O-C13-C14-C15
47	y	312	A1EB1	C26-C27-C28-O6
40	K	307	CLA	O1D-CGD-O2D-CED
40	B	306	CLA	CBA-CGA-O2A-C1
40	a	821	CLA	CBA-CGA-O2A-C1
40	a	852	CLA	C4-C3-C5-C6
40	b	810	CLA	C4-C3-C5-C6
40	b	812	CLA	CAA-CBA-CGA-O2A
40	P	305	CLA	C2-C3-C5-C6
42	N	317	DD6	C2-C1-C24-C25
44	K	314	A86	C5-C6-C8-C9
44	X	317	A86	C2-C1-C24-C25
44	Y	317	A86	C5-C6-C8-C9
40	o	310	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
40	T	317	CLA	C2A-CAA-CBA-CGA
40	l	203	CLA	O1D-CGD-O2D-CED
44	D	319	A86	C9-C10-C11-C12
44	F	312	A86	C9-C10-C11-C12
44	F	313	A86	C9-C10-C11-C12
44	Q	210	A86	C9-C10-C11-C12
44	o	316	A86	C9-C10-C11-C12
44	u	318	A86	C9-C10-C11-C12
47	p	323	A1EB1	C9-C10-C11-C12
47	t	314	A1EB1	C9-C10-C11-C12
47	u	322	A1EB1	C9-C10-C11-C12
43	E	321	LMG	C14-C15-C16-C17
40	o	304	CLA	C10-C11-C12-C13
40	A	303	CLA	C6-C7-C8-C10
40	D	309	CLA	C6-C7-C8-C10
40	E	307	CLA	C11-C10-C8-C7
40	E	310	CLA	C6-C7-C8-C10
40	I	206	CLA	C11-C10-C8-C7
40	P	308	CLA	C6-C7-C8-C10
40	a	842	CLA	C6-C7-C8-C10
40	a	851	CLA	C11-C12-C13-C15
40	b	814	CLA	C6-C7-C8-C10
40	b	818	CLA	C11-C12-C13-C15
40	b	822	CLA	C11-C12-C13-C15
40	q	311	CLA	C6-C7-C8-C10
40	v	312	CLA	C6-C7-C8-C10
40	p	305	CLA	C4C-C3C-CAC-CBC
47	t	313	A1EB1	C44-C45-C46-C47
40	F	307	CLA	C11-C12-C13-C14
40	A	301	CLA	C2C-C3C-CAC-CBC
40	R	305	CLA	O1A-CGA-O2A-C1
40	v	307	CLA	O1A-CGA-O2A-C1
41	S	310	KC2	CAA-CBA-CGA-O2A
40	B	302	CLA	C3A-C2A-CAA-CBA
40	R	305	CLA	C4-C3-C5-C6
40	X	312	CLA	C3A-C2A-CAA-CBA
40	w	303	CLA	C3A-C2A-CAA-CBA
40	x	307	CLA	C3A-C2A-CAA-CBA
40	z	314	CLA	C3A-C2A-CAA-CBA
46	I	215	SQD	C34-C35-C36-C37
40	b	818	CLA	C4C-C3C-CAC-CBC
47	T	320	A1EB1	C27-C28-O6-C42

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Mol	Chain	Res	Type	Atoms
40	S	302	CLA	C2A-CAA-CBA-CGA
40	C	306	CLA	C11-C10-C8-C9
40	E	308	CLA	C11-C10-C8-C9
40	F	306	CLA	C6-C7-C8-C9
40	T	310	CLA	C6-C7-C8-C9
40	a	813	CLA	C6-C7-C8-C9
40	b	818	CLA	C11-C10-C8-C9
40	x	308	CLA	C8-C10-C11-C12
40	K	301	CLA	O1D-CGD-O2D-CED
40	z	308	CLA	C10-C11-C12-C13
41	C	303	KC2	C1A-C2A-CAA-CBA
41	E	319	KC2	C3A-C2A-CAA-CBA
41	F	309	KC2	C3A-C2A-CAA-CBA
41	G	202	KC2	C1A-C2A-CAA-CBA
41	G	208	KC2	C1A-C2A-CAA-CBA
41	I	209	KC2	C3A-C2A-CAA-CBA
41	I	214	KC2	C1A-C2A-CAA-CBA
41	J	304	KC2	C3A-C2A-CAA-CBA
41	K	305	KC2	C1A-C2A-CAA-CBA
41	K	309	KC2	C3A-C2A-CAA-CBA
41	L	302	KC2	C3A-C2A-CAA-CBA
41	L	308	KC2	C3A-C2A-CAA-CBA
41	L	309	KC2	C1A-C2A-CAA-CBA
41	M	301	KC2	C3A-C2A-CAA-CBA
41	M	309	KC2	C3A-C2A-CAA-CBA
41	N	302	KC2	C1A-C2A-CAA-CBA
41	N	312	KC2	C1A-C2A-CAA-CBA
41	O	308	KC2	C1A-C2A-CAA-CBA
41	Q	216	KC2	C1A-C2A-CAA-CBA
41	R	302	KC2	C3A-C2A-CAA-CBA
41	R	303	KC2	C3A-C2A-CAA-CBA
41	R	308	KC2	C1A-C2A-CAA-CBA
41	S	309	KC2	C3A-C2A-CAA-CBA
41	W	302	KC2	C1A-C2A-CAA-CBA
41	W	310	KC2	C3A-C2A-CAA-CBA
41	X	309	KC2	C3A-C2A-CAA-CBA
41	Y	302	KC2	C1A-C2A-CAA-CBA
41	Z	302	KC2	C1A-C2A-CAA-CBA
41	o	302	KC2	C1A-C2A-CAA-CBA
41	o	308	KC2	C3A-C2A-CAA-CBA
41	o	309	KC2	C3A-C2A-CAA-CBA
41	p	303	KC2	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
41	p	304	KC2	C3A-C2A-CAA-CBA
41	q	302	KC2	C3A-C2A-CAA-CBA
41	u	303	KC2	C1A-C2A-CAA-CBA
41	u	304	KC2	C3A-C2A-CAA-CBA
41	v	302	KC2	C3A-C2A-CAA-CBA
41	w	301	KC2	C3A-C2A-CAA-CBA
41	x	303	KC2	C1A-C2A-CAA-CBA
41	z	303	KC2	C1A-C2A-CAA-CBA
44	N	321	A86	C26-C27-C29-C30
44	S	315	A86	C26-C27-C29-C30
44	X	317	A86	C26-C27-C29-C30
44	p	319	A86	C26-C27-C29-C30
44	p	320	A86	C26-C27-C29-C30
44	t	310	A86	C26-C27-C29-C30
44	u	318	A86	C26-C27-C29-C30
44	v	319	A86	C26-C27-C29-C30
44	w	310	A86	C26-C27-C29-C30
44	x	319	A86	C26-C27-C29-C30
44	y	310	A86	C26-C27-C29-C30
43	L	319	LMG	O1-C7-C8-O7
43	M	317	LMG	O7-C8-C9-O8
43	S	322	LMG	O1-C7-C8-O7
43	T	318	LMG	O7-C8-C9-O8
43	a	802	LMG	O7-C8-C9-O8
43	j	101	LMG	O7-C8-C9-O8
43	x	301	LMG	C12-C13-C14-C15
40	a	832	CLA	C5-C6-C7-C8
40	b	805	CLA	C10-C11-C12-C13
40	u	308	CLA	C10-C11-C12-C13
43	A	317	LMG	O1-C7-C8-C9
43	S	322	LMG	O1-C7-C8-C9
45	F	319	LHG	C4-C5-C6-O8
46	P	319	SQD	O6-C44-C45-C46
46	W	318	SQD	O6-C44-C45-C46
40	b	824	CLA	CAA-CBA-CGA-O2A
40	E	302	CLA	CAD-CBD-CGD-O2D
40	F	321	CLA	CAD-CBD-CGD-O2D
40	K	312	CLA	CAD-CBD-CGD-O2D
40	M	312	CLA	CAD-CBD-CGD-O2D
40	N	307	CLA	CAD-CBD-CGD-O2D
40	P	313	CLA	CAD-CBD-CGD-O2D
40	R	307	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
40	S	312	CLA	CAD-CBD-CGD-O2D
40	S	314	CLA	CAD-CBD-CGD-O2D
40	U	205	CLA	CAD-CBD-CGD-O2D
40	W	313	CLA	CAD-CBD-CGD-O2D
40	Z	313	CLA	CAD-CBD-CGD-O2D
40	a	806	CLA	CAD-CBD-CGD-O2D
40	a	815	CLA	CAD-CBD-CGD-O2D
40	a	832	CLA	CAD-CBD-CGD-O2D
40	a	836	CLA	CAD-CBD-CGD-O2D
40	a	839	CLA	CAD-CBD-CGD-O2D
40	b	818	CLA	CAD-CBD-CGD-O2D
40	b	819	CLA	CAD-CBD-CGD-O2D
40	b	839	CLA	CAD-CBD-CGD-O2D
40	b	840	CLA	CAD-CBD-CGD-O2D
40	l	205	CLA	CAD-CBD-CGD-O2D
40	p	312	CLA	CAD-CBD-CGD-O2D
40	q	310	CLA	CAD-CBD-CGD-O2D
40	t	304	CLA	CAD-CBD-CGD-O2D
40	u	307	CLA	CAD-CBD-CGD-O2D
40	u	312	CLA	CAD-CBD-CGD-O2D
40	v	310	CLA	CAD-CBD-CGD-O2D
40	v	313	CLA	CAD-CBD-CGD-O2D
40	w	304	CLA	CAD-CBD-CGD-O2D
40	x	307	CLA	CAD-CBD-CGD-O2D
40	x	314	CLA	CAD-CBD-CGD-O2D
40	y	304	CLA	CAD-CBD-CGD-O2D
41	J	304	KC2	CAD-CBD-CGD-O2D
41	T	311	KC2	CAD-CBD-CGD-O2D
41	Z	302	KC2	CAD-CBD-CGD-O2D
41	t	306	KC2	CAD-CBD-CGD-O2D
41	w	306	KC2	CAD-CBD-CGD-O2D
41	y	306	KC2	CAD-CBD-CGD-O2D
41	z	310	KC2	CAD-CBD-CGD-O2D
44	F	313	A86	C13-C14-C15-C20
44	G	209	A86	C13-C14-C15-C20
44	H	315	A86	C13-C14-C15-C20
44	P	321	A86	C13-C14-C15-C20
44	S	315	A86	C13-C14-C15-C20
44	Y	320	A86	C13-C14-C15-C20
44	Z	316	A86	C13-C14-C15-C20
44	o	316	A86	C13-C14-C15-C20
47	q	322	A1EB1	C13-C14-C15-C20

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Mol	Chain	Res	Type	Atoms
47	v	322	A1EB1	C13-C14-C15-C20
48	M	319	A1EB4	C13-C11-C12-O3
40	i	101	CLA	O1A-CGA-O2A-C1
40	l	204	CLA	C15-C16-C17-C18
41	J	304	KC2	CAA-CBA-CGA-O1A
41	S	310	KC2	CAA-CBA-CGA-O1A
40	t	307	CLA	O1D-CGD-O2D-CED
40	K	301	CLA	C2C-C3C-CAC-CBC
40	A	304	CLA	C3-C5-C6-C7
40	U	206	CLA	C2A-CAA-CBA-CGA
40	F	307	CLA	C10-C11-C12-C13
40	q	310	CLA	O1A-CGA-O2A-C1
40	y	309	CLA	O1A-CGA-O2A-C1
40	B	306	CLA	CHA-CBD-CGD-O1D
40	C	306	CLA	CHA-CBD-CGD-O1D
40	D	309	CLA	CAD-CBD-CGD-O1D
40	E	302	CLA	CAD-CBD-CGD-O1D
40	F	311	CLA	CAD-CBD-CGD-O1D
40	F	321	CLA	CAD-CBD-CGD-O1D
40	G	213	CLA	CHA-CBD-CGD-O1D
40	H	302	CLA	CHA-CBD-CGD-O2D
40	H	305	CLA	CHA-CBD-CGD-O1D
40	H	305	CLA	CHA-CBD-CGD-O2D
40	I	203	CLA	CHA-CBD-CGD-O1D
40	K	312	CLA	CAD-CBD-CGD-O1D
40	L	311	CLA	CAD-CBD-CGD-O1D
40	M	312	CLA	CAD-CBD-CGD-O1D
40	N	307	CLA	CAD-CBD-CGD-O1D
40	O	307	CLA	CAD-CBD-CGD-O1D
40	P	313	CLA	CAD-CBD-CGD-O1D
40	R	307	CLA	CAD-CBD-CGD-O1D
40	S	312	CLA	CAD-CBD-CGD-O1D
40	S	314	CLA	CAD-CBD-CGD-O1D
40	U	205	CLA	CAD-CBD-CGD-O1D
40	U	208	CLA	CHA-CBD-CGD-O1D
40	W	313	CLA	CAD-CBD-CGD-O1D
40	X	306	CLA	CHA-CBD-CGD-O1D
40	X	306	CLA	CHA-CBD-CGD-O2D
40	Z	313	CLA	CAD-CBD-CGD-O1D
40	a	805	CLA	CHA-CBD-CGD-O1D
40	a	805	CLA	CHA-CBD-CGD-O2D
40	a	806	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
40	a	809	CLA	CHA-CBD-CGD-O1D
40	a	809	CLA	CHA-CBD-CGD-O2D
40	a	815	CLA	CAD-CBD-CGD-O1D
40	a	832	CLA	CAD-CBD-CGD-O1D
40	a	833	CLA	CHA-CBD-CGD-O1D
40	a	836	CLA	CAD-CBD-CGD-O1D
40	a	839	CLA	CAD-CBD-CGD-O1D
40	b	818	CLA	CAD-CBD-CGD-O1D
40	b	819	CLA	CAD-CBD-CGD-O1D
40	b	826	CLA	CHA-CBD-CGD-O1D
40	b	839	CLA	CAD-CBD-CGD-O1D
40	b	840	CLA	CAD-CBD-CGD-O1D
40	l	204	CLA	CHA-CBD-CGD-O1D
40	l	205	CLA	CAD-CBD-CGD-O1D
40	o	313	CLA	CAD-CBD-CGD-O1D
40	q	306	CLA	CHA-CBD-CGD-O1D
40	q	306	CLA	CHA-CBD-CGD-O2D
40	q	310	CLA	CAD-CBD-CGD-O1D
40	t	304	CLA	CAD-CBD-CGD-O1D
40	t	307	CLA	CHA-CBD-CGD-O1D
40	t	307	CLA	CHA-CBD-CGD-O2D
40	u	307	CLA	CAD-CBD-CGD-O1D
40	u	312	CLA	CAD-CBD-CGD-O1D
40	v	306	CLA	CHA-CBD-CGD-O1D
40	v	306	CLA	CHA-CBD-CGD-O2D
40	v	310	CLA	CAD-CBD-CGD-O1D
40	v	313	CLA	CAD-CBD-CGD-O1D
40	w	304	CLA	CAD-CBD-CGD-O1D
40	w	309	CLA	CHA-CBD-CGD-O1D
40	w	309	CLA	CHA-CBD-CGD-O2D
40	x	307	CLA	CAD-CBD-CGD-O1D
40	x	314	CLA	CAD-CBD-CGD-O1D
40	y	304	CLA	CAD-CBD-CGD-O1D
40	y	309	CLA	CHA-CBD-CGD-O1D
41	J	304	KC2	CAD-CBD-CGD-O1D
41	O	309	KC2	CHA-CBD-CGD-O1D
41	Q	201	KC2	CHA-CBD-CGD-O1D
41	Q	201	KC2	CHA-CBD-CGD-O2D
41	R	303	KC2	CHA-CBD-CGD-O1D
41	T	311	KC2	CAD-CBD-CGD-O1D
41	Y	314	KC2	CHA-CBD-CGD-O1D
41	Y	314	KC2	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
41	Z	302	KC2	CAD-CBD-CGD-O1D
41	Z	303	KC2	CHA-CBD-CGD-O1D
41	Z	303	KC2	CHA-CBD-CGD-O2D
41	o	309	KC2	CHA-CBD-CGD-O1D
41	p	304	KC2	CHA-CBD-CGD-O1D
41	t	301	KC2	CHA-CBD-CGD-O1D
41	t	306	KC2	CAD-CBD-CGD-O1D
41	u	315	KC2	CHA-CBD-CGD-O1D
41	u	315	KC2	CHA-CBD-CGD-O2D
41	v	303	KC2	CHA-CBD-CGD-O1D
41	w	301	KC2	CHA-CBD-CGD-O1D
41	w	301	KC2	CHA-CBD-CGD-O2D
41	w	306	KC2	CAD-CBD-CGD-O1D
41	x	304	KC2	CHA-CBD-CGD-O1D
41	y	301	KC2	CHA-CBD-CGD-O1D
41	y	301	KC2	CHA-CBD-CGD-O2D
41	y	306	KC2	CAD-CBD-CGD-O1D
41	z	310	KC2	CAD-CBD-CGD-O1D
44	F	317	A86	C10-C11-C13-C14
44	G	209	A86	C10-C11-C13-C14
44	M	320	A86	C10-C11-C13-C14
44	O	312	A86	C10-C11-C13-C14
44	O	313	A86	C10-C11-C13-C14
44	S	316	A86	C10-C11-C13-C14
44	T	315	A86	C10-C11-C13-C14
44	Y	320	A86	C10-C11-C13-C14
44	Z	315	A86	C10-C11-C13-C14
44	q	324	A86	C10-C11-C13-C14
44	t	311	A86	C10-C11-C13-C14
44	u	319	A86	C10-C11-C13-C14
44	u	320	A86	C10-C11-C13-C14
44	v	325	A86	C10-C11-C13-C14
44	w	311	A86	C10-C11-C13-C14
44	w	316	A86	C10-C11-C13-C14
44	x	318	A86	C10-C11-C13-C14
44	x	319	A86	C10-C11-C13-C14
44	z	301	A86	C10-C11-C13-C14
44	z	315	A86	C10-C11-C13-C14
45	F	319	LHG	C4-O6-P-O3
45	F	319	LHG	C4-O6-P-O4
45	S	323	LHG	C4-O6-P-O5
45	a	848	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
45	a	849	LHG	C3-O3-P-O4
47	F	322	A1EB1	C10-C11-C13-C14
47	G	212	A1EB1	C10-C11-C13-C14
47	P	301	A1EB1	C10-C11-C13-C14
47	Z	321	A1EB1	C10-C11-C13-C14
47	t	313	A1EB1	C10-C11-C13-C14
47	t	314	A1EB1	C10-C11-C13-C14
40	p	302	CLA	C3-C5-C6-C7
40	N	305	CLA	C6-C7-C8-C10
40	Q	205	CLA	O1A-CGA-O2A-C1
43	E	301	LMG	O10-C28-O8-C9
40	b	823	CLA	C5-C6-C7-C8
43	E	321	LMG	C17-C18-C19-C20
40	W	308	CLA	C4-C3-C5-C6
40	b	822	CLA	C4-C3-C5-C6
40	A	309	CLA	C2B-C3B-CAB-CBB
40	B	302	CLA	C2B-C3B-CAB-CBB
40	C	302	CLA	C2B-C3B-CAB-CBB
40	E	302	CLA	C2B-C3B-CAB-CBB
40	E	311	CLA	C2B-C3B-CAB-CBB
40	F	310	CLA	C2B-C3B-CAB-CBB
40	I	201	CLA	C2B-C3B-CAB-CBB
40	J	302	CLA	C2B-C3B-CAB-CBB
40	L	310	CLA	C2B-C3B-CAB-CBB
40	N	306	CLA	C2B-C3B-CAB-CBB
40	N	310	CLA	C2B-C3B-CAB-CBB
40	P	312	CLA	C2B-C3B-CAB-CBB
40	P	313	CLA	C2B-C3B-CAB-CBB
40	S	301	CLA	C2B-C3B-CAB-CBB
40	S	319	CLA	C2B-C3B-CAB-CBB
40	U	202	CLA	C2B-C3B-CAB-CBB
40	a	811	CLA	C2B-C3B-CAB-CBB
40	a	814	CLA	C2B-C3B-CAB-CBB
40	a	830	CLA	C2B-C3B-CAB-CBB
40	a	840	CLA	C2B-C3B-CAB-CBB
40	a	841	CLA	C2B-C3B-CAB-CBB
40	a	851	CLA	C2B-C3B-CAB-CBB
40	b	829	CLA	C2B-C3B-CAB-CBB
40	f	204	CLA	C2B-C3B-CAB-CBB
40	l	203	CLA	C2B-C3B-CAB-CBB
40	o	310	CLA	C2B-C3B-CAB-CBB
40	p	305	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
40	u	308	CLA	C2B-C3B-CAB-CBB
40	v	306	CLA	C2B-C3B-CAB-CBB
40	x	308	CLA	C2B-C3B-CAB-CBB
40	y	302	CLA	C2B-C3B-CAB-CBB
40	y	304	CLA	C2B-C3B-CAB-CBB
40	y	309	CLA	C2B-C3B-CAB-CBB
49	b	846	BCR	C23-C24-C25-C30
49	b	847	BCR	C1-C6-C7-C8
40	F	321	CLA	C2-C3-C5-C6
40	R	307	CLA	C2-C3-C5-C6
40	W	313	CLA	C2-C3-C5-C6
40	M	312	CLA	C8-C10-C11-C12
40	a	811	CLA	C10-C11-C12-C13
42	N	316	DD6	C12-C11-C13-C14
44	N	321	A86	C7-C6-C8-C9
47	Z	320	A1EB1	C7-C6-C8-C9
40	K	304	CLA	C8-C10-C11-C12
40	a	806	CLA	C16-C17-C18-C20
40	z	305	CLA	C11-C12-C13-C14
41	o	302	KC2	O1D-CGD-O2D-CED
44	C	311	A86	C12-C11-C13-C14
44	F	313	A86	C12-C11-C13-C14
44	G	211	A86	C12-C11-C13-C14
44	O	313	A86	C12-C11-C13-C14
44	P	316	A86	C12-C11-C13-C14
44	R	313	A86	C12-C11-C13-C14
44	S	316	A86	C12-C11-C13-C14
44	T	312	A86	C12-C11-C13-C14
44	W	316	A86	C12-C11-C13-C14
44	X	319	A86	C12-C11-C13-C14
44	X	320	A86	C12-C11-C13-C14
44	Z	315	A86	C12-C11-C13-C14
44	o	315	A86	C12-C11-C13-C14
44	p	318	A86	C12-C11-C13-C14
44	p	319	A86	C12-C11-C13-C14
44	p	321	A86	C12-C11-C13-C14
44	q	319	A86	C12-C11-C13-C14
44	q	324	A86	C12-C11-C13-C14
44	t	311	A86	C12-C11-C13-C14
44	u	320	A86	C12-C11-C13-C14
44	v	319	A86	C12-C11-C13-C14
44	v	325	A86	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
44	w	310	A86	C12-C11-C13-C14
44	x	318	A86	C12-C11-C13-C14
44	z	301	A86	C12-C11-C13-C14
44	z	315	A86	C12-C11-C13-C14
47	G	212	A1EB1	C12-C11-C13-C14
47	K	315	A1EB1	C12-C11-C13-C14
47	P	301	A1EB1	C12-C11-C13-C14
47	Z	321	A1EB1	C12-C11-C13-C14
47	w	313	A1EB1	C12-C11-C13-C14
47	y	313	A1EB1	C12-C11-C13-C14
40	Q	202	CLA	O1A-CGA-O2A-C1
47	v	322	A1EB1	C44-C45-C46-C47
44	o	314	A86	C33-C34-O4-C38
40	A	304	CLA	C8-C10-C11-C12
40	q	311	CLA	C13-C15-C16-C17
40	P	308	CLA	C3-C5-C6-C7
43	F	318	LMG	C9-C8-O7-C10
40	a	829	CLA	C8-C10-C11-C12
40	b	803	CLA	C15-C16-C17-C18
40	b	820	CLA	C8-C10-C11-C12
40	p	307	CLA	C5-C6-C7-C8
43	l	201	LMG	C32-C33-C34-C35
47	y	313	A1EB1	C25-C26-C27-C29
40	b	824	CLA	C16-C17-C18-C20
40	l	202	CLA	C16-C17-C18-C20
40	a	832	CLA	C10-C11-C12-C13
40	u	308	CLA	C8-C10-C11-C12
40	U	208	CLA	CBA-CGA-O2A-C1
40	b	819	CLA	CBA-CGA-O2A-C1
40	A	303	CLA	C11-C12-C13-C14
40	F	303	CLA	C6-C7-C8-C9
40	N	307	CLA	C6-C7-C8-C9
40	X	311	CLA	C11-C12-C13-C14
40	a	824	CLA	C11-C12-C13-C14
40	a	829	CLA	C14-C13-C15-C16
40	b	803	CLA	C11-C10-C8-C9
40	b	812	CLA	C11-C10-C8-C9
40	b	835	CLA	C14-C13-C15-C16
40	o	311	CLA	C11-C12-C13-C14
40	x	312	CLA	C6-C7-C8-C9
40	z	307	CLA	C6-C7-C8-C9
40	z	312	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
40	H	301	CLA	O1D-CGD-O2D-CED
41	A	310	KC2	CAA-CBA-CGA-O1A
40	M	312	CLA	C11-C10-C8-C7
40	b	817	CLA	C12-C13-C15-C16
40	l	205	CLA	C6-C7-C8-C10
40	z	308	CLA	C6-C7-C8-C10
40	b	838	CLA	C10-C11-C12-C13
40	a	840	CLA	C6-C7-C8-C9
40	b	824	CLA	C16-C17-C18-C19
40	o	306	CLA	C11-C12-C13-C14
40	Q	208	CLA	C10-C11-C12-C13
40	S	305	CLA	CBA-CGA-O2A-C1
47	K	315	A1EB1	O6-C42-C44-C45
41	T	303	KC2	CAA-CBA-CGA-O2A
52	b	850	DGD	C2E-C1E-O5D-C6D
40	V	202	CLA	C4-C3-C5-C6
40	o	307	CLA	O1A-CGA-O2A-C1
40	D	303	CLA	C2C-C3C-CAC-CBC
40	a	838	CLA	C6-C7-C8-C10
40	P	312	CLA	C8-C10-C11-C12
40	H	301	CLA	C2C-C3C-CAC-CBC
45	F	319	LHG	C27-C28-C29-C30
40	W	306	CLA	C10-C11-C12-C13
45	F	319	LHG	O7-C5-C6-O8
46	F	320	SQD	O47-C45-C46-O48
41	T	308	KC2	CAA-CBA-CGA-O1A
41	T	308	KC2	CAA-CBA-CGA-O2A
40	A	301	CLA	C4C-C3C-CAC-CBC
40	V	201	CLA	C10-C11-C12-C13
40	J	305	CLA	C6-C7-C8-C9
43	T	318	LMG	C31-C32-C33-C34
40	a	826	CLA	C2A-CAA-CBA-CGA
41	J	304	KC2	CAA-CBA-CGA-O2A
40	K	307	CLA	C2-C1-O2A-CGA
40	l	205	CLA	C4-C3-C5-C6
43	L	319	LMG	O1-C7-C8-C9
43	M	317	LMG	C7-C8-C9-O8
44	X	319	A86	C9-C10-C11-C12
46	I	215	SQD	O47-C7-C8-C9
40	P	305	CLA	C11-C12-C13-C15
40	Z	307	CLA	C11-C12-C13-C15
40	o	306	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
50	b	849	PQN	C21-C22-C23-C25
47	Z	320	A1EB1	C5-C6-C8-C9
49	l	207	BCR	C11-C12-C13-C14
40	q	305	CLA	C5-C6-C7-C8
40	q	307	CLA	O1A-CGA-O2A-C1
40	l	202	CLA	C8-C10-C11-C12
40	x	308	CLA	C5-C6-C7-C8
40	B	307	CLA	C2A-CAA-CBA-CGA
40	J	318	CLA	C2A-CAA-CBA-CGA
40	q	313	CLA	C2A-CAA-CBA-CGA
41	T	303	KC2	CAA-CBA-CGA-O1A
43	A	317	LMG	C11-C12-C13-C14
43	D	318	LMG	C12-C13-C14-C15
40	a	828	CLA	C10-C11-C12-C13
40	S	305	CLA	C2-C3-C5-C6
40	b	810	CLA	C2-C3-C5-C6
40	k	201	CLA	C2-C3-C5-C6
41	J	304	KC2	C2C-C3C-CAC-CBC
41	R	311	KC2	C2B-C3B-CAB-CBB
41	t	306	KC2	O1D-CGD-O2D-CED
40	U	203	CLA	CBA-CGA-O2A-C1
42	C	312	DD6	C27-C29-C30-C31
44	M	315	A86	C13-C14-C15-C16
44	O	312	A86	C13-C14-C15-C16
44	R	313	A86	C13-C14-C15-C16
44	T	319	A86	C13-C14-C15-C16
44	X	319	A86	C13-C14-C15-C16
44	Y	315	A86	C13-C14-C15-C16
44	Y	321	A86	C13-C14-C15-C16
44	o	314	A86	C13-C14-C15-C16
44	u	318	A86	C13-C14-C15-C16
44	w	316	A86	C13-C14-C15-C16
47	q	321	A1EB1	C13-C14-C15-C16
47	v	321	A1EB1	C13-C14-C15-C16
47	v	323	A1EB1	C13-C14-C15-C16
40	Z	305	CLA	C6-C7-C8-C9
40	A	309	CLA	C6-C7-C8-C9
40	D	307	CLA	C6-C7-C8-C9
40	N	304	CLA	C6-C7-C8-C9
40	O	306	CLA	C6-C7-C8-C9
40	X	311	CLA	C11-C10-C8-C9
40	a	804	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
40	b	806	CLA	C14-C13-C15-C16
40	E	311	CLA	CBA-CGA-O2A-C1
40	V	201	CLA	CBA-CGA-O2A-C1
40	E	309	CLA	C4B-C3B-CAB-CBB
40	R	310	CLA	C4B-C3B-CAB-CBB
40	T	310	CLA	C4B-C3B-CAB-CBB
40	U	204	CLA	C4B-C3B-CAB-CBB
40	b	811	CLA	C4B-C3B-CAB-CBB
40	j	102	CLA	C4B-C3B-CAB-CBB
40	l	204	CLA	C4B-C3B-CAB-CBB
40	u	311	CLA	C4B-C3B-CAB-CBB
40	x	307	CLA	C4B-C3B-CAB-CBB
40	x	313	CLA	C4B-C3B-CAB-CBB
40	z	305	CLA	C4B-C3B-CAB-CBB
40	z	314	CLA	C4B-C3B-CAB-CBB
40	E	302	CLA	C2C-C3C-CAC-CBC
40	D	310	CLA	C11-C12-C13-C15
40	q	312	CLA	C11-C12-C13-C14
40	p	311	CLA	CBA-CGA-O2A-C1
40	t	307	CLA	CBA-CGA-O2A-C1
40	u	311	CLA	CBA-CGA-O2A-C1
41	A	310	KC2	CAA-CBA-CGA-O2A
40	Y	306	CLA	C5-C6-C7-C8
40	b	835	CLA	C13-C15-C16-C17
40	G	213	CLA	C2A-CAA-CBA-CGA
40	A	309	CLA	C4-C3-C5-C6
40	b	832	CLA	C4-C3-C5-C6
40	b	838	CLA	C4-C3-C5-C6
40	o	305	CLA	C4-C3-C5-C6
40	D	304	CLA	C2-C3-C5-C6
40	V	202	CLA	C2-C3-C5-C6
40	W	308	CLA	C2-C3-C5-C6
40	l	205	CLA	C2-C3-C5-C6
41	C	303	KC2	C4B-C3B-CAB-CBB
41	E	319	KC2	C4C-C3C-CAC-CBC
41	H	303	KC2	C4B-C3B-CAB-CBB
41	H	303	KC2	C4C-C3C-CAC-CBC
41	J	304	KC2	C4B-C3B-CAB-CBB
41	K	302	KC2	C4B-C3B-CAB-CBB
41	K	303	KC2	C4C-C3C-CAC-CBC
41	K	305	KC2	C4C-C3C-CAC-CBC
41	L	302	KC2	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
41	L	313	KC2	C4C-C3C-CAC-CBC
41	M	302	KC2	C4C-C3C-CAC-CBC
41	M	303	KC2	C4B-C3B-CAB-CBB
41	N	309	KC2	C4C-C3C-CAC-CBC
41	N	312	KC2	C4C-C3C-CAC-CBC
41	O	302	KC2	C4C-C3C-CAC-CBC
41	P	302	KC2	C4B-C3B-CAB-CBB
41	P	304	KC2	C4B-C3B-CAB-CBB
41	P	309	KC2	C4C-C3C-CAC-CBC
41	P	310	KC2	C4B-C3B-CAB-CBB
41	R	302	KC2	C4C-C3C-CAC-CBC
41	R	303	KC2	C4B-C3B-CAB-CBB
41	T	308	KC2	C4B-C3B-CAB-CBB
41	W	309	KC2	C4B-C3B-CAB-CBB
41	X	308	KC2	C4B-C3B-CAB-CBB
41	X	309	KC2	C4C-C3C-CAC-CBC
41	Y	314	KC2	C4B-C3B-CAB-CBB
41	Z	303	KC2	C4B-C3B-CAB-CBB
41	Z	308	KC2	C4B-C3B-CAB-CBB
41	Z	309	KC2	C4B-C3B-CAB-CBB
41	o	302	KC2	C4C-C3C-CAC-CBC
41	o	308	KC2	C4C-C3C-CAC-CBC
41	o	309	KC2	C4C-C3C-CAC-CBC
41	p	310	KC2	C4C-C3C-CAC-CBC
41	q	302	KC2	C4C-C3C-CAC-CBC
41	t	306	KC2	C4C-C3C-CAC-CBC
41	u	309	KC2	C4C-C3C-CAC-CBC
41	u	310	KC2	C4C-C3C-CAC-CBC
41	w	306	KC2	C4B-C3B-CAB-CBB
41	x	310	KC2	C4C-C3C-CAC-CBC
41	y	301	KC2	C4C-C3C-CAC-CBC
41	y	306	KC2	C4C-C3C-CAC-CBC
41	z	309	KC2	C4C-C3C-CAC-CBC
41	z	310	KC2	C4C-C3C-CAC-CBC
47	L	318	A1EB1	C25-C26-C27-C28
40	W	305	CLA	C11-C10-C8-C7
40	b	839	CLA	C6-C7-C8-C10
52	b	850	DGD	O1A-C1A-O1G-C1G
48	W	319	A1EB4	C39-C43-C44-C45
43	L	319	LMG	C31-C32-C33-C34
40	Z	310	CLA	C6-C7-C8-C9
50	b	849	PQN	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
43	a	802	LMG	C15-C16-C17-C18
40	K	304	CLA	C5-C6-C7-C8
40	Y	301	CLA	O1A-CGA-O2A-C1
40	J	308	CLA	C3A-C2A-CAA-CBA
40	J	310	CLA	C3A-C2A-CAA-CBA
40	L	311	CLA	C3A-C2A-CAA-CBA
40	P	311	CLA	C3A-C2A-CAA-CBA
40	S	302	CLA	C4-C3-C5-C6
40	S	311	CLA	C3A-C2A-CAA-CBA
40	X	310	CLA	C3A-C2A-CAA-CBA
40	Z	306	CLA	C3A-C2A-CAA-CBA
40	Z	310	CLA	C3A-C2A-CAA-CBA
40	a	820	CLA	C3A-C2A-CAA-CBA
40	f	202	CLA	C3A-C2A-CAA-CBA
40	o	306	CLA	C3A-C2A-CAA-CBA
40	q	306	CLA	C3A-C2A-CAA-CBA
40	t	307	CLA	C3A-C2A-CAA-CBA
40	u	314	CLA	C3A-C2A-CAA-CBA
40	v	306	CLA	C3A-C2A-CAA-CBA
40	v	313	CLA	C3A-C2A-CAA-CBA
40	y	309	CLA	C3A-C2A-CAA-CBA
40	z	311	CLA	C3A-C2A-CAA-CBA
41	y	306	KC2	O1D-CGD-O2D-CED
43	T	318	LMG	C30-C31-C32-C33
43	x	301	LMG	C30-C31-C32-C33
40	O	306	CLA	CAA-CBA-CGA-O2A
40	b	822	CLA	C2-C3-C5-C6
40	I	204	CLA	C4C-C3C-CAC-CBC
40	a	851	CLA	C13-C15-C16-C17
49	b	844	BCR	C20-C21-C22-C37
49	f	206	BCR	C35-C13-C14-C15
49	l	207	BCR	C11-C10-C9-C34
40	E	314	CLA	C2C-C3C-CAC-CBC
40	J	305	CLA	C5-C6-C7-C8
43	A	317	LMG	C17-C18-C19-C20
40	J	302	CLA	CBD-CGD-O2D-CED
43	S	322	LMG	C35-C36-C37-C38
40	O	307	CLA	C2-C1-O2A-CGA
40	Q	203	CLA	C2-C1-O2A-CGA
40	a	821	CLA	C2-C1-O2A-CGA
40	a	839	CLA	C2-C1-O2A-CGA
40	E	306	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
42	v	320	DD6	C-C1-C24-C25
44	o	314	A86	C7-C6-C8-C9
45	a	848	LHG	C18-C19-C20-C21
40	R	304	CLA	C4-C3-C5-C6
40	a	828	CLA	C13-C15-C16-C17
46	I	215	SQD	C25-C26-C27-C28
40	b	828	CLA	C5-C6-C7-C8
42	D	317	DD6	C5-C6-C8-C9
42	Y	322	DD6	C2-C1-C24-C25
40	P	312	CLA	C4-C3-C5-C6
40	k	201	CLA	C4-C3-C5-C6
40	a	852	CLA	C2-C3-C5-C6
40	U	204	CLA	C2-C1-O2A-CGA
40	H	301	CLA	C4C-C3C-CAC-CBC
40	b	817	CLA	C13-C15-C16-C17
44	L	314	A86	C12-C11-C13-O
44	M	320	A86	C12-C11-C13-O
44	O	313	A86	C12-C11-C13-O
44	Q	215	A86	C12-C11-C13-O
44	R	313	A86	C12-C11-C13-O
44	X	316	A86	C12-C11-C13-O
44	Y	315	A86	C12-C11-C13-O
44	Z	315	A86	C12-C11-C13-O
44	p	319	A86	C12-C11-C13-O
44	u	316	A86	C12-C11-C13-O
44	v	319	A86	C12-C11-C13-O
44	w	315	A86	C12-C11-C13-O
47	p	324	A1EB1	C12-C11-C13-O
47	w	313	A1EB1	C12-C11-C13-O
41	X	309	KC2	CAA-CBA-CGA-O1A
40	Z	307	CLA	C5-C6-C7-C8
40	b	832	CLA	C8-C10-C11-C12
40	o	305	CLA	C5-C6-C7-C8
40	B	306	CLA	O1A-CGA-O2A-C1
40	S	301	CLA	O1A-CGA-O2A-C1
40	A	304	CLA	C11-C12-C13-C14
40	a	828	CLA	C11-C10-C8-C9
40	a	841	CLA	C6-C7-C8-C9
40	b	803	CLA	C14-C13-C15-C16
40	b	815	CLA	C11-C10-C8-C9
40	b	826	CLA	C11-C12-C13-C14
40	b	838	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
40	l	204	CLA	C11-C12-C13-C14
45	S	323	LHG	O1-C1-C2-C3
40	p	305	CLA	CBD-CGD-O2D-CED
40	u	313	CLA	CBD-CGD-O2D-CED
40	x	312	CLA	CBD-CGD-O2D-CED
40	K	301	CLA	C4C-C3C-CAC-CBC
40	b	819	CLA	C15-C16-C17-C18
47	t	313	A1EB1	C45-C46-C47-C48
43	D	318	LMG	C14-C15-C16-C17
40	M	310	CLA	C4-C3-C5-C6
40	U	203	CLA	C4-C3-C5-C6
40	S	305	CLA	CAA-CBA-CGA-O2A
45	a	849	LHG	C11-C10-C9-C8
40	b	824	CLA	C2A-CAA-CBA-CGA
40	A	311	CLA	C1A-C2A-CAA-CBA
40	E	309	CLA	C1A-C2A-CAA-CBA
40	L	306	CLA	C1A-C2A-CAA-CBA
40	W	308	CLA	C1A-C2A-CAA-CBA
40	X	301	CLA	C1A-C2A-CAA-CBA
40	X	312	CLA	C1A-C2A-CAA-CBA
40	a	826	CLA	C1A-C2A-CAA-CBA
40	b	818	CLA	C1A-C2A-CAA-CBA
40	b	826	CLA	C1A-C2A-CAA-CBA
40	f	202	CLA	C1A-C2A-CAA-CBA
40	k	202	CLA	C1A-C2A-CAA-CBA
40	q	307	CLA	C1A-C2A-CAA-CBA
40	q	311	CLA	C1A-C2A-CAA-CBA
40	w	303	CLA	C1A-C2A-CAA-CBA
40	x	307	CLA	C1A-C2A-CAA-CBA
40	z	324	CLA	C1A-C2A-CAA-CBA
44	O	312	A86	C10-C11-C13-O
44	O	313	A86	C10-C11-C13-O
44	R	313	A86	C10-C11-C13-O
44	R	315	A86	C10-C11-C13-O
44	T	312	A86	C10-C11-C13-O
44	T	315	A86	C10-C11-C13-O
44	W	316	A86	C10-C11-C13-O
44	X	320	A86	C10-C11-C13-O
44	X	321	A86	C10-C11-C13-O
44	Y	319	A86	C10-C11-C13-O
44	Z	315	A86	C10-C11-C13-O
44	o	316	A86	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
44	p	318	A86	C10-C11-C13-O
44	p	319	A86	C10-C11-C13-O
44	q	315	A86	C10-C11-C13-O
44	q	319	A86	C10-C11-C13-O
44	v	315	A86	C10-C11-C13-O
44	v	319	A86	C10-C11-C13-O
44	w	315	A86	C10-C11-C13-O
47	K	315	A1EB1	C10-C11-C13-O
47	v	324	A1EB1	C10-C11-C13-O
47	w	313	A1EB1	C10-C11-C13-O
47	y	312	A1EB1	C10-C11-C13-O
49	b	844	BCR	C20-C21-C22-C23
49	f	206	BCR	C12-C13-C14-C15
49	l	207	BCR	C11-C10-C9-C8
40	x	311	CLA	CBA-CGA-O2A-C1
47	z	323	A1EB1	C42-C44-C45-C46
40	v	310	CLA	O1A-CGA-O2A-C1
40	A	308	CLA	C2B-C3B-CAB-CBB
40	B	303	CLA	C2B-C3B-CAB-CBB
40	C	305	CLA	C2B-C3B-CAB-CBB
40	D	303	CLA	C2B-C3B-CAB-CBB
40	D	308	CLA	C2B-C3B-CAB-CBB
40	D	312	CLA	C2B-C3B-CAB-CBB
40	E	303	CLA	C2B-C3B-CAB-CBB
40	E	306	CLA	C2B-C3B-CAB-CBB
40	E	310	CLA	C2B-C3B-CAB-CBB
40	E	314	CLA	C2B-C3B-CAB-CBB
40	F	301	CLA	C2B-C3B-CAB-CBB
40	F	305	CLA	C2B-C3B-CAB-CBB
40	F	321	CLA	C2B-C3B-CAB-CBB
40	G	201	CLA	C2B-C3B-CAB-CBB
40	H	311	CLA	C2B-C3B-CAB-CBB
40	I	208	CLA	C2B-C3B-CAB-CBB
40	J	309	CLA	C2B-C3B-CAB-CBB
40	J	312	CLA	C2B-C3B-CAB-CBB
40	M	312	CLA	C2B-C3B-CAB-CBB
40	N	311	CLA	C2B-C3B-CAB-CBB
40	O	307	CLA	C2B-C3B-CAB-CBB
40	O	316	CLA	C2B-C3B-CAB-CBB
40	P	305	CLA	C2B-C3B-CAB-CBB
40	P	308	CLA	C2B-C3B-CAB-CBB
40	P	311	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
40	Q	203	CLA	C2B-C3B-CAB-CBB
40	R	310	CLA	C2B-C3B-CAB-CBB
40	U	204	CLA	C2B-C3B-CAB-CBB
40	W	305	CLA	C2B-C3B-CAB-CBB
40	W	306	CLA	C2B-C3B-CAB-CBB
40	W	307	CLA	C2B-C3B-CAB-CBB
40	X	311	CLA	C2B-C3B-CAB-CBB
40	Y	301	CLA	C2B-C3B-CAB-CBB
40	Y	307	CLA	C2B-C3B-CAB-CBB
40	Y	310	CLA	C2B-C3B-CAB-CBB
40	a	806	CLA	C2B-C3B-CAB-CBB
40	a	820	CLA	C2B-C3B-CAB-CBB
40	a	829	CLA	C2B-C3B-CAB-CBB
40	a	833	CLA	C2B-C3B-CAB-CBB
40	a	834	CLA	C2B-C3B-CAB-CBB
40	a	838	CLA	C2B-C3B-CAB-CBB
40	b	813	CLA	C2B-C3B-CAB-CBB
40	b	834	CLA	C2B-C3B-CAB-CBB
40	b	839	CLA	C2B-C3B-CAB-CBB
40	b	840	CLA	C2B-C3B-CAB-CBB
40	i	101	CLA	C2B-C3B-CAB-CBB
40	k	201	CLA	C2B-C3B-CAB-CBB
40	l	204	CLA	C2B-C3B-CAB-CBB
40	o	304	CLA	C2B-C3B-CAB-CBB
40	p	308	CLA	C2B-C3B-CAB-CBB
40	t	307	CLA	C2B-C3B-CAB-CBB
40	u	311	CLA	C2B-C3B-CAB-CBB
40	w	304	CLA	C2B-C3B-CAB-CBB
40	w	309	CLA	C2B-C3B-CAB-CBB
40	x	302	CLA	C2B-C3B-CAB-CBB
40	x	311	CLA	C2B-C3B-CAB-CBB
40	x	312	CLA	C2B-C3B-CAB-CBB
40	z	305	CLA	C2B-C3B-CAB-CBB
40	z	311	CLA	C2B-C3B-CAB-CBB
40	z	312	CLA	C2B-C3B-CAB-CBB
40	z	313	CLA	C2B-C3B-CAB-CBB
49	a	844	BCR	C23-C24-C25-C30
49	a	846	BCR	C23-C24-C25-C30
49	b	846	BCR	C1-C6-C7-C8
49	b	847	BCR	C23-C24-C25-C26
49	f	206	BCR	C23-C24-C25-C30
49	k	203	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
49	l	208	BCR	C23-C24-C25-C30
49	r	201	BCR	C23-C24-C25-C26
40	Y	313	CLA	CBA-CGA-O2A-C1
40	y	304	CLA	CBA-CGA-O2A-C1
40	u	302	CLA	C10-C11-C12-C13
48	P	320	A1EB4	C43-C44-C45-C46
40	b	803	CLA	C3-C5-C6-C7
40	i	101	CLA	CBD-CGD-O2D-CED
44	G	211	A86	C9-C10-C11-C12
44	N	315	A86	C9-C10-C11-C12
44	S	316	A86	C9-C10-C11-C12
44	t	310	A86	C9-C10-C11-C12
44	t	311	A86	C9-C10-C11-C12
40	F	321	CLA	C4-C3-C5-C6
40	J	312	CLA	C4-C3-C5-C6
40	M	311	CLA	C4-C3-C5-C6
40	M	312	CLA	C4-C3-C5-C6
40	Z	311	CLA	C4-C3-C5-C6
43	D	318	LMG	C15-C16-C17-C18
40	A	309	CLA	C2-C3-C5-C6
40	M	311	CLA	C2-C3-C5-C6
40	b	838	CLA	C2-C3-C5-C6
40	b	826	CLA	C16-C17-C18-C19
45	F	319	LHG	C11-C12-C13-C14
40	A	304	CLA	C12-C13-C15-C16
40	M	305	CLA	C6-C7-C8-C10
40	P	312	CLA	C6-C7-C8-C10
40	W	307	CLA	C11-C12-C13-C15
40	X	311	CLA	C6-C7-C8-C10
40	a	811	CLA	C6-C7-C8-C10
40	a	816	CLA	C11-C10-C8-C7
40	a	842	CLA	C11-C12-C13-C15
40	b	806	CLA	C12-C13-C15-C16
40	o	311	CLA	C11-C12-C13-C15
40	v	307	CLA	C6-C7-C8-C10
40	x	306	CLA	C6-C7-C8-C10
40	z	312	CLA	C11-C10-C8-C7
40	Z	311	CLA	C15-C16-C17-C18
45	a	849	LHG	O7-C5-C6-O8
46	F	320	SQD	O6-C44-C45-O47
40	A	304	CLA	C13-C15-C16-C17
40	b	842	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
43	D	318	LMG	C28-C29-C30-C31
47	G	212	A1EB1	C-C1-C24-C25
49	l	206	BCR	C11-C12-C13-C35
40	a	821	CLA	O1A-CGA-O2A-C1
40	D	304	CLA	C4-C3-C5-C6
40	L	304	CLA	C4-C3-C5-C6
40	Q	205	CLA	C4-C3-C5-C6
40	k	202	CLA	C4-C3-C5-C6
40	w	304	CLA	CBA-CGA-O2A-C1
40	a	815	CLA	C3-C5-C6-C7
50	b	849	PQN	C18-C20-C21-C22
40	P	312	CLA	C2-C3-C5-C6
40	Z	311	CLA	C2-C3-C5-C6
40	b	832	CLA	C2-C3-C5-C6
40	f	201	CLA	C2-C3-C5-C6
40	o	305	CLA	C2-C3-C5-C6
44	w	316	A86	C9-C10-C11-C13
47	G	212	A1EB1	C9-C10-C11-C13
40	D	312	CLA	C2-C1-O2A-CGA
40	Y	306	CLA	C2-C1-O2A-CGA
40	z	308	CLA	C2-C1-O2A-CGA
45	a	848	LHG	C17-C18-C19-C20
41	w	306	KC2	CBD-CGD-O2D-CED
40	P	312	CLA	C10-C11-C12-C13
40	l	202	CLA	C15-C16-C17-C18
40	l	205	CLA	C5-C6-C7-C8
43	M	317	LMG	C15-C16-C17-C18
45	a	849	LHG	C8-C7-O7-C5
43	P	318	LMG	O6-C5-C6-O5
40	b	841	CLA	C6-C7-C8-C9
40	Y	306	CLA	C10-C11-C12-C13
40	G	213	CLA	C4C-C3C-CAC-CBC
40	W	311	CLA	O1D-CGD-O2D-CED
40	z	307	CLA	CBA-CGA-O2A-C1
43	T	318	LMG	C34-C35-C36-C37
40	A	306	CLA	C4-C3-C5-C6
40	D	301	CLA	C4-C3-C5-C6
40	f	201	CLA	C4-C3-C5-C6
40	o	307	CLA	C4-C3-C5-C6
40	D	301	CLA	C2-C3-C5-C6
40	S	302	CLA	C2-C3-C5-C6
40	Y	301	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
46	W	318	SQD	O10-C23-O48-C46
40	a	839	CLA	C13-C15-C16-C17
40	S	305	CLA	O1A-CGA-O2A-C1
40	u	308	CLA	CAA-CBA-CGA-O2A
40	b	819	CLA	O1A-CGA-O2A-C1
43	l	201	LMG	O10-C28-O8-C9
43	F	318	LMG	C35-C36-C37-C38
40	E	307	CLA	C2A-CAA-CBA-CGA
40	o	305	CLA	C2A-CAA-CBA-CGA
47	o	322	A1EB1	O6-C42-C44-C45
42	I	211	DD6	C27-C29-C30-C31
42	J	317	DD6	C27-C29-C30-C31
42	O	314	DD6	C27-C29-C30-C31
42	P	315	DD6	C27-C29-C30-C31
42	w	312	DD6	C27-C29-C30-C31
42	z	322	DD6	C27-C29-C30-C31
40	Y	307	CLA	C4-C3-C5-C6
40	a	836	CLA	C4-C3-C5-C6
40	b	825	CLA	C4-C3-C5-C6
40	o	301	CLA	C4-C3-C5-C6
40	z	308	CLA	C4-C3-C5-C6
40	p	308	CLA	CAA-CBA-CGA-O2A
40	A	309	CLA	C5-C6-C7-C8
40	a	826	CLA	C5-C6-C7-C8
40	p	308	CLA	C10-C11-C12-C13
43	S	322	LMG	C32-C33-C34-C35
40	D	303	CLA	C4B-C3B-CAB-CBB
40	D	308	CLA	C4B-C3B-CAB-CBB
40	E	310	CLA	C4B-C3B-CAB-CBB
40	G	201	CLA	C4B-C3B-CAB-CBB
40	I	202	CLA	C4B-C3B-CAB-CBB
40	I	208	CLA	C4B-C3B-CAB-CBB
40	M	312	CLA	C4B-C3B-CAB-CBB
40	N	311	CLA	C4B-C3B-CAB-CBB
40	O	310	CLA	C4B-C3B-CAB-CBB
40	O	316	CLA	C4B-C3B-CAB-CBB
40	P	308	CLA	C4B-C3B-CAB-CBB
40	S	311	CLA	C4B-C3B-CAB-CBB
40	Z	304	CLA	C4B-C3B-CAB-CBB
40	b	820	CLA	C4B-C3B-CAB-CBB
40	b	834	CLA	C4B-C3B-CAB-CBB
40	p	313	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
40	Z	312	CLA	O1A-CGA-O2A-C1
40	Z	306	CLA	O1D-CGD-O2D-CED
47	x	322	A1EB1	C45-C46-C47-C48
40	x	308	CLA	CAA-CBA-CGA-O2A
40	U	208	CLA	C4C-C3C-CAC-CBC
40	b	808	CLA	CBD-CGD-O2D-CED
41	x	303	KC2	CBD-CGD-O2D-CED
40	B	304	CLA	O1D-CGD-O2D-CED
47	Z	321	A1EB1	C42-C44-C45-C46
40	I	207	CLA	CAA-CBA-CGA-O2A
40	A	306	CLA	C2-C3-C5-C6
52	b	850	DGD	O6E-C1E-O5D-C6D
40	X	301	CLA	C5-C6-C7-C8
40	A	303	CLA	C11-C10-C8-C7
40	D	302	CLA	C11-C10-C8-C7
40	T	304	CLA	C11-C10-C8-C7
40	a	821	CLA	C11-C10-C8-C7
40	v	311	CLA	C6-C7-C8-C10
40	S	314	CLA	CAA-CBA-CGA-O2A
40	T	317	CLA	CAA-CBA-CGA-O2A
43	F	318	LMG	C31-C32-C33-C34
42	B	305	DD6	C5-C6-C8-C9
40	E	307	CLA	C11-C10-C8-C9
40	E	310	CLA	C6-C7-C8-C9
40	K	308	CLA	C6-C7-C8-C9
40	M	311	CLA	C11-C12-C13-C14
40	P	308	CLA	C11-C10-C8-C9
40	S	306	CLA	C6-C7-C8-C9
40	S	307	CLA	C6-C7-C8-C9
40	a	829	CLA	C11-C10-C8-C9
40	a	833	CLA	C6-C7-C8-C9
40	b	827	CLA	C11-C10-C8-C9
40	b	837	CLA	C11-C10-C8-C9
43	E	320	LMG	C8-C7-O1-C1
40	o	301	CLA	CAA-CBA-CGA-O2A
40	L	311	CLA	C2A-CAA-CBA-CGA
40	U	208	CLA	C2A-CAA-CBA-CGA
40	a	831	CLA	C2A-CAA-CBA-CGA
40	E	306	CLA	C2-C1-O2A-CGA
40	I	201	CLA	C2-C1-O2A-CGA
40	N	305	CLA	C2-C1-O2A-CGA
40	S	308	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
40	a	822	CLA	C2-C1-O2A-CGA
40	b	810	CLA	C2-C1-O2A-CGA
40	b	827	CLA	C2-C1-O2A-CGA
40	b	830	CLA	C2-C1-O2A-CGA
40	x	307	CLA	C2-C1-O2A-CGA
40	z	312	CLA	C2-C1-O2A-CGA
40	i	101	CLA	C3-C5-C6-C7
40	a	832	CLA	C16-C17-C18-C19
40	J	308	CLA	CBA-CGA-O2A-C1
40	a	829	CLA	CBA-CGA-O2A-C1
40	E	302	CLA	C3A-C2A-CAA-CBA
40	G	213	CLA	C3A-C2A-CAA-CBA
40	J	303	CLA	C3A-C2A-CAA-CBA
40	P	313	CLA	C3A-C2A-CAA-CBA
40	Y	306	CLA	C3A-C2A-CAA-CBA
40	b	818	CLA	C3A-C2A-CAA-CBA
40	l	204	CLA	C3A-C2A-CAA-CBA
41	I	214	KC2	C2C-C3C-CAC-CBC
41	P	302	KC2	C2C-C3C-CAC-CBC
41	P	304	KC2	C2B-C3B-CAB-CBB
41	W	303	KC2	C2B-C3B-CAB-CBB
41	W	303	KC2	C2C-C3C-CAC-CBC
41	Y	302	KC2	C2C-C3C-CAC-CBC
41	t	301	KC2	C2B-C3B-CAB-CBB
41	t	308	KC2	C2B-C3B-CAB-CBB
41	u	309	KC2	C2B-C3B-CAB-CBB
41	w	307	KC2	C2C-C3C-CAC-CBC
40	E	302	CLA	C4C-C3C-CAC-CBC
40	a	821	CLA	C13-C15-C16-C17
45	S	323	LHG	C9-C10-C11-C12
46	W	318	SQD	C24-C23-O48-C46
40	A	305	CLA	O2A-C1-C2-C3
45	a	849	LHG	C6-C5-O7-C7
40	E	314	CLA	C4C-C3C-CAC-CBC
40	F	310	CLA	CAA-CBA-CGA-O2A
46	I	215	SQD	C24-C25-C26-C27
44	p	318	A86	C9-C10-C11-C12
40	X	312	CLA	C2A-CAA-CBA-CGA
40	z	306	CLA	C2A-CAA-CBA-CGA
40	o	311	CLA	CBA-CGA-O2A-C1
43	D	318	LMG	C29-C28-O8-C9
42	A	316	DD6	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
42	F	316	DD6	C13-C14-C15-O1
42	J	301	DD6	C13-C14-C15-O1
45	a	848	LHG	O6-C4-C5-O7
40	D	310	CLA	C5-C6-C7-C8
40	C	304	CLA	CBA-CGA-O2A-C1
40	T	310	CLA	CBD-CGD-O2D-CED
40	V	201	CLA	O1A-CGA-O2A-C1
40	H	307	CLA	C10-C11-C12-C13
41	I	214	KC2	C4B-C3B-CAB-CBB
41	K	302	KC2	C4C-C3C-CAC-CBC
41	K	303	KC2	C4B-C3B-CAB-CBB
41	K	309	KC2	C4B-C3B-CAB-CBB
41	L	313	KC2	C4B-C3B-CAB-CBB
41	M	309	KC2	C4B-C3B-CAB-CBB
41	N	309	KC2	C4B-C3B-CAB-CBB
41	P	302	KC2	C4C-C3C-CAC-CBC
41	P	303	KC2	C4C-C3C-CAC-CBC
41	R	308	KC2	C4B-C3B-CAB-CBB
41	R	311	KC2	C4B-C3B-CAB-CBB
41	S	303	KC2	C4C-C3C-CAC-CBC
41	T	303	KC2	C4B-C3B-CAB-CBB
41	T	308	KC2	C4C-C3C-CAC-CBC
41	T	309	KC2	C4B-C3B-CAB-CBB
41	T	311	KC2	C4B-C3B-CAB-CBB
41	U	201	KC2	C4B-C3B-CAB-CBB
41	W	303	KC2	C4B-C3B-CAB-CBB
41	W	309	KC2	C4C-C3C-CAC-CBC
41	Y	308	KC2	C4B-C3B-CAB-CBB
41	Y	309	KC2	C4B-C3B-CAB-CBB
41	o	303	KC2	C4B-C3B-CAB-CBB
41	p	303	KC2	C4C-C3C-CAC-CBC
41	p	309	KC2	C4B-C3B-CAB-CBB
41	p	309	KC2	C4C-C3C-CAC-CBC
41	t	301	KC2	C4B-C3B-CAB-CBB
41	t	308	KC2	C4B-C3B-CAB-CBB
41	w	306	KC2	C4C-C3C-CAC-CBC
41	w	307	KC2	C4C-C3C-CAC-CBC
41	x	309	KC2	C4B-C3B-CAB-CBB
41	y	301	KC2	C4B-C3B-CAB-CBB
41	y	307	KC2	C4B-C3B-CAB-CBB
41	z	309	KC2	C4B-C3B-CAB-CBB
45	F	319	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
41	X	309	KC2	CAA-CBA-CGA-O2A
40	A	311	CLA	CBA-CGA-O2A-C1
45	F	319	LHG	C11-C10-C9-C8
40	W	306	CLA	C4-C3-C5-C6
40	a	810	CLA	C4-C3-C5-C6
40	y	303	CLA	C2A-CAA-CBA-CGA
47	v	321	A1EB1	C11-C10-C9-C8
40	j	102	CLA	C2-C1-O2A-CGA
40	N	305	CLA	C6-C7-C8-C9
46	I	215	SQD	C31-C32-C33-C34
40	w	305	CLA	C4C-C3C-CAC-CBC
40	v	305	CLA	C5-C6-C7-C8
41	N	312	KC2	CAA-CBA-CGA-O1A
40	L	305	CLA	CAA-CBA-CGA-O2A
40	W	308	CLA	CAA-CBA-CGA-O2A
40	b	814	CLA	CAA-CBA-CGA-O2A
47	T	320	A1EB1	O6-C42-C44-C45
40	A	306	CLA	C6-C7-C8-C9
40	W	306	CLA	C11-C10-C8-C9
40	W	313	CLA	C6-C7-C8-C9
40	a	811	CLA	C11-C12-C13-C14
40	a	842	CLA	C6-C7-C8-C9
40	b	814	CLA	C6-C7-C8-C9
40	b	815	CLA	C6-C7-C8-C9
40	b	840	CLA	C11-C10-C8-C9
40	z	308	CLA	C11-C10-C8-C9
40	A	303	CLA	CAA-CBA-CGA-O2A
40	U	204	CLA	CAA-CBA-CGA-O2A
40	W	306	CLA	CAA-CBA-CGA-O2A
40	u	306	CLA	CAA-CBA-CGA-O2A
40	z	306	CLA	CAA-CBA-CGA-O2A
43	u	301	LMG	O7-C10-C11-C12
40	t	307	CLA	O1A-CGA-O2A-C1
41	w	306	KC2	CAA-CBA-CGA-O1A
44	W	301	A86	C2-C1-C24-C25
49	a	843	BCR	C21-C22-C23-C24
44	P	314	A86	C13-C14-C15-O1
44	P	316	A86	C13-C14-C15-O1
44	P	317	A86	C13-C14-C15-O1
44	Q	215	A86	C13-C14-C15-O1
44	R	315	A86	C13-C14-C15-O1
44	X	317	A86	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
44	Y	319	A86	C13-C14-C15-O1
44	o	315	A86	C13-C14-C15-O1
44	o	317	A86	C13-C14-C15-O1
44	o	318	A86	C13-C14-C15-O1
44	p	317	A86	C13-C14-C15-O1
44	p	321	A86	C13-C14-C15-O1
44	q	317	A86	C13-C14-C15-O1
44	q	324	A86	C13-C14-C15-O1
44	t	316	A86	C13-C14-C15-O1
44	u	317	A86	C13-C14-C15-O1
44	v	317	A86	C13-C14-C15-O1
44	v	325	A86	C13-C14-C15-O1
44	x	317	A86	C13-C14-C15-O1
44	z	316	A86	C13-C14-C15-O1
44	z	320	A86	C13-C14-C15-O1
47	p	324	A1EB1	C13-C14-C15-O1
47	q	323	A1EB1	C13-C14-C15-O1
47	u	323	A1EB1	C13-C14-C15-O1
47	x	322	A1EB1	C13-C14-C15-O1
40	F	301	CLA	CAA-CBA-CGA-O2A
40	J	311	CLA	CAA-CBA-CGA-O2A
40	H	310	CLA	CBA-CGA-O2A-C1
40	G	206	CLA	C2A-CAA-CBA-CGA
40	b	811	CLA	C2A-CAA-CBA-CGA
40	A	304	CLA	C11-C10-C8-C7
40	E	309	CLA	C11-C10-C8-C7
40	P	313	CLA	C6-C7-C8-C10
40	S	306	CLA	C6-C7-C8-C10
40	b	835	CLA	C11-C12-C13-C15
40	b	838	CLA	C11-C10-C8-C7
40	b	841	CLA	C6-C7-C8-C10
40	q	307	CLA	C6-C7-C8-C10
40	a	803	CLA	C5-C6-C7-C8
44	O	312	A86	C9-C10-C11-C13
44	t	316	A86	C9-C10-C11-C13
44	w	310	A86	C9-C10-C11-C13
44	z	317	A86	C9-C10-C11-C13
40	b	822	CLA	C16-C17-C18-C19
40	B	306	CLA	C2B-C3B-CAB-CBB
40	D	307	CLA	C2B-C3B-CAB-CBB
40	D	309	CLA	C2B-C3B-CAB-CBB
40	E	307	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
40	E	309	CLA	C2B-C3B-CAB-CBB
40	F	308	CLA	C2B-C3B-CAB-CBB
40	I	202	CLA	C2B-C3B-CAB-CBB
40	K	307	CLA	C2B-C3B-CAB-CBB
40	M	306	CLA	C2B-C3B-CAB-CBB
40	M	311	CLA	C2B-C3B-CAB-CBB
40	O	310	CLA	C2B-C3B-CAB-CBB
40	R	306	CLA	C2B-C3B-CAB-CBB
40	R	316	CLA	C2B-C3B-CAB-CBB
40	S	311	CLA	C2B-C3B-CAB-CBB
40	T	317	CLA	C2B-C3B-CAB-CBB
40	W	311	CLA	C2B-C3B-CAB-CBB
40	W	313	CLA	C2B-C3B-CAB-CBB
40	Y	311	CLA	C2B-C3B-CAB-CBB
40	b	814	CLA	C2B-C3B-CAB-CBB
40	j	102	CLA	C2B-C3B-CAB-CBB
40	p	313	CLA	C2B-C3B-CAB-CBB
40	q	312	CLA	C2B-C3B-CAB-CBB
40	v	312	CLA	C2B-C3B-CAB-CBB
40	x	313	CLA	C2B-C3B-CAB-CBB
49	a	844	BCR	C23-C24-C25-C26
49	a	846	BCR	C23-C24-C25-C26
49	b	846	BCR	C23-C24-C25-C26
49	b	847	BCR	C5-C6-C7-C8
49	f	206	BCR	C23-C24-C25-C26
49	i	102	BCR	C23-C24-C25-C26
49	l	208	BCR	C23-C24-C25-C26
40	t	309	CLA	CAA-CBA-CGA-O2A
40	B	306	CLA	C2-C1-O2A-CGA
40	C	306	CLA	C2-C1-O2A-CGA
40	D	307	CLA	C2-C1-O2A-CGA
40	K	304	CLA	C2-C1-O2A-CGA
40	Q	205	CLA	C2-C1-O2A-CGA
40	Z	306	CLA	C2-C1-O2A-CGA
40	a	820	CLA	C2-C1-O2A-CGA
40	b	837	CLA	C2-C1-O2A-CGA
40	l	203	CLA	C2-C1-O2A-CGA
52	b	850	DGD	C4D-C5D-C6D-O5D
40	W	307	CLA	C15-C16-C17-C18
40	J	302	CLA	CAA-CBA-CGA-O2A
47	v	323	A1EB1	O6-C42-C44-C45
40	a	826	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
40	M	311	CLA	C10-C11-C12-C13
47	K	315	A1EB1	C29-C27-C28-O6
47	P	301	A1EB1	C29-C27-C28-O6
47	t	315	A1EB1	C29-C27-C28-O6
47	w	313	A1EB1	C29-C27-C28-O6
40	Q	203	CLA	CBA-CGA-O2A-C1
40	u	302	CLA	C3-C5-C6-C7
40	O	307	CLA	CAA-CBA-CGA-O2A
40	b	818	CLA	CAA-CBA-CGA-O2A
47	q	323	A1EB1	O6-C42-C44-C45
40	a	836	CLA	C2-C3-C5-C6
40	p	302	CLA	C10-C11-C12-C13
40	t	307	CLA	C5-C6-C7-C8
40	A	309	CLA	C2A-CAA-CBA-CGA
40	C	307	CLA	C2A-CAA-CBA-CGA
40	a	828	CLA	C2A-CAA-CBA-CGA
40	B	301	CLA	C2-C1-O2A-CGA
40	A	302	CLA	C5-C6-C7-C8
41	N	312	KC2	CAA-CBA-CGA-O2A
48	P	320	A1EB4	C45-C46-C47-C51
40	B	304	CLA	CAA-CBA-CGA-O2A
40	O	305	CLA	CAA-CBA-CGA-O2A
40	S	319	CLA	CAA-CBA-CGA-O2A
40	b	803	CLA	CAA-CBA-CGA-O2A
40	b	807	CLA	CAA-CBA-CGA-O2A
40	b	809	CLA	CAA-CBA-CGA-O2A
40	b	810	CLA	CAA-CBA-CGA-O2A
40	q	313	CLA	CAA-CBA-CGA-O2A
40	y	302	CLA	CAA-CBA-CGA-O2A
40	X	304	CLA	C2-C1-O2A-CGA
43	D	318	LMG	C16-C17-C18-C19
52	b	850	DGD	C5B-C6B-C7B-C8B
40	Z	305	CLA	C6-C7-C8-C10
40	a	832	CLA	C16-C17-C18-C20
40	b	806	CLA	C8-C10-C11-C12
40	M	307	CLA	C5-C6-C7-C8
40	o	307	CLA	C5-C6-C7-C8
40	H	302	CLA	CAA-CBA-CGA-O2A
40	M	306	CLA	CAA-CBA-CGA-O2A
40	a	838	CLA	CAA-CBA-CGA-O2A
43	A	317	LMG	O8-C28-C29-C30
43	p	301	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
47	P	301	A1EB1	O6-C42-C44-C45
40	z	324	CLA	C2-C1-O2A-CGA
44	X	315	A86	C35-C34-O4-C38
40	F	301	CLA	C4-C3-C5-C6
40	G	204	CLA	C4-C3-C5-C6
43	W	317	LMG	C15-C16-C17-C18
40	p	306	CLA	CAA-CBA-CGA-O2A
47	O	317	A1EB1	O6-C42-C44-C45
40	p	308	CLA	C8-C10-C11-C12
40	b	805	CLA	C3-C5-C6-C7
40	b	807	CLA	C5-C6-C7-C8
41	w	306	KC2	CAA-CBA-CGA-O2A
40	a	822	CLA	C2A-CAA-CBA-CGA
40	j	102	CLA	C2A-CAA-CBA-CGA
40	I	203	CLA	CAA-CBA-CGA-O2A
40	I	206	CLA	CAA-CBA-CGA-O2A
40	b	816	CLA	CAA-CBA-CGA-O2A
40	U	208	CLA	O1A-CGA-O2A-C1
45	a	848	LHG	C27-C28-C29-C30
40	A	305	CLA	C6-C7-C8-C9
40	D	309	CLA	C6-C7-C8-C9
40	M	312	CLA	C11-C10-C8-C9
40	P	308	CLA	C6-C7-C8-C9
40	b	818	CLA	C11-C12-C13-C14
40	b	822	CLA	C11-C12-C13-C14
40	b	842	CLA	C11-C10-C8-C9
40	q	311	CLA	C6-C7-C8-C9
40	C	306	CLA	C13-C15-C16-C17
40	S	307	CLA	CAA-CBA-CGA-O2A
40	b	808	CLA	CAA-CBA-CGA-O2A
40	t	305	CLA	CAA-CBA-CGA-O2A
52	b	850	DGD	O2G-C1B-C2B-C3B
40	O	306	CLA	C10-C11-C12-C13
40	o	301	CLA	C10-C11-C12-C13
40	B	303	CLA	C1A-C2A-CAA-CBA
40	D	307	CLA	C4B-C3B-CAB-CBB
40	E	307	CLA	C4B-C3B-CAB-CBB
40	E	314	CLA	C4B-C3B-CAB-CBB
40	F	305	CLA	C4B-C3B-CAB-CBB
40	H	305	CLA	C4B-C3B-CAB-CBB
40	H	307	CLA	C4B-C3B-CAB-CBB
40	H	308	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
40	I	207	CLA	C4B-C3B-CAB-CBB
40	J	307	CLA	C4B-C3B-CAB-CBB
40	J	312	CLA	C4B-C3B-CAB-CBB
40	P	312	CLA	C1A-C2A-CAA-CBA
40	Q	209	CLA	C1A-C2A-CAA-CBA
40	R	306	CLA	C4B-C3B-CAB-CBB
40	Z	301	CLA	C1A-C2A-CAA-CBA
40	Z	305	CLA	C4B-C3B-CAB-CBB
40	Z	307	CLA	C1A-C2A-CAA-CBA
40	a	806	CLA	C4B-C3B-CAB-CBB
40	a	808	CLA	C4B-C3B-CAB-CBB
40	a	813	CLA	C4B-C3B-CAB-CBB
40	a	823	CLA	C1A-C2A-CAA-CBA
40	b	816	CLA	C4B-C3B-CAB-CBB
40	f	201	CLA	C4B-C3B-CAB-CBB
40	l	204	CLA	C1A-C2A-CAA-CBA
40	p	306	CLA	C4B-C3B-CAB-CBB
40	p	307	CLA	C4B-C3B-CAB-CBB
40	q	306	CLA	C1A-C2A-CAA-CBA
40	q	312	CLA	C1A-C2A-CAA-CBA
40	q	312	CLA	C4B-C3B-CAB-CBB
40	t	303	CLA	C1A-C2A-CAA-CBA
40	u	306	CLA	C4B-C3B-CAB-CBB
40	v	306	CLA	C1A-C2A-CAA-CBA
40	x	306	CLA	C4B-C3B-CAB-CBB
40	x	311	CLA	C4B-C3B-CAB-CBB
40	x	312	CLA	C1A-C2A-CAA-CBA
40	y	303	CLA	C4B-C3B-CAB-CBB
40	z	314	CLA	C1A-C2A-CAA-CBA
44	L	314	A86	O-C13-C14-C15
44	P	317	A86	O-C13-C14-C15
44	T	315	A86	O-C13-C14-C15
44	p	320	A86	O-C13-C14-C15
44	u	318	A86	O-C13-C14-C15
44	w	311	A86	O-C13-C14-C15
44	w	316	A86	O-C13-C14-C15
44	x	318	A86	O-C13-C14-C15
47	K	315	A1EB1	O-C13-C14-C15
47	o	322	A1EB1	O-C13-C14-C15
47	t	314	A1EB1	O-C13-C14-C15
47	v	323	A1EB1	O-C13-C14-C15
52	b	850	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
40	P	313	CLA	C4-C3-C5-C6
40	a	824	CLA	C5-C6-C7-C8
40	C	306	CLA	CAA-CBA-CGA-O2A
40	H	305	CLA	CAA-CBA-CGA-O2A
40	W	311	CLA	CAA-CBA-CGA-O2A
40	a	813	CLA	CAA-CBA-CGA-O2A
40	a	831	CLA	CAA-CBA-CGA-O2A
40	a	852	CLA	CAA-CBA-CGA-O2A
45	a	848	LHG	O8-C23-C24-C25
46	F	320	SQD	O47-C7-C8-C9
45	a	848	LHG	O7-C5-C6-O8
42	A	313	DD6	C10-C11-C13-C14
42	k	204	DD6	C2-C1-C24-C25
42	u	321	DD6	C10-C11-C13-C14
44	N	321	A86	C5-C6-C8-C9
44	Q	210	A86	C5-C6-C8-C9
44	t	316	A86	C2-C1-C24-C25
47	Y	323	A1EB1	C2-C1-C24-C25
49	b	848	BCR	C7-C8-C9-C10
49	l	208	BCR	C17-C18-C19-C20
40	N	311	CLA	CBA-CGA-O2A-C1
40	a	833	CLA	CBA-CGA-O2A-C1
40	F	307	CLA	C8-C10-C11-C12
40	D	306	CLA	CAA-CBA-CGA-O2A
40	I	205	CLA	CAA-CBA-CGA-O2A
40	J	307	CLA	CAA-CBA-CGA-O2A
40	X	310	CLA	CAA-CBA-CGA-O2A
40	Z	305	CLA	CAA-CBA-CGA-O2A
40	q	312	CLA	CAA-CBA-CGA-O2A
40	w	305	CLA	CAA-CBA-CGA-O2A
40	y	305	CLA	CAA-CBA-CGA-O2A
40	F	310	CLA	CBD-CGD-O2D-CED
40	B	306	CLA	C2A-CAA-CBA-CGA
40	b	814	CLA	C2A-CAA-CBA-CGA
40	u	306	CLA	C4C-C3C-CAC-CBC
40	v	307	CLA	C8-C10-C11-C12
40	E	311	CLA	O1A-CGA-O2A-C1
43	P	318	LMG	C29-C30-C31-C32
40	a	820	CLA	C11-C12-C13-C14
40	b	840	CLA	C16-C17-C18-C20
43	x	301	LMG	O7-C10-C11-C12
47	t	315	A1EB1	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
40	a	830	CLA	CAA-CBA-CGA-O1A
40	a	826	CLA	C10-C11-C12-C13
40	M	305	CLA	C5-C6-C7-C8
40	N	311	CLA	C2-C1-O2A-CGA
40	S	314	CLA	C2-C1-O2A-CGA
40	V	201	CLA	C2-C1-O2A-CGA
40	X	305	CLA	C2-C1-O2A-CGA
40	a	850	CLA	C2-C1-O2A-CGA
40	p	307	CLA	C2-C1-O2A-CGA
40	u	307	CLA	C2-C1-O2A-CGA
40	K	306	CLA	CAA-CBA-CGA-O2A
40	a	820	CLA	CAA-CBA-CGA-O2A
40	a	821	CLA	CAA-CBA-CGA-O2A
40	M	307	CLA	C6-C7-C8-C10
40	M	311	CLA	C11-C12-C13-C15
40	M	312	CLA	C6-C7-C8-C10
40	W	308	CLA	C6-C7-C8-C10
40	b	812	CLA	C6-C7-C8-C10
40	l	202	CLA	C11-C10-C8-C7
40	l	204	CLA	C6-C7-C8-C10
40	Z	311	CLA	CBA-CGA-O2A-C1
40	k	202	CLA	C2-C3-C5-C6
40	Q	206	CLA	C10-C11-C12-C13
40	P	307	CLA	C10-C11-C12-C13
40	I	201	CLA	C16-C17-C18-C20
40	u	312	CLA	C11-C12-C13-C15
40	A	307	CLA	O2A-C1-C2-C3
40	M	304	CLA	O2A-C1-C2-C3
40	N	304	CLA	O2A-C1-C2-C3
40	U	203	CLA	O2A-C1-C2-C3
40	z	311	CLA	O2A-C1-C2-C3
45	a	849	LHG	C4-C5-O7-C7
40	a	824	CLA	C13-C15-C16-C17
40	F	303	CLA	CAA-CBA-CGA-O2A
47	t	315	A1EB1	O6-C42-C44-C45
40	a	821	CLA	C15-C16-C17-C18
40	a	850	CLA	C15-C16-C17-C18
48	W	319	A1EB4	C10-C11-C12-O3
40	H	311	CLA	C2A-CAA-CBA-CGA
40	Q	209	CLA	C2A-CAA-CBA-CGA
40	b	810	CLA	C5-C6-C7-C8
40	Y	305	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
40	b	842	CLA	CAA-CBA-CGA-O2A
40	z	305	CLA	CAA-CBA-CGA-O2A
43	E	301	LMG	O7-C10-C11-C12
40	u	306	CLA	CAA-CBA-CGA-O1A
43	l	201	LMG	O10-C28-C29-C30
47	q	323	A1EB1	O43-C42-C44-C45
40	w	309	CLA	CBA-CGA-O2A-C1
40	x	313	CLA	CBA-CGA-O2A-C1
43	p	301	LMG	C30-C31-C32-C33
40	B	306	CLA	C3A-C2A-CAA-CBA
40	C	302	CLA	C3A-C2A-CAA-CBA
40	E	303	CLA	C3A-C2A-CAA-CBA
40	H	309	CLA	C3A-C2A-CAA-CBA
40	P	312	CLA	C3A-C2A-CAA-CBA
40	R	310	CLA	C3A-C2A-CAA-CBA
40	S	301	CLA	C3A-C2A-CAA-CBA
40	S	314	CLA	C3A-C2A-CAA-CBA
40	T	310	CLA	C3A-C2A-CAA-CBA
40	W	308	CLA	C3A-C2A-CAA-CBA
40	a	823	CLA	C3A-C2A-CAA-CBA
40	b	827	CLA	C3A-C2A-CAA-CBA
40	b	832	CLA	C3A-C2A-CAA-CBA
40	p	308	CLA	C3A-C2A-CAA-CBA
40	t	303	CLA	C3A-C2A-CAA-CBA
40	x	302	CLA	C3A-C2A-CAA-CBA
40	z	312	CLA	C3A-C2A-CAA-CBA
40	H	302	CLA	CAA-CBA-CGA-O1A
40	H	305	CLA	CAA-CBA-CGA-O1A
40	L	305	CLA	CAA-CBA-CGA-O1A
40	S	307	CLA	CAA-CBA-CGA-O1A
40	W	306	CLA	CAA-CBA-CGA-O1A
40	D	303	CLA	C10-C11-C12-C13
40	Y	310	CLA	C6-C7-C8-C9
40	z	312	CLA	C11-C12-C13-C15
40	O	310	CLA	CBD-CGD-O2D-CED
43	L	319	LMG	C11-C12-C13-C14
40	O	307	CLA	CAA-CBA-CGA-O1A
40	U	203	CLA	O1A-CGA-O2A-C1
45	a	848	LHG	C26-C27-C28-C29
43	u	301	LMG	C15-C16-C17-C18
47	G	212	A1EB1	C44-C45-C46-C47
40	D	305	CLA	CGD-CBD-CHA-C4D

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Mol	Chain	Res	Type	Atoms
40	Q	209	CLA	CAA-CBA-CGA-O2A
40	S	306	CLA	CAA-CBA-CGA-O2A
40	b	835	CLA	CAA-CBA-CGA-O2A
40	x	306	CLA	CAA-CBA-CGA-O2A
40	b	809	CLA	CAA-CBA-CGA-O1A
40	P	313	CLA	CBA-CGA-O2A-C1
40	A	303	CLA	C6-C7-C8-C9
40	T	304	CLA	C6-C7-C8-C9
40	a	811	CLA	C11-C10-C8-C9
40	x	306	CLA	C6-C7-C8-C9
40	o	312	CLA	CAA-CBA-CGA-O2A
40	B	304	CLA	CAA-CBA-CGA-O1A
40	a	852	CLA	CAA-CBA-CGA-O1A
40	b	818	CLA	CAA-CBA-CGA-O1A
40	q	313	CLA	CAA-CBA-CGA-O1A
40	z	306	CLA	CAA-CBA-CGA-O1A
43	x	301	LMG	O9-C10-C11-C12
47	P	301	A1EB1	O43-C42-C44-C45
47	v	323	A1EB1	O43-C42-C44-C45
45	a	848	LHG	C11-C10-C9-C8
47	q	321	A1EB1	C11-C10-C9-C8
40	L	306	CLA	O1D-CGD-O2D-CED
40	q	312	CLA	C11-C12-C13-C15
40	P	307	CLA	C8-C10-C11-C12
40	P	308	CLA	C10-C11-C12-C13
40	x	312	CLA	C10-C11-C12-C13
40	M	306	CLA	CAA-CBA-CGA-O1A
40	b	807	CLA	CAA-CBA-CGA-O1A
40	b	810	CLA	CAA-CBA-CGA-O1A
45	S	323	LHG	O10-C23-C24-C25
40	T	305	CLA	CAA-CBA-CGA-O2A
40	t	304	CLA	CAA-CBA-CGA-O2A
40	w	304	CLA	CAA-CBA-CGA-O2A
43	E	320	LMG	O8-C28-C29-C30
40	M	310	CLA	C2-C3-C5-C6
41	K	303	KC2	C1A-C2A-CAA-CBA
41	K	303	KC2	C3A-C2A-CAA-CBA
41	K	305	KC2	C3A-C2A-CAA-CBA
41	L	309	KC2	C3A-C2A-CAA-CBA
41	L	313	KC2	C1A-C2A-CAA-CBA
41	M	302	KC2	C1A-C2A-CAA-CBA
41	M	308	KC2	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
41	N	303	KC2	C3A-C2A-CAA-CBA
41	N	308	KC2	C3A-C2A-CAA-CBA
41	N	312	KC2	C3A-C2A-CAA-CBA
41	O	302	KC2	C1A-C2A-CAA-CBA
41	O	309	KC2	C1A-C2A-CAA-CBA
41	P	304	KC2	C1A-C2A-CAA-CBA
41	P	310	KC2	C3A-C2A-CAA-CBA
41	R	308	KC2	C3A-C2A-CAA-CBA
41	R	309	KC2	C3A-C2A-CAA-CBA
41	S	303	KC2	C1A-C2A-CAA-CBA
41	S	304	KC2	C1A-C2A-CAA-CBA
41	S	304	KC2	C3A-C2A-CAA-CBA
41	T	308	KC2	C1A-C2A-CAA-CBA
41	T	308	KC2	C3A-C2A-CAA-CBA
41	T	311	KC2	C3A-C2A-CAA-CBA
41	W	302	KC2	C3A-C2A-CAA-CBA
41	W	303	KC2	C1A-C2A-CAA-CBA
41	W	304	KC2	C3A-C2A-CAA-CBA
41	W	309	KC2	C3A-C2A-CAA-CBA
41	X	302	KC2	C1A-C2A-CAA-CBA
41	X	308	KC2	C1A-C2A-CAA-CBA
41	p	310	KC2	C3A-C2A-CAA-CBA
41	q	303	KC2	C1A-C2A-CAA-CBA
41	q	308	KC2	C1A-C2A-CAA-CBA
41	u	309	KC2	C1A-C2A-CAA-CBA
41	u	310	KC2	C3A-C2A-CAA-CBA
41	v	308	KC2	C1A-C2A-CAA-CBA
41	x	310	KC2	C3A-C2A-CAA-CBA
41	z	304	KC2	C1A-C2A-CAA-CBA
41	z	304	KC2	C3A-C2A-CAA-CBA
41	z	309	KC2	C1A-C2A-CAA-CBA
42	B	305	DD6	C13-C14-C15-C16
42	I	211	DD6	C13-C14-C15-C16
42	K	311	DD6	C13-C14-C15-C16
44	Y	320	A86	C26-C27-C29-C30
40	J	308	CLA	O1A-CGA-O2A-C1
40	A	303	CLA	CAA-CBA-CGA-O1A
40	D	306	CLA	CAA-CBA-CGA-O1A
40	J	302	CLA	CAA-CBA-CGA-O1A
40	S	319	CLA	CAA-CBA-CGA-O1A
40	X	304	CLA	CAA-CBA-CGA-O1A
40	b	803	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
40	q	307	CLA	CAA-CBA-CGA-O1A
40	t	305	CLA	CAA-CBA-CGA-O1A
40	y	305	CLA	CAA-CBA-CGA-O1A
43	p	301	LMG	O9-C10-C11-C12
45	a	848	LHG	O10-C23-C24-C25
40	N	311	CLA	CAA-CBA-CGA-O2A
40	R	304	CLA	CAA-CBA-CGA-O2A
40	a	804	CLA	CAA-CBA-CGA-O2A
40	H	309	CLA	C5-C6-C7-C8
40	b	812	CLA	C8-C10-C11-C12
44	F	313	A86	C2-C1-C24-C25
44	Y	320	A86	C5-C6-C8-C9
44	o	315	A86	C5-C6-C8-C9
44	u	318	A86	C2-C1-C24-C25
44	x	317	A86	C2-C1-C24-C25
40	I	206	CLA	CAA-CBA-CGA-O1A
40	U	204	CLA	CAA-CBA-CGA-O1A
40	a	831	CLA	CAA-CBA-CGA-O1A
40	y	302	CLA	CAA-CBA-CGA-O1A
40	z	305	CLA	CAA-CBA-CGA-O1A
47	O	317	A1EB1	O43-C42-C44-C45
40	l	203	CLA	C8-C10-C11-C12
47	R	317	A1EB1	C45-C46-C47-C48
40	J	311	CLA	CAA-CBA-CGA-O1A
40	W	311	CLA	CAA-CBA-CGA-O1A
40	a	820	CLA	CAA-CBA-CGA-O1A
40	b	816	CLA	CAA-CBA-CGA-O1A
40	p	306	CLA	CAA-CBA-CGA-O1A
43	E	320	LMG	O10-C28-C29-C30
40	T	310	CLA	CAA-CBA-CGA-O2A
40	X	304	CLA	CAA-CBA-CGA-O2A
40	b	801	CLA	CAA-CBA-CGA-O2A
40	q	307	CLA	CAA-CBA-CGA-O2A
43	l	201	LMG	O8-C28-C29-C30
40	t	304	CLA	C2A-CAA-CBA-CGA
41	K	305	KC2	CAA-CBA-CGA-O1A
41	K	305	KC2	CAA-CBA-CGA-O2A
40	D	305	CLA	CGD-CBD-CHA-C1A
44	P	317	A86	C12-C11-C13-O
44	R	312	A86	C12-C11-C13-O
44	T	312	A86	C12-C11-C13-O
44	W	314	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
44	W	316	A86	C12-C11-C13-O
44	p	316	A86	C12-C11-C13-O
44	p	318	A86	C12-C11-C13-O
44	q	319	A86	C12-C11-C13-O
44	u	318	A86	C12-C11-C13-O
44	x	316	A86	C12-C11-C13-O
44	z	320	A86	C12-C11-C13-O
46	F	320	SQD	O6-C44-C45-C46
47	K	315	A1EB1	C12-C11-C13-O
47	v	324	A1EB1	C12-C11-C13-O
47	y	312	A1EB1	C12-C11-C13-O
47	y	313	A1EB1	C12-C11-C13-O
40	F	301	CLA	CAA-CBA-CGA-O1A
40	I	203	CLA	CAA-CBA-CGA-O1A
40	J	307	CLA	CAA-CBA-CGA-O1A
40	O	305	CLA	CAA-CBA-CGA-O1A
46	F	320	SQD	O49-C7-C8-C9
40	a	810	CLA	C5-C6-C7-C8
40	f	205	CLA	CAA-CBA-CGA-O2A
40	Q	205	CLA	C2-C3-C5-C6
40	T	310	CLA	C2-C3-C5-C6
41	I	214	KC2	C2B-C3B-CAB-CBB
41	L	302	KC2	C2B-C3B-CAB-CBB
41	N	313	KC2	C2B-C3B-CAB-CBB
41	P	309	KC2	C2B-C3B-CAB-CBB
41	Q	216	KC2	C2B-C3B-CAB-CBB
41	R	308	KC2	C2C-C3C-CAC-CBC
41	T	303	KC2	C2B-C3B-CAB-CBB
41	U	201	KC2	C2B-C3B-CAB-CBB
41	Z	308	KC2	C2C-C3C-CAC-CBC
41	w	301	KC2	C2C-C3C-CAC-CBC
41	z	304	KC2	C2C-C3C-CAC-CBC
41	z	309	KC2	C2B-C3B-CAB-CBB
40	a	811	CLA	CBD-CGD-O2D-CED
40	a	824	CLA	CAA-CBA-CGA-O1A
40	a	838	CLA	CAA-CBA-CGA-O1A
40	v	307	CLA	CAA-CBA-CGA-O1A
40	w	305	CLA	CAA-CBA-CGA-O1A
40	x	306	CLA	CAA-CBA-CGA-O1A
43	a	801	LMG	C17-C18-C19-C20
40	A	306	CLA	CAD-CBD-CGD-O2D
40	A	307	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
40	D	303	CLA	CAD-CBD-CGD-O2D
40	D	306	CLA	CAD-CBD-CGD-O2D
40	E	305	CLA	CAD-CBD-CGD-O2D
40	M	311	CLA	CAD-CBD-CGD-O2D
40	O	310	CLA	CAD-CBD-CGD-O2D
40	P	305	CLA	CAD-CBD-CGD-O2D
40	a	840	CLA	CAD-CBD-CGD-O2D
40	u	302	CLA	CAD-CBD-CGD-O2D
40	u	305	CLA	CAD-CBD-CGD-O2D
40	u	308	CLA	CAD-CBD-CGD-O2D
40	w	308	CLA	CAD-CBD-CGD-O2D
40	w	309	CLA	CAD-CBD-CGD-O2D
41	R	308	KC2	CAD-CBD-CGD-O2D
41	S	303	KC2	CAD-CBD-CGD-O2D
41	W	304	KC2	CAD-CBD-CGD-O2D
41	X	303	KC2	CAD-CBD-CGD-O2D
41	Y	308	KC2	CAD-CBD-CGD-O2D
44	X	318	A86	C13-C14-C15-C20
47	L	318	A1EB1	C13-C14-C15-C20
47	q	321	A1EB1	C13-C14-C15-C20
47	v	321	A1EB1	C13-C14-C15-C20
48	W	319	A1EB4	C13-C11-C12-O3
40	o	306	CLA	C8-C10-C11-C12
40	a	824	CLA	CAA-CBA-CGA-O2A
40	o	305	CLA	CAA-CBA-CGA-O2A
43	E	301	LMG	O9-C10-C11-C12
52	b	850	DGD	O1B-C1B-C2B-C3B
40	G	204	CLA	C5-C6-C7-C8
40	p	311	CLA	O1A-CGA-O2A-C1
40	R	304	CLA	C2-C1-O2A-CGA
40	Z	310	CLA	C2-C1-O2A-CGA
40	w	303	CLA	C2-C1-O2A-CGA
40	X	310	CLA	CAA-CBA-CGA-O1A
40	b	808	CLA	CAA-CBA-CGA-O1A
40	q	312	CLA	CAA-CBA-CGA-O1A
40	f	201	CLA	CAA-CBA-CGA-O2A
47	Z	319	A1EB1	O6-C42-C44-C45
40	P	313	CLA	C11-C12-C13-C14
40	u	312	CLA	C11-C12-C13-C14
40	v	312	CLA	C11-C12-C13-C14
40	H	302	CLA	C2A-CAA-CBA-CGA
40	a	841	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
40	N	311	CLA	CAA-CBA-CGA-O1A
40	Q	209	CLA	CAA-CBA-CGA-O1A
40	Z	305	CLA	CAA-CBA-CGA-O1A
40	Z	304	CLA	C6-C7-C8-C10
40	M	305	CLA	C4C-C3C-CAC-CBC
40	A	307	CLA	CAA-CBA-CGA-O2A
40	E	314	CLA	CAA-CBA-CGA-O2A
40	L	307	CLA	CAA-CBA-CGA-O2A
40	N	305	CLA	CAA-CBA-CGA-O2A
40	P	307	CLA	CAA-CBA-CGA-O2A
40	U	203	CLA	CAA-CBA-CGA-O2A
40	l	203	CLA	CAA-CBA-CGA-O2A
40	o	306	CLA	CAA-CBA-CGA-O2A
40	w	309	CLA	CAA-CBA-CGA-O2A
40	z	311	CLA	CAA-CBA-CGA-O2A
47	L	318	A1EB1	O6-C42-C44-C45
40	b	822	CLA	C8-C10-C11-C12
40	P	313	CLA	C11-C12-C13-C15
40	X	310	CLA	O1D-CGD-O2D-CED
40	Y	305	CLA	CAA-CBA-CGA-O1A
47	v	323	A1EB1	C44-C45-C46-C47
40	I	202	CLA	CAA-CBA-CGA-O2A
40	P	306	CLA	CAA-CBA-CGA-O2A
40	R	306	CLA	CAA-CBA-CGA-O2A
40	T	306	CLA	CAA-CBA-CGA-O2A
40	Z	307	CLA	CAA-CBA-CGA-O2A
40	i	101	CLA	CAA-CBA-CGA-O2A
40	y	304	CLA	CAA-CBA-CGA-O2A
43	x	301	LMG	O8-C28-C29-C30
47	w	314	A1EB1	O6-C42-C44-C45
40	I	205	CLA	CAA-CBA-CGA-O1A
40	L	307	CLA	CAA-CBA-CGA-O1A
40	T	305	CLA	CAA-CBA-CGA-O1A
40	l	203	CLA	CAA-CBA-CGA-O1A
47	t	315	A1EB1	O43-C42-C44-C45
47	w	314	A1EB1	O43-C42-C44-C45

All (21) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	t	311	A86	C31-C32-C33-C34-C35-C36
44	X	314	A86	C31-C32-C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
44	C	311	A86	C31-C32-C33-C34-C35-C36
44	Z	317	A86	C31-C32-C33-C34-C35-C36
44	Z	316	A86	C31-C32-C33-C34-C35-C36
44	M	315	A86	C31-C32-C33-C34-C35-C36
47	v	321	A1EB1	C31-C32-C33-C34-C35-C36
44	T	315	A86	C31-C32-C33-C34-C35-C36
47	o	321	A1EB1	C31-C32-C33-C34-C35-C36
47	S	321	A1EB1	C31-C32-C33-C34-C35-C36
44	z	316	A86	C31-C32-C33-C34-C35-C36
44	q	316	A86	C31-C32-C33-C34-C35-C36
47	v	323	A1EB1	C31-C32-C33-C34-C35-C36
47	S	320	A1EB1	C31-C32-C33-C34-C35-C36
47	q	321	A1EB1	C31-C32-C33-C34-C35-C36
47	t	314	A1EB1	C31-C32-C33-C34-C35-C36
44	z	318	A86	C31-C32-C33-C34-C35-C36
47	K	315	A1EB1	C31-C32-C33-C34-C35-C36
47	O	317	A1EB1	C31-C32-C33-C34-C35-C36
44	w	315	A86	C31-C32-C33-C34-C35-C36
44	v	316	A86	C31-C32-C33-C34-C35-C36

264 monomers are involved in 562 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	K	301	CLA	2	0
40	Q	206	CLA	9	0
40	H	307	CLA	1	0
40	W	305	CLA	1	0
44	D	319	A86	1	0
40	o	307	CLA	1	0
40	U	203	CLA	1	0
40	w	308	CLA	5	0
41	N	302	KC2	1	0
40	F	306	CLA	1	0
42	x	320	DD6	2	0
44	P	317	A86	1	0
40	J	318	CLA	2	0
42	O	314	DD6	1	0
40	V	201	CLA	2	0
40	a	824	CLA	1	0
40	S	308	CLA	3	0
42	H	312	DD6	1	0
40	M	307	CLA	1	0
47	x	322	A1EB1	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	a	809	CLA	1	0
49	f	206	BCR	4	0
42	u	321	DD6	1	0
44	X	317	A86	3	0
40	A	305	CLA	3	0
42	J	315	DD6	1	0
40	b	820	CLA	1	0
42	I	210	DD6	1	0
40	L	305	CLA	1	0
49	b	846	BCR	1	0
41	w	307	KC2	1	0
47	P	301	A1EB1	9	0
47	t	315	A1EB1	1	0
40	Q	204	CLA	1	0
40	N	304	CLA	1	0
40	D	304	CLA	1	0
40	a	819	CLA	21	0
40	b	810	CLA	2	0
40	z	305	CLA	3	0
40	A	311	CLA	3	0
40	H	301	CLA	1	0
40	f	202	CLA	3	0
40	C	307	CLA	2	0
41	X	303	KC2	1	0
47	K	315	A1EB1	1	0
40	a	815	CLA	12	0
40	Q	207	CLA	1	0
42	p	322	DD6	1	0
43	D	318	LMG	1	0
41	T	308	KC2	1	0
44	W	301	A86	1	0
40	b	826	CLA	1	0
41	z	304	KC2	1	0
43	u	301	LMG	1	0
40	b	834	CLA	2	0
40	b	839	CLA	1	0
40	S	319	CLA	1	0
47	v	324	A1EB1	4	0
40	L	306	CLA	7	0
40	i	101	CLA	4	0
47	q	322	A1EB1	1	0
40	D	307	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	t	308	KC2	1	0
42	N	316	DD6	1	0
42	Y	322	DD6	9	0
40	v	311	CLA	1	0
44	y	310	A86	1	0
40	S	312	CLA	6	0
46	P	319	SQD	5	0
40	z	306	CLA	1	0
49	b	847	BCR	1	0
40	b	824	CLA	2	0
40	A	302	CLA	2	0
42	v	320	DD6	1	0
40	C	302	CLA	1	0
40	G	213	CLA	2	0
40	o	311	CLA	1	0
41	W	310	KC2	1	0
44	Y	315	A86	1	0
44	Q	210	A86	1	0
40	a	850	CLA	1	0
40	b	828	CLA	1	0
43	x	301	LMG	5	0
40	N	306	CLA	1	0
40	v	312	CLA	2	0
40	E	311	CLA	6	0
43	E	321	LMG	3	0
40	E	307	CLA	12	0
40	a	814	CLA	1	0
40	a	823	CLA	1	0
40	w	305	CLA	1	0
41	y	306	KC2	7	0
41	M	303	KC2	1	0
40	o	301	CLA	1	0
41	T	301	KC2	1	0
43	E	320	LMG	2	0
40	l	202	CLA	2	0
40	y	302	CLA	1	0
44	L	314	A86	1	0
40	z	302	CLA	1	0
46	W	318	SQD	4	0
44	t	310	A86	1	0
41	O	301	KC2	1	0
41	Y	308	KC2	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	a	832	CLA	2	0
40	P	306	CLA	1	0
42	Q	214	DD6	1	0
44	o	315	A86	1	0
42	L	315	DD6	15	0
43	j	101	LMG	13	0
47	t	314	A1EB1	1	0
40	v	301	CLA	1	0
44	W	314	A86	1	0
47	u	322	A1EB1	1	0
47	x	321	A1EB1	1	0
40	p	305	CLA	1	0
40	S	301	CLA	9	0
41	Z	309	KC2	1	0
42	P	315	DD6	5	0
40	a	842	CLA	1	0
40	b	807	CLA	1	0
41	C	303	KC2	1	0
40	D	303	CLA	1	0
40	l	203	CLA	1	0
42	M	314	DD6	1	0
40	a	817	CLA	1	0
44	M	315	A86	1	0
40	b	803	CLA	1	0
44	G	209	A86	3	0
40	R	305	CLA	1	0
47	Z	321	A1EB1	1	0
42	w	312	DD6	26	0
40	M	305	CLA	1	0
41	Z	303	KC2	1	0
49	r	201	BCR	1	0
40	k	202	CLA	16	0
40	b	833	CLA	1	0
44	p	318	A86	1	0
40	o	312	CLA	2	0
41	t	306	KC2	14	0
49	m	101	BCR	4	0
41	Q	201	KC2	2	0
40	X	304	CLA	2	0
40	P	305	CLA	3	0
40	a	816	CLA	1	0
40	p	306	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	C	310	DD6	1	0
42	B	305	DD6	1	0
47	v	322	A1EB1	1	0
40	a	830	CLA	1	0
40	F	307	CLA	4	0
47	p	324	A1EB1	1	0
40	B	307	CLA	3	0
40	W	312	CLA	2	0
42	F	314	DD6	1	0
40	D	311	CLA	2	0
40	b	809	CLA	3	0
40	P	313	CLA	1	0
46	k	205	SQD	3	0
40	b	827	CLA	1	0
41	Q	216	KC2	8	0
40	E	306	CLA	8	0
42	y	311	DD6	17	0
42	o	320	DD6	2	0
40	Z	305	CLA	1	0
49	l	208	BCR	1	0
41	L	303	KC2	1	0
40	S	313	CLA	1	0
44	Z	316	A86	1	0
45	S	323	LHG	2	0
40	W	311	CLA	1	0
40	A	308	CLA	4	0
40	G	201	CLA	1	0
40	L	312	CLA	1	0
42	t	312	DD6	29	0
49	a	845	BCR	1	0
40	R	306	CLA	1	0
40	S	314	CLA	1	0
40	q	311	CLA	2	0
40	k	201	CLA	1	0
40	N	305	CLA	1	0
41	P	303	KC2	1	0
40	b	832	CLA	2	0
40	f	205	CLA	4	0
40	E	302	CLA	1	0
40	l	205	CLA	1	0
47	y	313	A1EB1	4	0
40	K	306	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	x	306	CLA	1	0
40	a	835	CLA	1	0
40	L	307	CLA	1	0
40	T	305	CLA	1	0
40	S	305	CLA	5	0
44	z	319	A86	1	0
43	a	802	LMG	1	0
50	b	849	PQN	2	0
49	l	207	BCR	3	0
41	w	306	KC2	12	0
40	G	203	CLA	1	0
44	Y	320	A86	1	0
40	b	802	CLA	2	0
40	t	305	CLA	1	0
47	p	323	A1EB1	1	0
40	b	829	CLA	2	0
42	D	317	DD6	1	0
40	b	813	CLA	2	0
48	W	319	A1EB4	7	0
46	I	215	SQD	2	0
43	a	801	LMG	2	0
40	b	819	CLA	1	0
40	a	808	CLA	1	0
40	y	305	CLA	1	0
40	K	308	CLA	2	0
41	M	301	KC2	1	0
41	y	307	KC2	1	0
40	F	301	CLA	7	0
42	J	316	DD6	15	0
46	F	320	SQD	2	0
40	x	305	CLA	1	0
42	I	212	DD6	1	0
52	b	850	DGD	7	0
40	Z	306	CLA	1	0
42	L	317	DD6	17	0
46	M	318	SQD	1	0
40	V	202	CLA	4	0
40	b	806	CLA	3	0
40	D	306	CLA	1	0
44	w	316	A86	1	0
40	b	835	CLA	3	0
40	A	306	CLA	12	0

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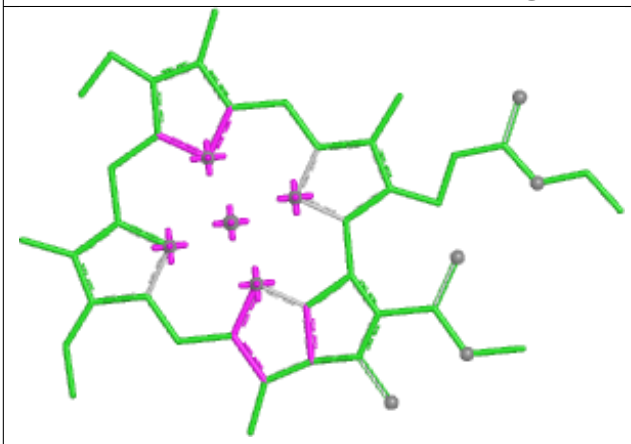
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	v	308	KC2	1	0
40	C	306	CLA	1	0
41	T	303	KC2	1	0
47	u	323	A1EB1	1	0
44	Y	319	A86	1	0
43	E	301	LMG	1	0
40	E	303	CLA	4	0
49	a	843	BCR	5	0
42	A	316	DD6	10	0
42	v	318	DD6	4	0
40	E	308	CLA	4	0
40	P	308	CLA	6	0
40	F	305	CLA	1	0
44	N	315	A86	7	0
41	o	308	KC2	1	0
42	q	320	DD6	1	0
40	N	310	CLA	1	0
40	W	306	CLA	1	0
49	a	846	BCR	1	0
49	i	102	BCR	3	0
40	D	305	CLA	1	0
50	a	847	PQN	1	0
42	q	318	DD6	6	0
42	W	315	DD6	1	0
40	y	308	CLA	5	0
40	x	312	CLA	1	0
40	j	102	CLA	2	0
40	J	309	CLA	12	0
48	P	320	A1EB4	4	0
40	K	307	CLA	1	0
40	b	814	CLA	3	0
40	a	841	CLA	2	0
40	M	311	CLA	1	0
47	T	320	A1EB1	1	0

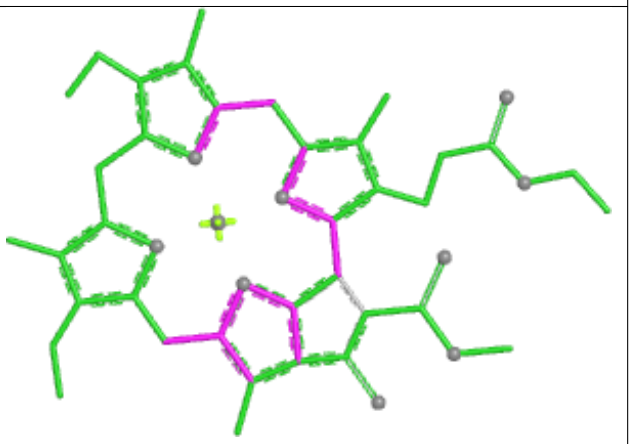
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

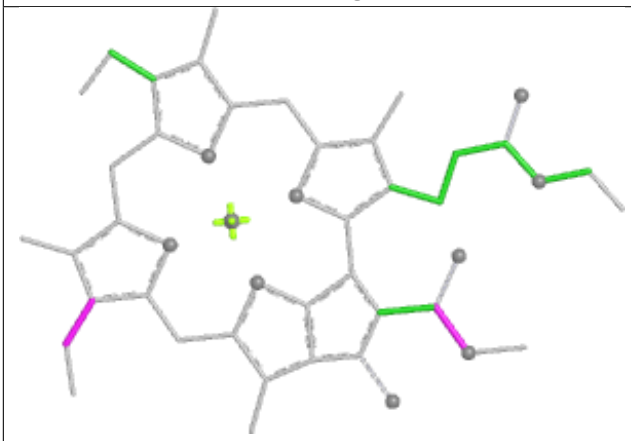
Ligand CLA K 301



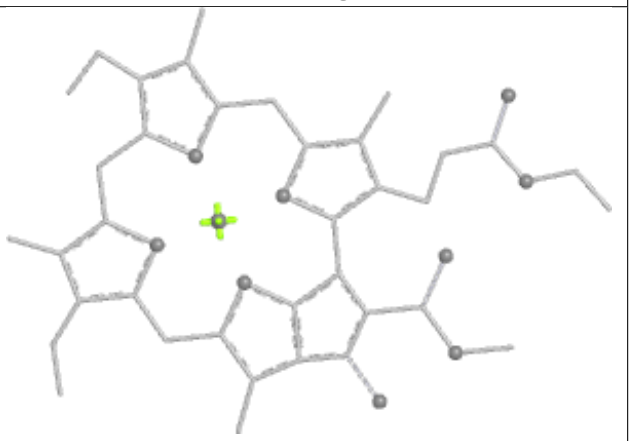
Bond lengths



Bond angles

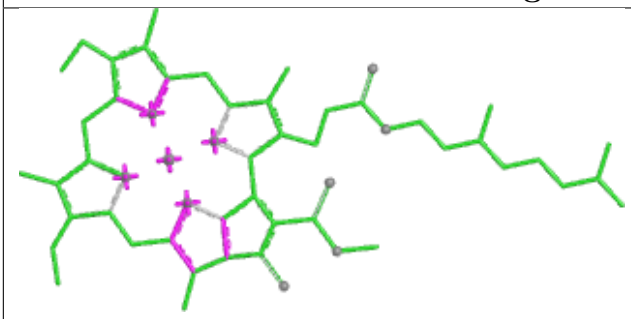


Torsions

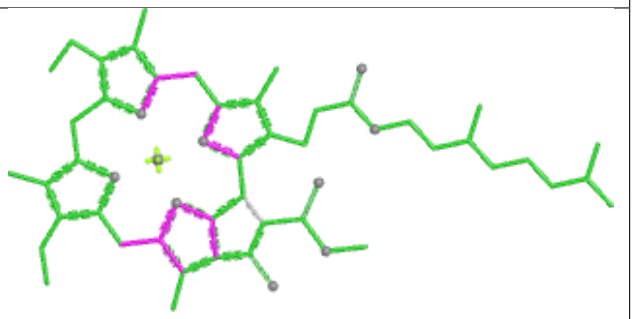


Rings

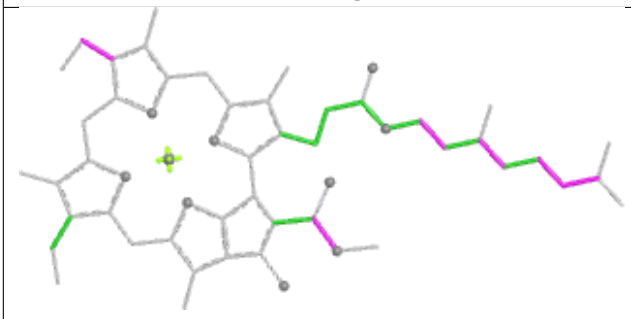
Ligand CLA Y 310



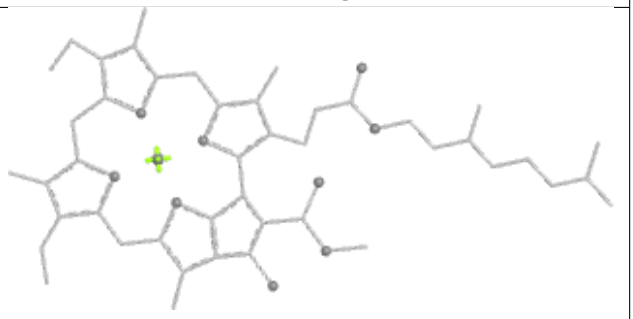
Bond lengths



Bond angles

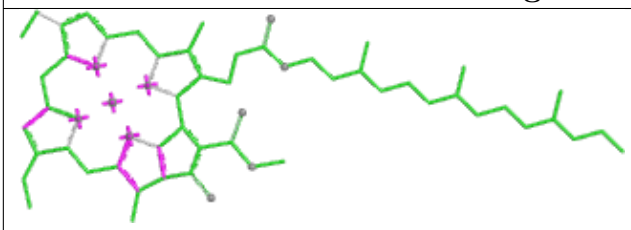


Torsions

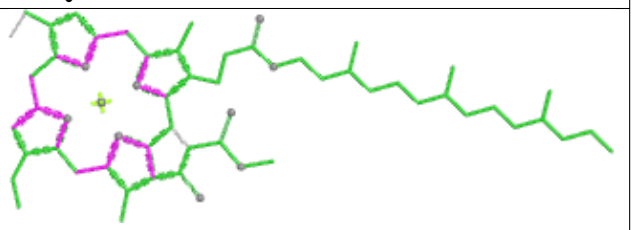


Rings

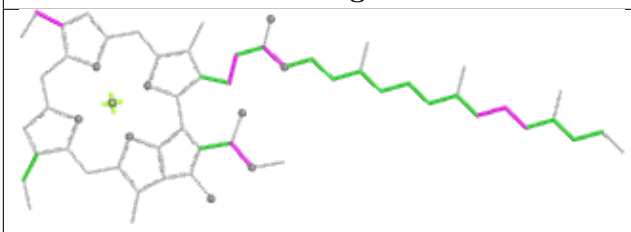
Ligand CLA Q 206



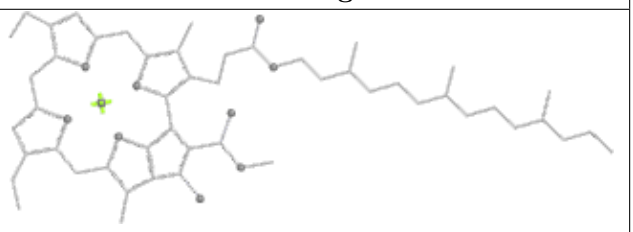
Bond lengths



Bond angles

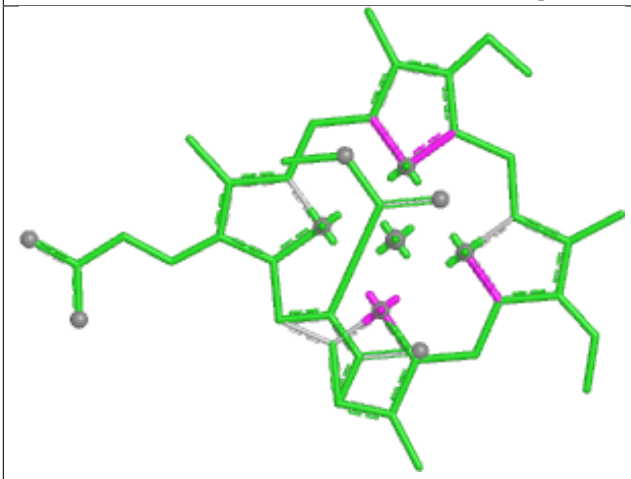


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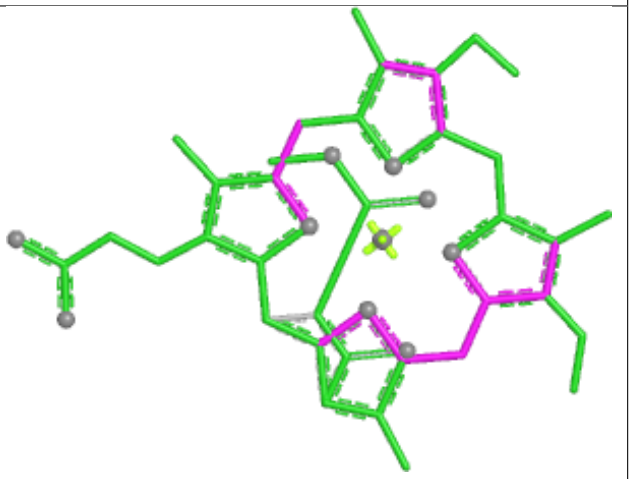


Rings

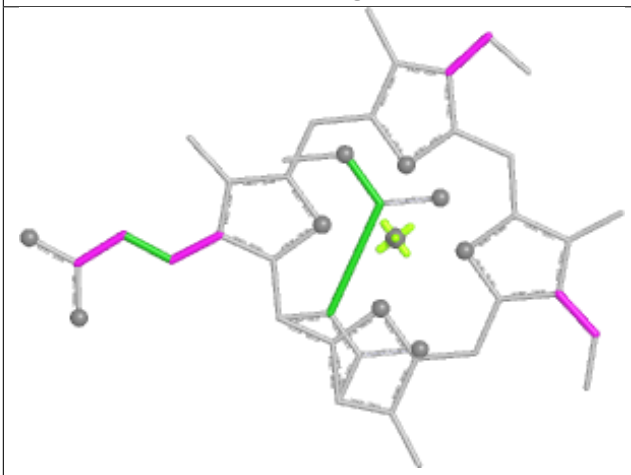
Ligand KC2 I 209



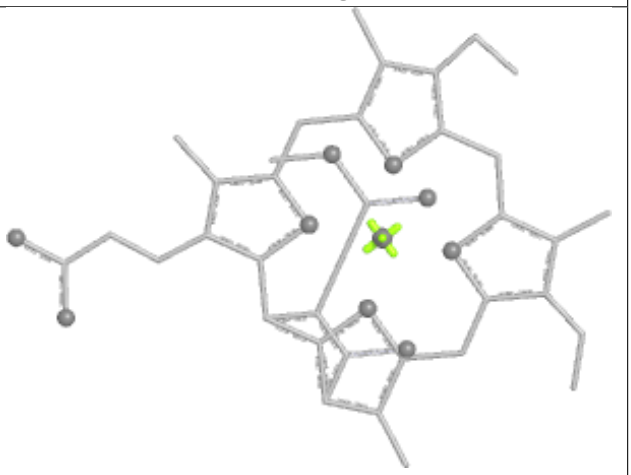
Bond lengths



Bond angles

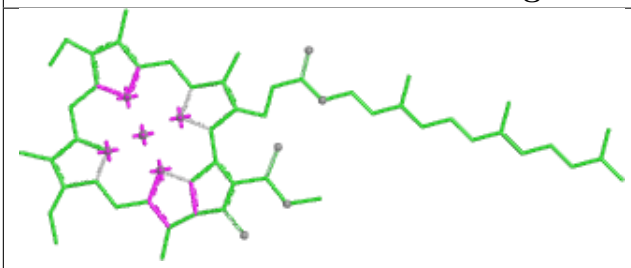


Torsions

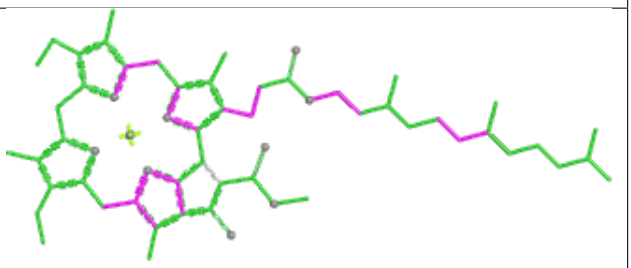


Rings

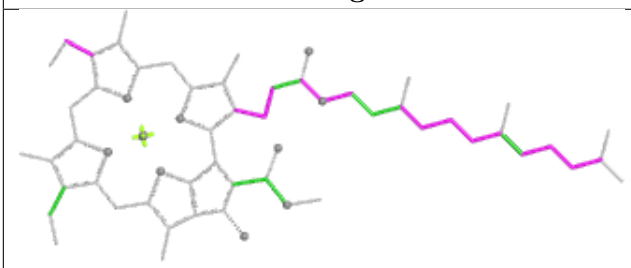
Ligand CLA H 307



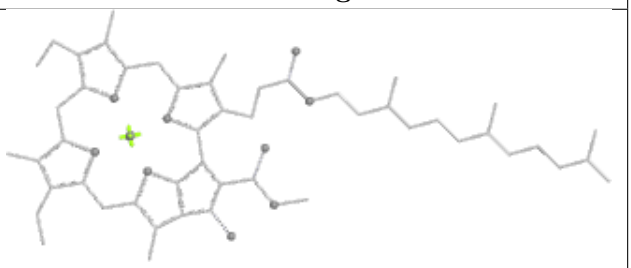
Bond lengths



Bond angles

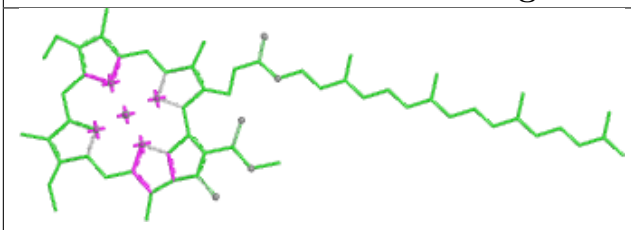


Torsions

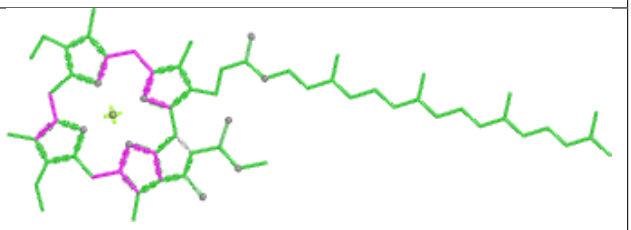


Rings

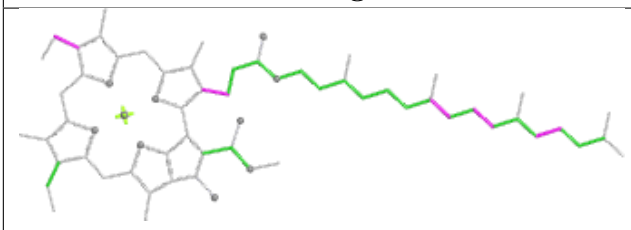
Ligand CLA W 305



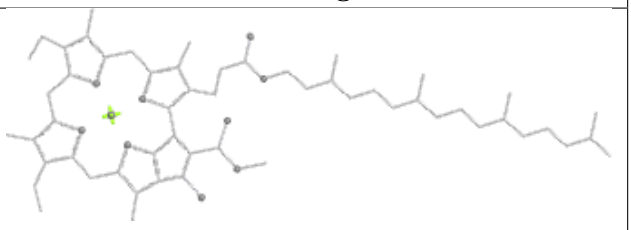
Bond lengths



Bond angles

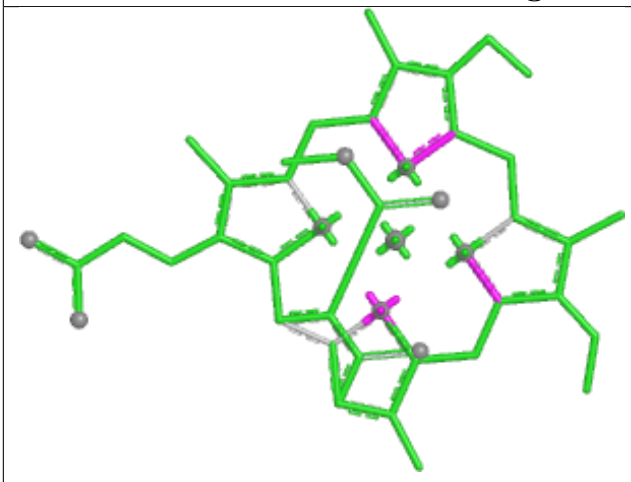


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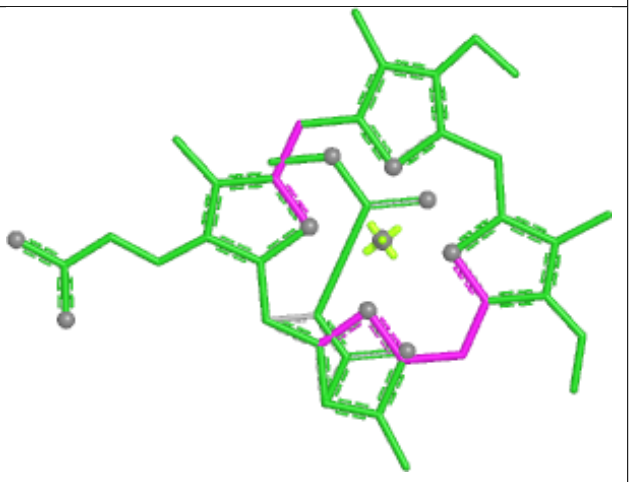


Rings

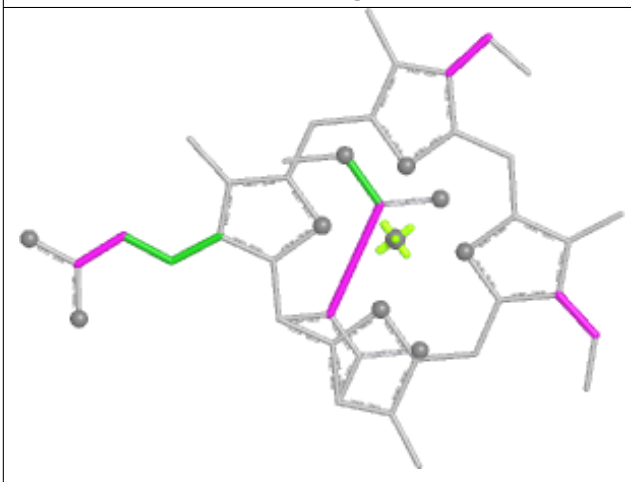
Ligand KC2 R 311



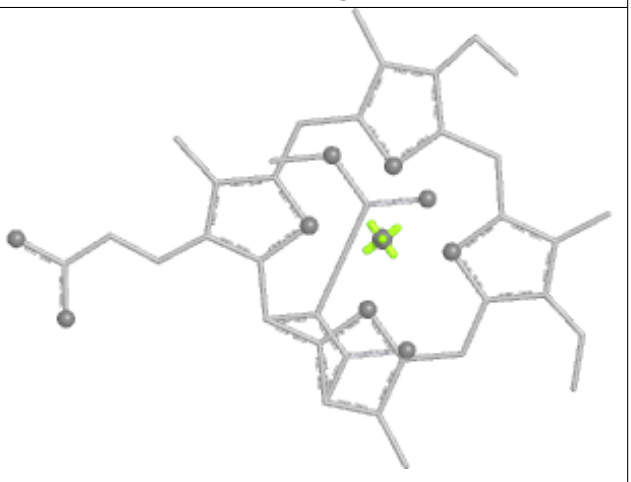
Bond lengths



Bond angles

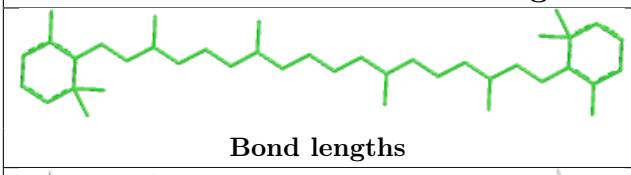


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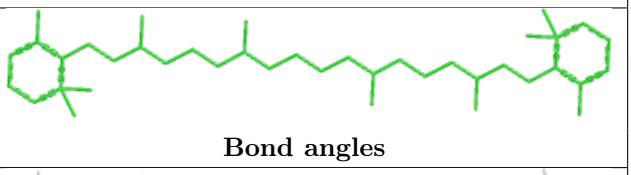


Rings

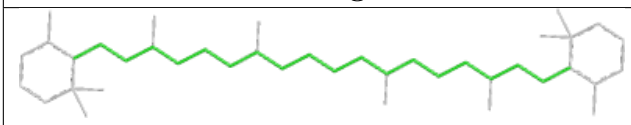
Ligand BCR f 203



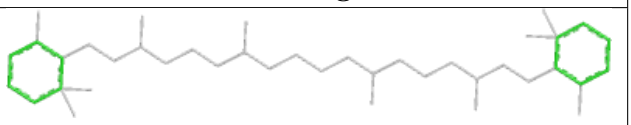
Bond lengths



Bond angles

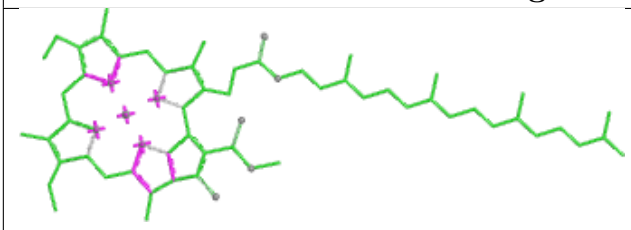


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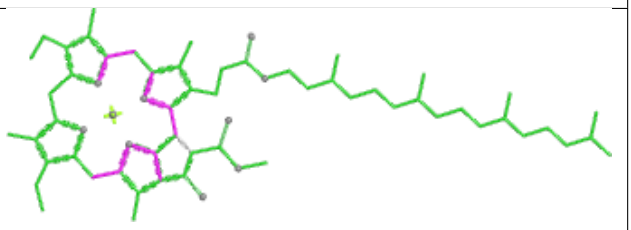


Rings

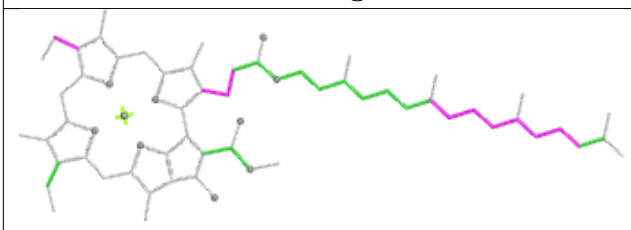
Ligand CLA a 828



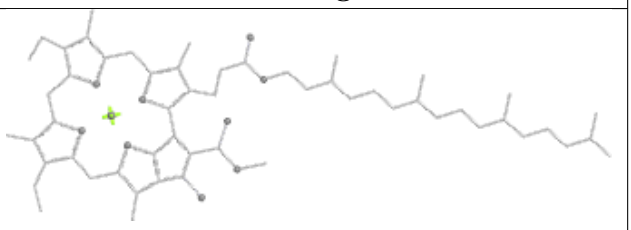
Bond lengths



Bond angles

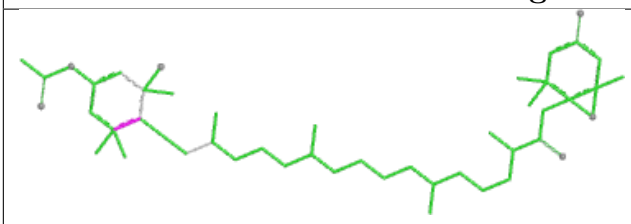


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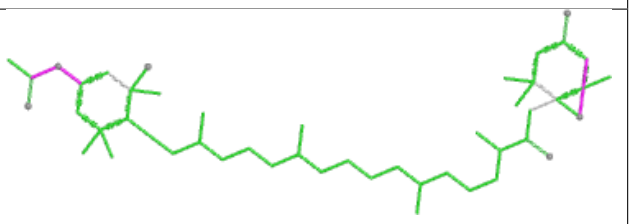


Rings

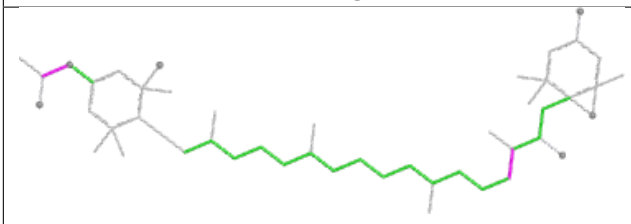
Ligand A86 D 319



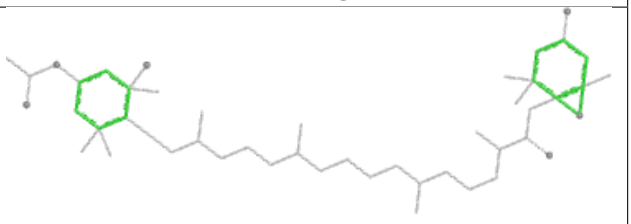
Bond lengths



Bond angles

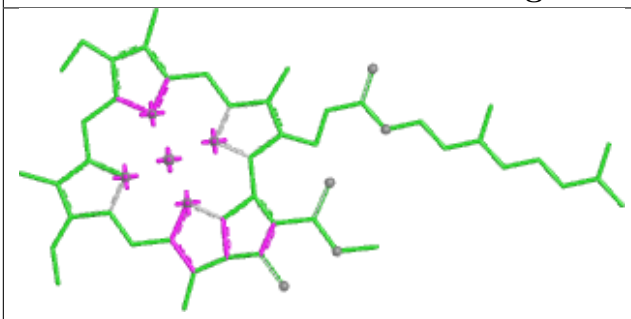


Torsions

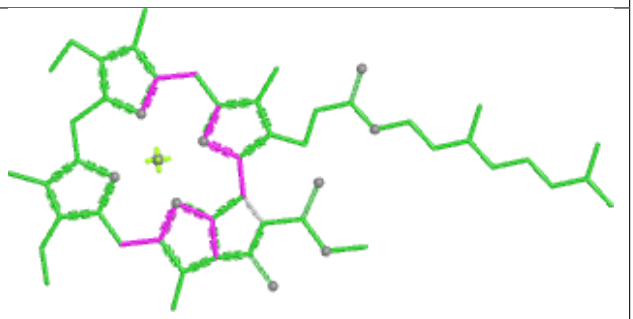


Rings

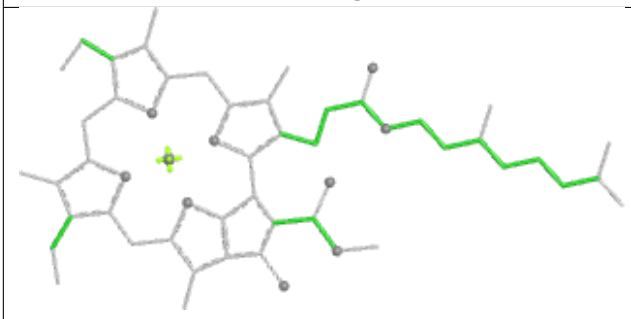
Ligand CLA E 304



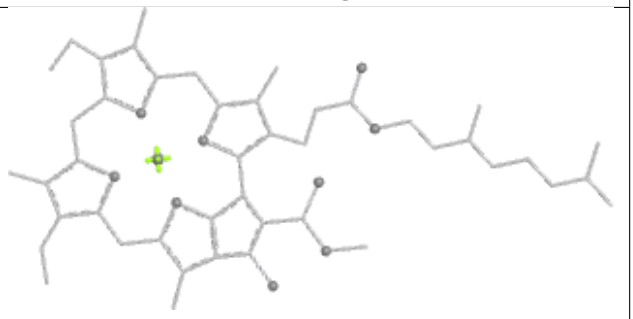
Bond lengths



Bond angles

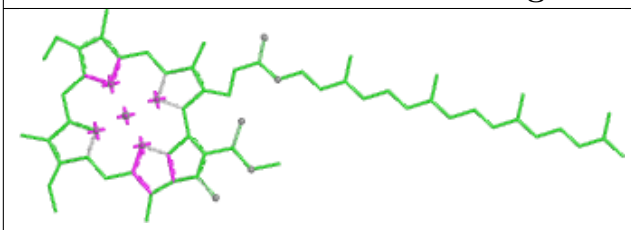


Torsions

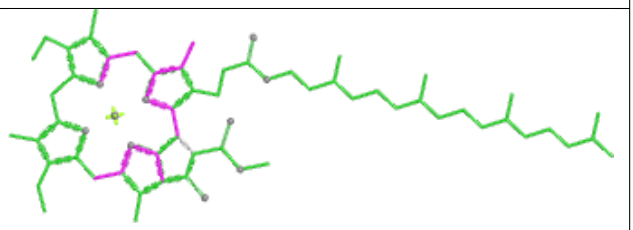


Rings

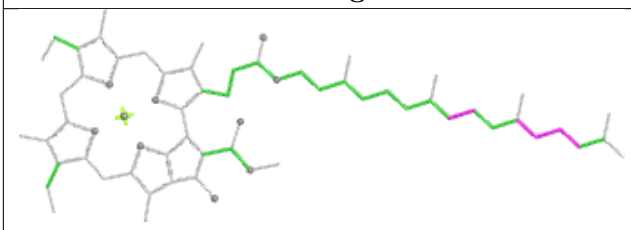
Ligand CLA b 821



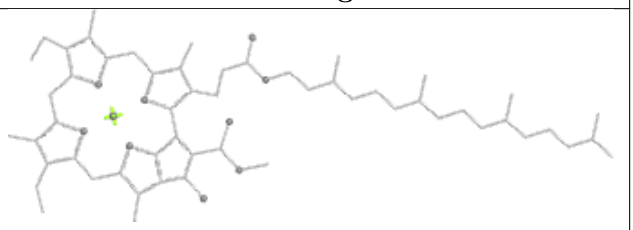
Bond lengths



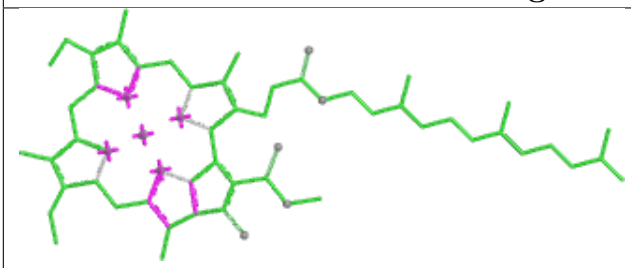
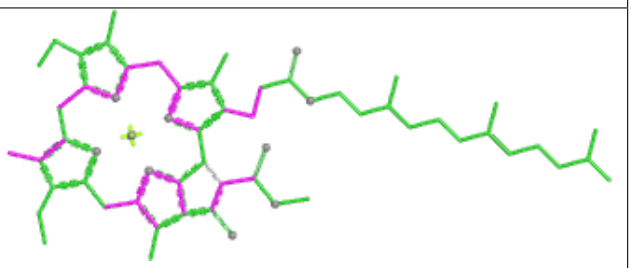
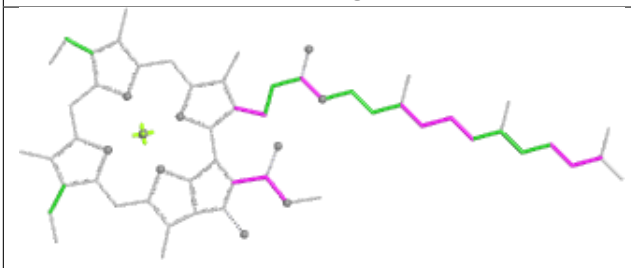
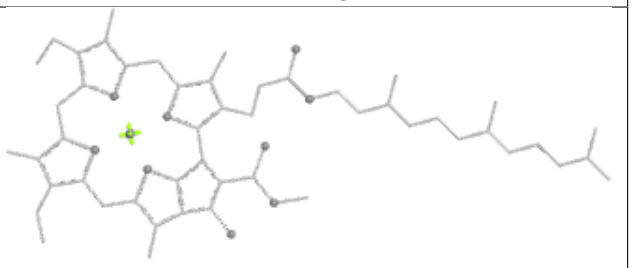
Bond angles

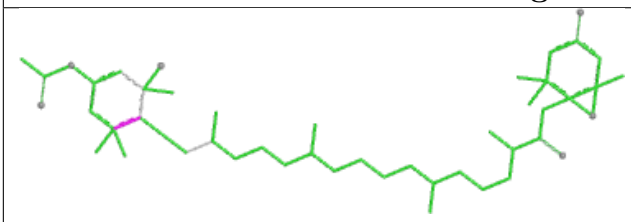
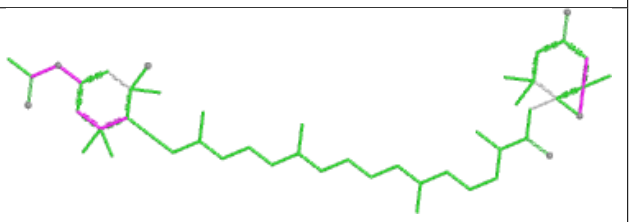
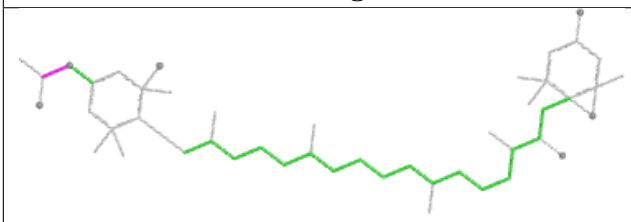
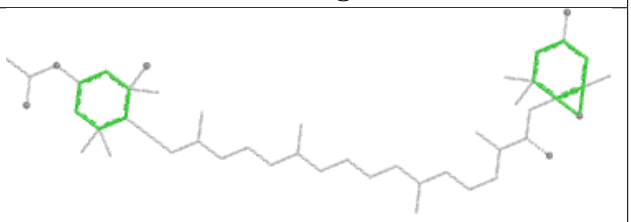


Torsions

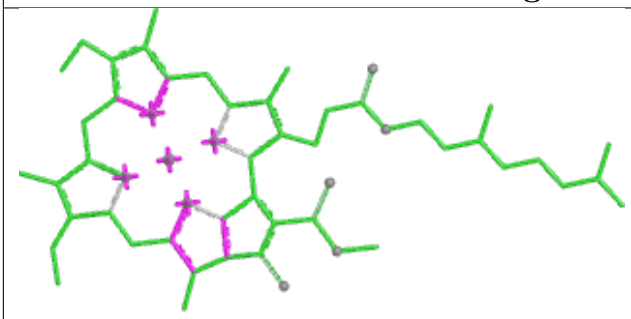


Rings

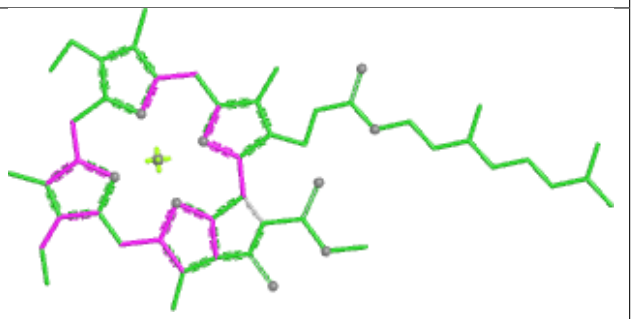
Ligand CLA o 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 T 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

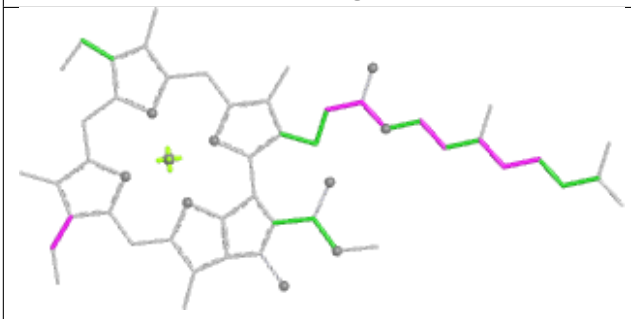
Ligand CLA U 203



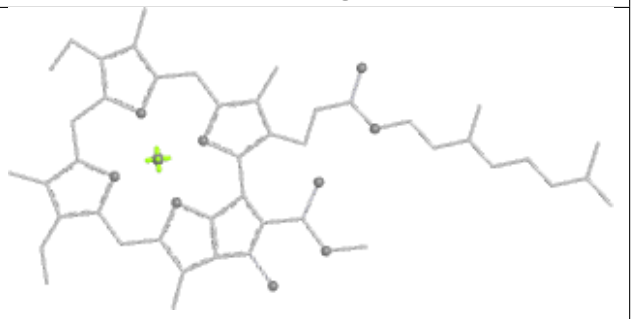
Bond lengths



Bond angles

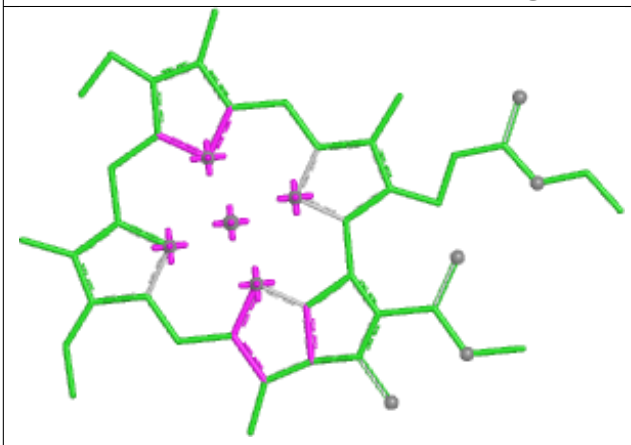


Torsions

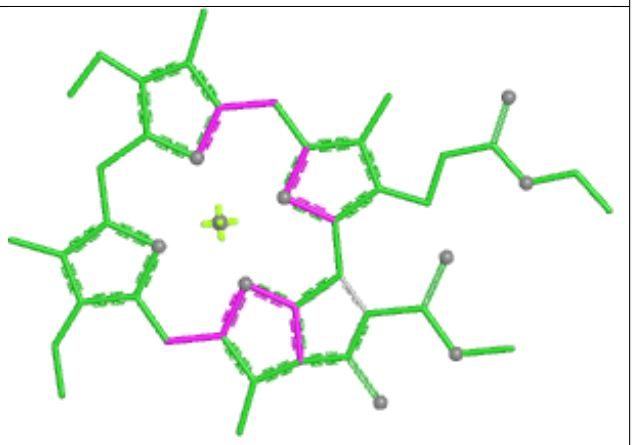


Rings

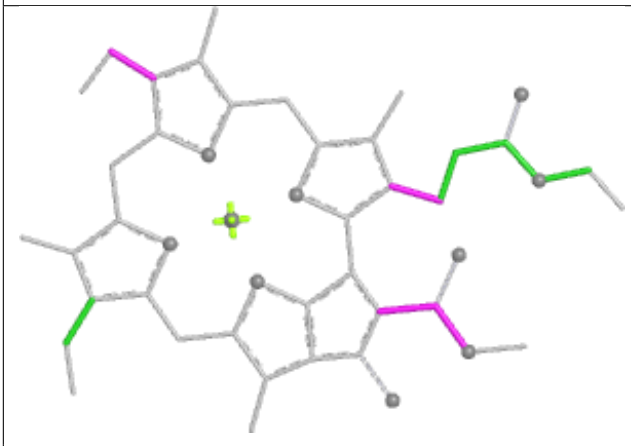
Ligand CLA w 308



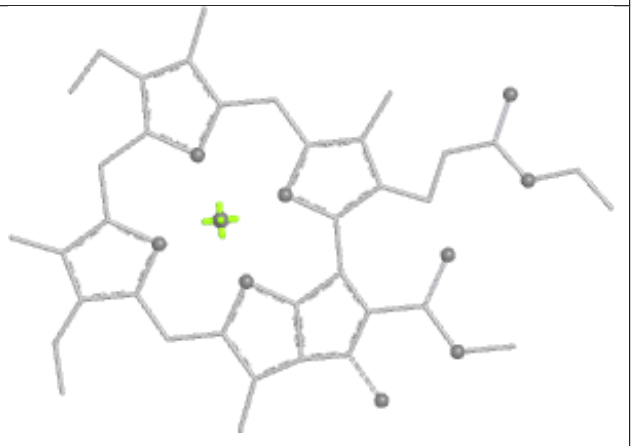
Bond lengths



Bond angles

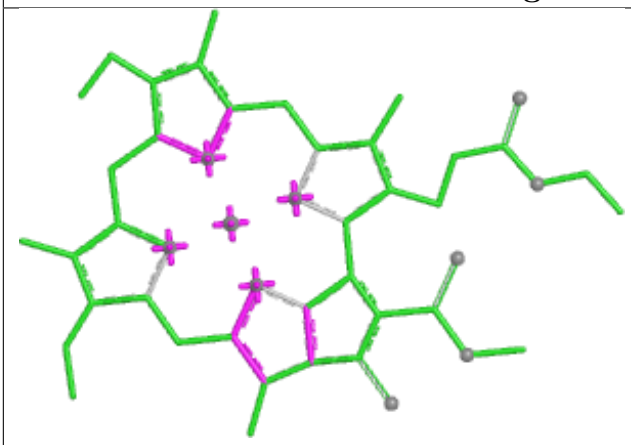


Torsions

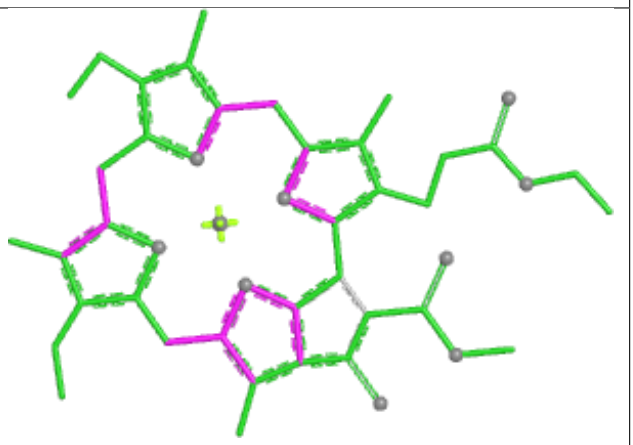


Rings

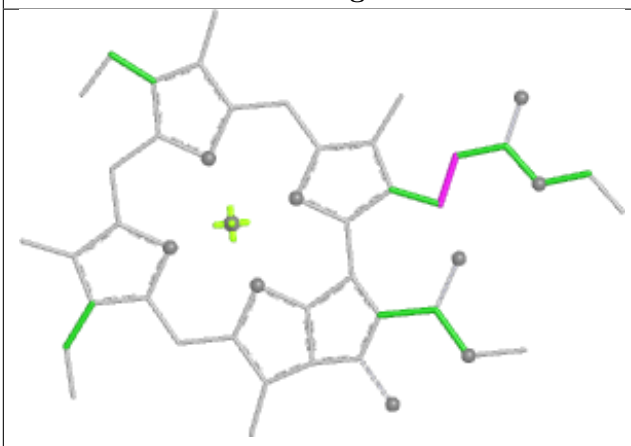
Ligand CLA U 206



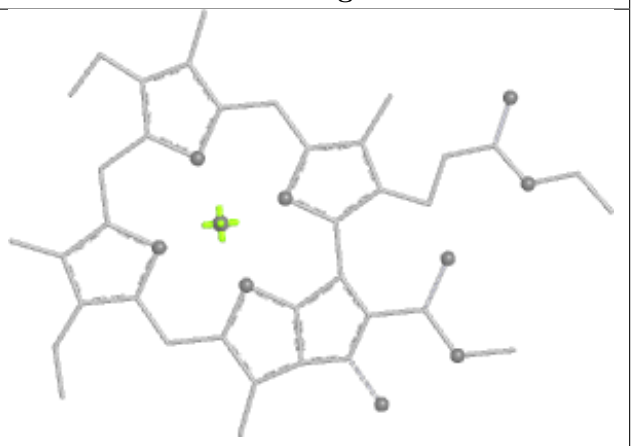
Bond lengths



Bond angles

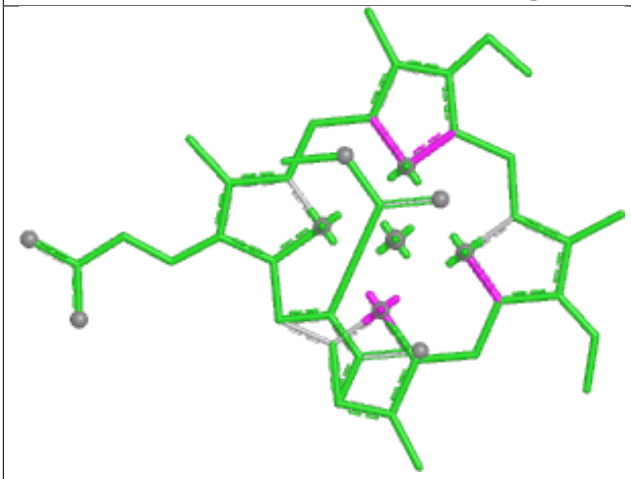


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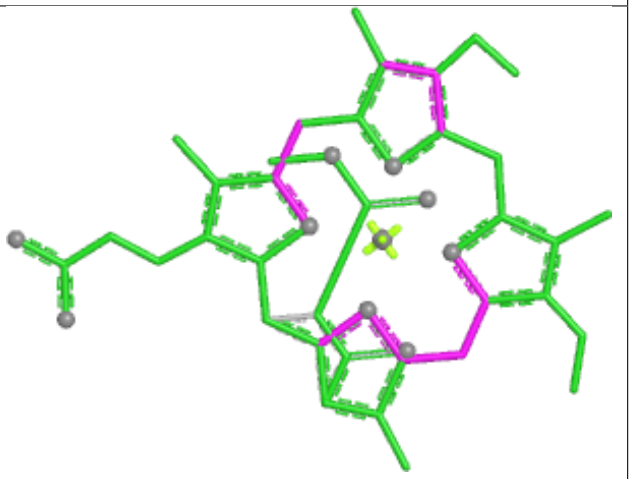


Rings

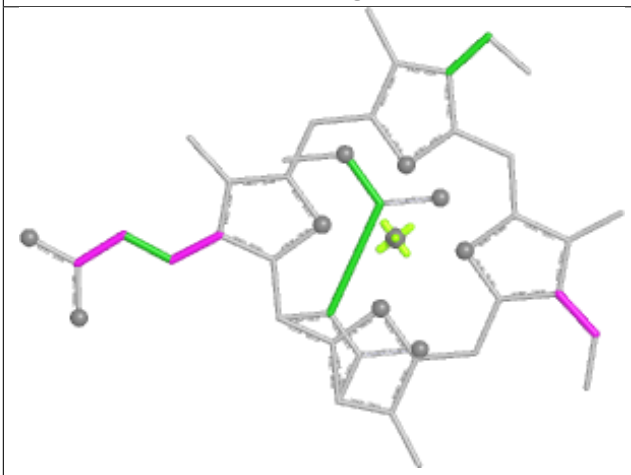
Ligand KC2 N 302



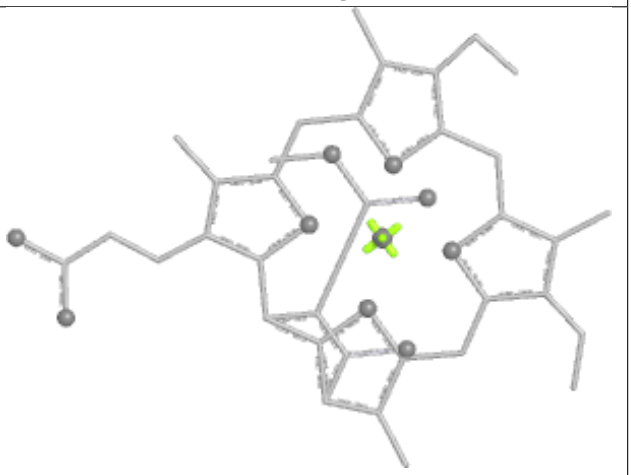
Bond lengths



Bond angles

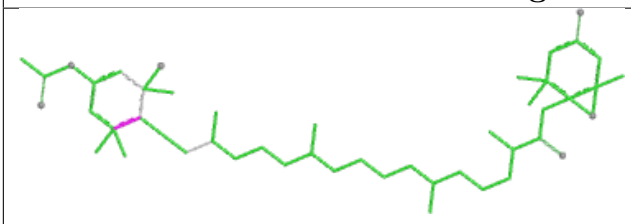


Torsions

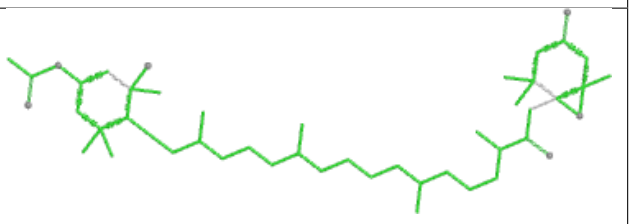


Rings

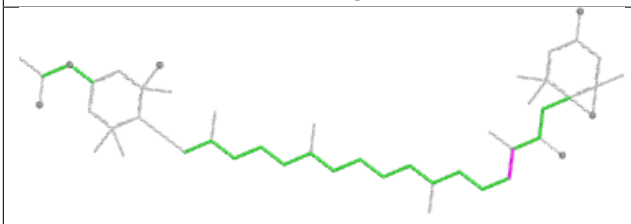
Ligand A86 N 318



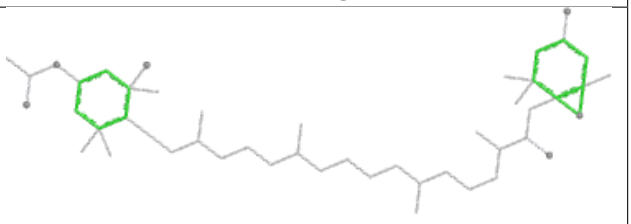
Bond lengths



Bond angles

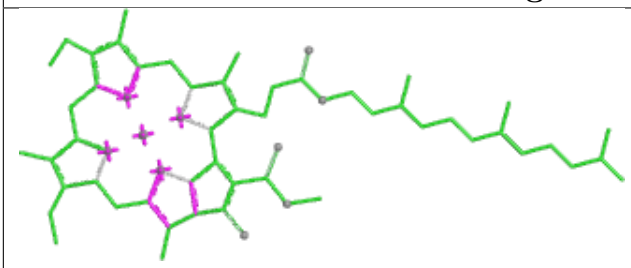


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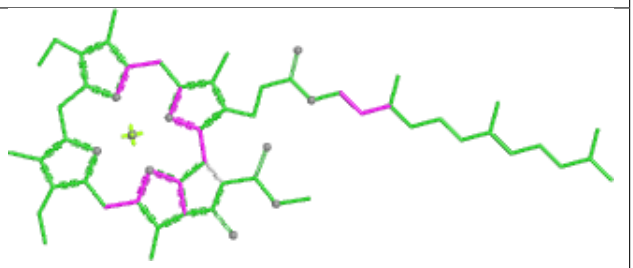


Rings

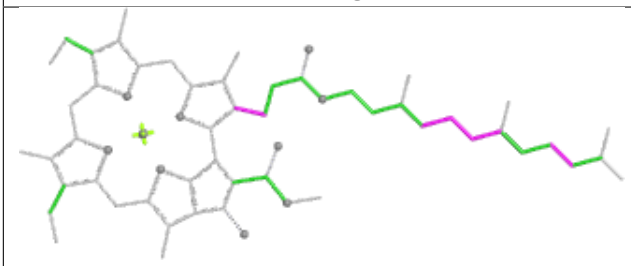
Ligand CLA F 306



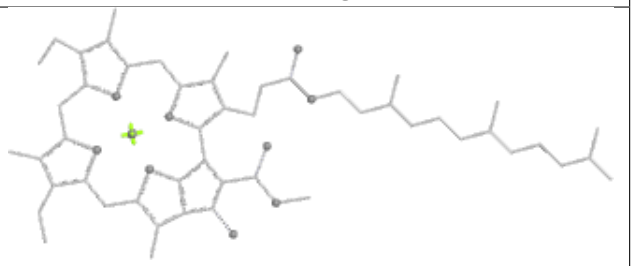
Bond lengths



Bond angles

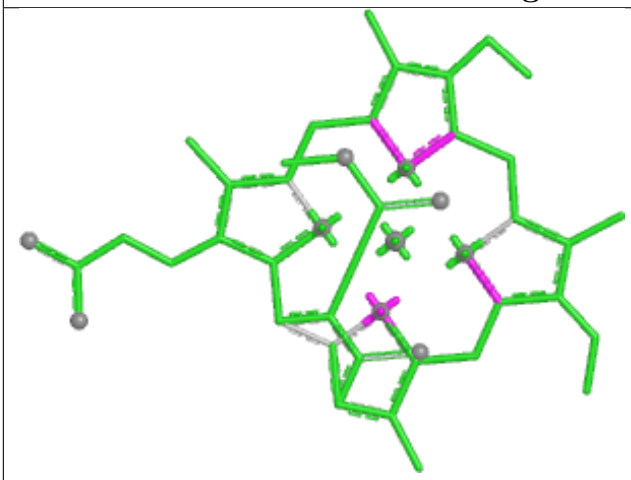


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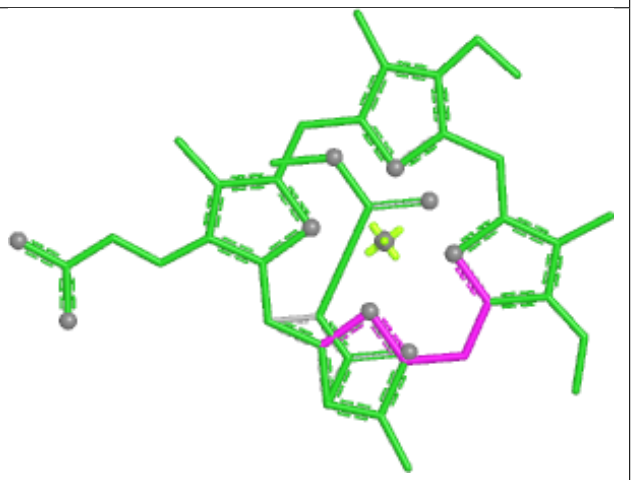


Rings

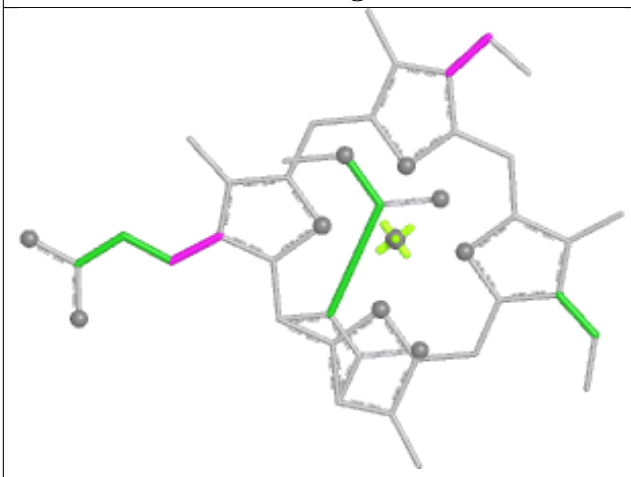
Ligand KC2 M 309



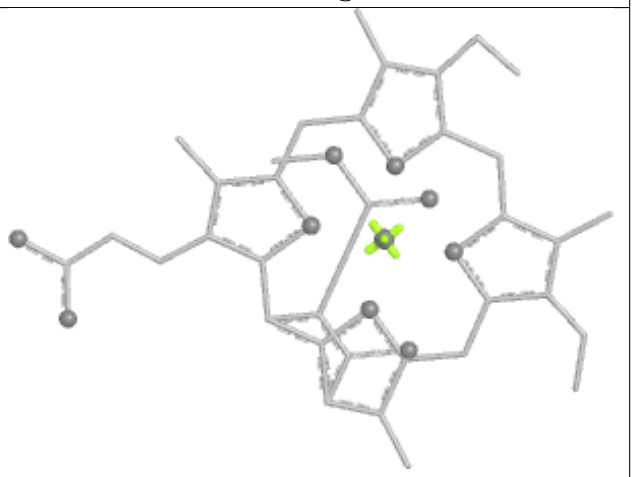
Bond lengths



Bond angles

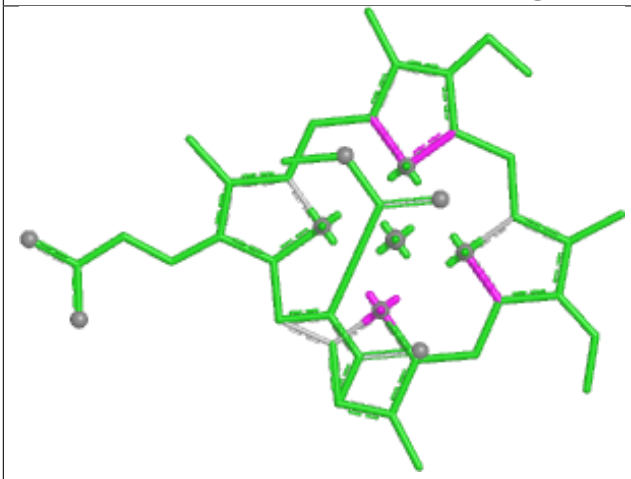


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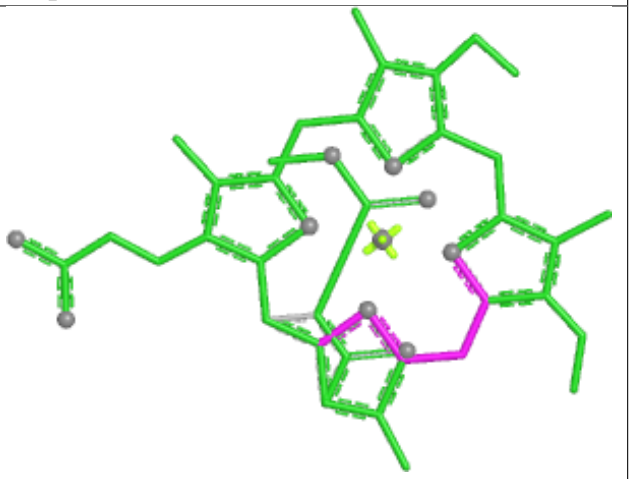


Rings

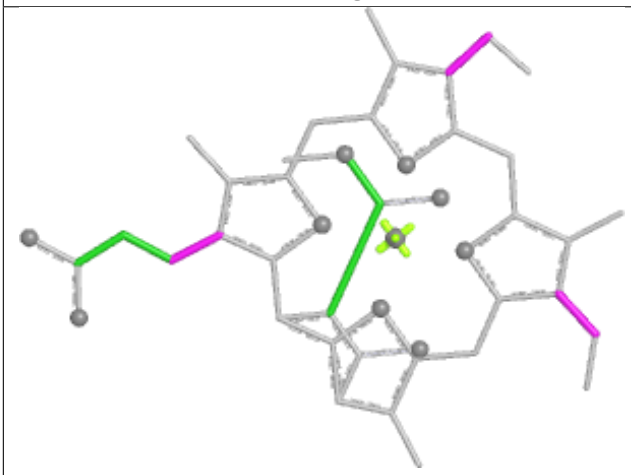
Ligand KC2 p 310



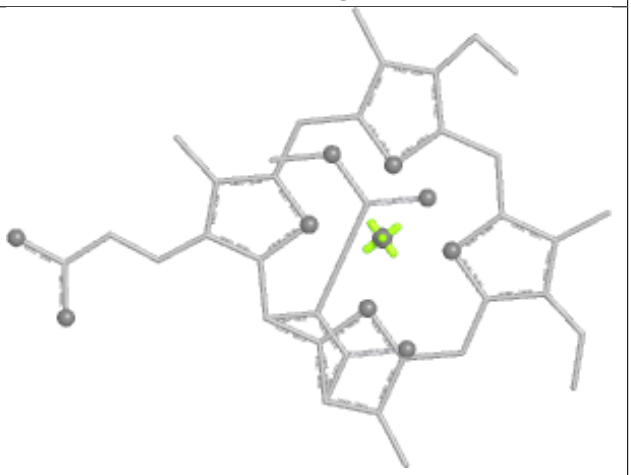
Bond lengths



Bond angles

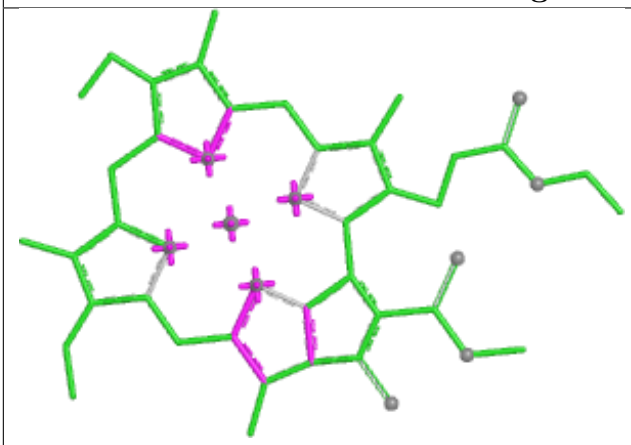


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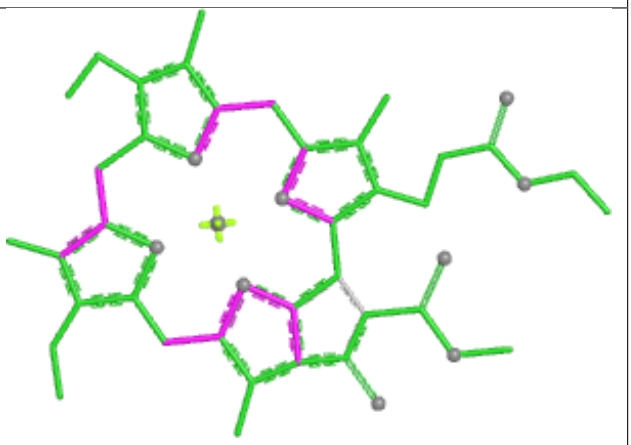


Rings

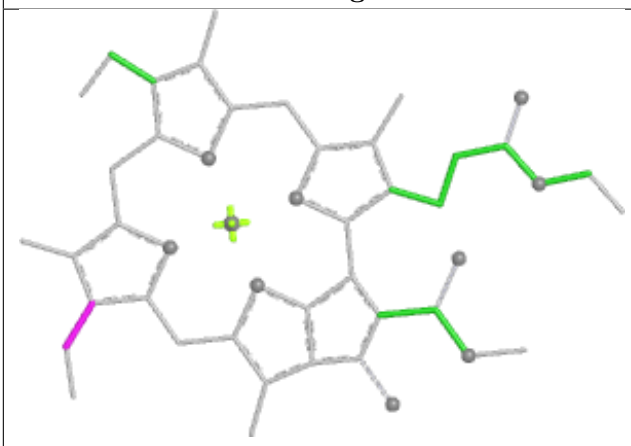
Ligand CLA I 204



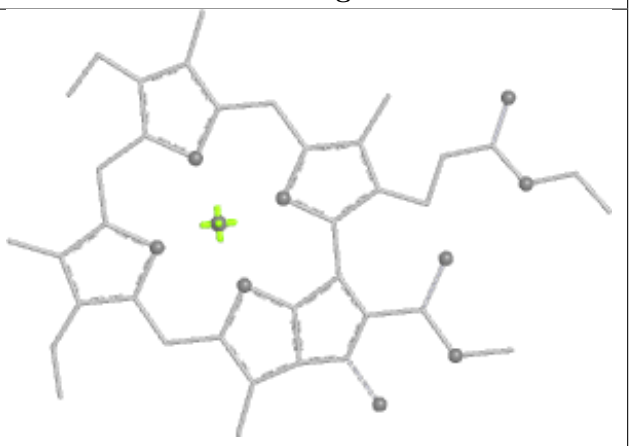
Bond lengths



Bond angles

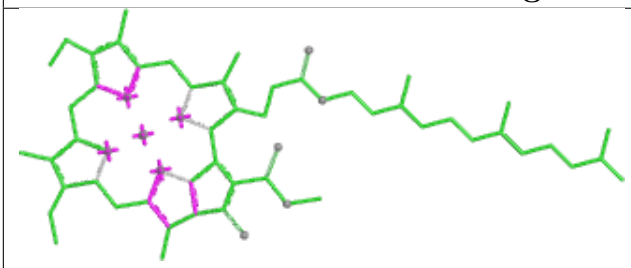


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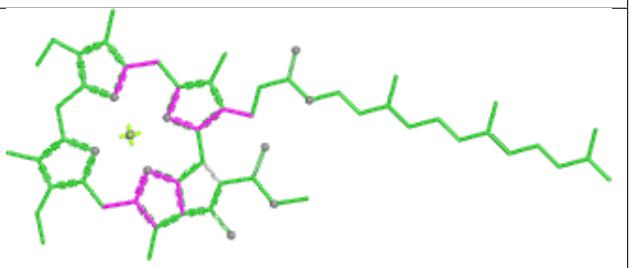


Rings

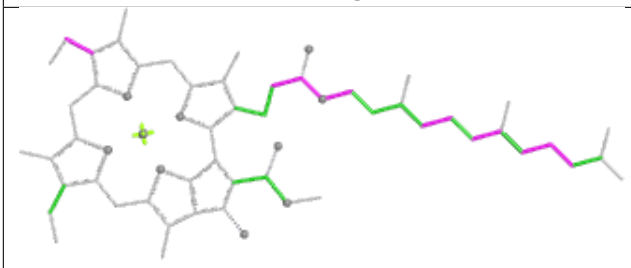
Ligand CLA N 311



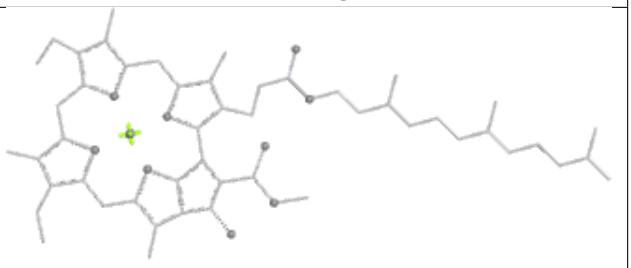
Bond lengths



Bond angles

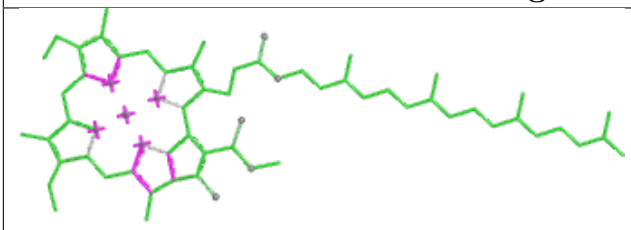


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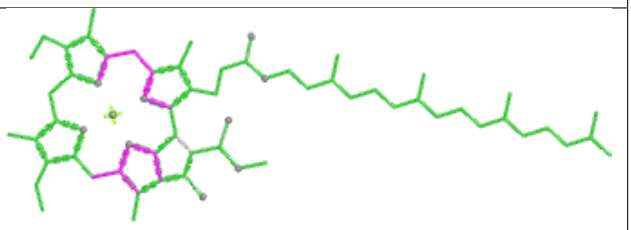


Rings

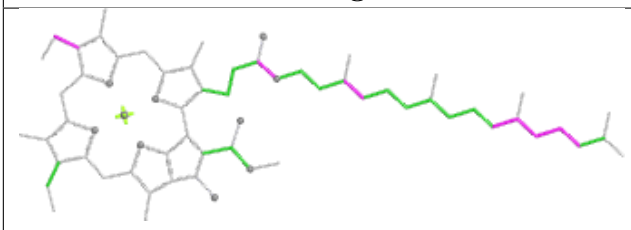
Ligand CLA a 851



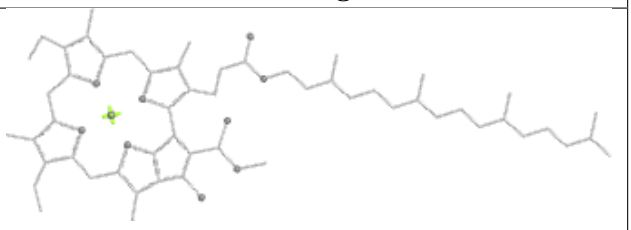
Bond lengths



Bond angles

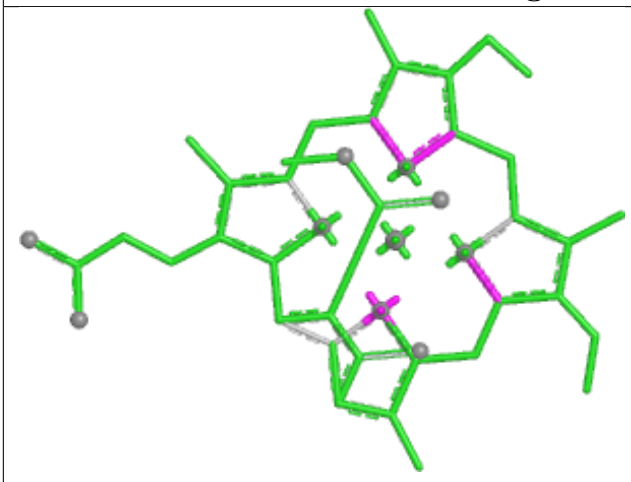


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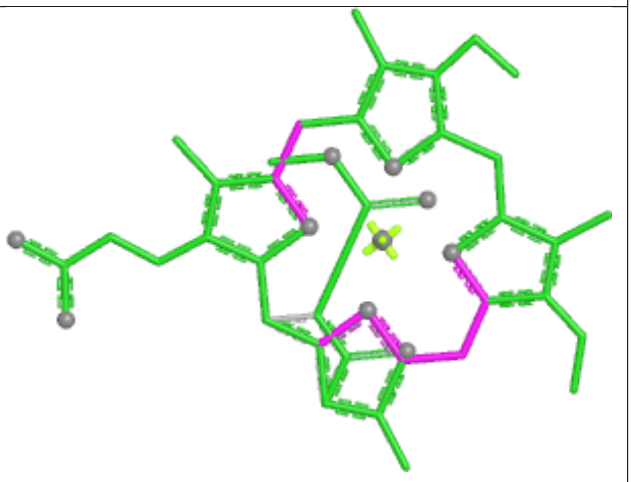


Rings

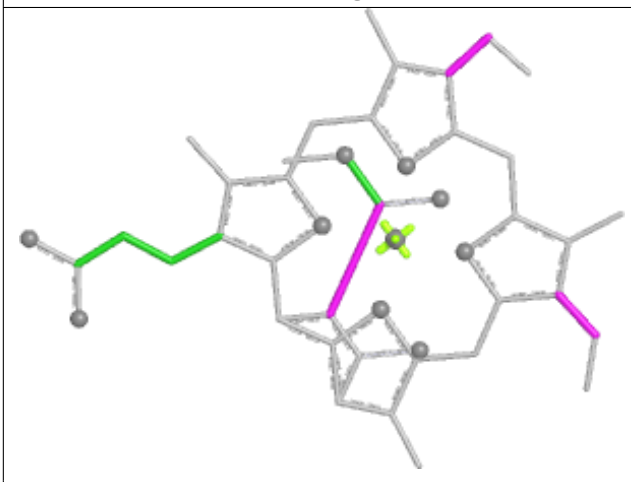
Ligand KC2 U 201



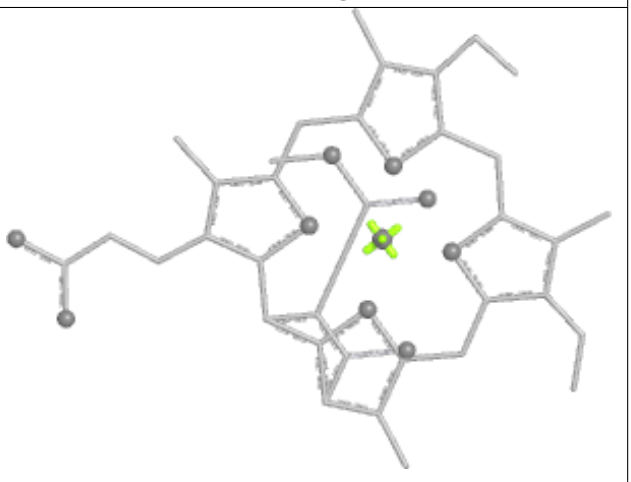
Bond lengths



Bond angles

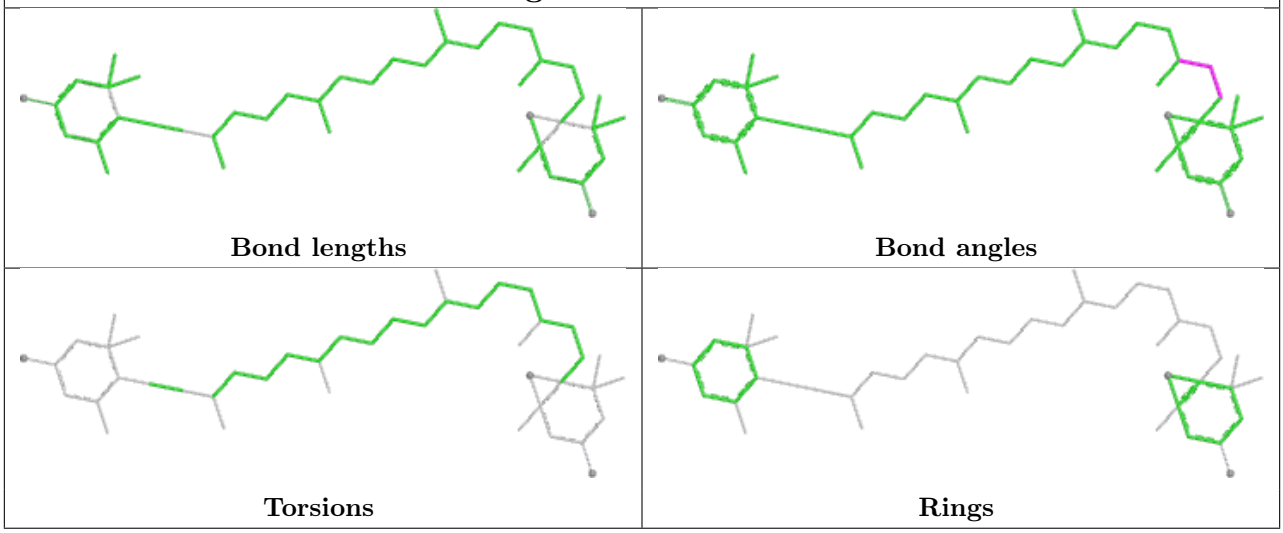


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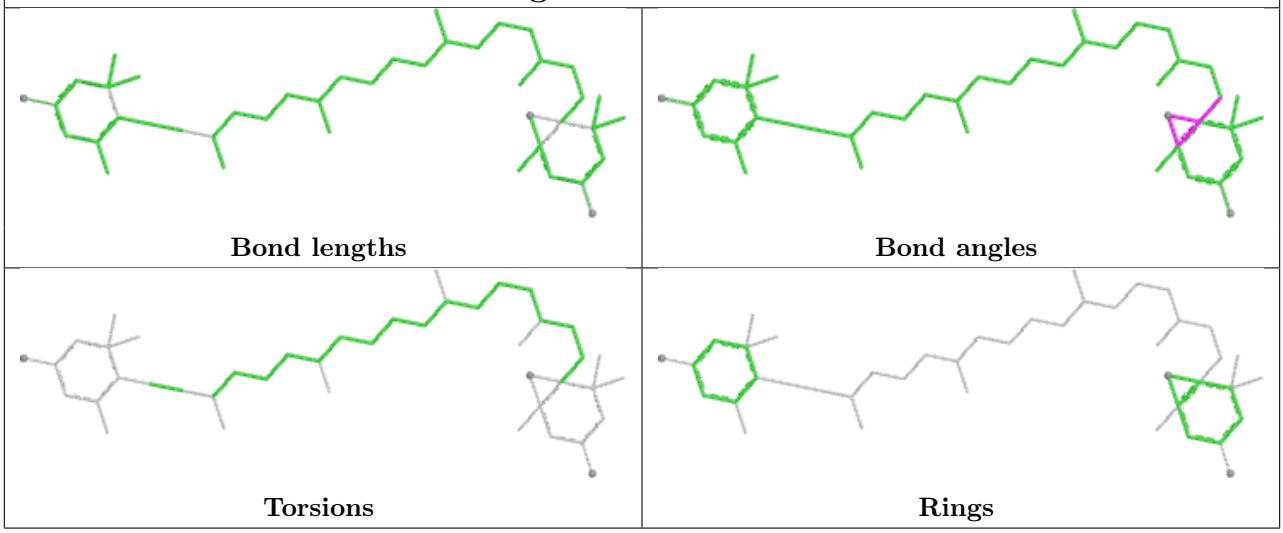


Rings

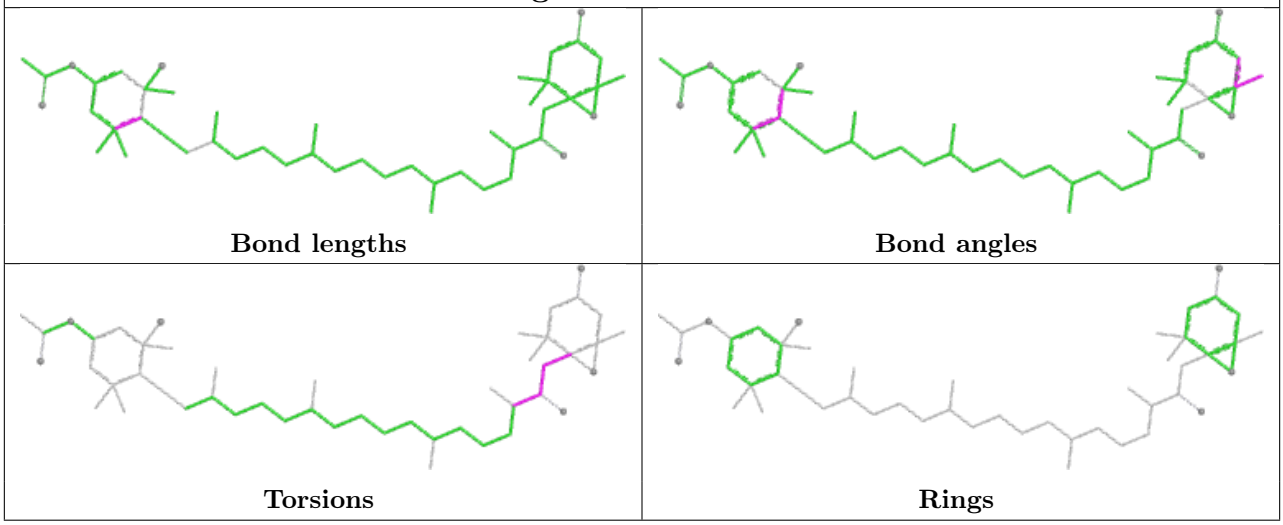
Ligand DD6 A 315



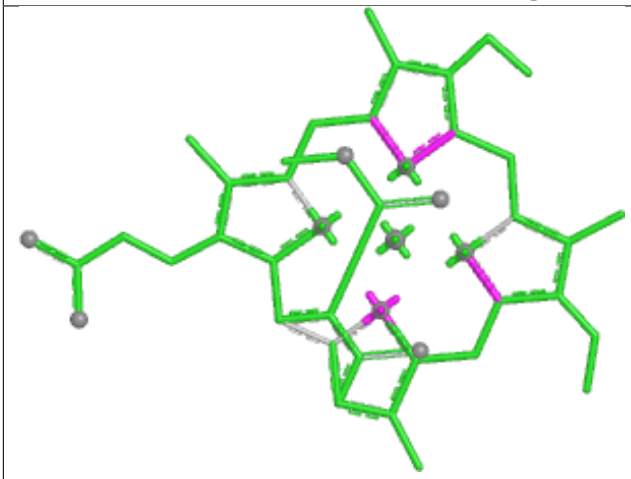
Ligand DD6 x 320



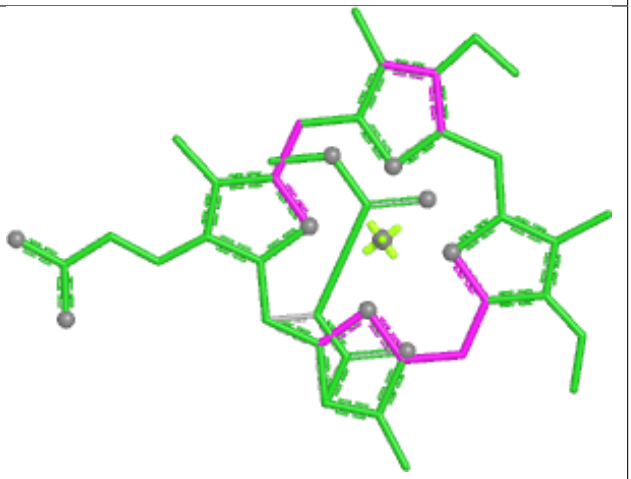
Ligand A86 P 317



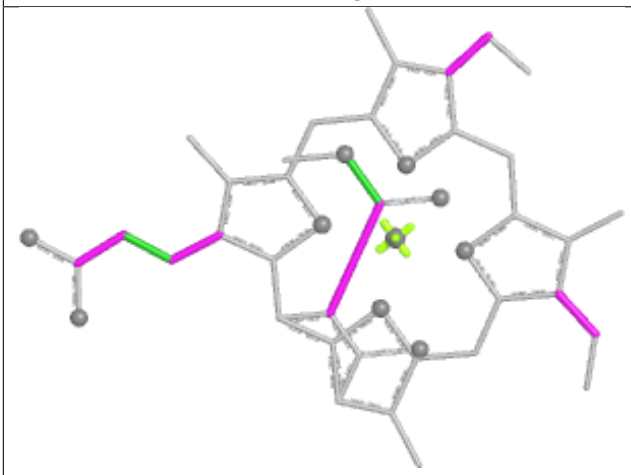
Ligand KC2 K 303



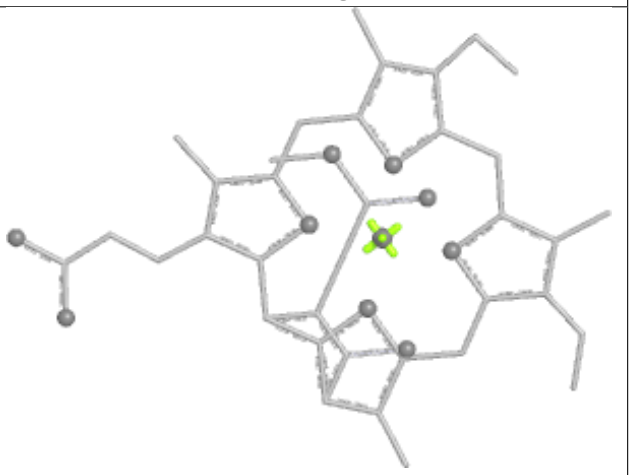
Bond lengths



Bond angles

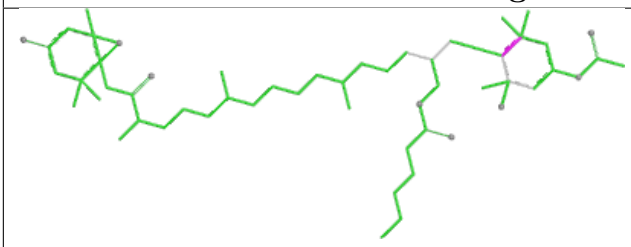


Torsions

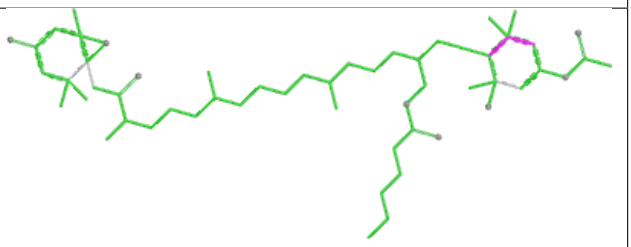


Rings

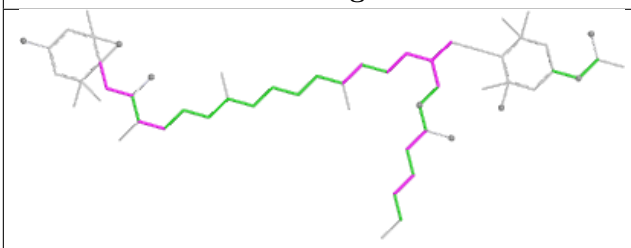
Ligand A1EB1 v 323



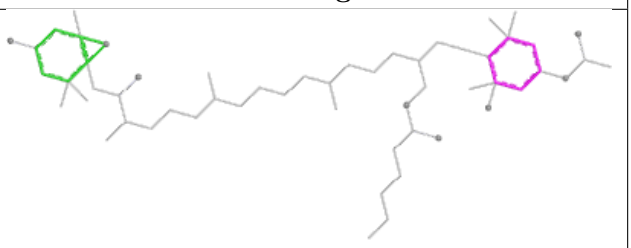
Bond lengths



Bond angles

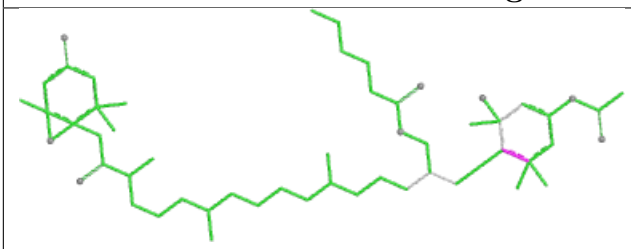


Torsions

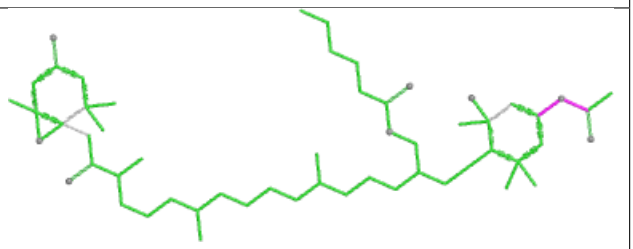


Rings

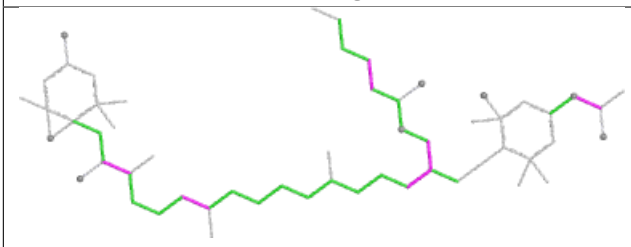
Ligand A1EB1 w 313



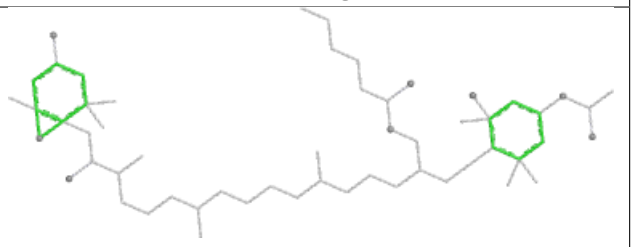
Bond lengths



Bond angles

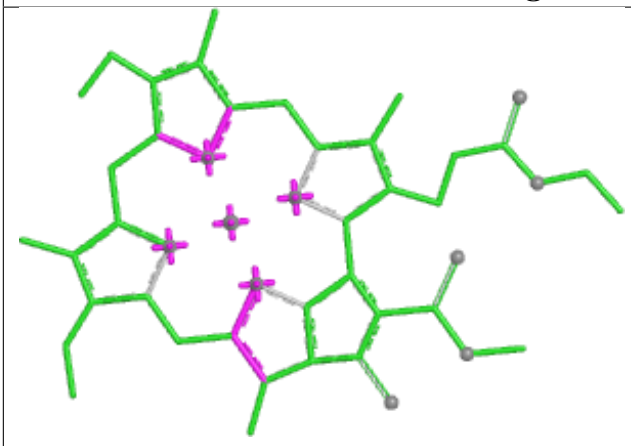


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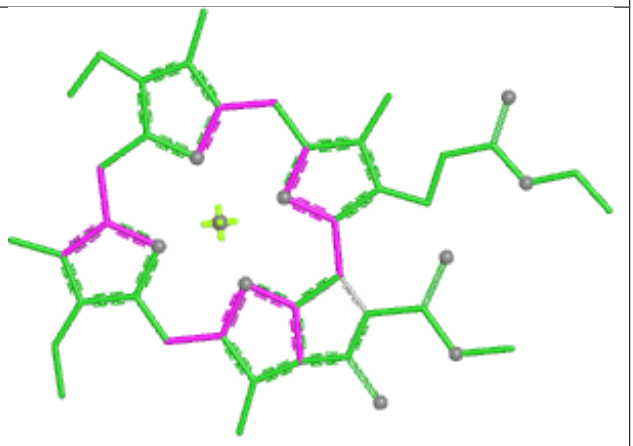


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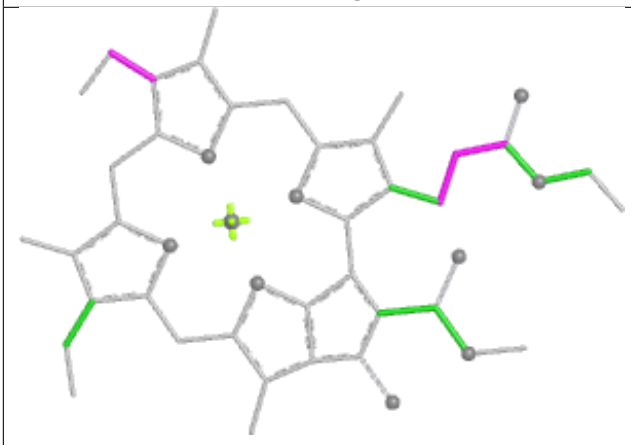
Ligand CLA T 317



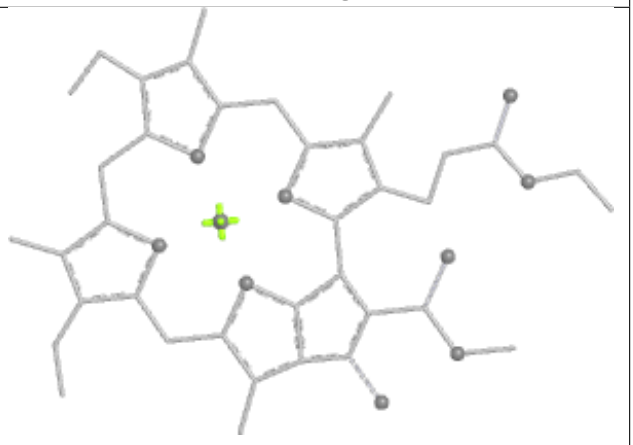
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Bond angles

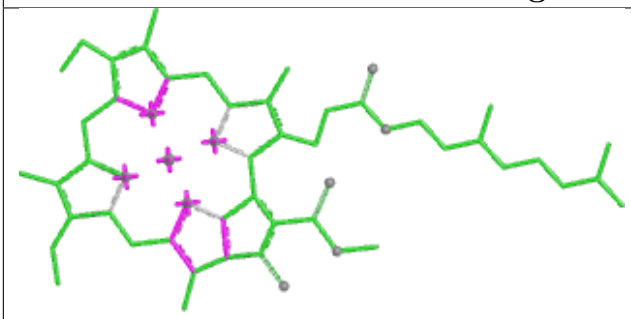


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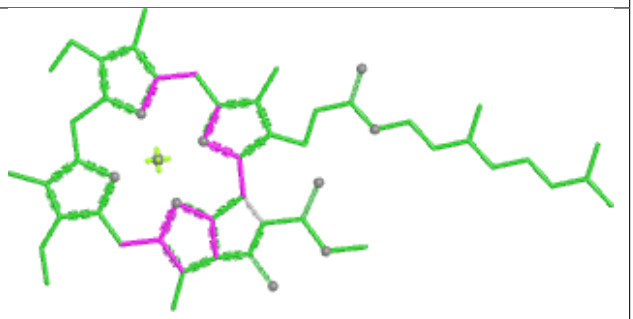


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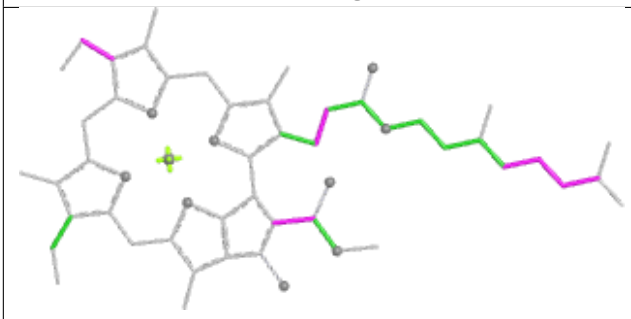
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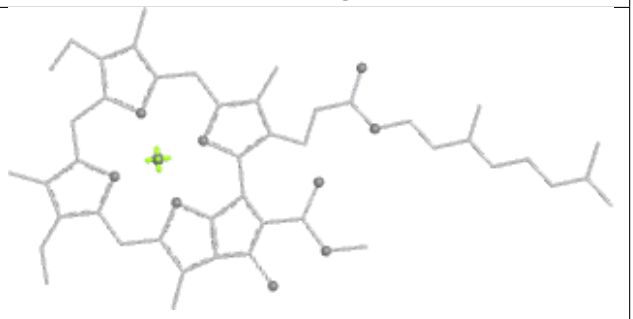
Bond lengths



Bond angles

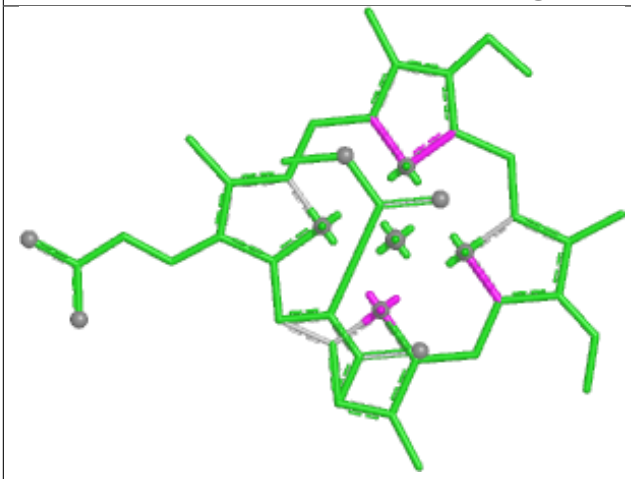


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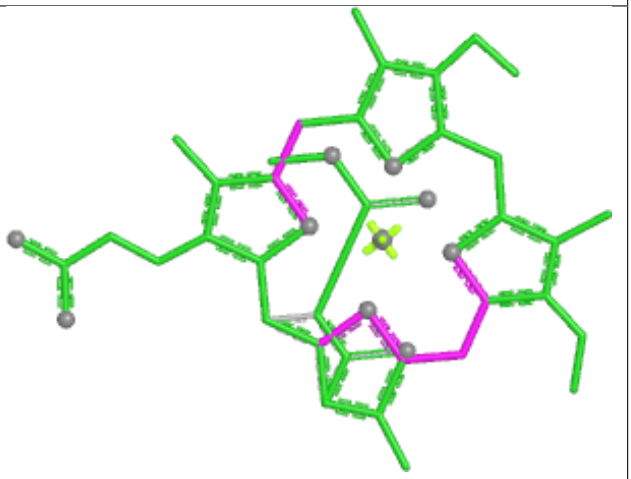


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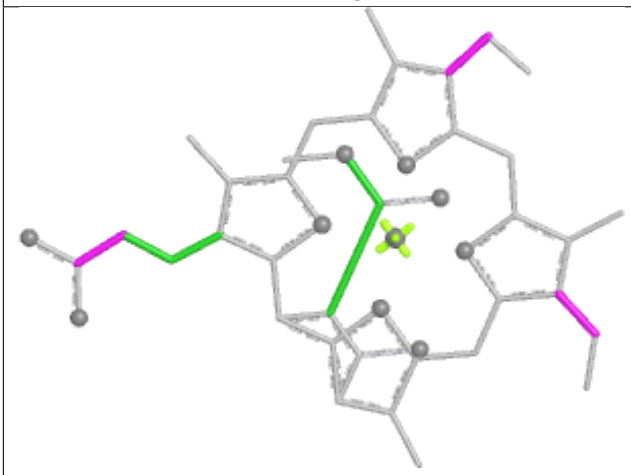
Ligand KC2 x 315



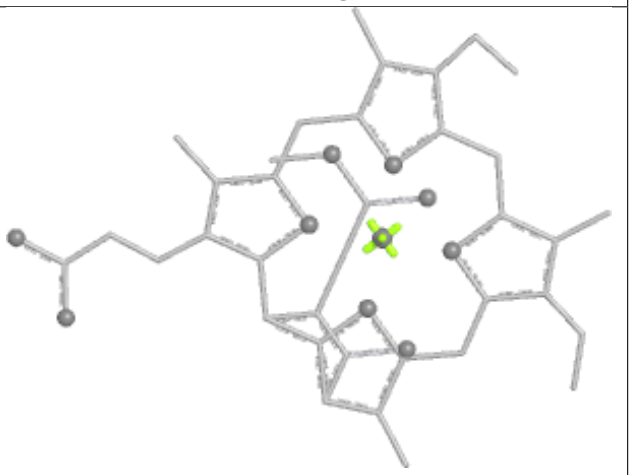
Bond lengths



Bond angles

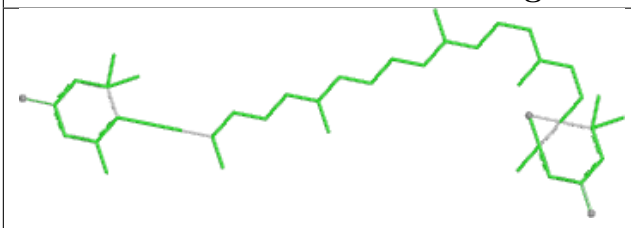


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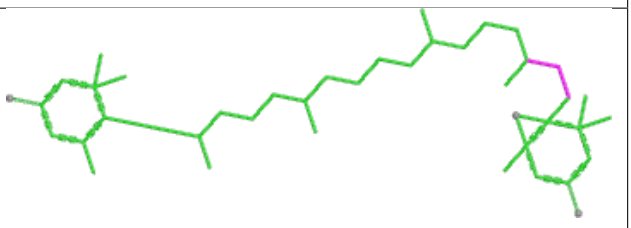


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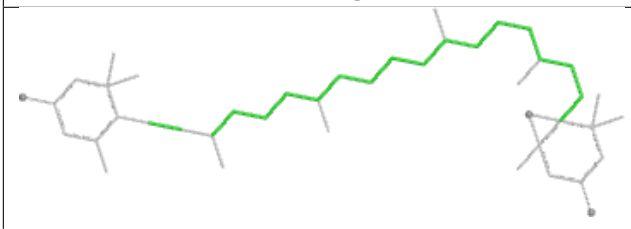
Ligand DD6 U 211



Bond lengths



Bond angles

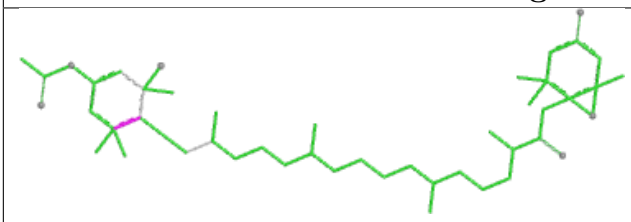


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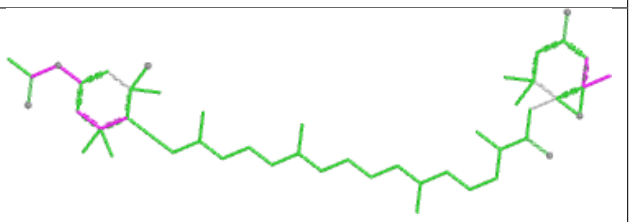


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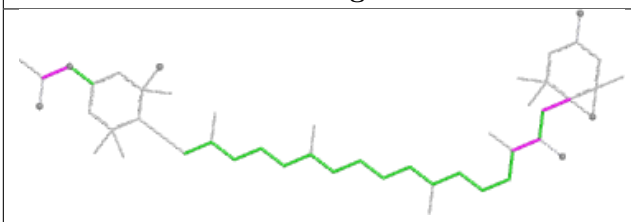
Ligand A86 R 312



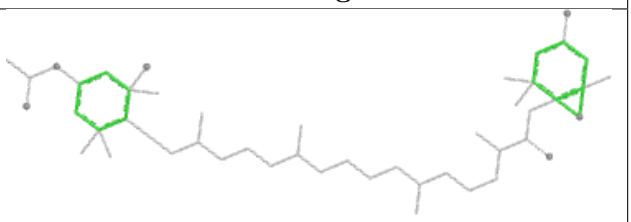
Bond lengths



Bond angles

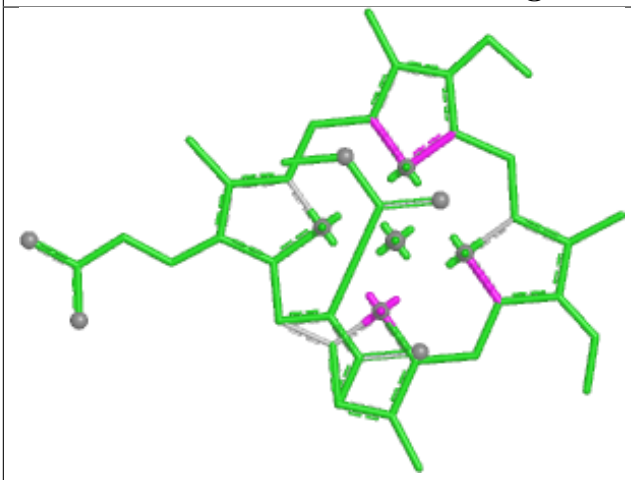


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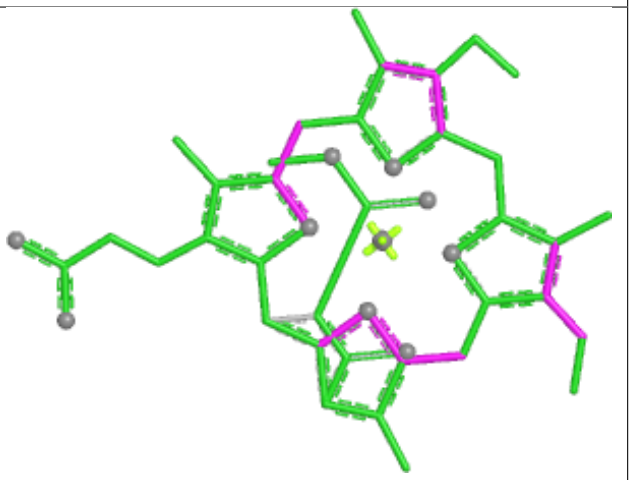


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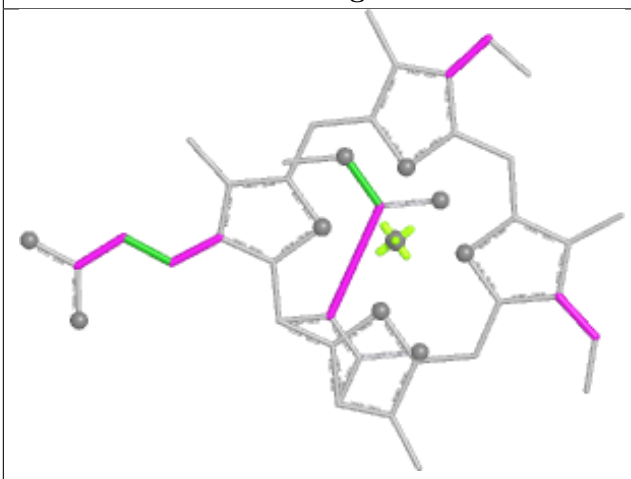
Ligand KC2 R 303



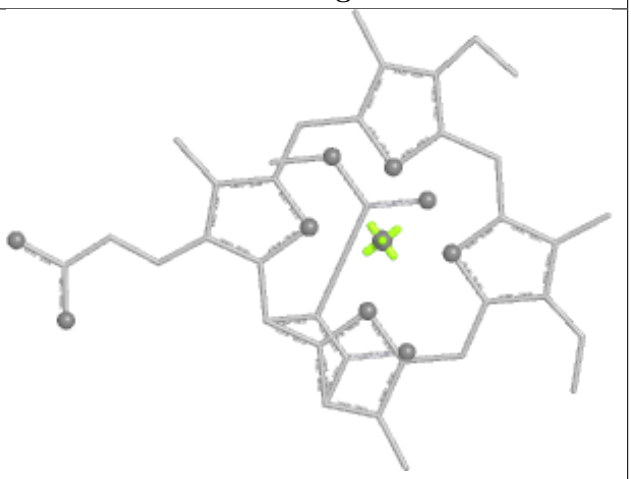
Bond lengths



Bond angles

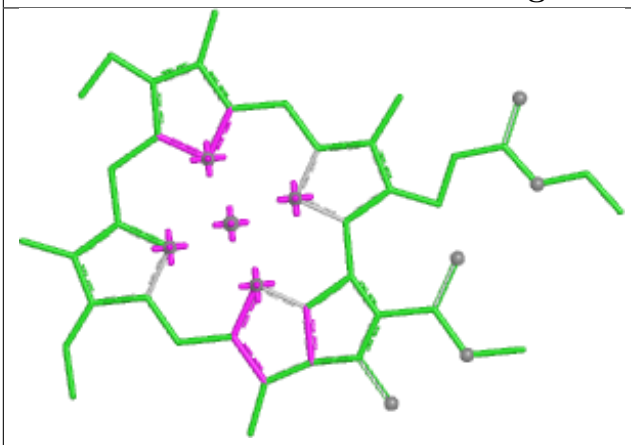


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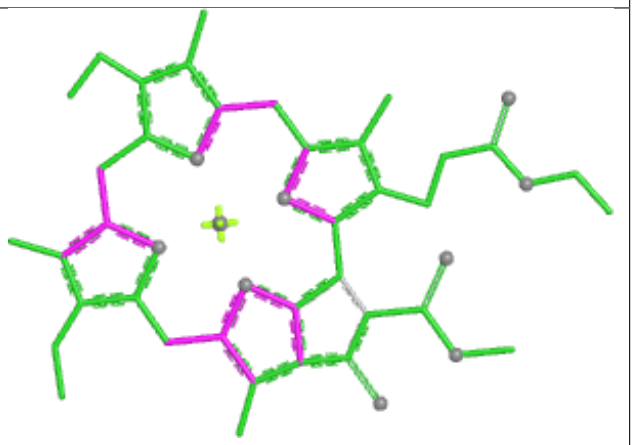


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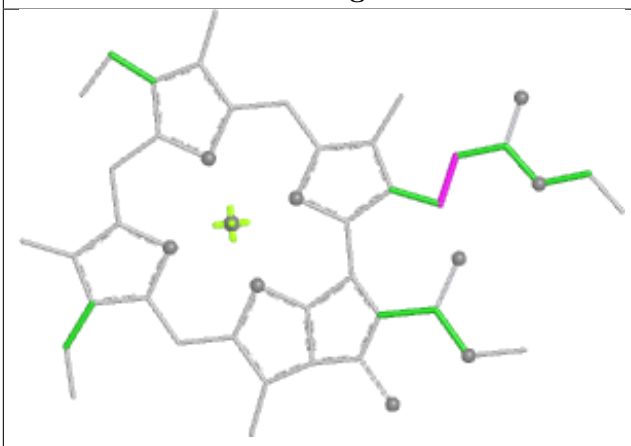
Ligand CLA J 318



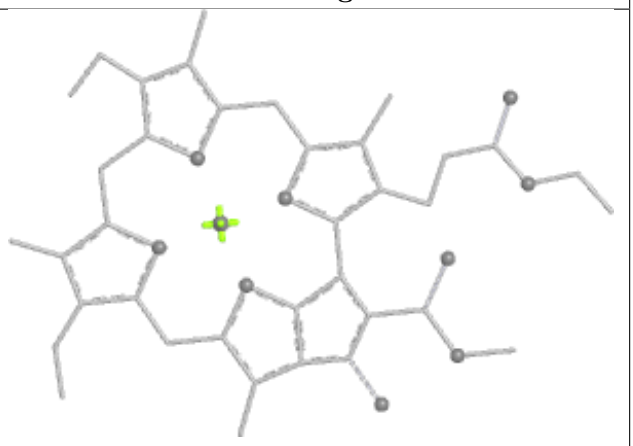
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Bond angles

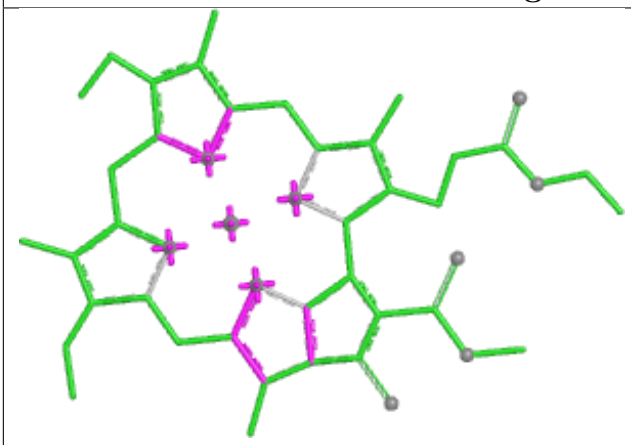


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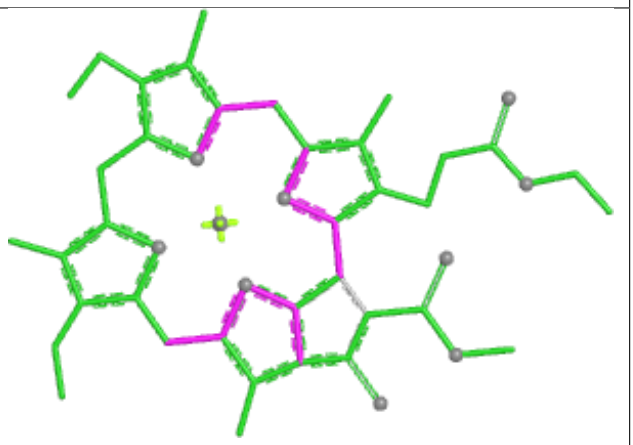


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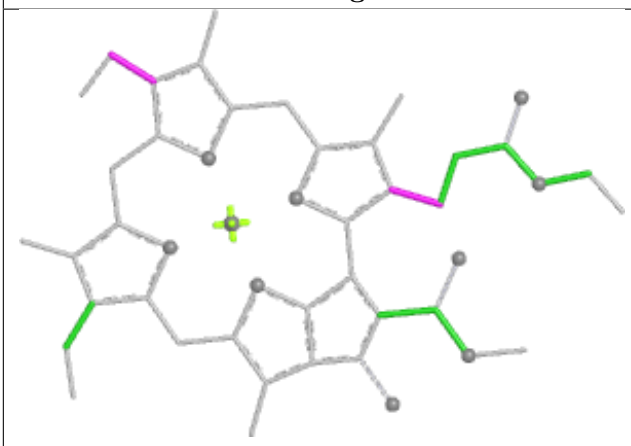
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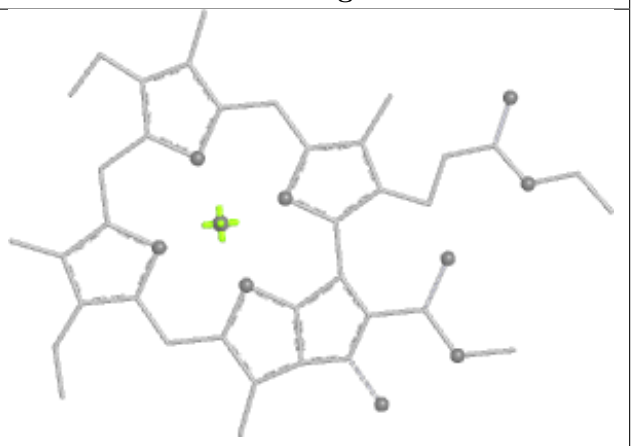
Bond lengths



Bond angles

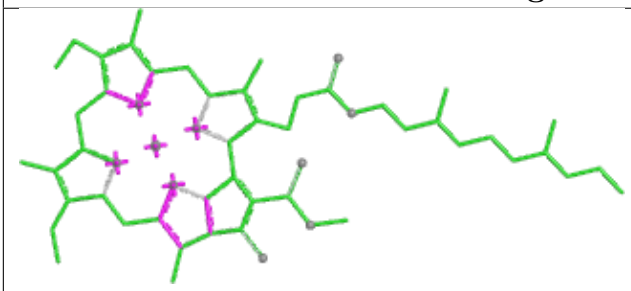


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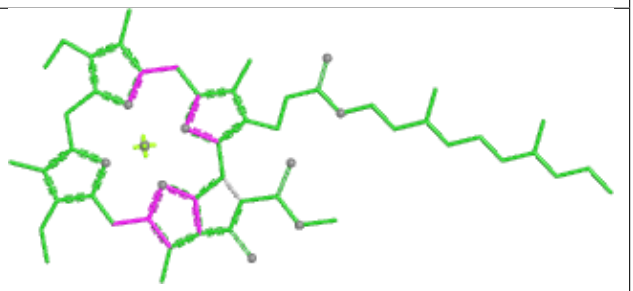


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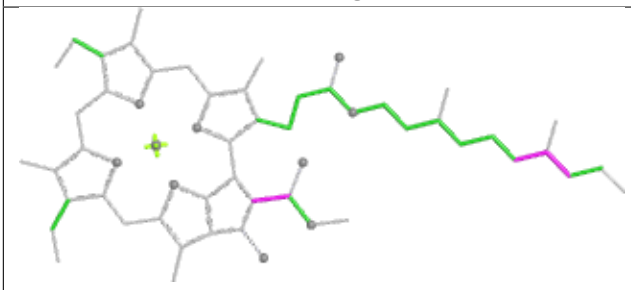
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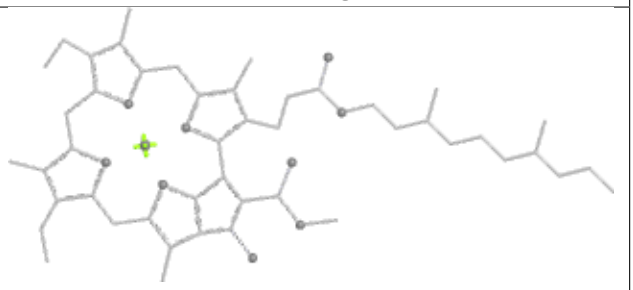
Bond lengths



Bond angles

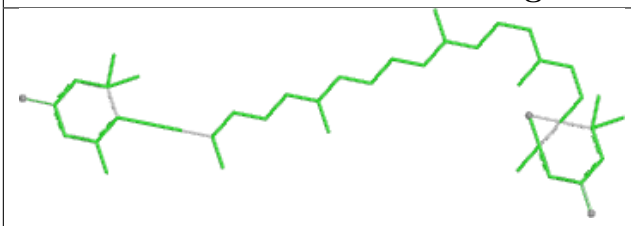


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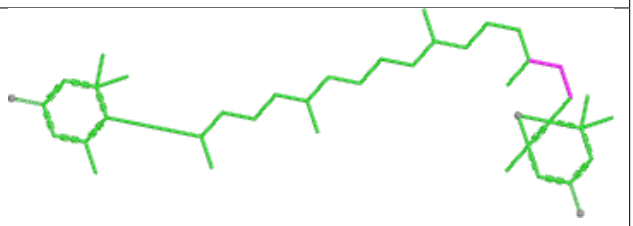


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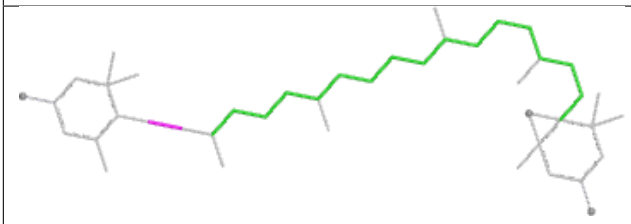
Ligand DD6 O 314



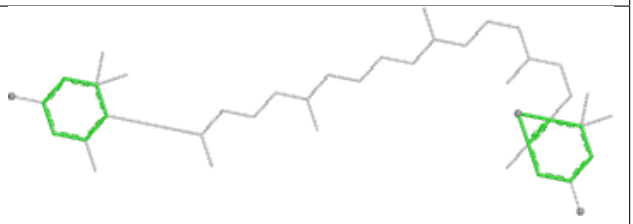
Bond lengths



Bond angles

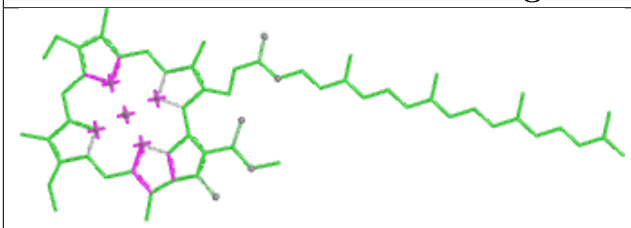


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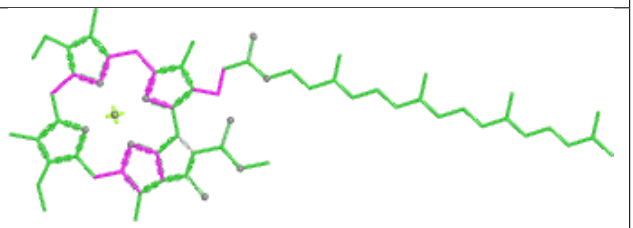


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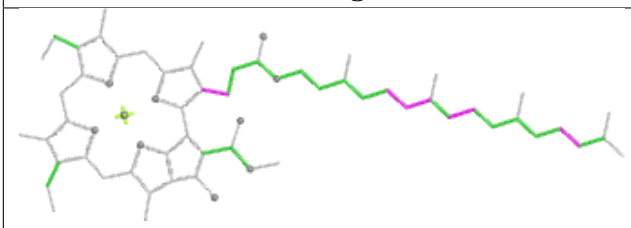
Ligand CLA O 304



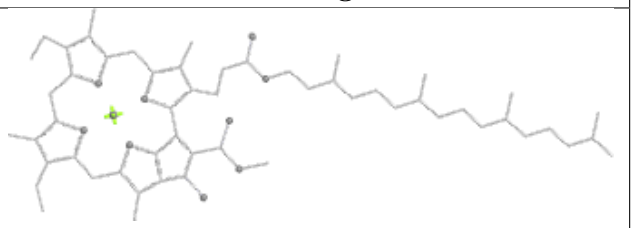
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Bond angles

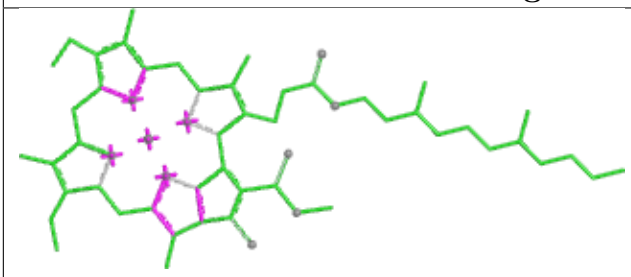


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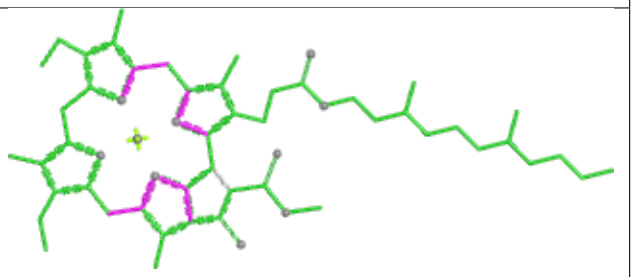


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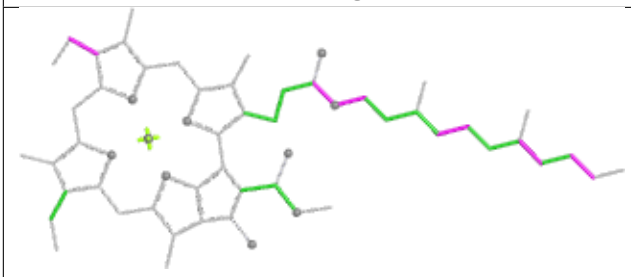
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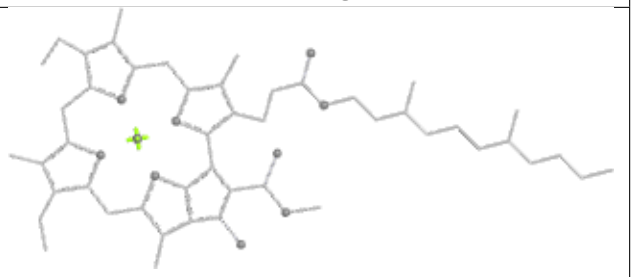
Bond lengths



Bond angles

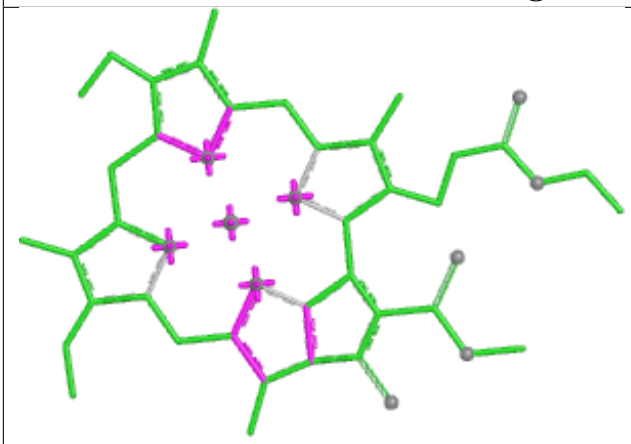


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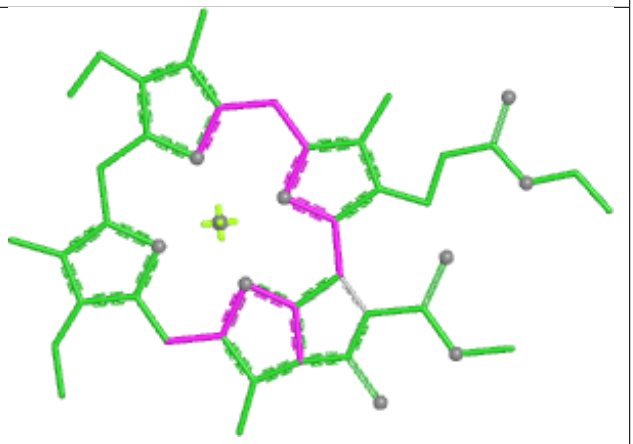


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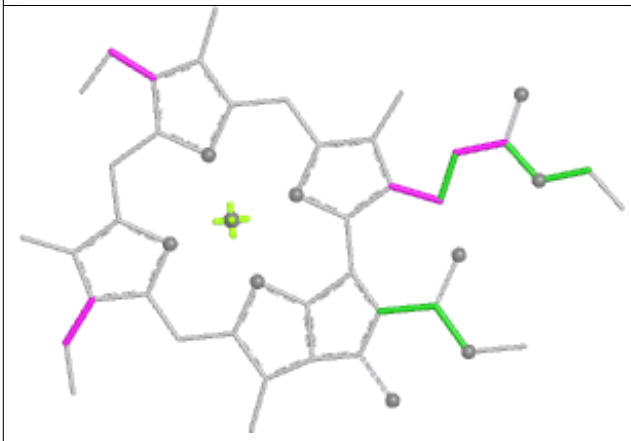
Ligand CLA u 306



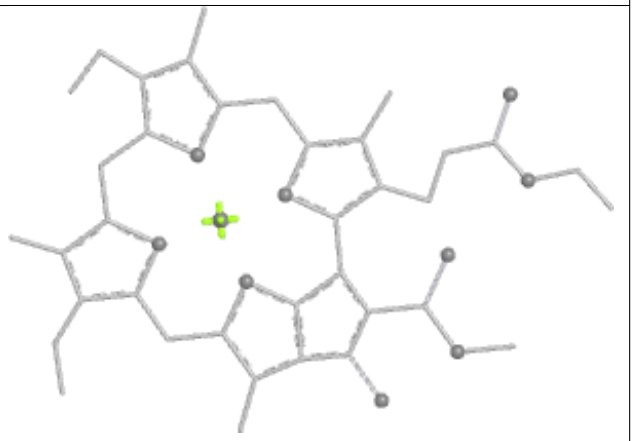
Bond lengths



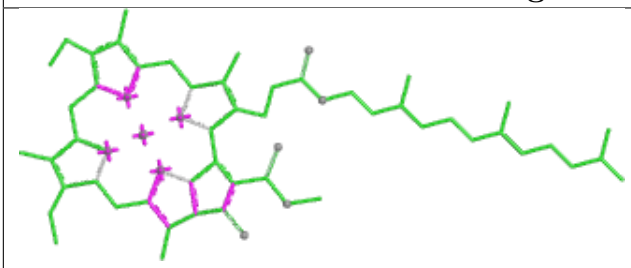
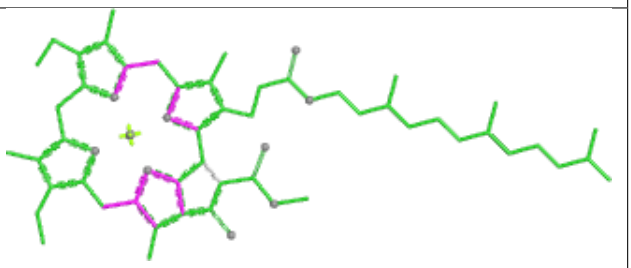
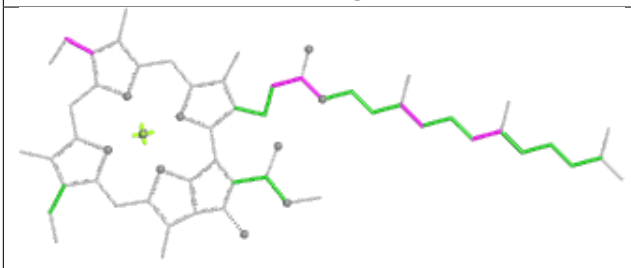
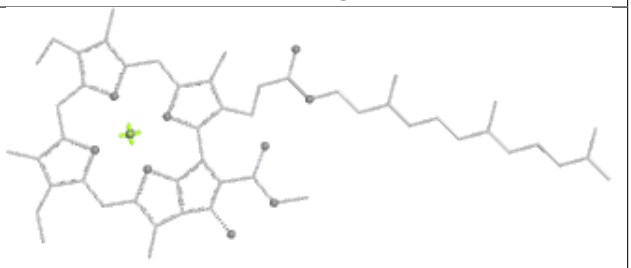
Bond angles

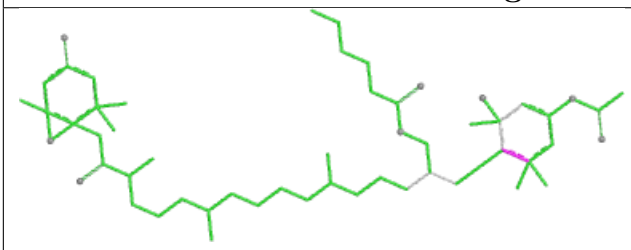
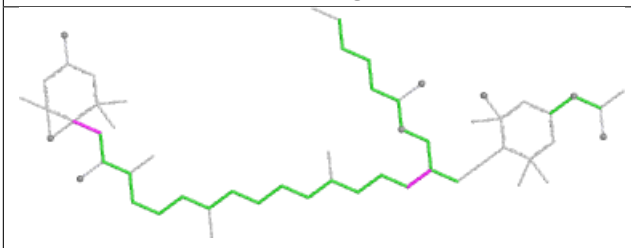
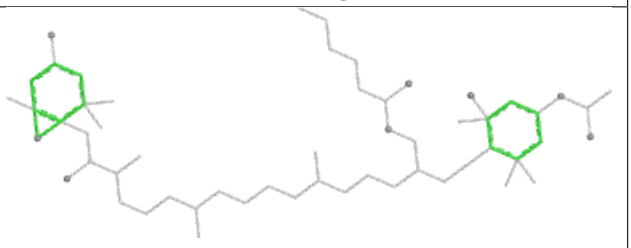


Torsions

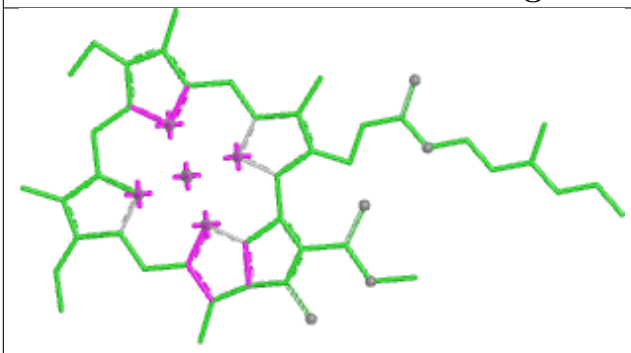


Rings

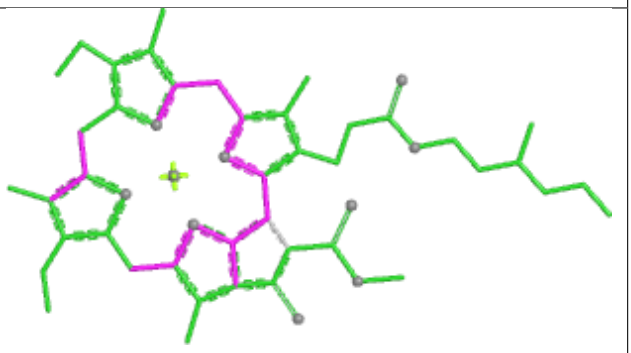
Ligand CLA S 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A1EB1 K 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

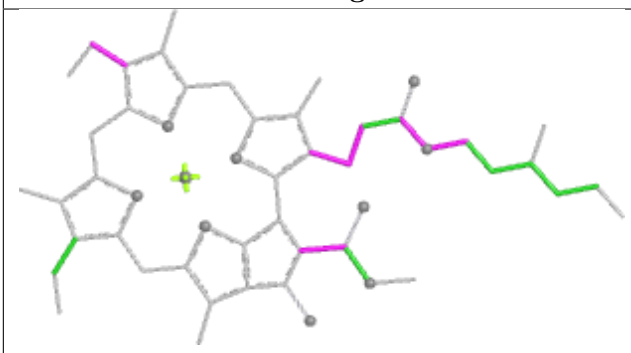
Ligand CLA B 306



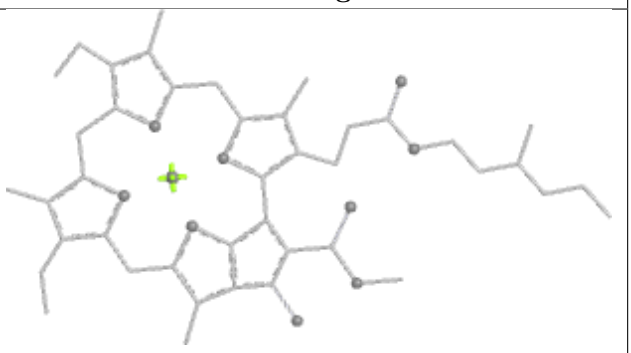
Bond lengths



Bond angles

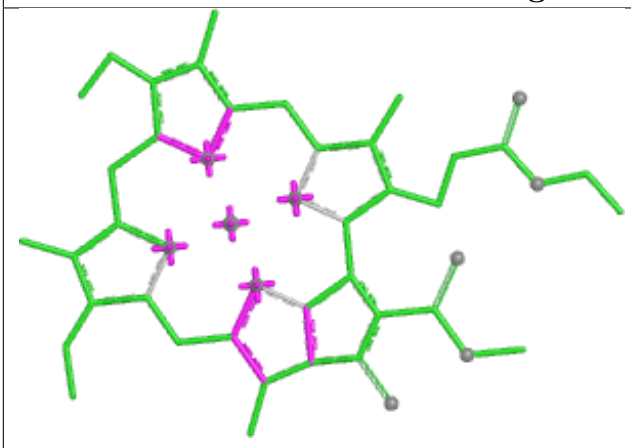


Torsions

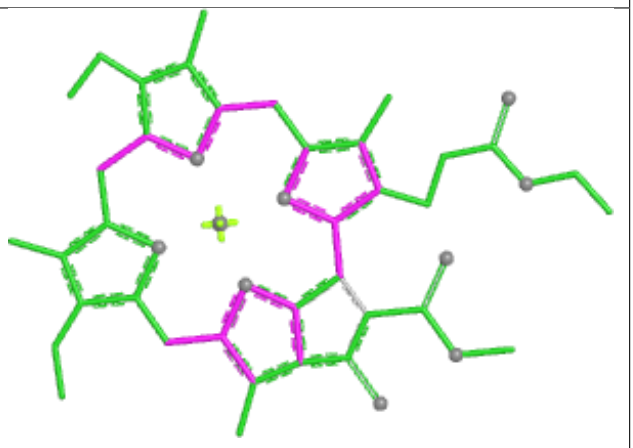


Rings

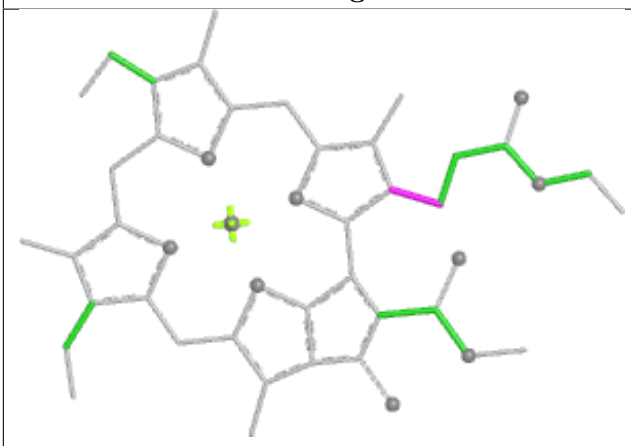
Ligand CLA J 310



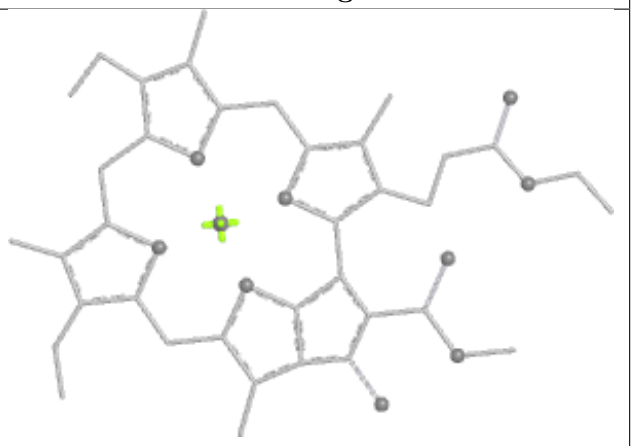
Bond lengths



Bond angles

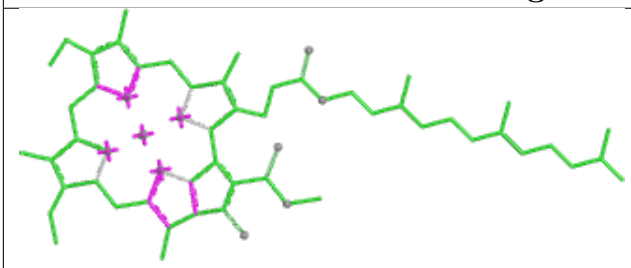


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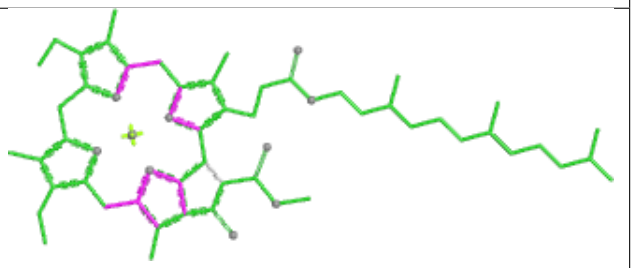


Rings

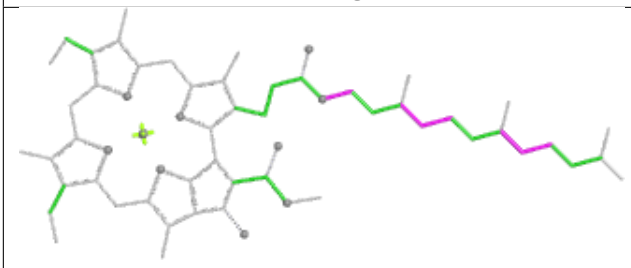
Ligand CLA b 837



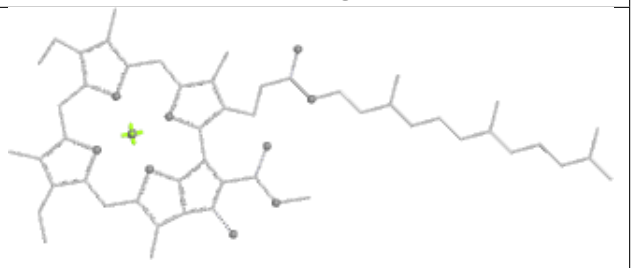
Bond lengths



Bond angles

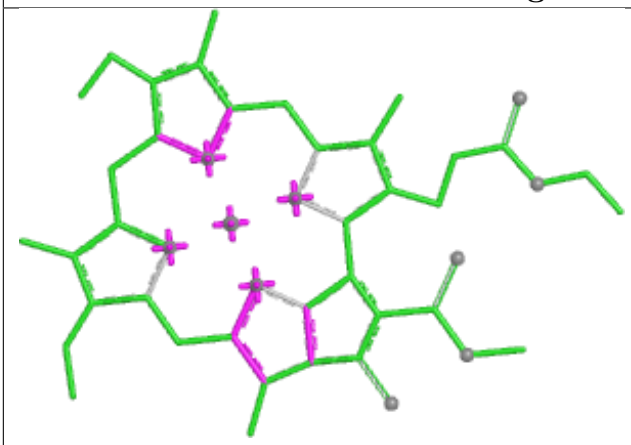


Torsions

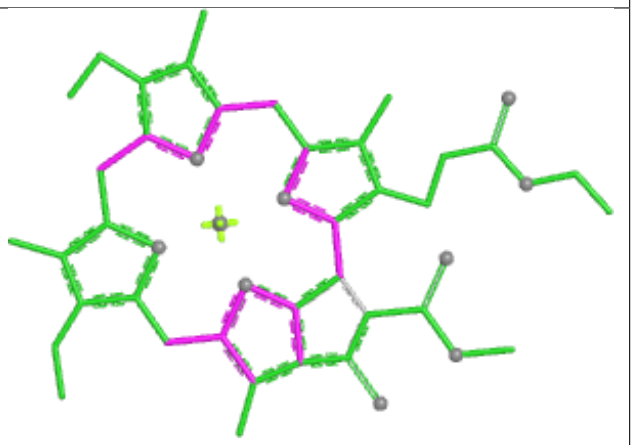


Rings

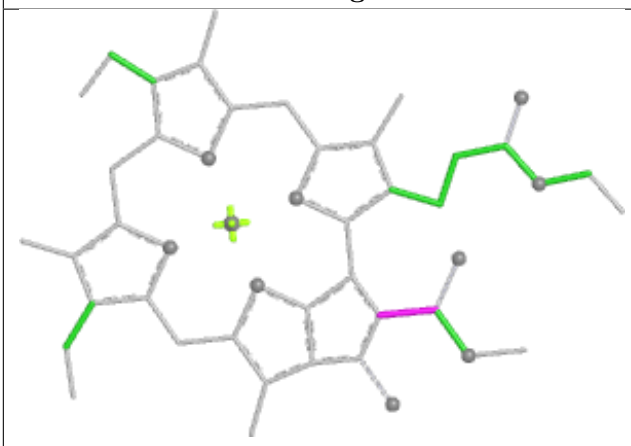
Ligand CLA u 305



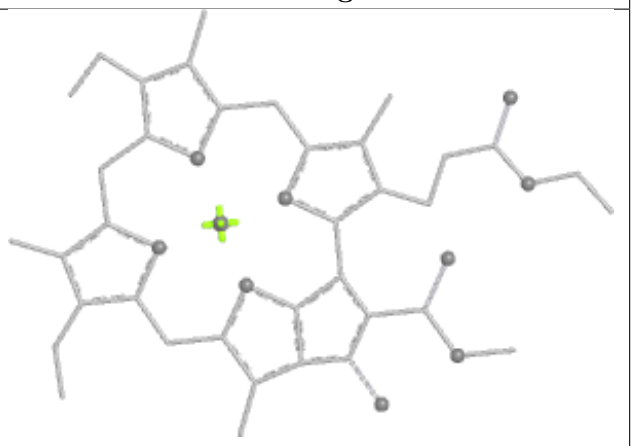
Bond lengths



Bond angles

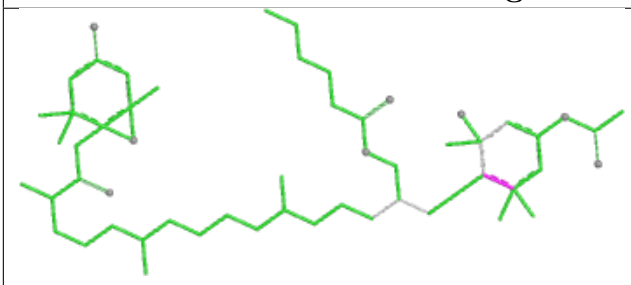


Torsions

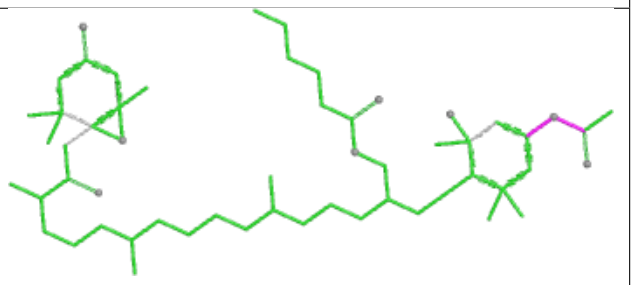


Rings

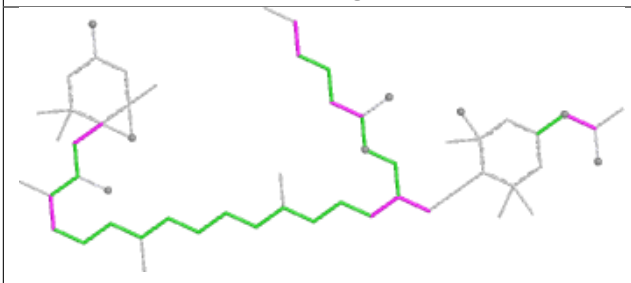
Ligand A1EB1 w 314



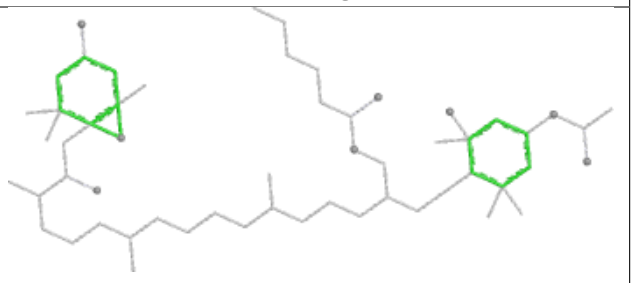
Bond lengths



Bond angles

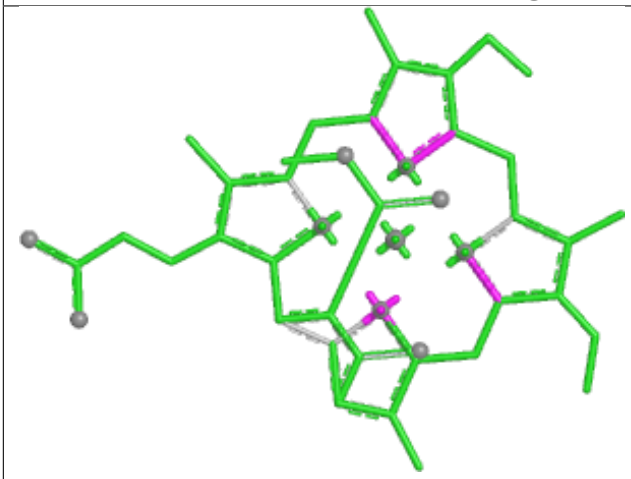


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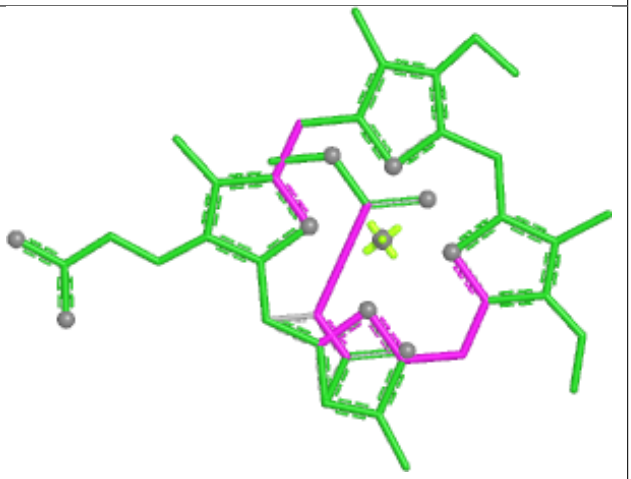


Rings

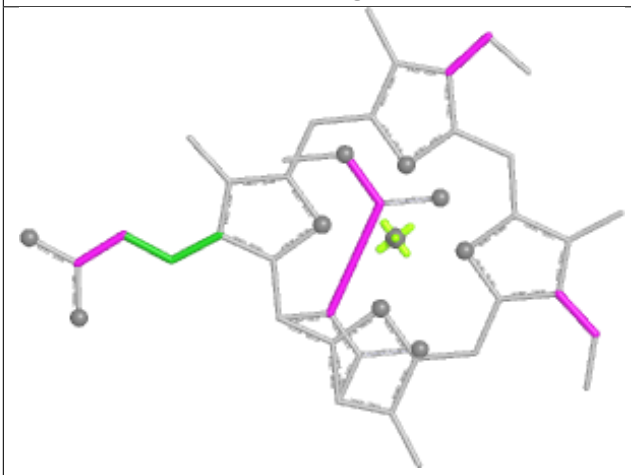
Ligand KC2 Y 314



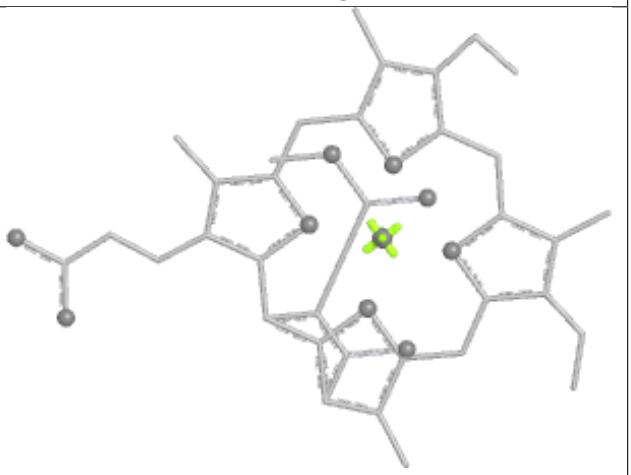
Bond lengths



Bond angles

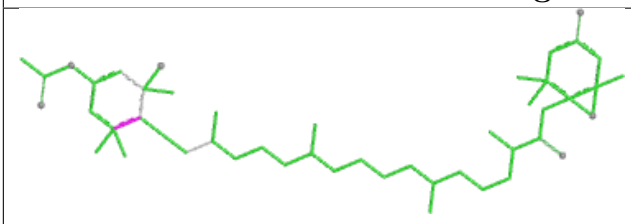


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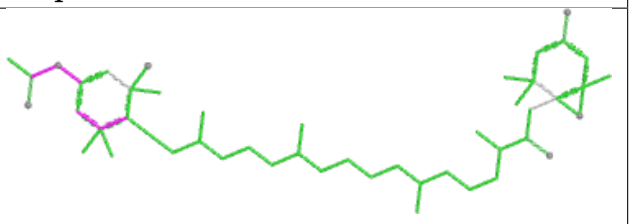


Rings

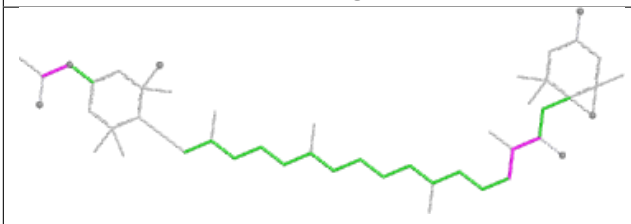
Ligand A86 q 315



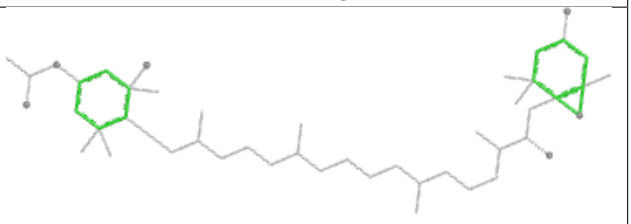
Bond lengths



Bond angles

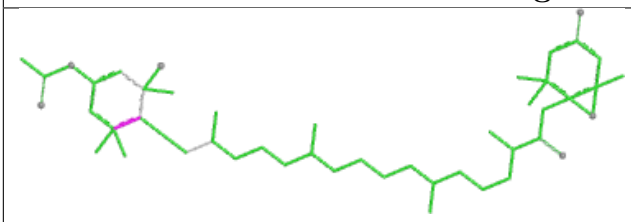


Torsions

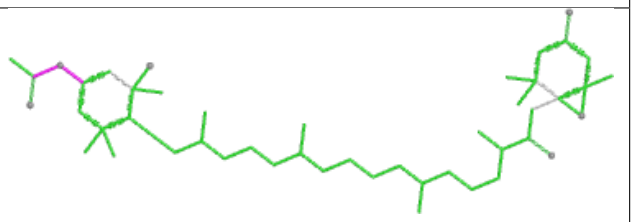


Rings

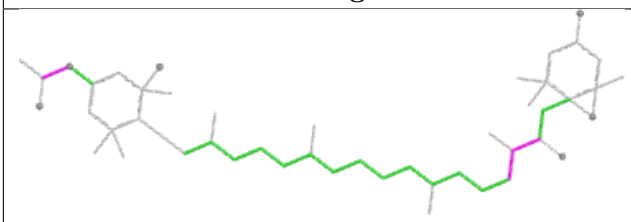
Ligand A86 v 315



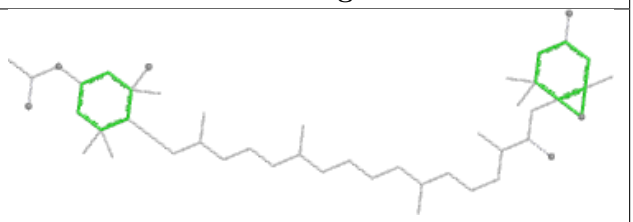
Bond lengths



Bond angles

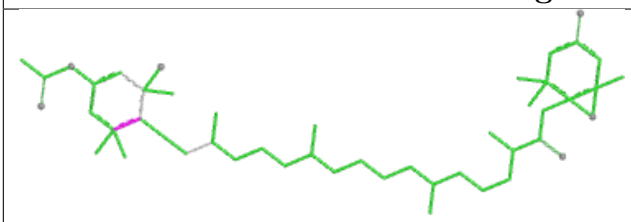


Torsions

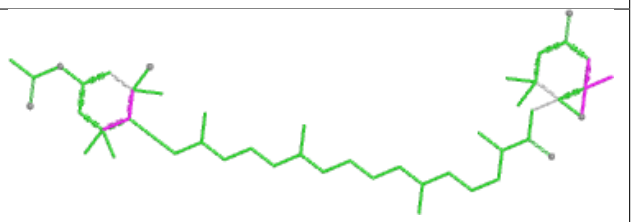


Rings

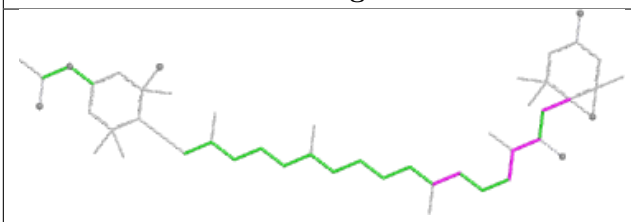
Ligand A86 z 316



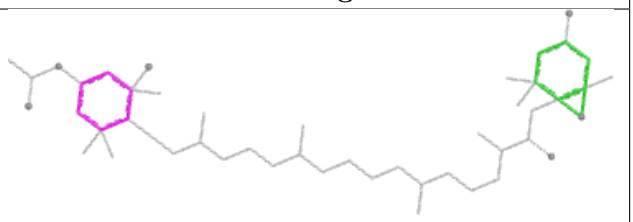
Bond lengths



Bond angles

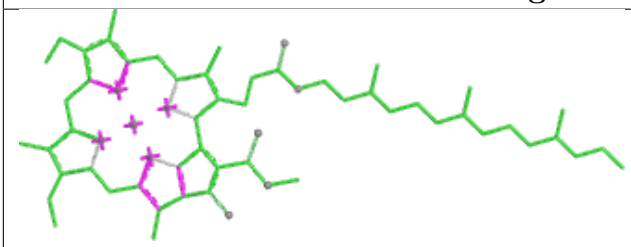


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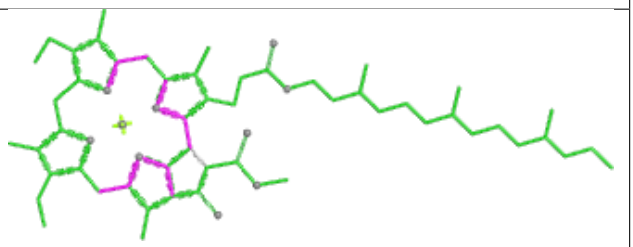


Rings

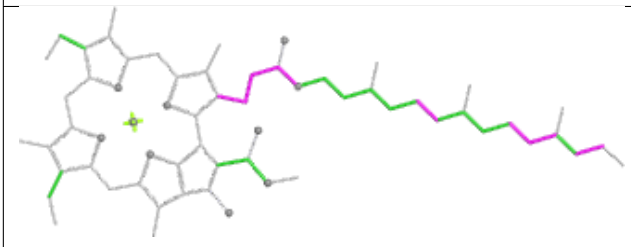
Ligand CLA a 824



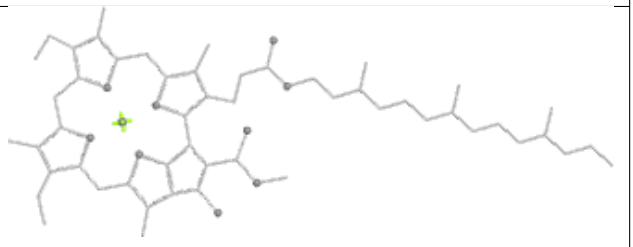
Bond lengths



Bond angles

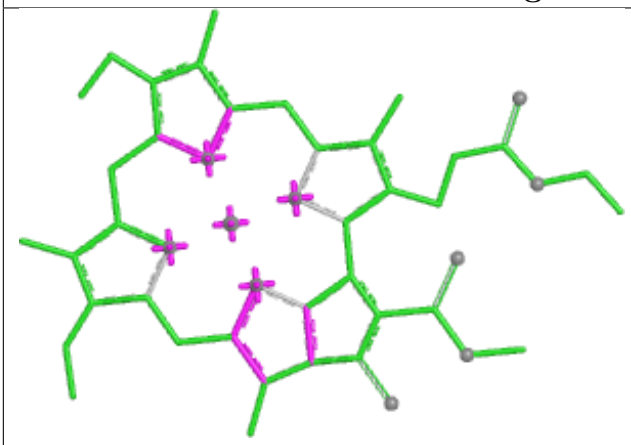


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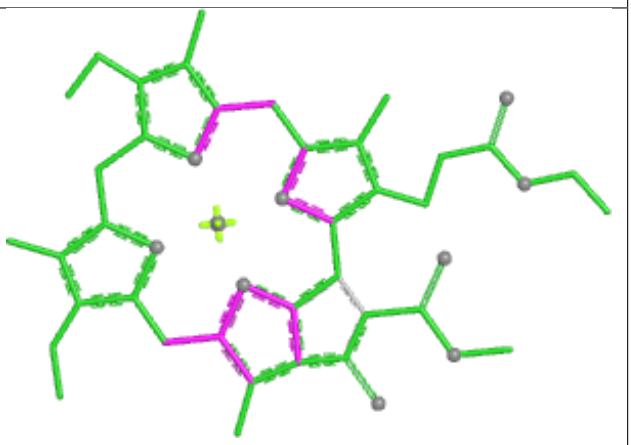


Rings

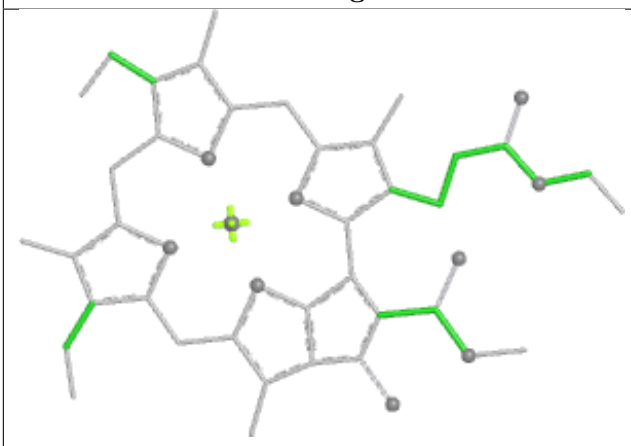
Ligand CLA w 302



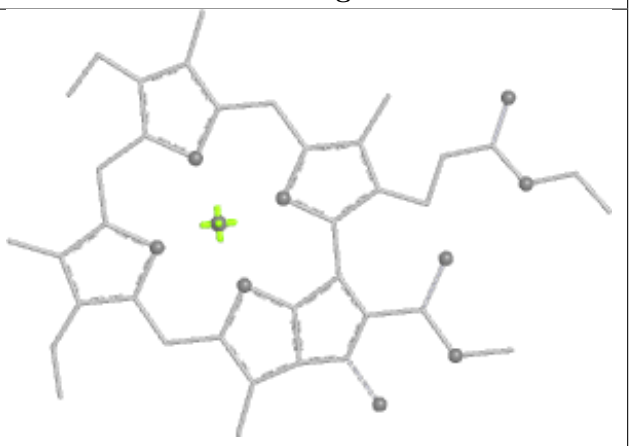
Bond lengths



Bond angles

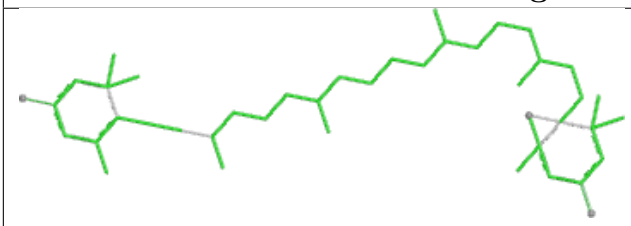


Torsions



Rings

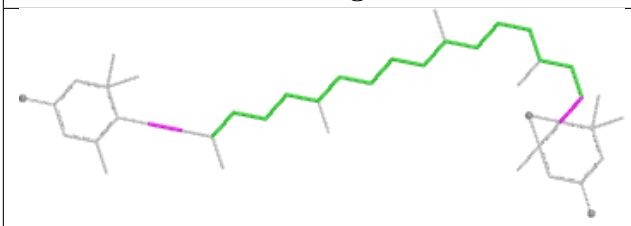
Ligand DD6 z 322



Bond lengths



Bond angles

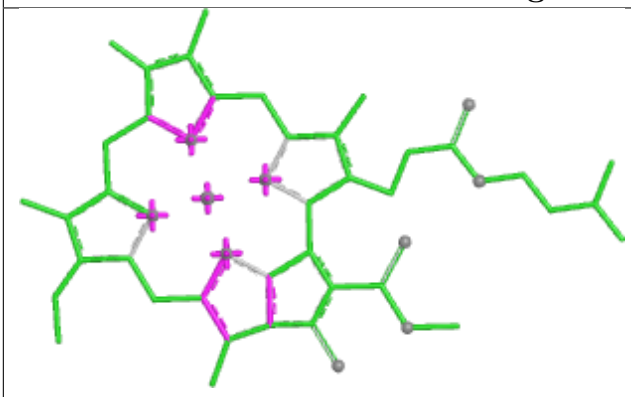


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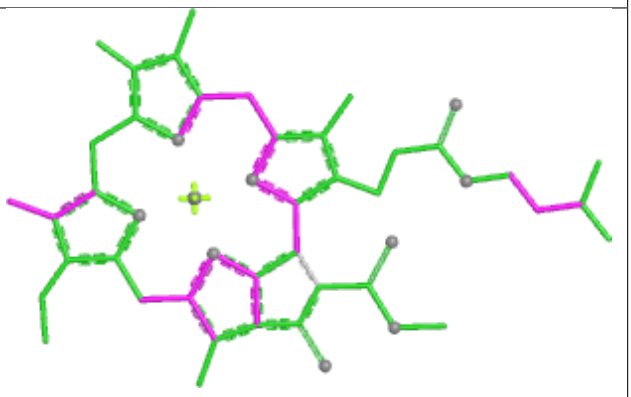


Rings

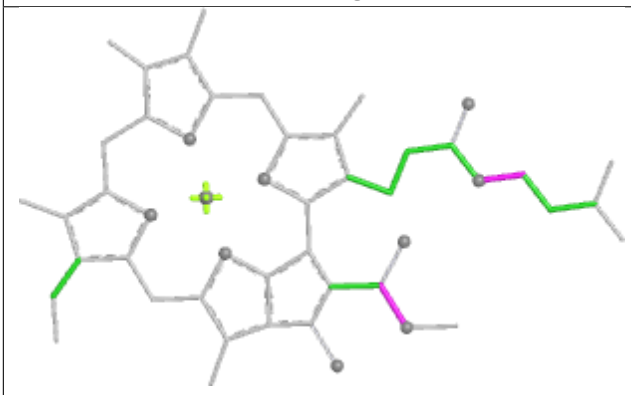
Ligand CLA S 308



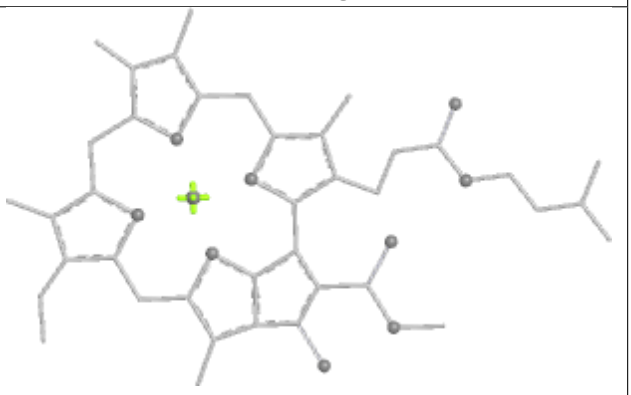
Bond lengths



Bond angles



Torsions



Rings

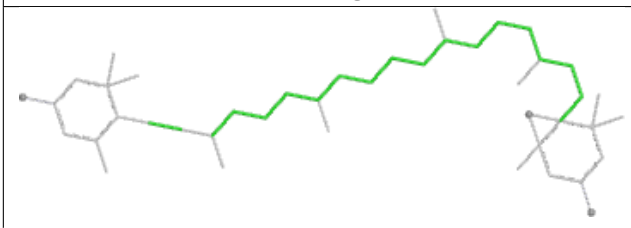
Ligand DD6 H 312



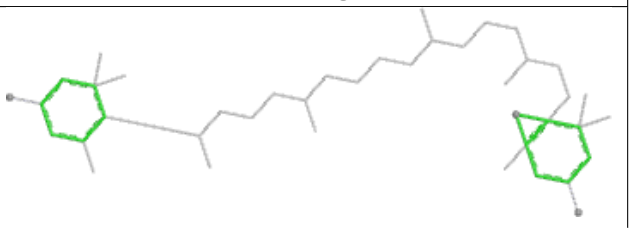
Bond lengths



Bond angles

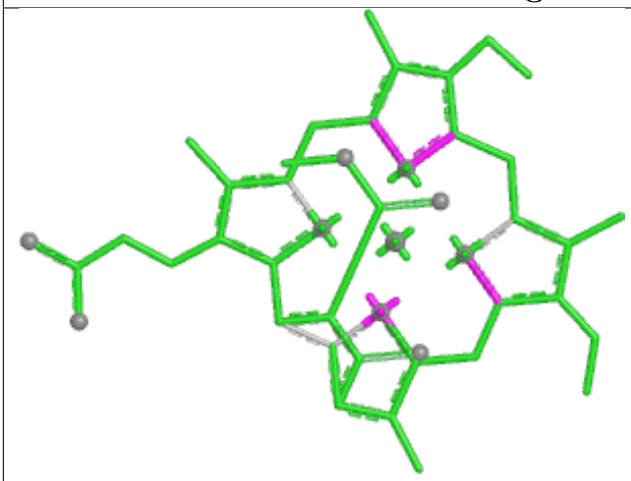


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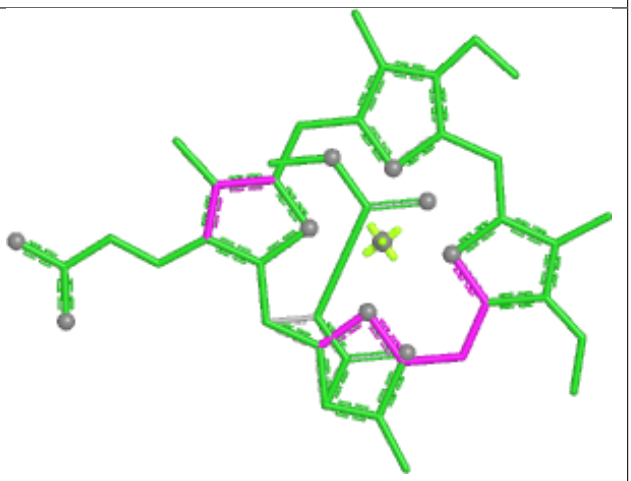


Rings

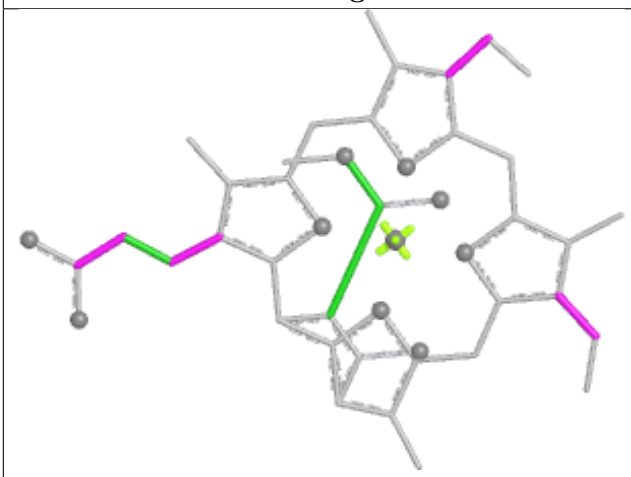
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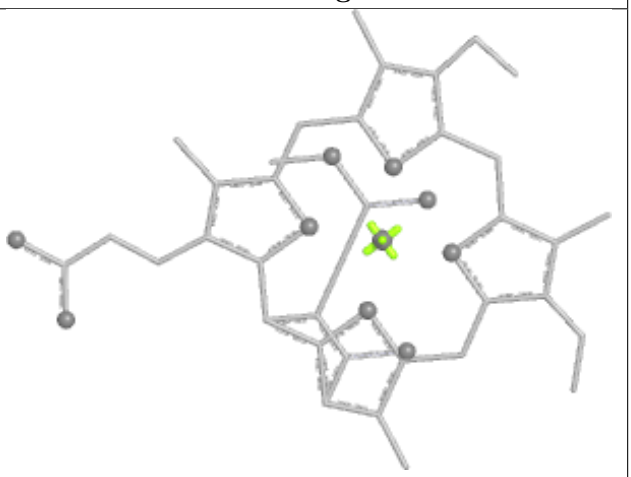
Bond lengths



Bond angles

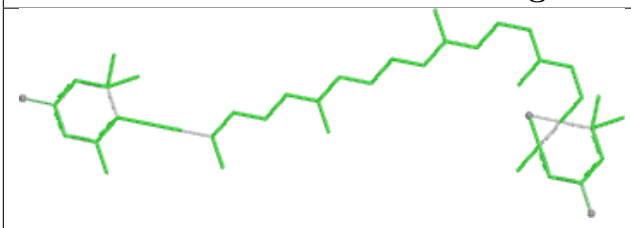


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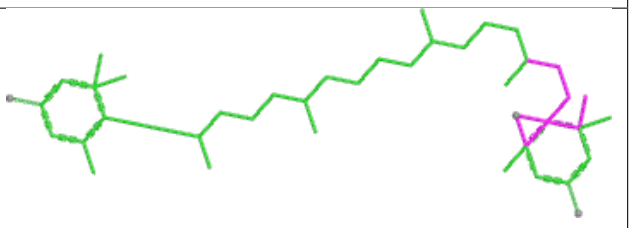


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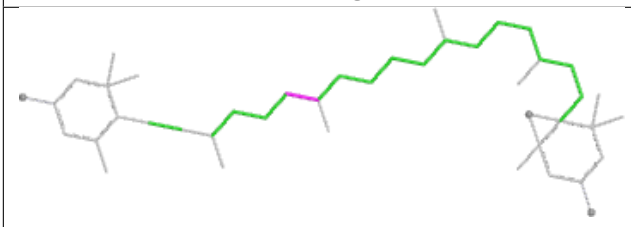
Ligand DD6 k 204



Bond lengths



Bond angles

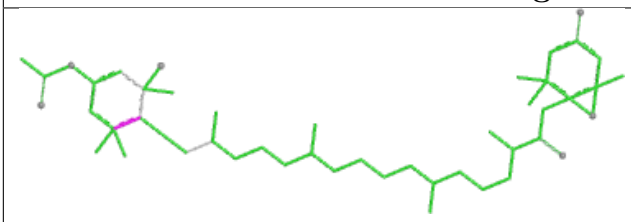


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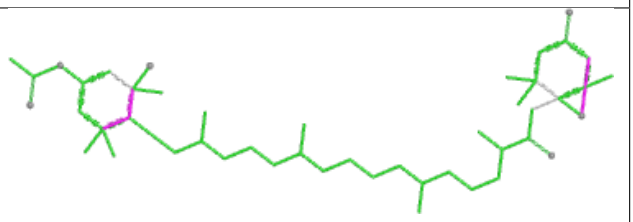


Rings

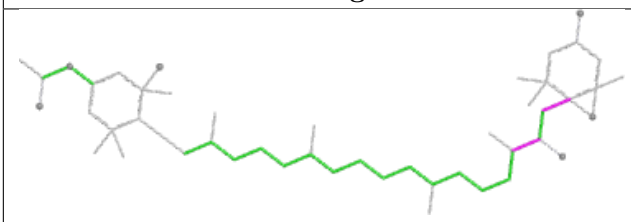
Ligand A86 u 320



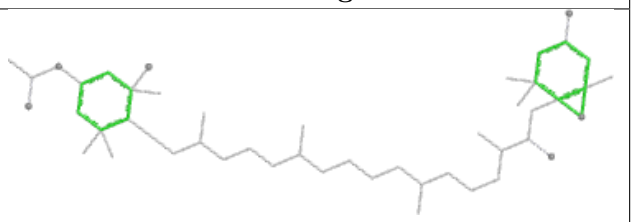
Bond lengths



Bond angles

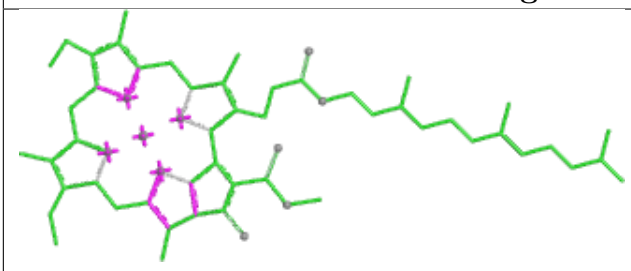


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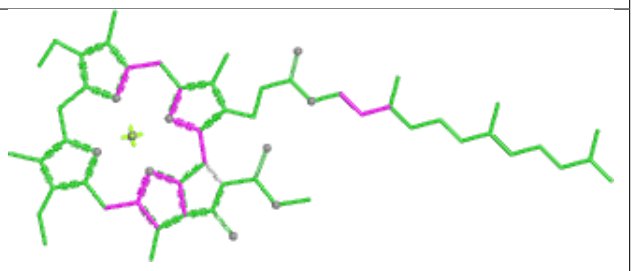


Rings

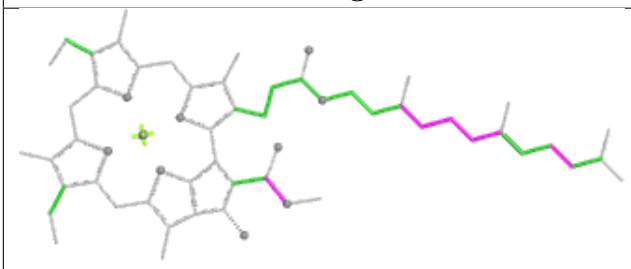
Ligand CLA M 307



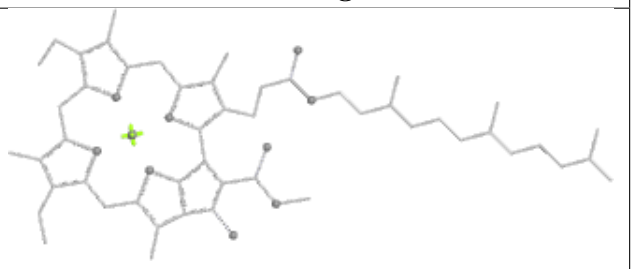
Bond lengths



Bond angles

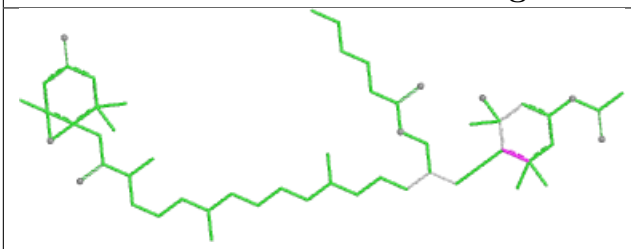


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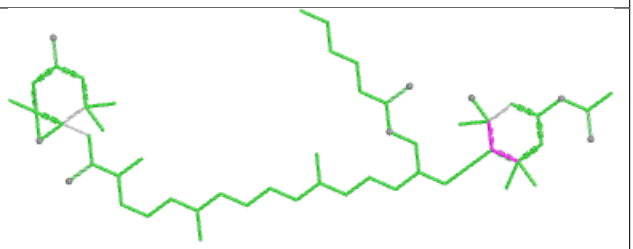


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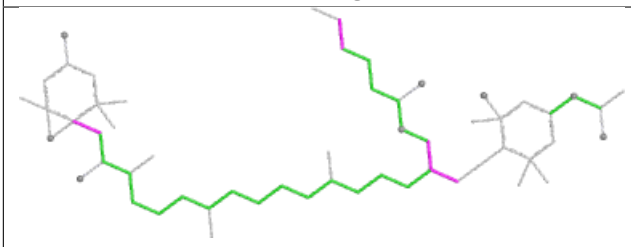
Ligand A1EB1 x 322



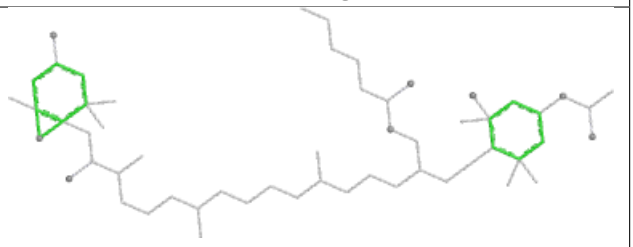
Bond lengths



Bond angles

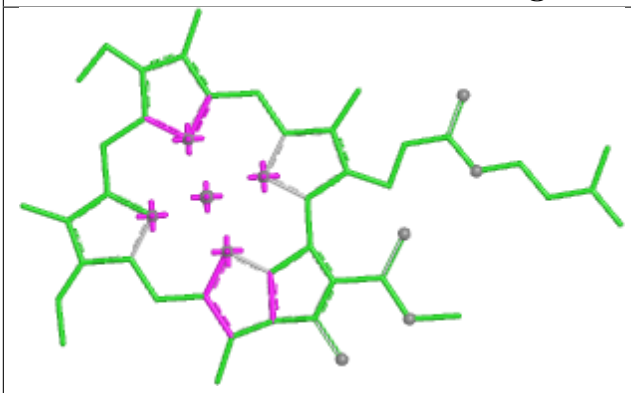


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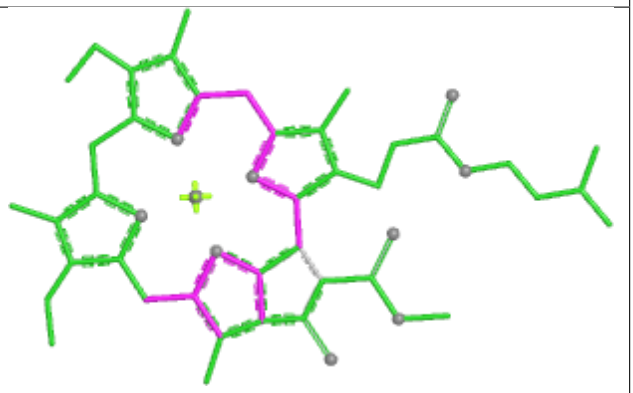


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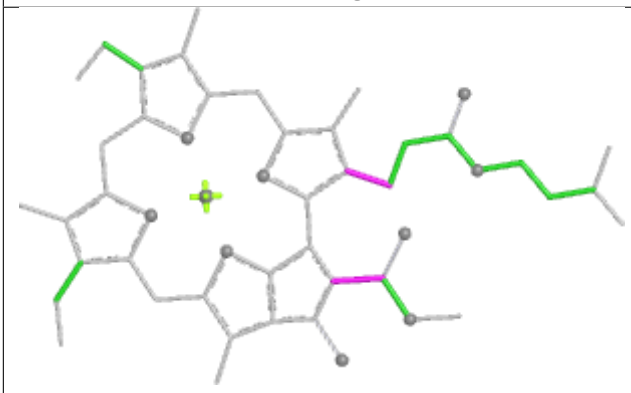
Ligand CLA a 809



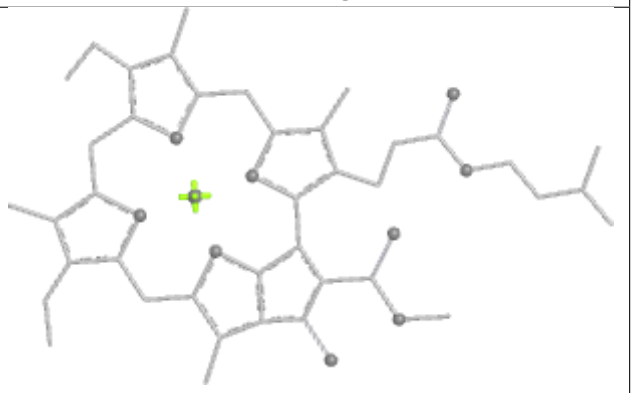
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Bond angles

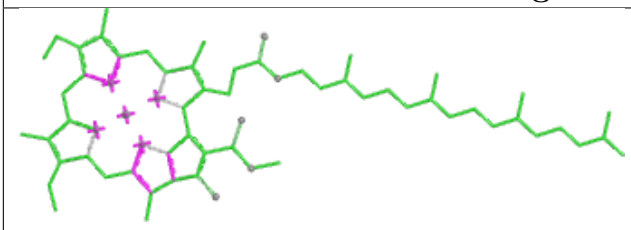


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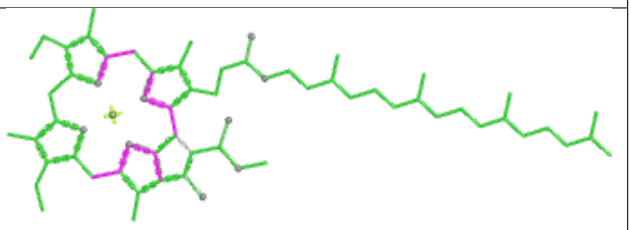


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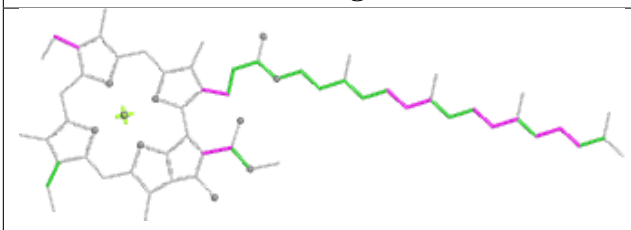
Ligand CLA l 204



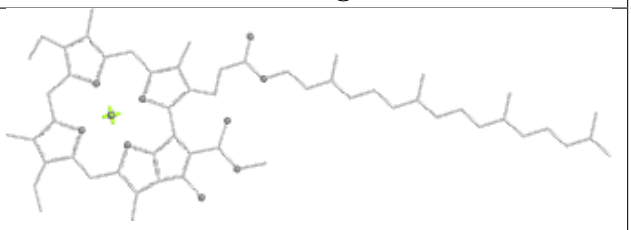
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Bond angles

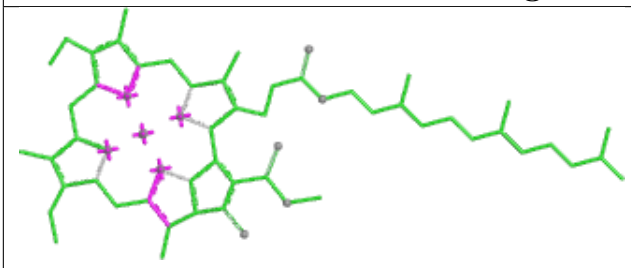


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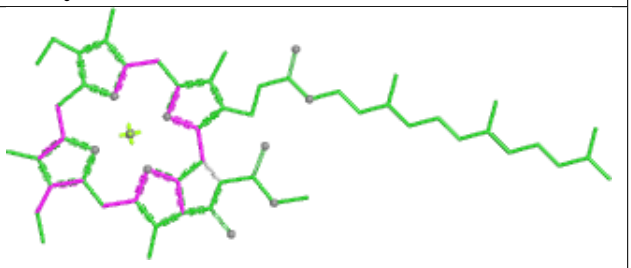


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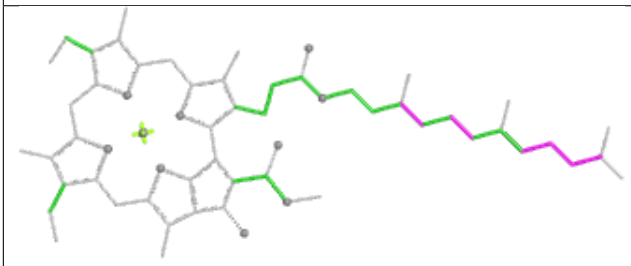
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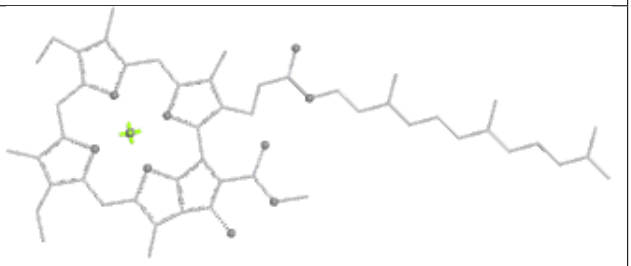
Bond lengths



Bond angles



Torsions



Rings

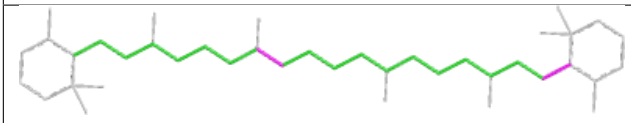
Ligand BCR f 206



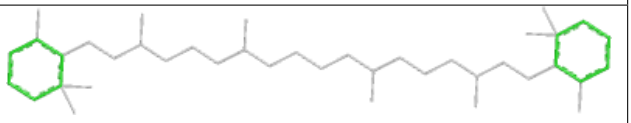
Bond lengths



Bond angles

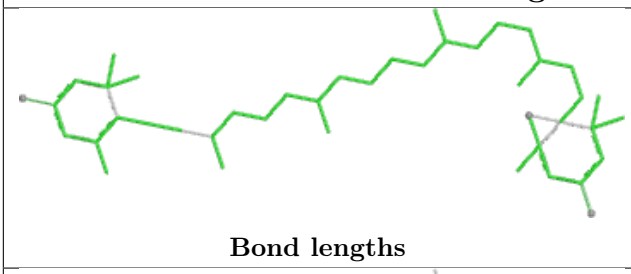


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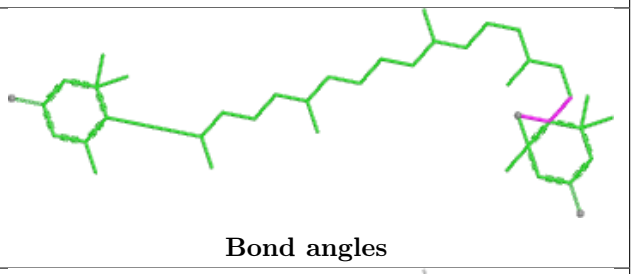


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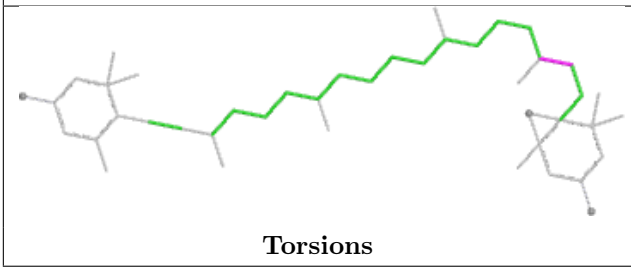
Ligand DD6 u 321



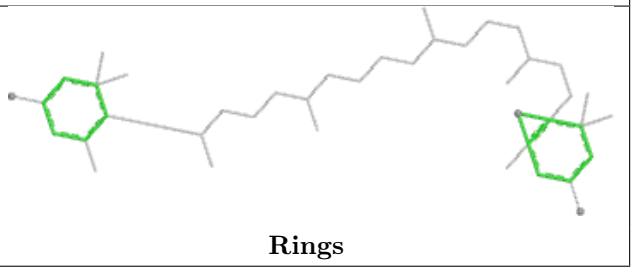
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Bond angles

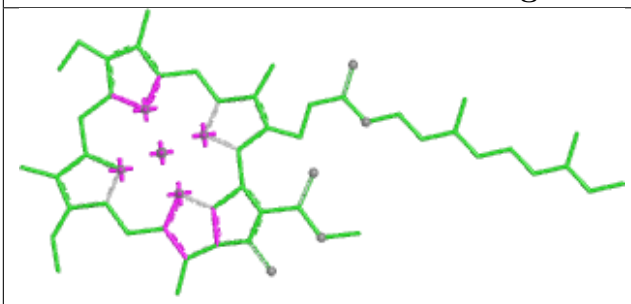


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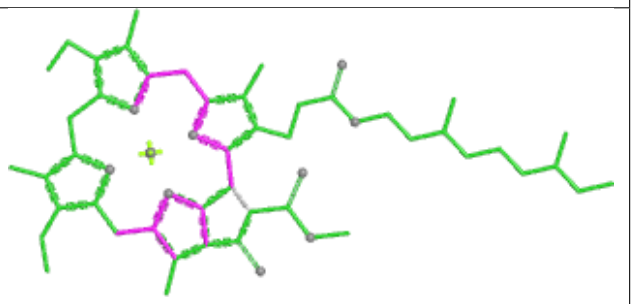


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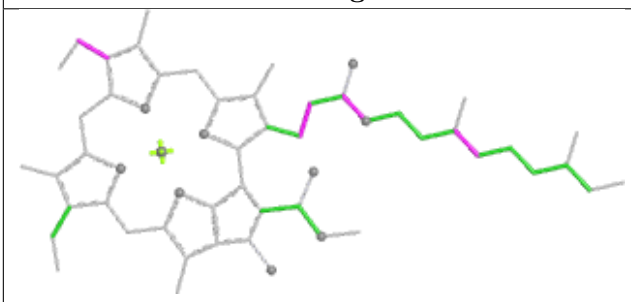
Ligand CLA M 310



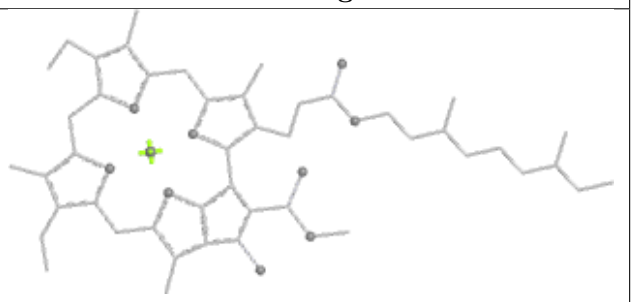
Bond lengths



Bond angles

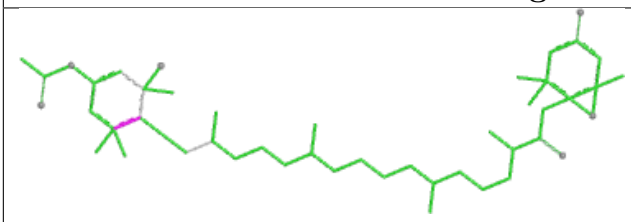


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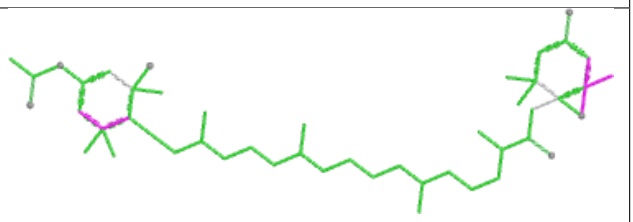


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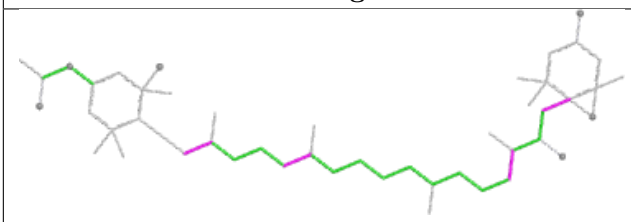
Ligand A86 X 317



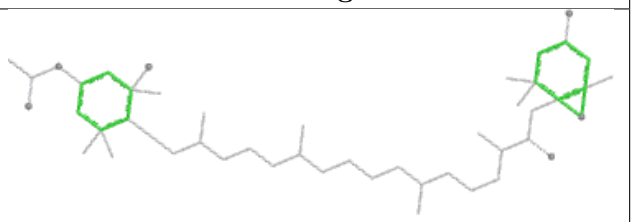
Bond lengths



Bond angles

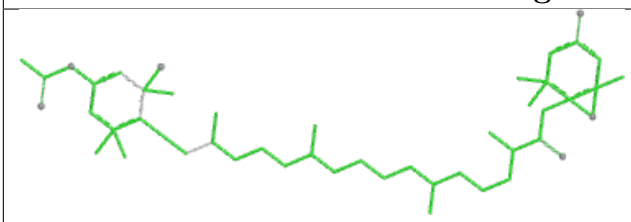


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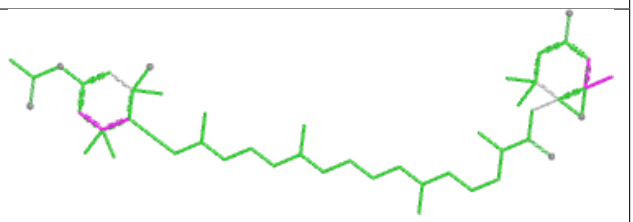


Rings

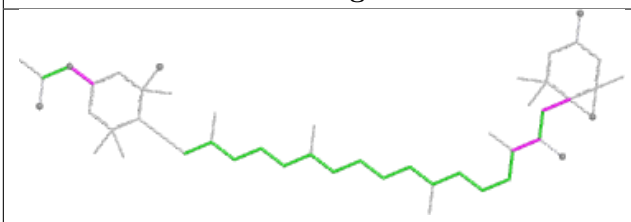
Ligand A86 v 325



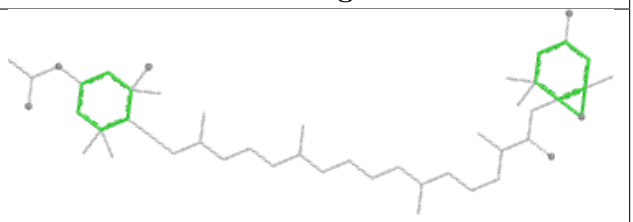
Bond lengths



Bond angles

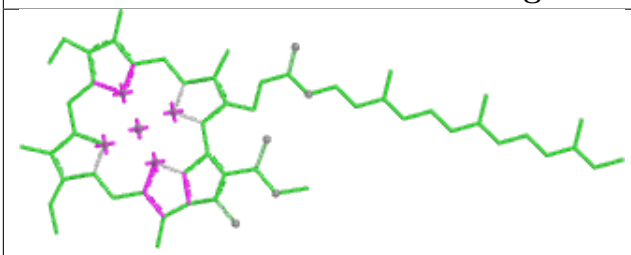


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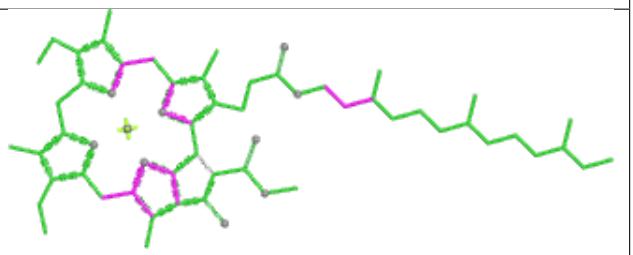


Rings

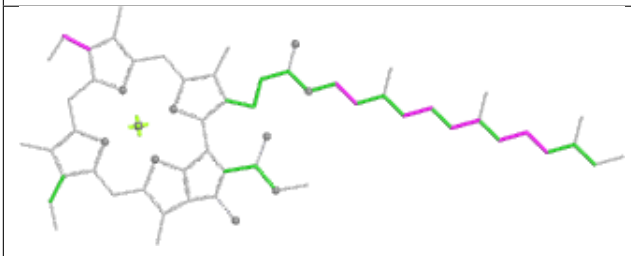
Ligand CLA A 305



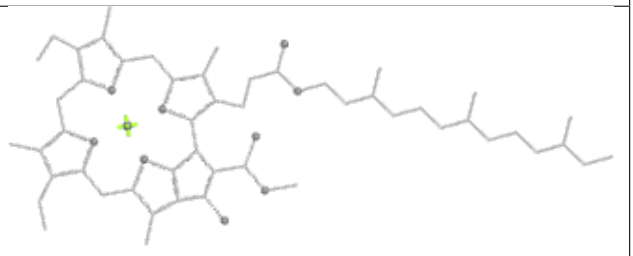
Bond lengths



Bond angles

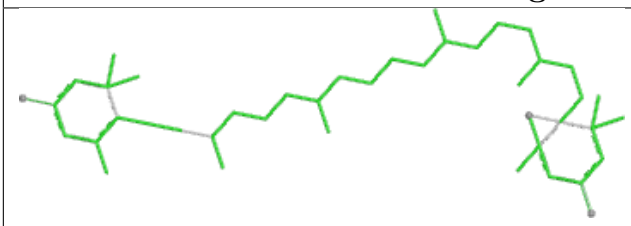


Torsions

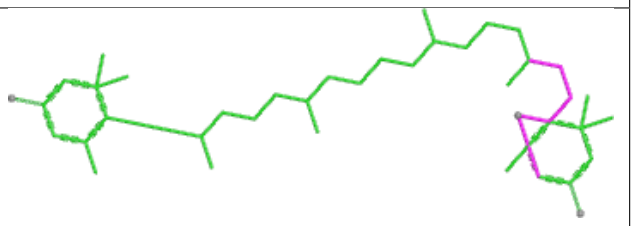


Rings

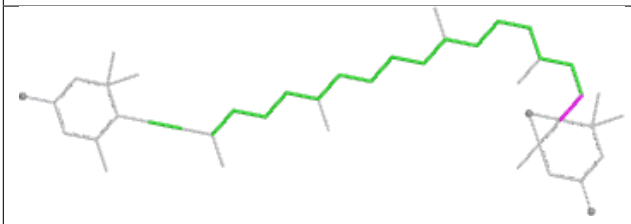
Ligand DD6 J 315



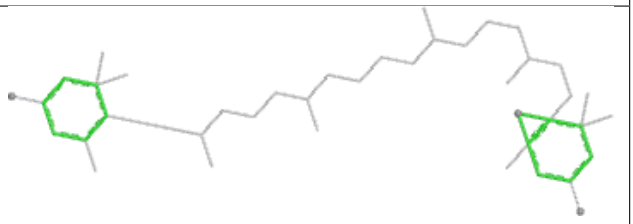
Bond lengths



Bond angles

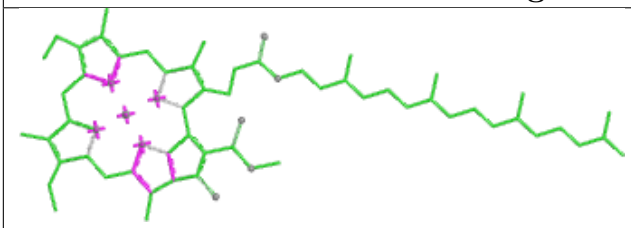


Torsions

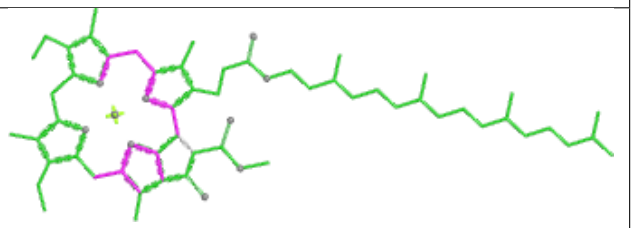


Rings

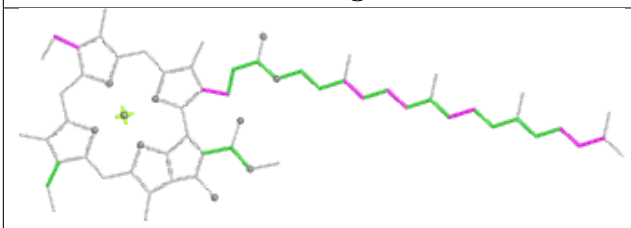
Ligand CLA b 820



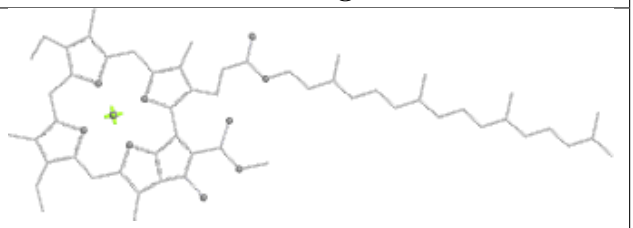
Bond lengths



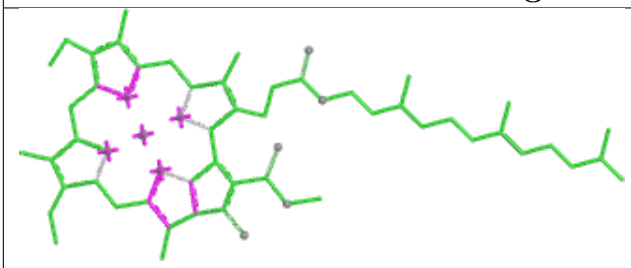
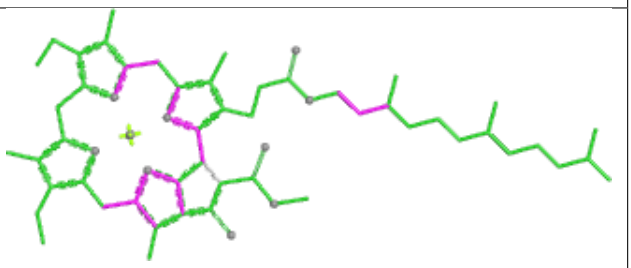
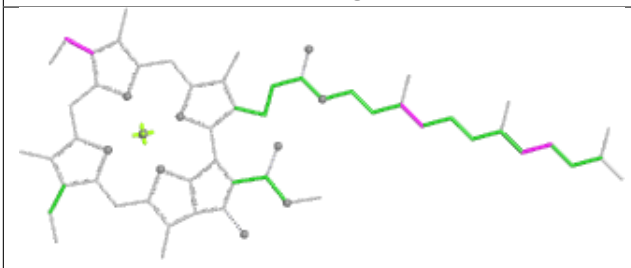
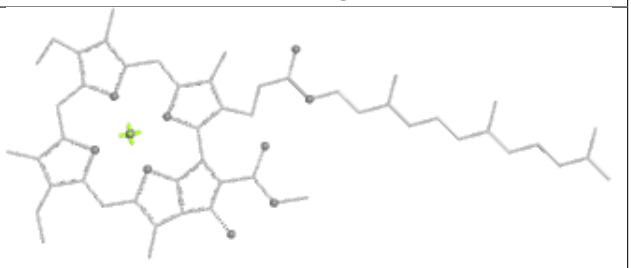
Bond angles

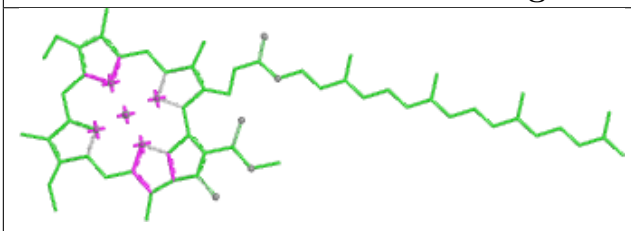
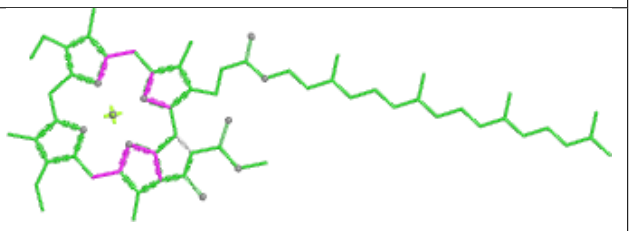
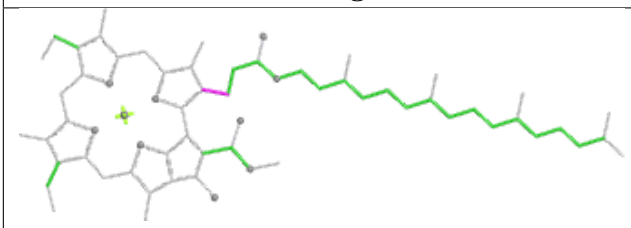
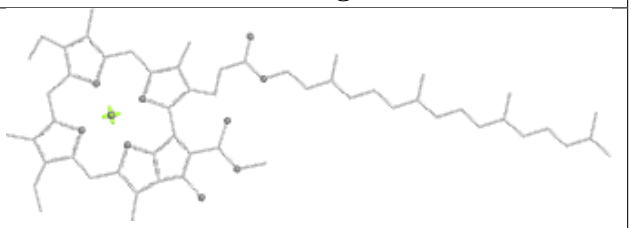


Torsions

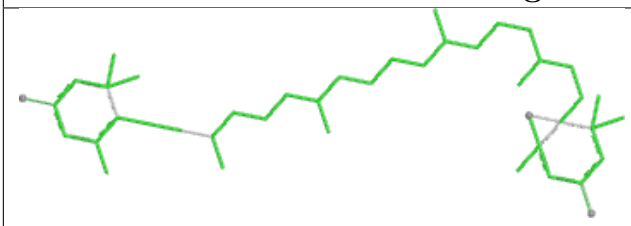


Rings

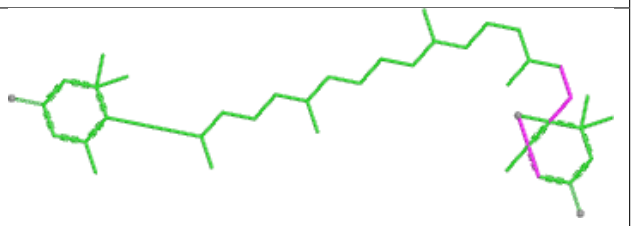
Ligand CLA C 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

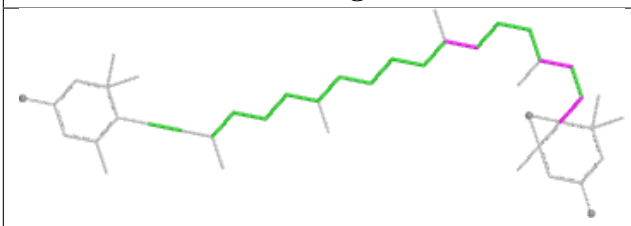
Ligand DD6 H 313



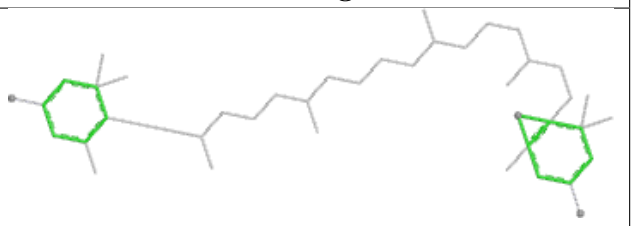
Bond lengths



Bond angles

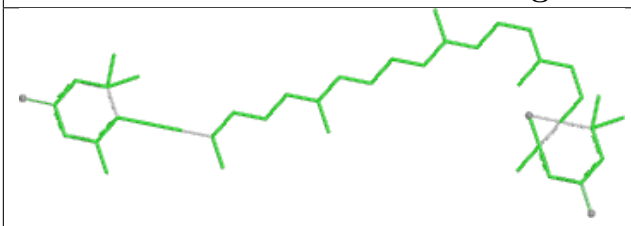


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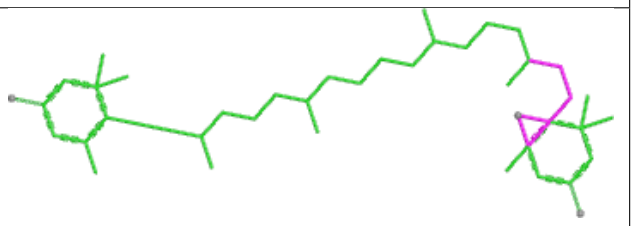


Rings

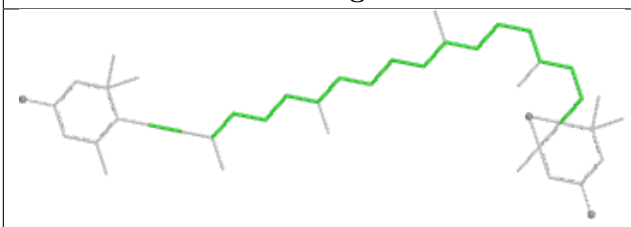
Ligand DD6 I 210



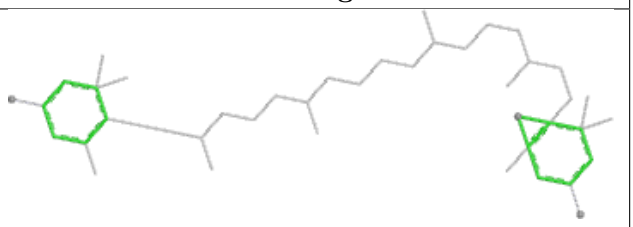
Bond lengths



Bond angles

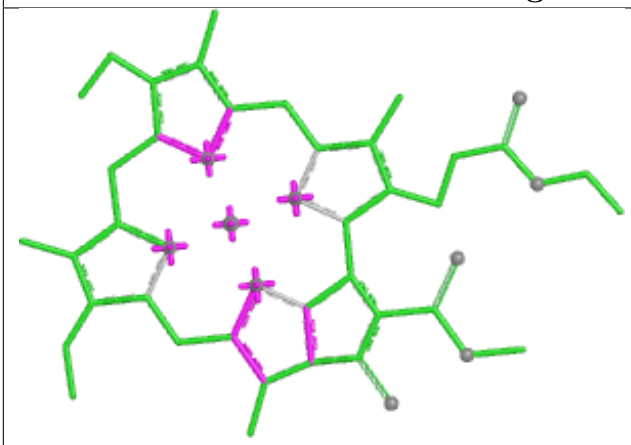


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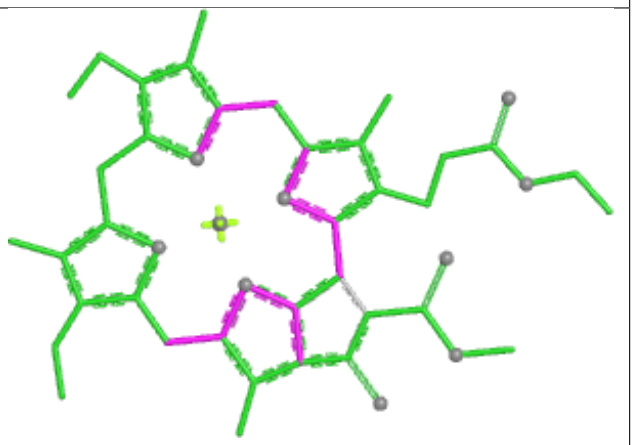


Rings

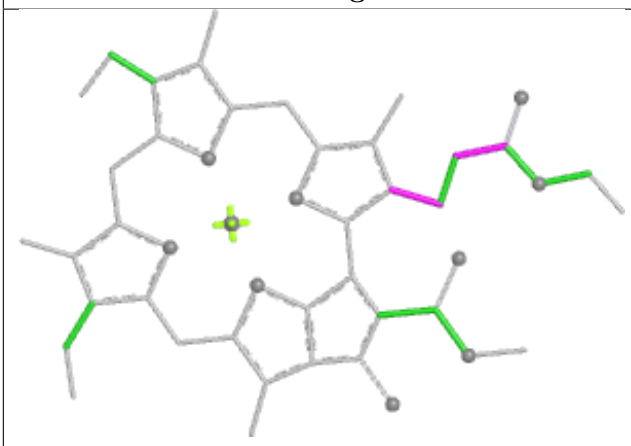
Ligand CLA L 305



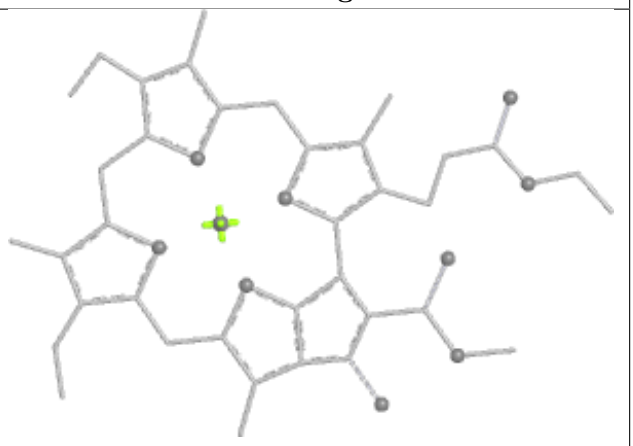
Bond lengths



Bond angles

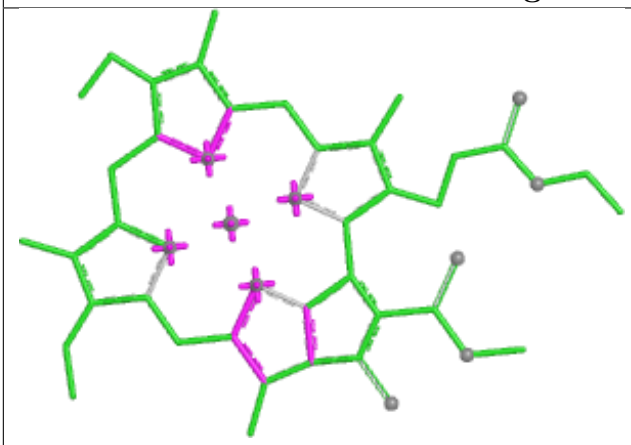


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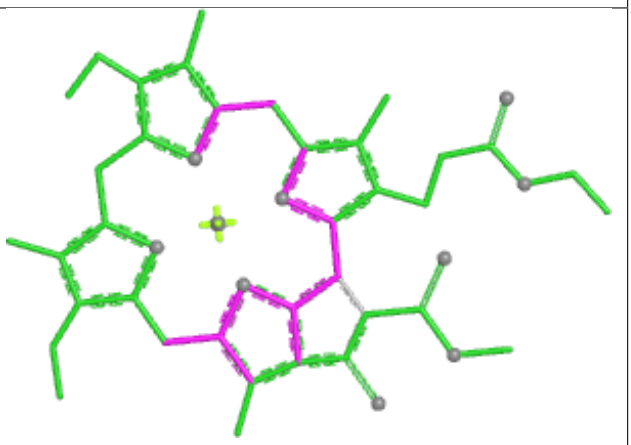


Rings

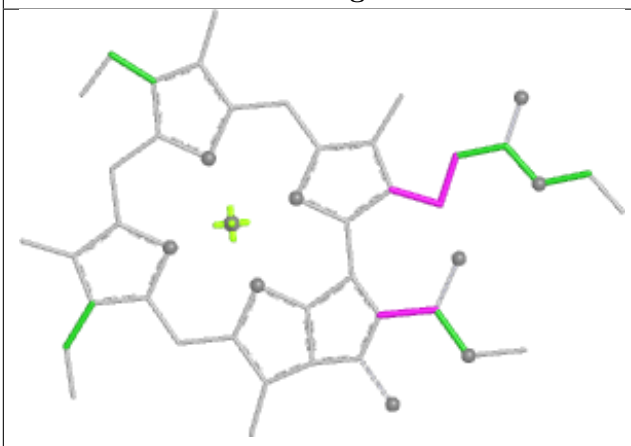
Ligand CLA X 312



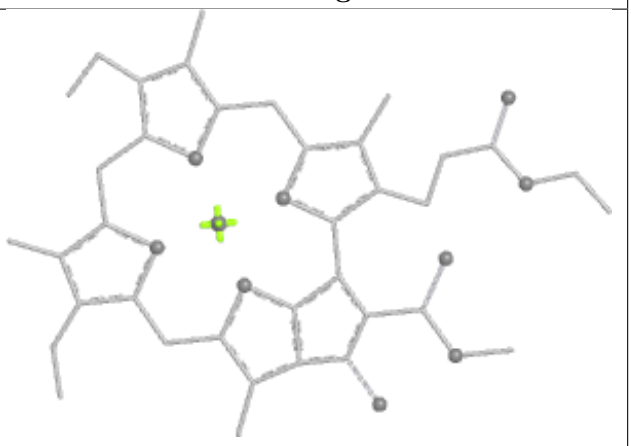
Bond lengths



Bond angles



Torsions



Rings

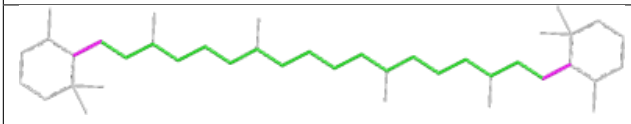
Ligand BCR b 846



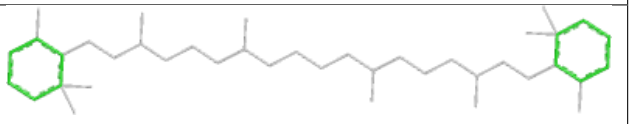
Bond lengths



Bond angles

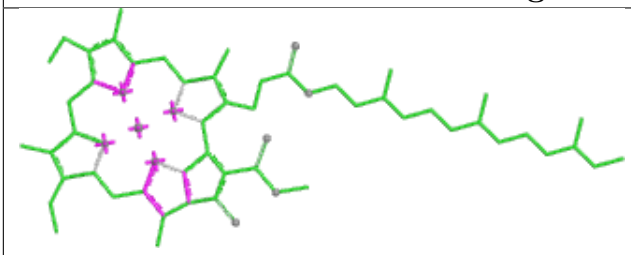


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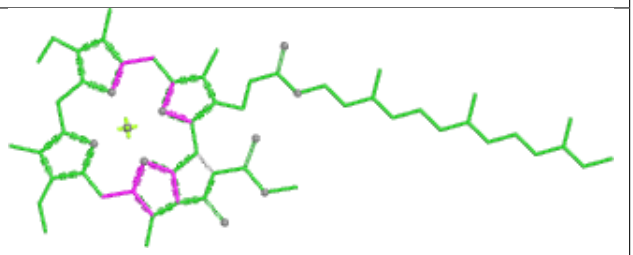


Rings

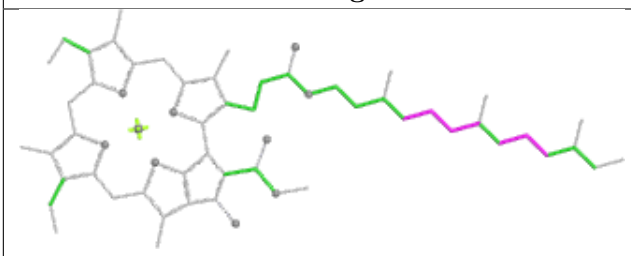
Ligand CLA b 805



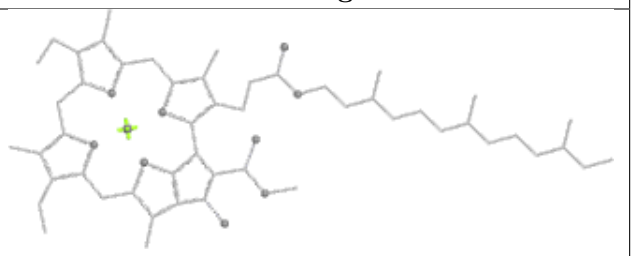
Bond lengths



Bond angles

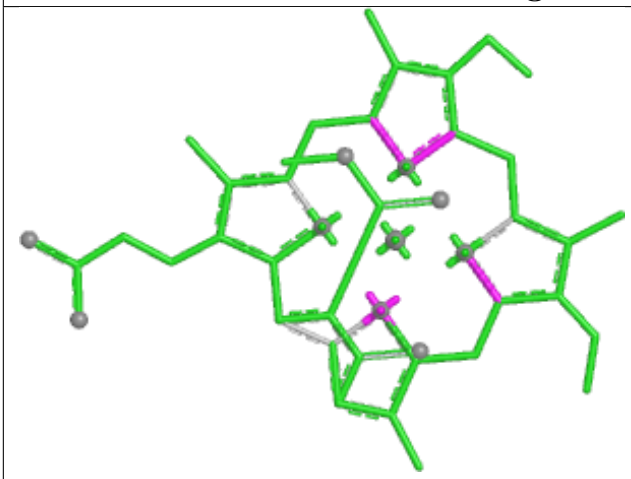


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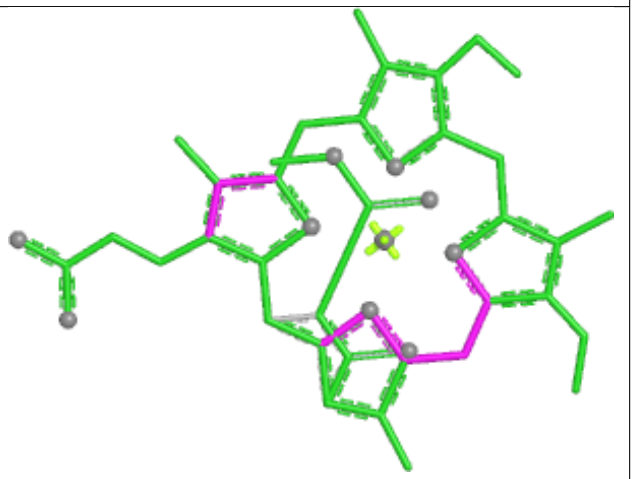


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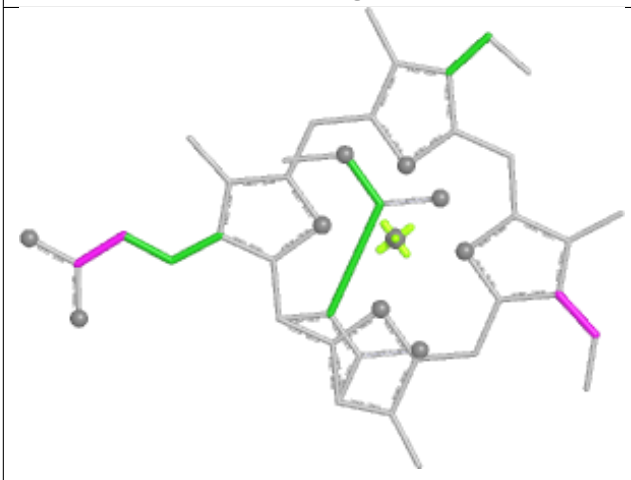
Ligand KC2 w 307



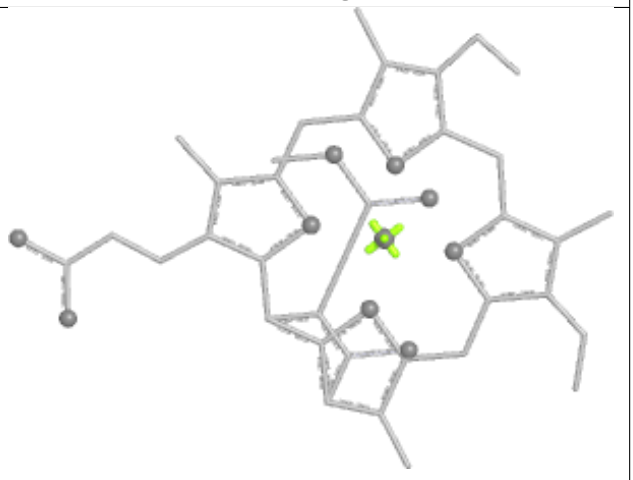
Bond lengths



Bond angles

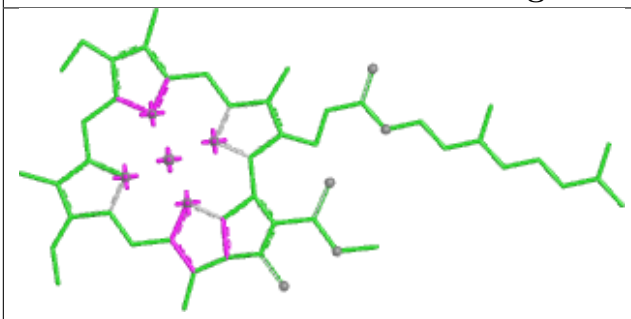


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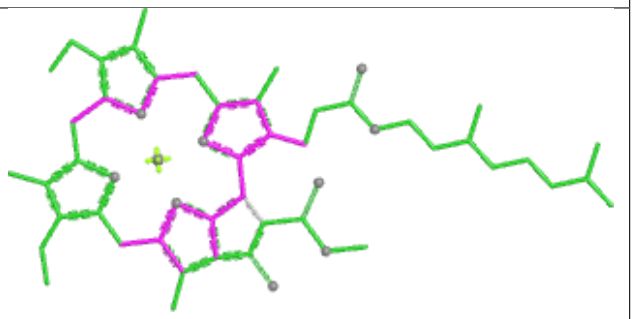


Rings

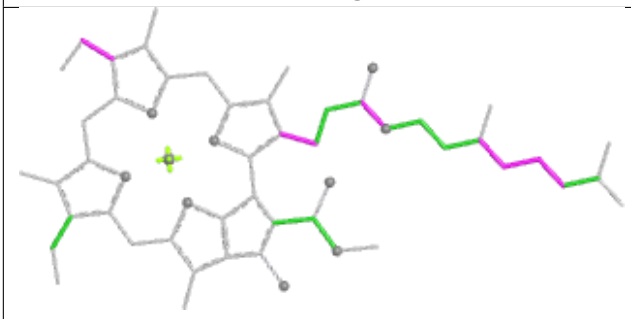
Ligand CLA u 311



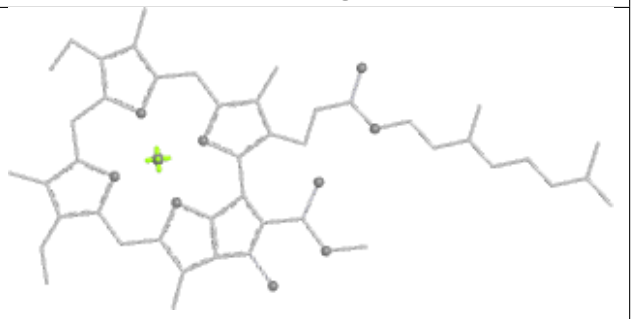
Bond lengths



Bond angles

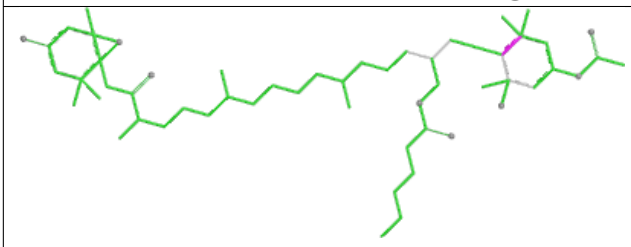


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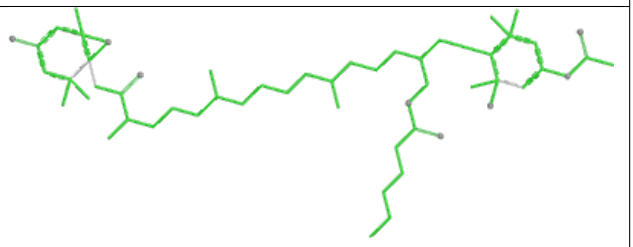


Rings

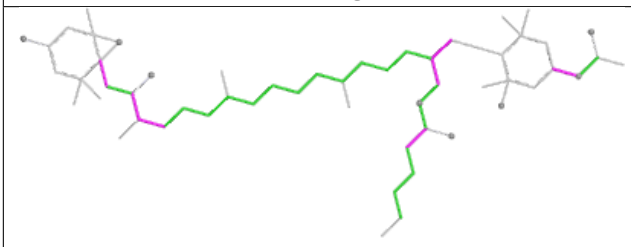
Ligand A1EB1 P 301



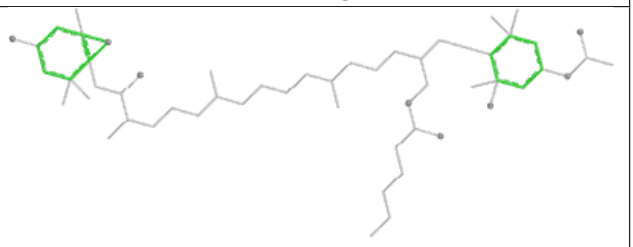
Bond lengths



Bond angles

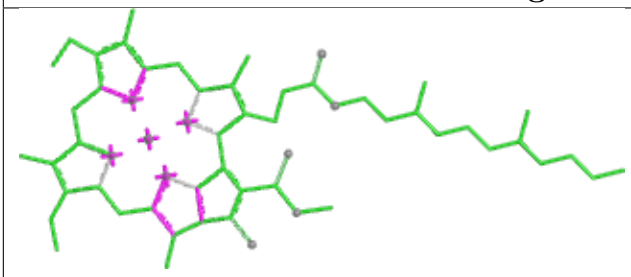


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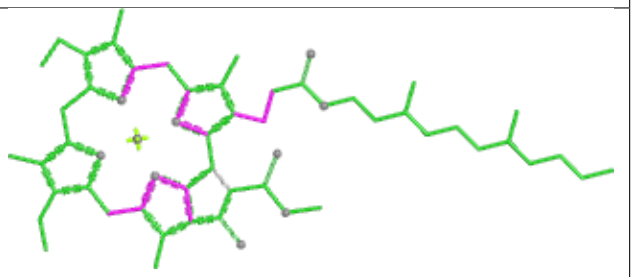


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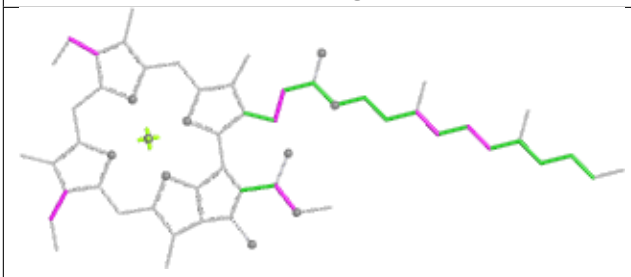
Ligand CLA J 312



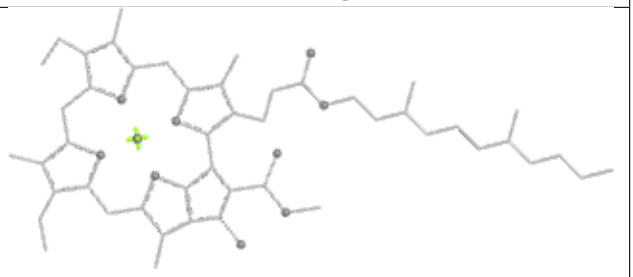
Bond lengths



Bond angles



Torsions



Rings

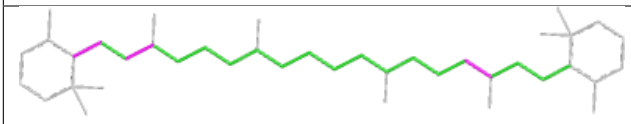
Ligand BCR b 844



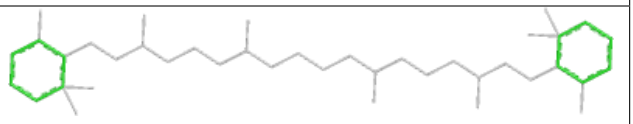
Bond lengths



Bond angles

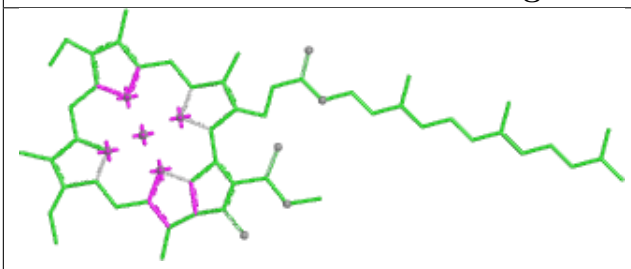


Torsions

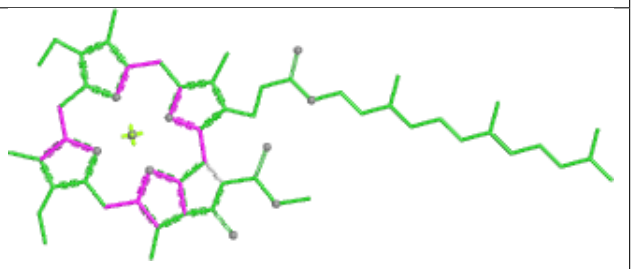


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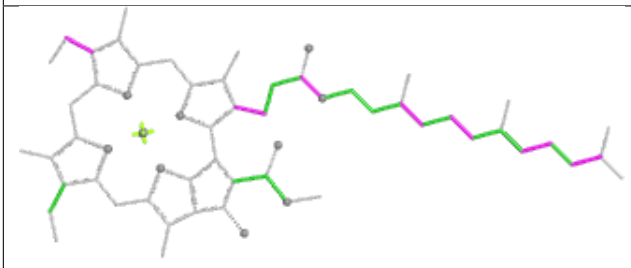
Ligand CLA D 310



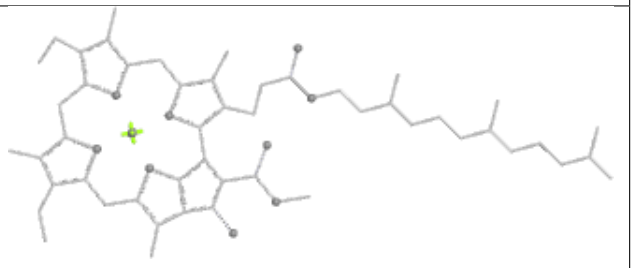
Bond lengths



Bond angles

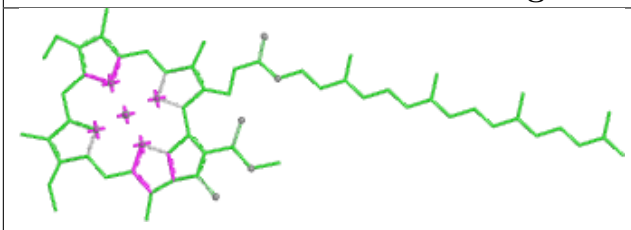


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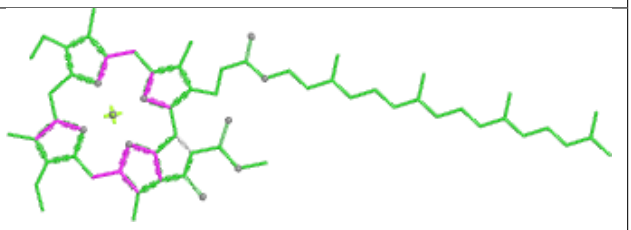


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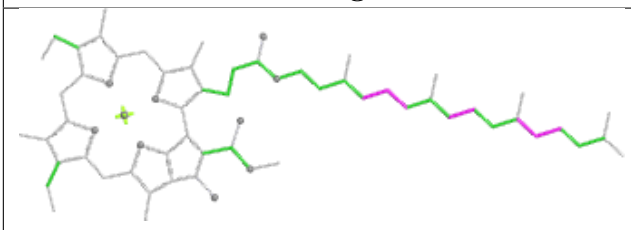
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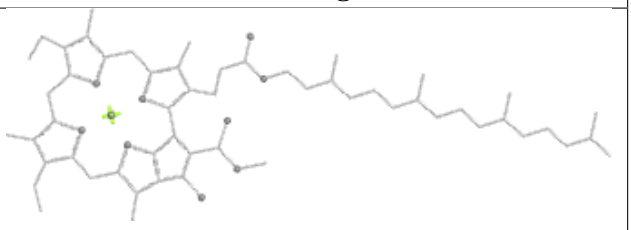
Bond lengths



Bond angles

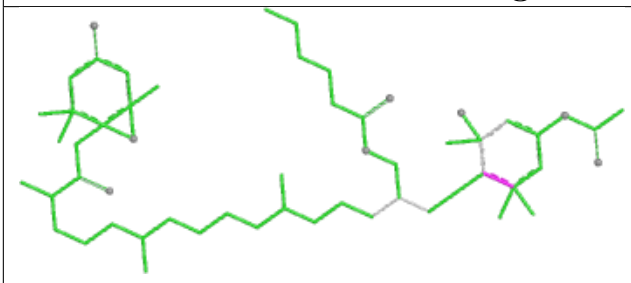


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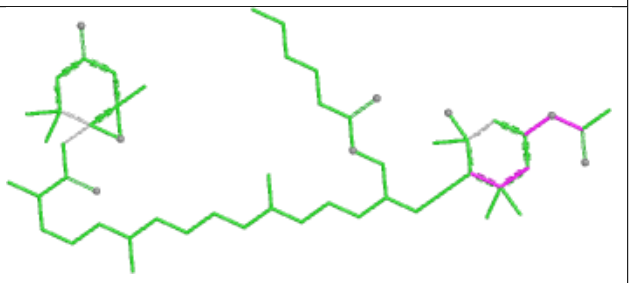


Rings

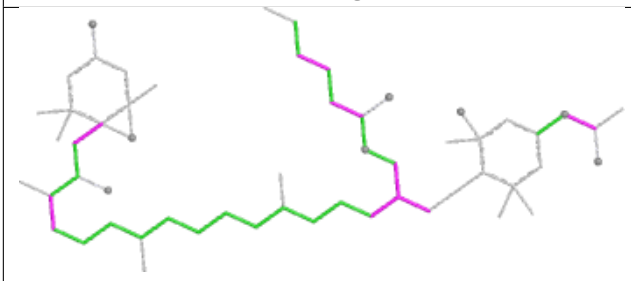
Ligand A1EB1 t 315



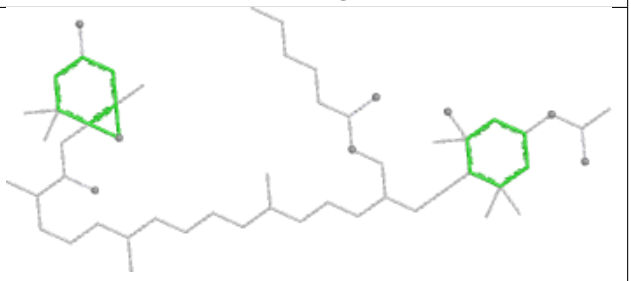
Bond lengths



Bond angles

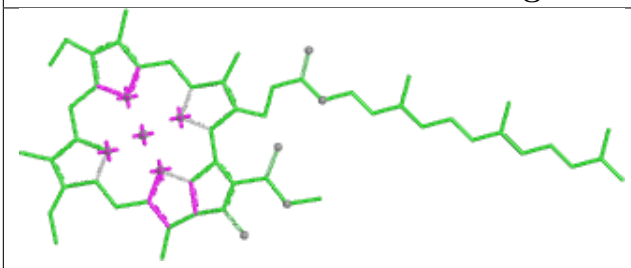


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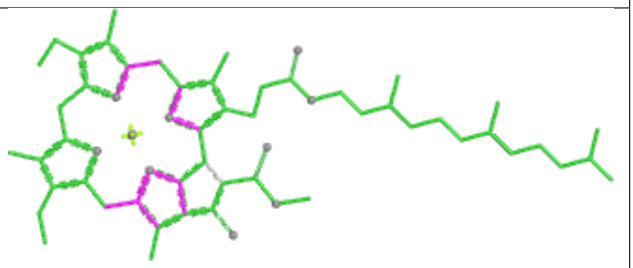


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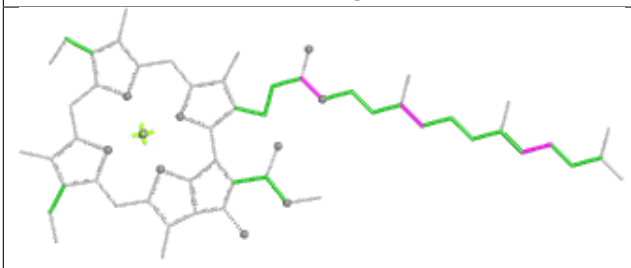
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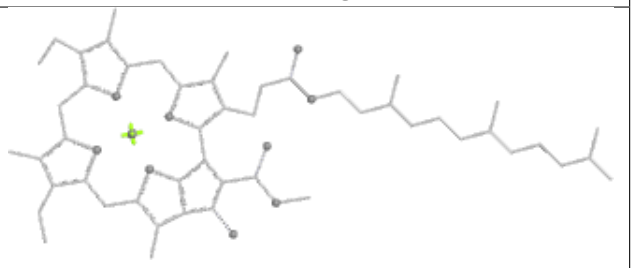
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Bond angles

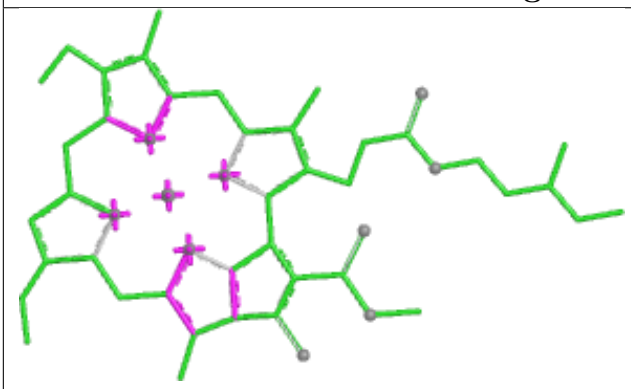


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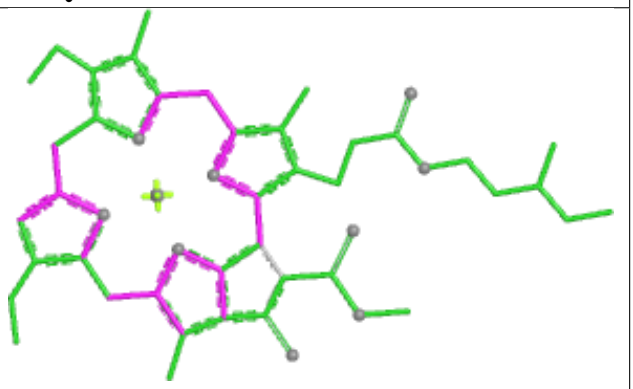


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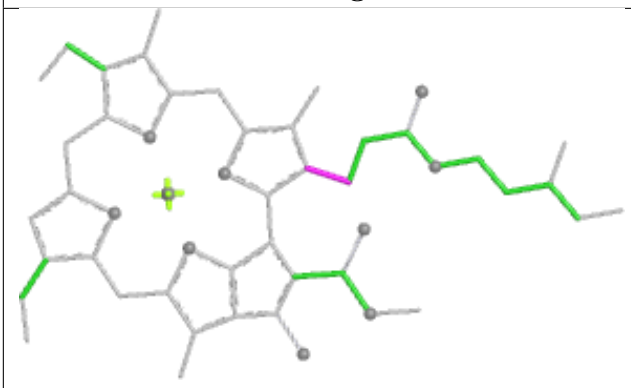
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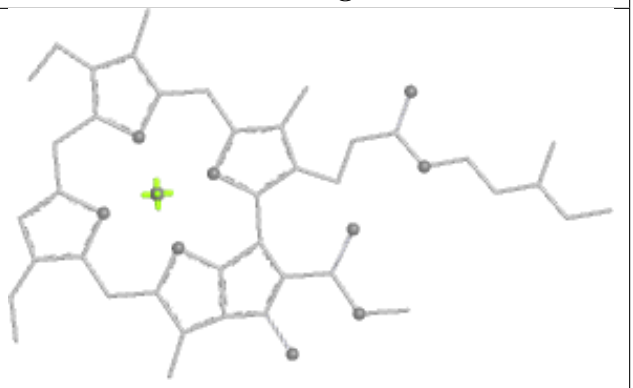
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Bond angles

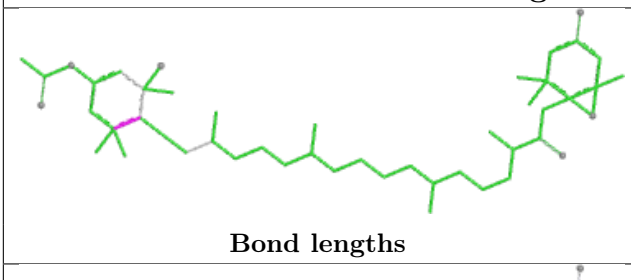


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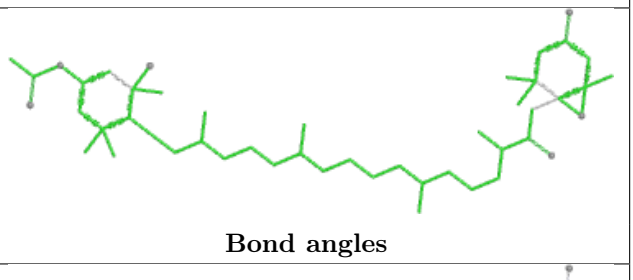


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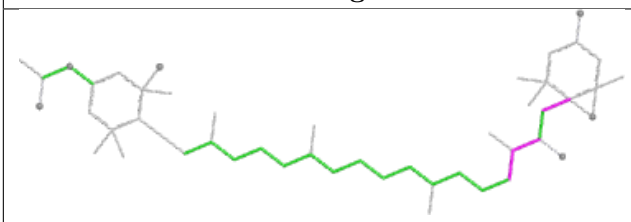
Ligand A86 R 313



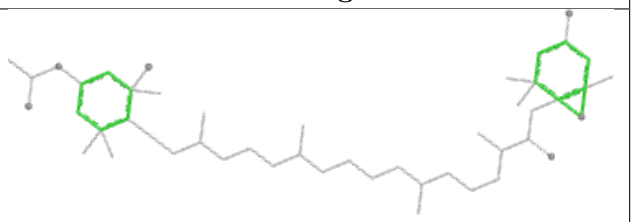
Bond lengths



Bond angles

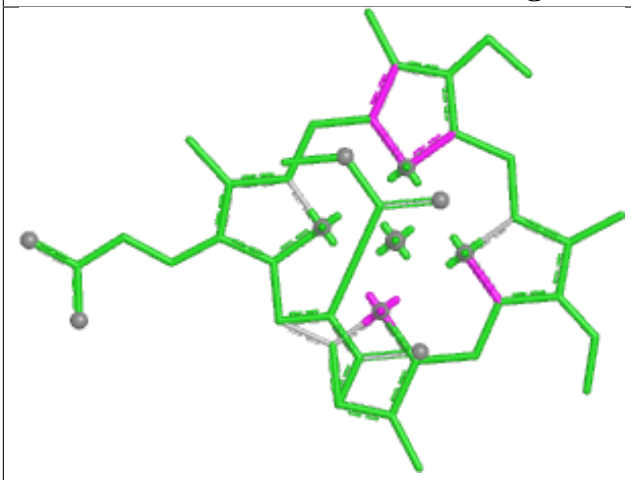


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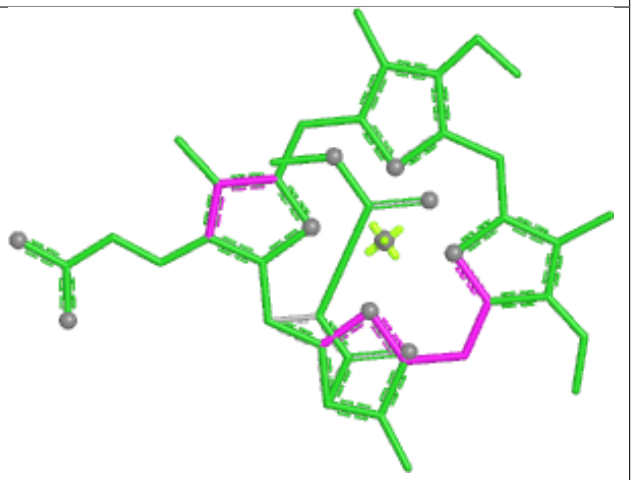


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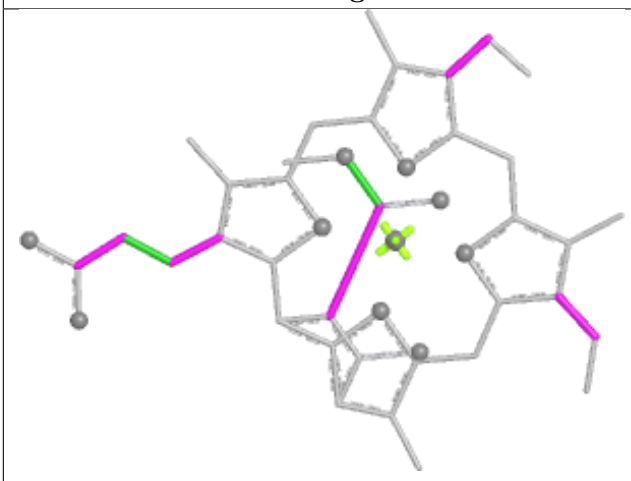
Ligand KC2 O 302



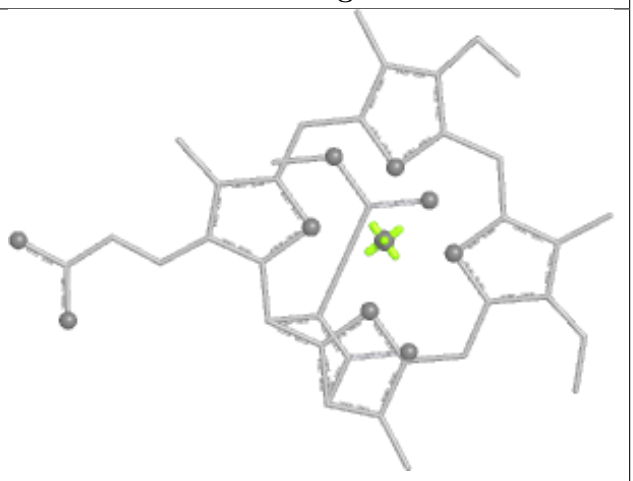
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Bond angles

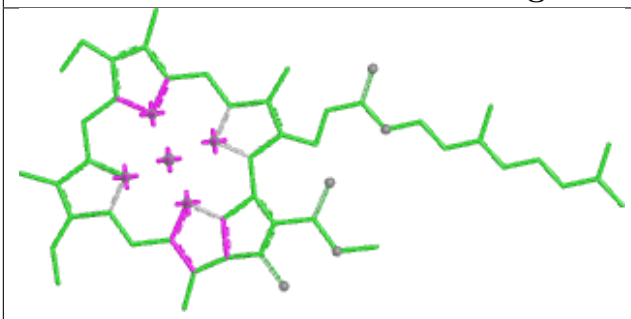


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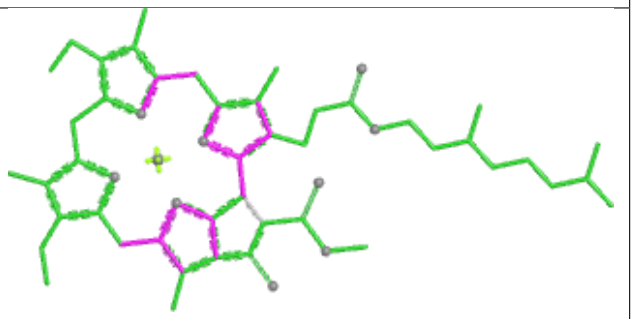


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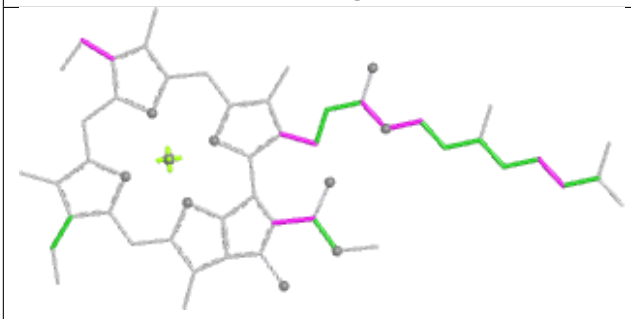
Ligand CLA x 307



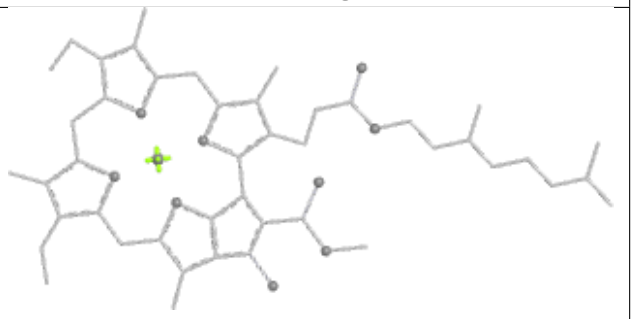
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Bond angles

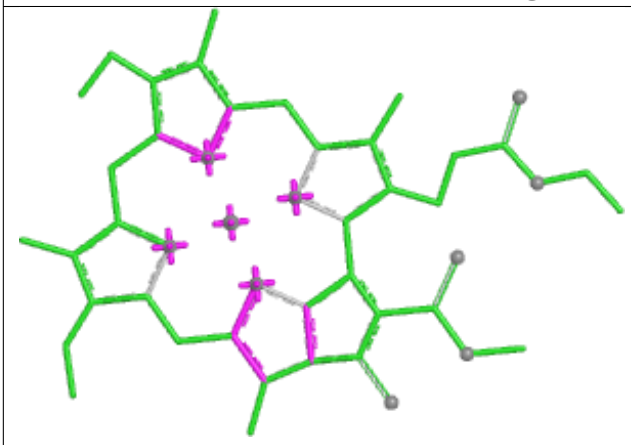


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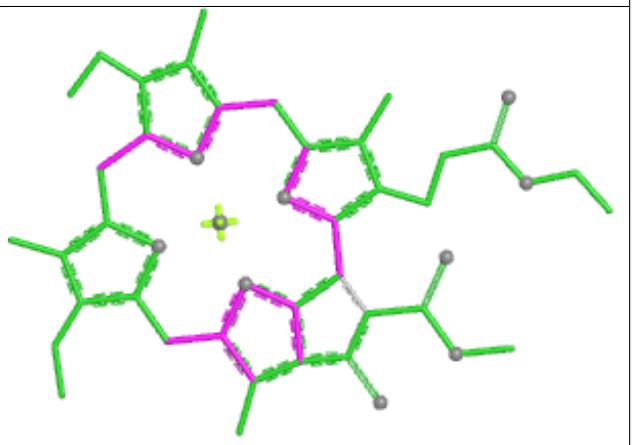


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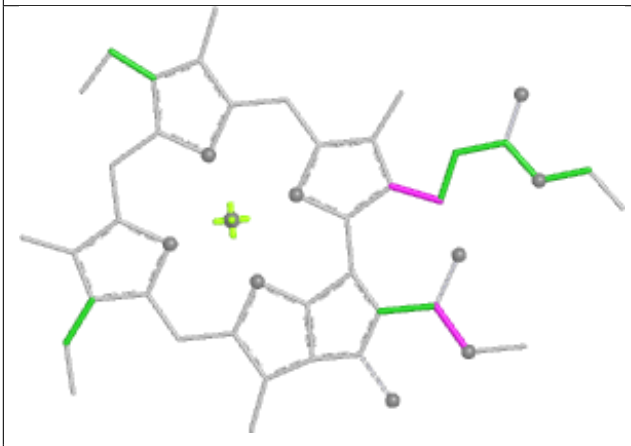
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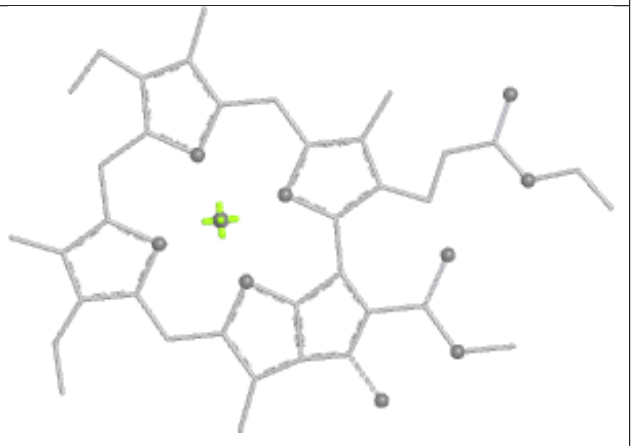
Bond lengths



Bond angles

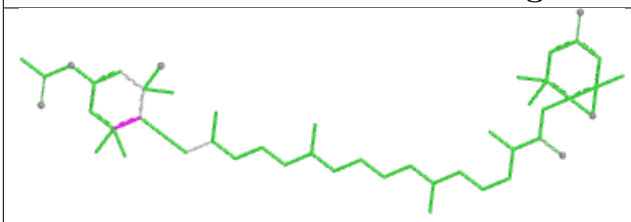


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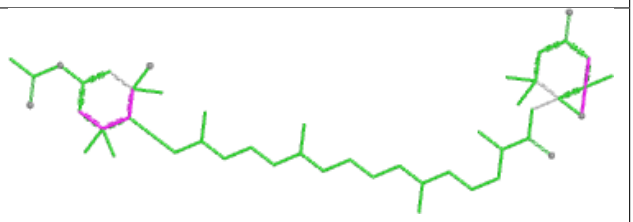


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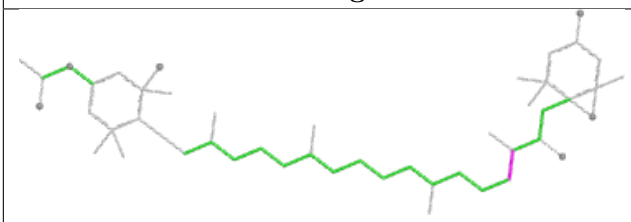
Ligand A86 M 316



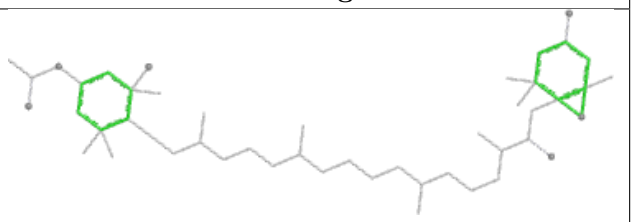
Bond lengths



Bond angles

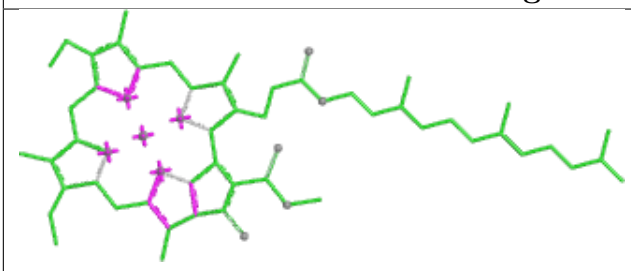


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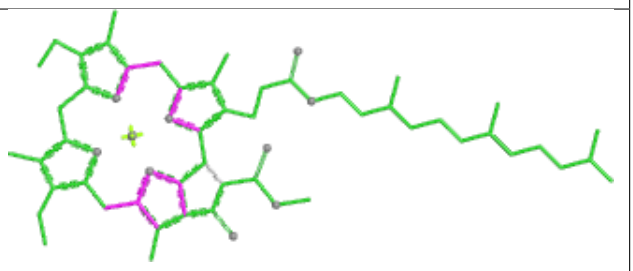


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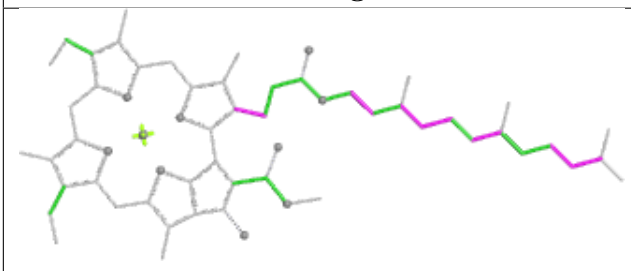
Ligand CLA N 304



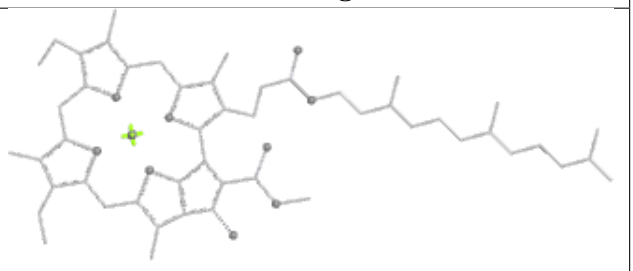
Bond lengths



Bond angles

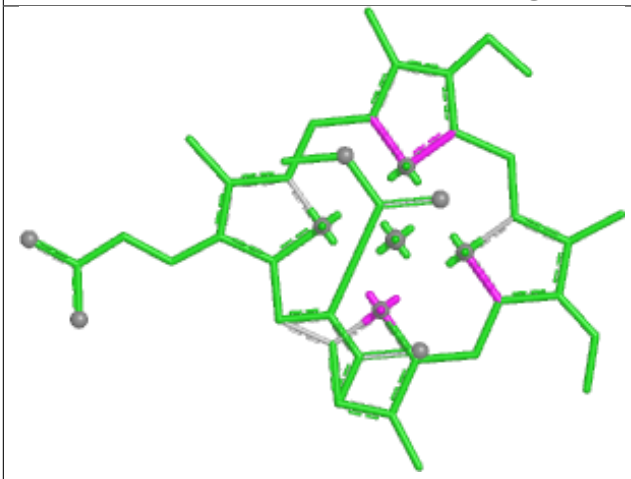


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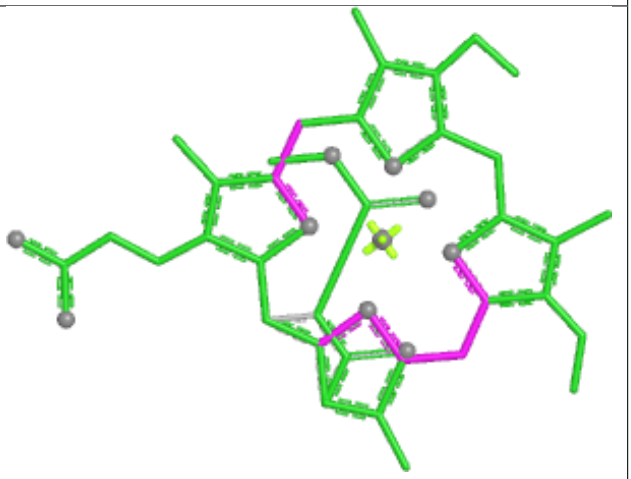


Rings

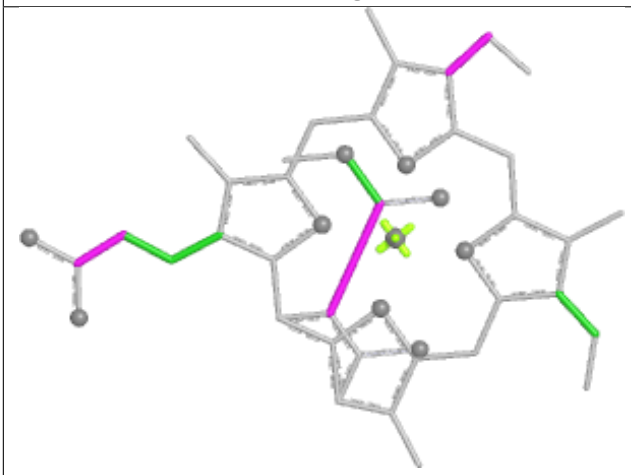
Ligand KC2 Y 303



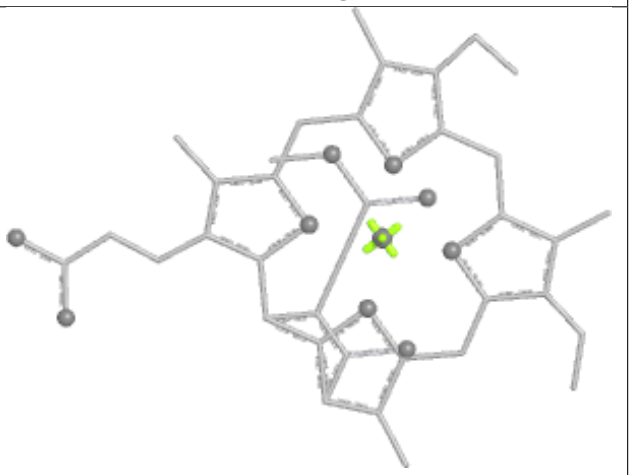
Bond lengths



Bond angles

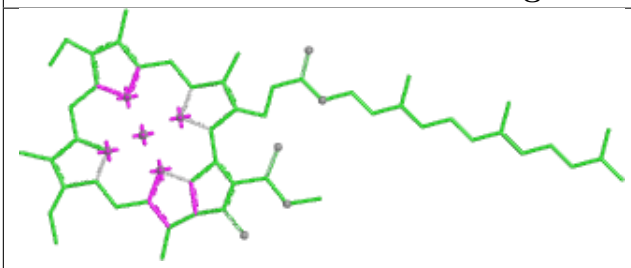


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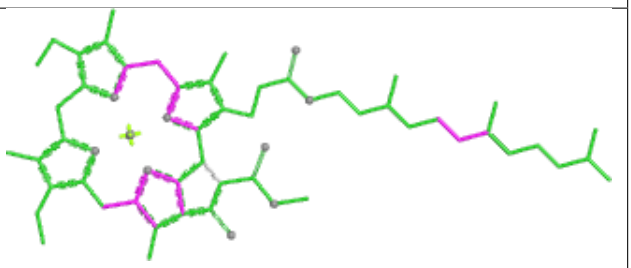


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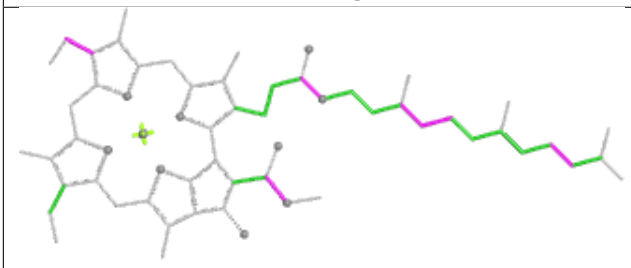
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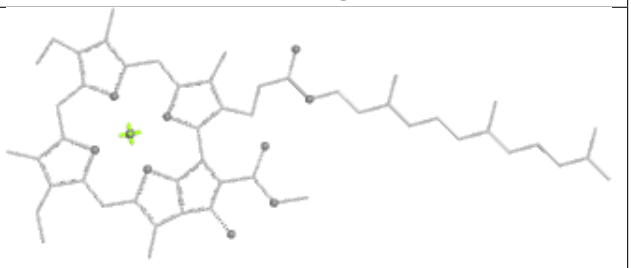
Bond lengths



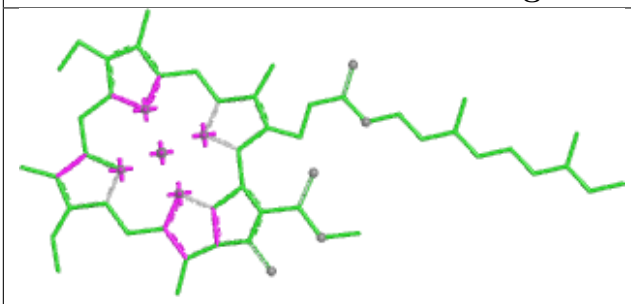
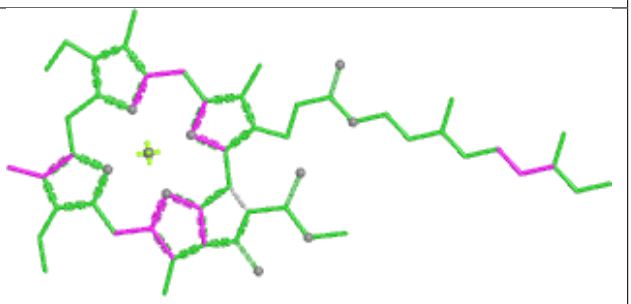
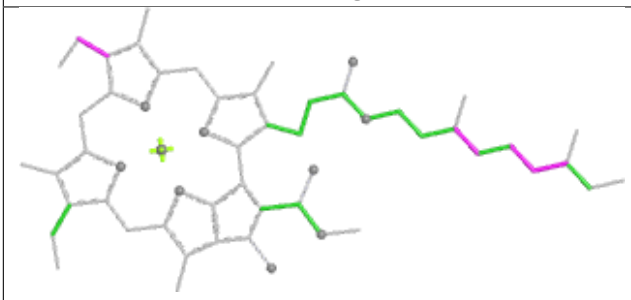
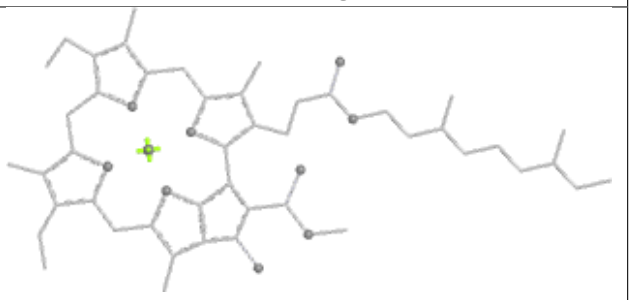
Bond angles

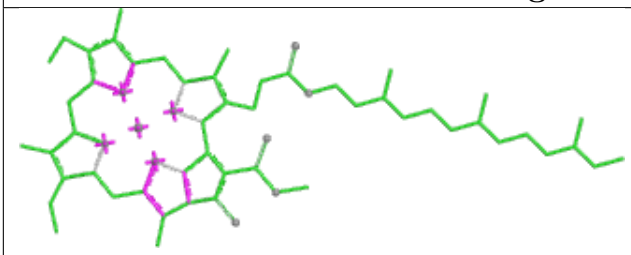
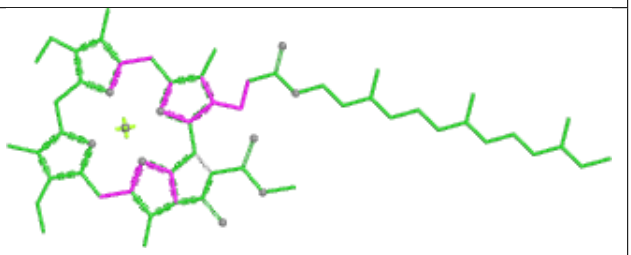
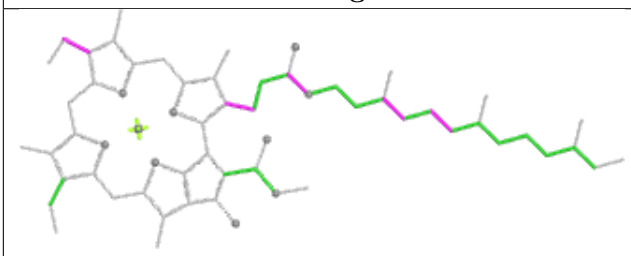
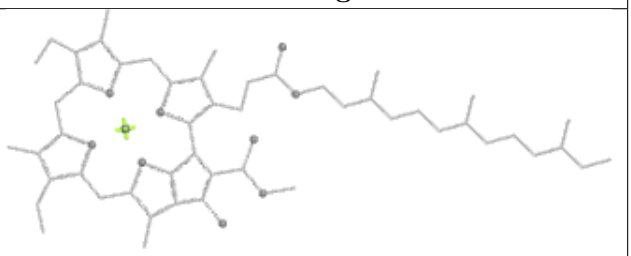


Torsions

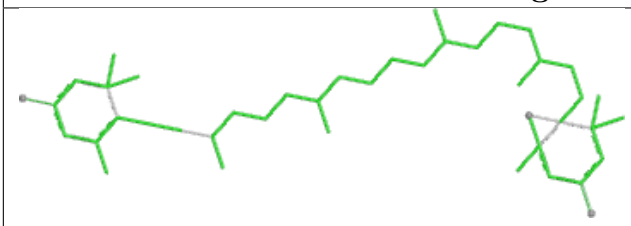


Rings

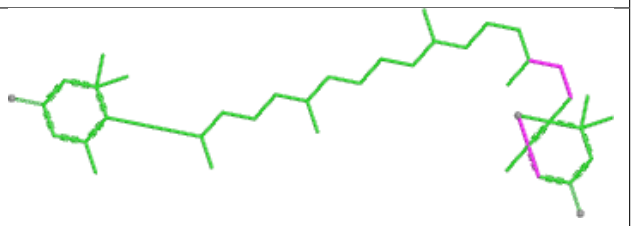
Ligand CLA D 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

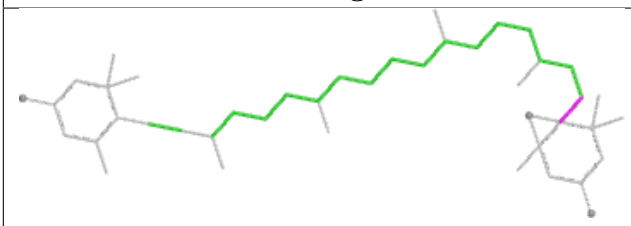
Ligand DD6 I 213



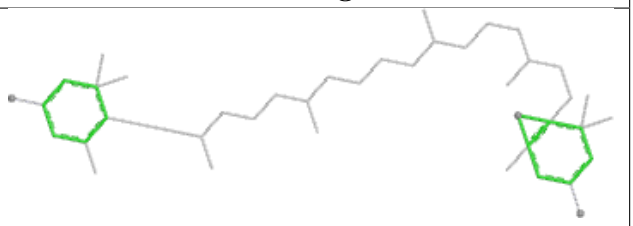
Bond lengths



Bond angles

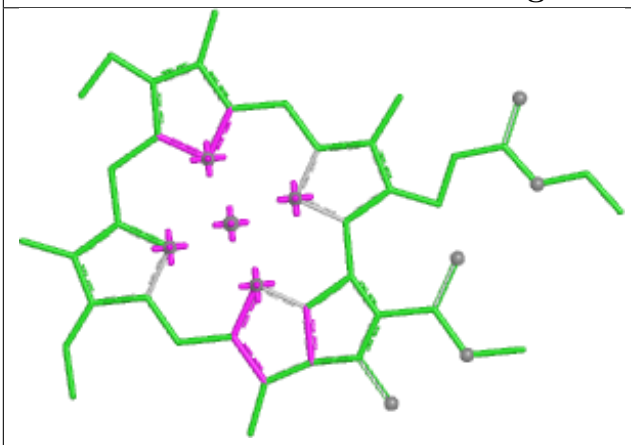


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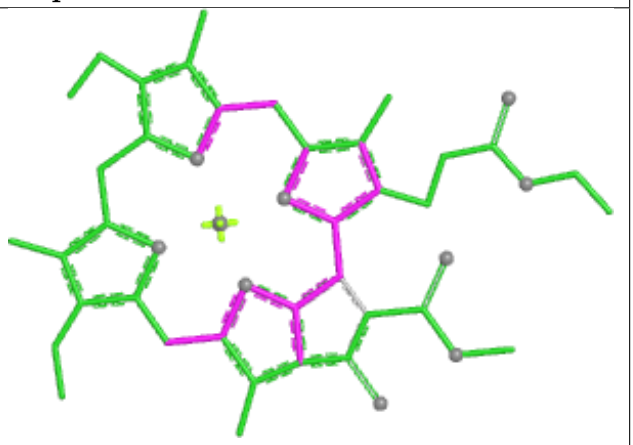


Rings

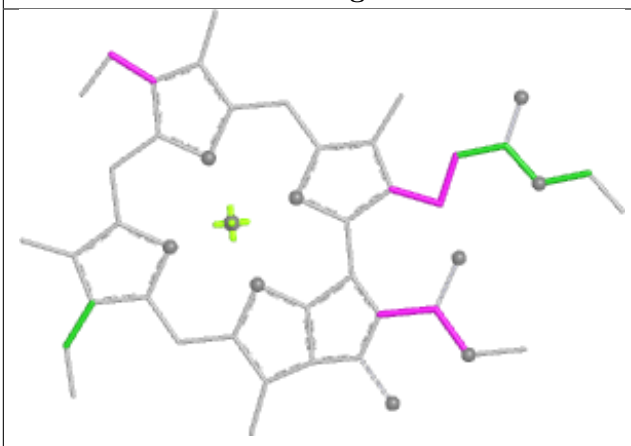
Ligand CLA p 314



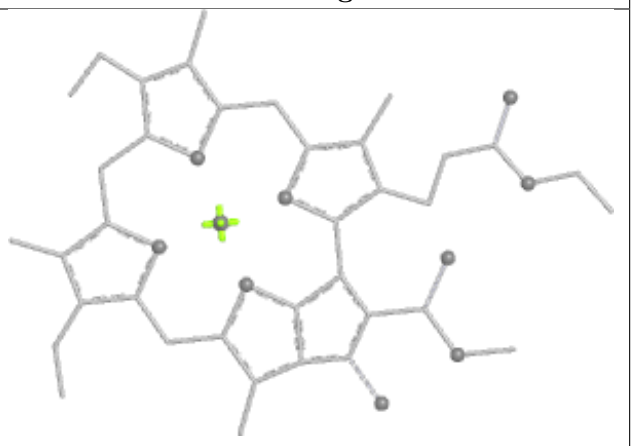
Bond lengths



Bond angles

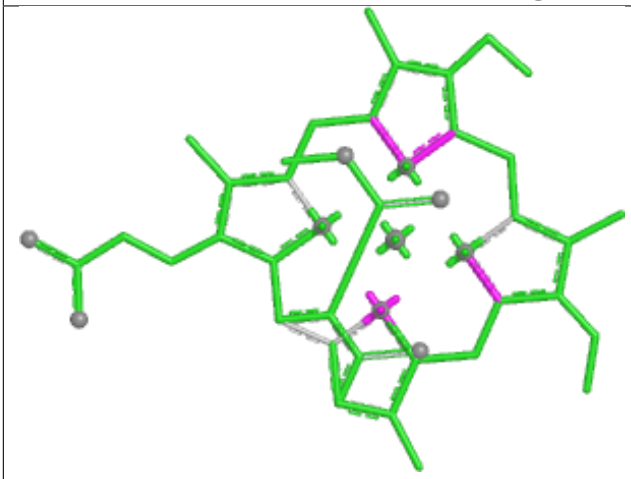


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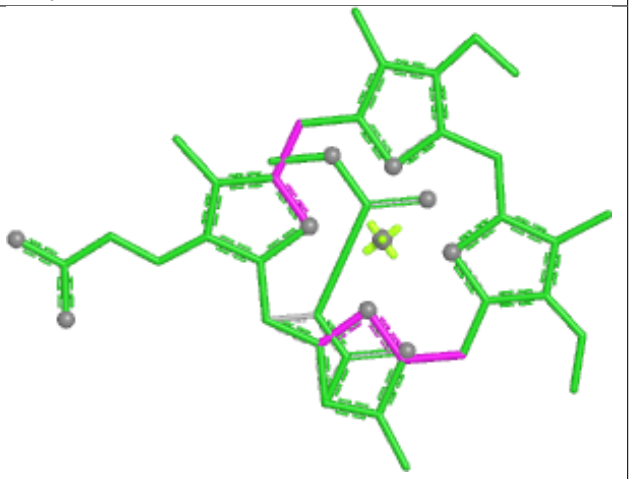


Rings

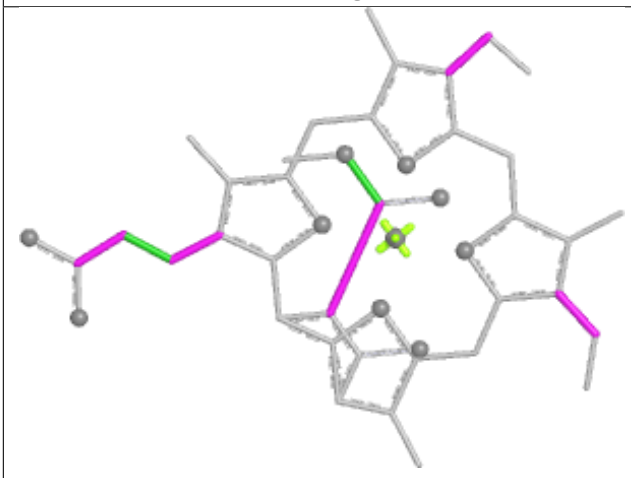
Ligand KC2 y 301



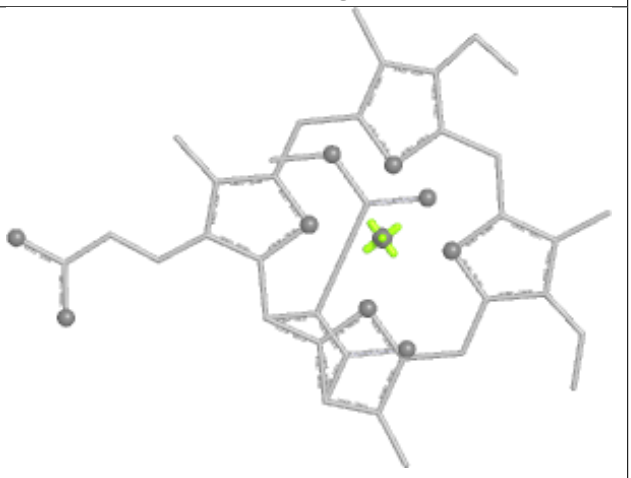
Bond lengths



Bond angles

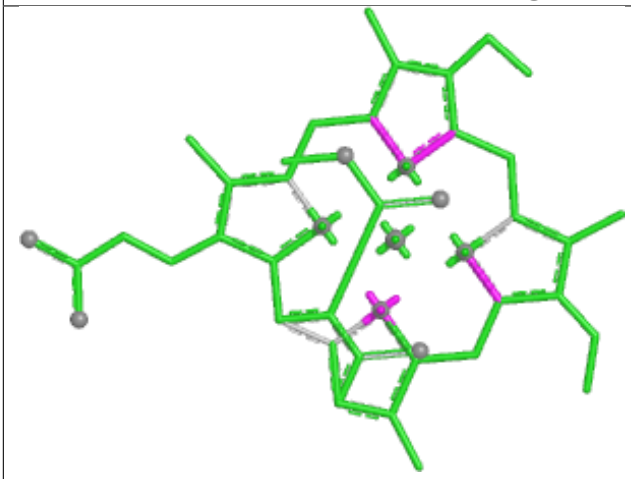


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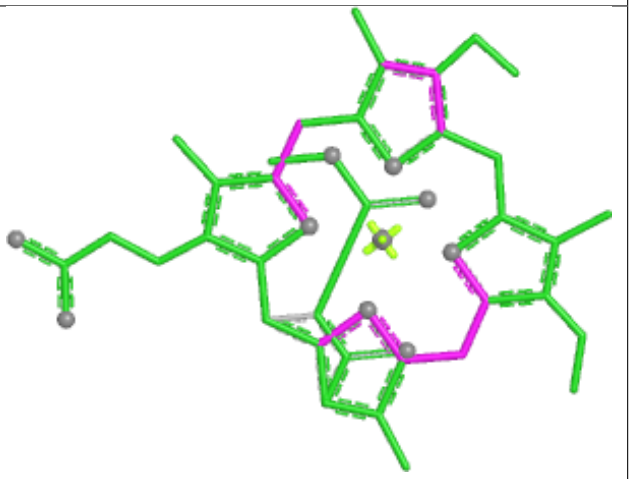


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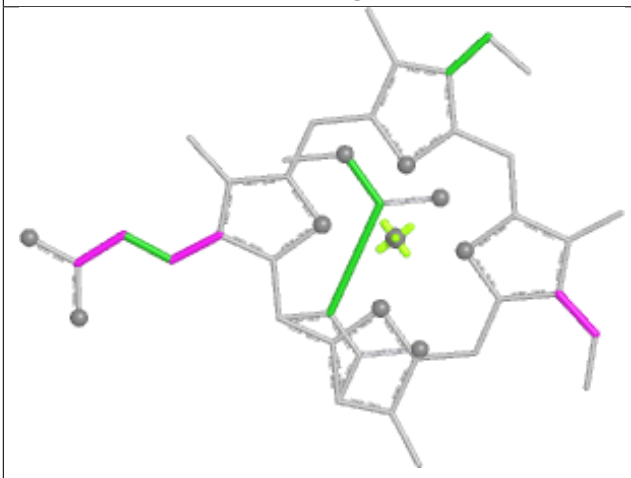
Ligand KC2 Y 302



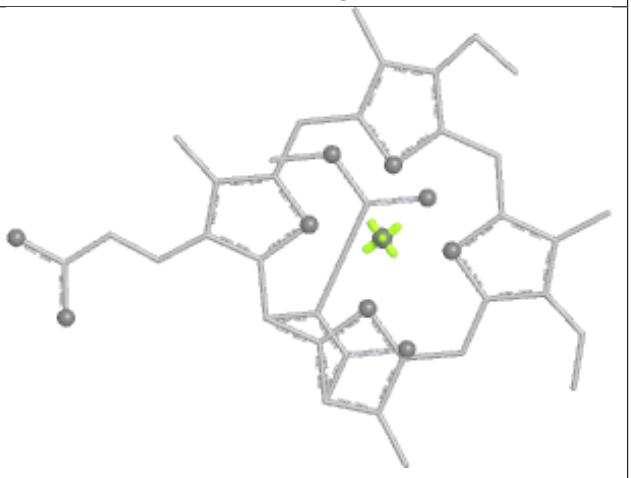
Bond lengths



Bond angles

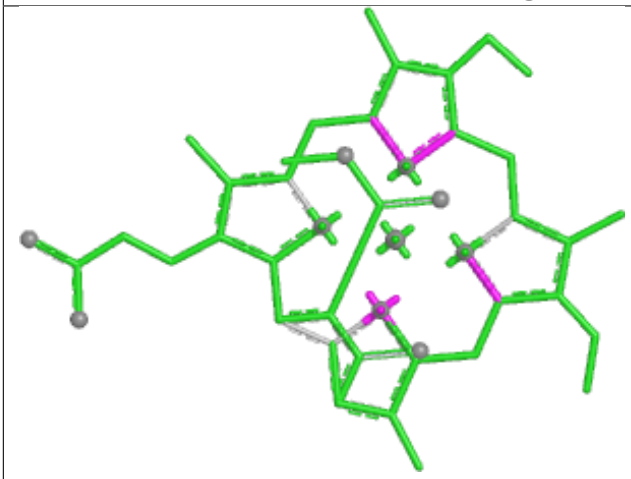


Torsions

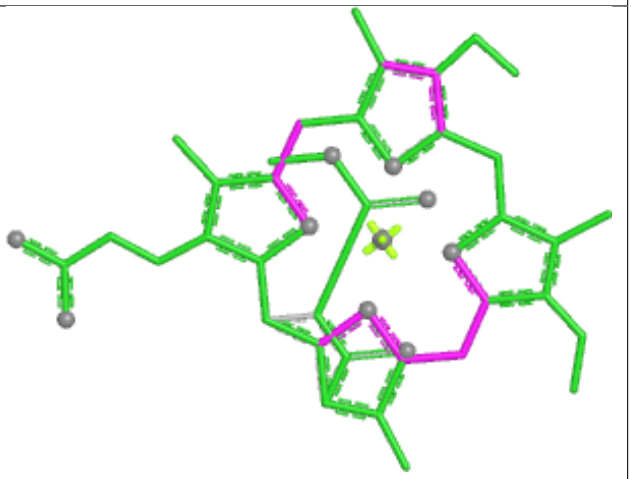


Rings

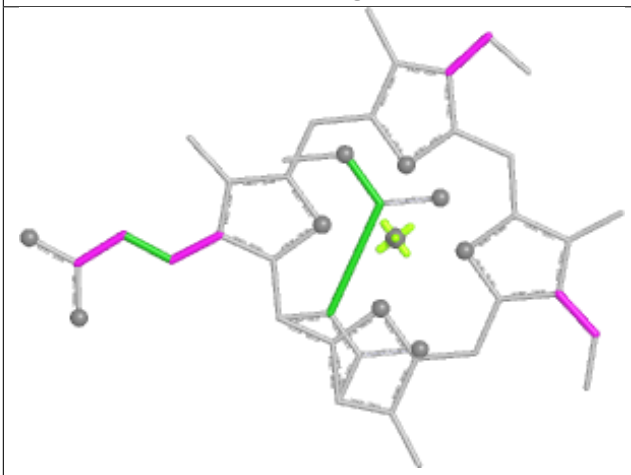
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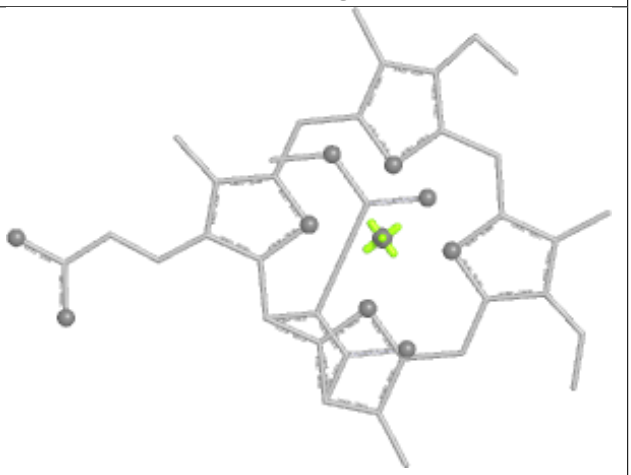
Bond lengths



Bond angles

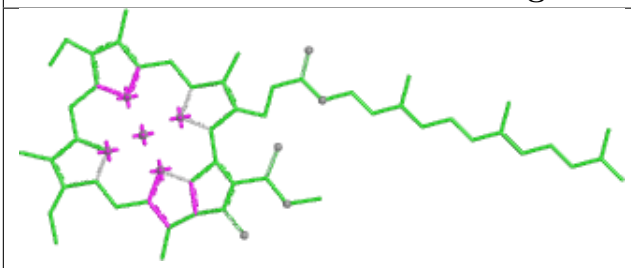


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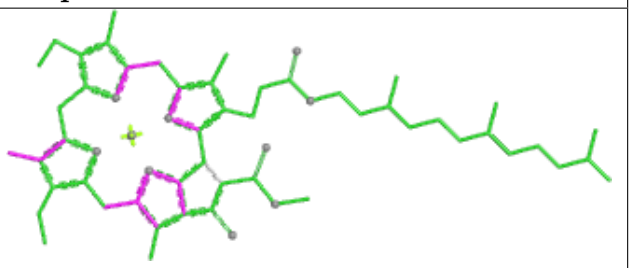


Rings

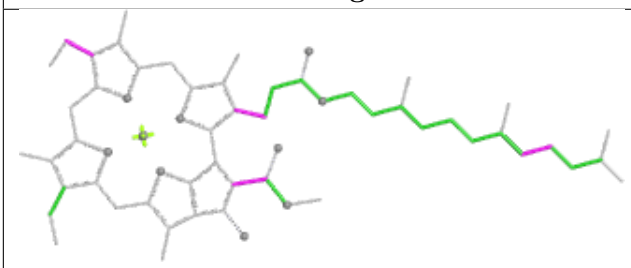
Ligand CLA q 306



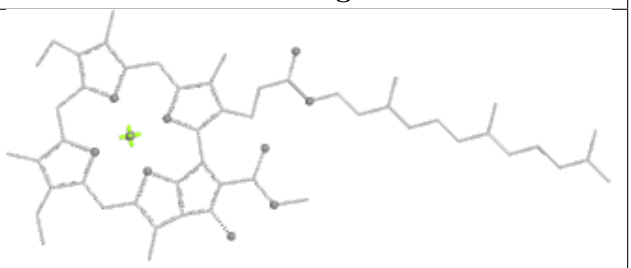
Bond lengths



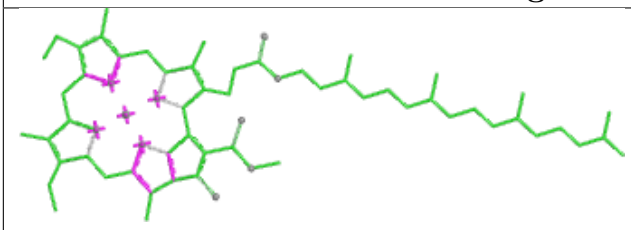
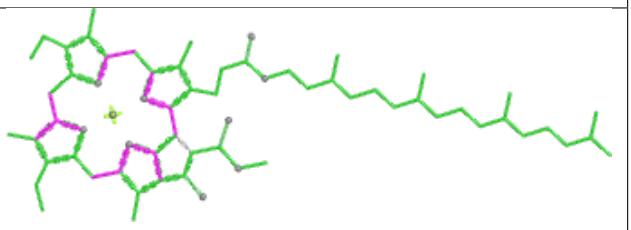
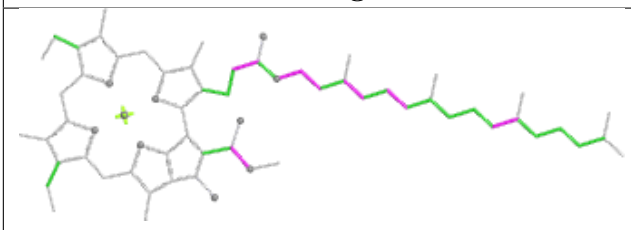
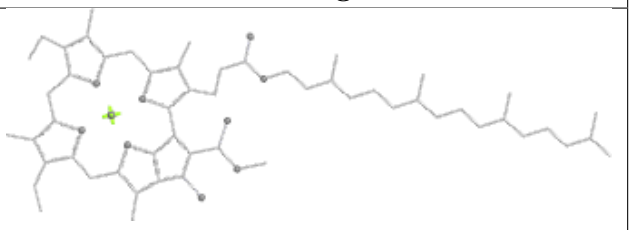
Bond angles

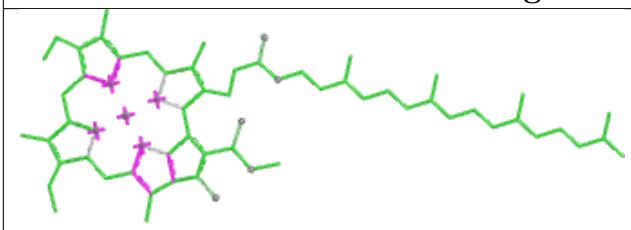
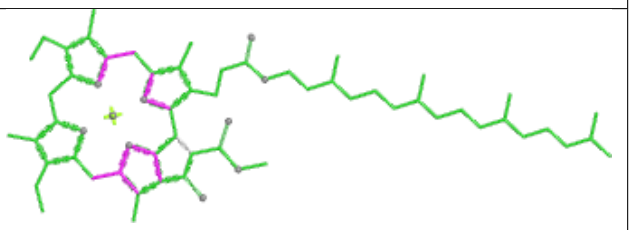
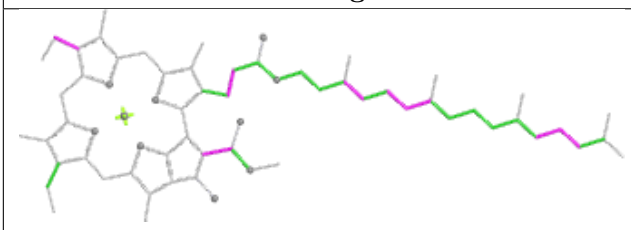
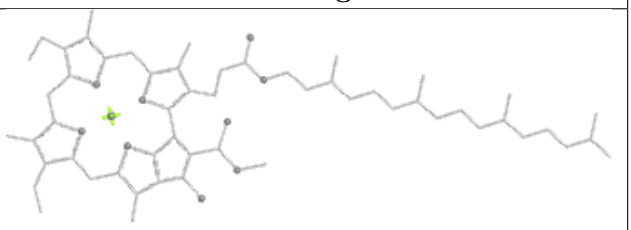


Torsions

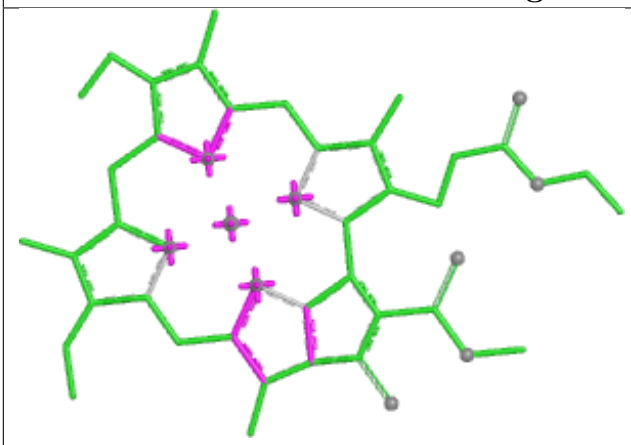


Rings

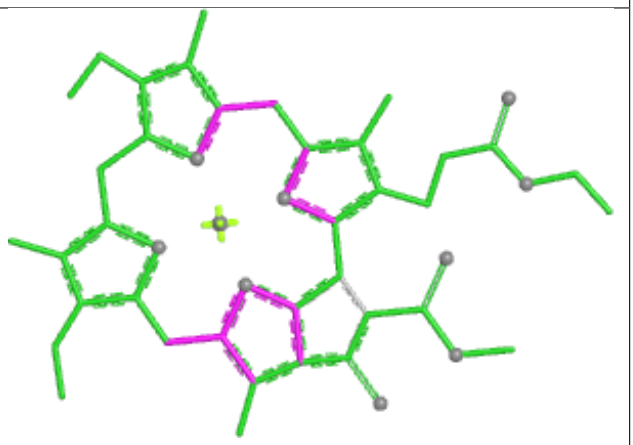
Ligand CLA b 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

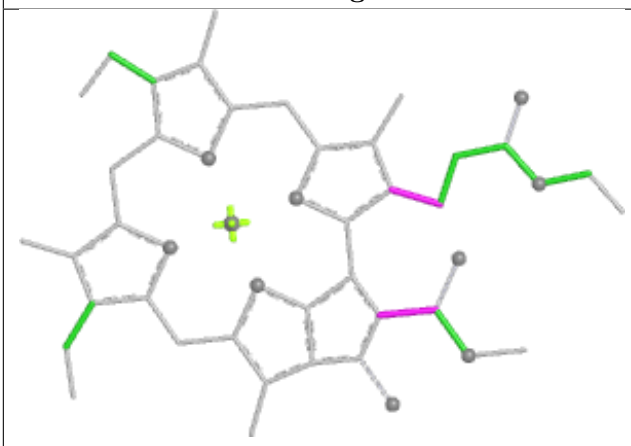
Ligand CLA F 311



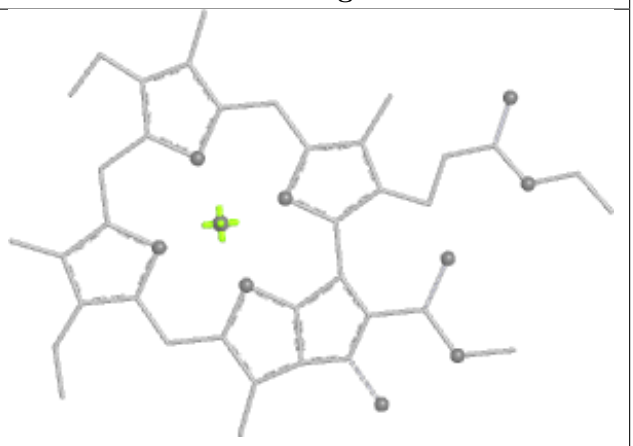
Bond lengths



Bond angles

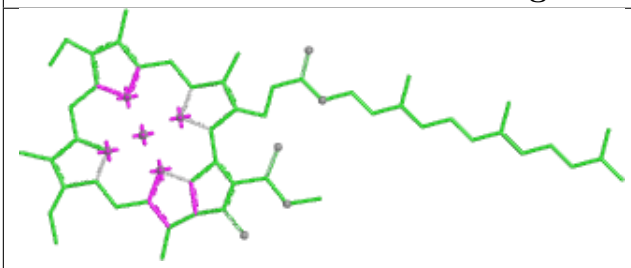


Torsions

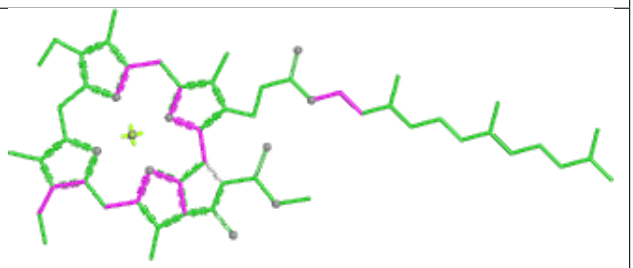


Rings

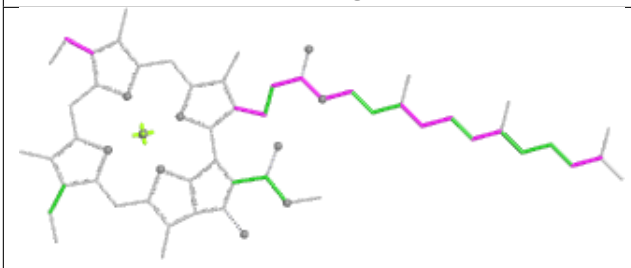
Ligand CLA z 305



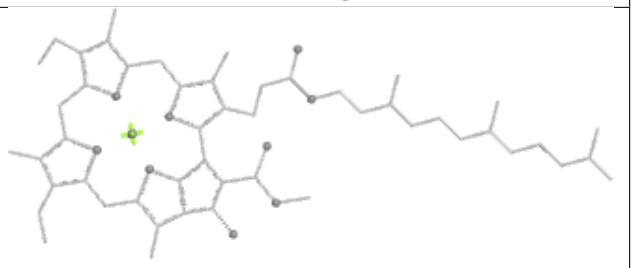
Bond lengths



Bond angles

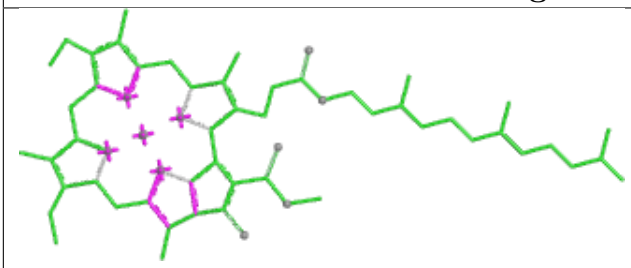


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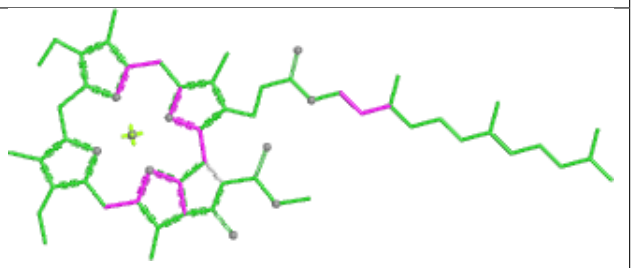


Rings

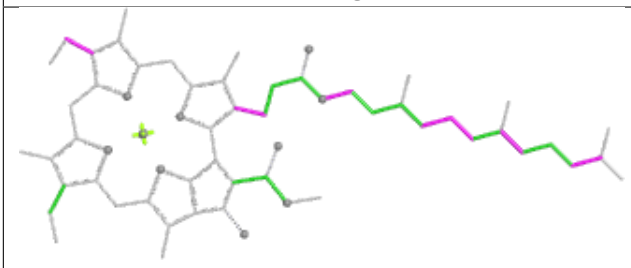
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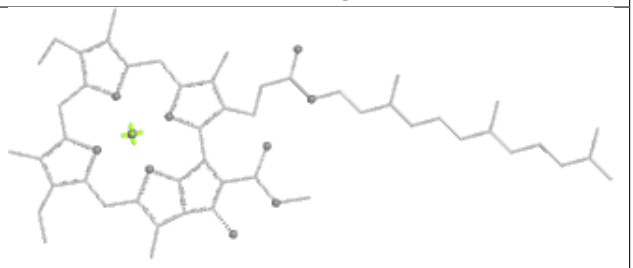
Bond lengths



Bond angles

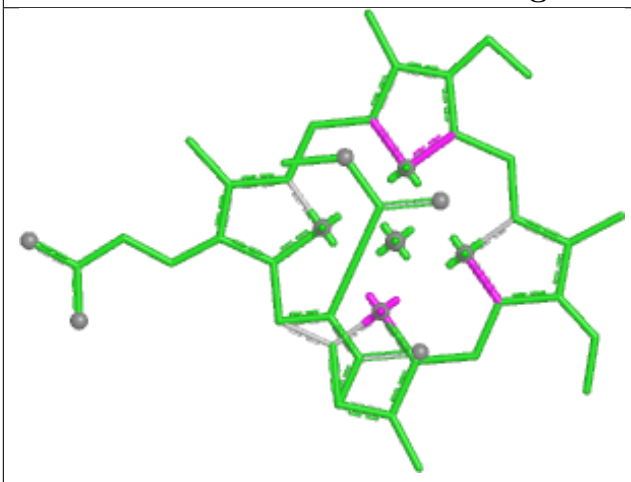


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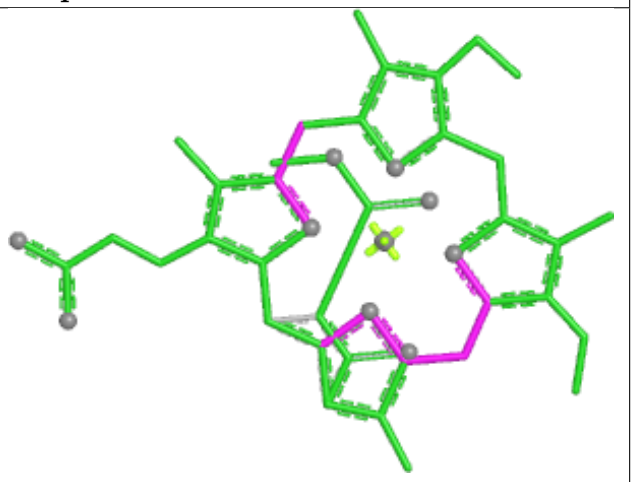


Rings

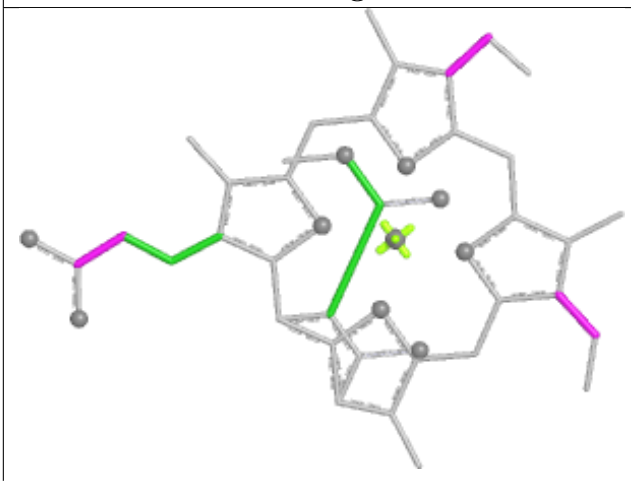
Ligand KC2 q 309



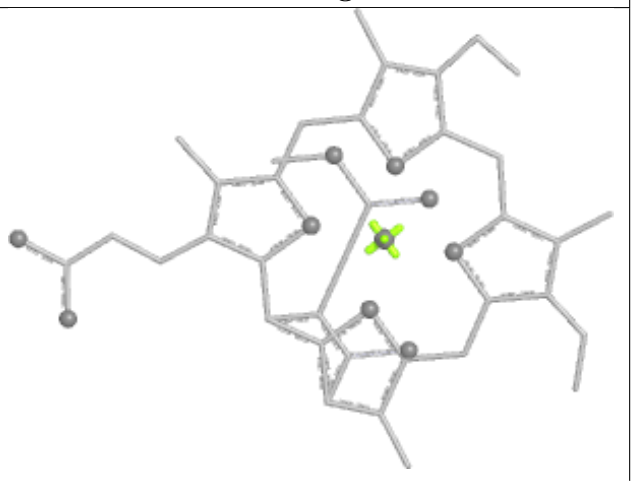
Bond lengths



Bond angles

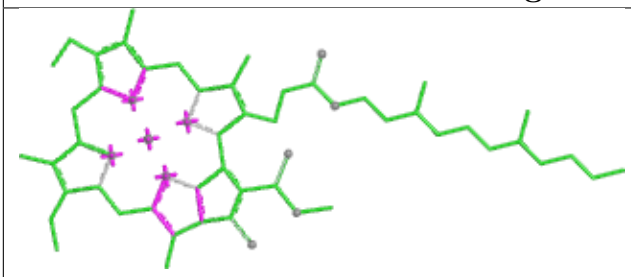


Torsions

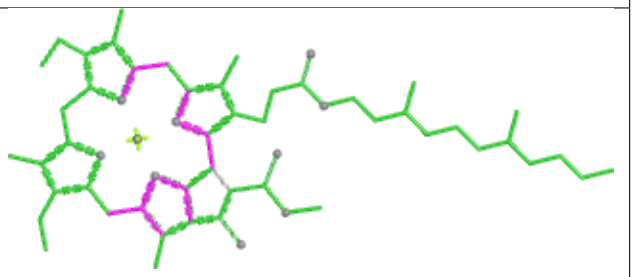


Rings

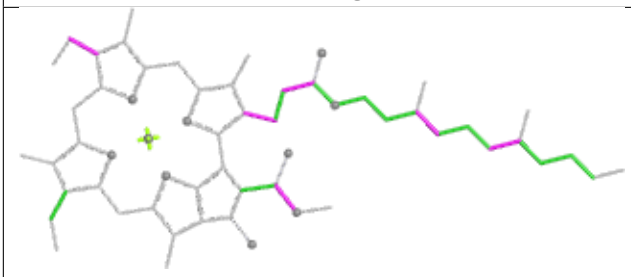
Ligand CLA T 310



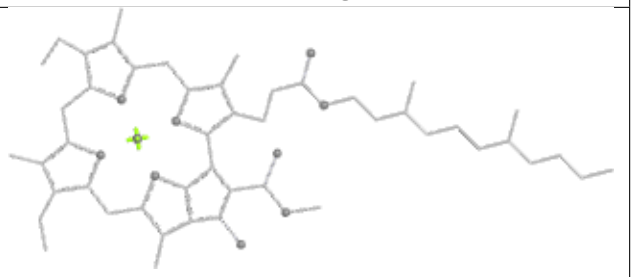
Bond lengths



Bond angles

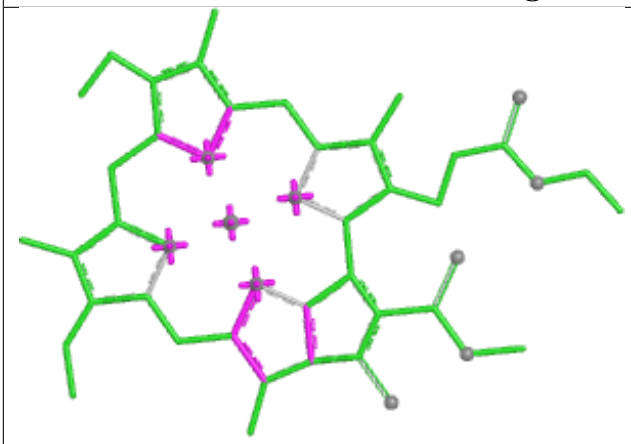


Torsions

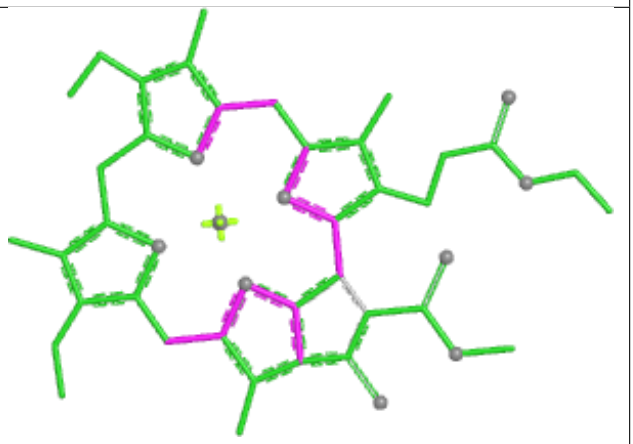


Rings

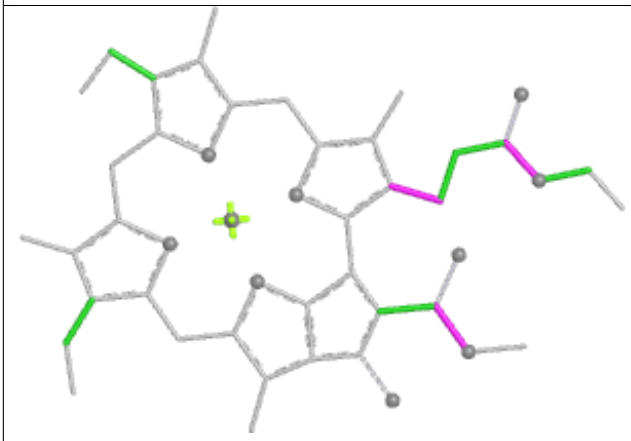
Ligand CLA A 311



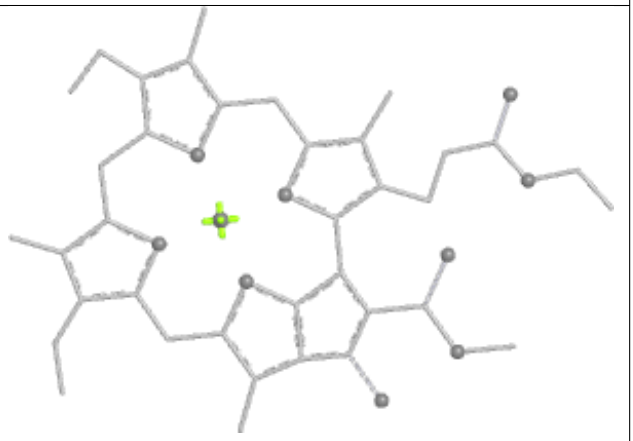
Bond lengths



Bond angles

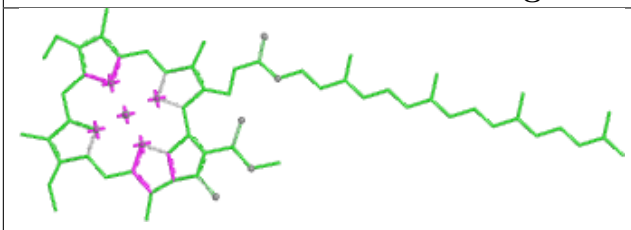


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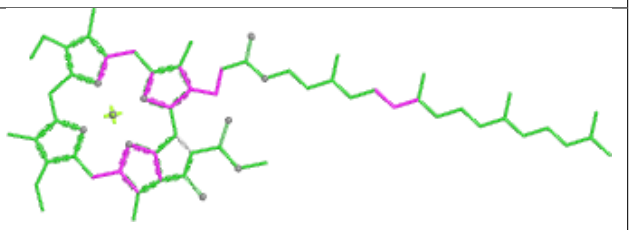


Rings

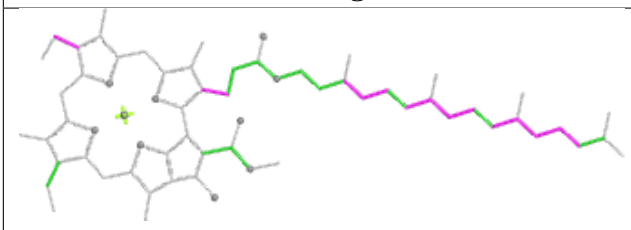
Ligand CLA A 304



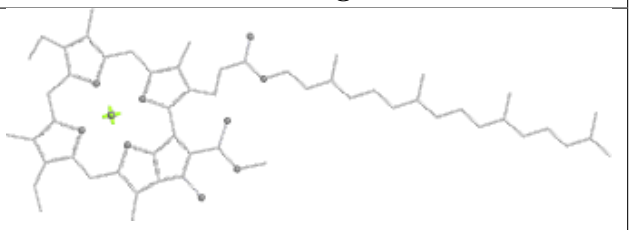
Bond lengths



Bond angles

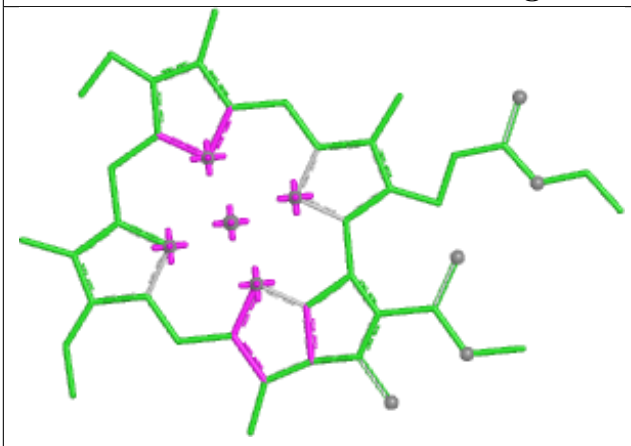


Torsions

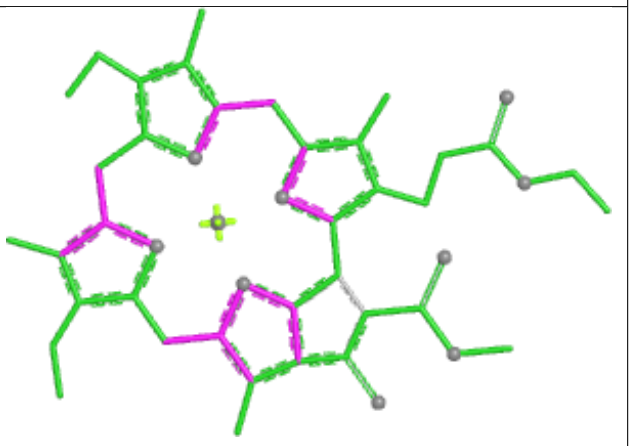


Rings

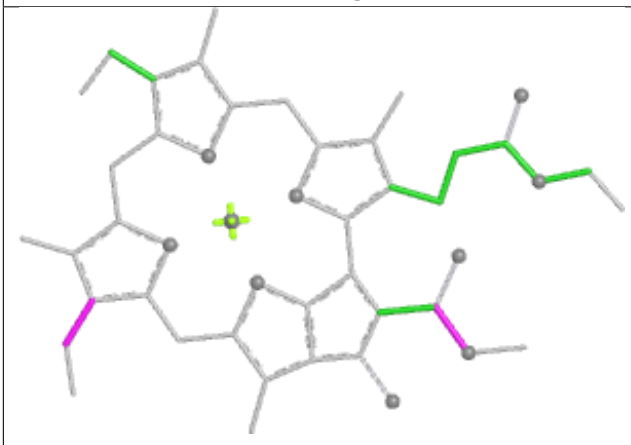
Ligand CLA H 301



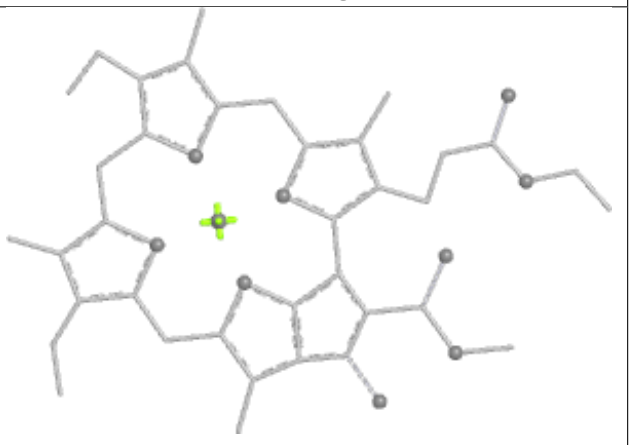
Bond lengths



Bond angles

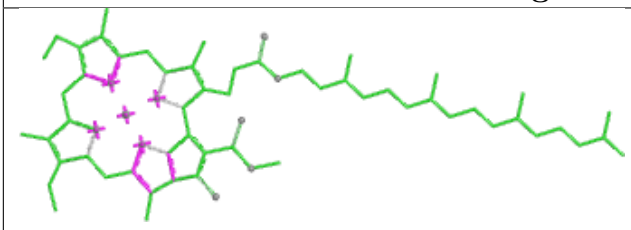


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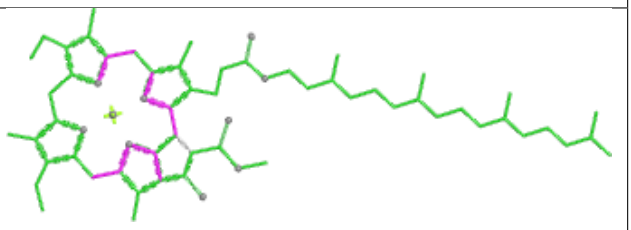


Rings

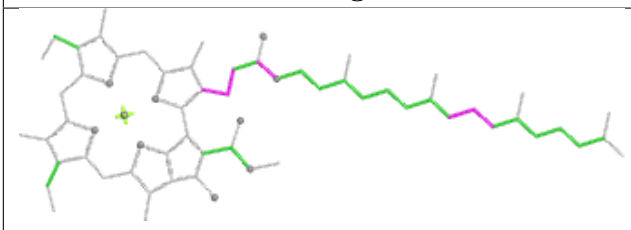
Ligand CLA f 202



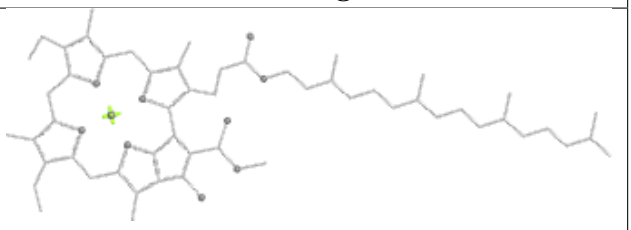
Bond lengths



Bond angles

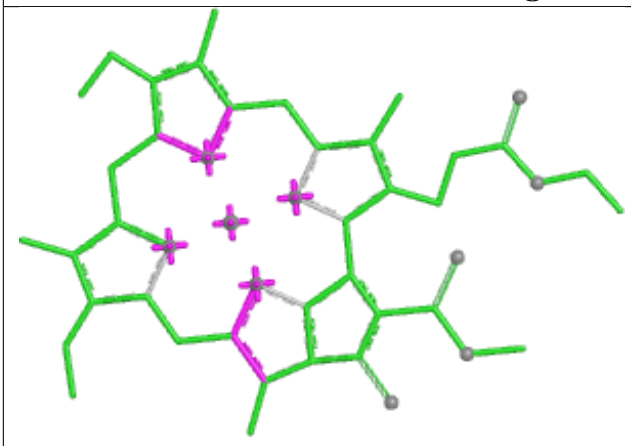


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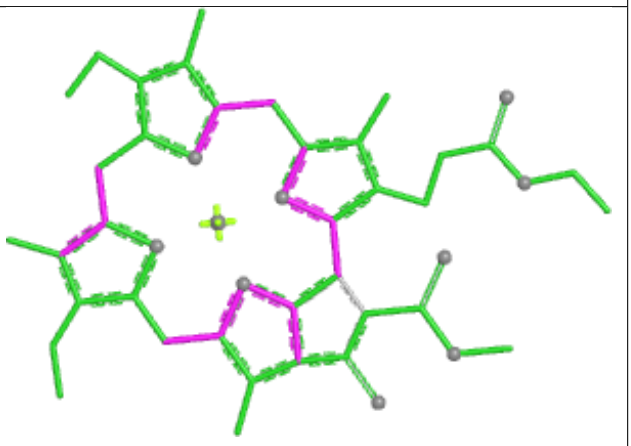


Rings

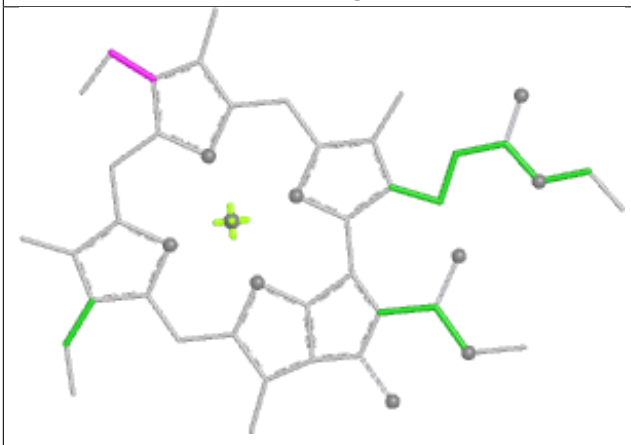
Ligand CLA R 316



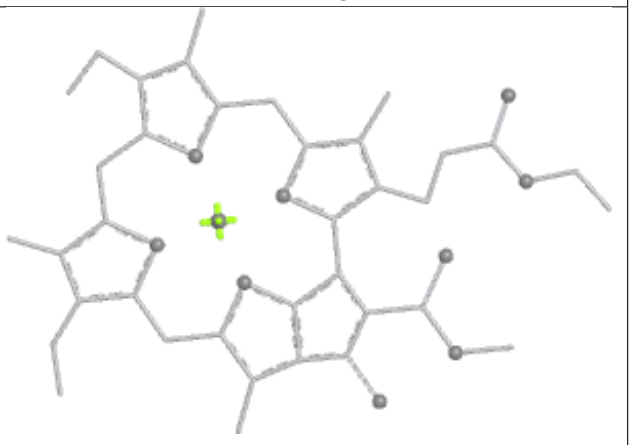
Bond lengths



Bond angles

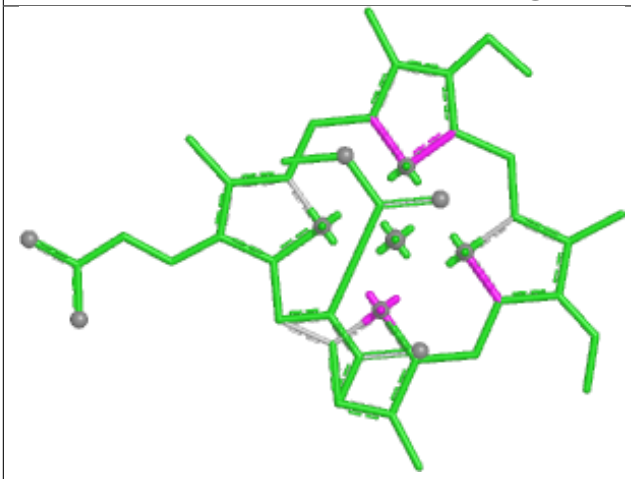


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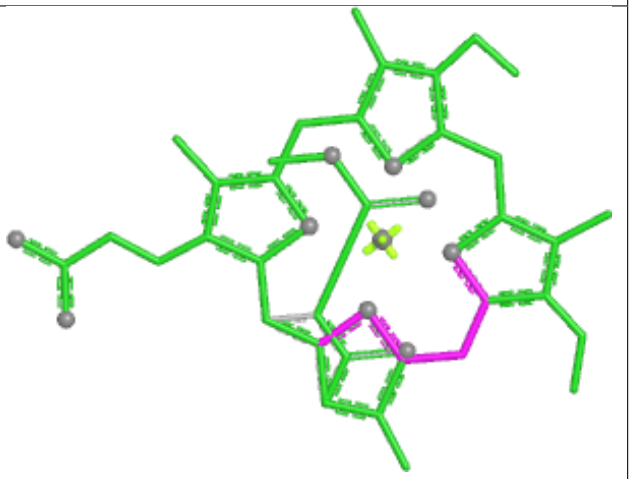


Rings

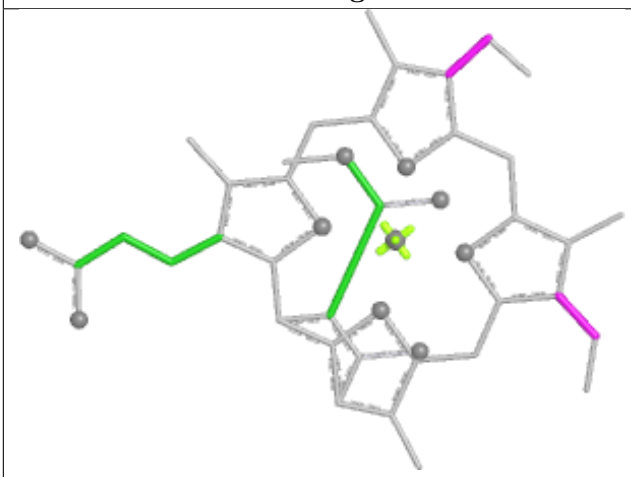
Ligand KC2 T 309



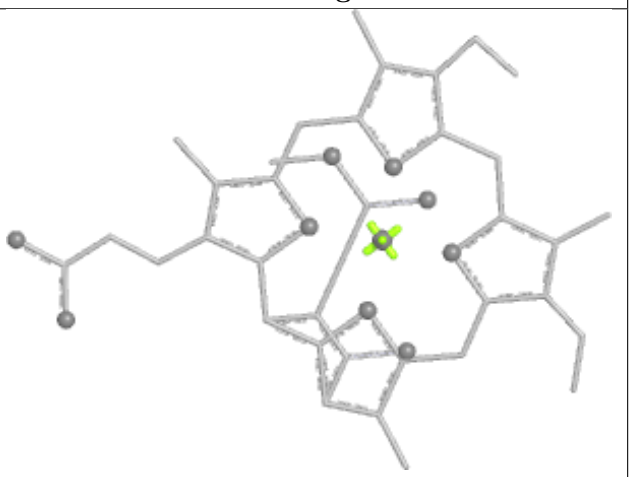
Bond lengths



Bond angles

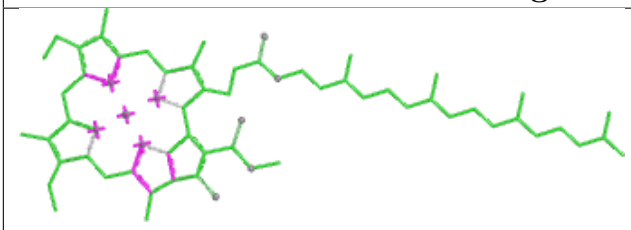


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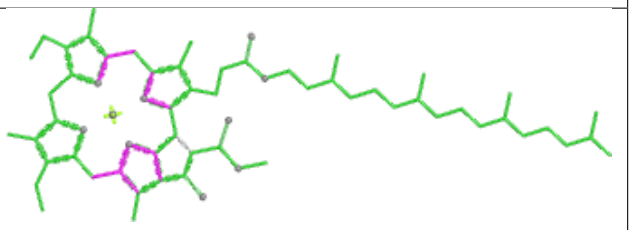


Rings

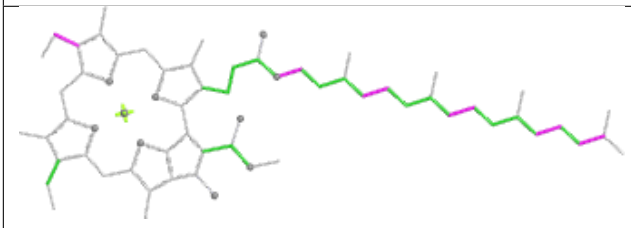
Ligand CLA I 201



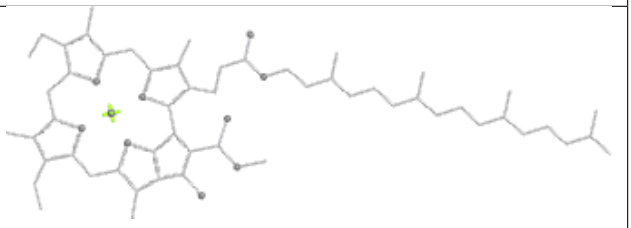
Bond lengths



Bond angles

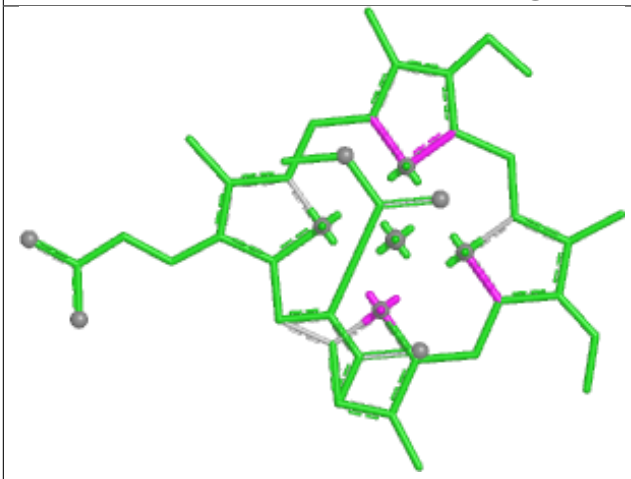


Torsions

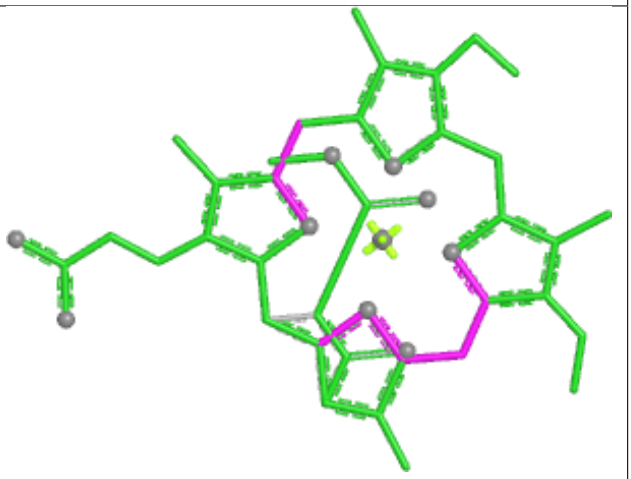


Rings

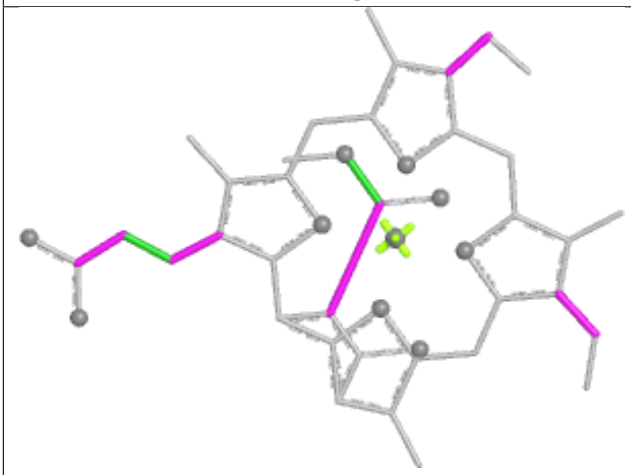
Ligand KC2 T 311



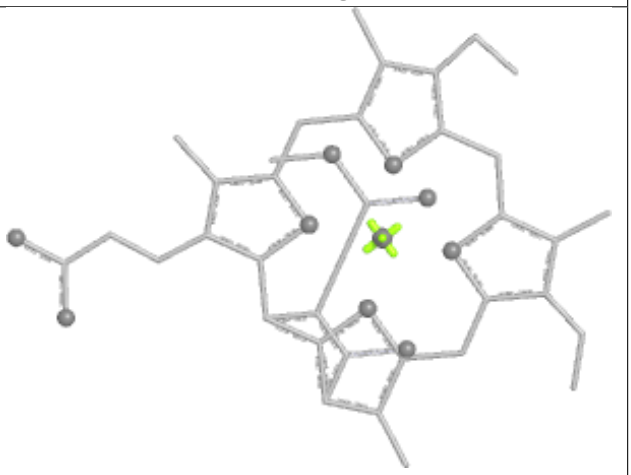
Bond lengths



Bond angles

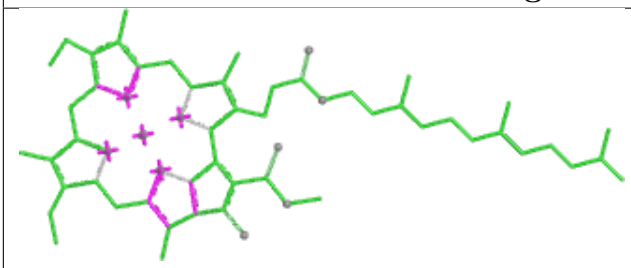


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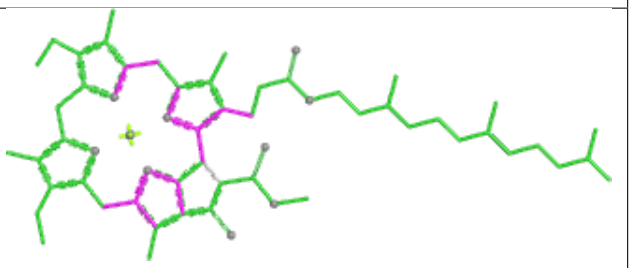


Rings

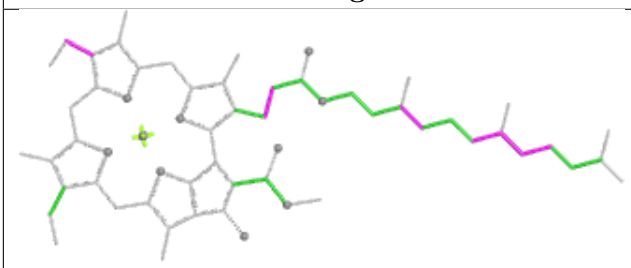
Ligand CLA C 307



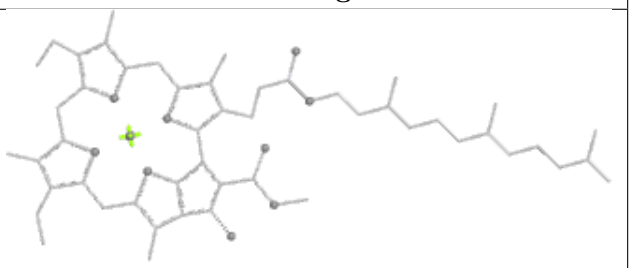
Bond lengths



Bond angles

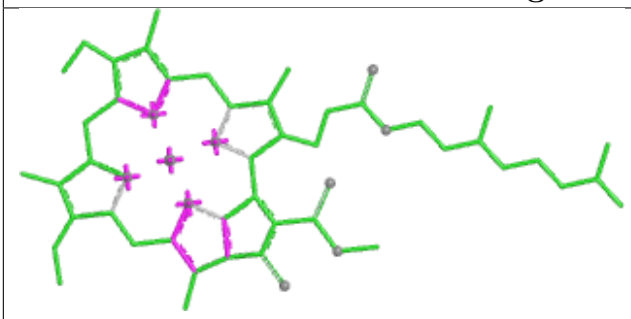


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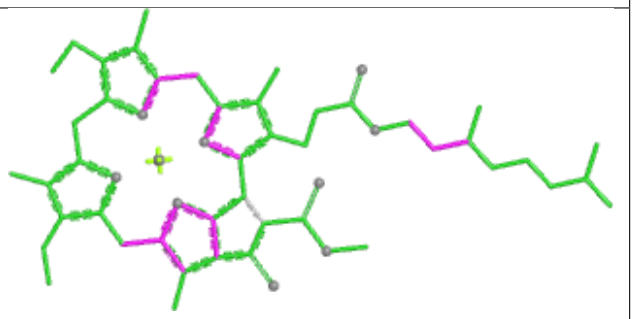


Rings

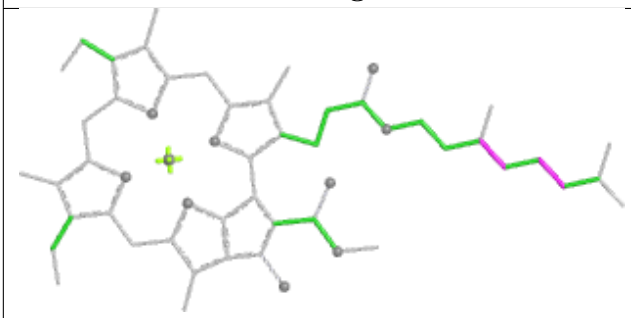
Ligand CLA b 823



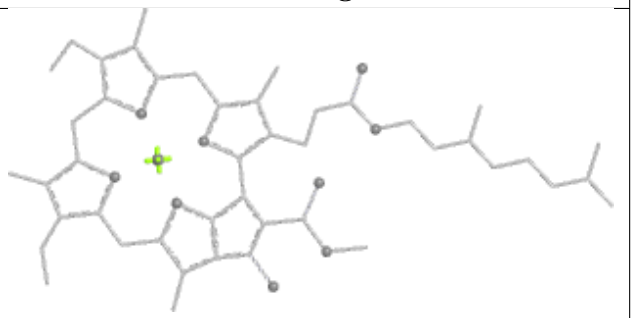
Bond lengths



Bond angles

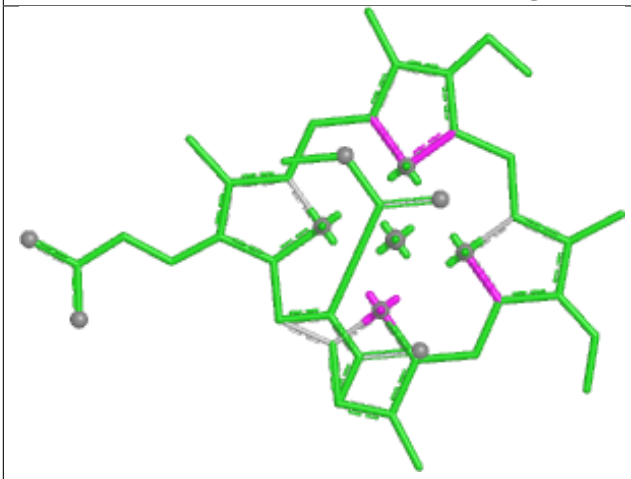


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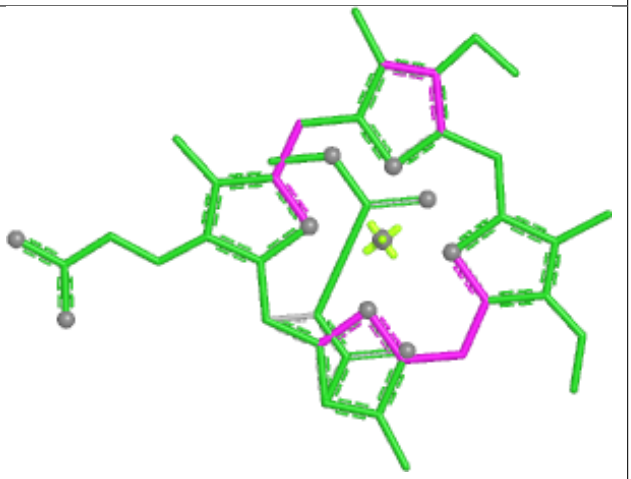


Rings

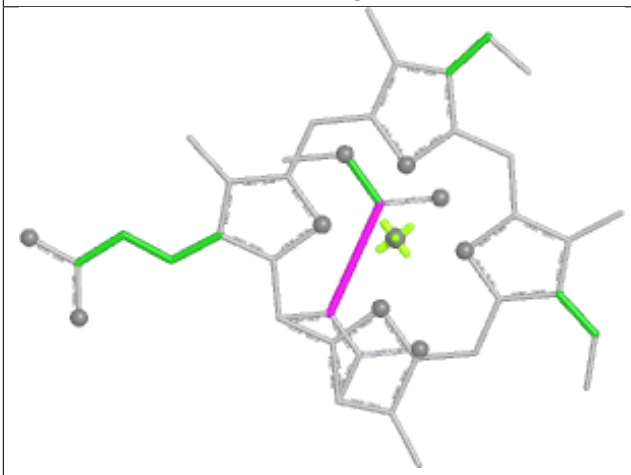
Ligand KC2 X 303



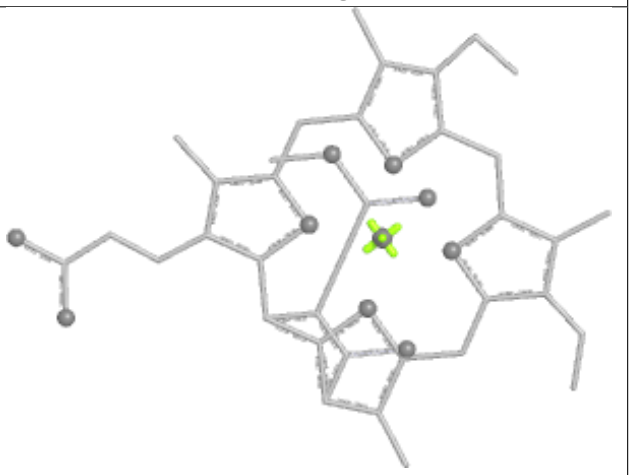
Bond lengths



Bond angles

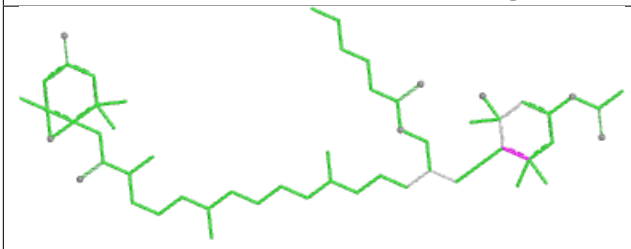


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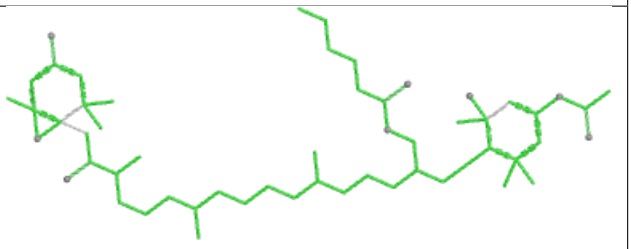


Rings

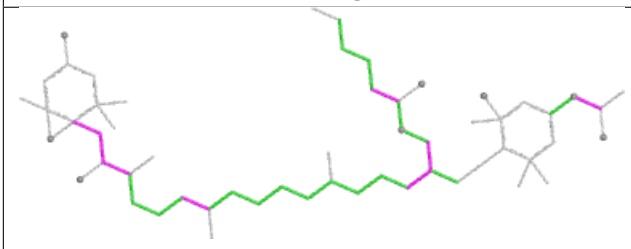
Ligand A1EB1 K 315



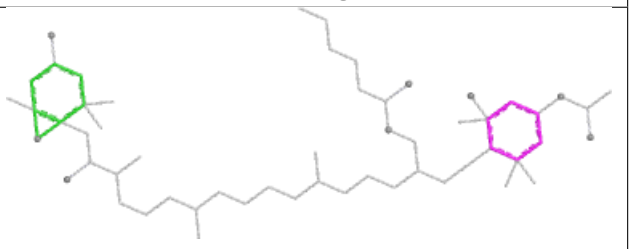
Bond lengths



Bond angles

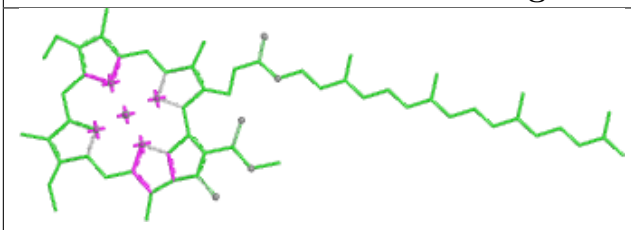


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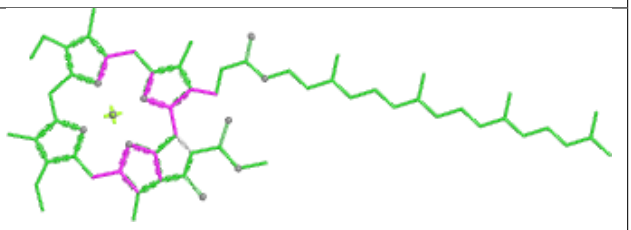


Rings

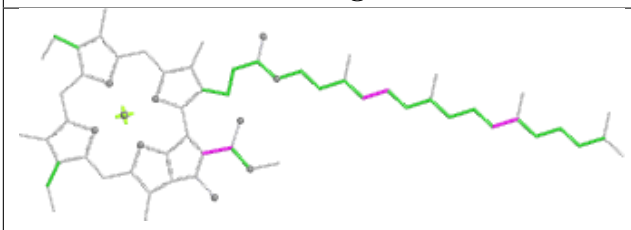
Ligand CLA a 815



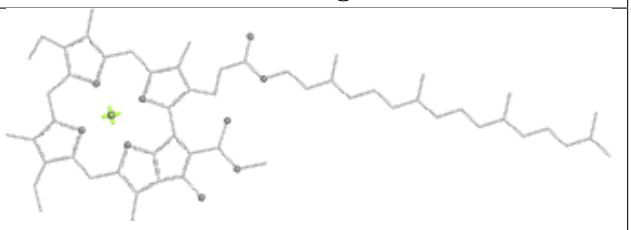
Bond lengths



Bond angles

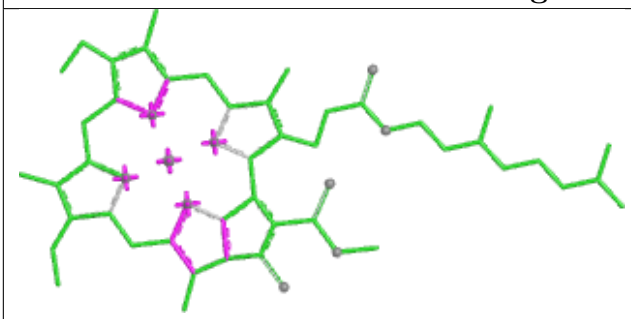


Torsions

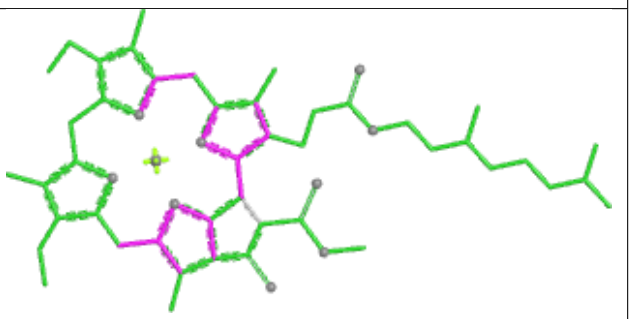


Rings

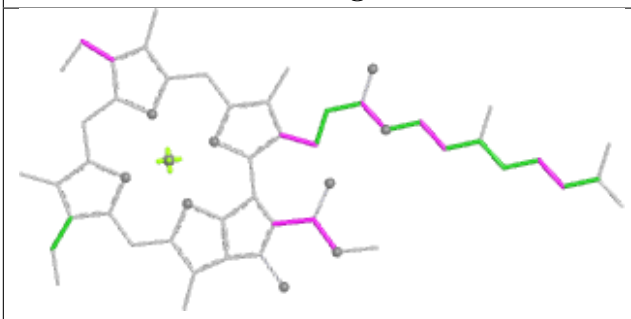
Ligand CLA t 307



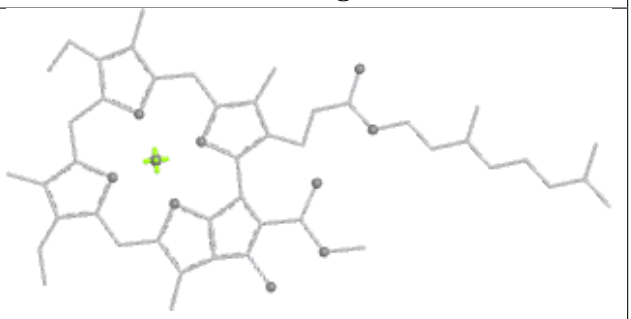
Bond lengths



Bond angles

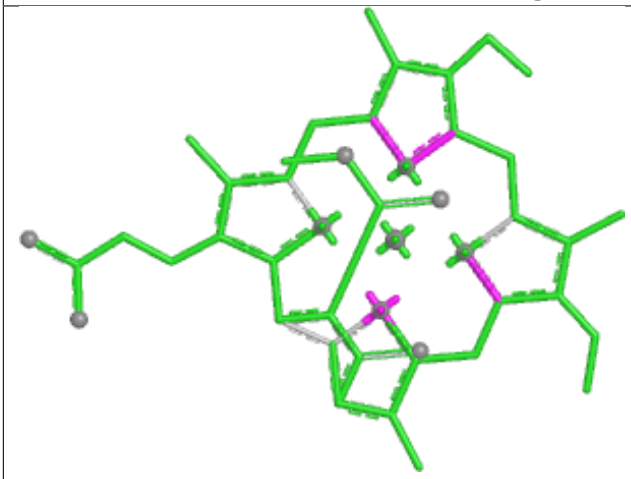


Torsions

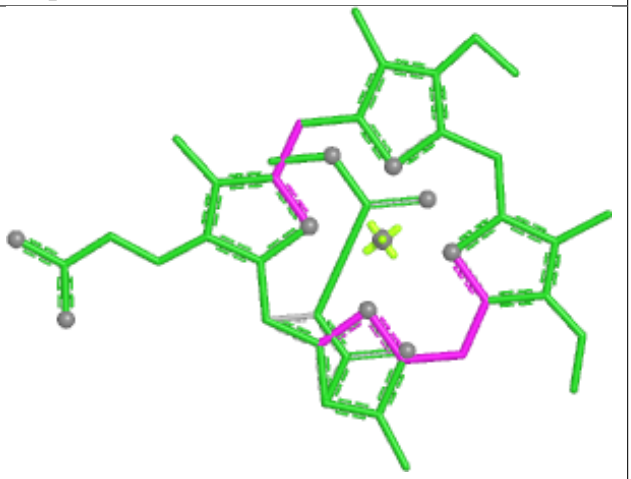


Rings

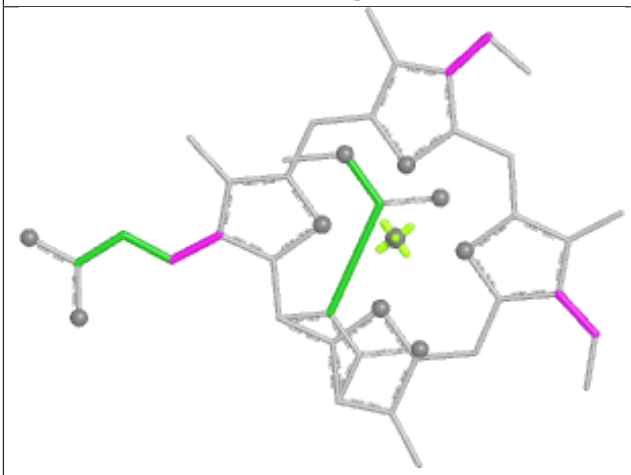
Ligand KC2 p 309



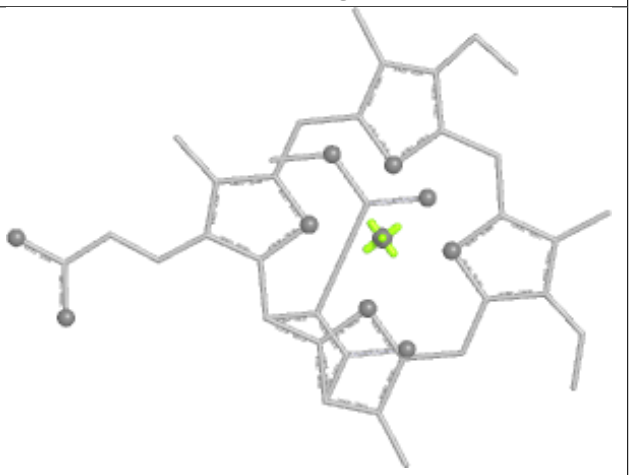
Bond lengths



Bond angles

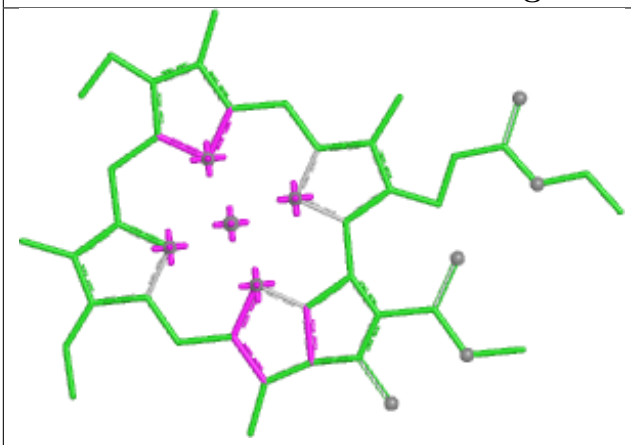


Torsions

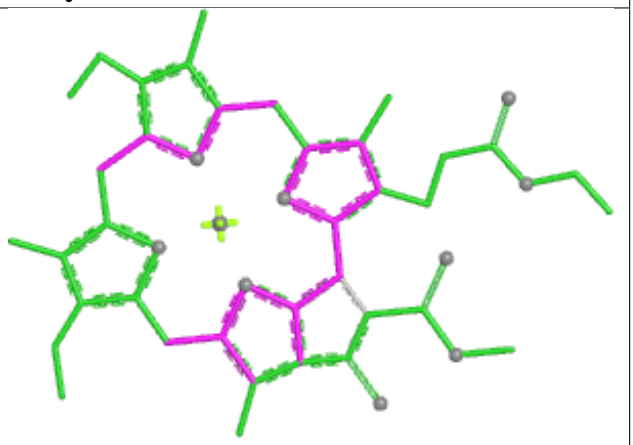


Rings

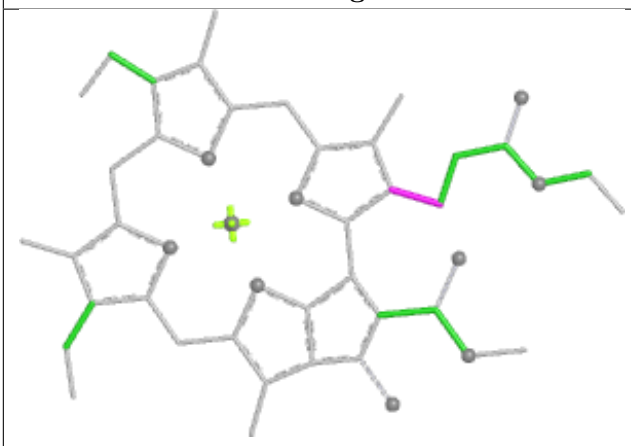
Ligand CLA Q 207



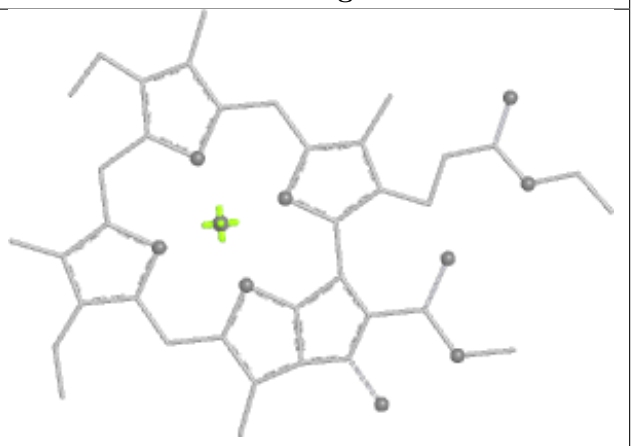
Bond lengths



Bond angles

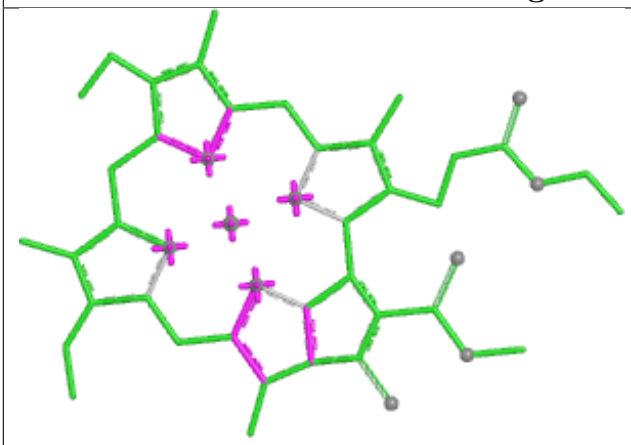


Torsions

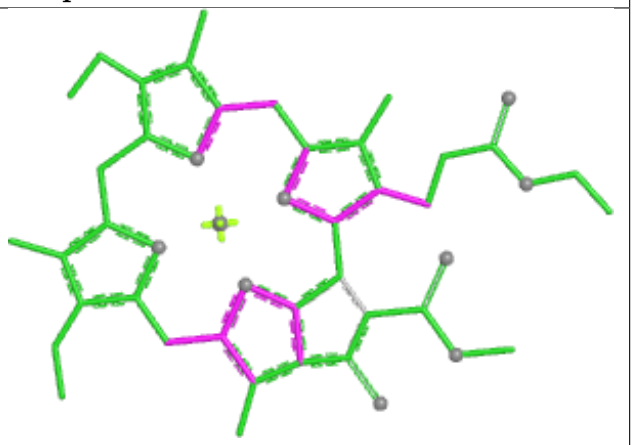


Rings

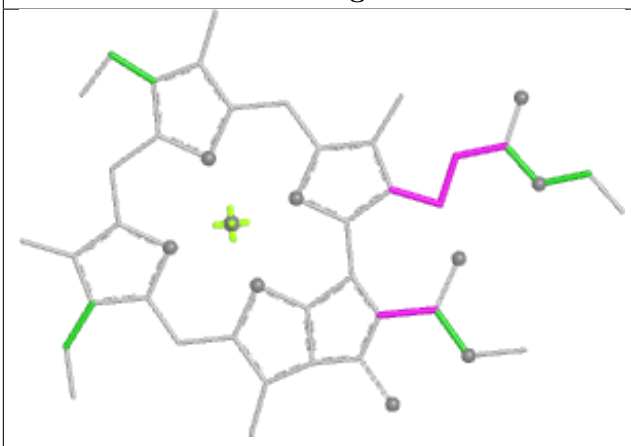
Ligand CLA q 313



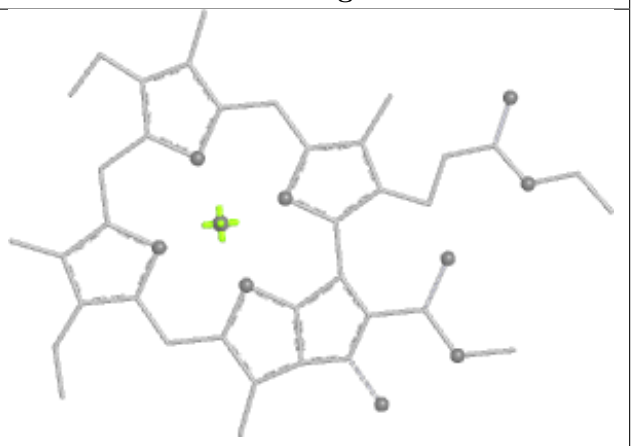
Bond lengths



Bond angles

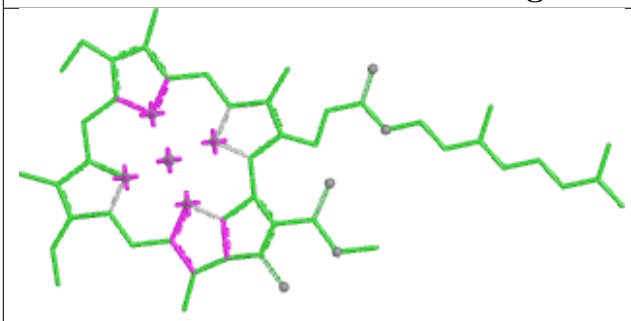


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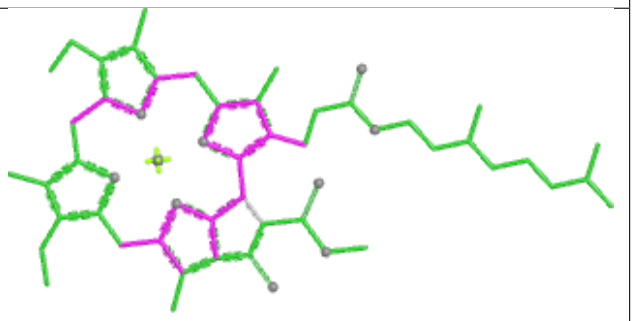


Rings

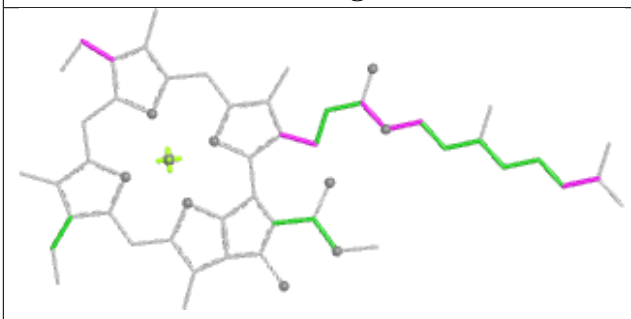
Ligand CLA Z 310



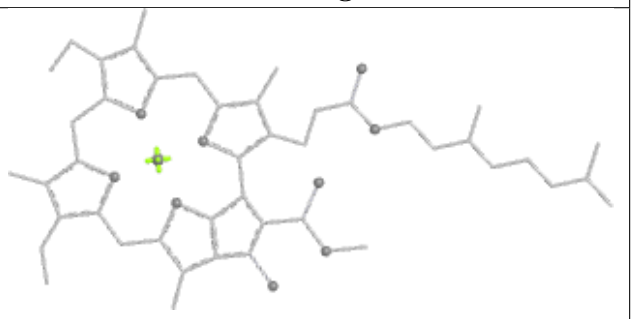
Bond lengths



Bond angles

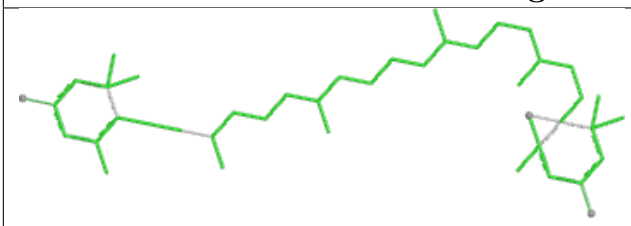


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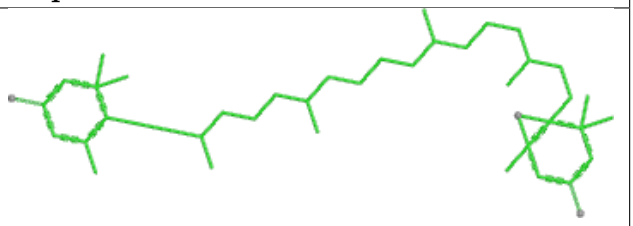


Rings

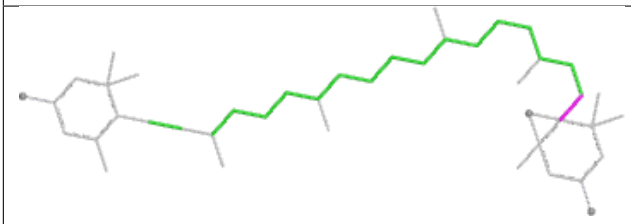
Ligand DD6 p 322



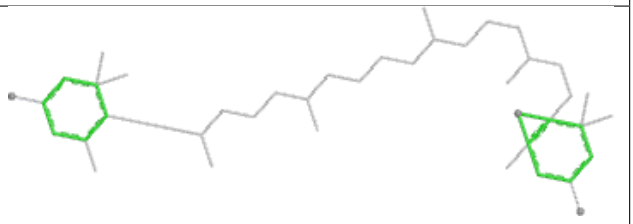
Bond lengths



Bond angles

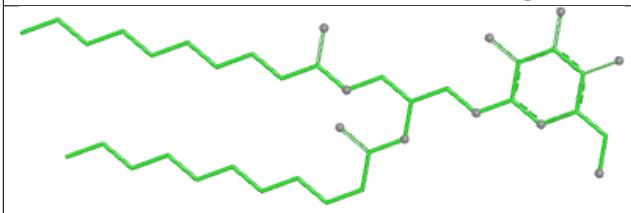


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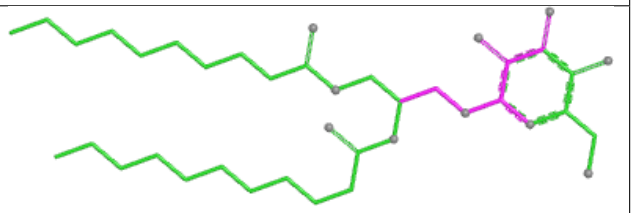


Rings

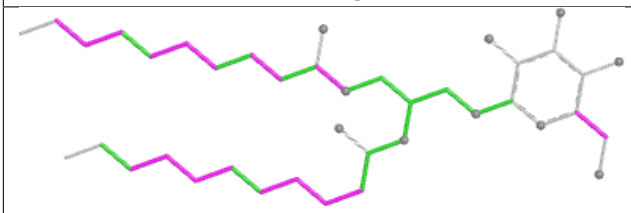
Ligand LMG D 318



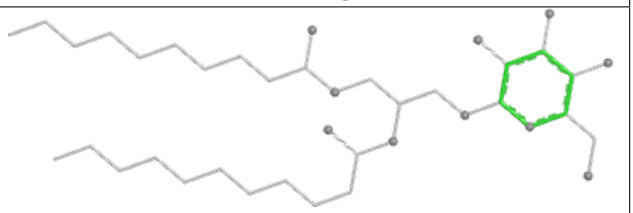
Bond lengths



Bond angles

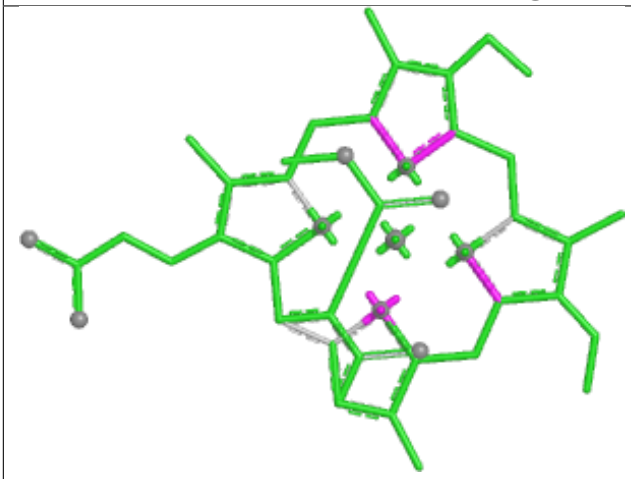


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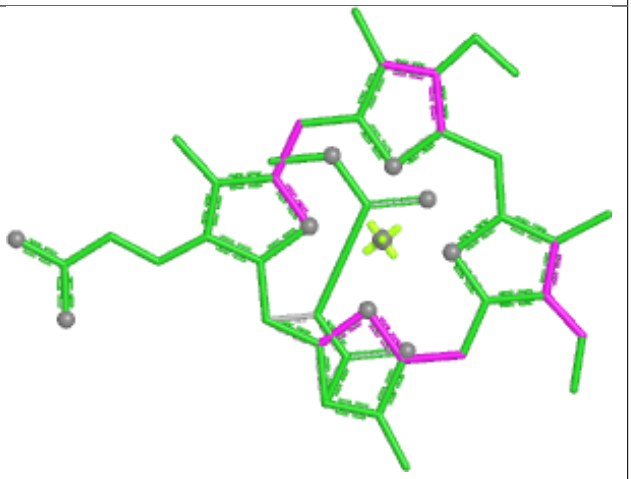


Rings

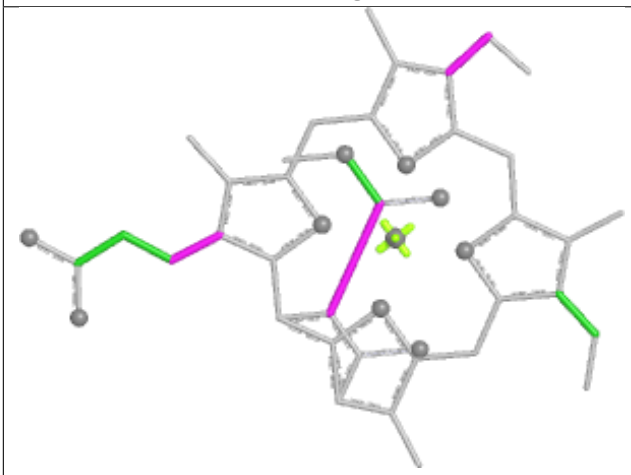
Ligand KC2 P 304



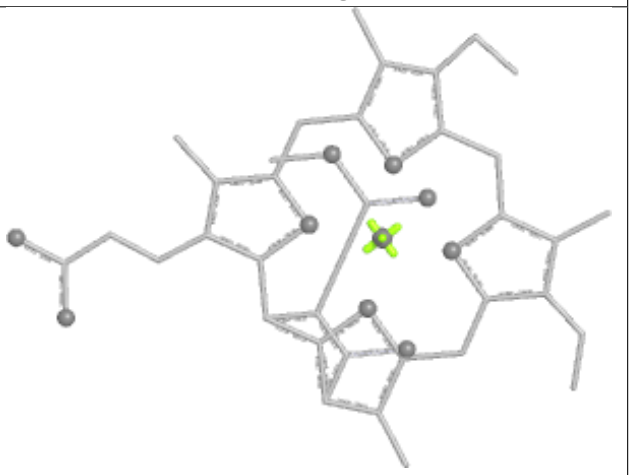
Bond lengths



Bond angles

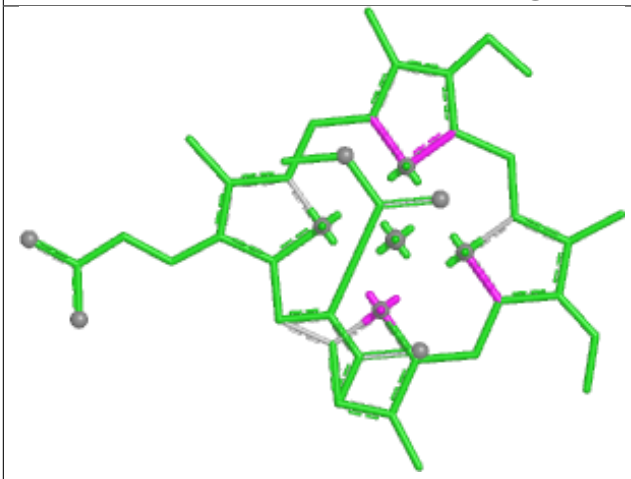


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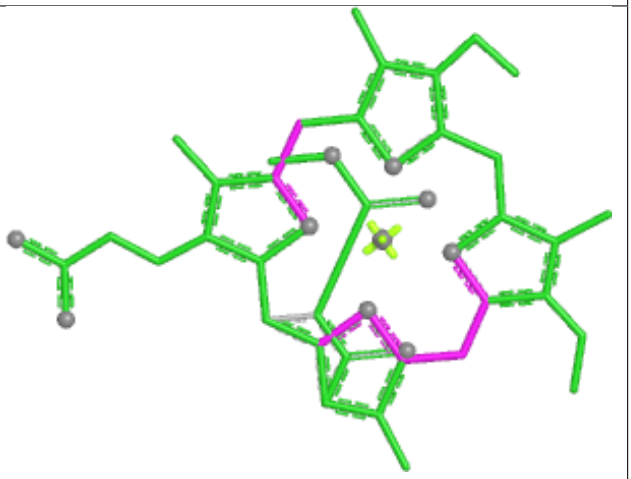


Rings

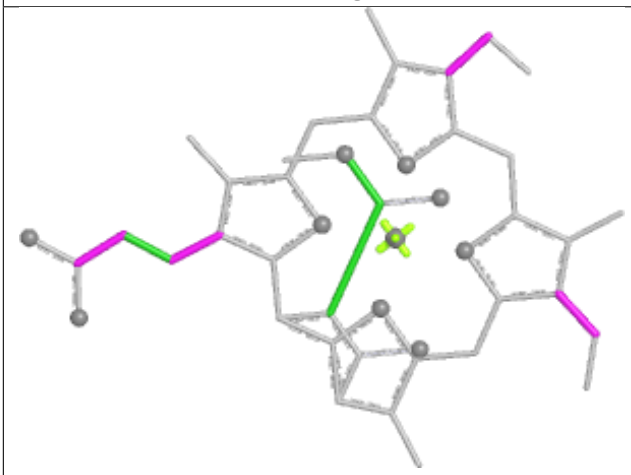
Ligand KC2 T 308



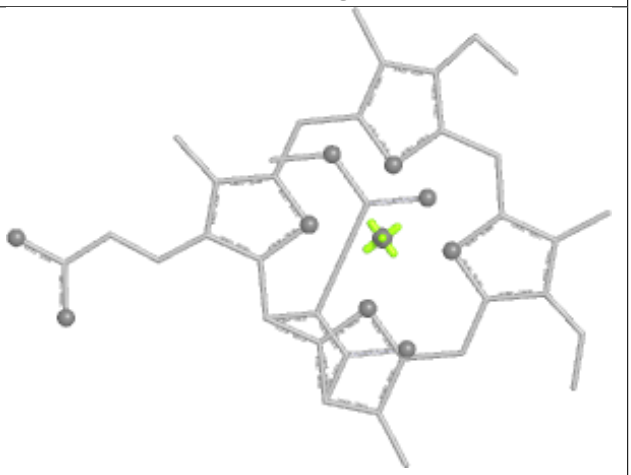
Bond lengths



Bond angles

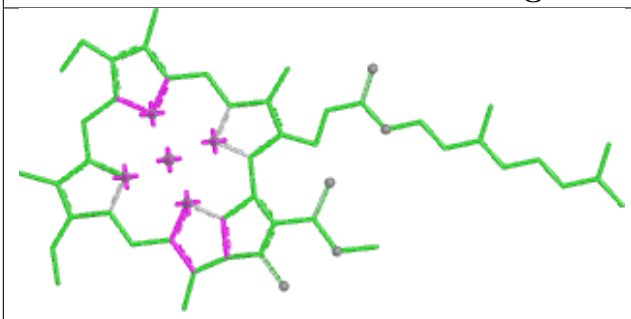


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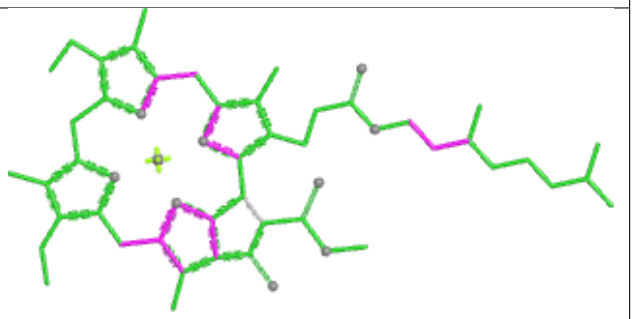


Rings

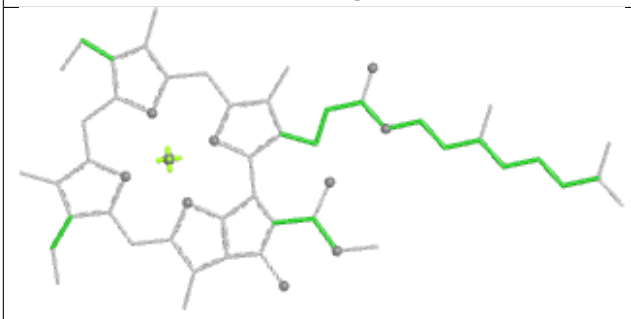
Ligand CLA T 307



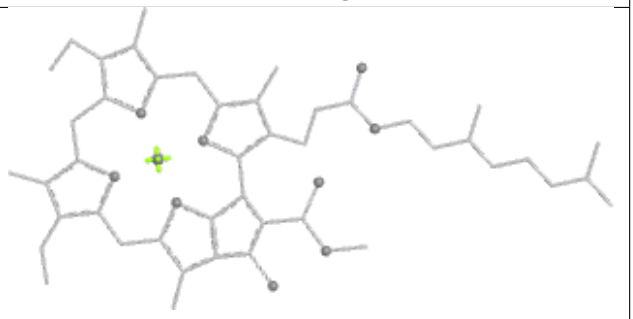
Bond lengths



Bond angles

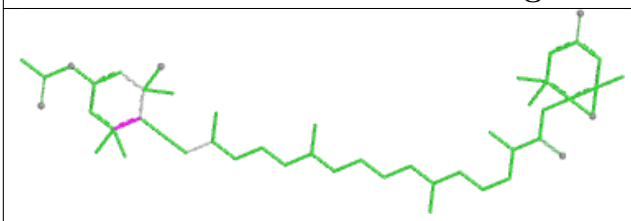


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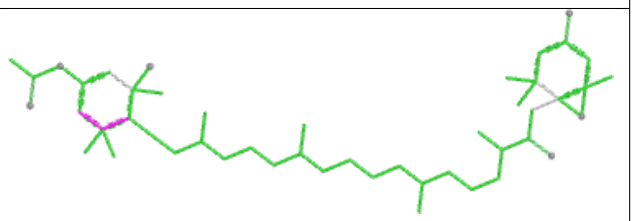


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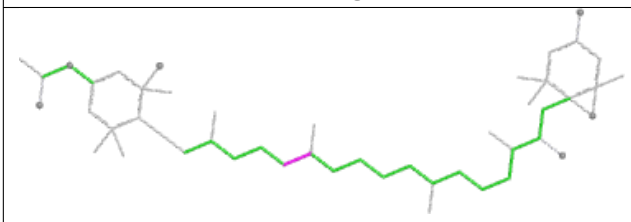
Ligand A86 W 301



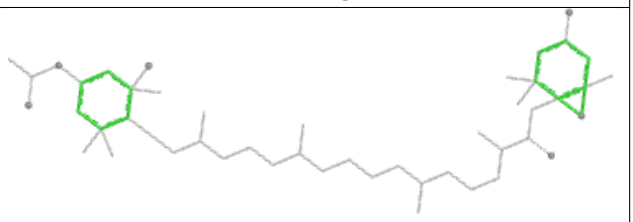
Bond lengths



Bond angles

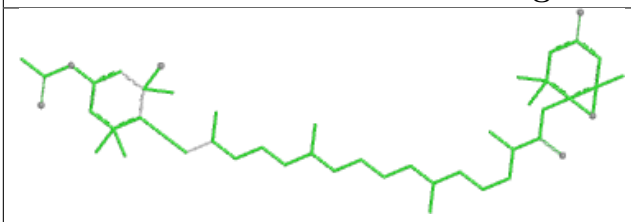


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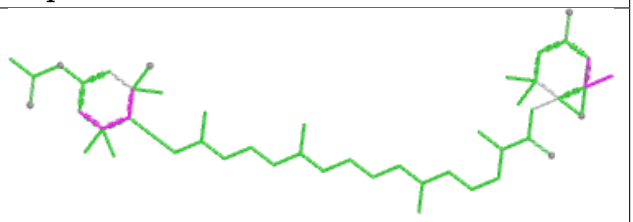


Rings

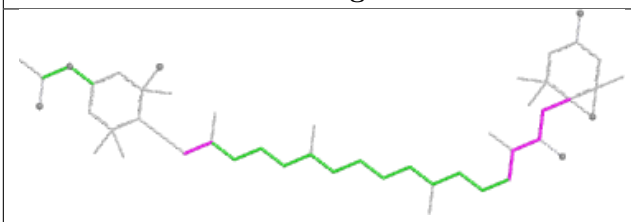
Ligand A86 p 320



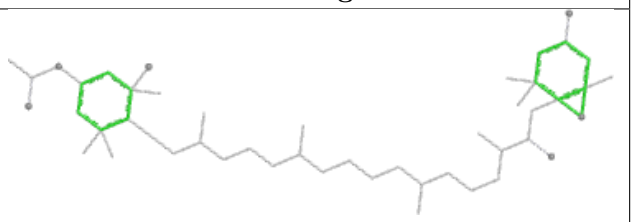
Bond lengths



Bond angles

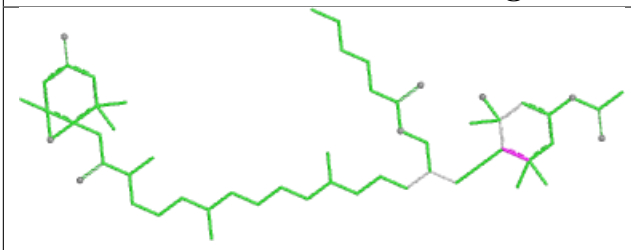


Torsions



Rings

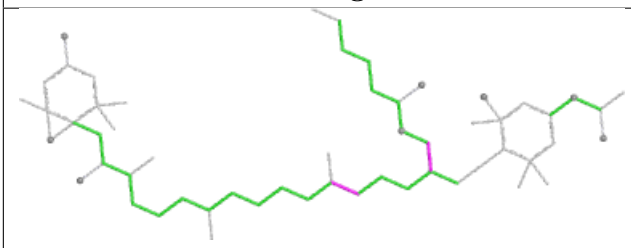
Ligand A1EB1 Y 323



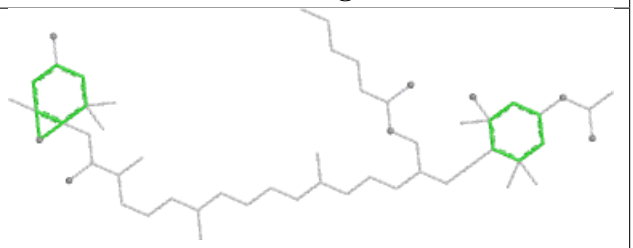
Bond lengths



Bond angles

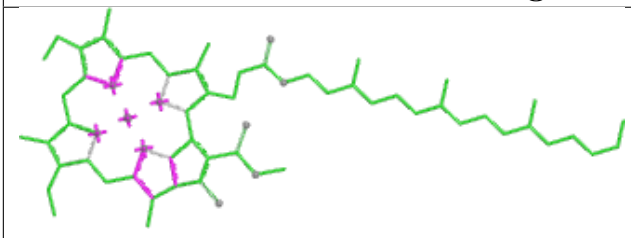


Torsions

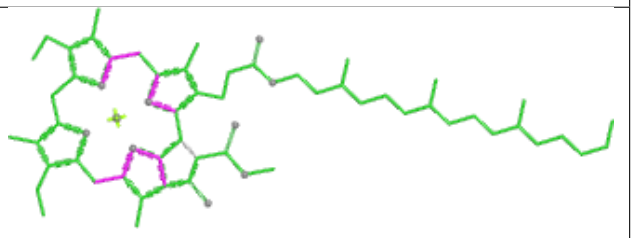


Rings

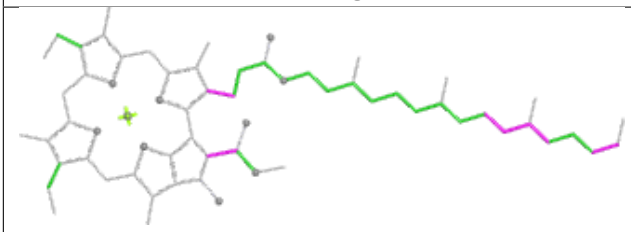
Ligand CLA b 826



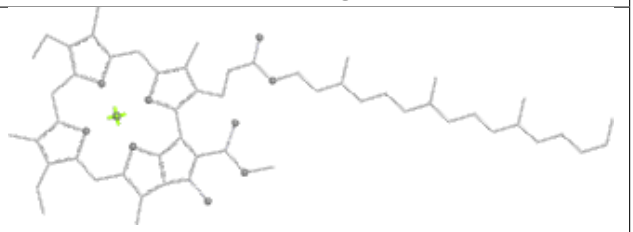
Bond lengths



Bond angles

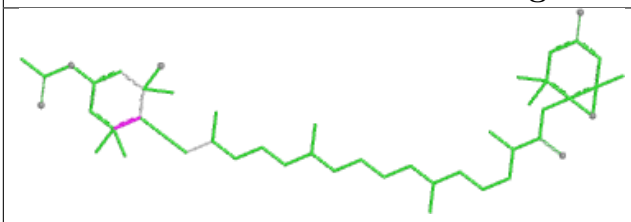


Torsions

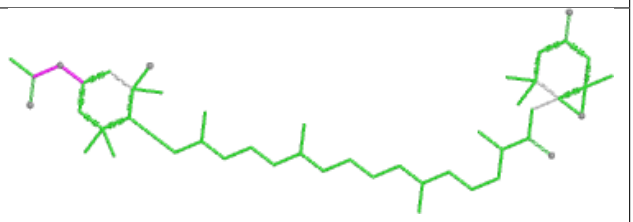


Rings

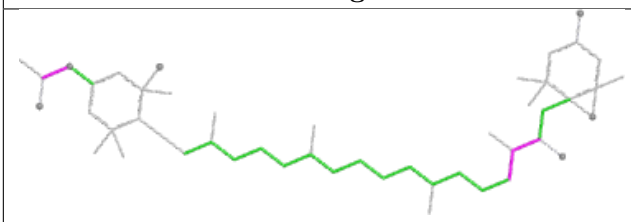
Ligand A86 G 211



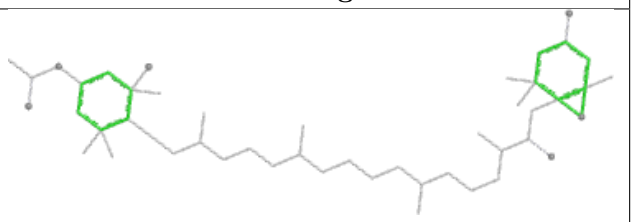
Bond lengths



Bond angles

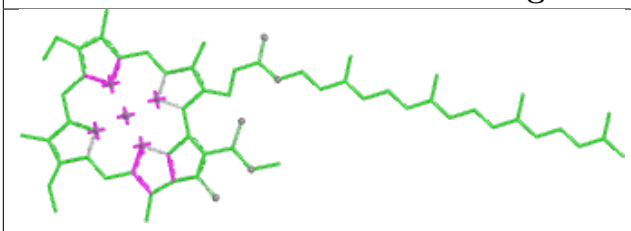


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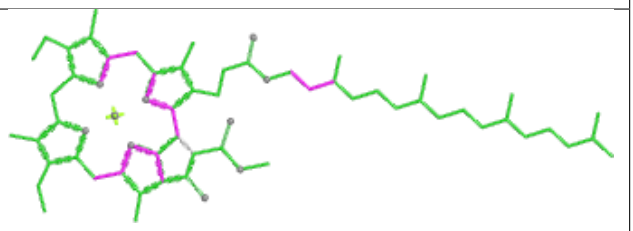


Rings

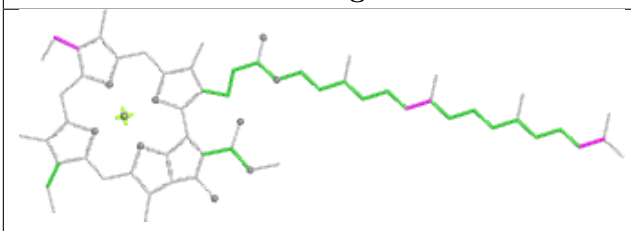
Ligand CLA b 841



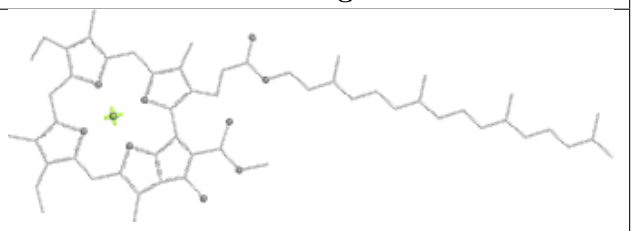
Bond lengths



Bond angles

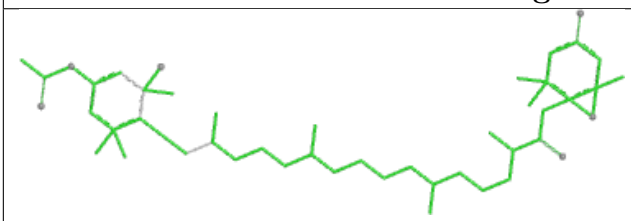


Torsions

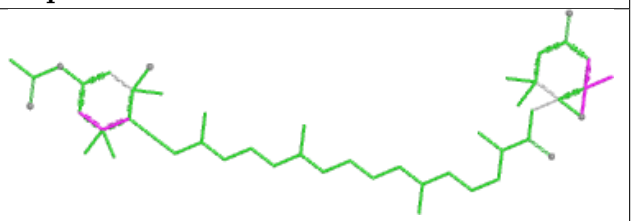


Rings

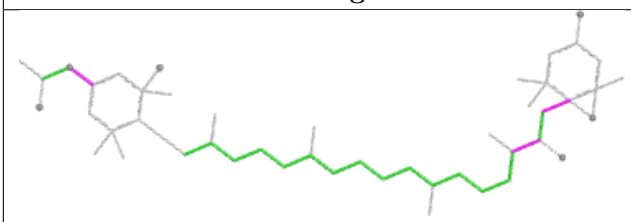
Ligand A86 p 321



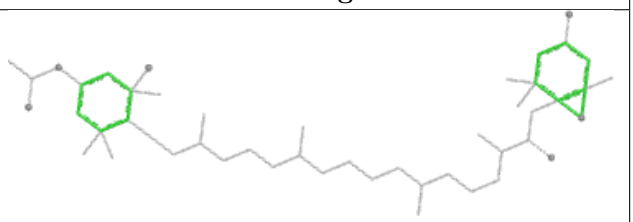
Bond lengths



Bond angles

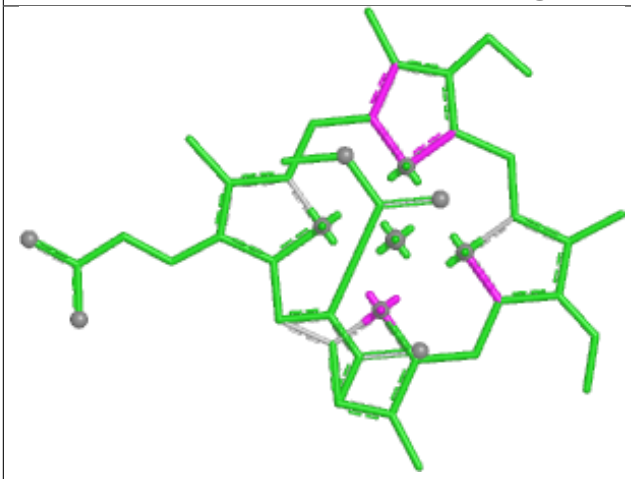


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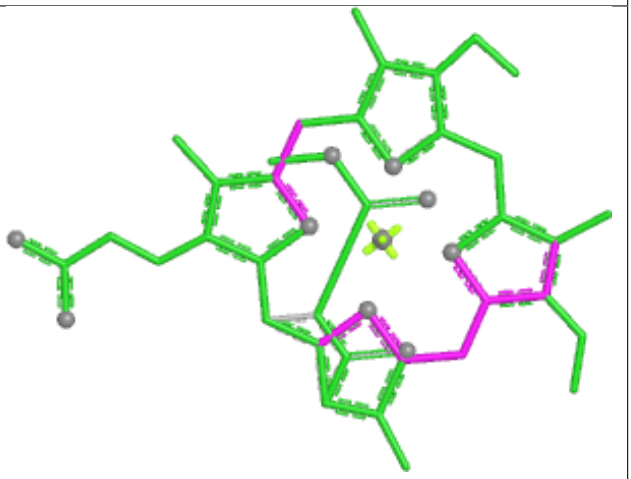


Rings

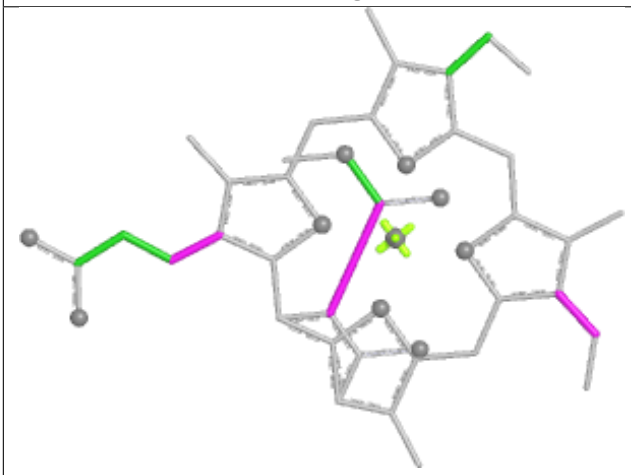
Ligand KC2 z 304



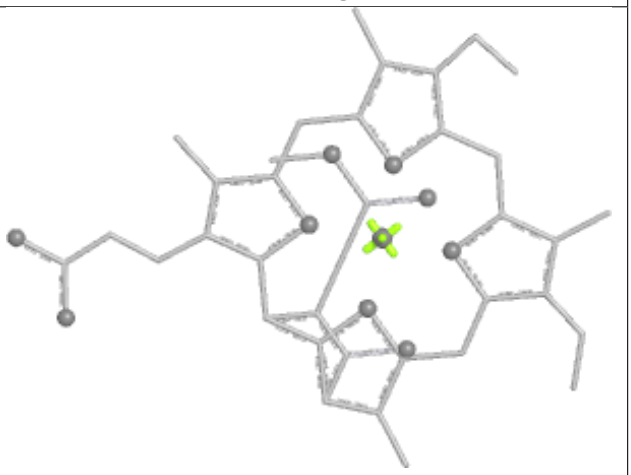
Bond lengths



Bond angles

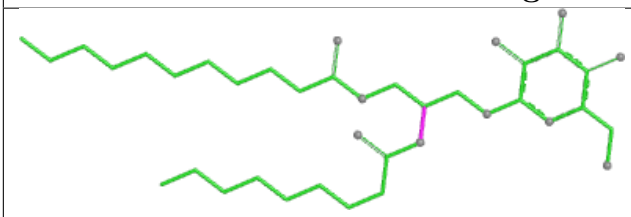


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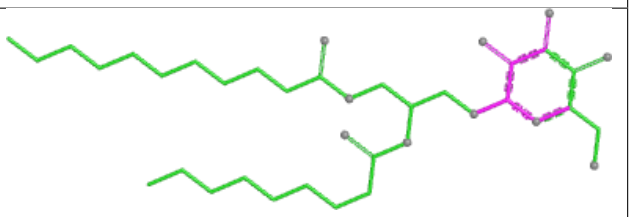


Rings

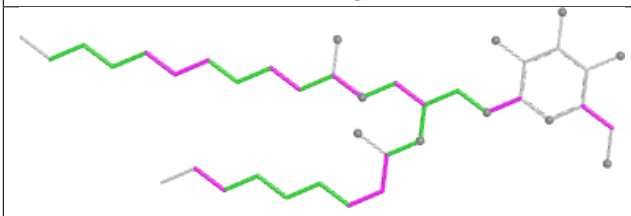
Ligand LMG u 301



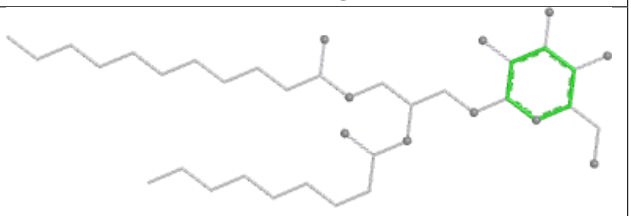
Bond lengths



Bond angles

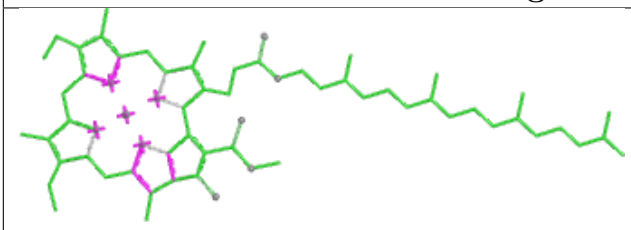


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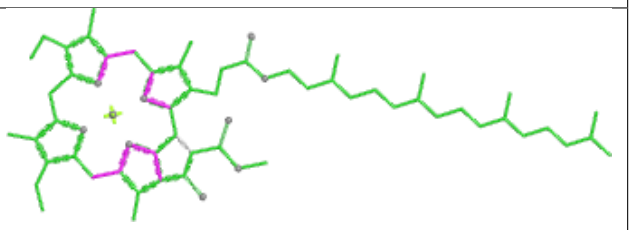


Rings

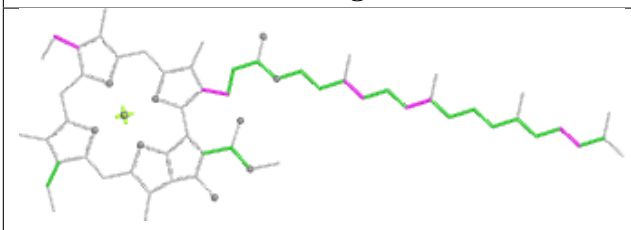
Ligand CLA b 834



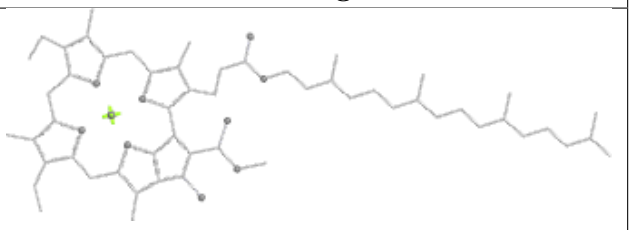
Bond lengths



Bond angles

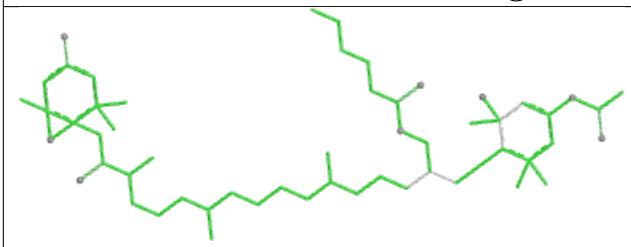


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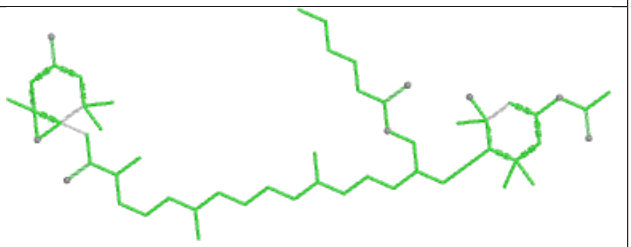


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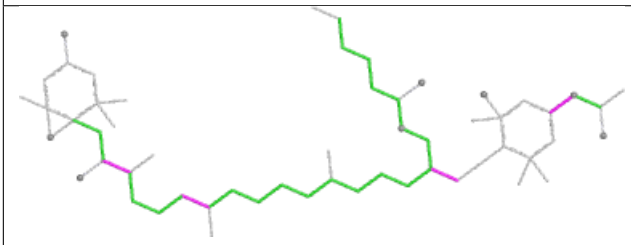
Ligand A1EB1 Z 320



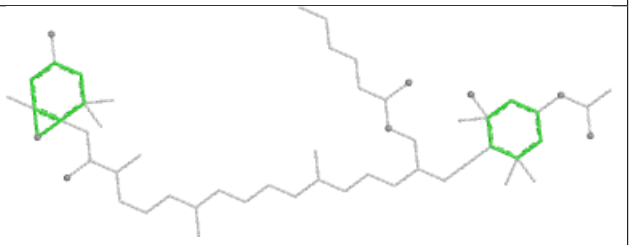
Bond lengths



Bond angles

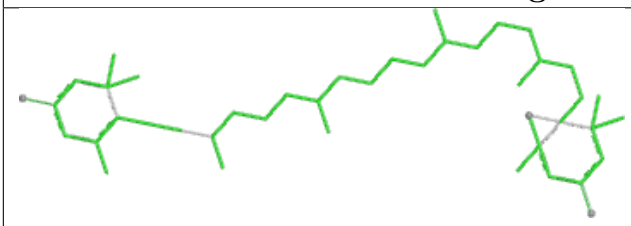


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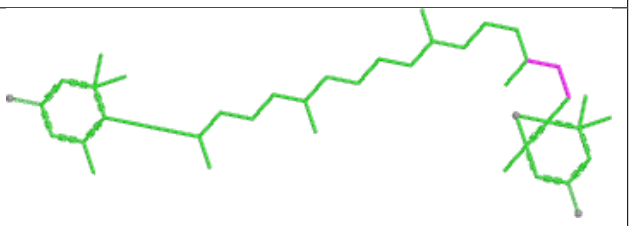


Rings

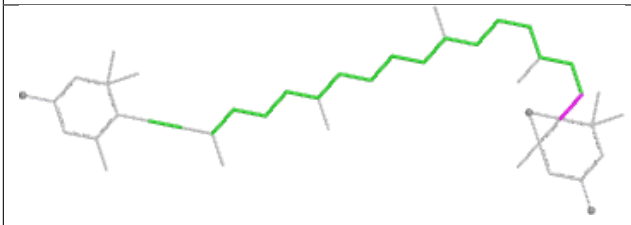
Ligand DD6 J 313



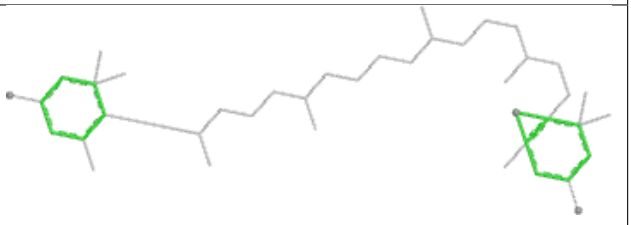
Bond lengths



Bond angles

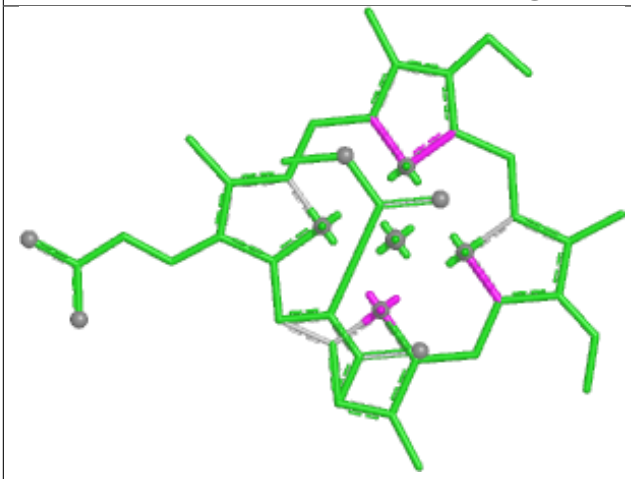


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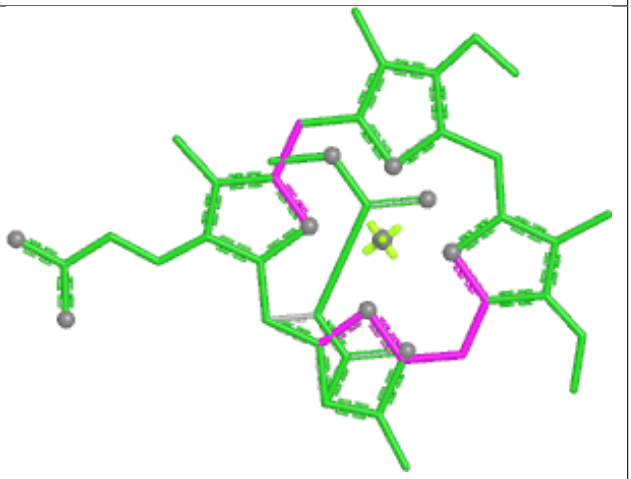


Rings

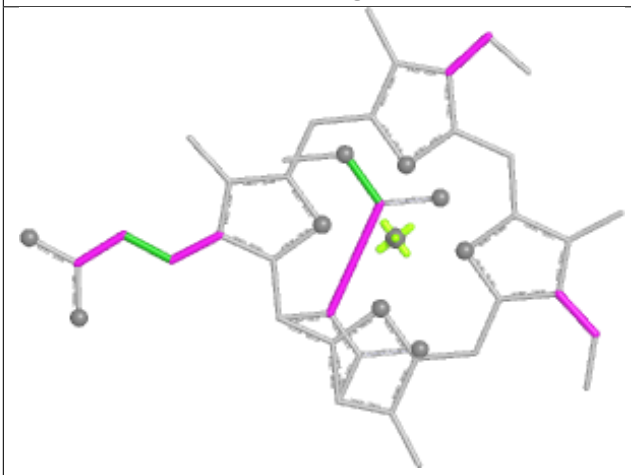
Ligand KC2 w 301



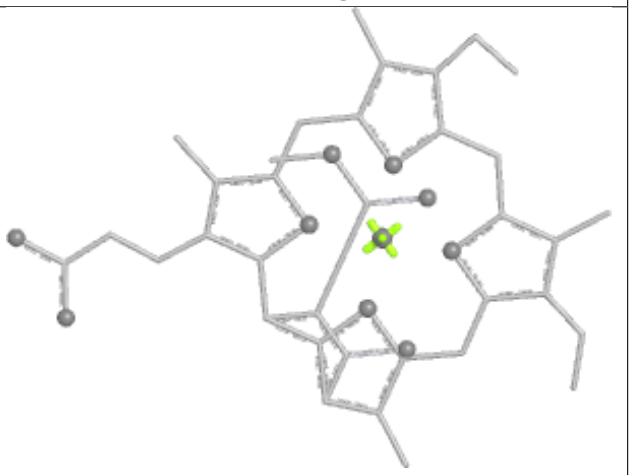
Bond lengths



Bond angles

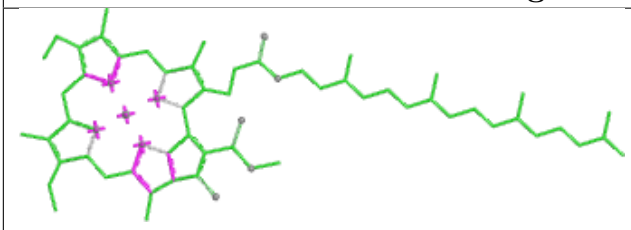


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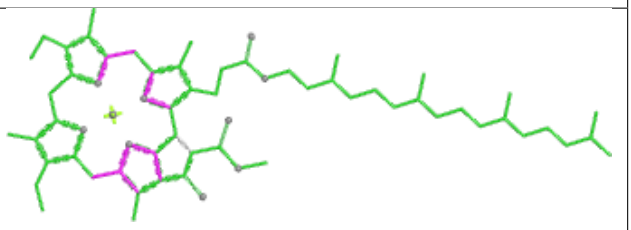


Rings

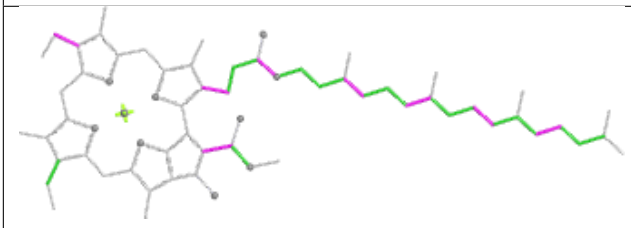
Ligand CLA b 839



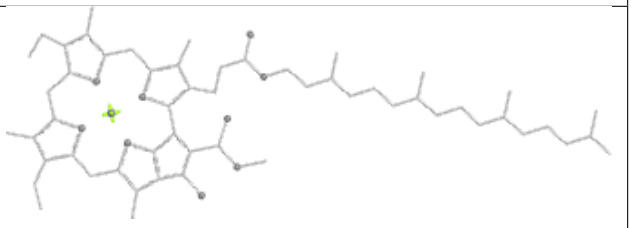
Bond lengths



Bond angles

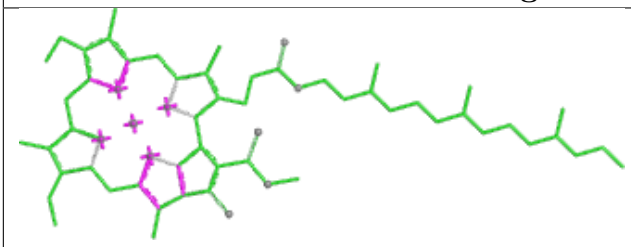


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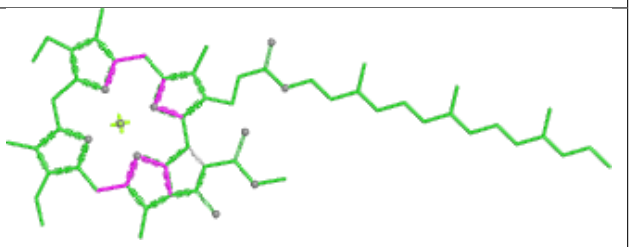


Rings

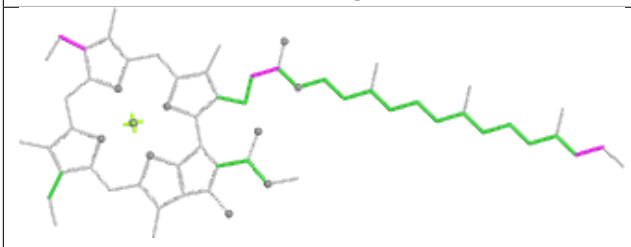
Ligand CLA M 306



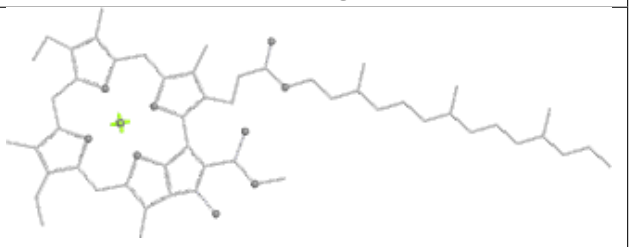
Bond lengths



Bond angles

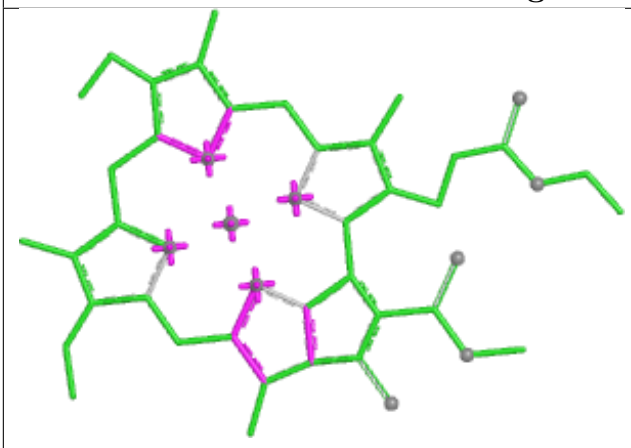


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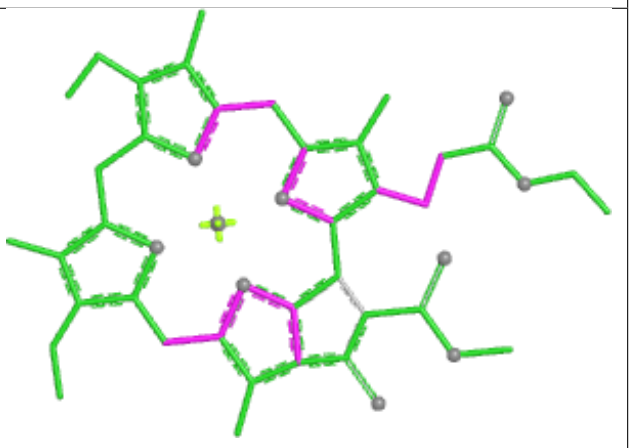


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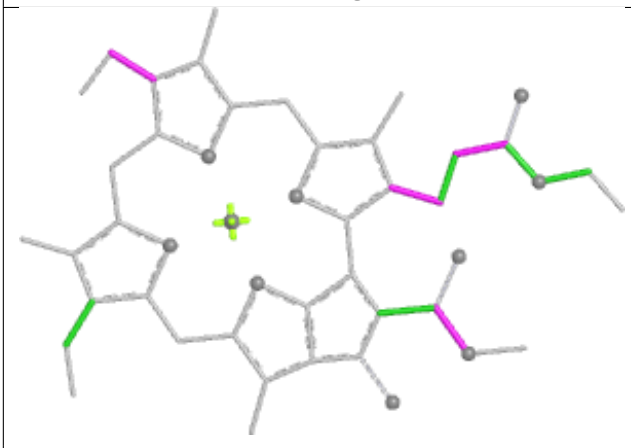
Ligand CLA S 319



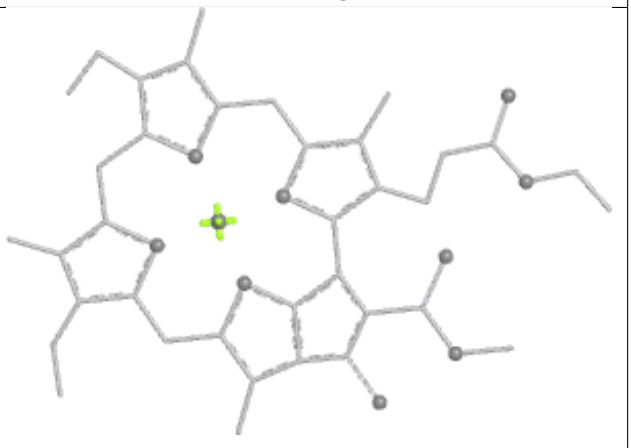
Bond lengths



Bond angles

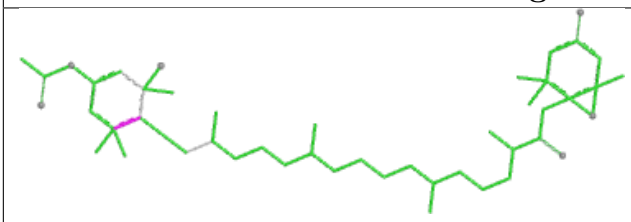


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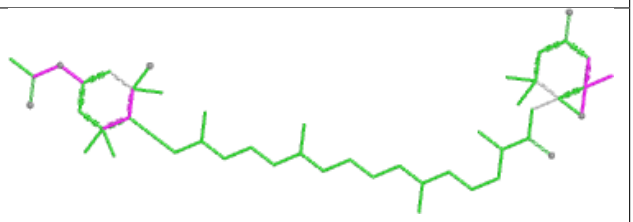


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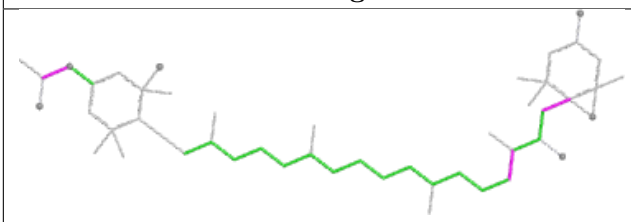
Ligand A86 X 318



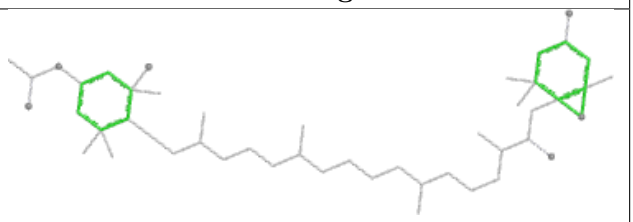
Bond lengths



Bond angles

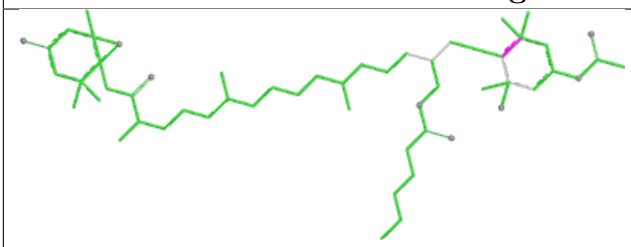


Torsions

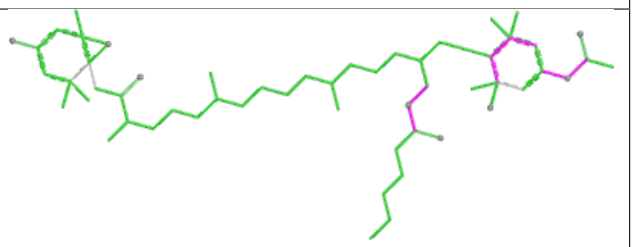


Rings

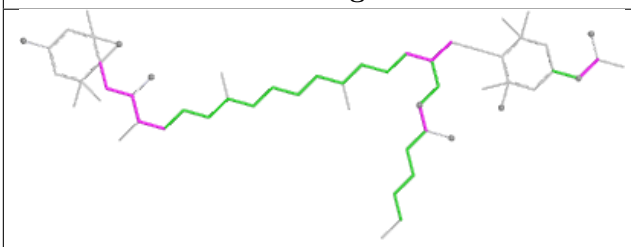
Ligand A1EB1 v 324



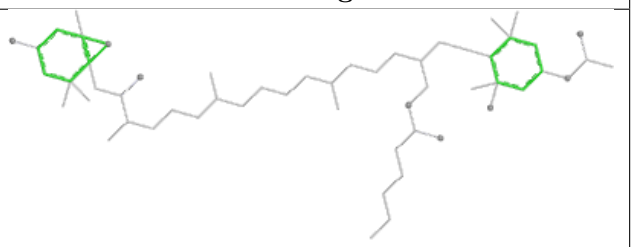
Bond lengths



Bond angles

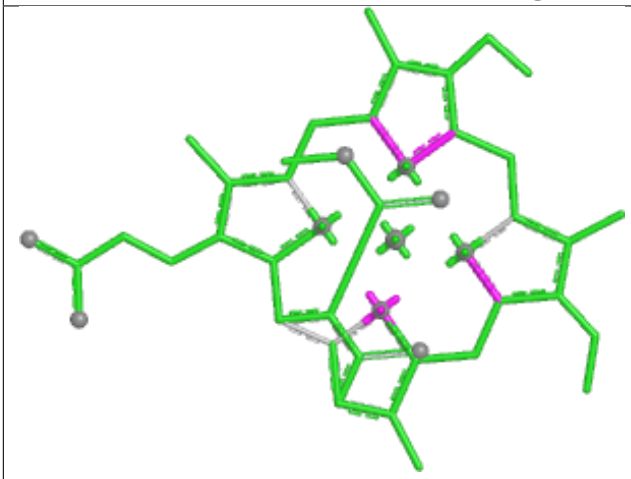


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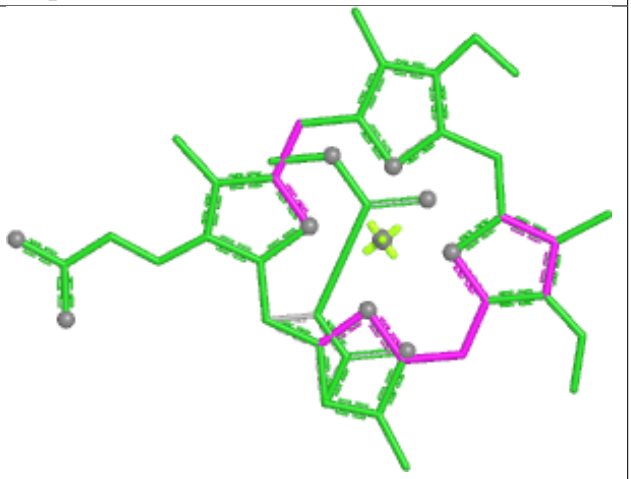


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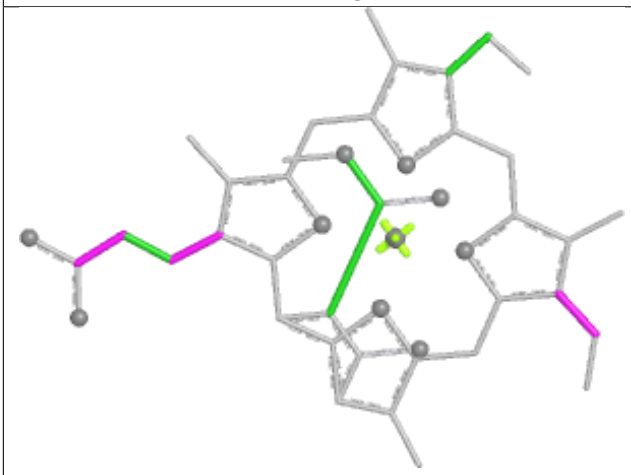
Ligand KC2 p 303



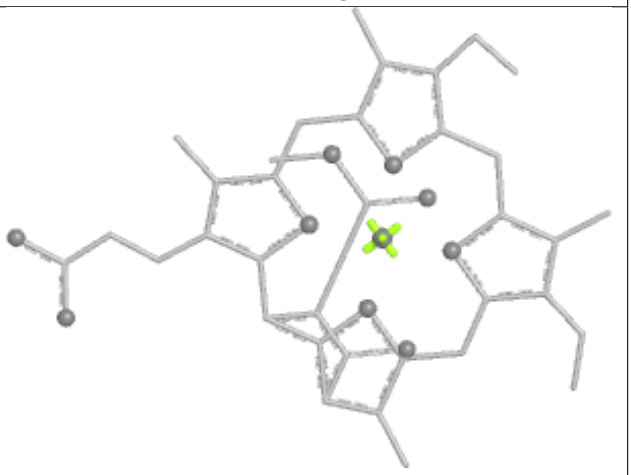
Bond lengths



Bond angles

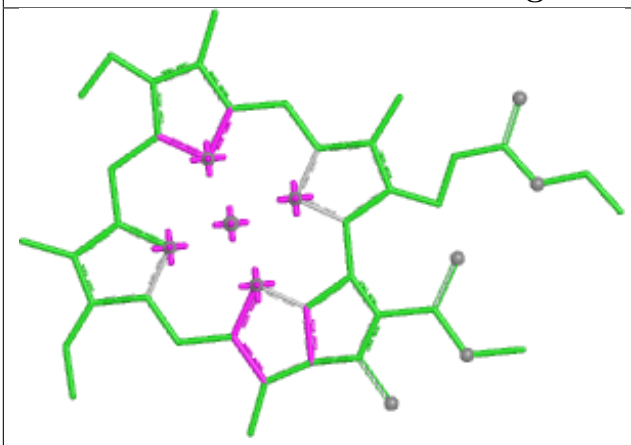


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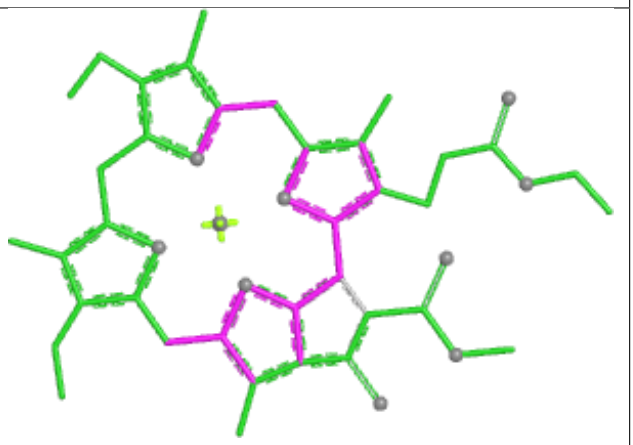


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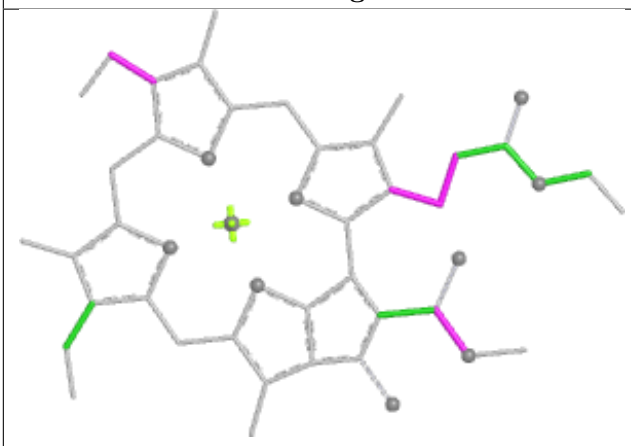
Ligand CLA L 306



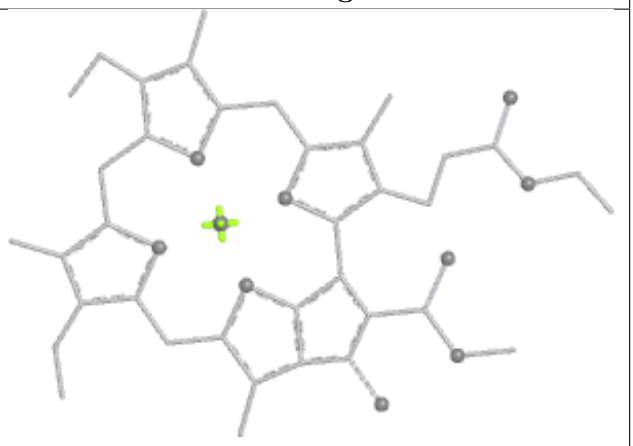
Bond lengths



Bond angles

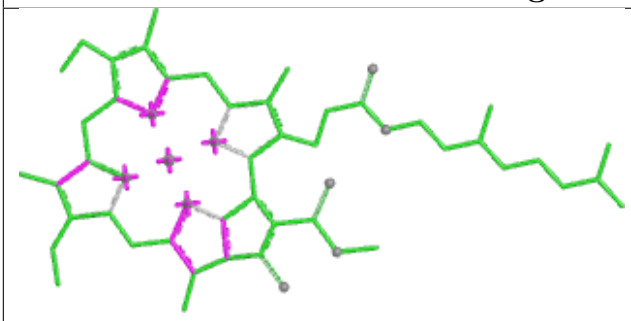


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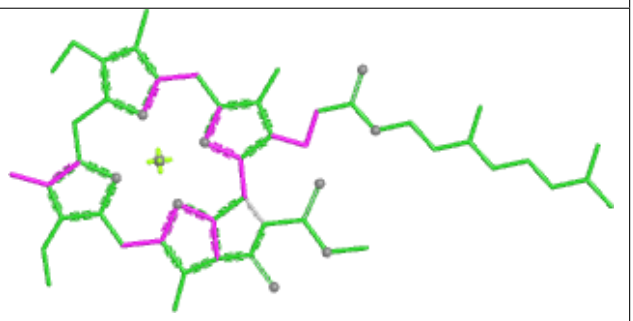


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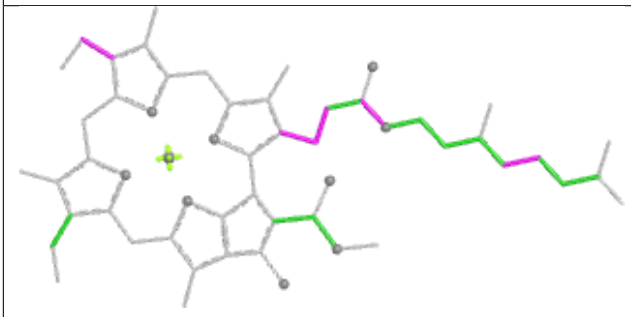
Ligand CLA J 308



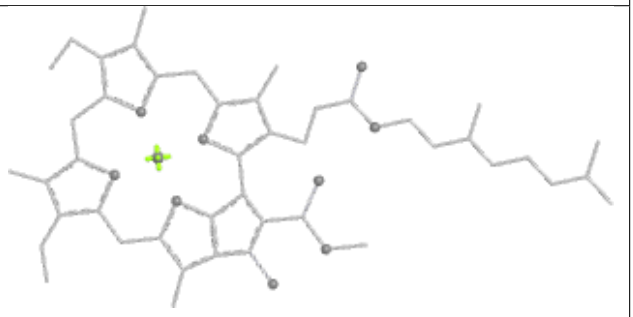
Bond lengths



Bond angles

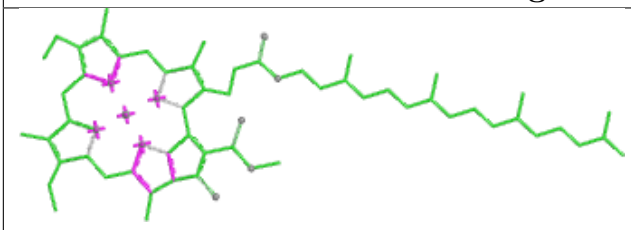


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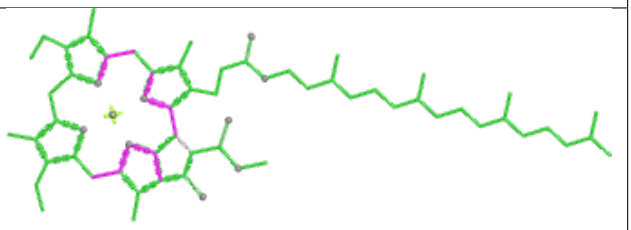


Rings

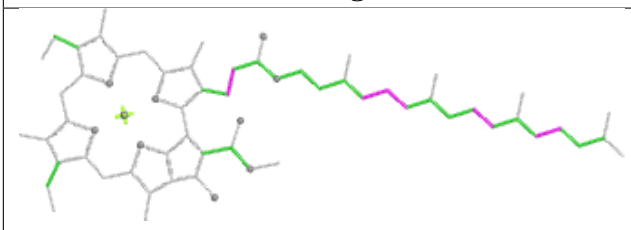
Ligand CLA a 825



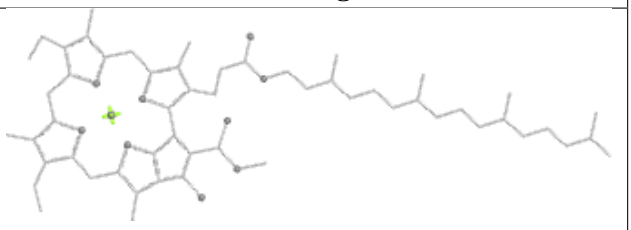
Bond lengths



Bond angles

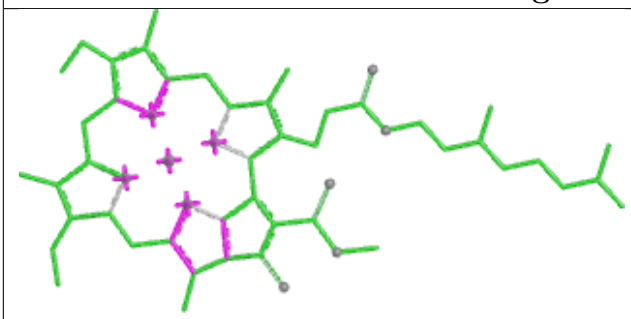


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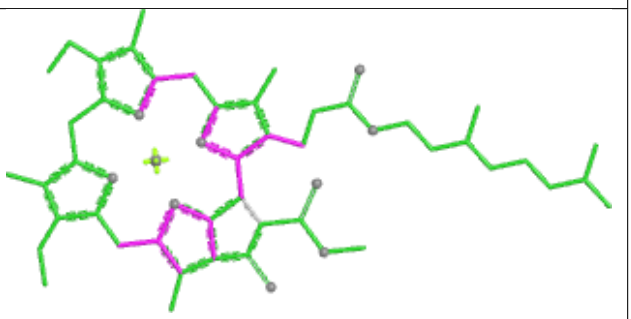


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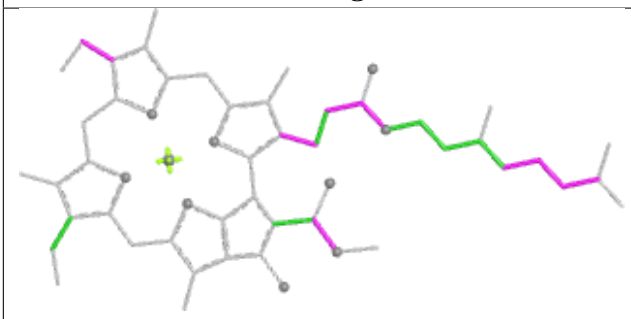
Ligand CLA i 101



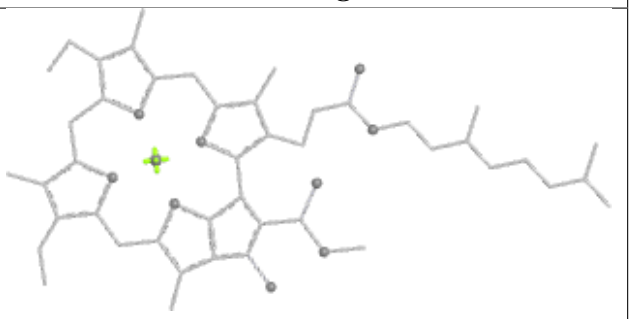
Bond lengths



Bond angles

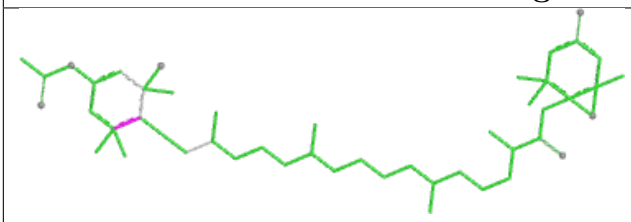


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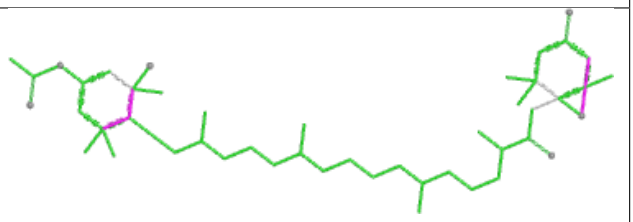


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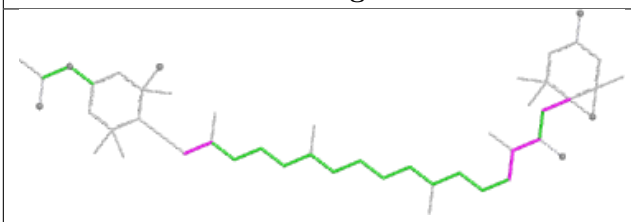
Ligand A86 S 315



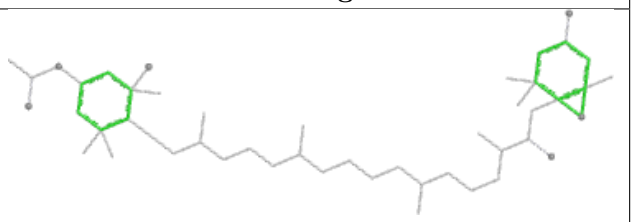
Bond lengths



Bond angles

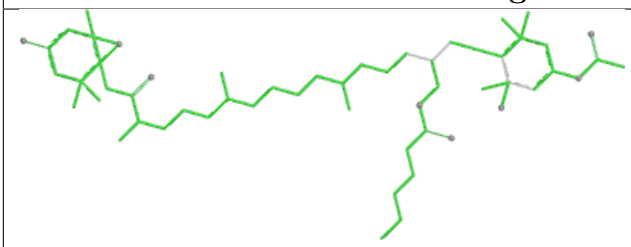


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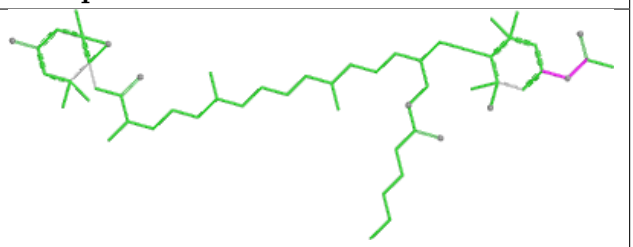


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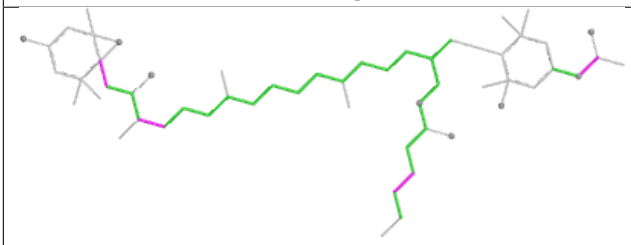
Ligand A1EB1 q 322



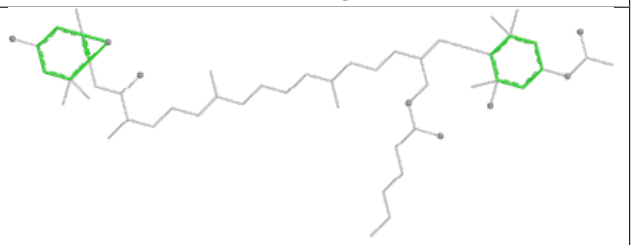
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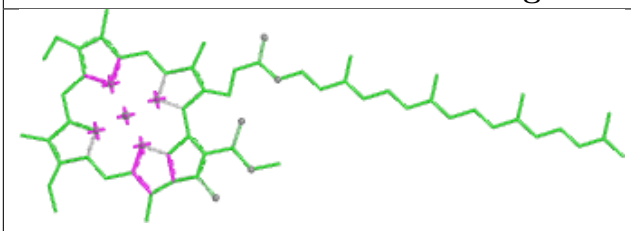


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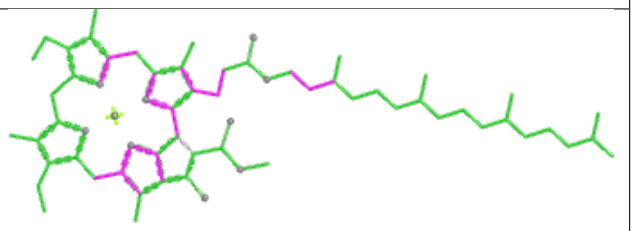


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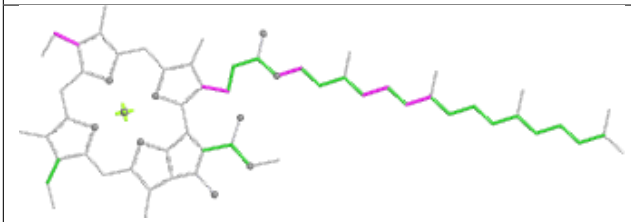
Ligand CLA D 307



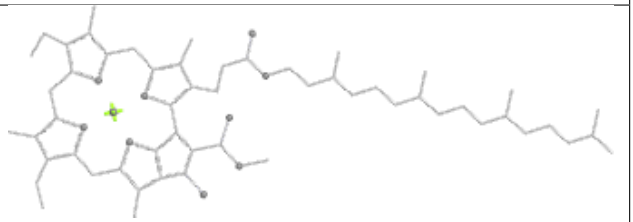
Bond lengths



Bond angles

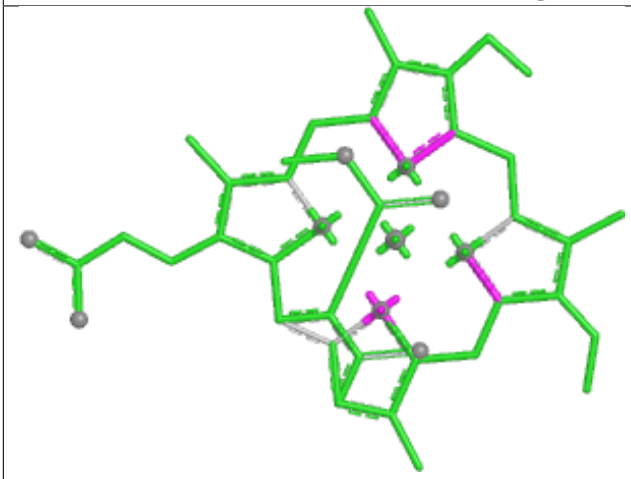


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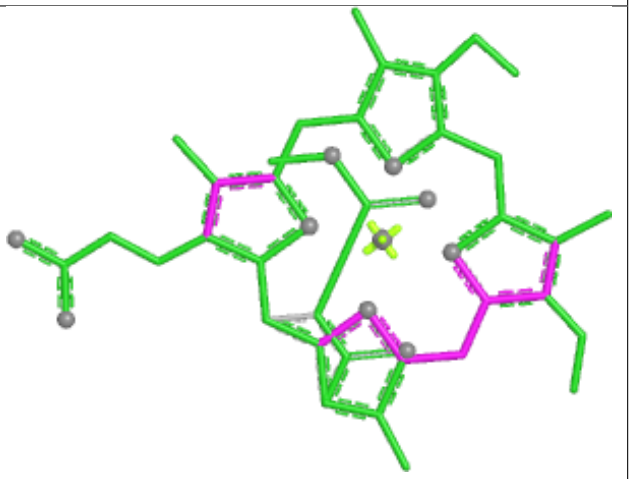


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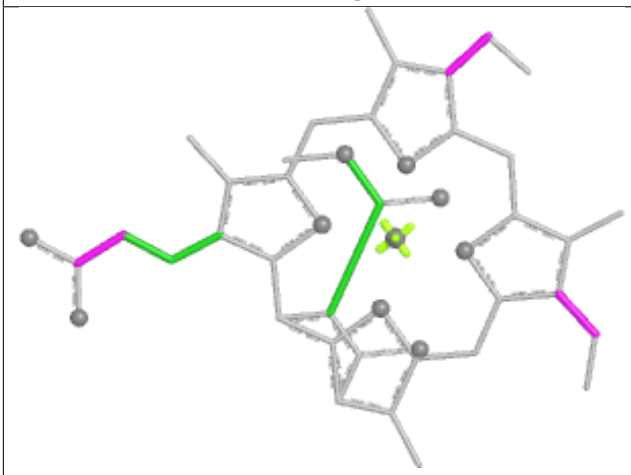
Ligand KC2 t 308



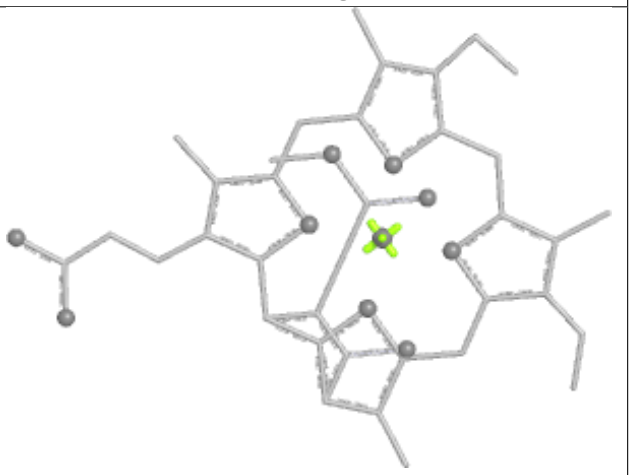
Bond lengths



Bond angles

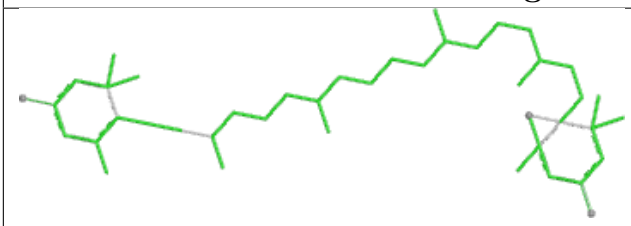


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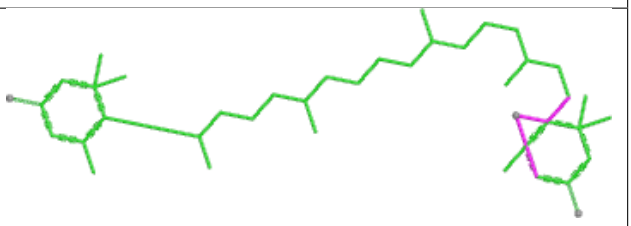


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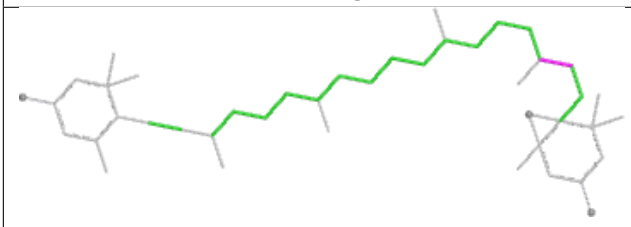
Ligand DD6 N 316



Bond lengths



Bond angles

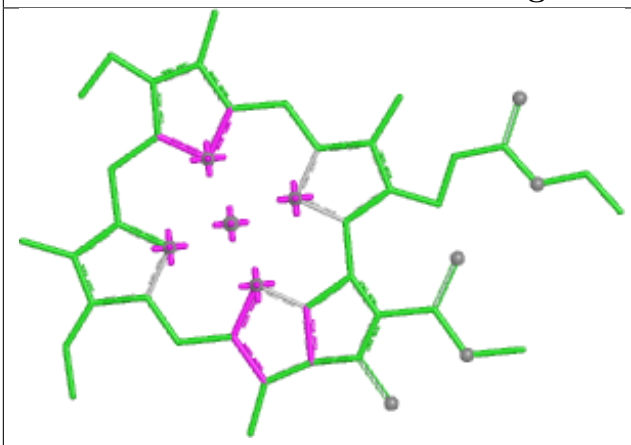


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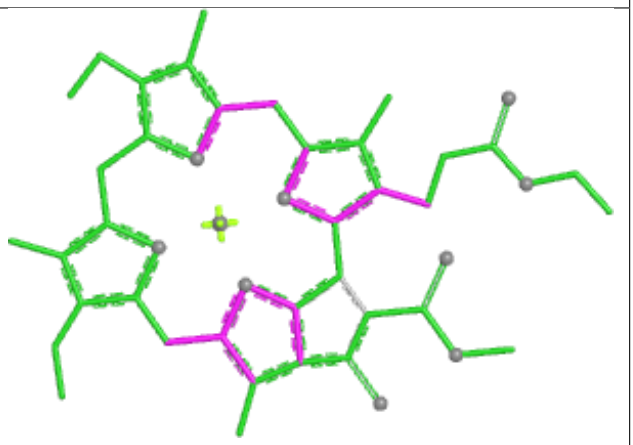


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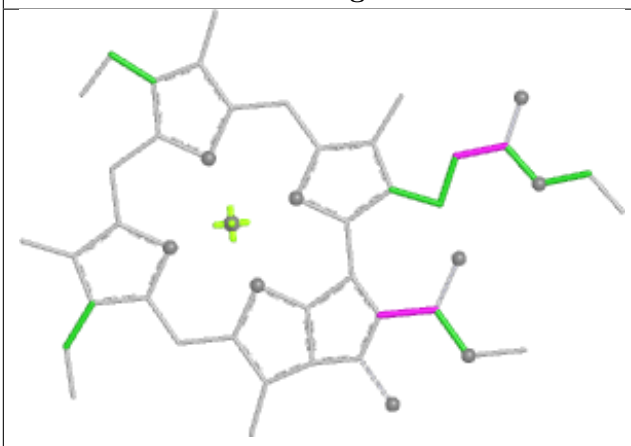
Ligand CLA J 311



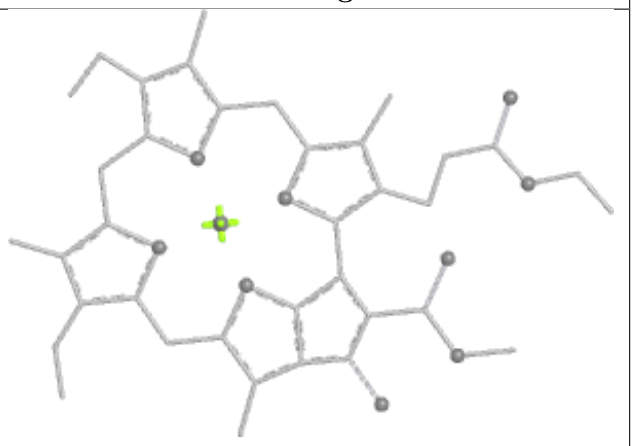
Bond lengths



Bond angles

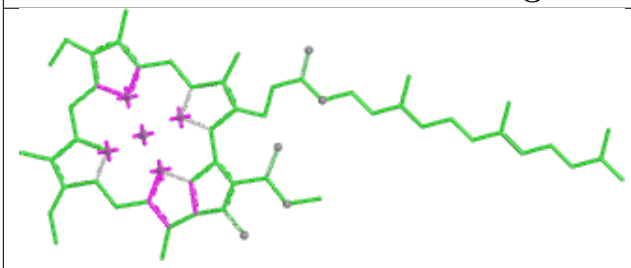


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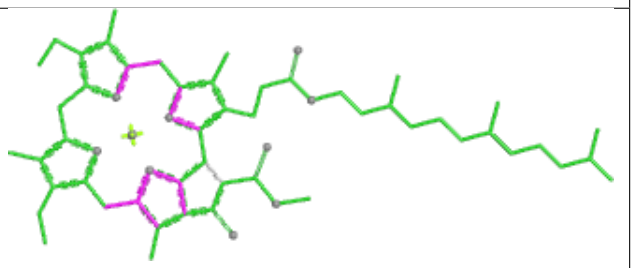


Rings

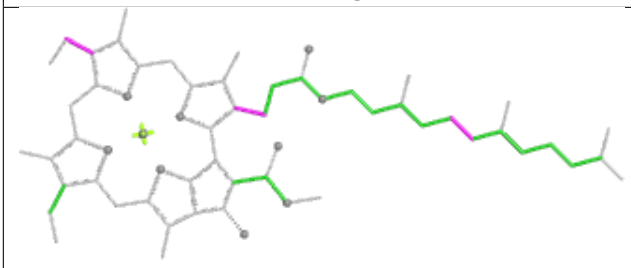
Ligand CLA X 301



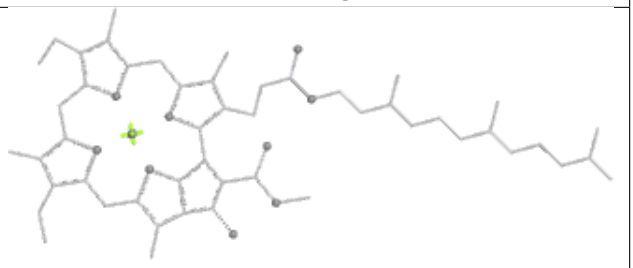
Bond lengths



Bond angles

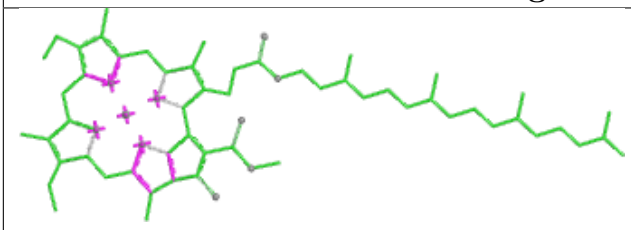


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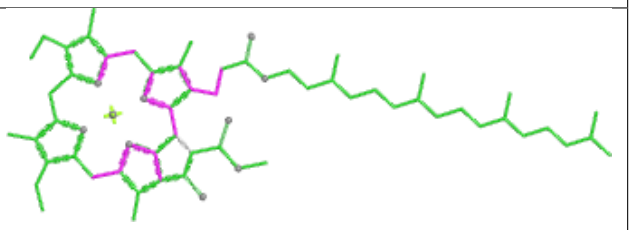


Rings

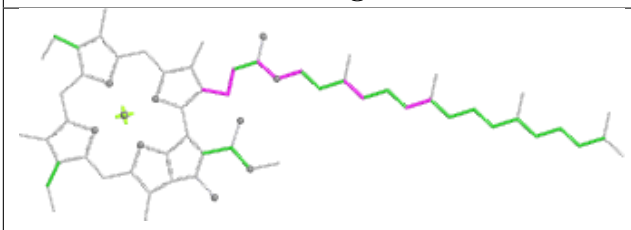
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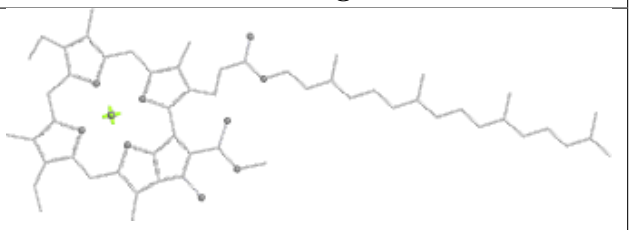
Bond lengths



Bond angles

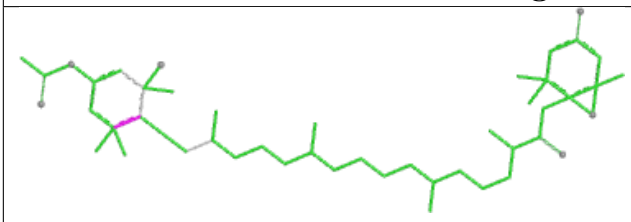


Torsions

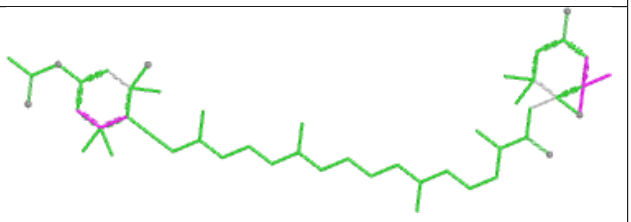


Rings

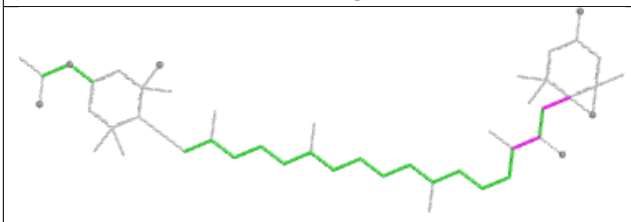
Ligand A86 T 312



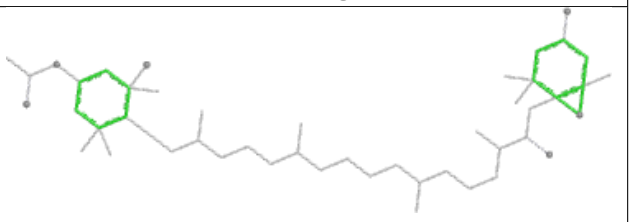
Bond lengths



Bond angles

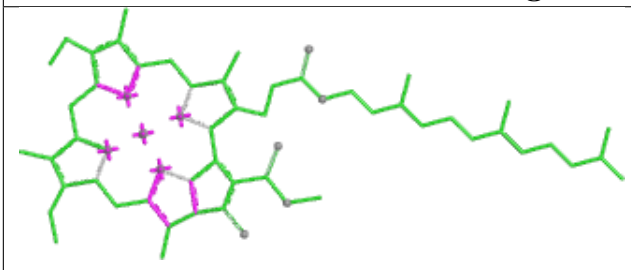


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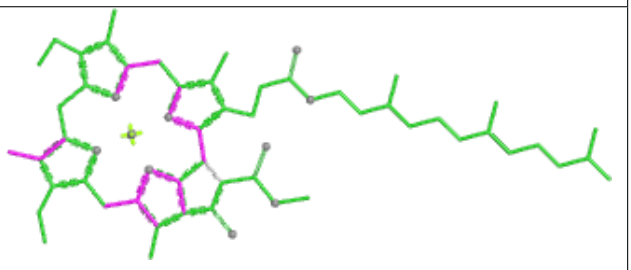


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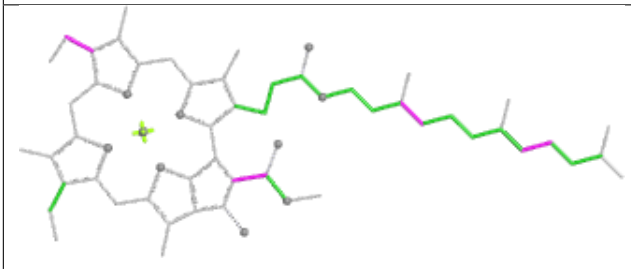
Ligand CLA E 305



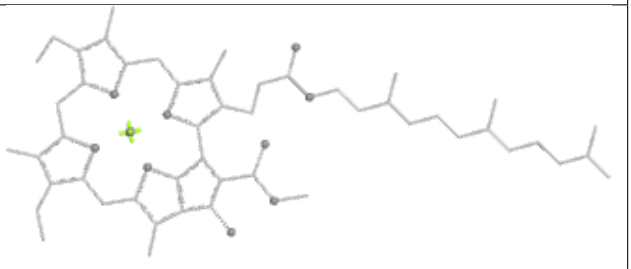
Bond lengths



Bond angles

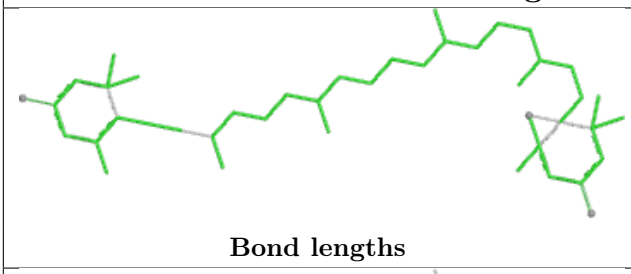


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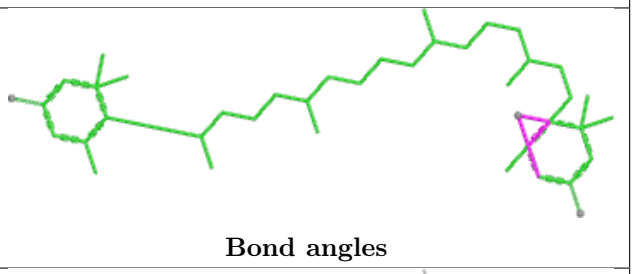


Rings

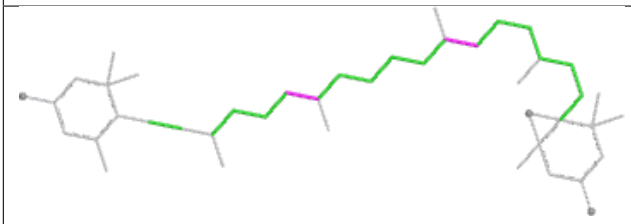
Ligand DD6 Y 322



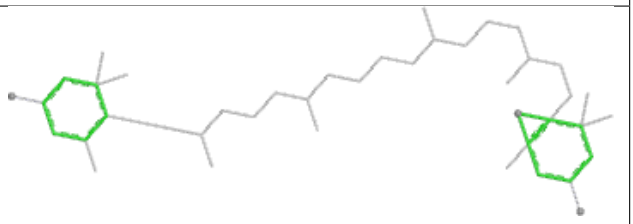
Bond lengths



Bond angles

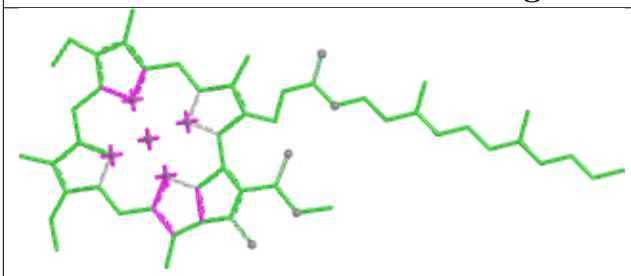


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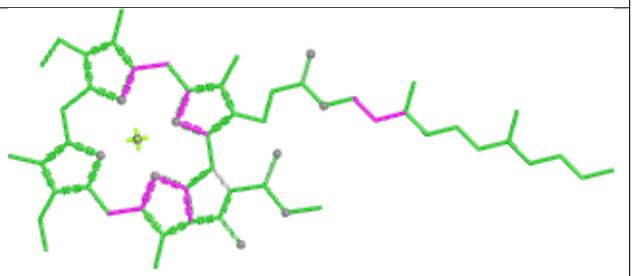


Rings

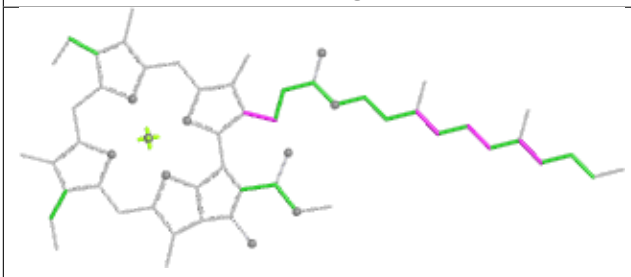
Ligand CLA D 302



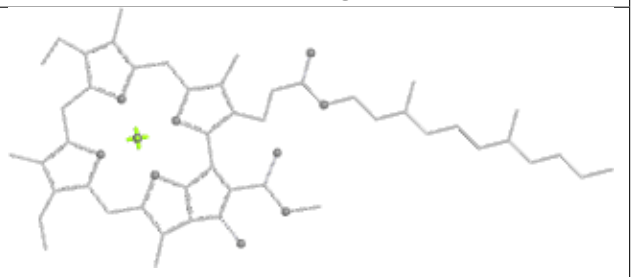
Bond lengths



Bond angles

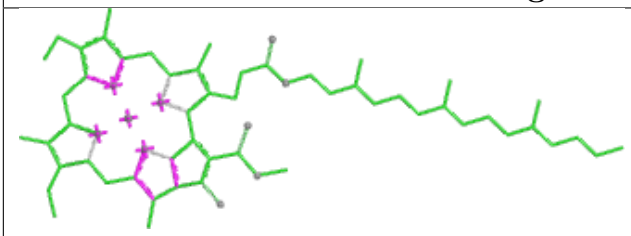


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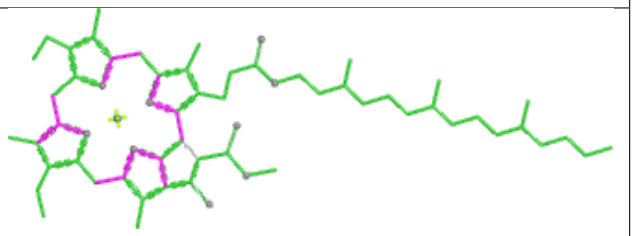


Rings

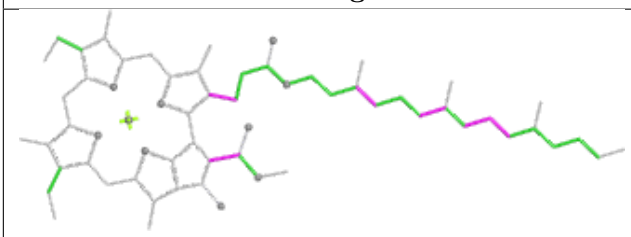
Ligand CLA v 311



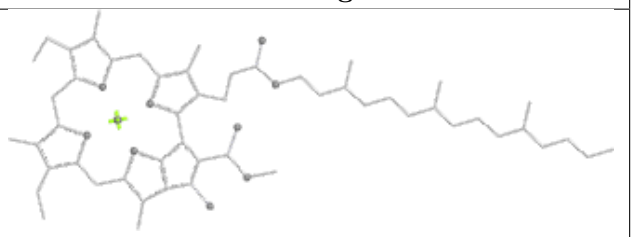
Bond lengths



Bond angles

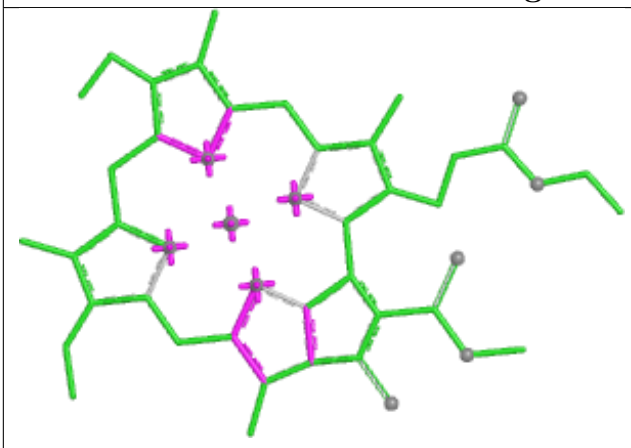


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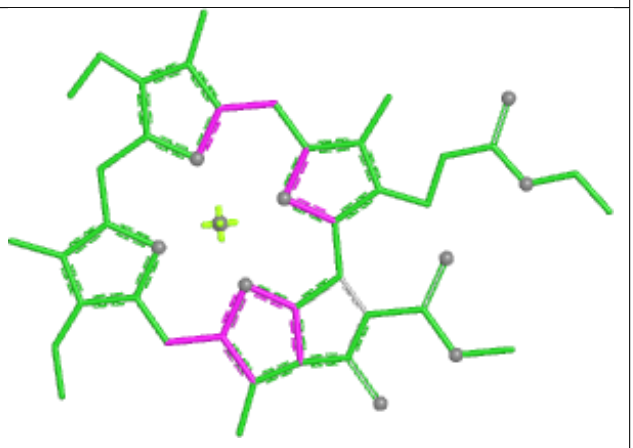


Rings

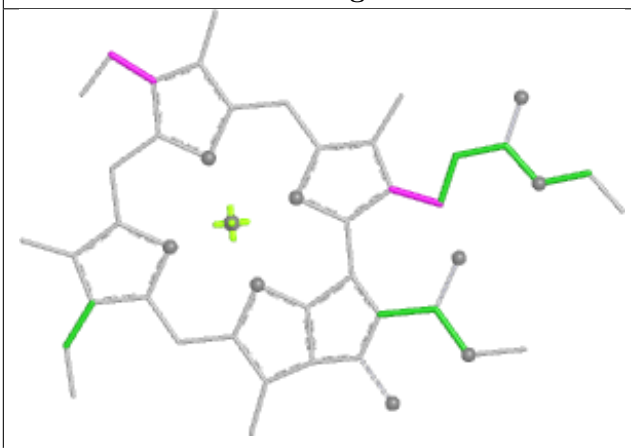
Ligand CLA B 303



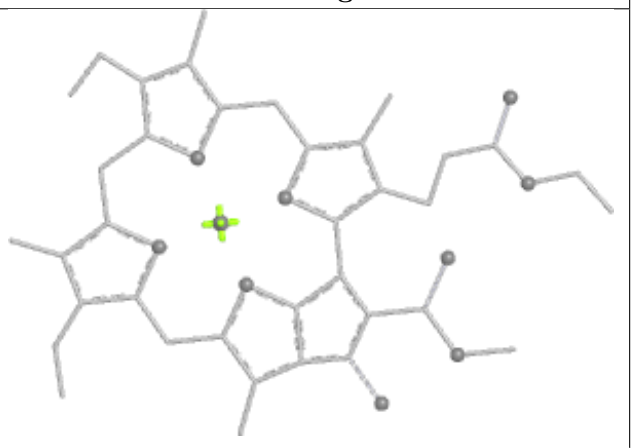
Bond lengths



Bond angles

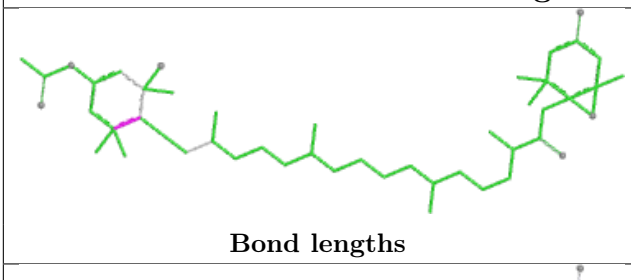


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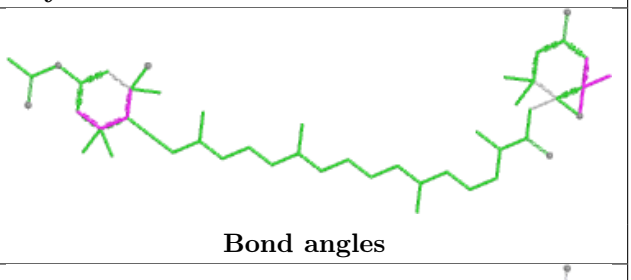


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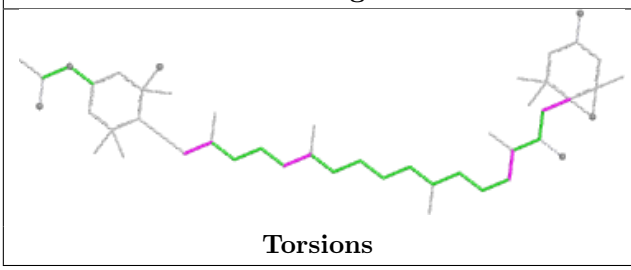
Ligand A86 y 310



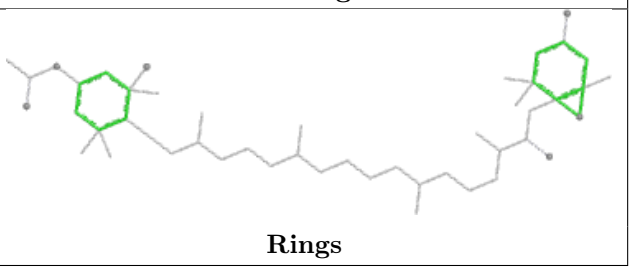
Bond lengths



Bond angles

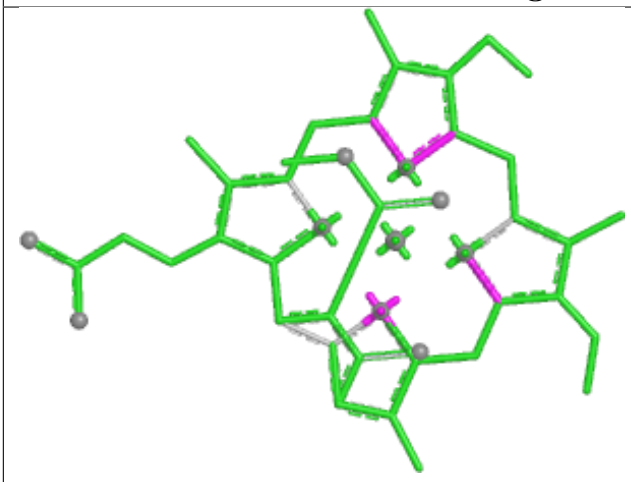


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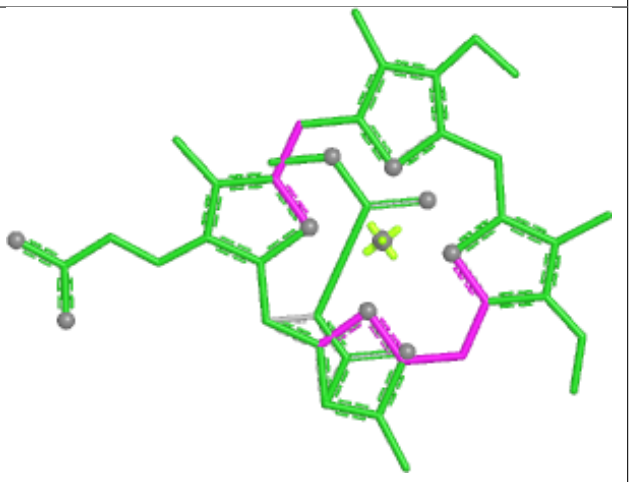


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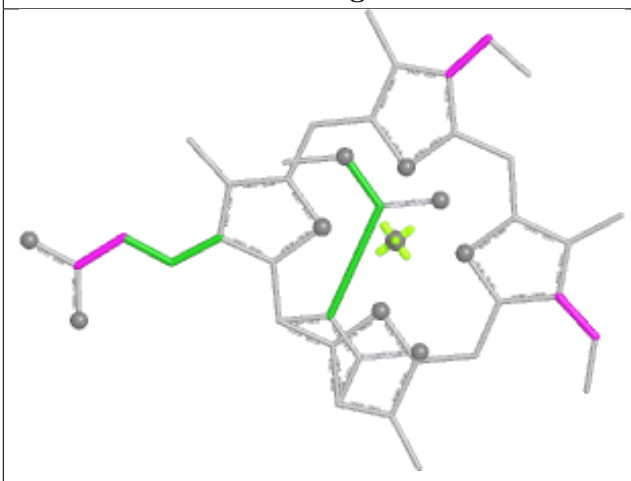
Ligand KC2 P 309



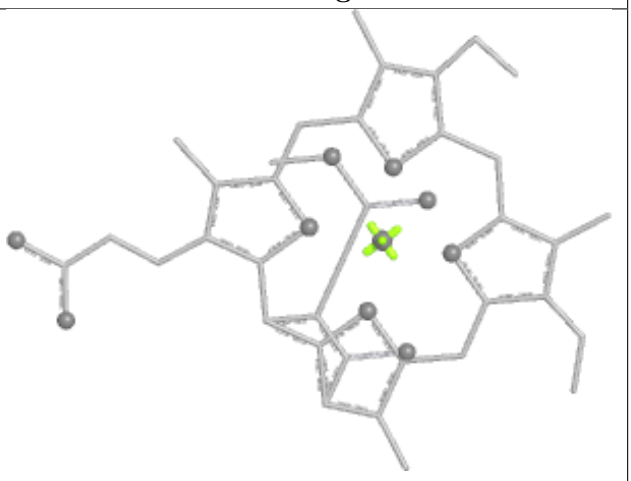
Bond lengths



Bond angles

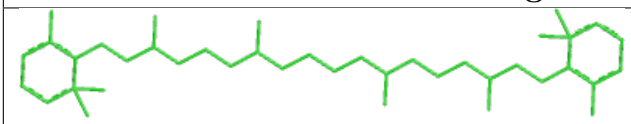


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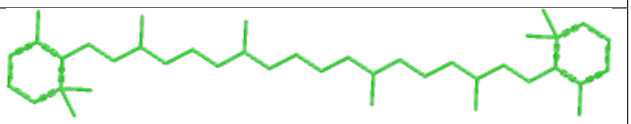


Rings

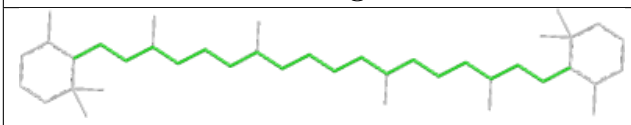
Ligand BCR b 843



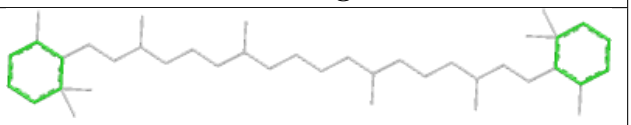
Bond lengths



Bond angles

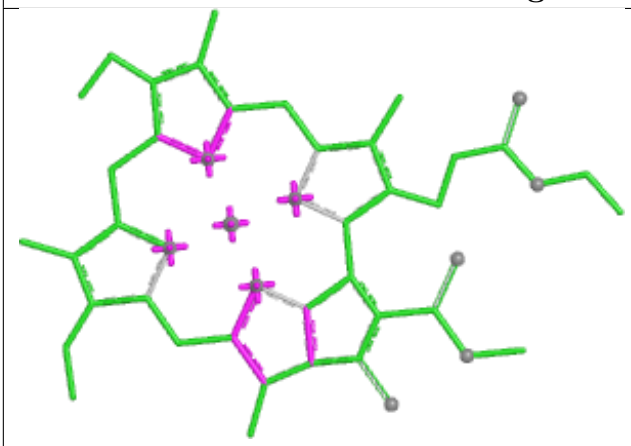


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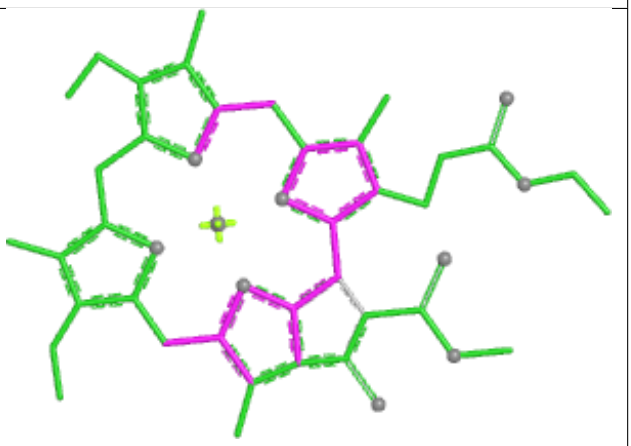


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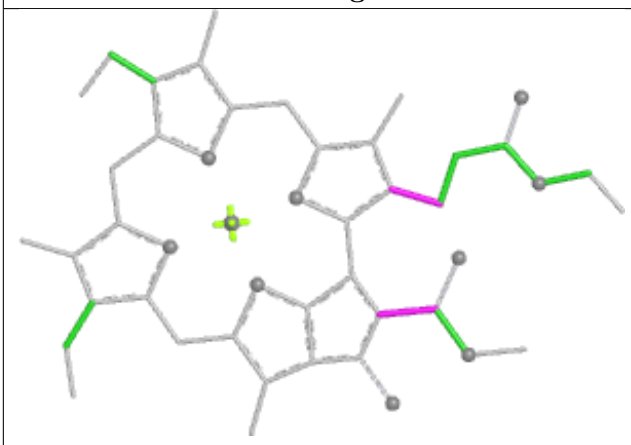
Ligand CLA S 312



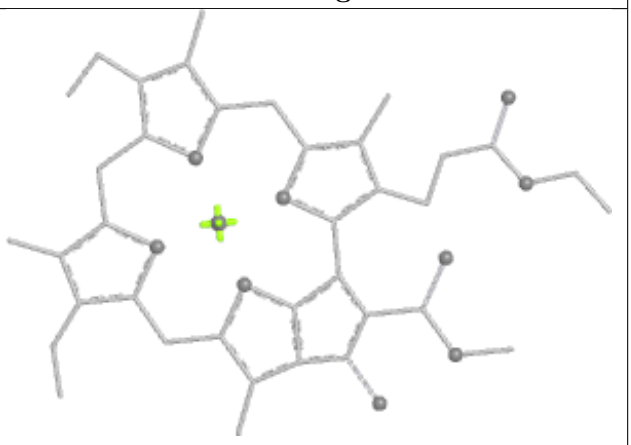
Bond lengths



Bond angles

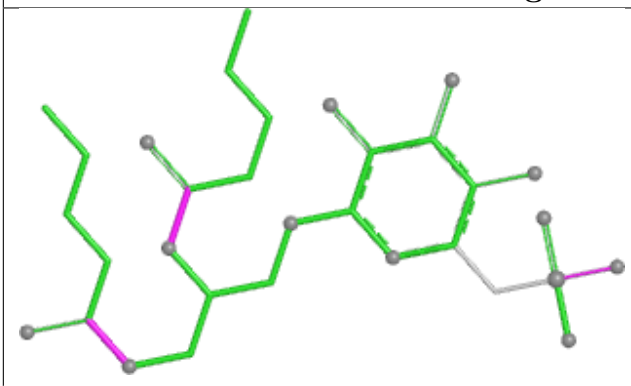


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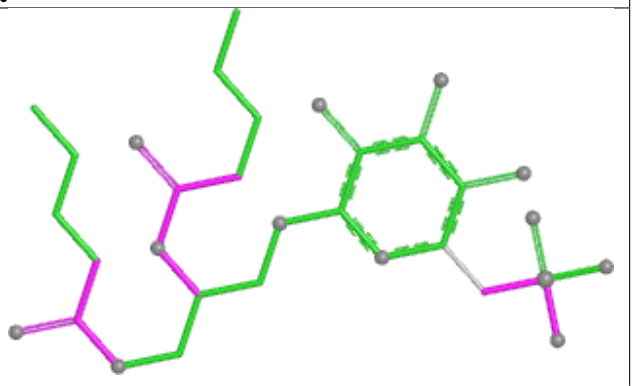


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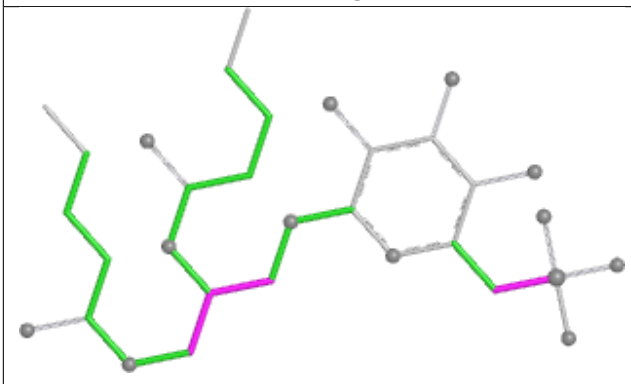
Ligand SQD P 319



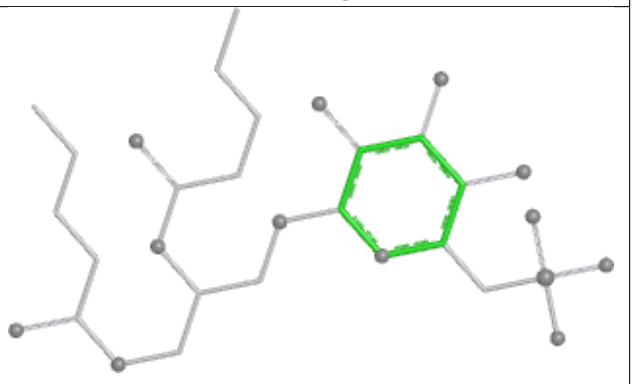
Bond lengths



Bond angles

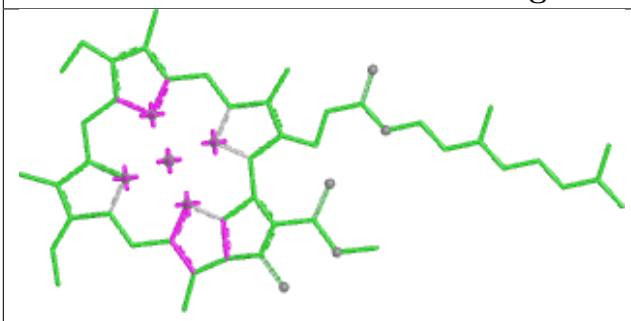


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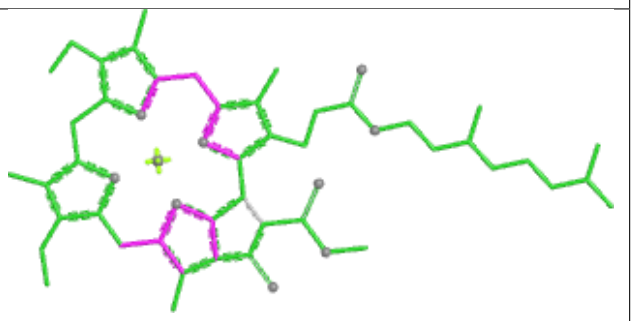


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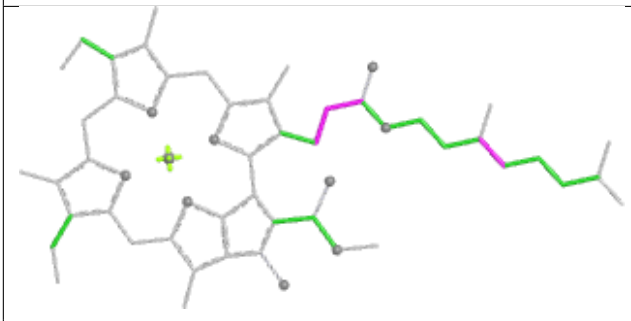
Ligand CLA z 306



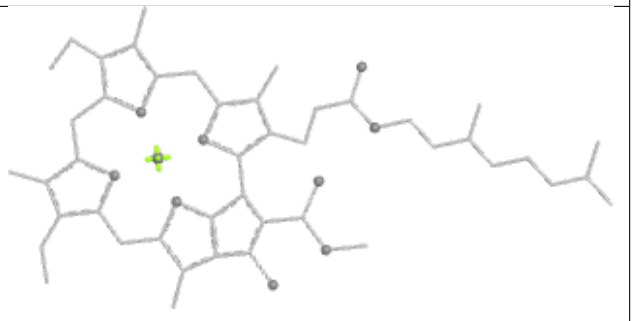
Bond lengths



Bond angles

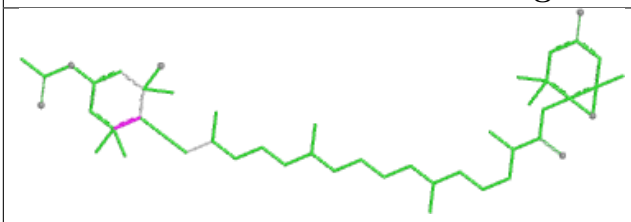


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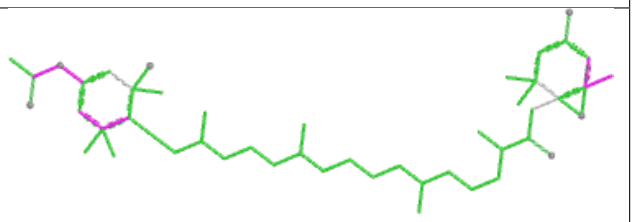


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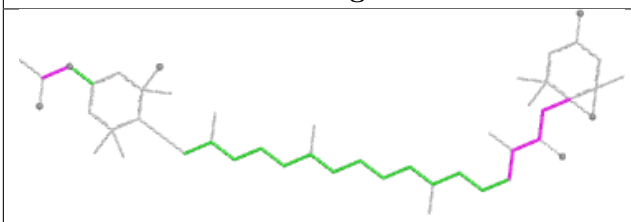
Ligand A86 o 316



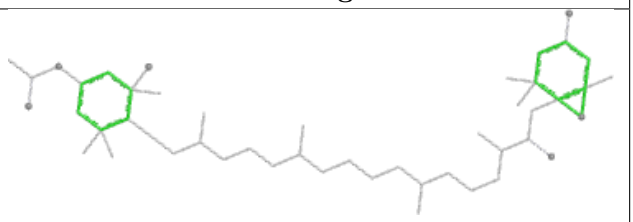
Bond lengths



Bond angles



Torsions

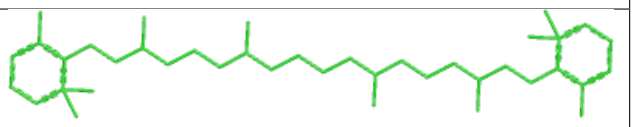


Rings

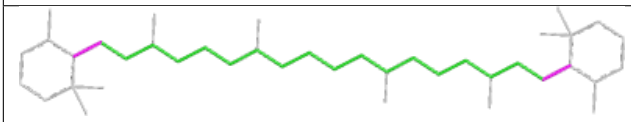
Ligand BCR b 847



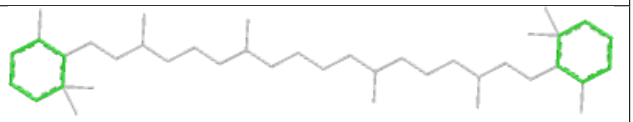
Bond lengths



Bond angles

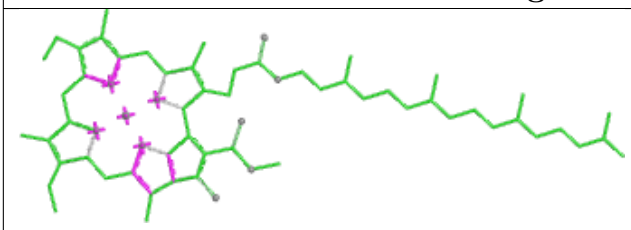


Torsions

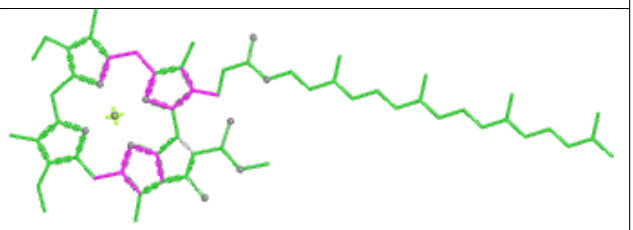


Rings

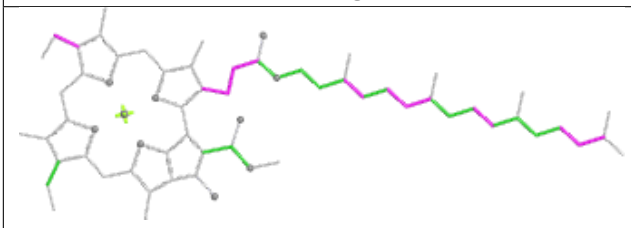
Ligand CLA b 824



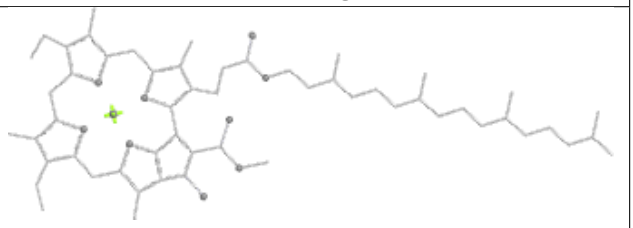
Bond lengths



Bond angles

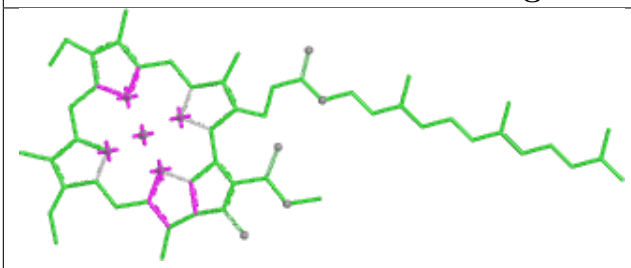


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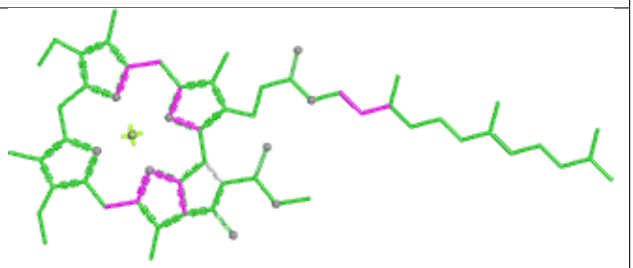


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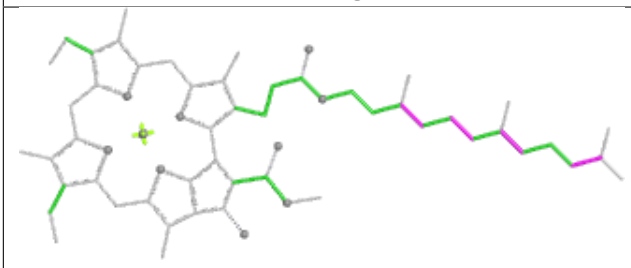
Ligand CLA A 302



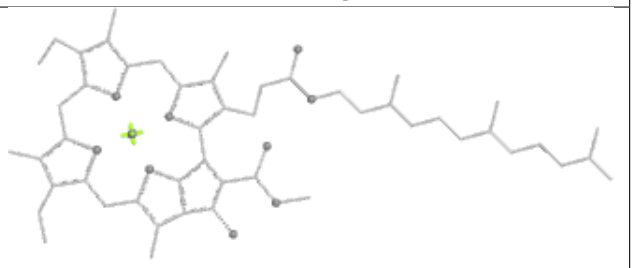
Bond lengths



Bond angles

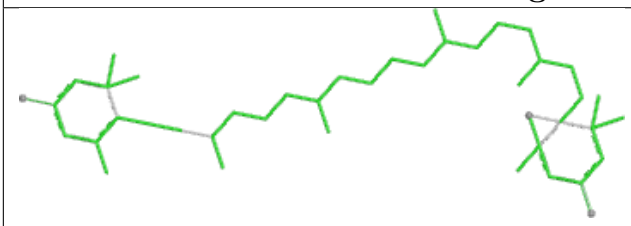


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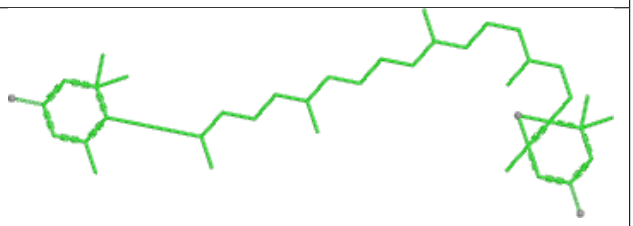


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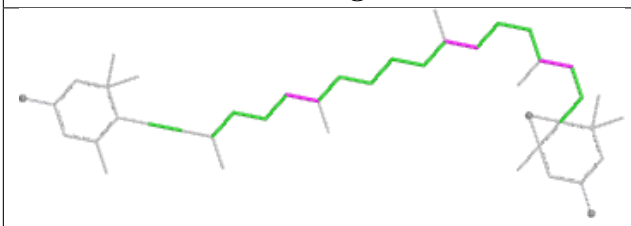
Ligand DD6 v 320



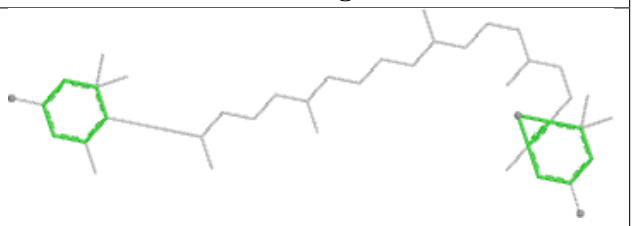
Bond lengths



Bond angles

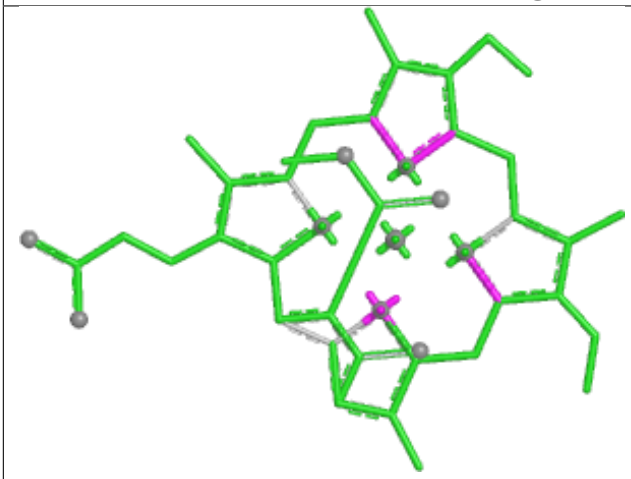


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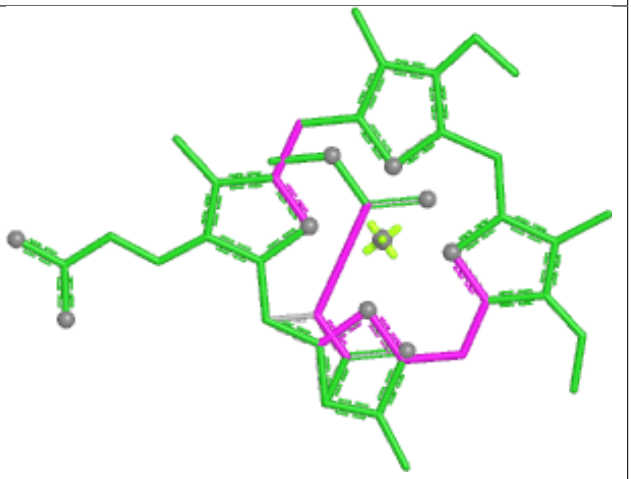


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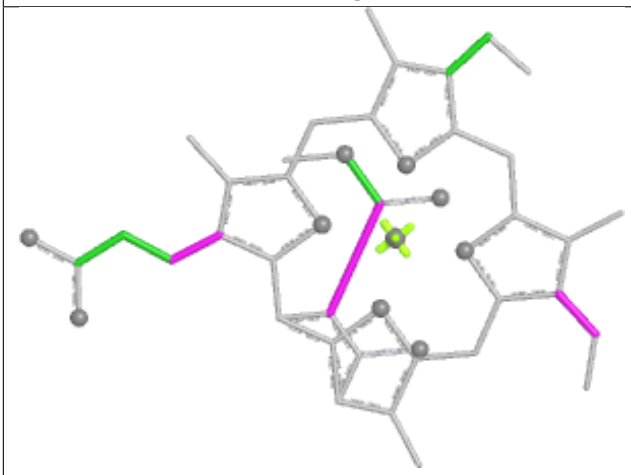
Ligand KC2 S 303



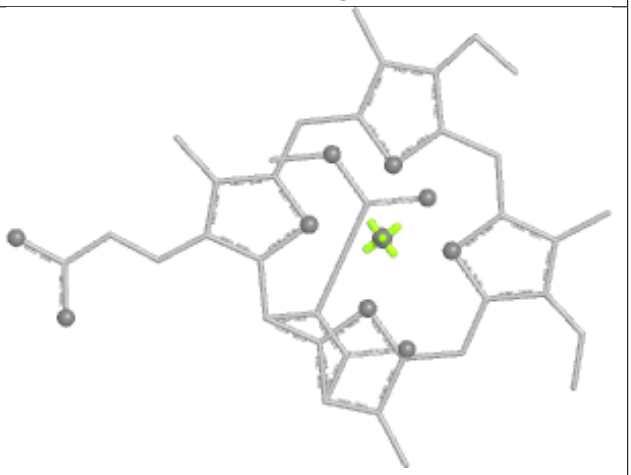
Bond lengths



Bond angles

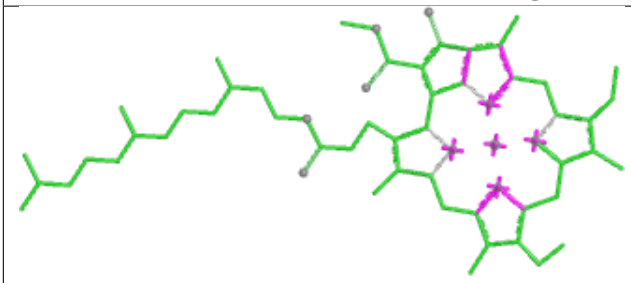


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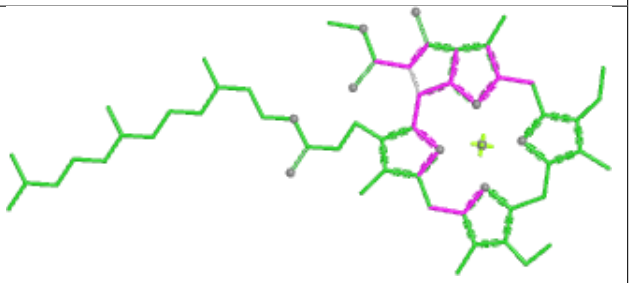


Rings

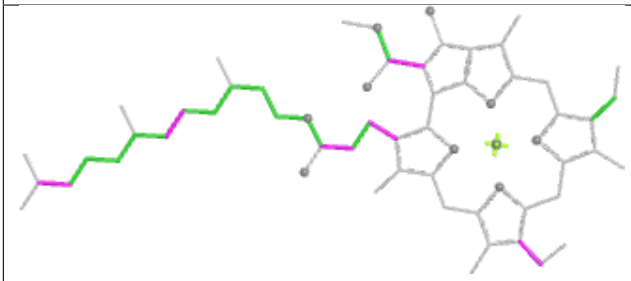
Ligand CLA Z 307



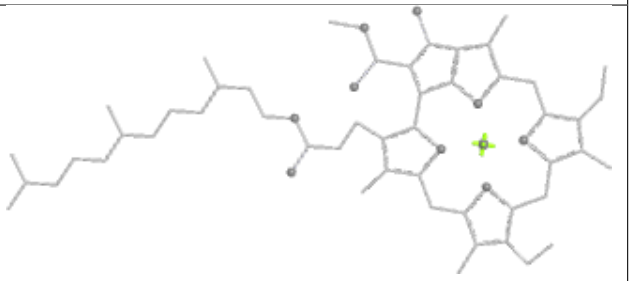
Bond lengths



Bond angles

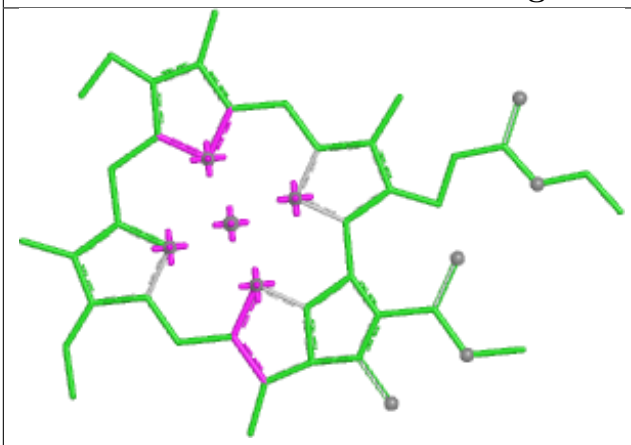


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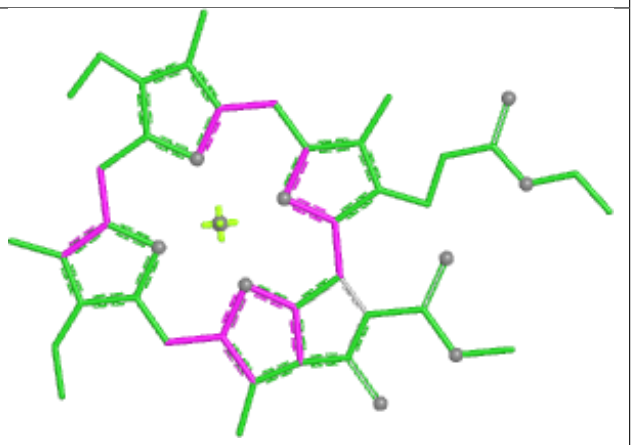


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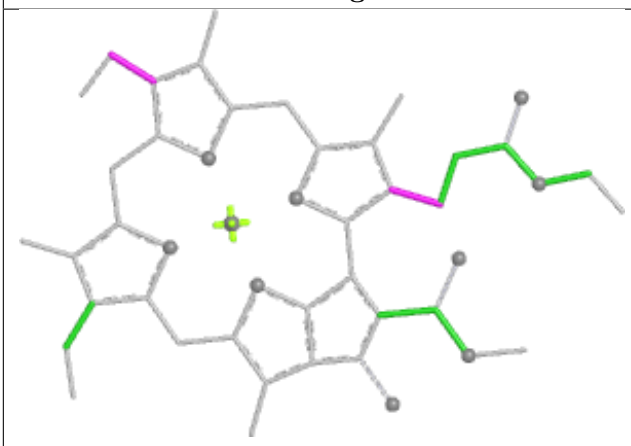
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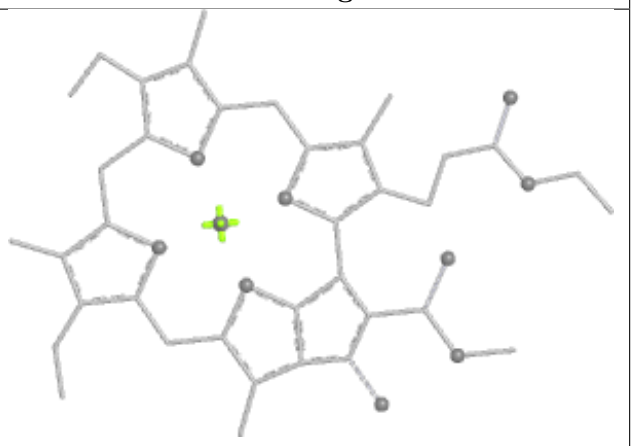
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Bond angles

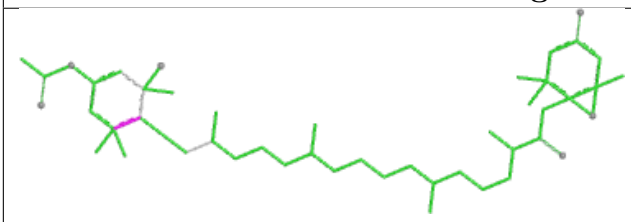


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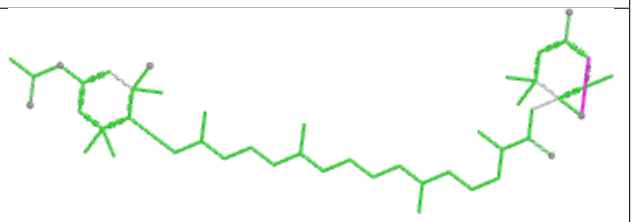


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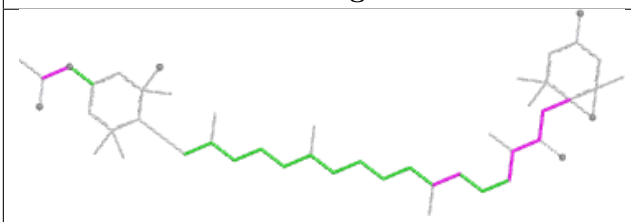
Ligand A86 T 315



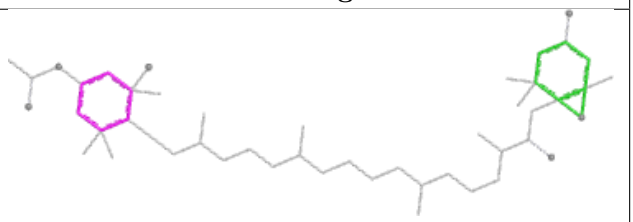
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Bond angles

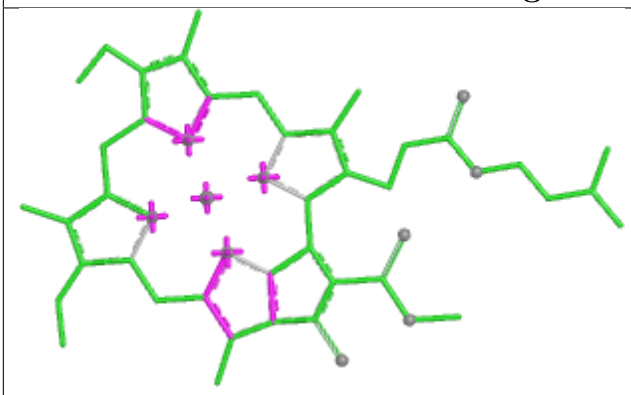


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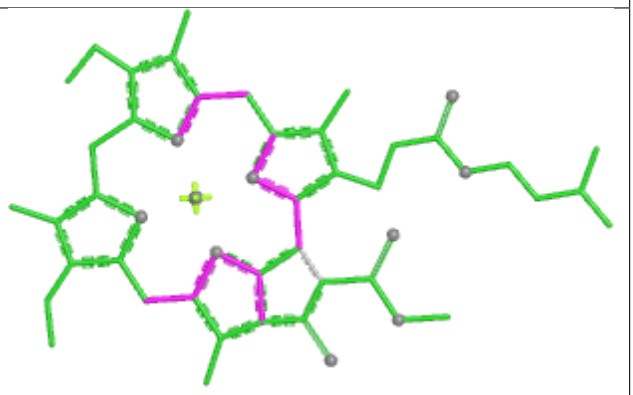


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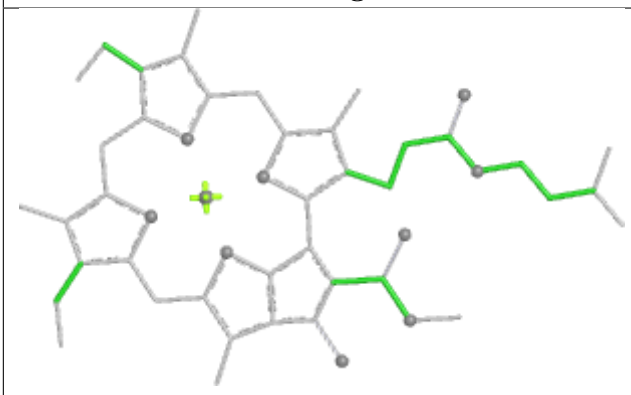
Ligand CLA H 306



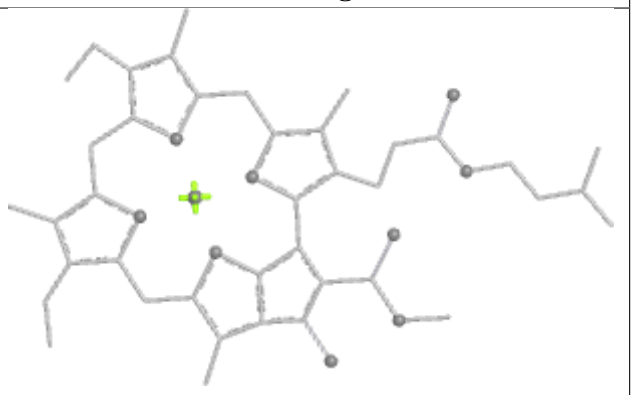
Bond lengths



Bond angles

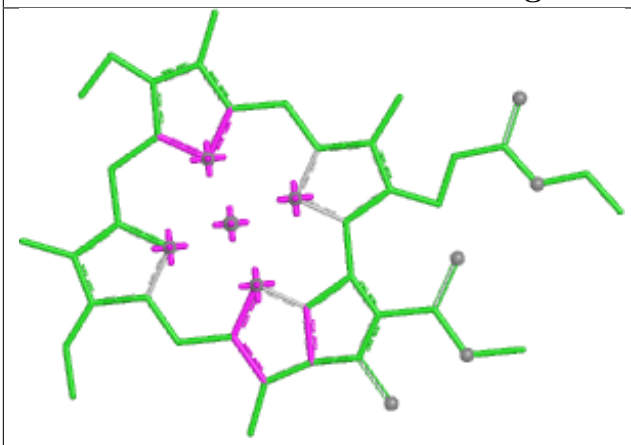


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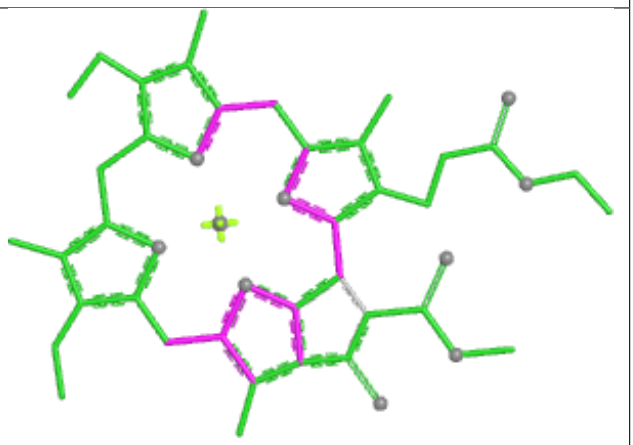


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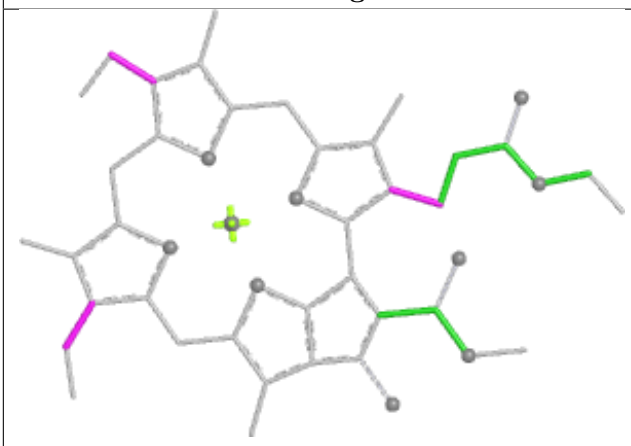
Ligand CLA C 302



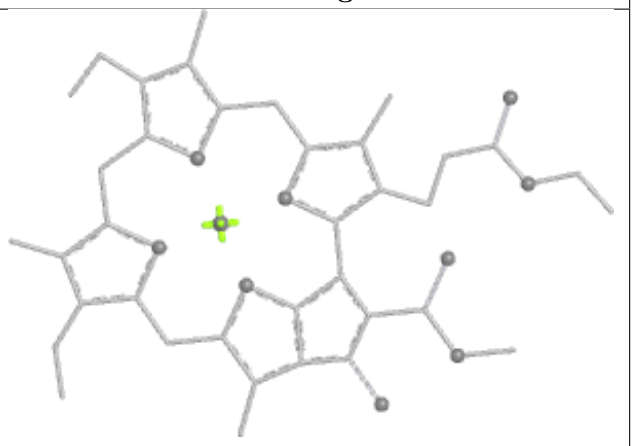
Bond lengths



Bond angles

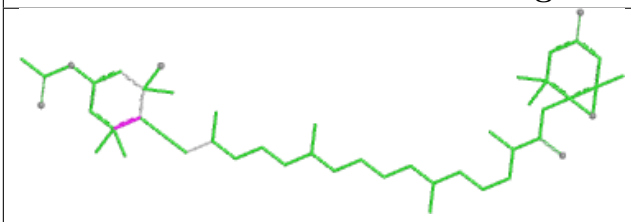


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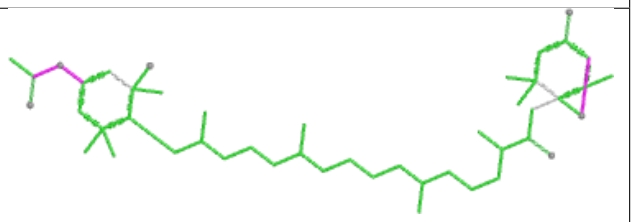


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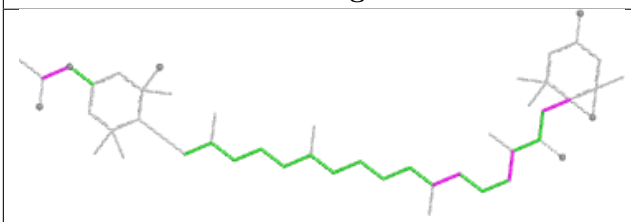
Ligand A86 z 317



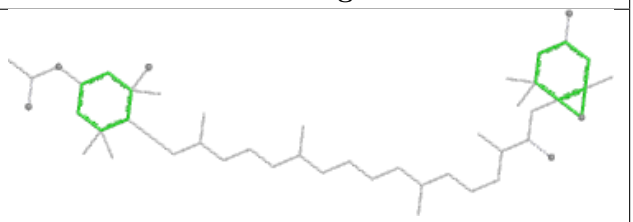
Bond lengths



Bond angles

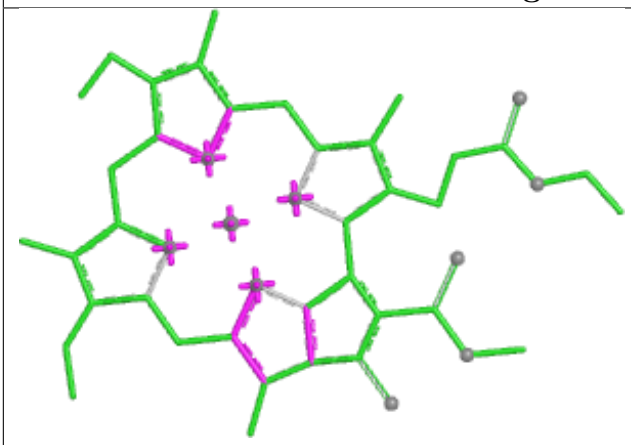


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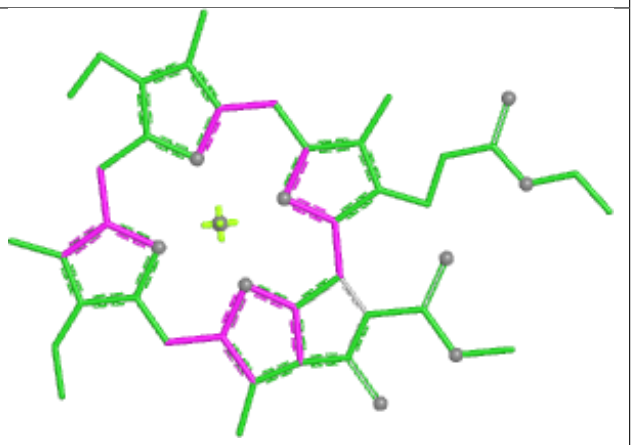


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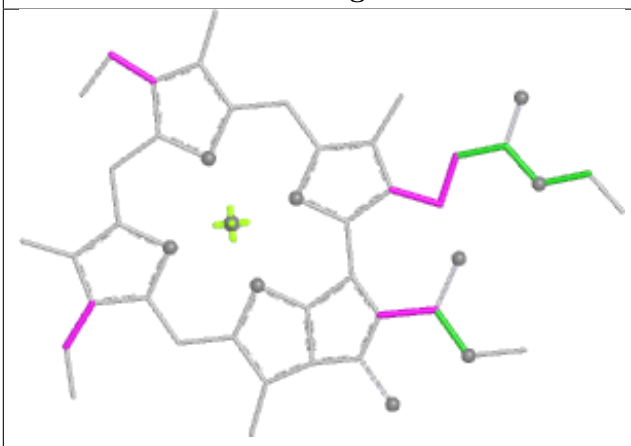
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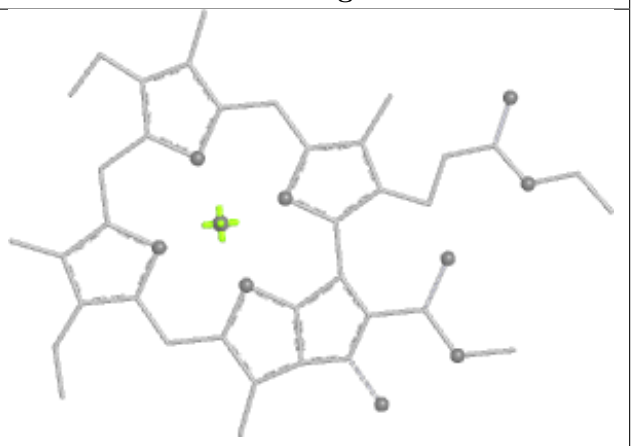
Bond lengths



Bond angles

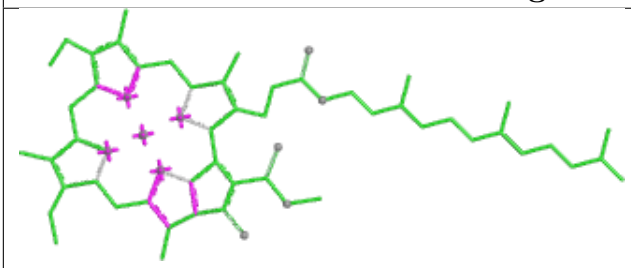


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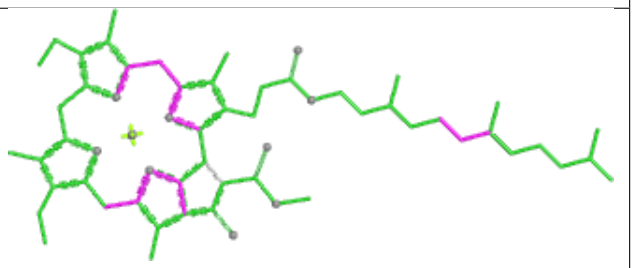


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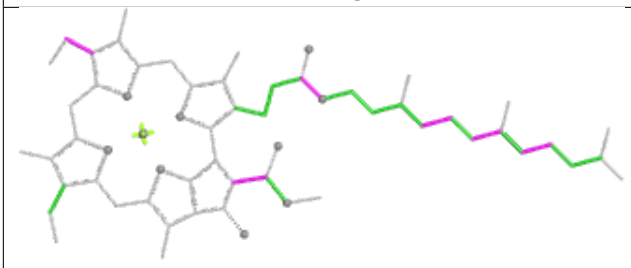
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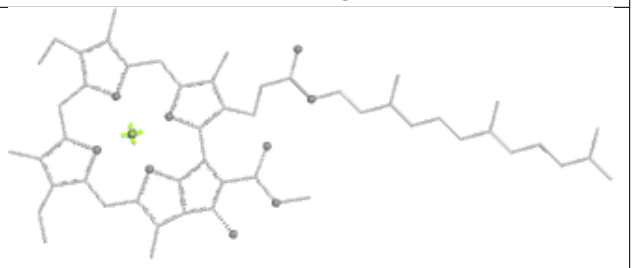
Bond lengths



Bond angles

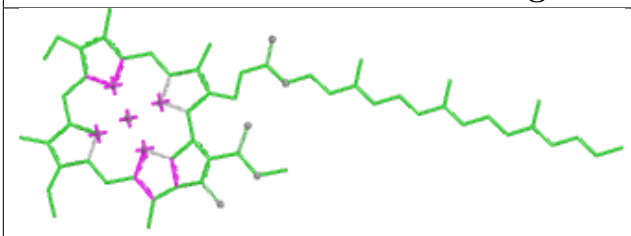


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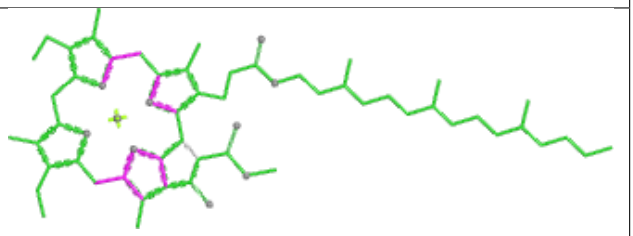


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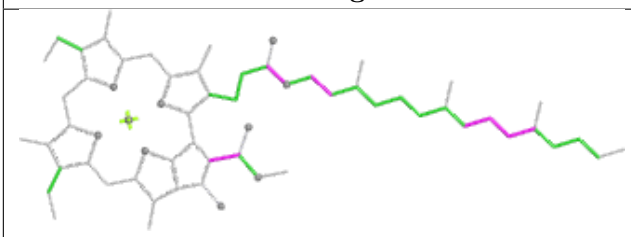
Ligand CLA o 311



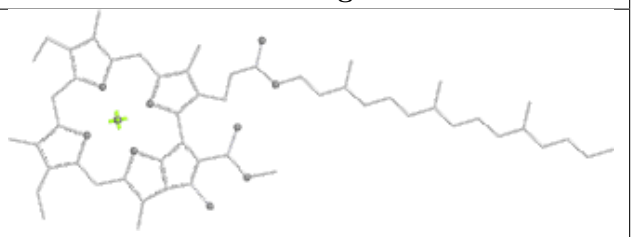
Bond lengths



Bond angles

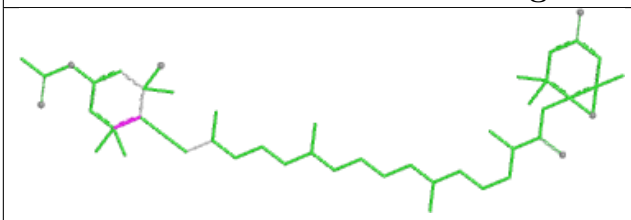


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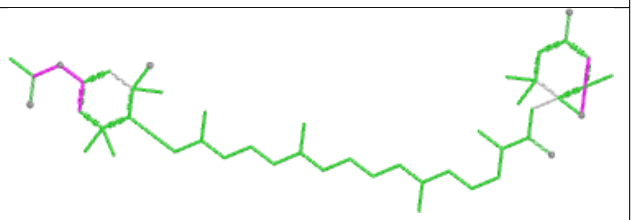


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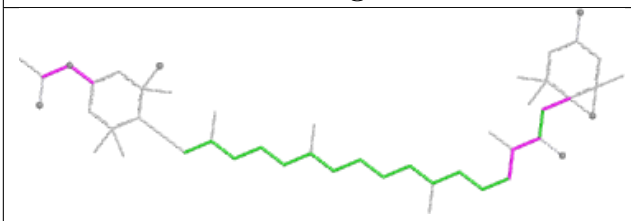
Ligand A86 R 315



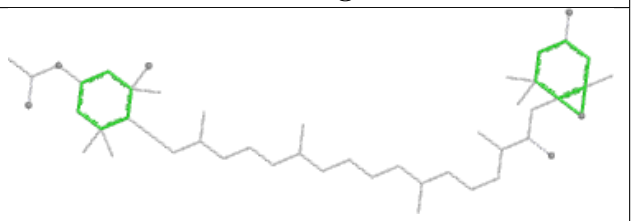
Bond lengths



Bond angles

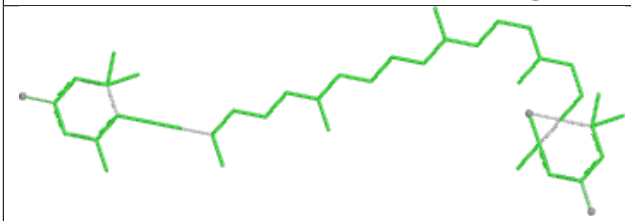


Torsions

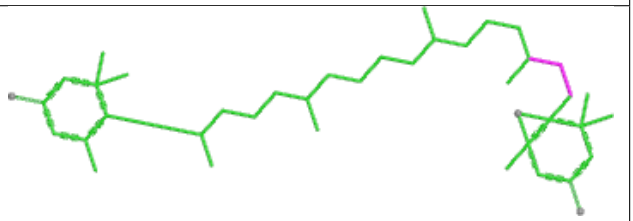


Rings

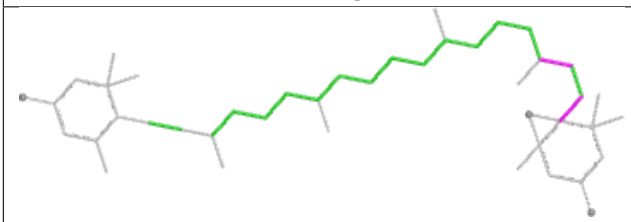
Ligand DD6 F 315



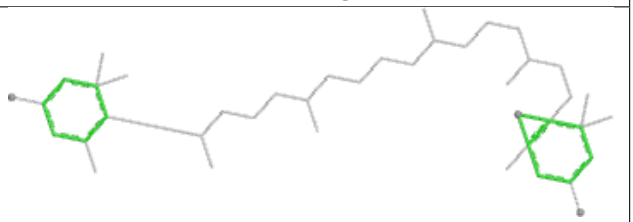
Bond lengths



Bond angles

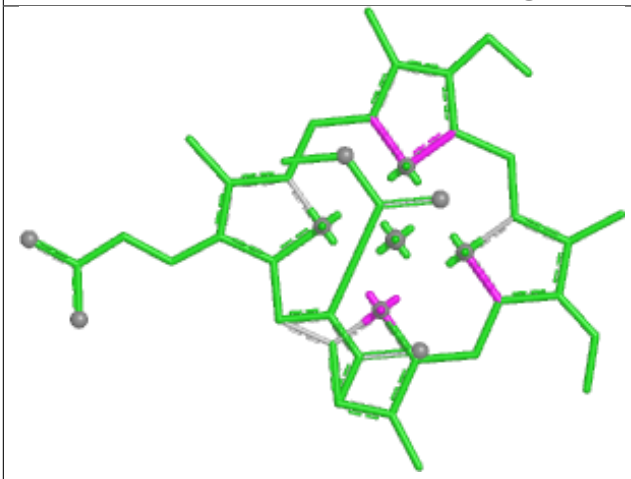


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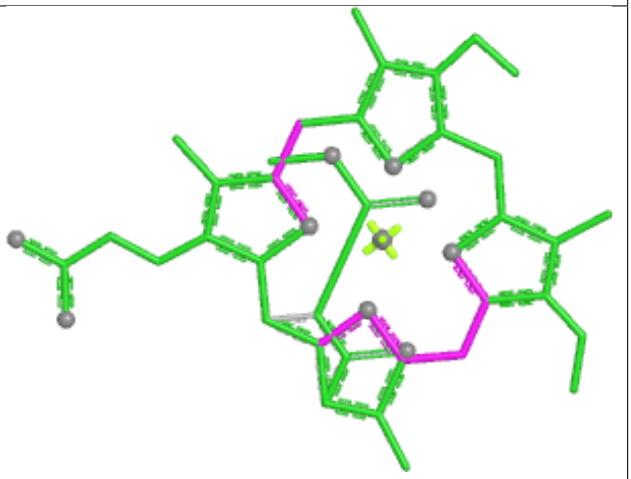


Rings

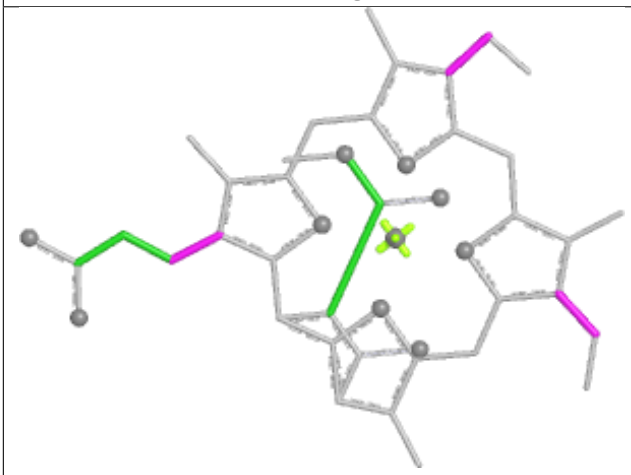
Ligand KC2 W 310



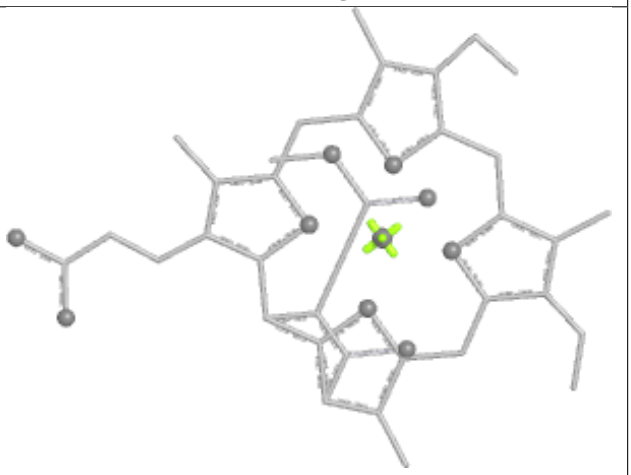
Bond lengths



Bond angles

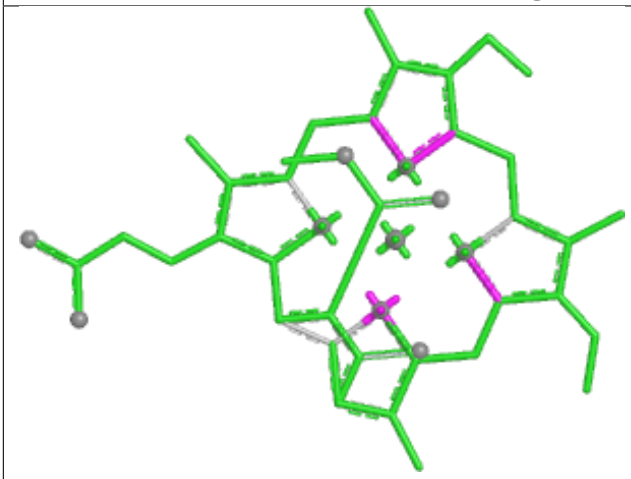


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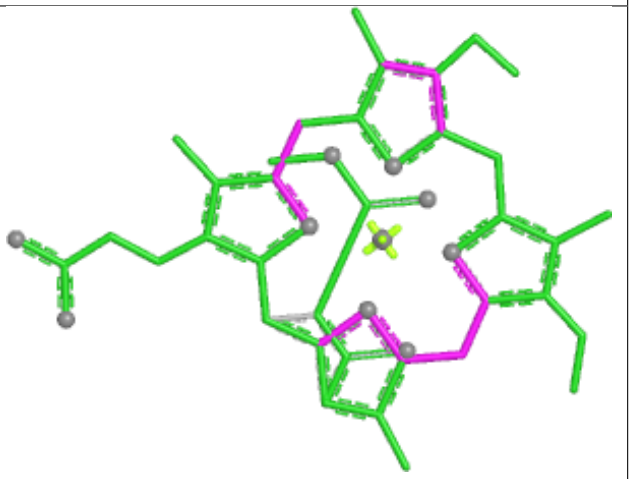


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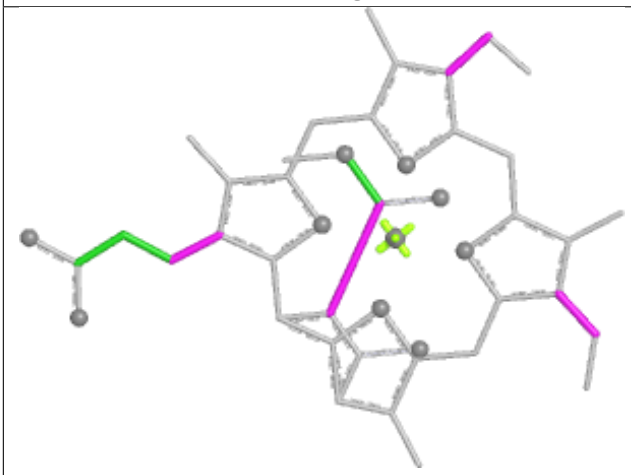
Ligand KC2 L 302



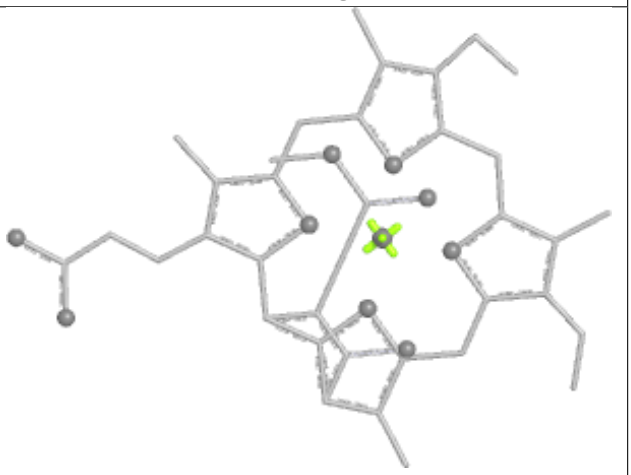
Bond lengths



Bond angles

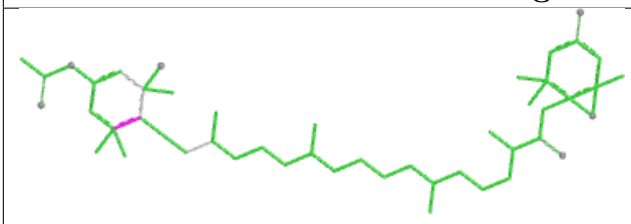


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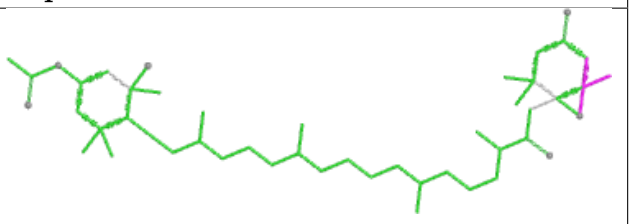


Rings

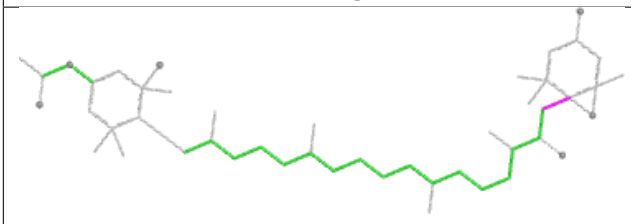
Ligand A86 p 317



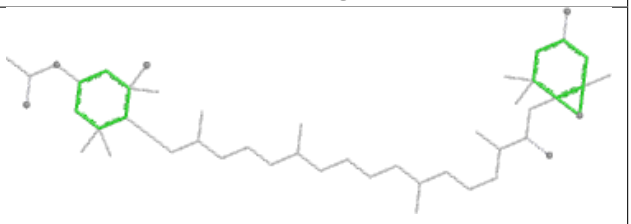
Bond lengths



Bond angles

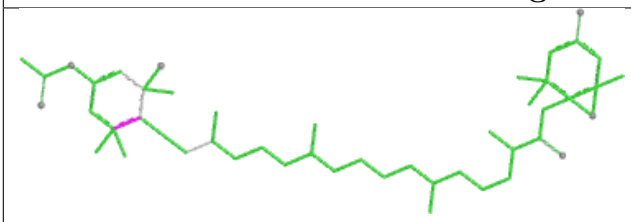


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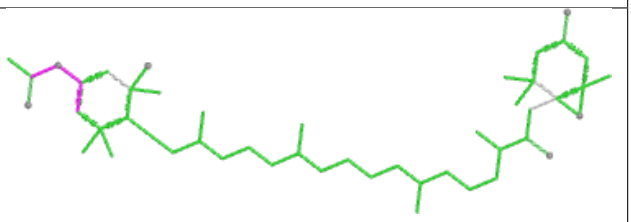


Rings

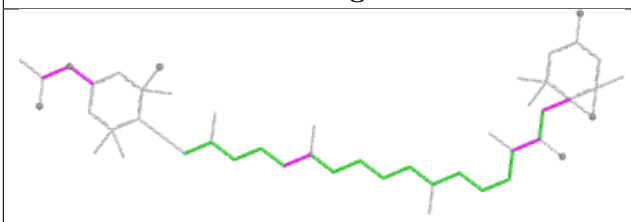
Ligand A86 Y 315



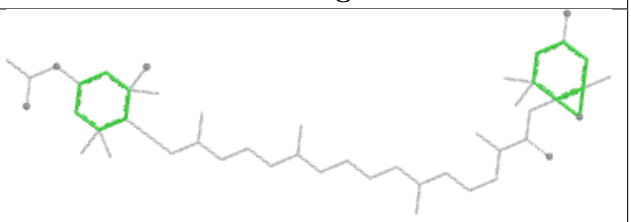
Bond lengths



Bond angles

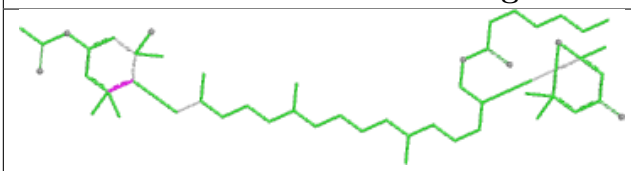


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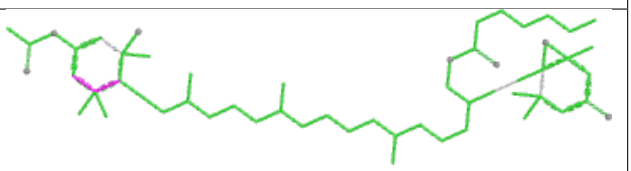


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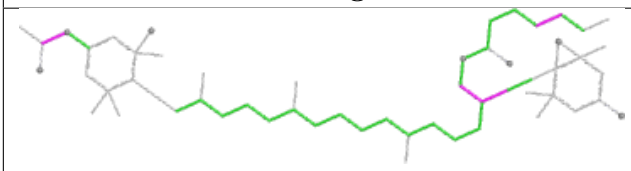
Ligand A1EB4 M 319



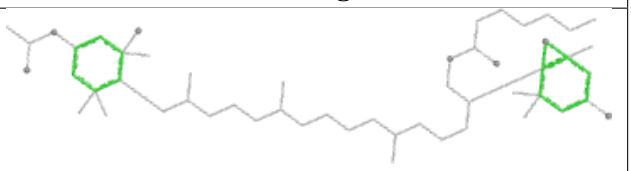
Bond lengths



Bond angles

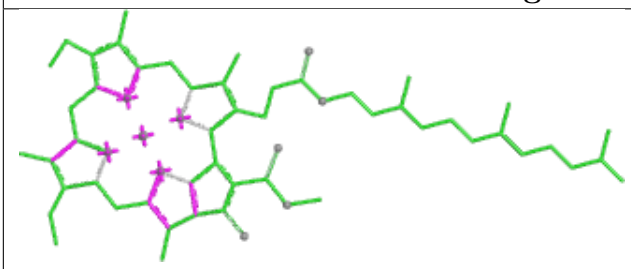


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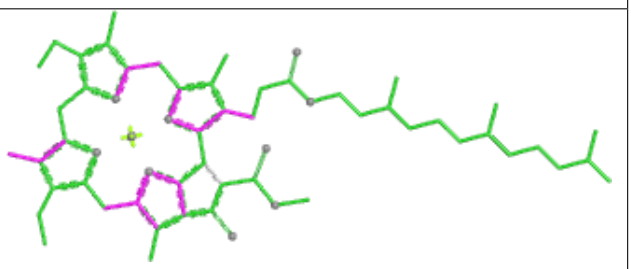


Rings

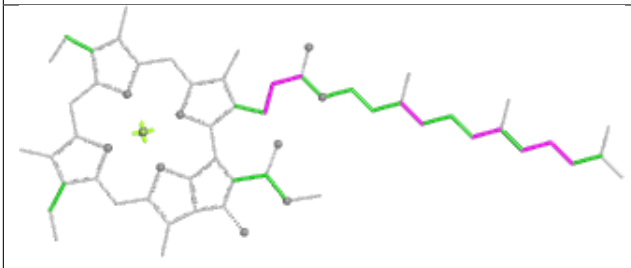
Ligand CLA O 306



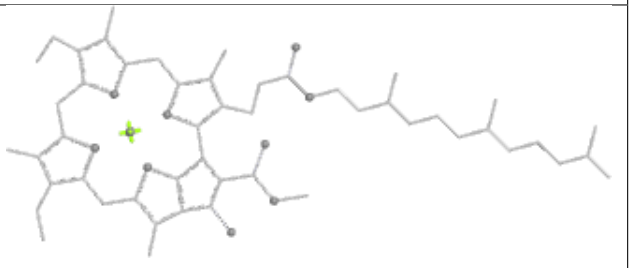
Bond lengths



Bond angles

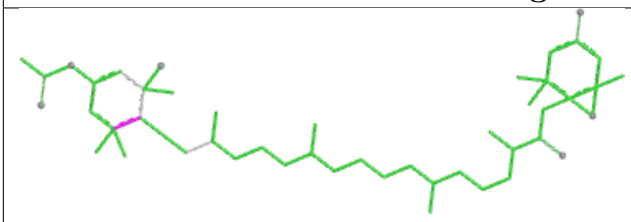


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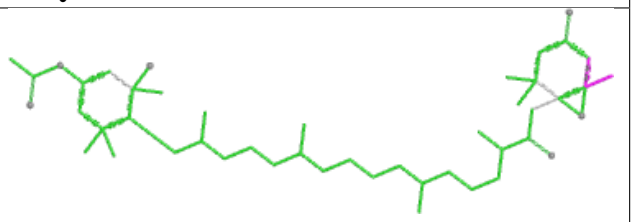


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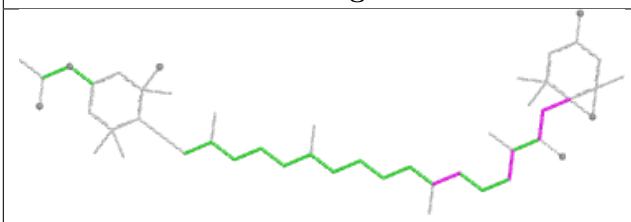
Ligand A86 Q 210



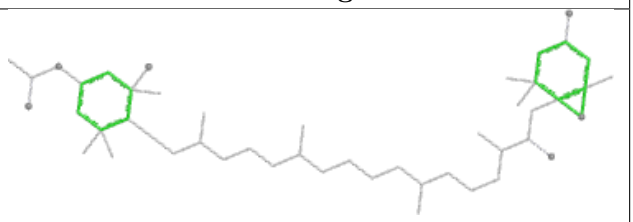
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Bond angles

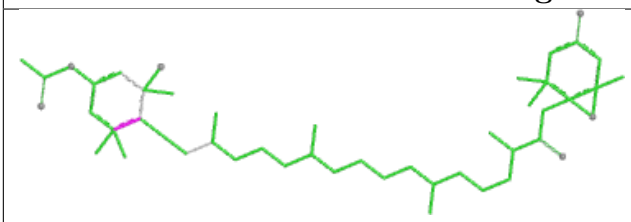


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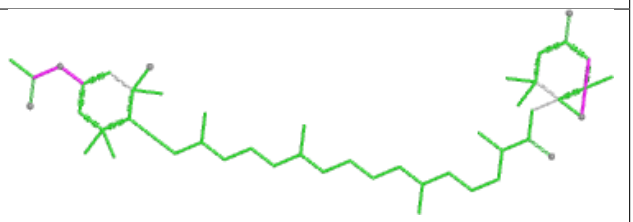


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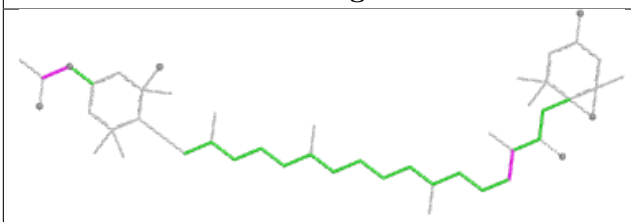
Ligand A86 z 318



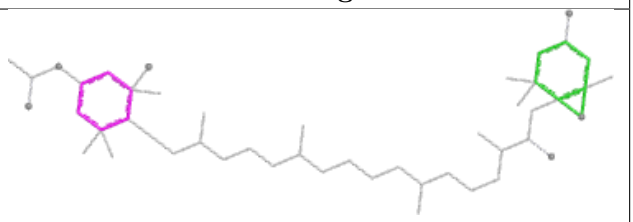
Bond lengths



Bond angles

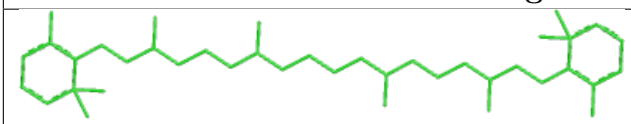


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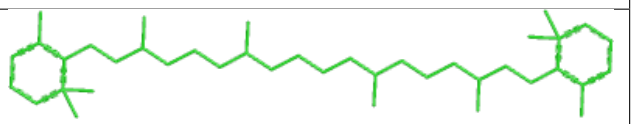


Rings

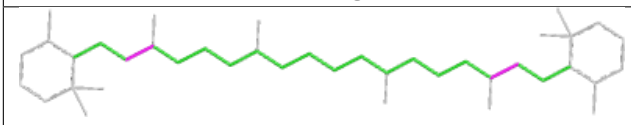
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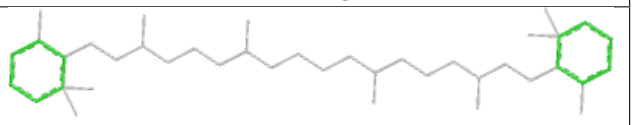
Bond lengths



Bond angles

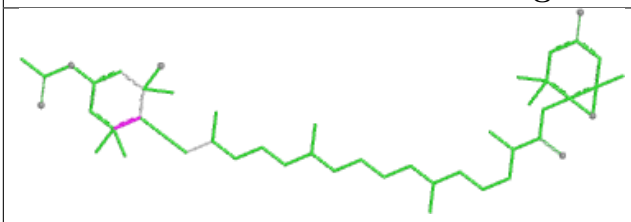


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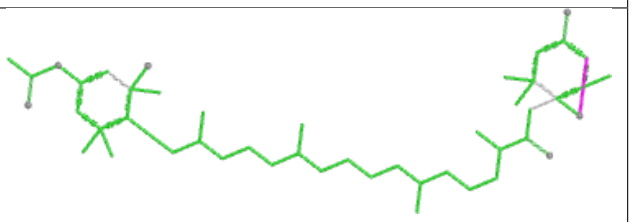


Rings

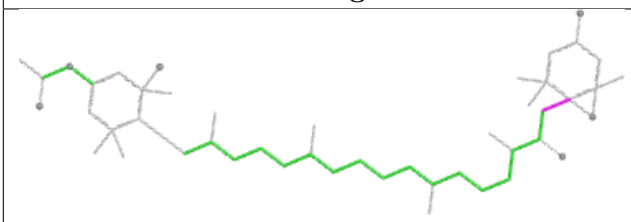
Ligand A86 v 317



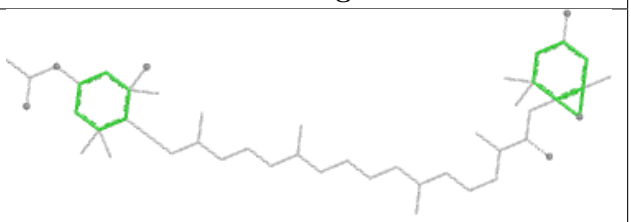
Bond lengths



Bond angles

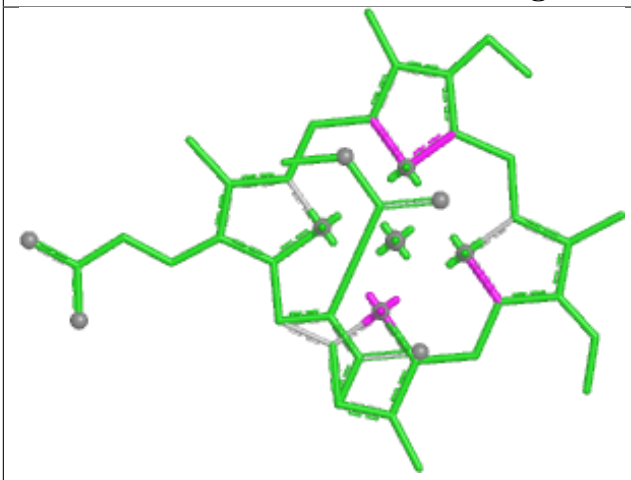


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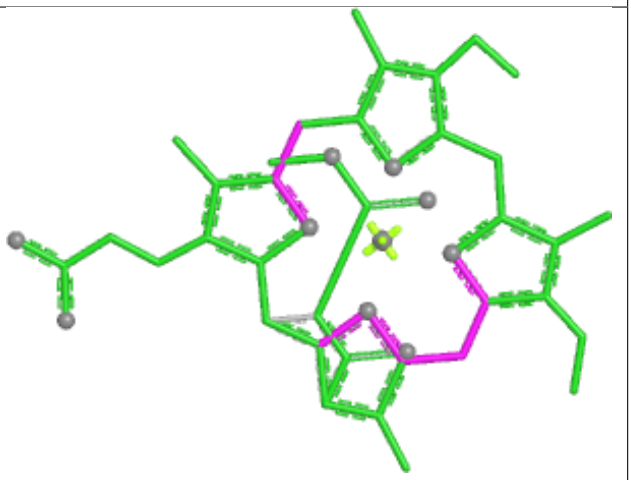


Rings

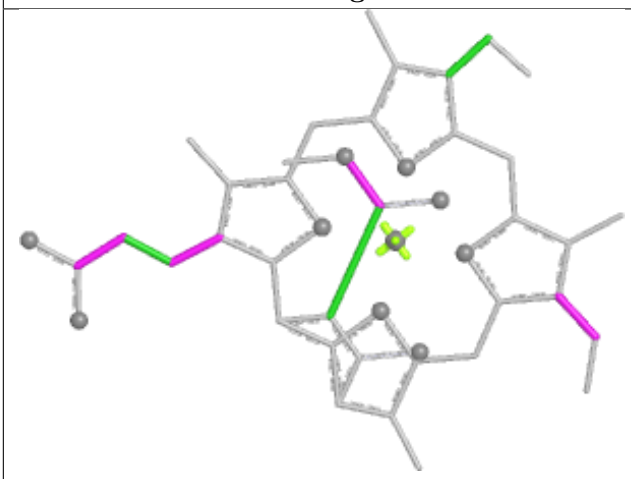
Ligand KC2 x 303



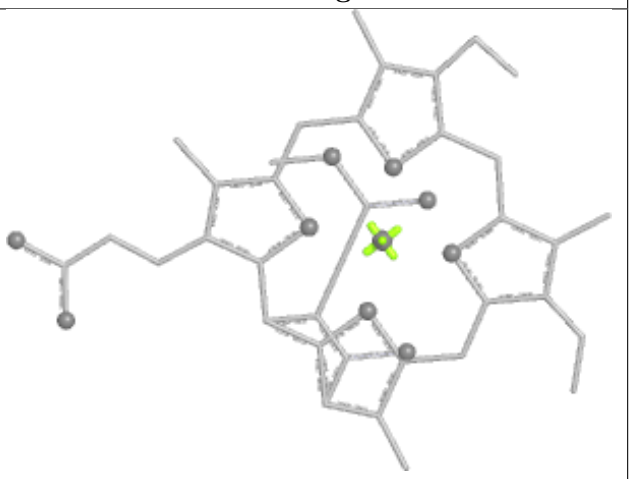
Bond lengths



Bond angles

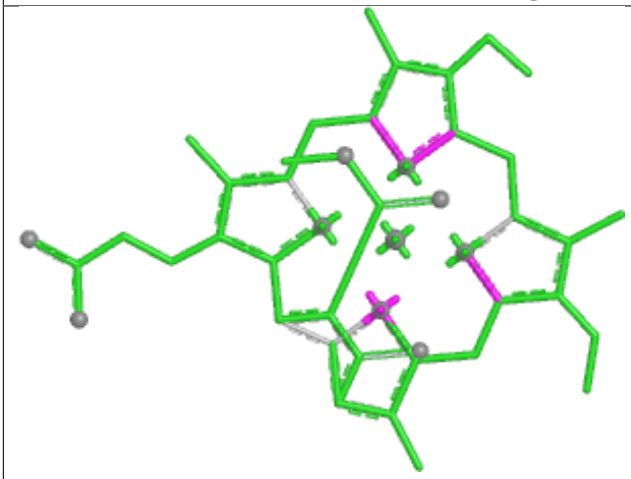


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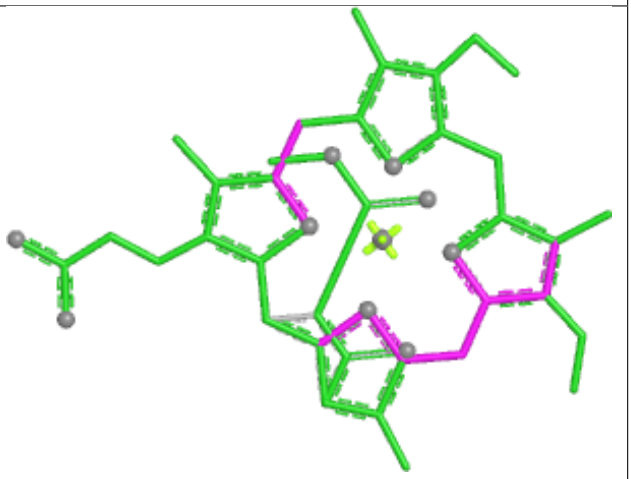


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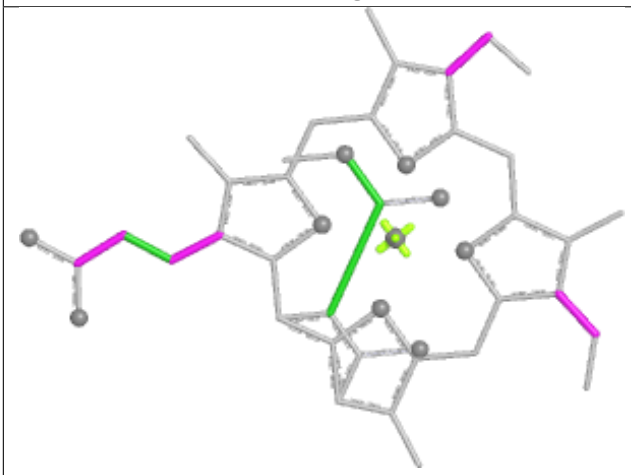
Ligand KC2 K 309



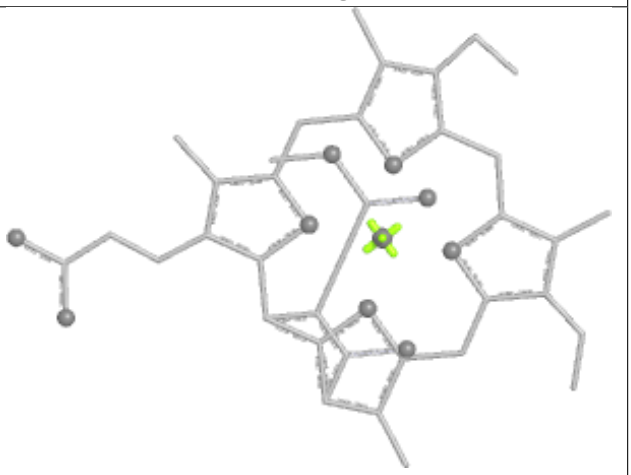
Bond lengths



Bond angles

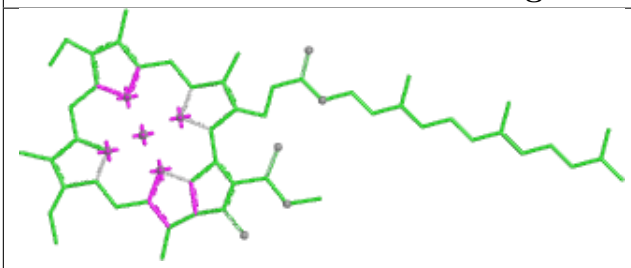


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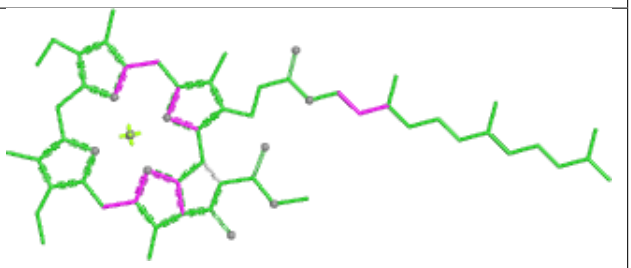


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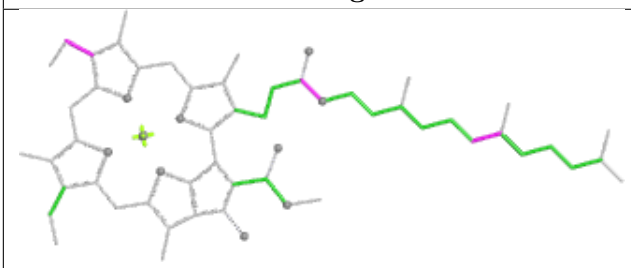
Ligand CLA E 310



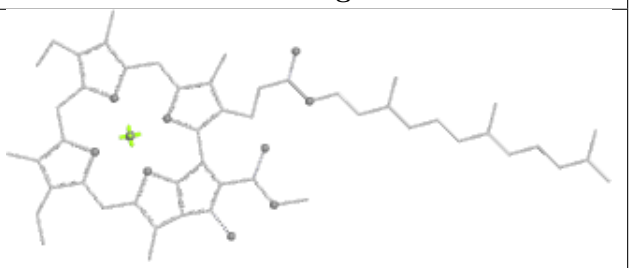
Bond lengths



Bond angles

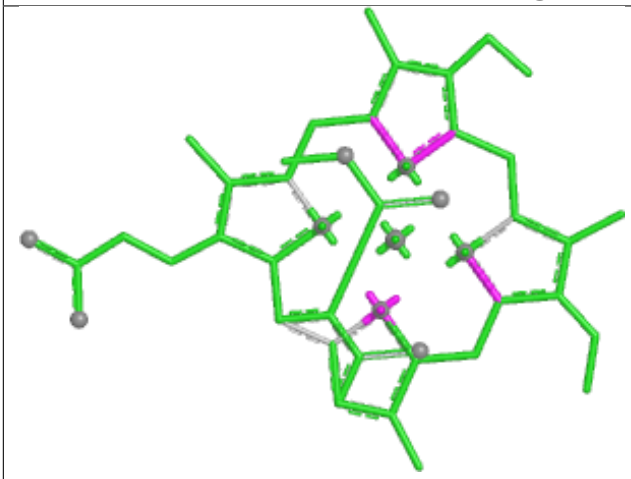


Torsions

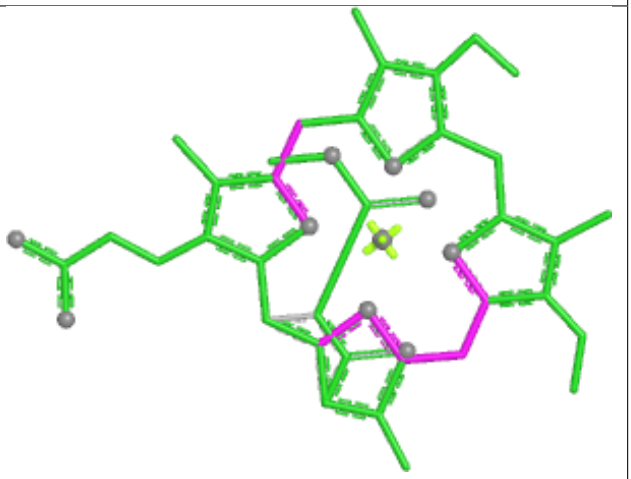


Rings

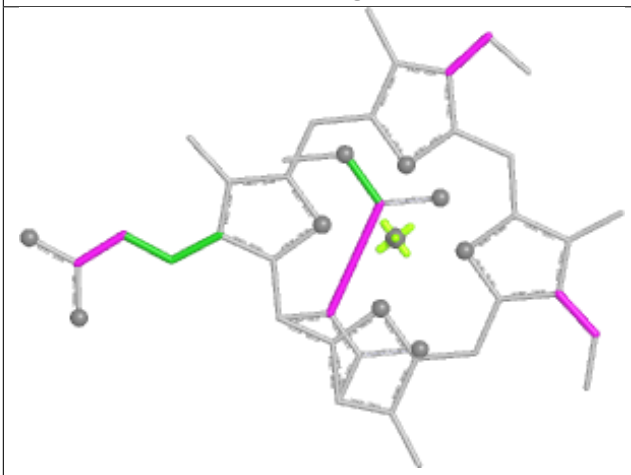
Ligand KC2 z 310



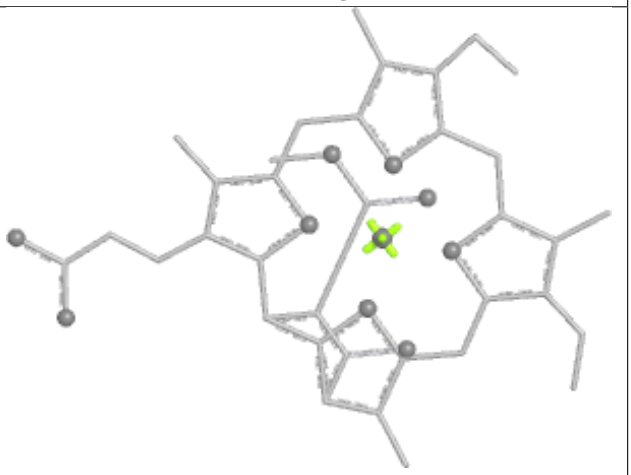
Bond lengths



Bond angles

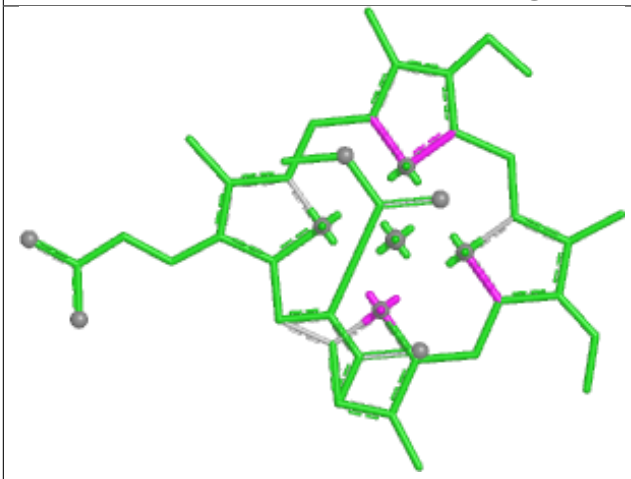


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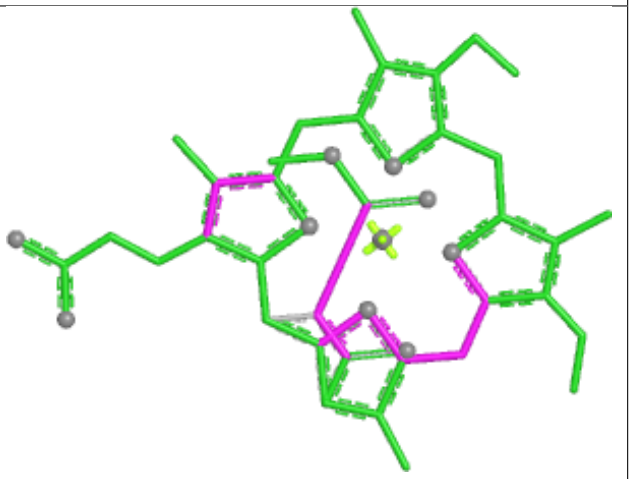


Rings

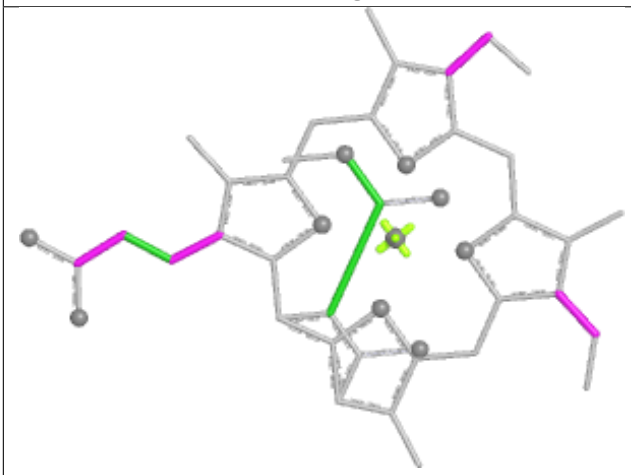
Ligand KC2 R 309



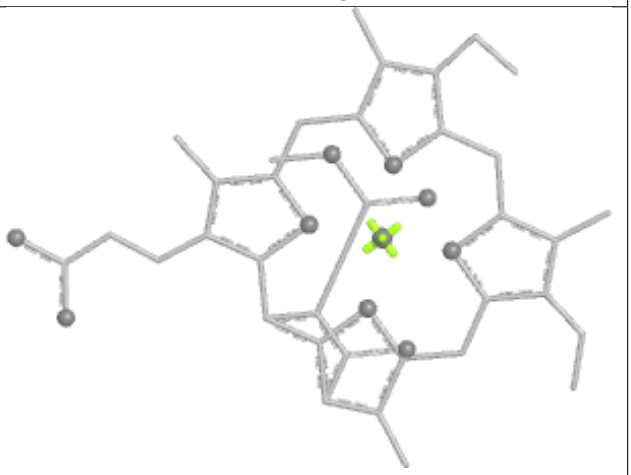
Bond lengths



Bond angles

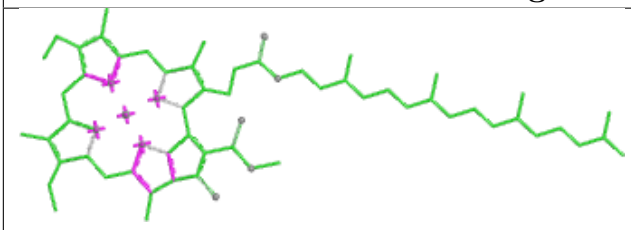


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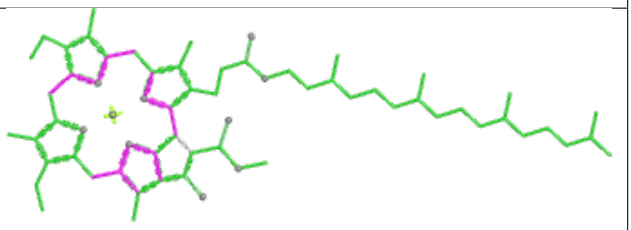


Rings

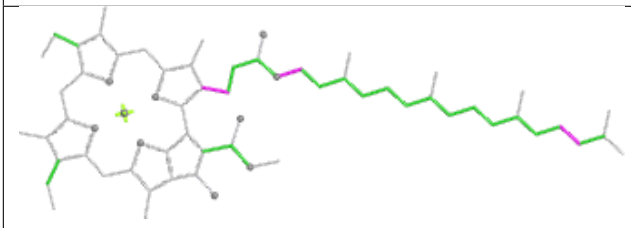
Ligand CLA a 850



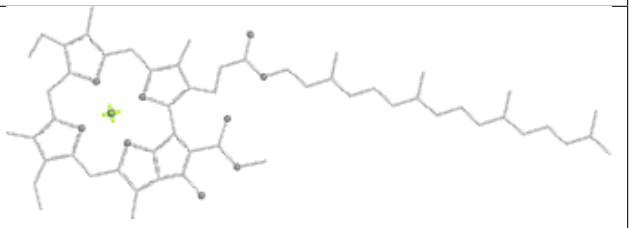
Bond lengths



Bond angles

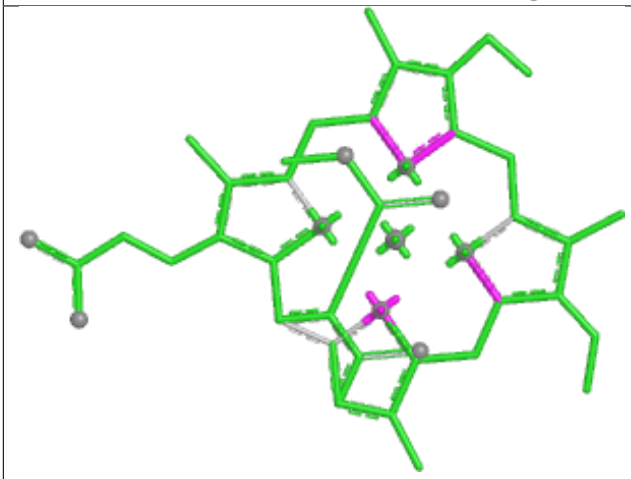


Torsions

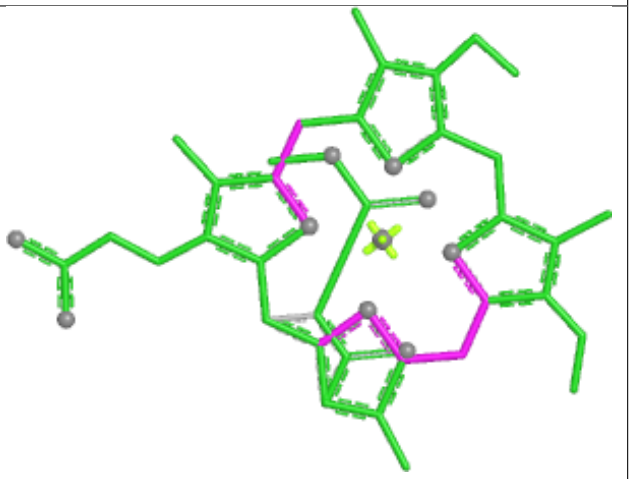


Rings

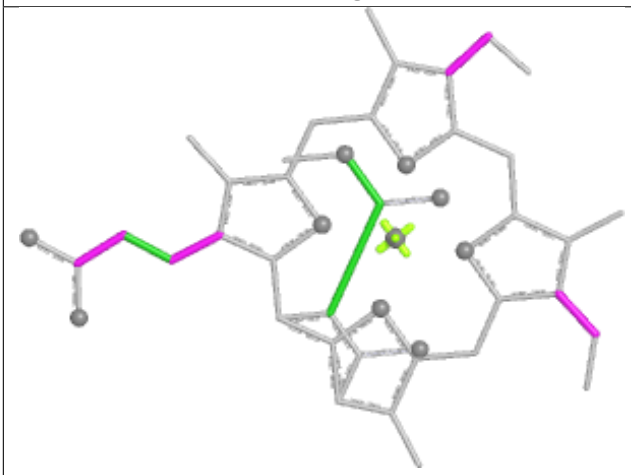
Ligand KC2 N 312



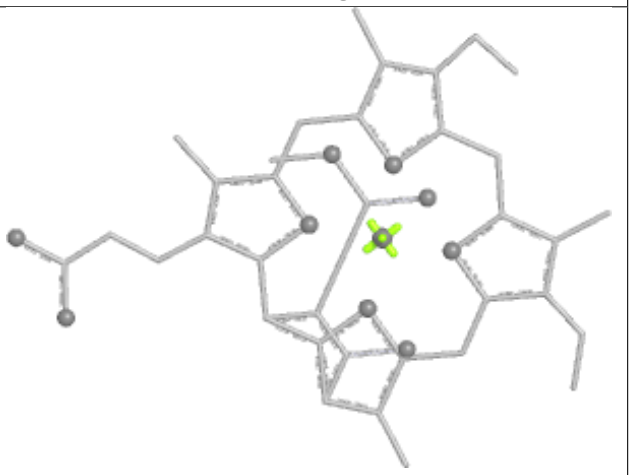
Bond lengths



Bond angles

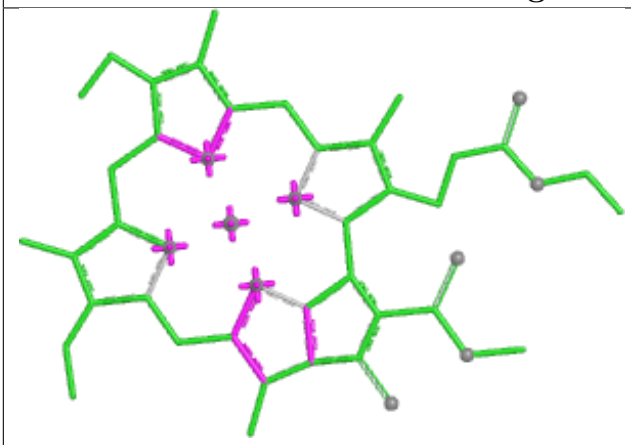


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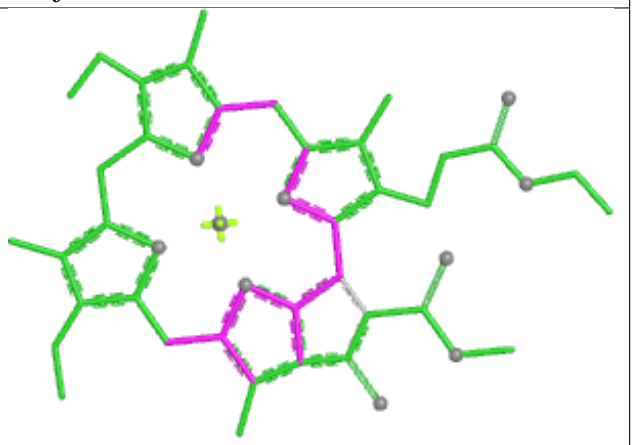


Rings

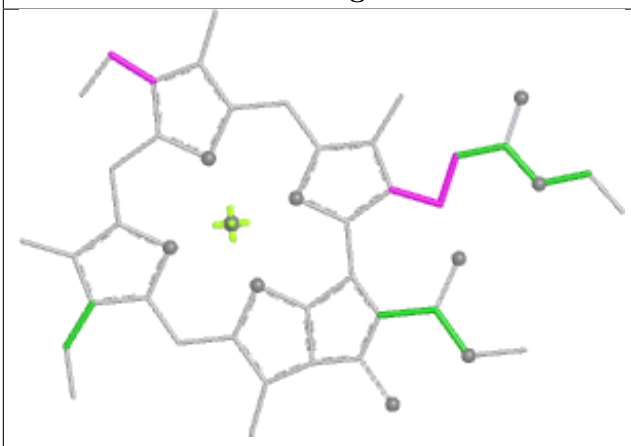
Ligand CLA y 303



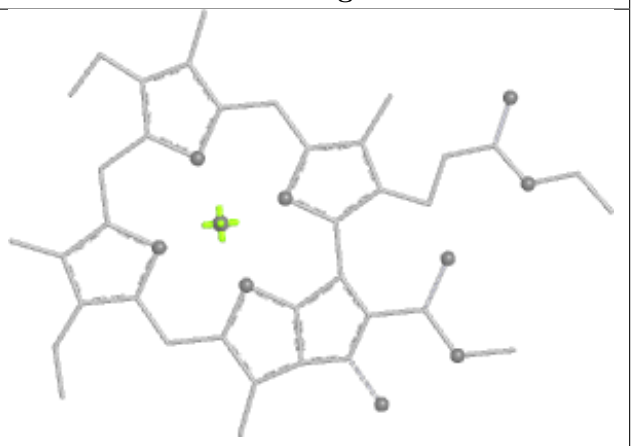
Bond lengths



Bond angles

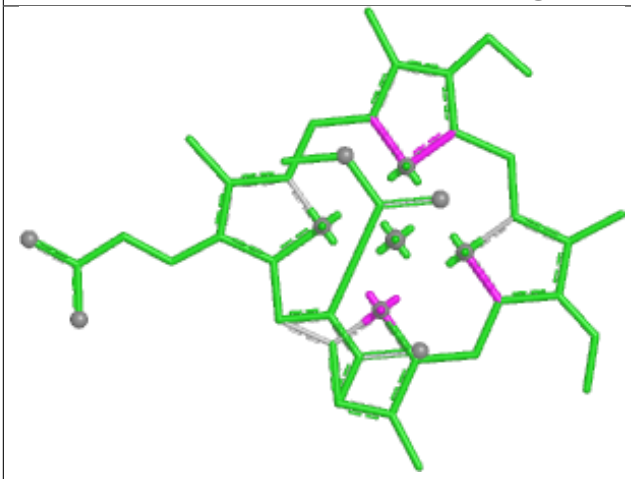


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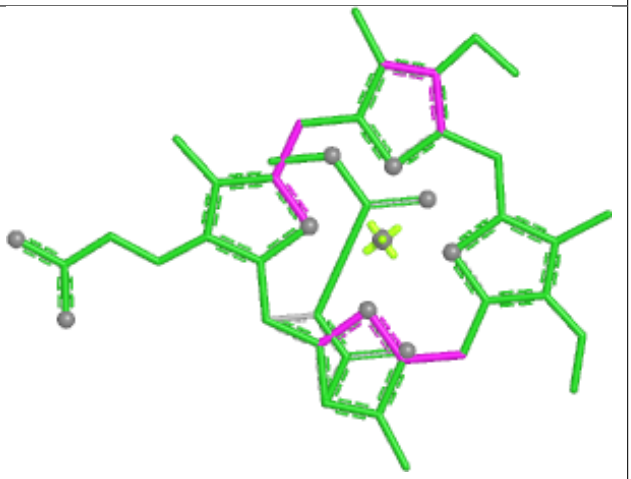


Rings

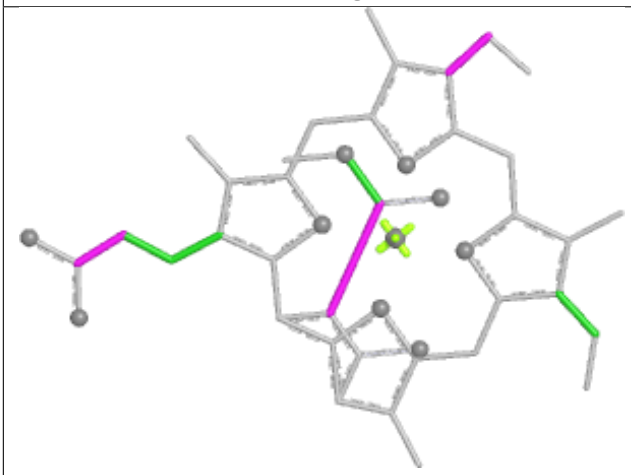
Ligand KC2 v 303



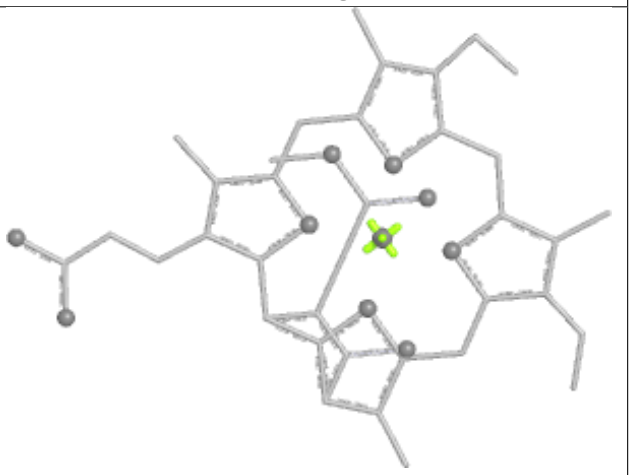
Bond lengths



Bond angles

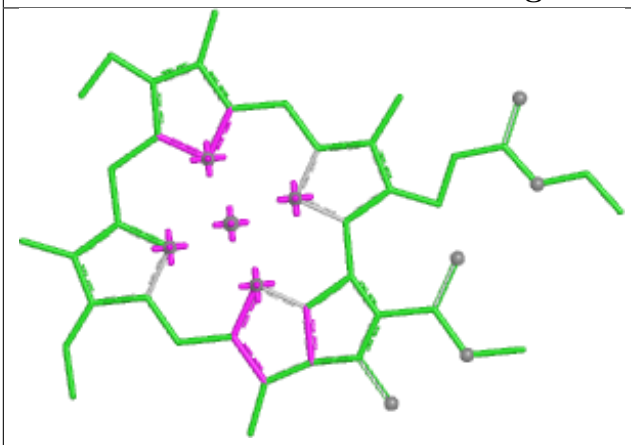


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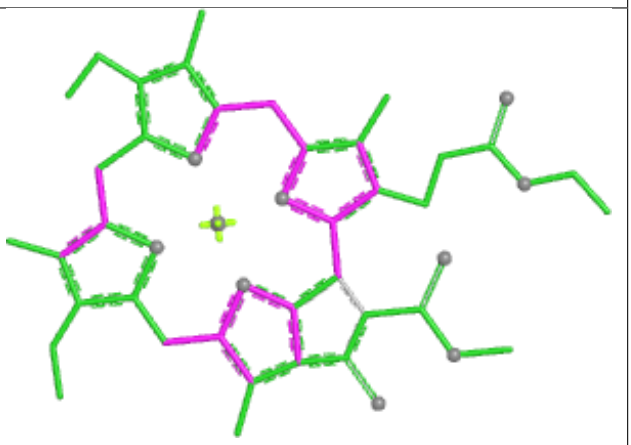


Rings

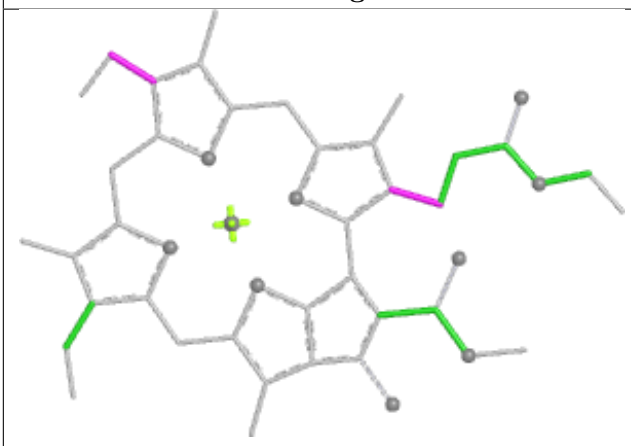
Ligand CLA P 311



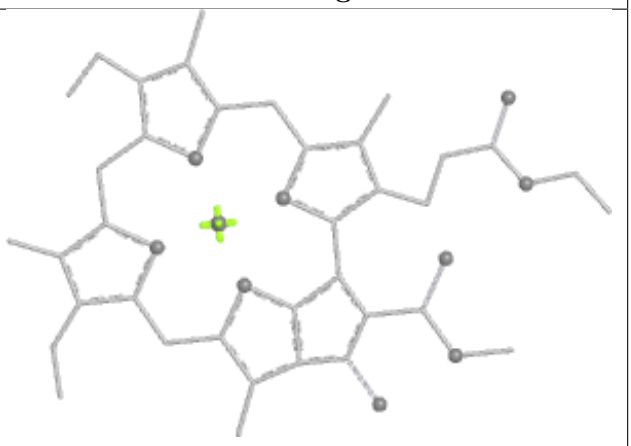
Bond lengths



Bond angles

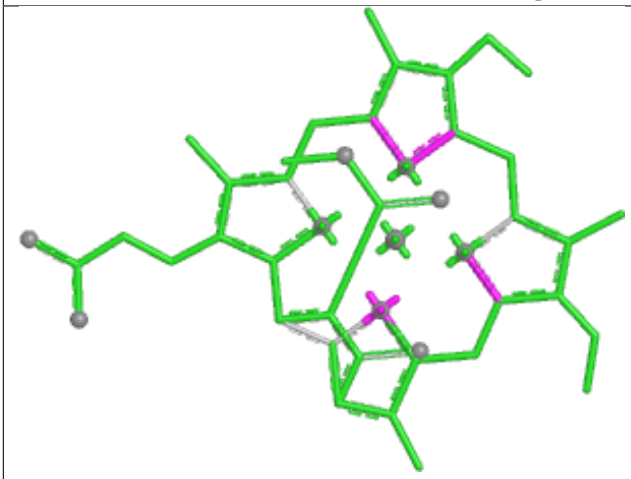


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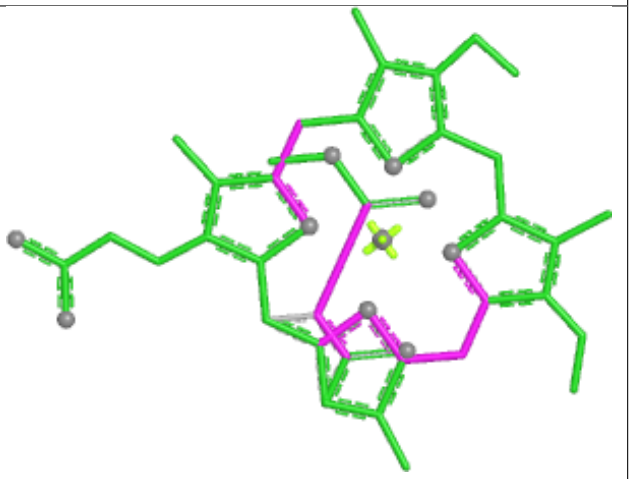


Rings

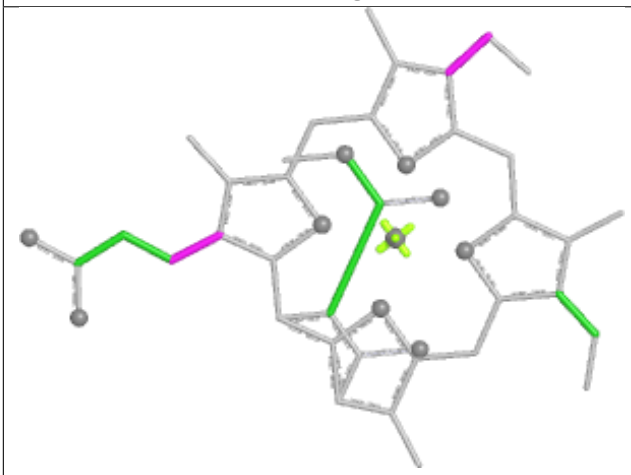
Ligand KC2 x 309



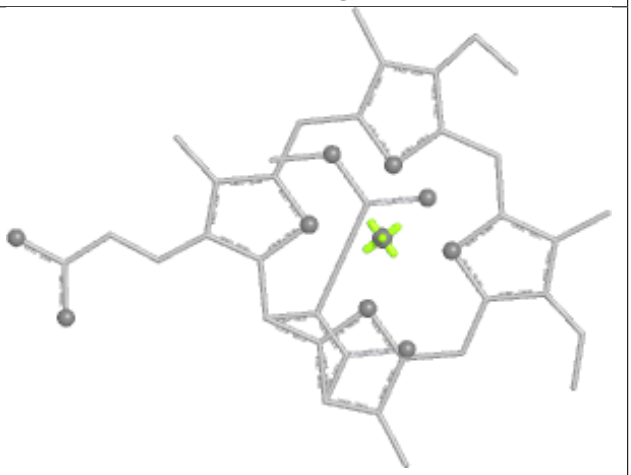
Bond lengths



Bond angles

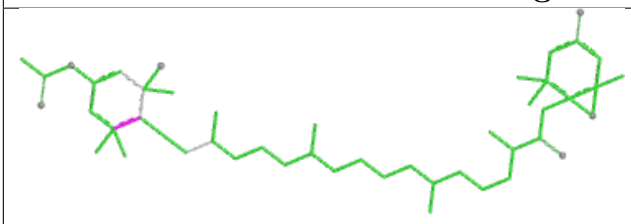


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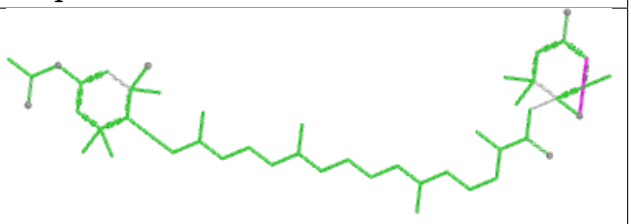


Rings

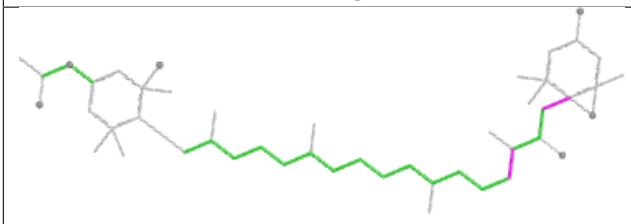
Ligand A86 q 316



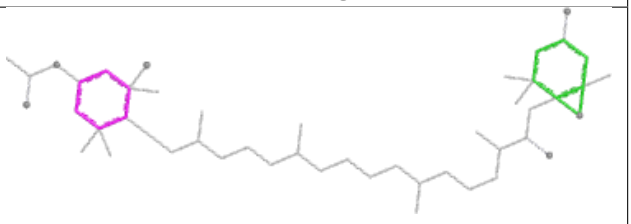
Bond lengths



Bond angles

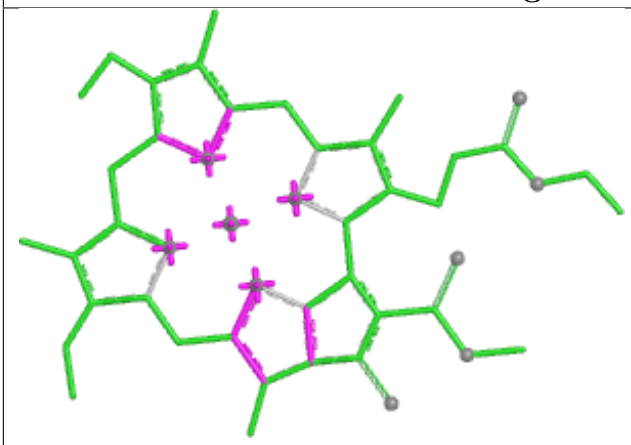


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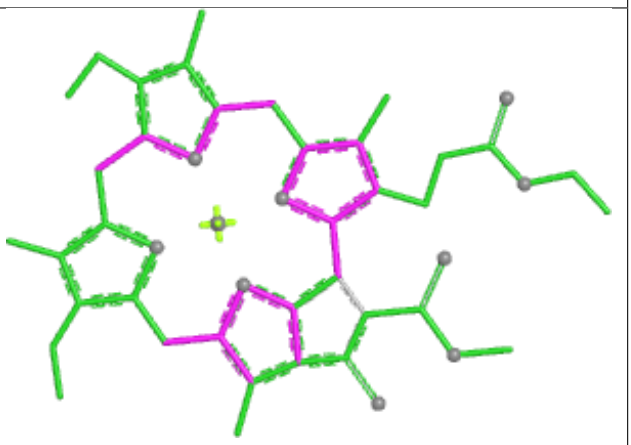


Rings

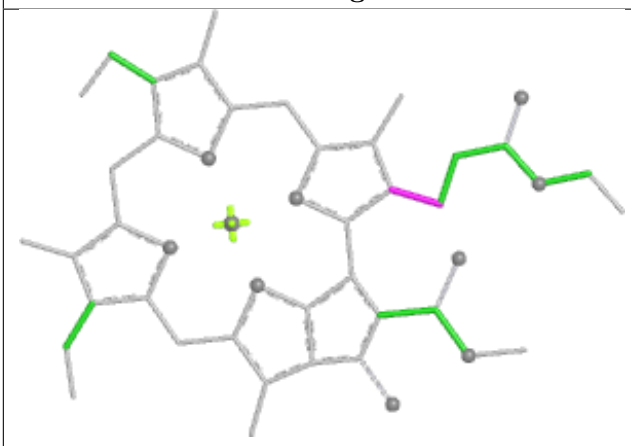
Ligand CLA Y 312



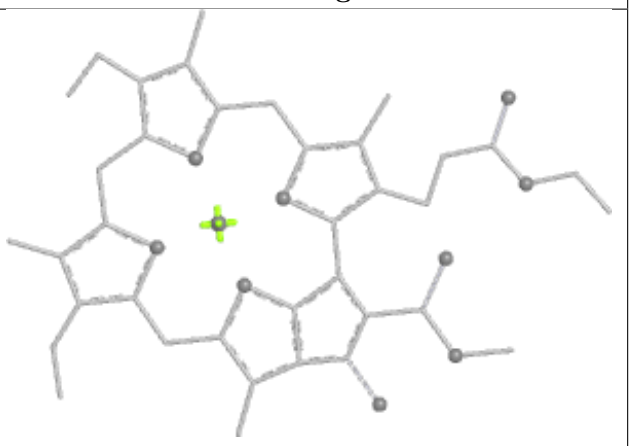
Bond lengths



Bond angles

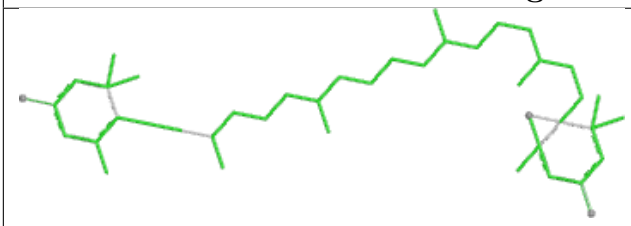


Torsions



Rings

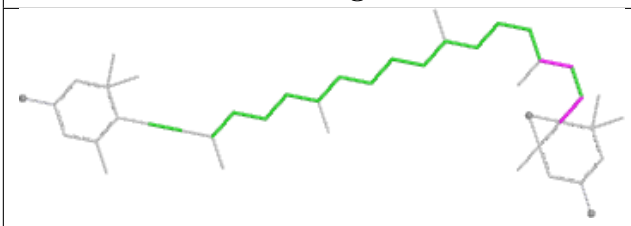
Ligand DD6 E 318



Bond lengths



Bond angles

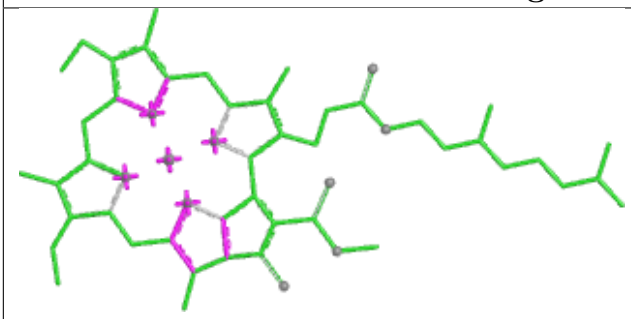


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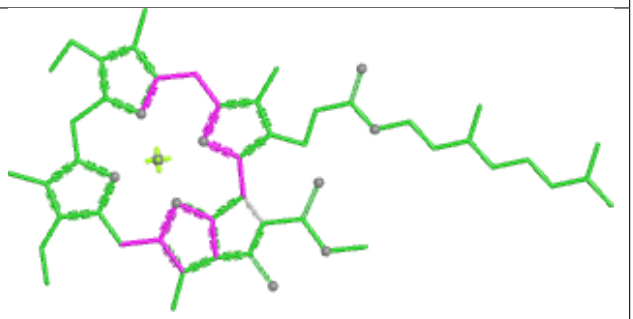


Rings

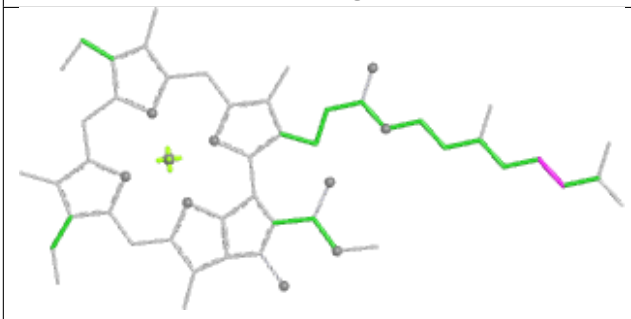
Ligand CLA b 828



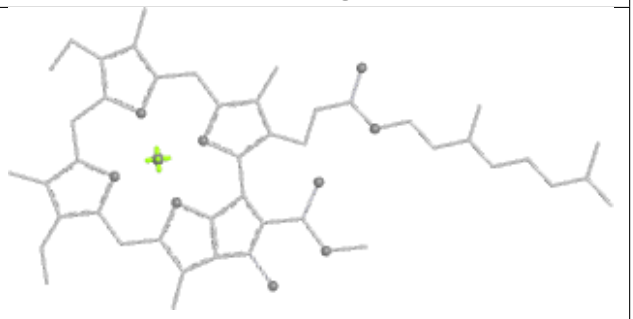
Bond lengths



Bond angles

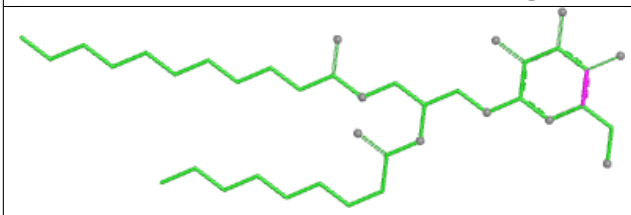


Torsions

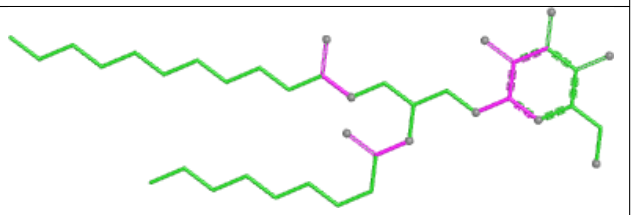


Rings

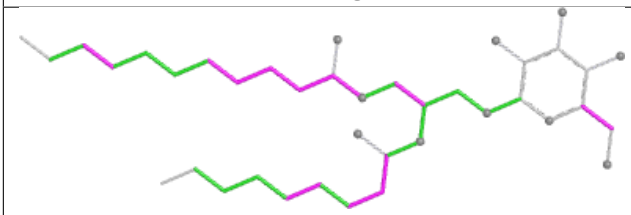
Ligand LMG x 301



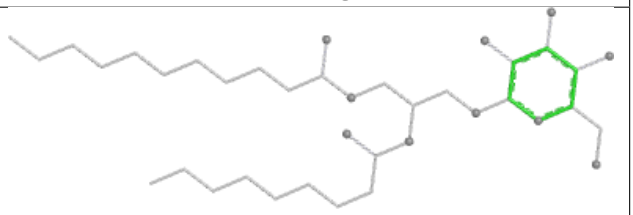
Bond lengths



Bond angles

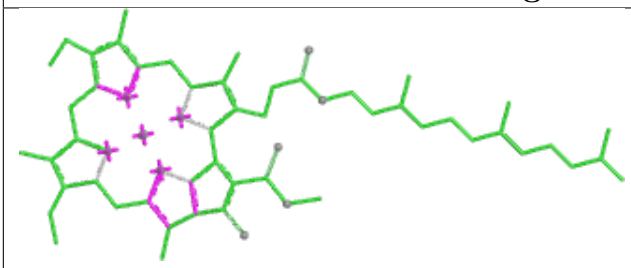


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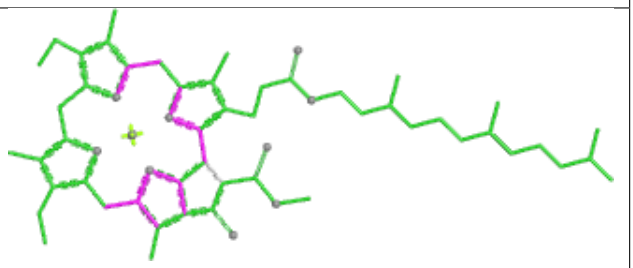


Rings

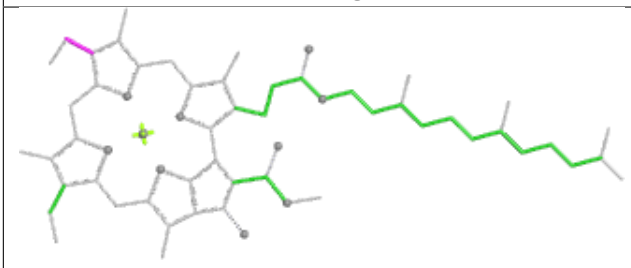
Ligand CLA N 306



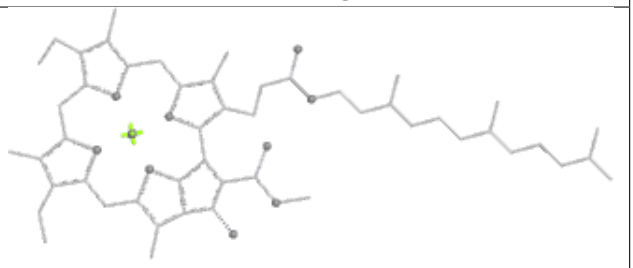
Bond lengths



Bond angles

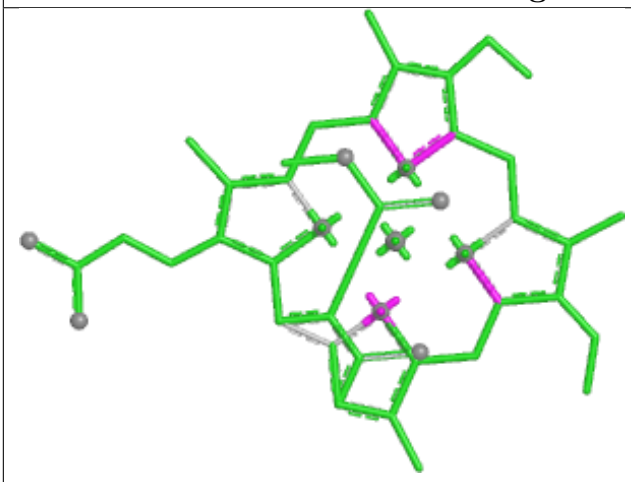


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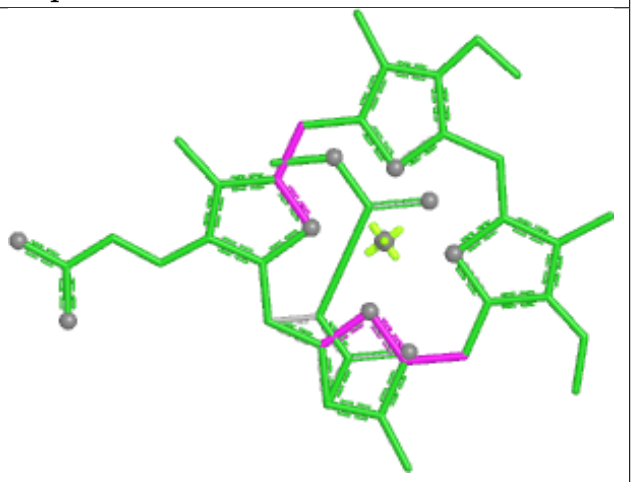


Rings

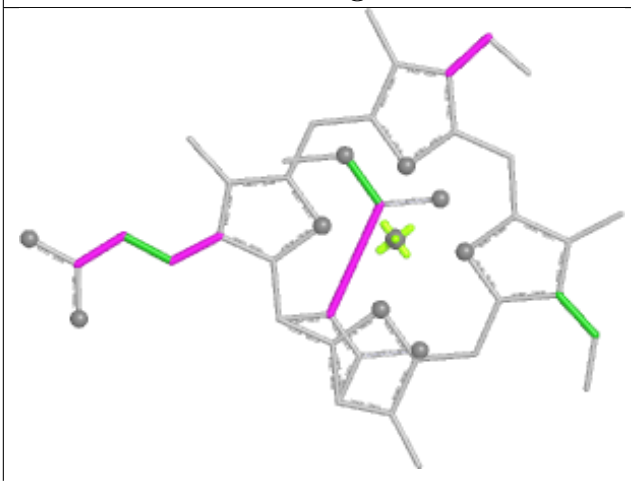
Ligand KC2 p 304



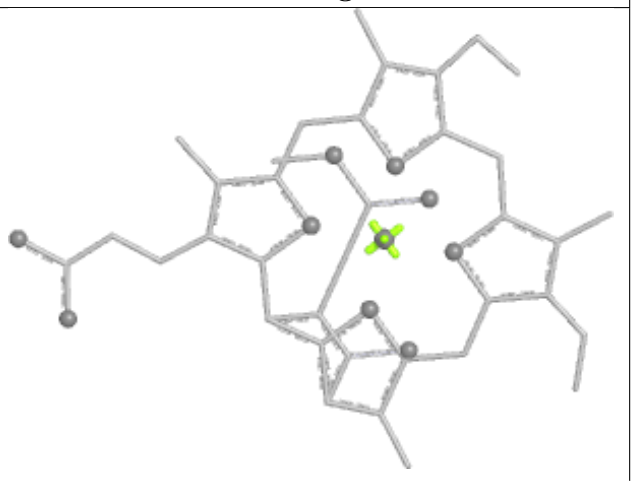
Bond lengths



Bond angles

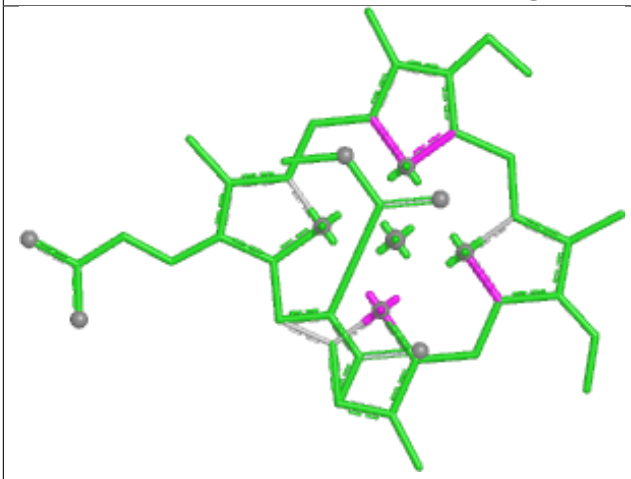


Torsions

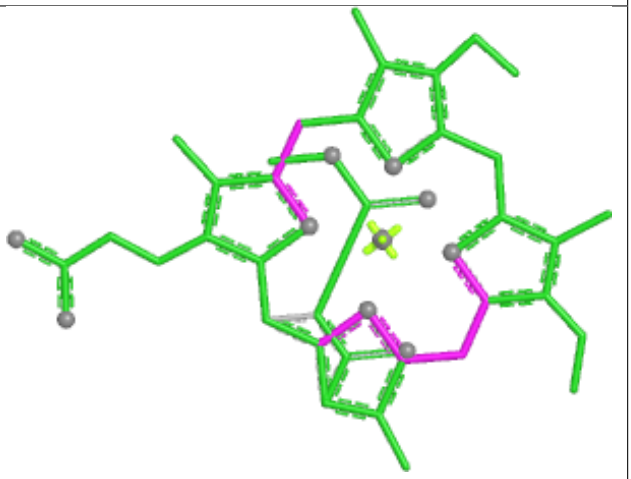


Rings

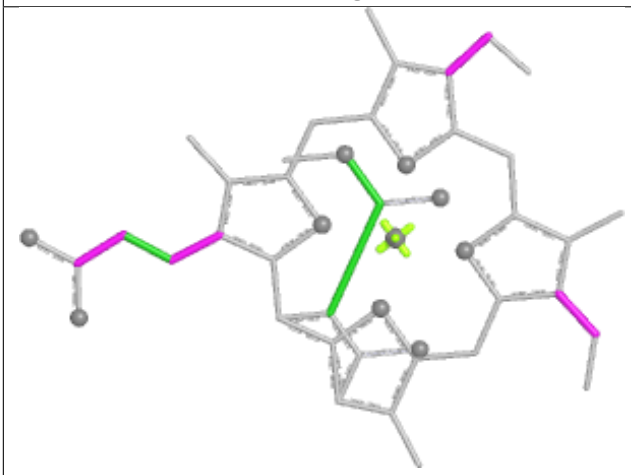
Ligand KC2 N 308



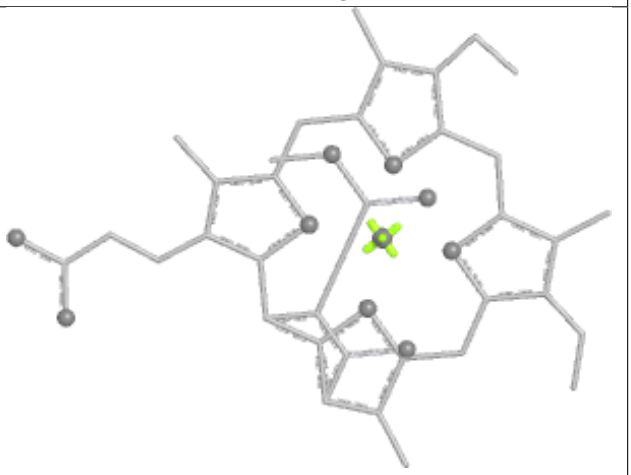
Bond lengths



Bond angles

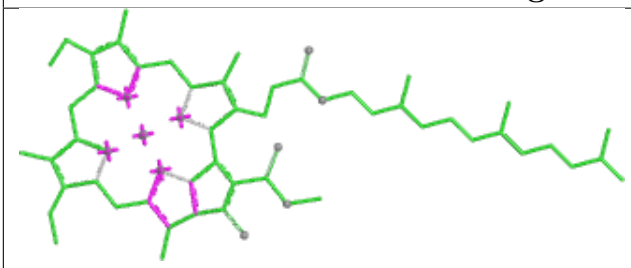


Torsions

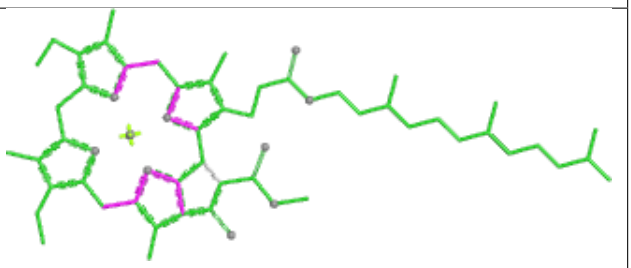


Rings

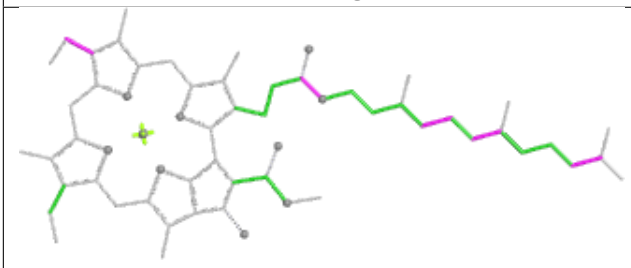
Ligand CLA v 312



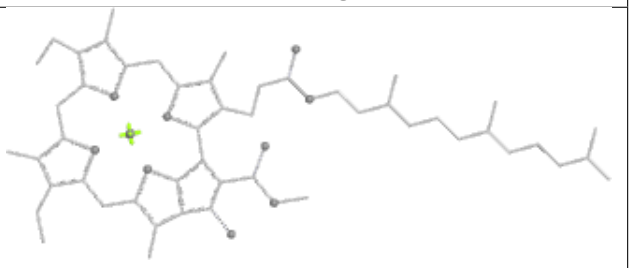
Bond lengths



Bond angles

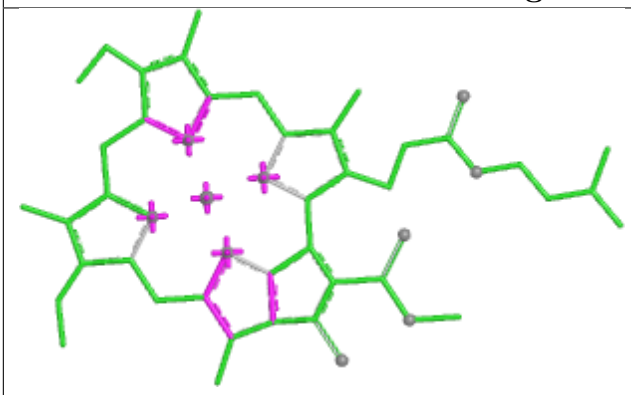


Torsions

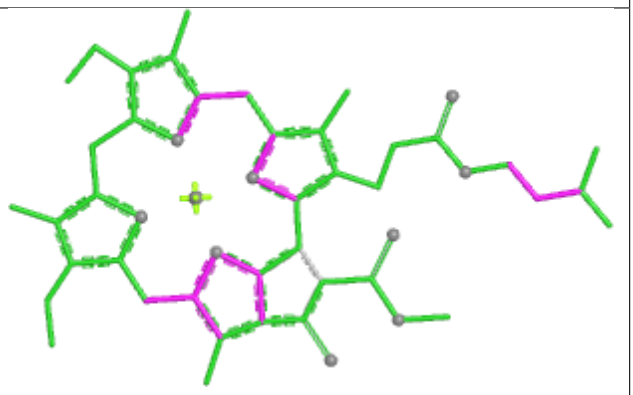


Rings

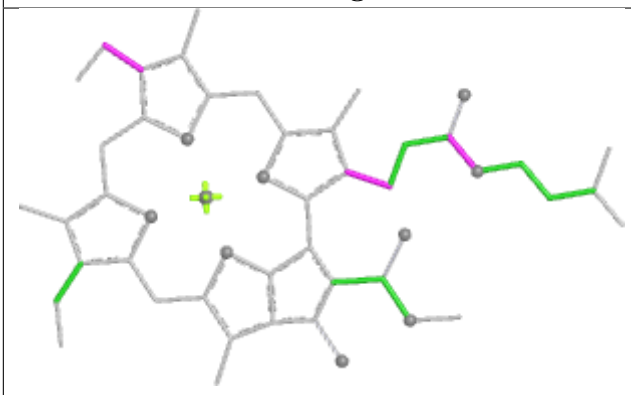
Ligand CLA E 311



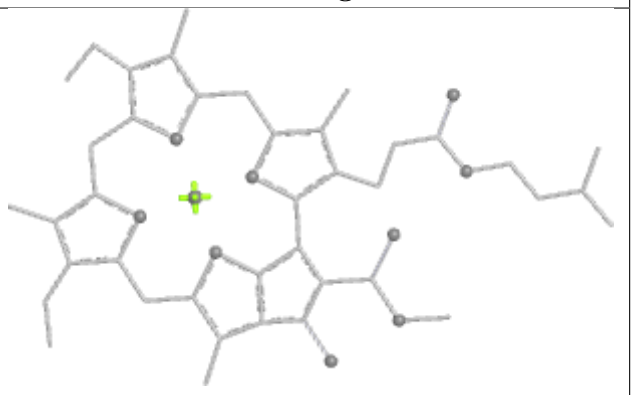
Bond lengths



Bond angles

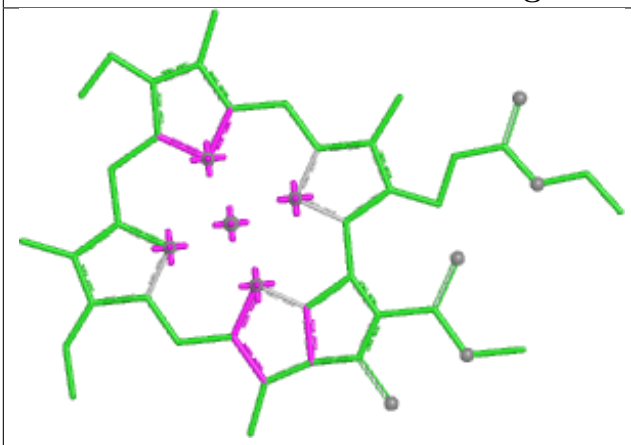


Torsions

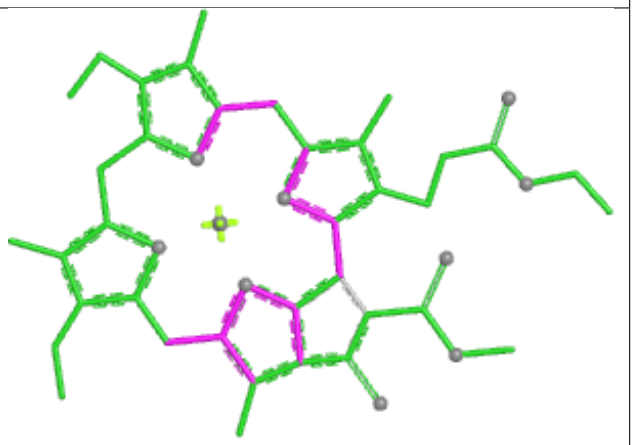


Rings

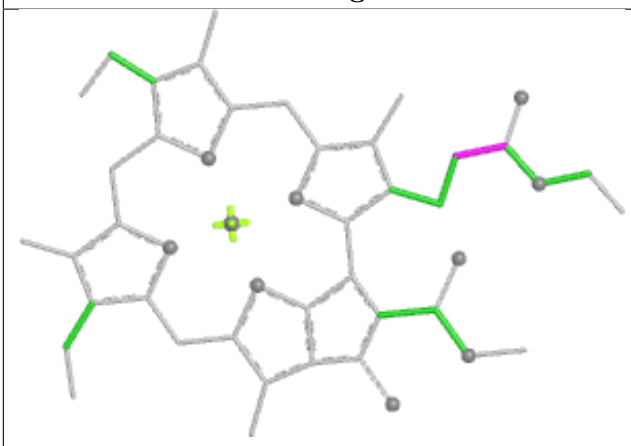
Ligand CLA O 305



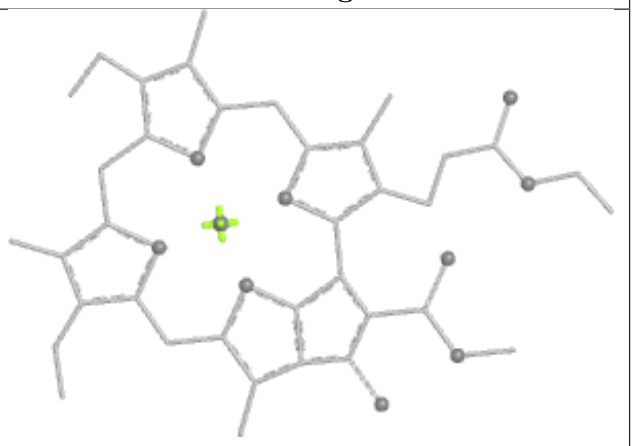
Bond lengths



Bond angles

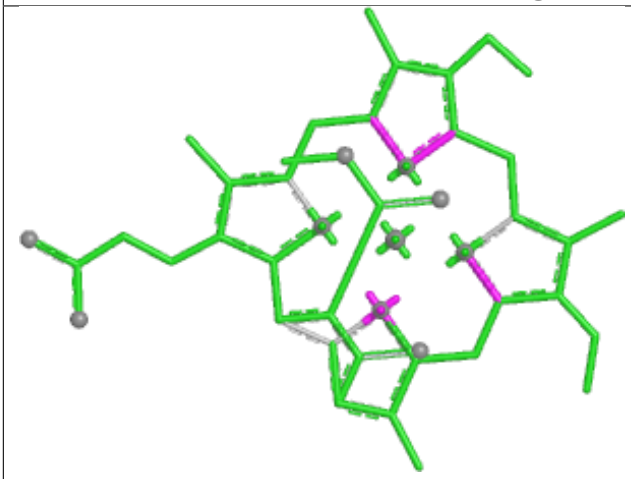


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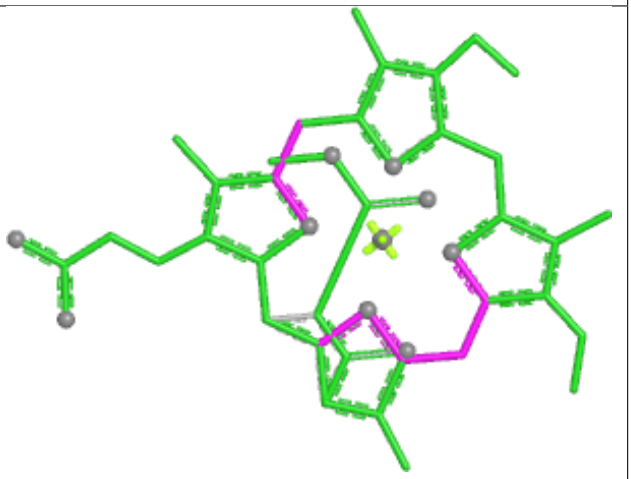


Rings

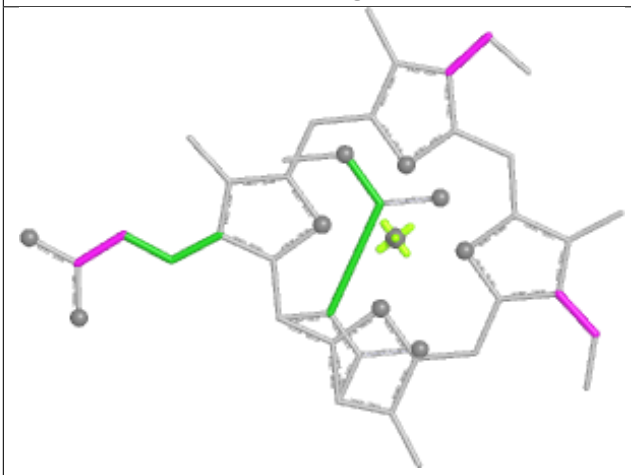
Ligand KC2 v 309



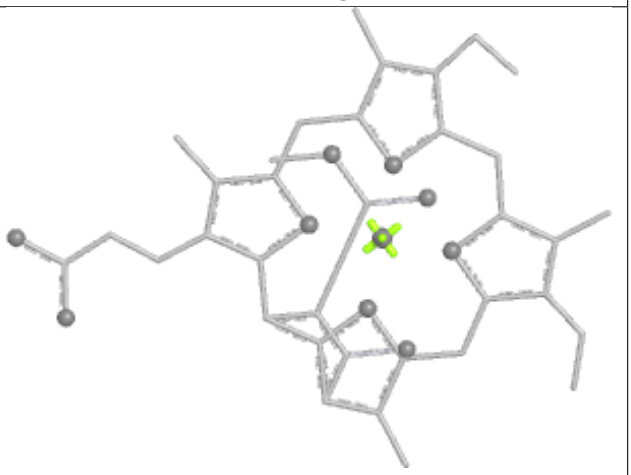
Bond lengths



Bond angles

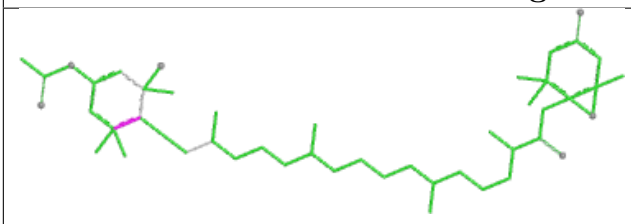


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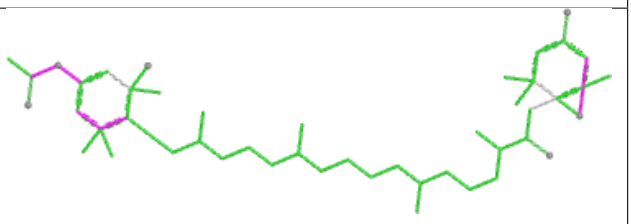


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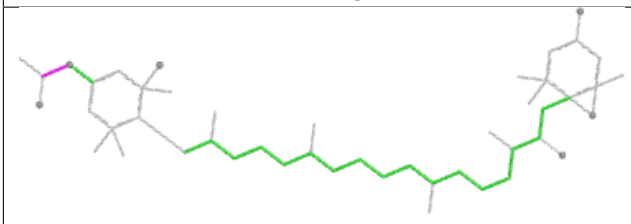
Ligand A86 U 210



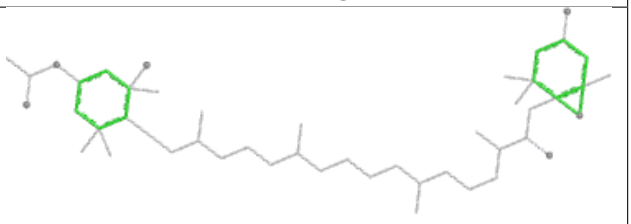
Bond lengths



Bond angles

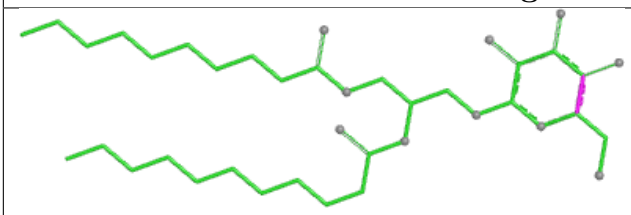


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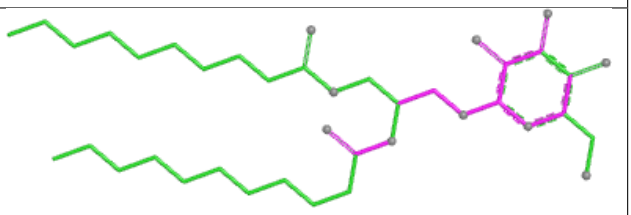


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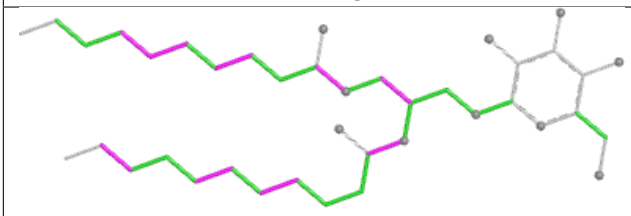
Ligand LMG E 321



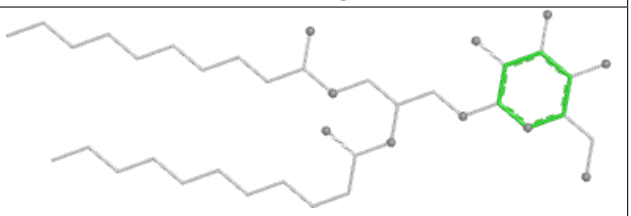
Bond lengths



Bond angles

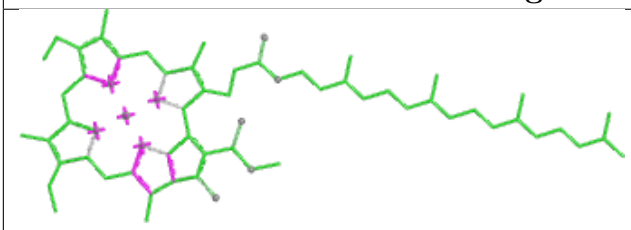


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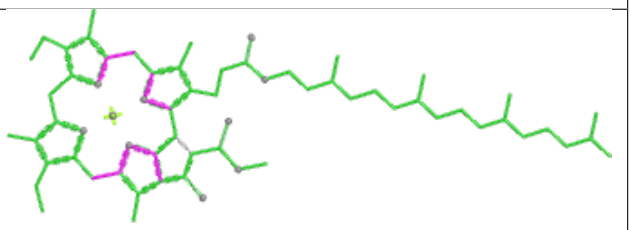


Rings

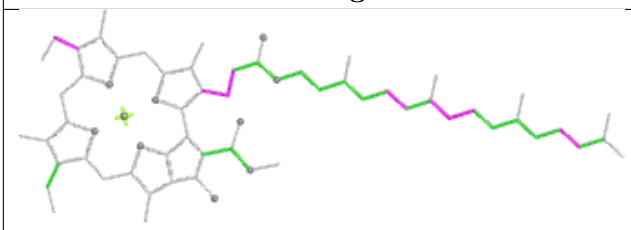
Ligand CLA E 307



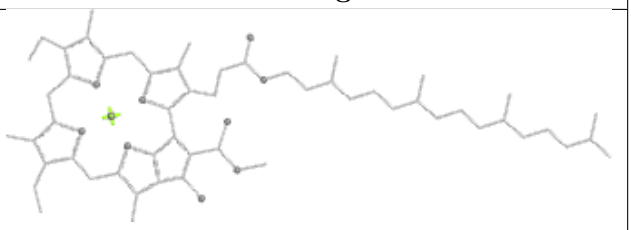
Bond lengths



Bond angles

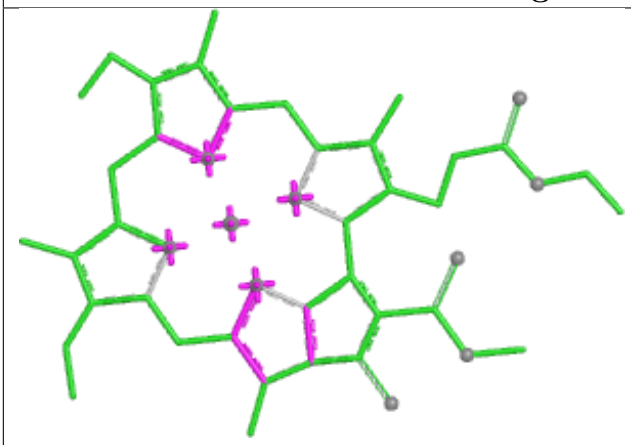


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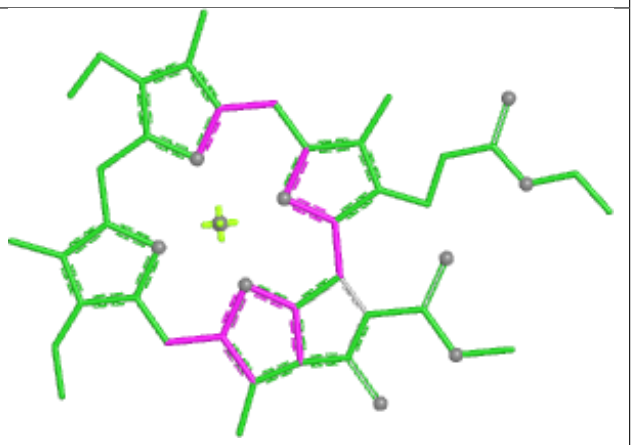


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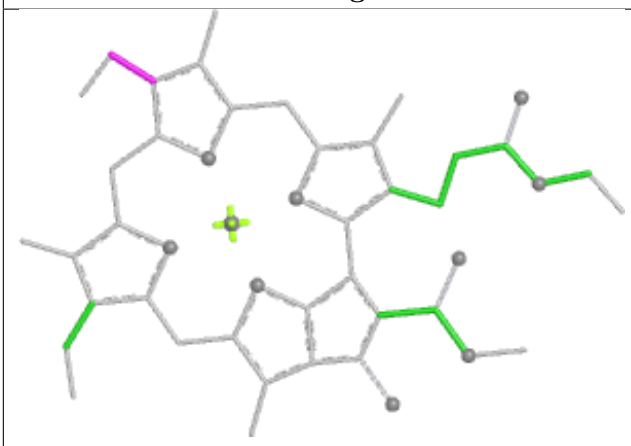
Ligand CLA f 204



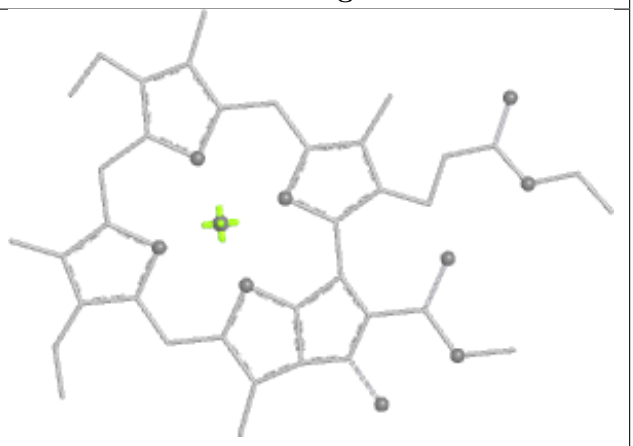
Bond lengths



Bond angles

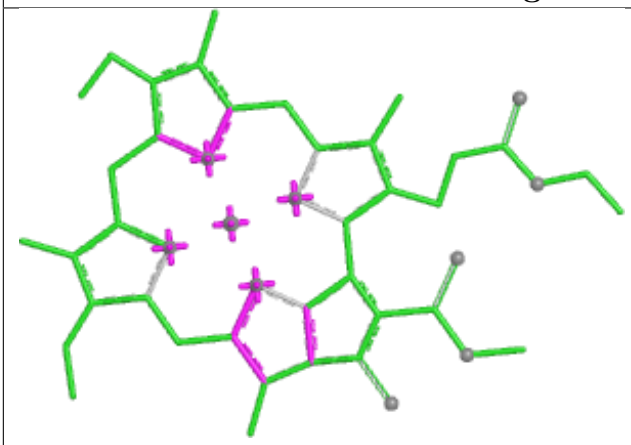


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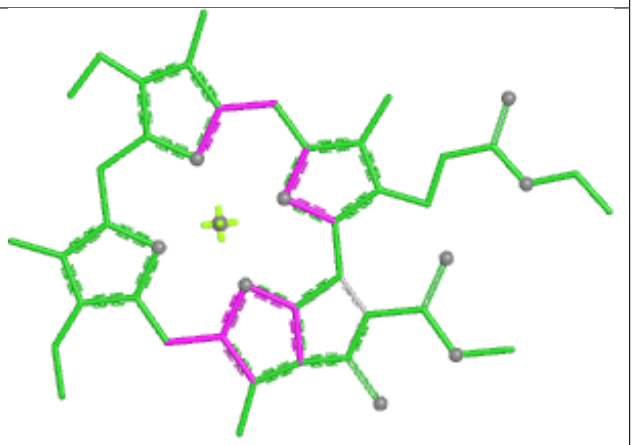


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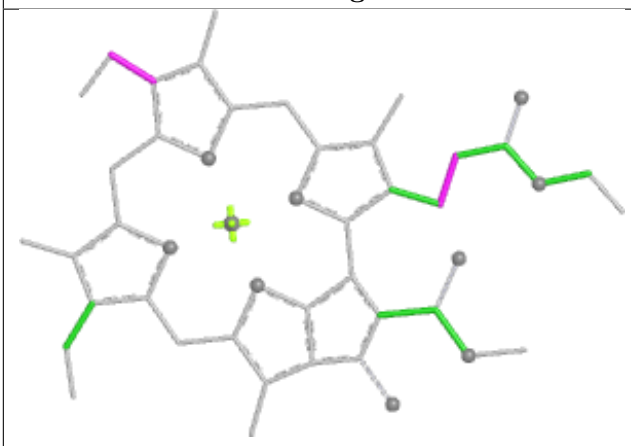
Ligand CLA H 311



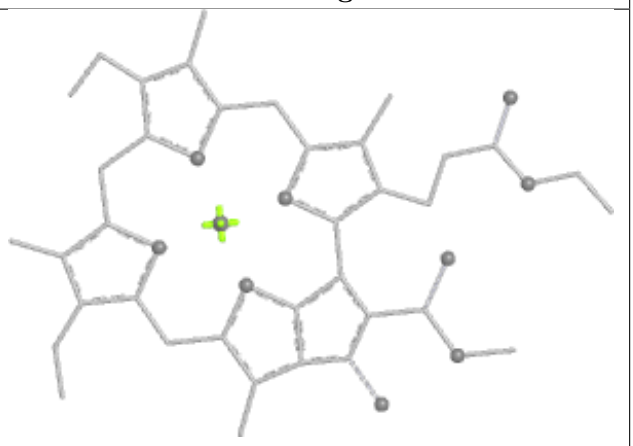
Bond lengths



Bond angles

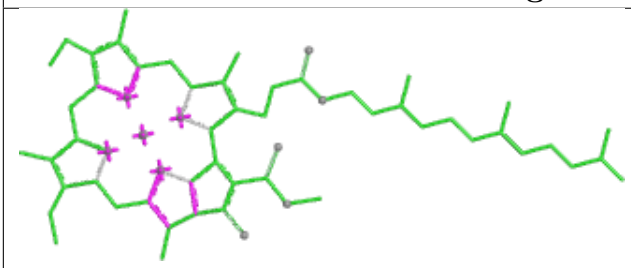


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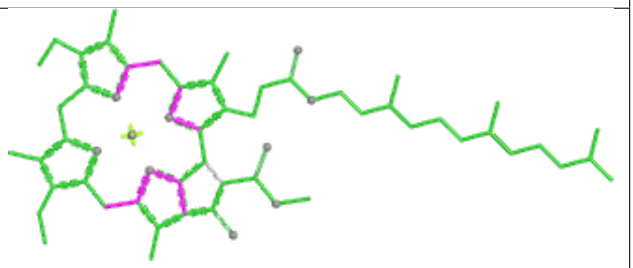


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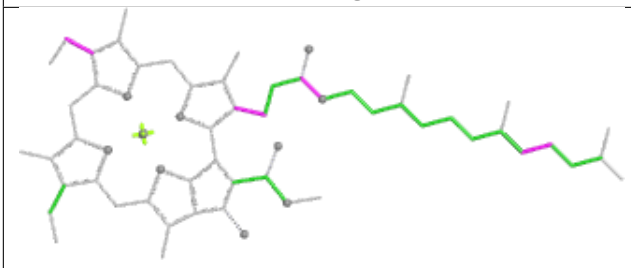
Ligand CLA Z 301



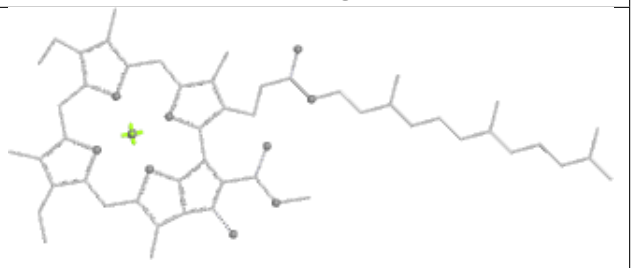
Bond lengths



Bond angles

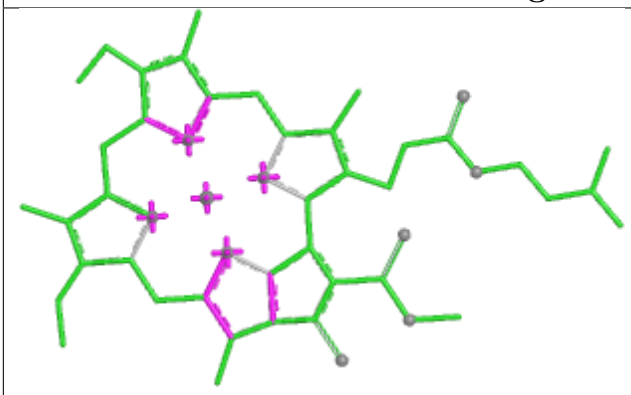


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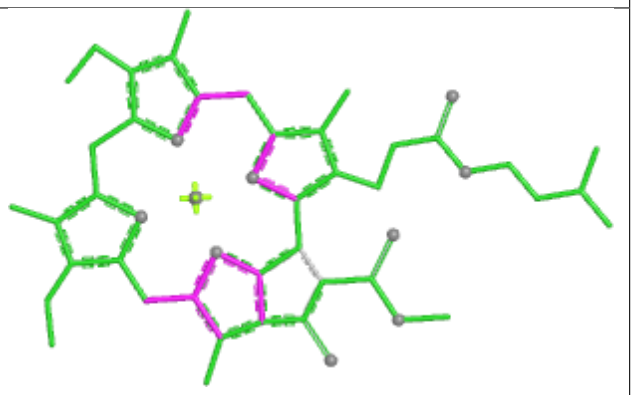


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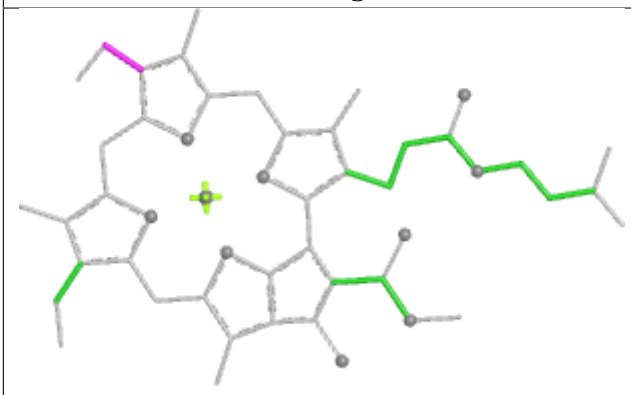
Ligand CLA a 814



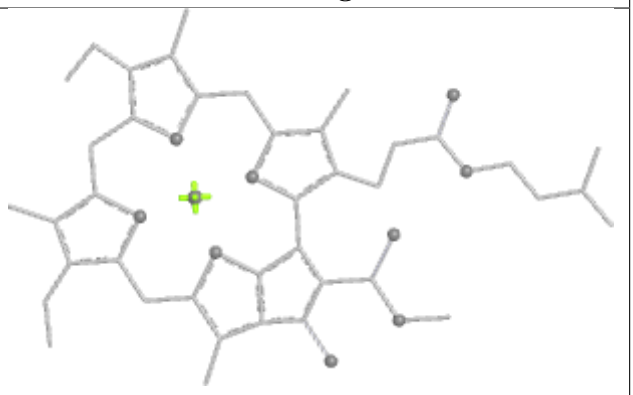
Bond lengths



Bond angles

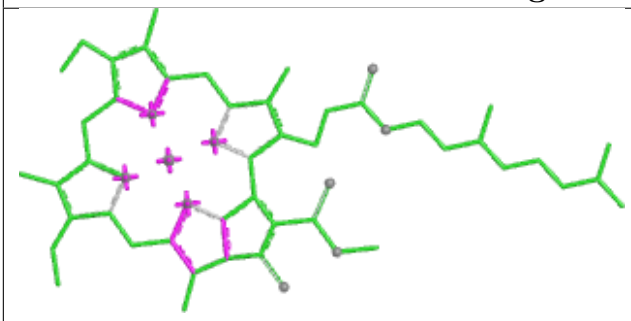


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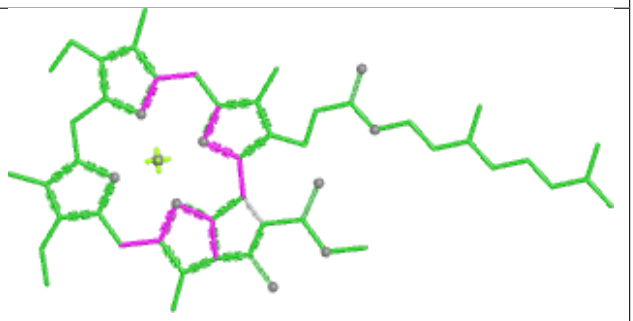


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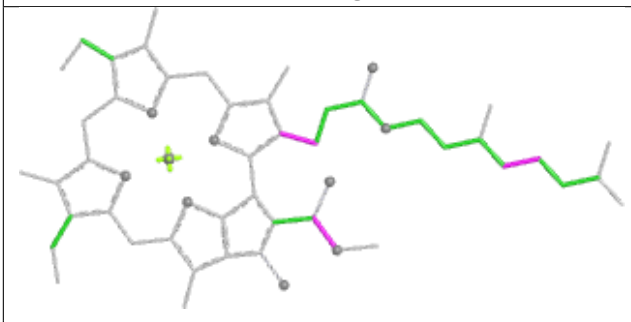
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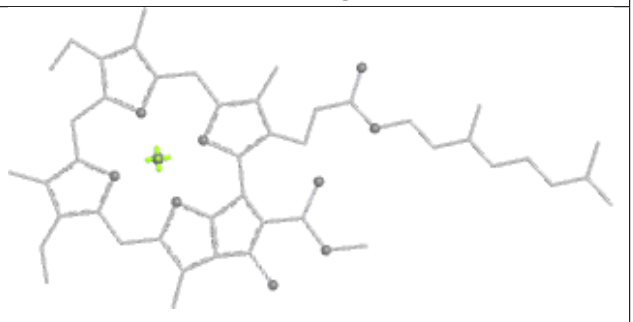
Bond lengths



Bond angles

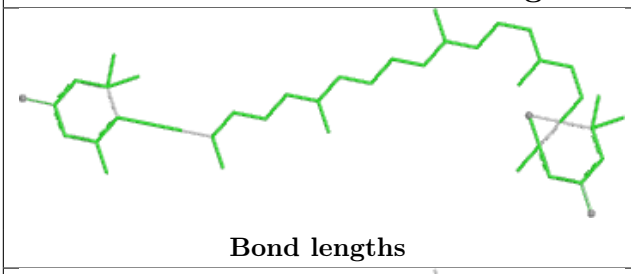


Torsions

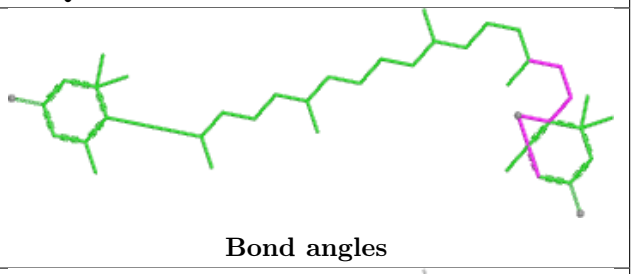


Rings

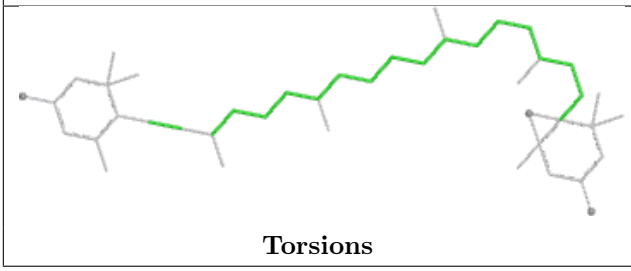
Ligand DD6 Q 213



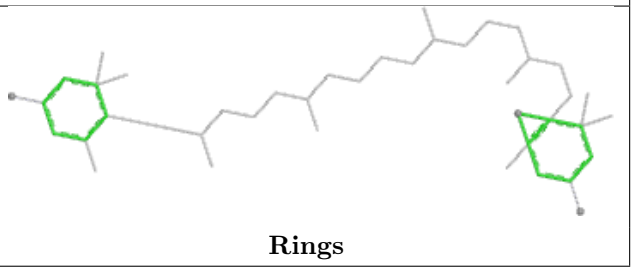
Bond lengths



Bond angles

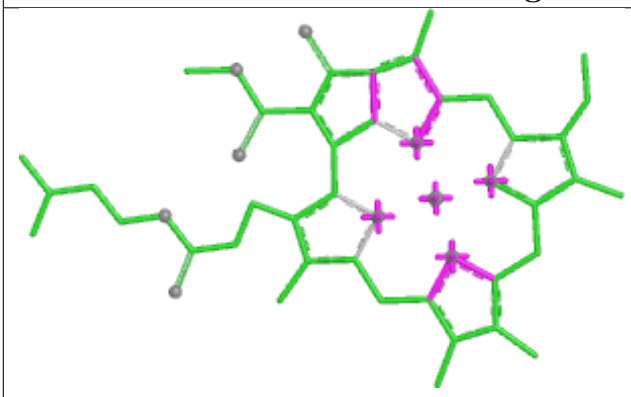


Torsions

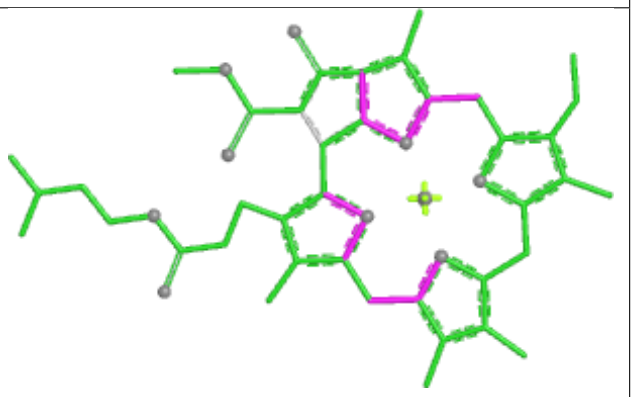


Rings

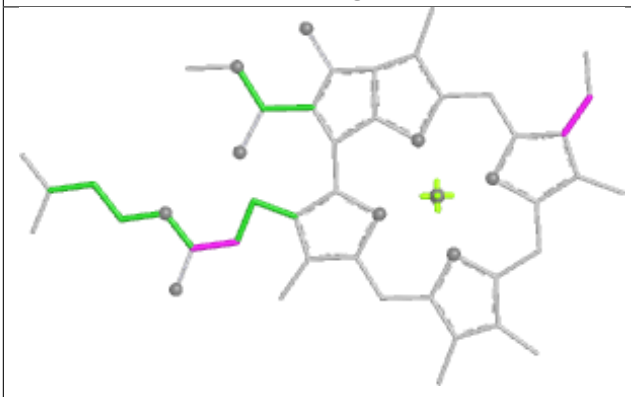
Ligand CLA w 305



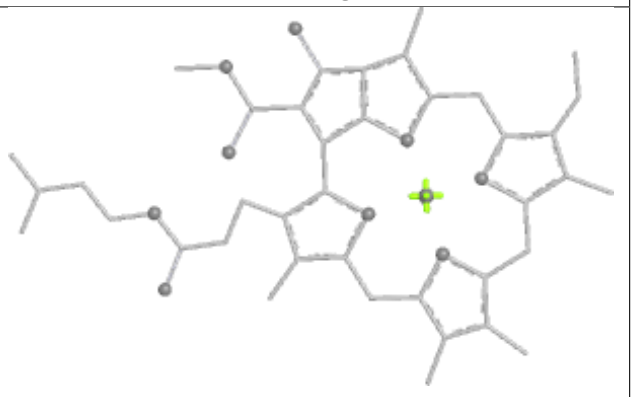
Bond lengths



Bond angles

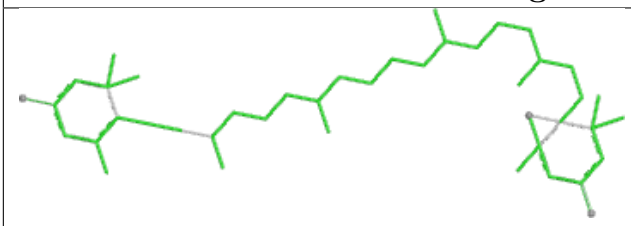


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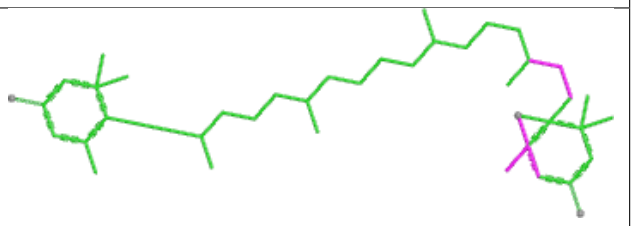


Rings

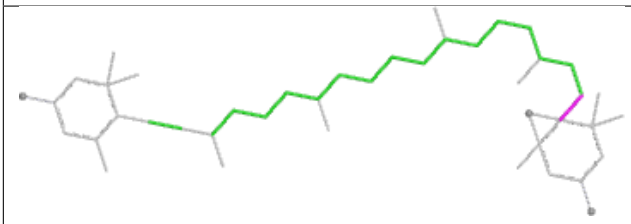
Ligand DD6 o 319



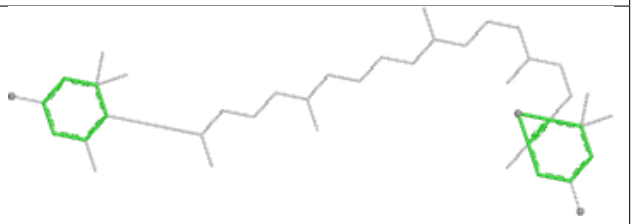
Bond lengths



Bond angles

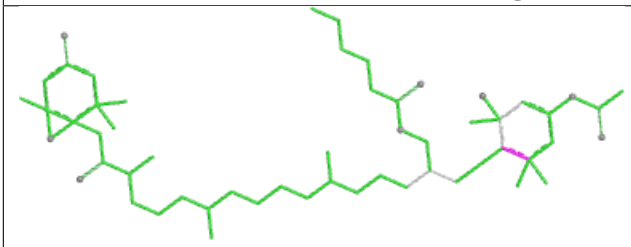


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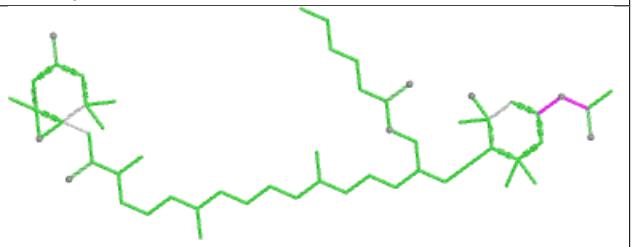


Rings

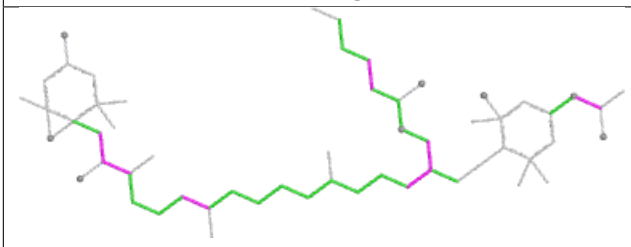
Ligand A1EB1 y 312



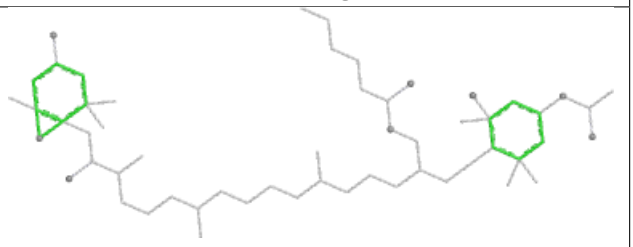
Bond lengths



Bond angles

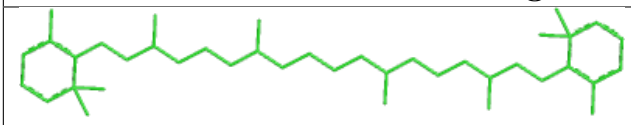


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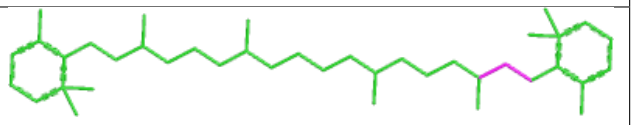


Rings

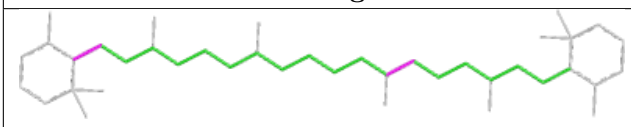
Ligand BCR k 203



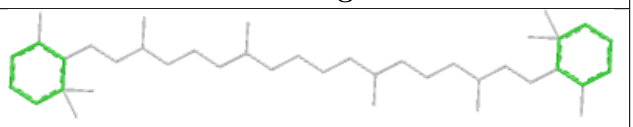
Bond lengths



Bond angles

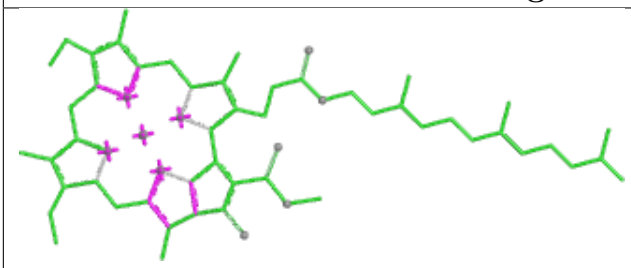


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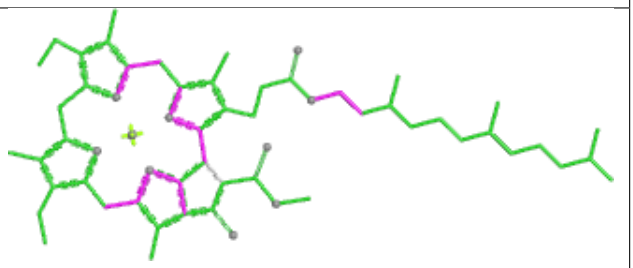


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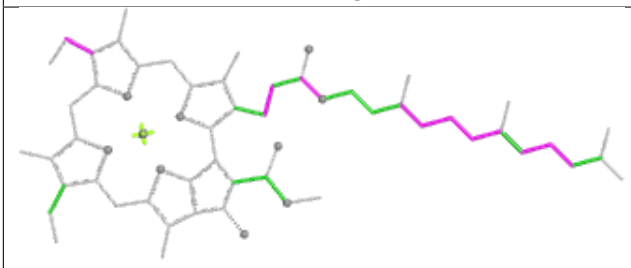
Ligand CLA S 302



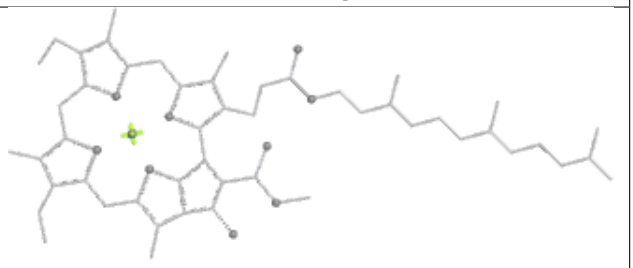
Bond lengths



Bond angles

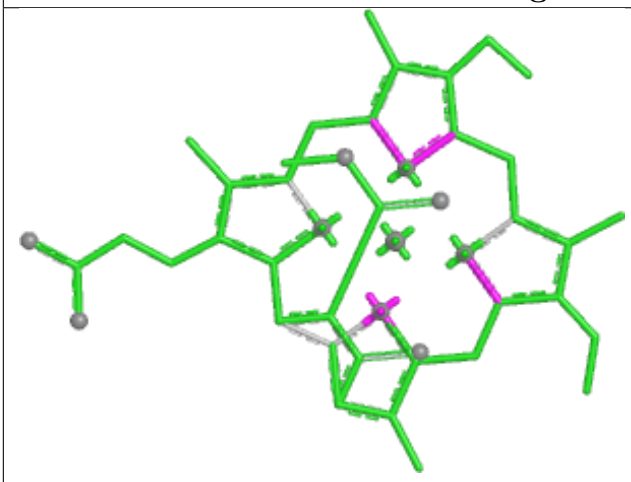


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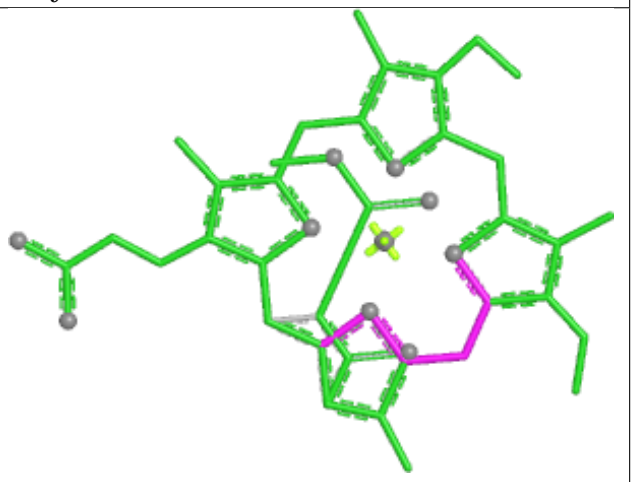


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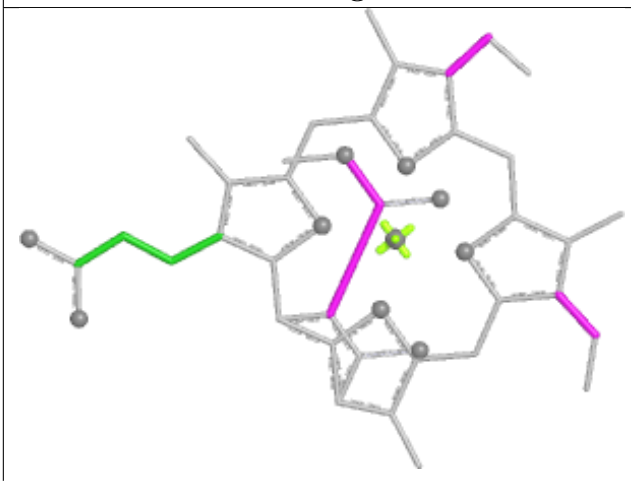
Ligand KC2 y 306



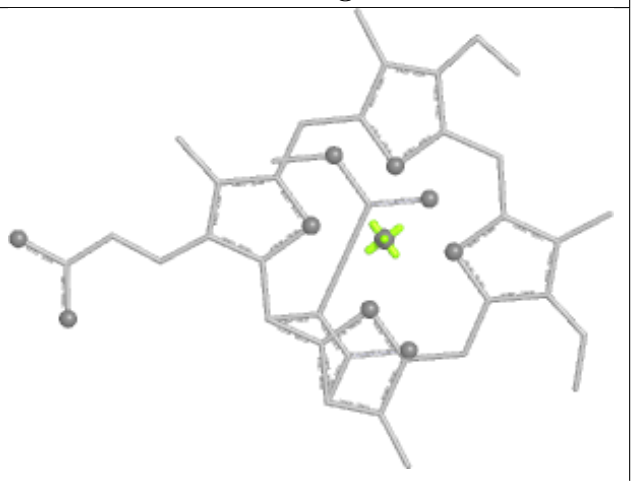
Bond lengths



Bond angles

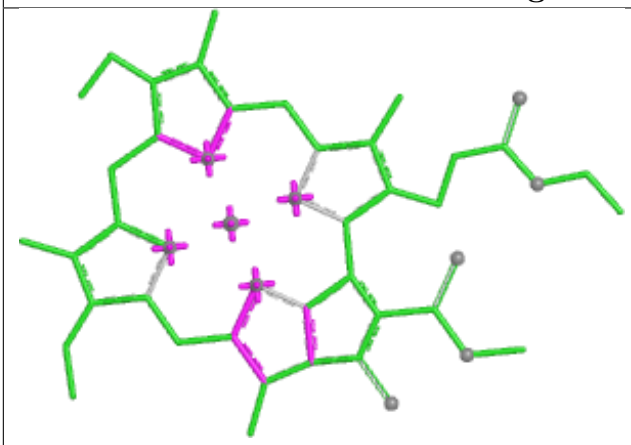


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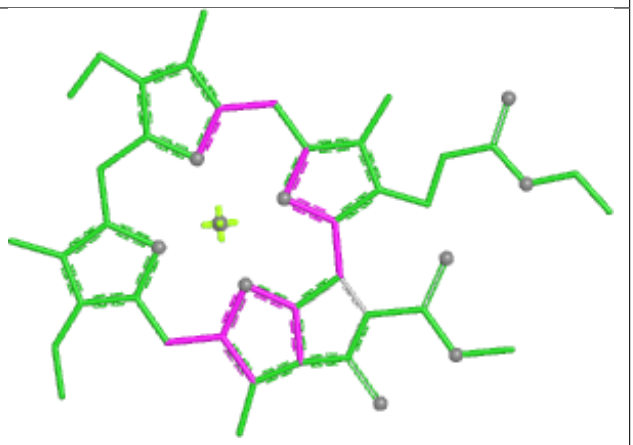


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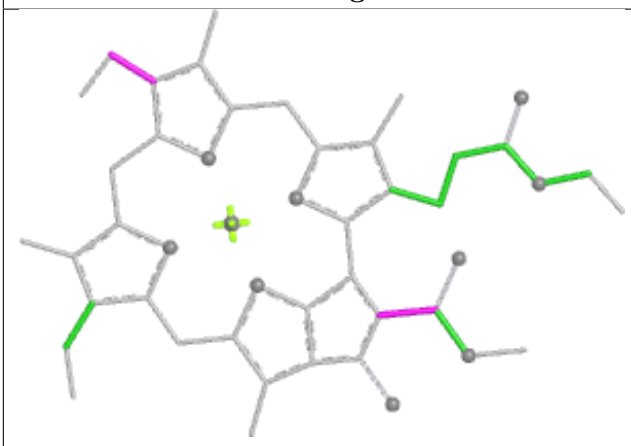
Ligand CLA x 314



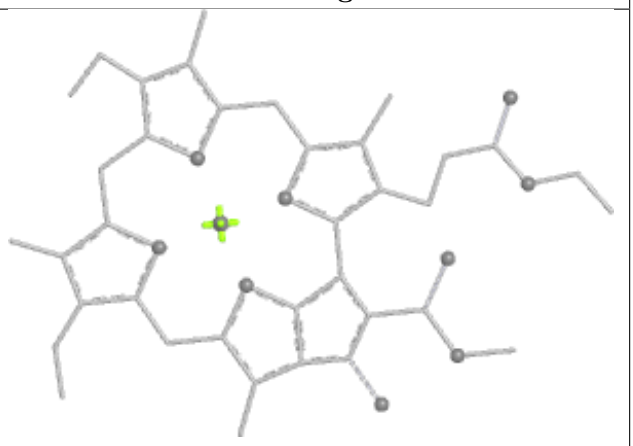
Bond lengths



Bond angles

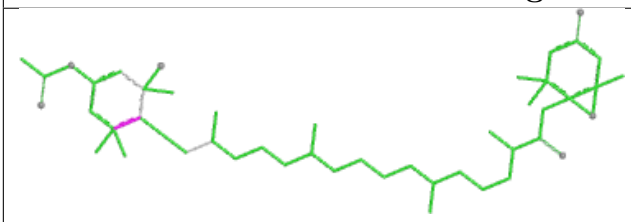


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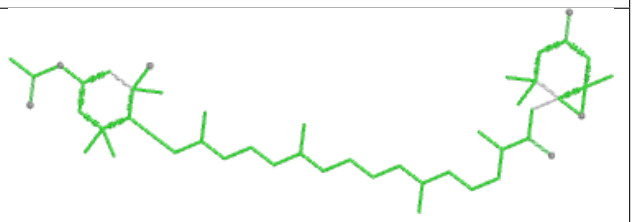


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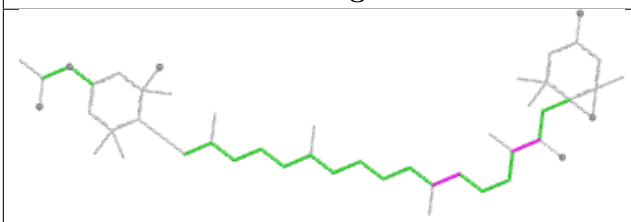
Ligand A86 M 320



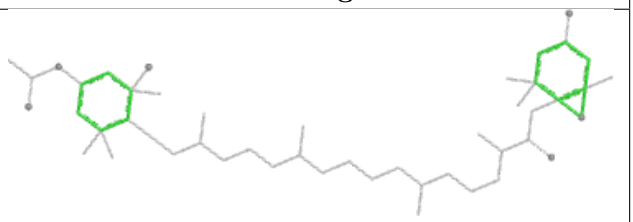
Bond lengths



Bond angles

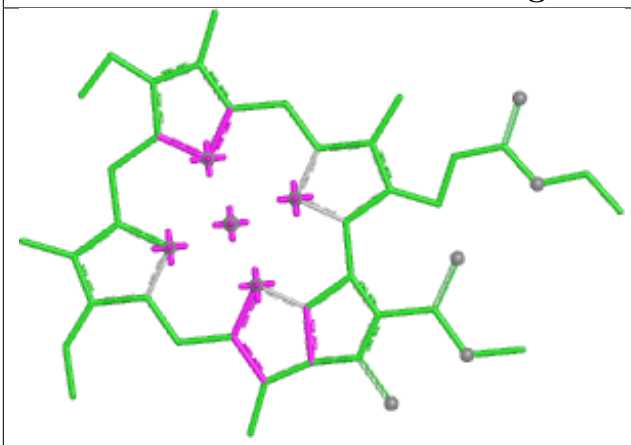


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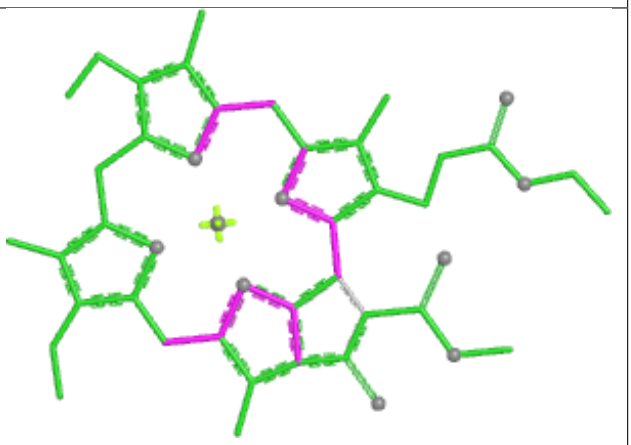


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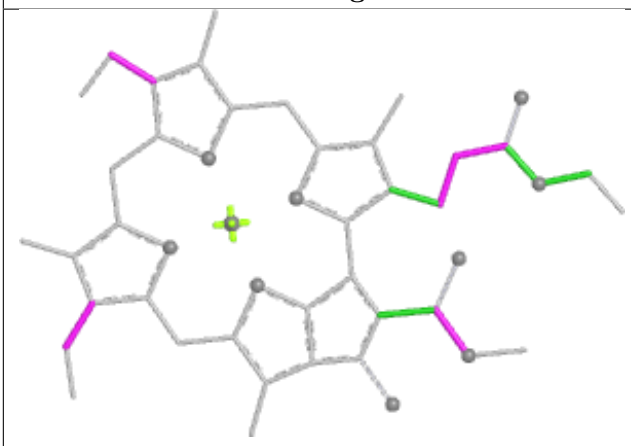
Ligand CLA J 302



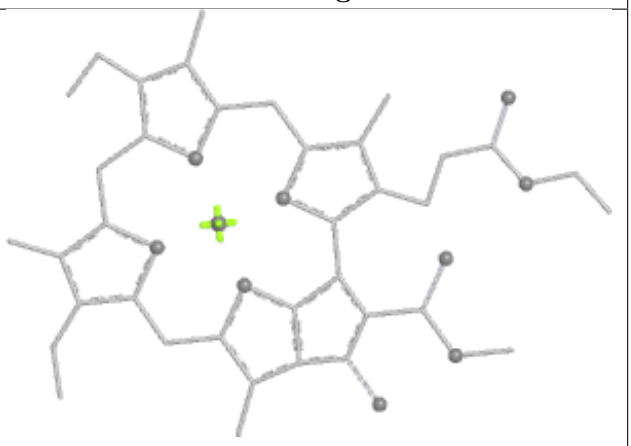
Bond lengths



Bond angles

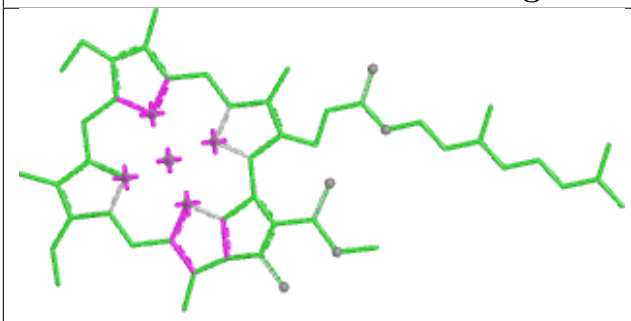


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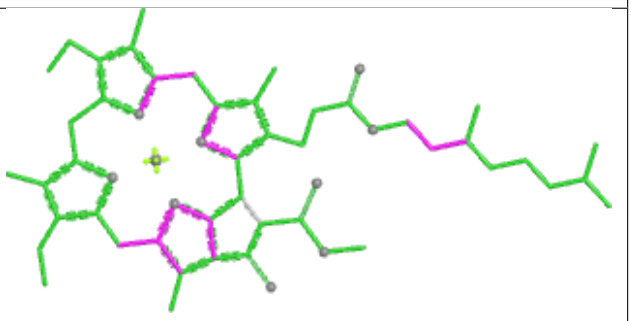


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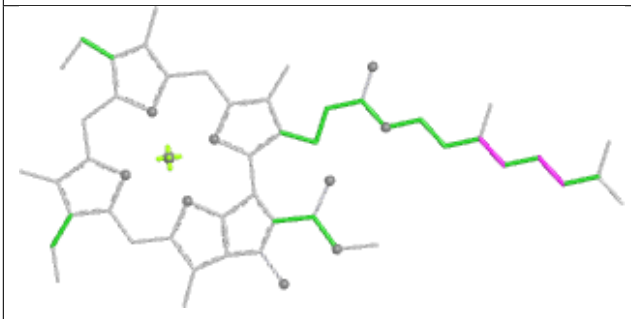
Ligand CLA G 204



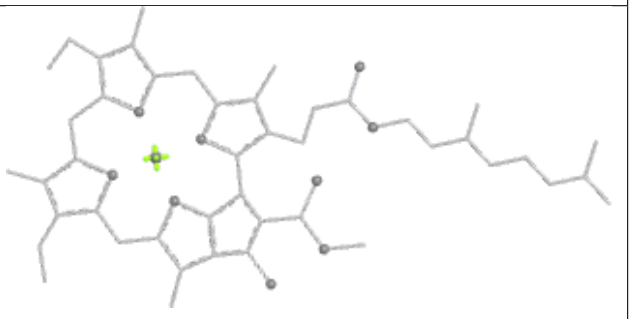
Bond lengths



Bond angles

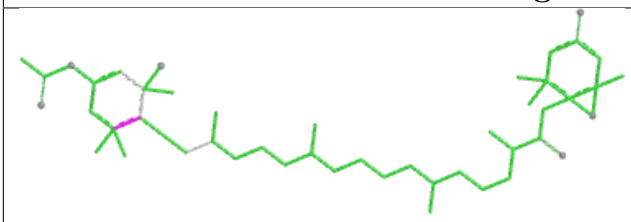


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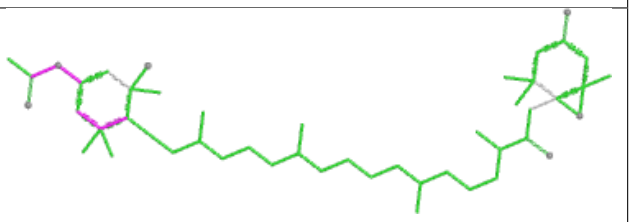


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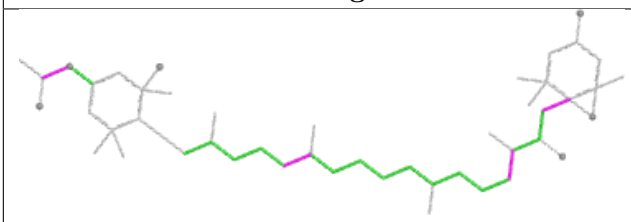
Ligand A86 x 317



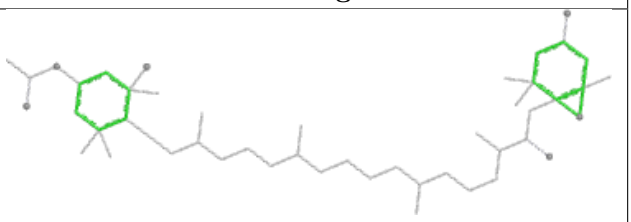
Bond lengths



Bond angles

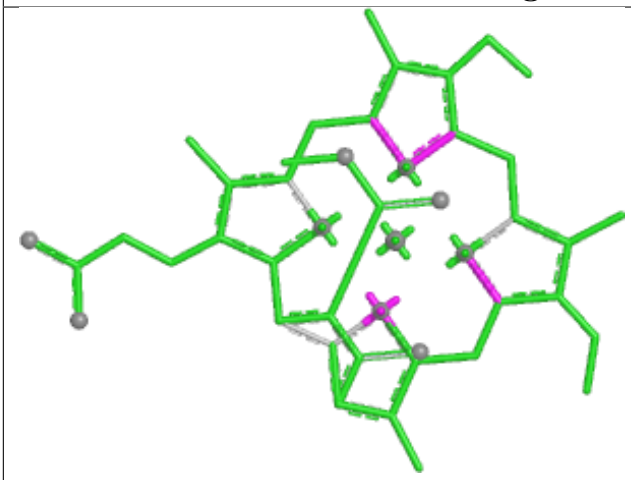


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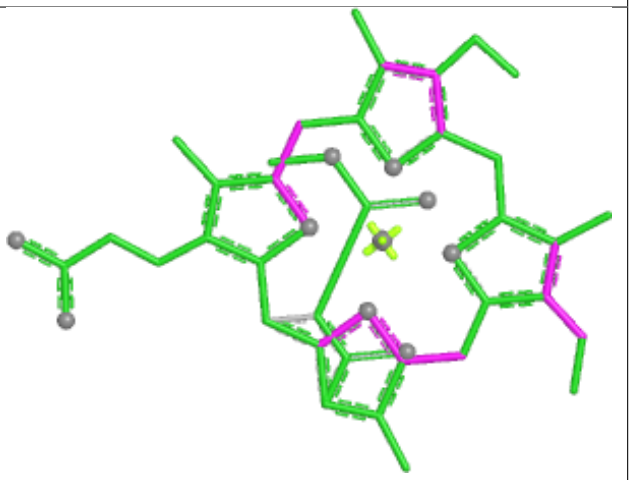


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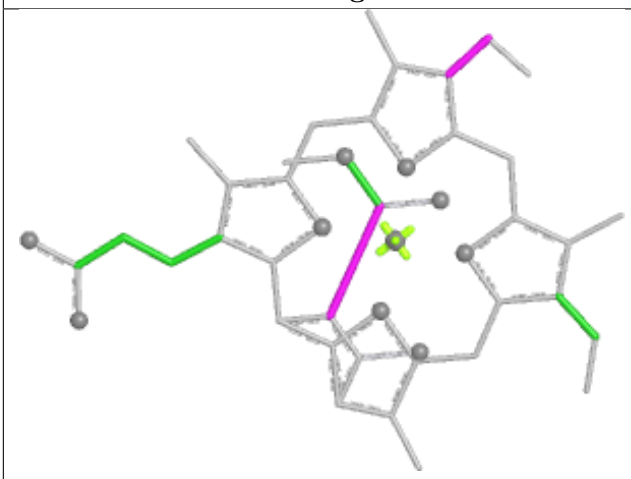
Ligand KC2 M 303



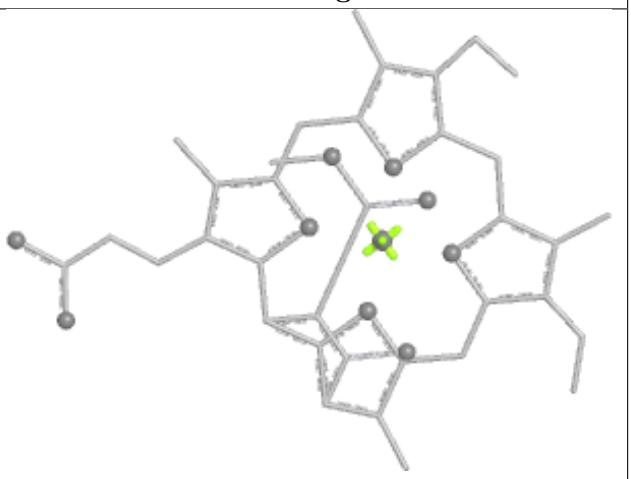
Bond lengths



Bond angles

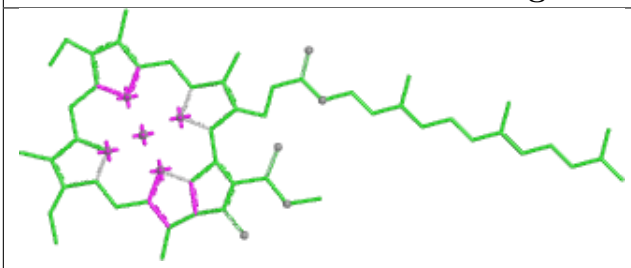


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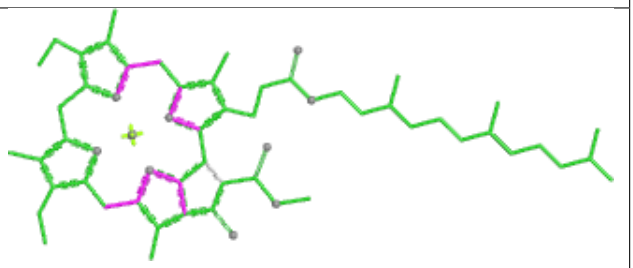


Rings

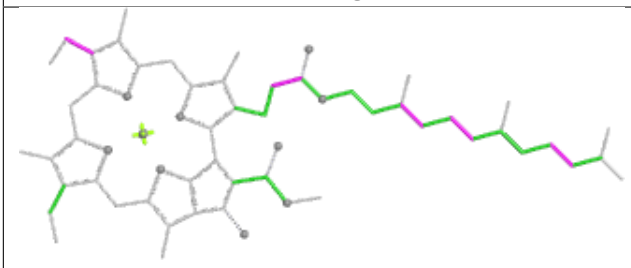
Ligand CLA o 301



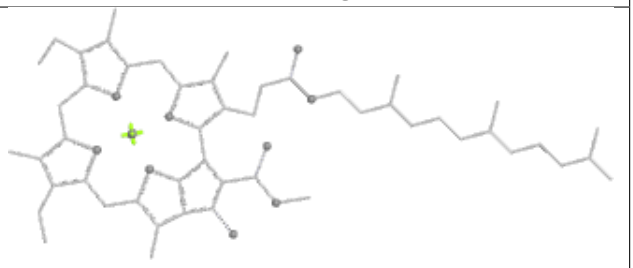
Bond lengths



Bond angles

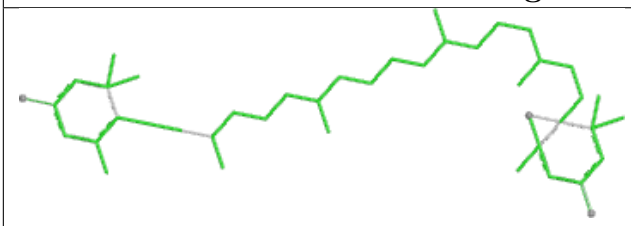


Torsions

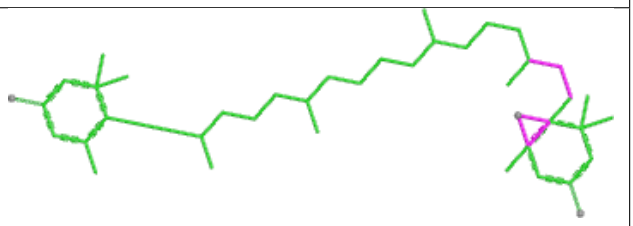


Rings

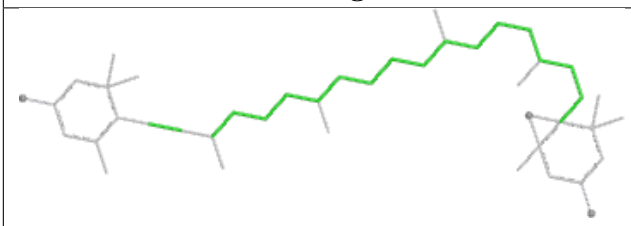
Ligand DD6 D 315



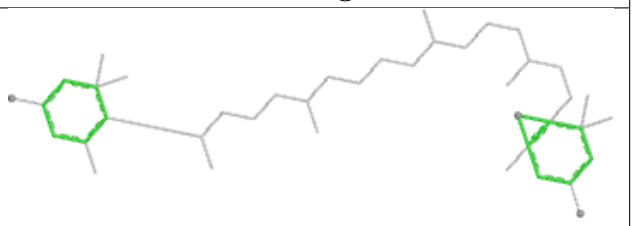
Bond lengths



Bond angles

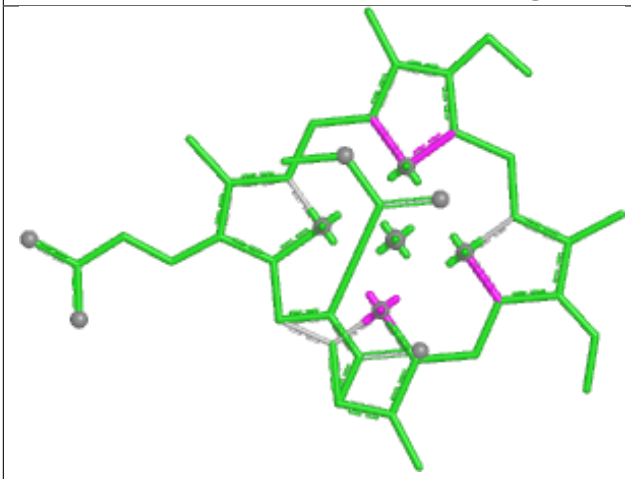


Torsions

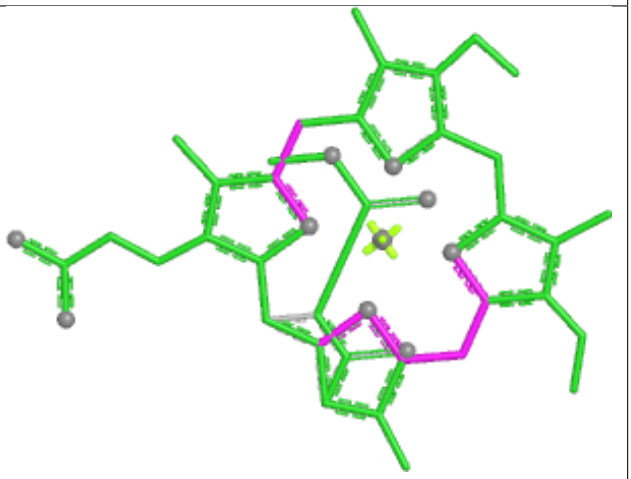


Rings

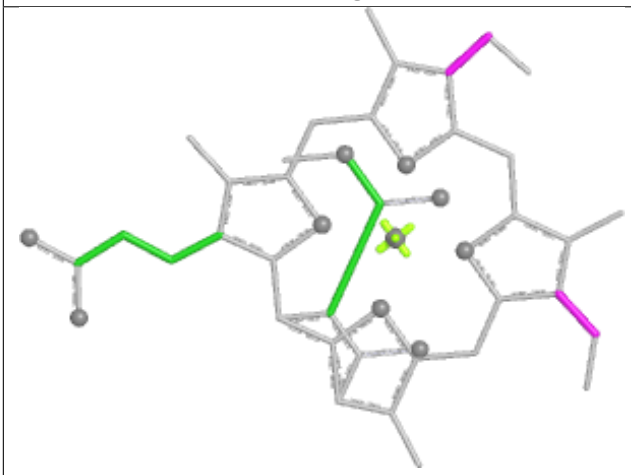
Ligand KC2 T 301



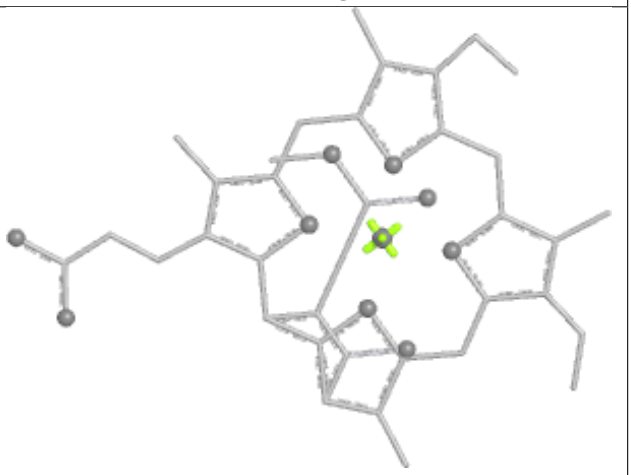
Bond lengths



Bond angles

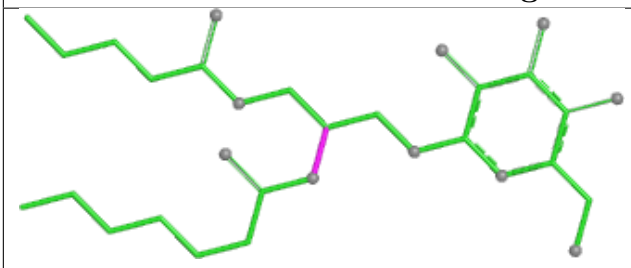


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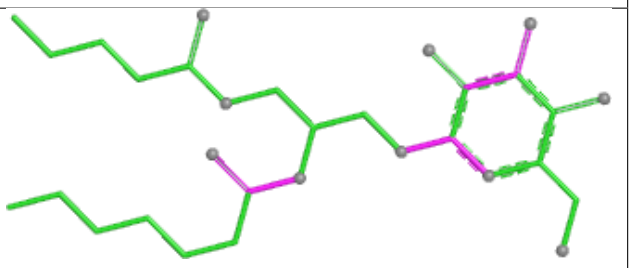


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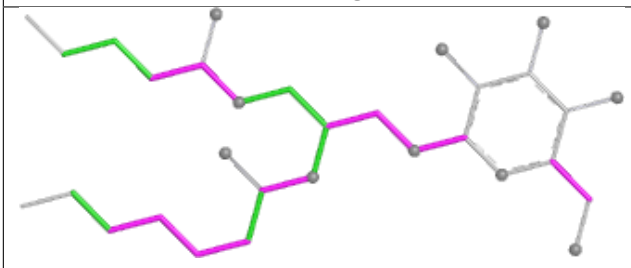
Ligand LMG E 320



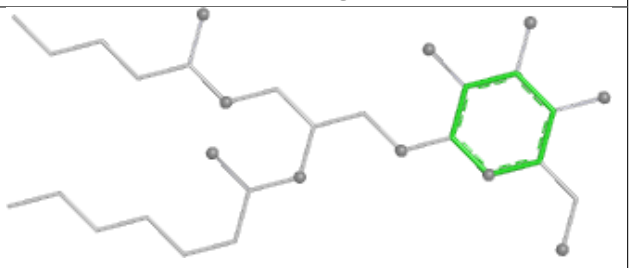
Bond lengths



Bond angles

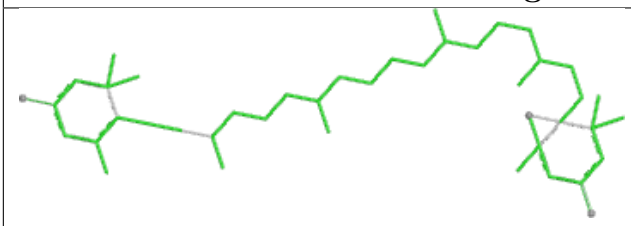


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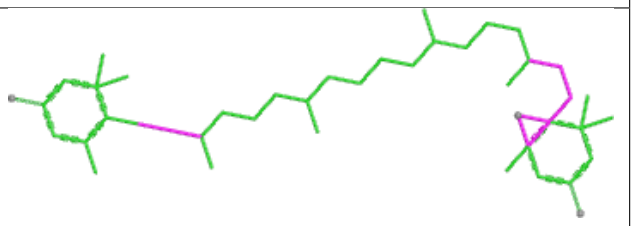


Rings

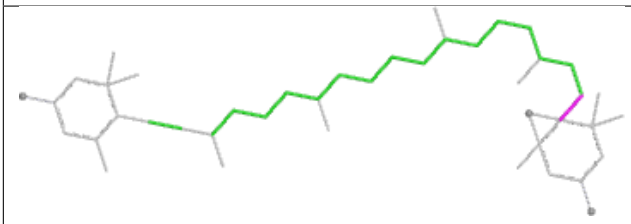
Ligand DD6 N 319



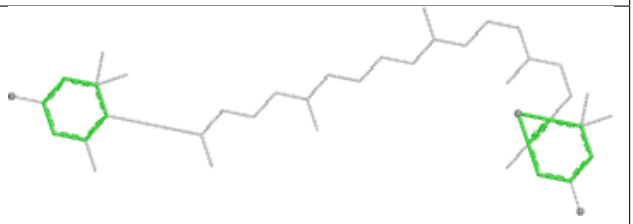
Bond lengths



Bond angles

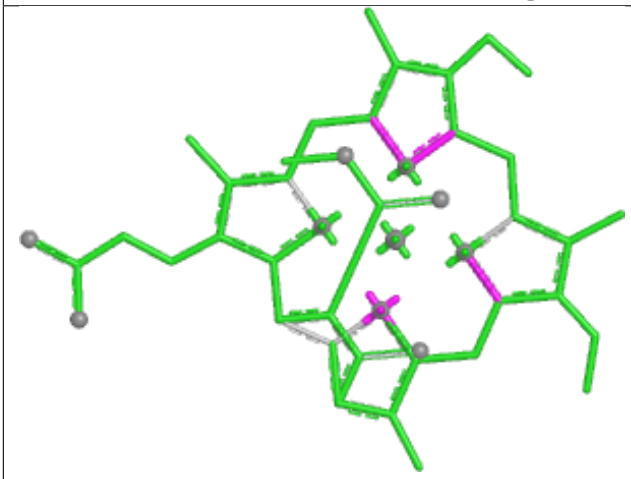


Torsions

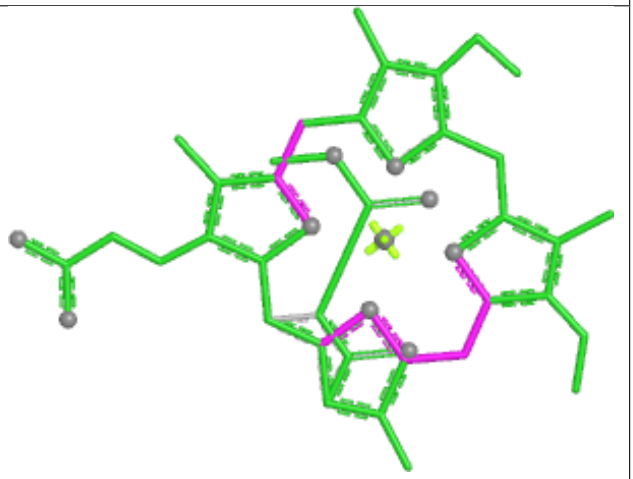


Rings

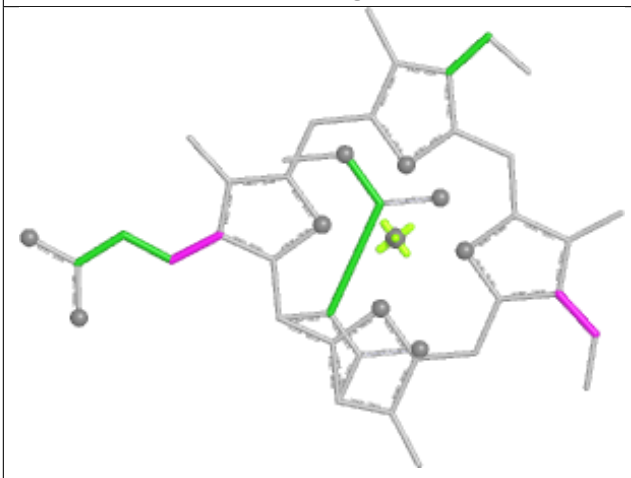
Ligand KC2 M 302



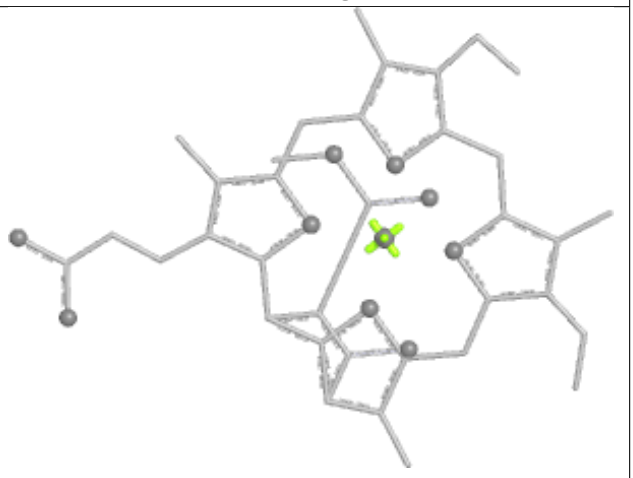
Bond lengths



Bond angles

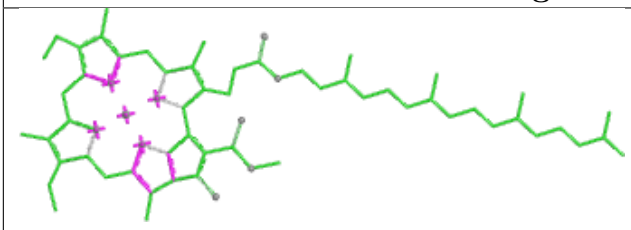


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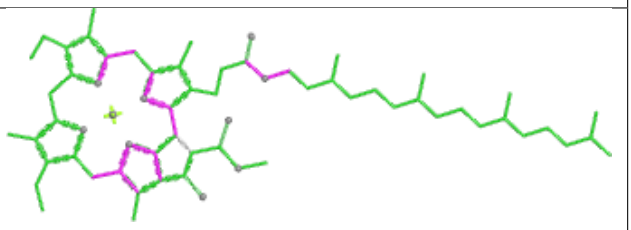


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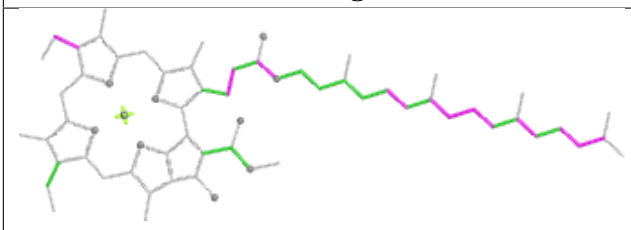
Ligand CLA l 202



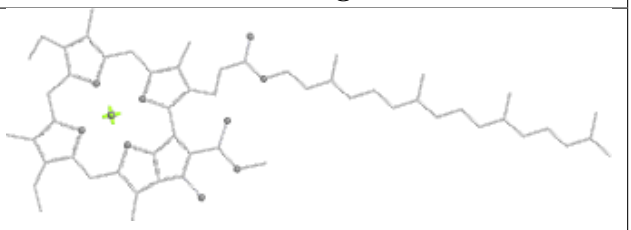
Bond lengths



Bond angles

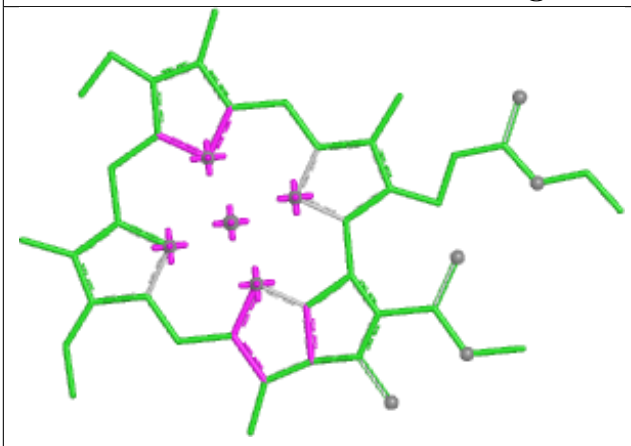


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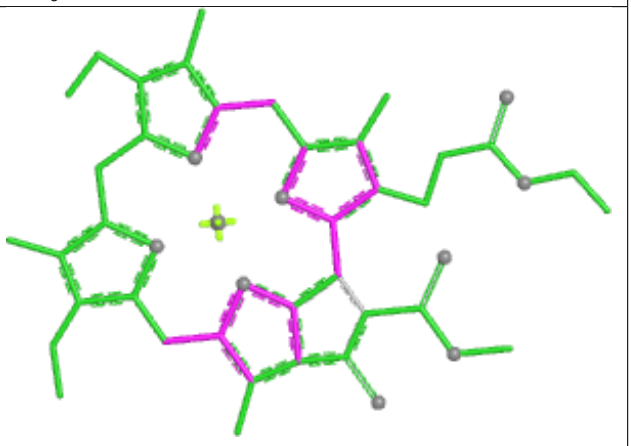


Rings

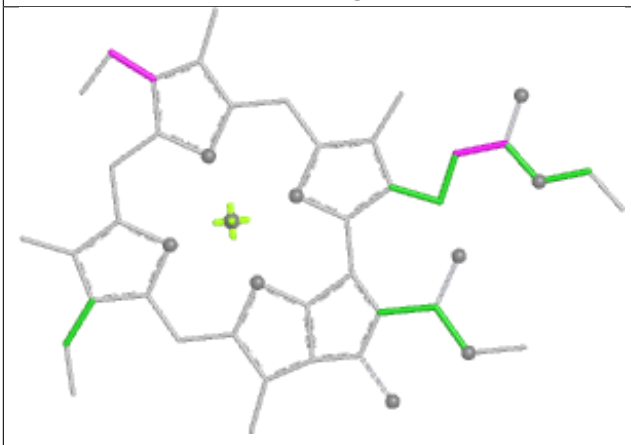
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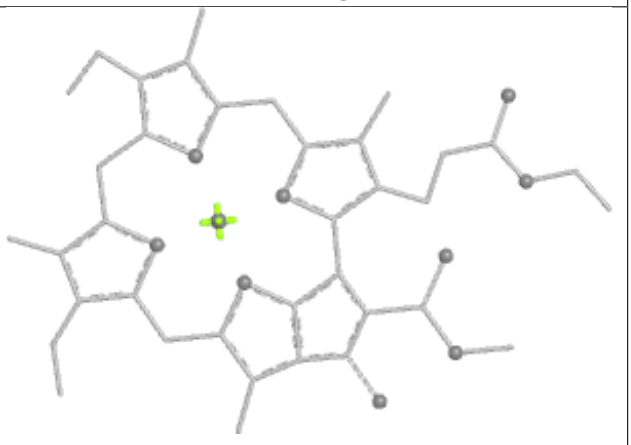
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Bond angles

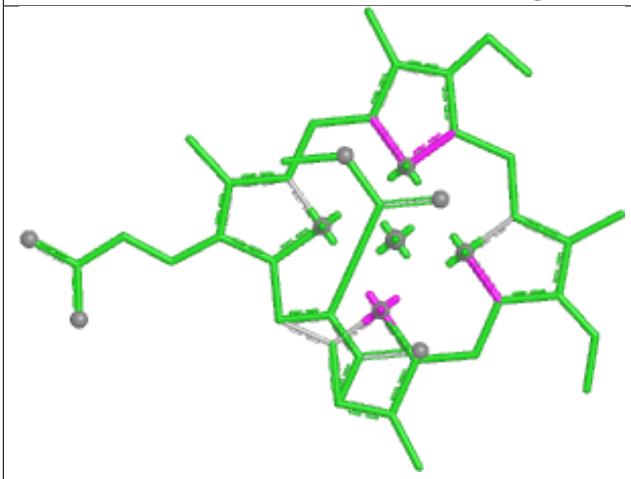


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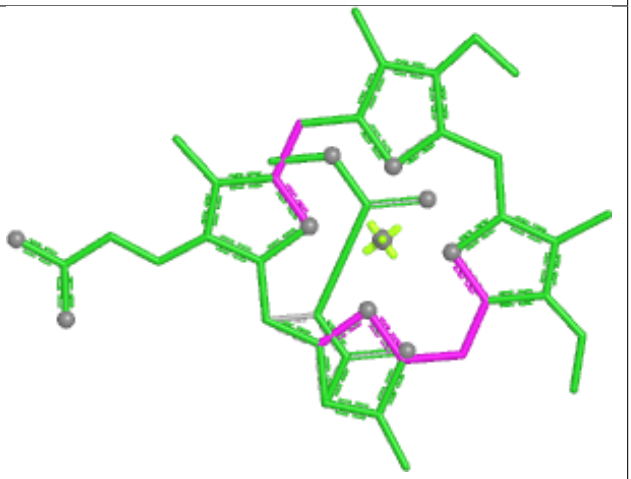


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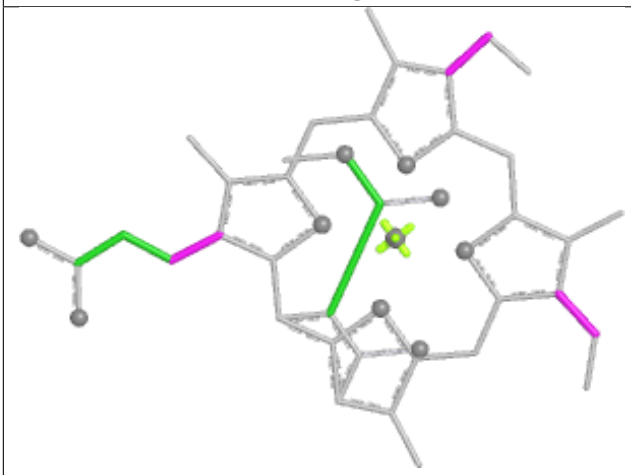
Ligand KC2 u 309



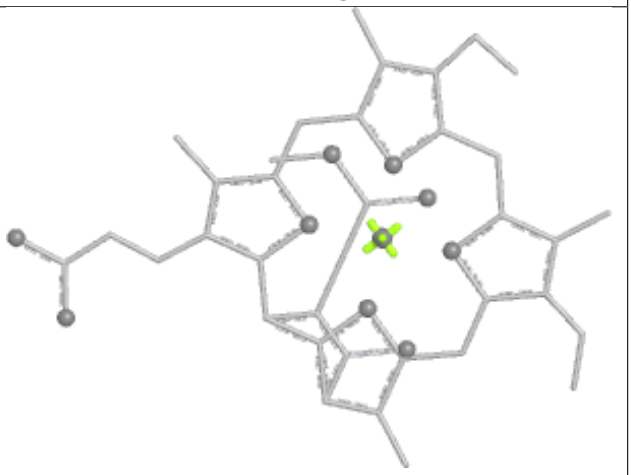
Bond lengths



Bond angles

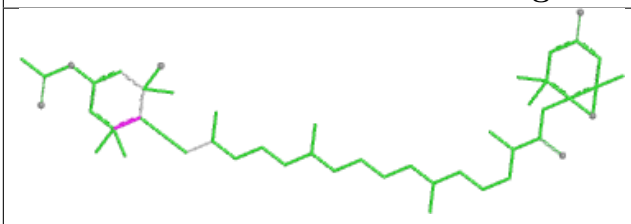


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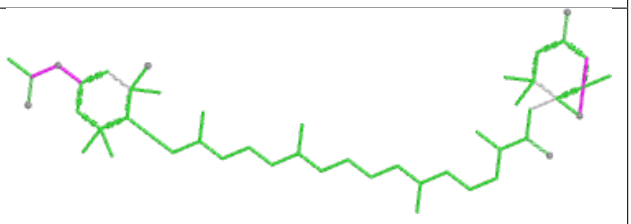


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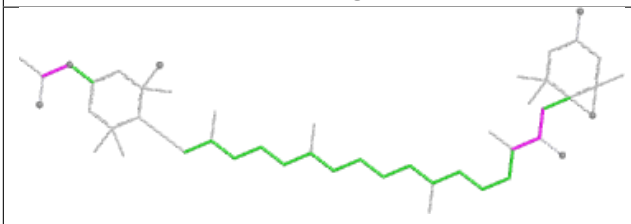
Ligand A86 L 314



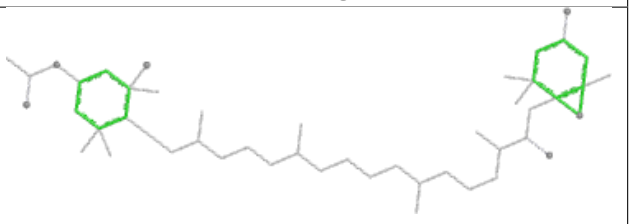
Bond lengths



Bond angles

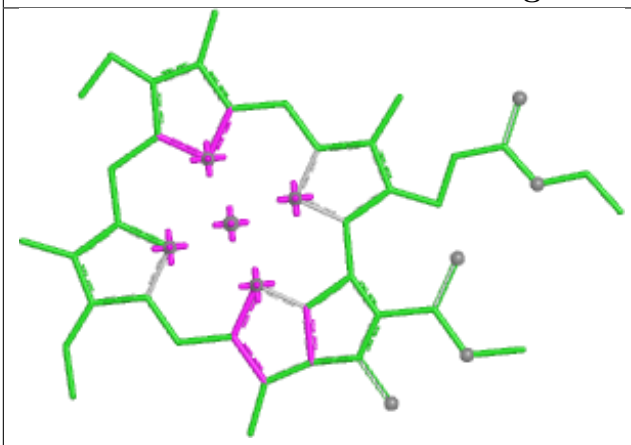


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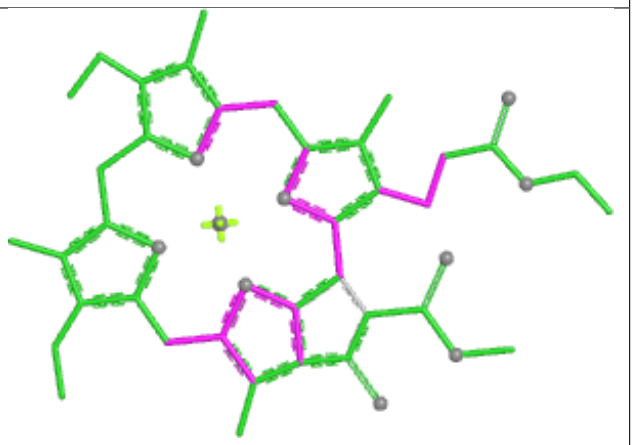


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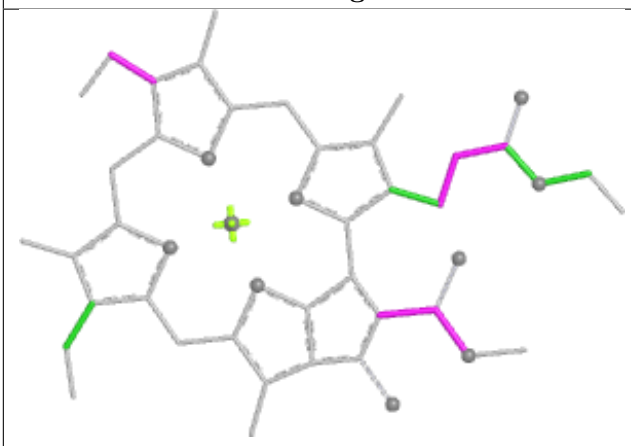
Ligand CLA H 302



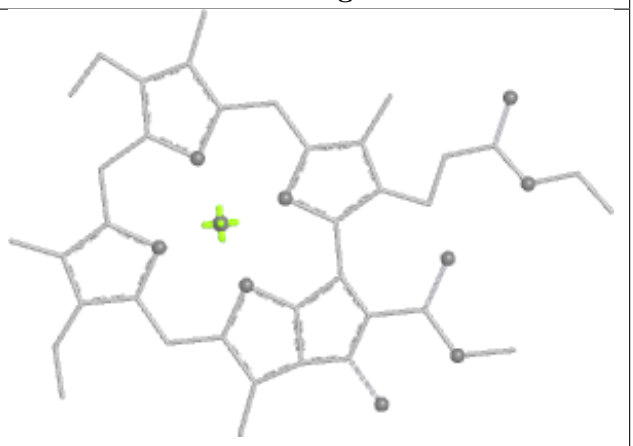
Bond lengths



Bond angles

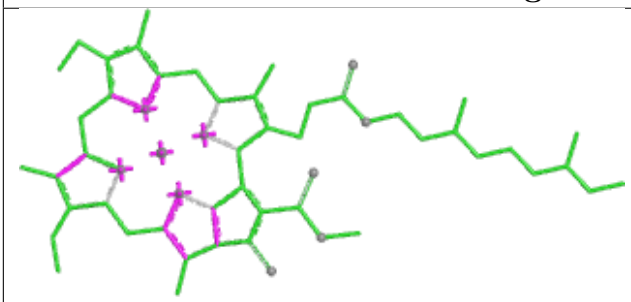


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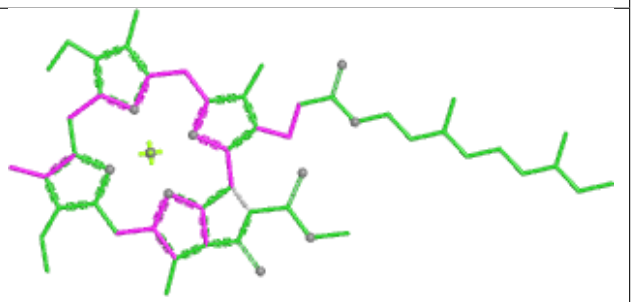


Rings

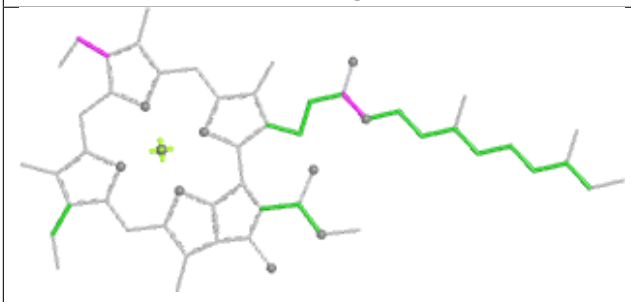
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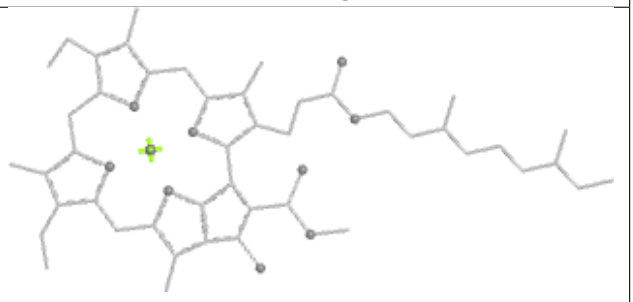
Bond lengths



Bond angles

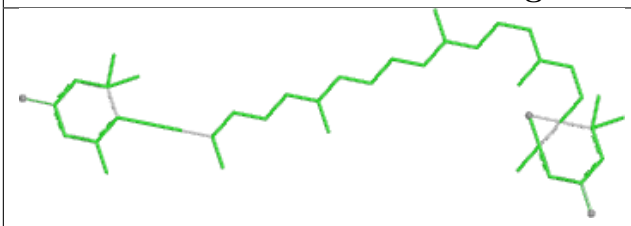


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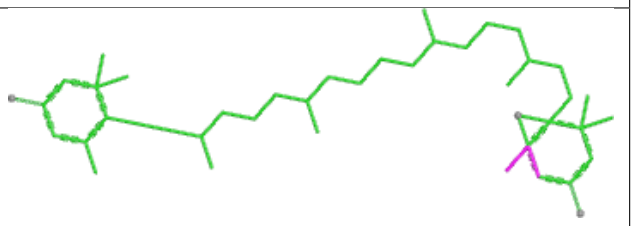


Rings

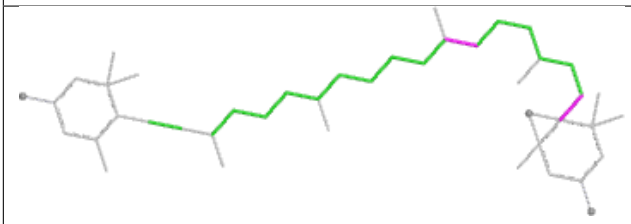
Ligand DD6 C 313



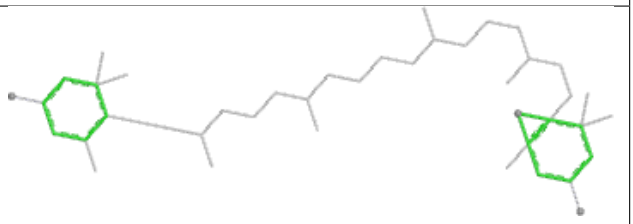
Bond lengths



Bond angles

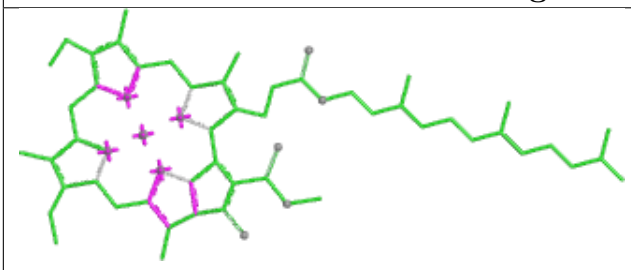


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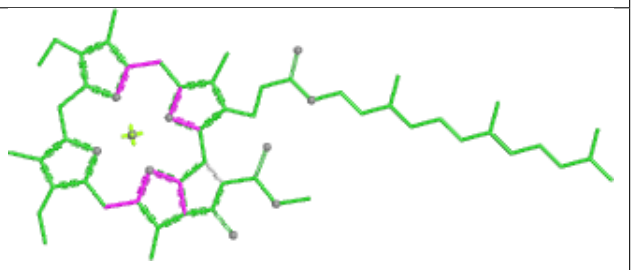


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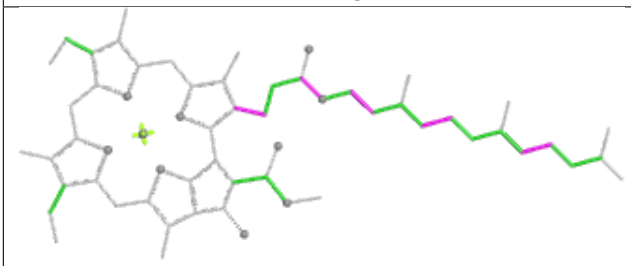
Ligand CLA z 302



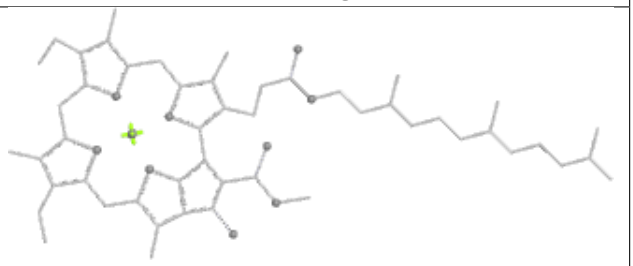
Bond lengths



Bond angles

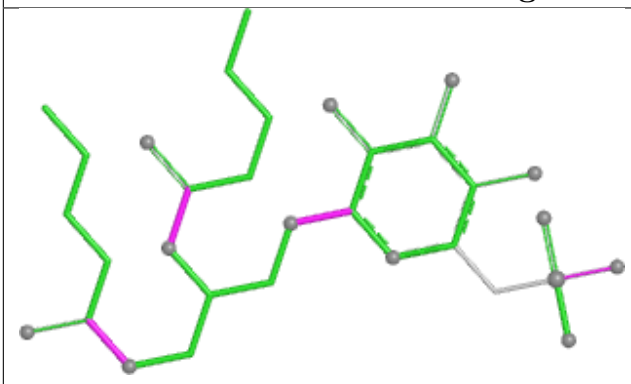


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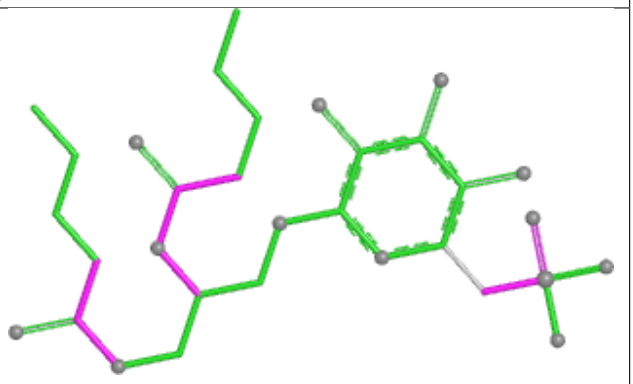


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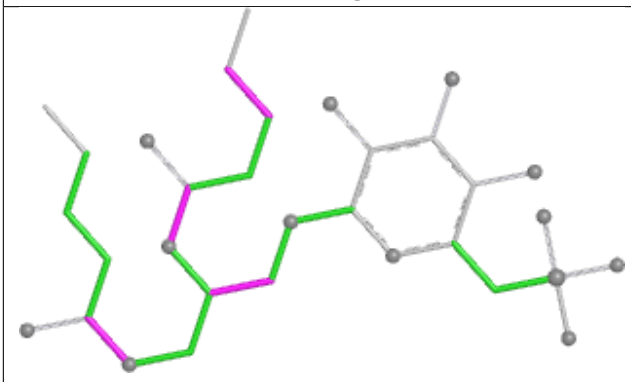
Ligand SQD W 318



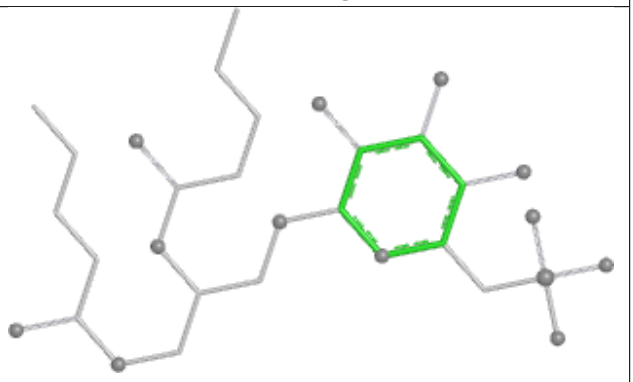
Bond lengths



Bond angles

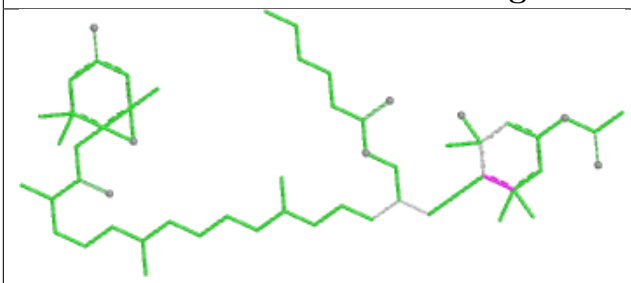


Torsions

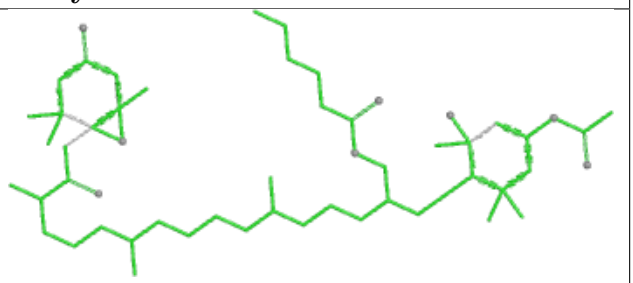


Rings

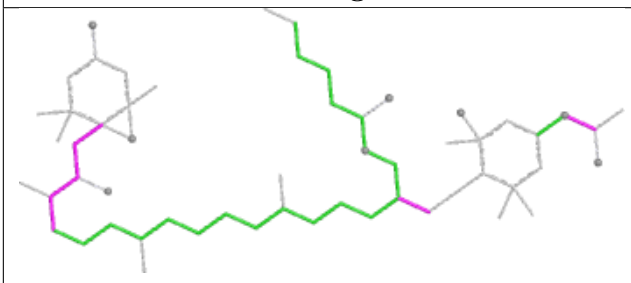
Ligand A1EB1 y 314



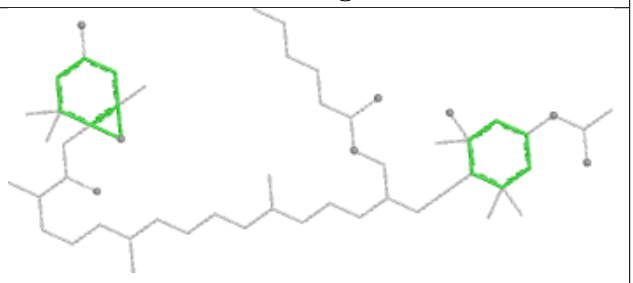
Bond lengths



Bond angles

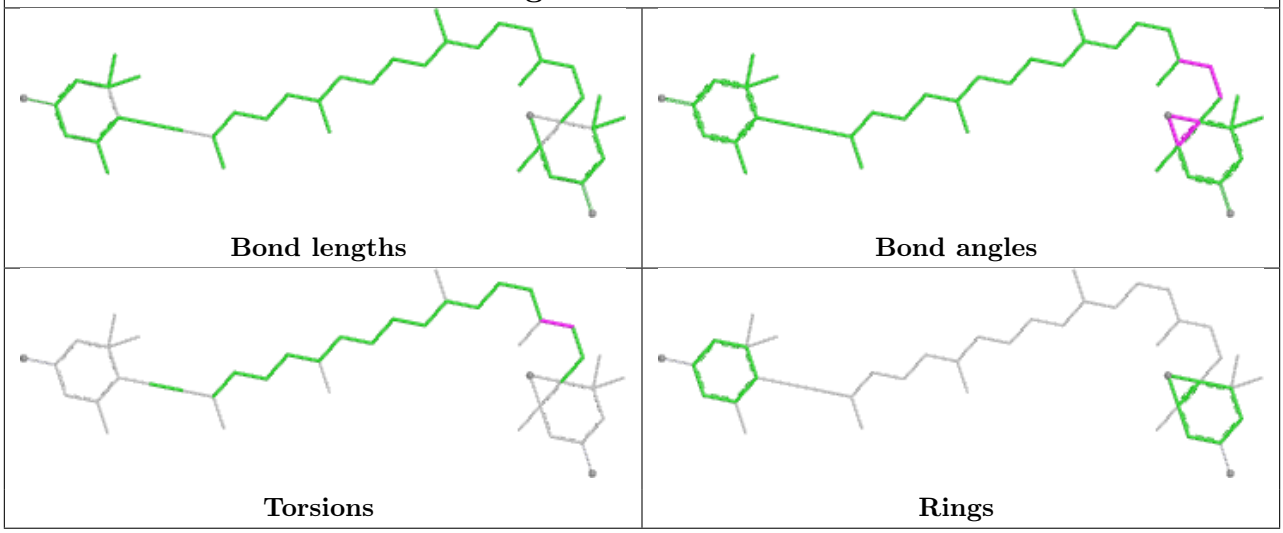


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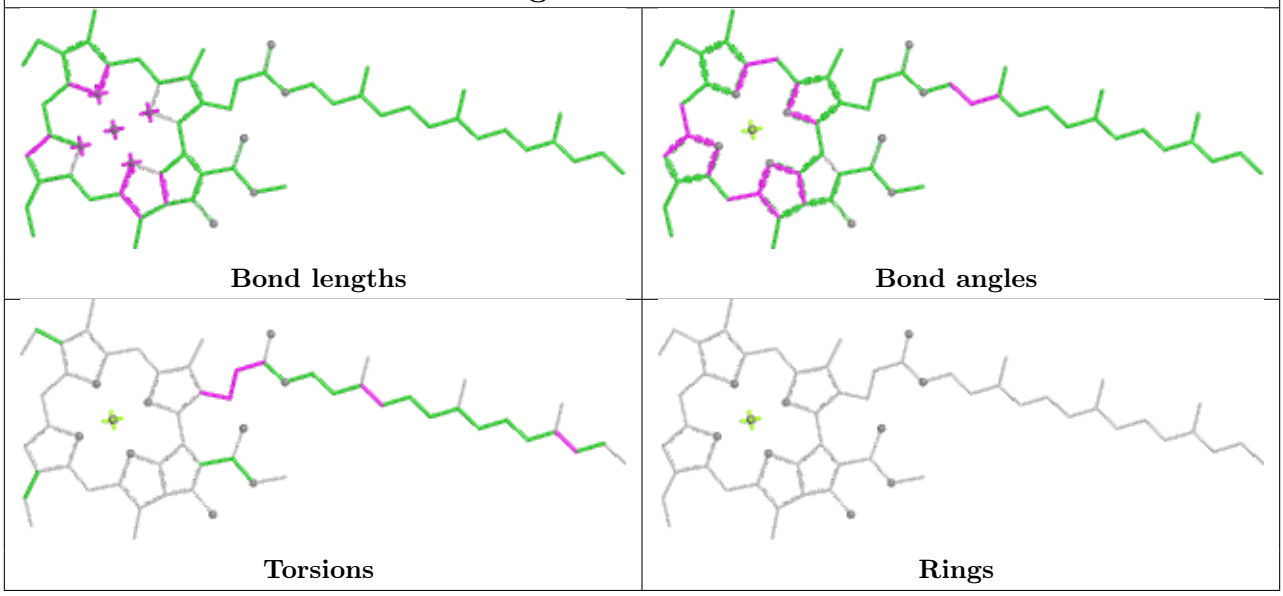


Rings

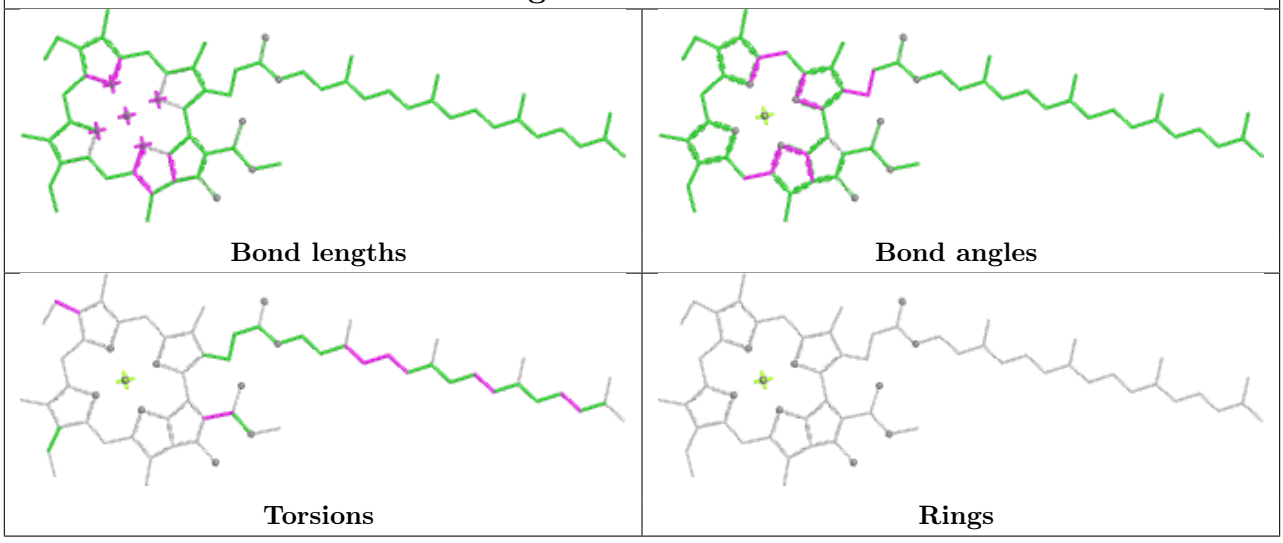
Ligand DD6 A 313



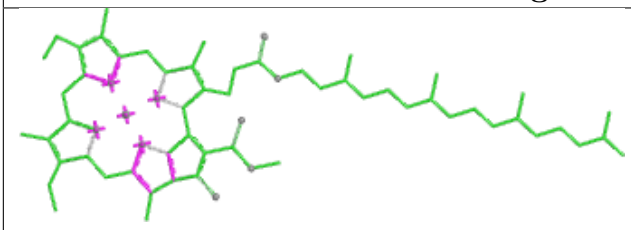
Ligand CLA a 804



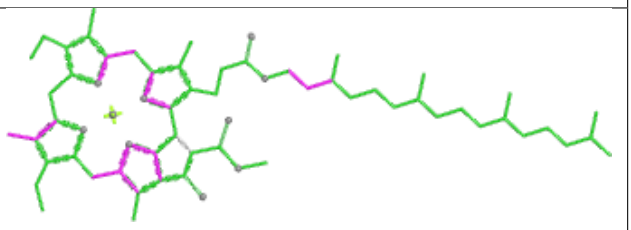
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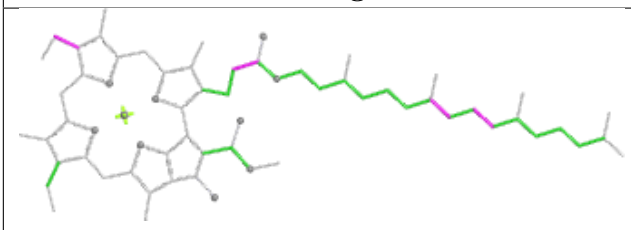
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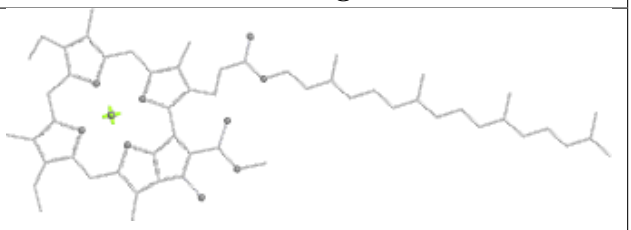
Bond lengths



Bond angles

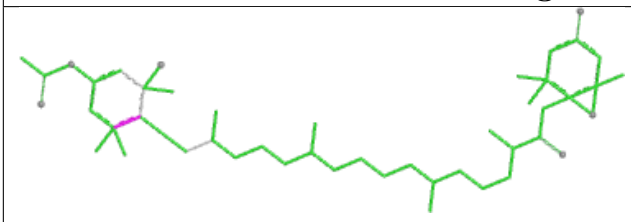


Torsions

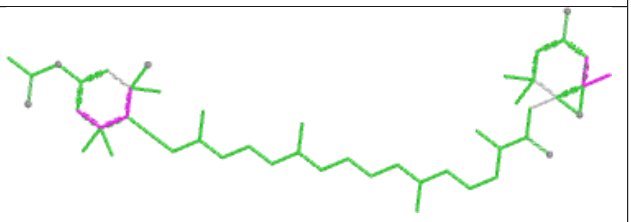


Rings

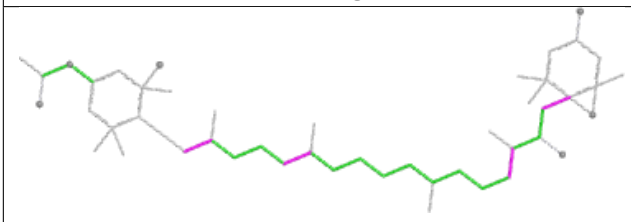
Ligand A86 t 310



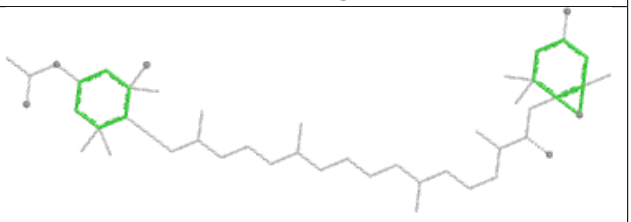
Bond lengths



Bond angles

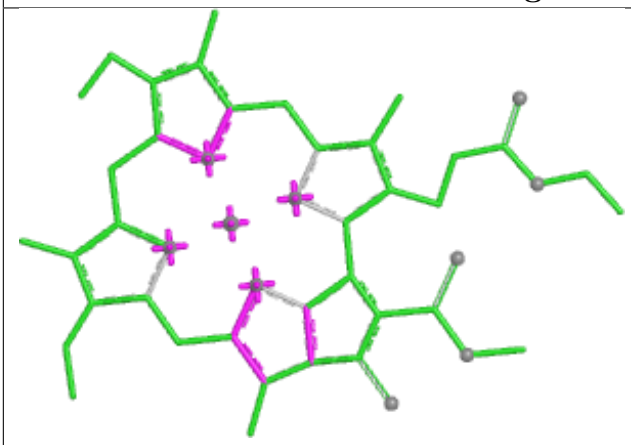


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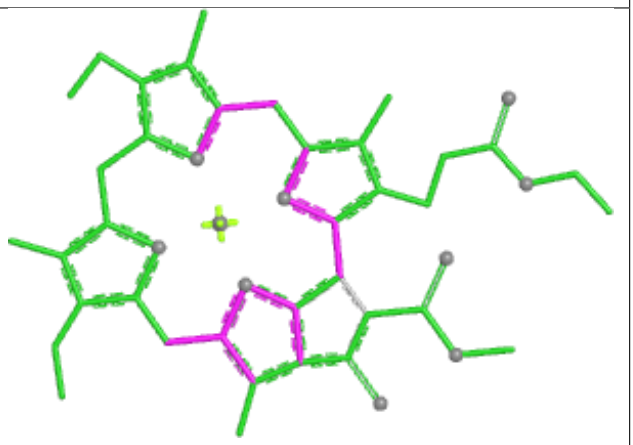


Rings

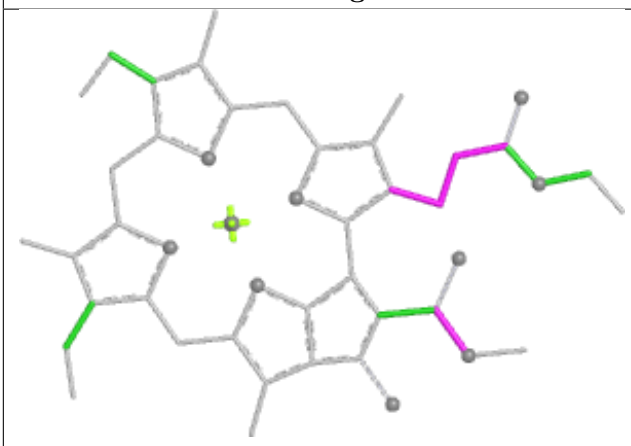
Ligand CLA B 304



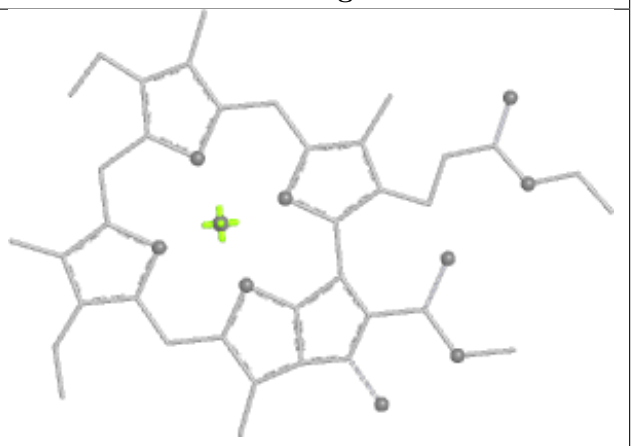
Bond lengths



Bond angles

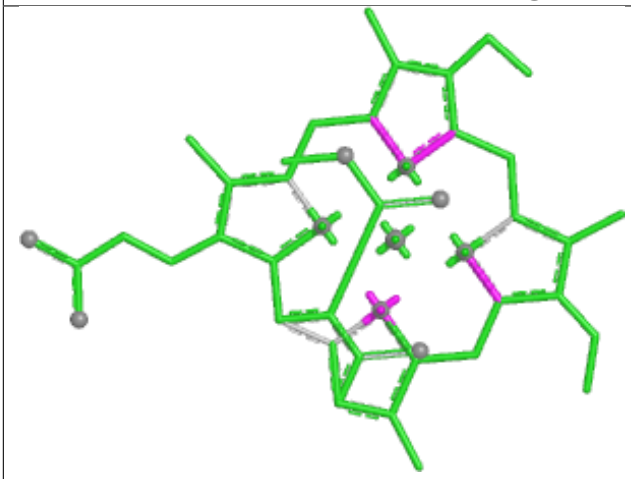


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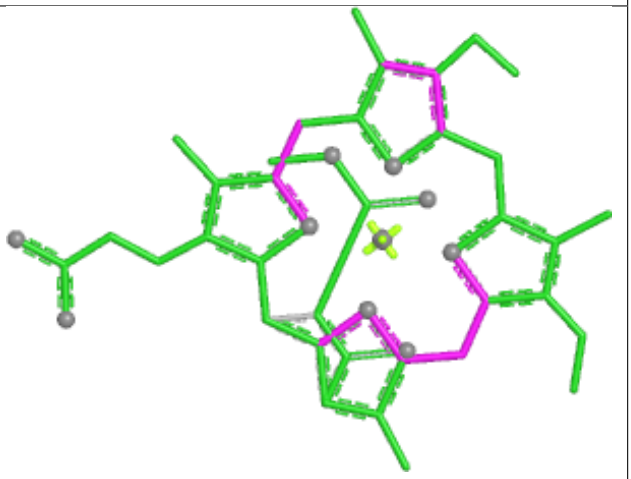


Rings

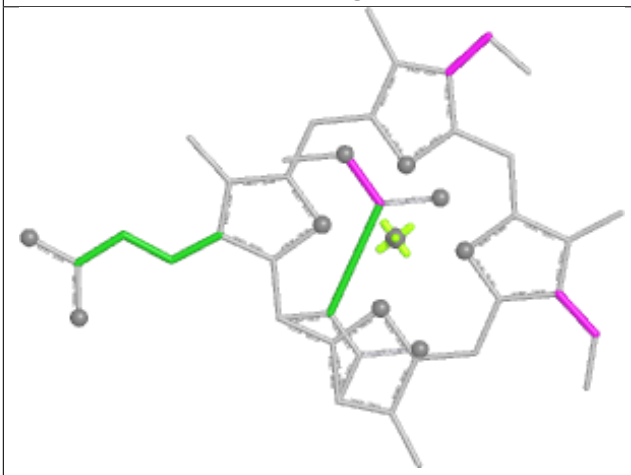
Ligand KC2 O 301



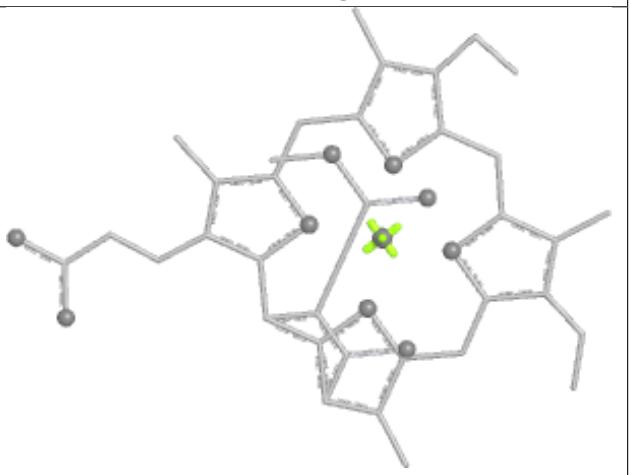
Bond lengths



Bond angles

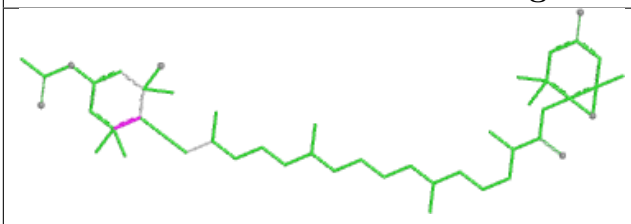


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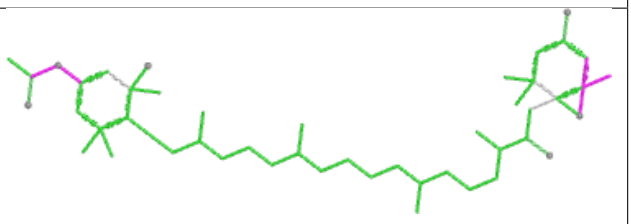


Rings

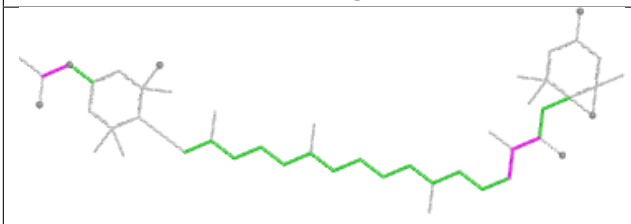
Ligand A86 X 321



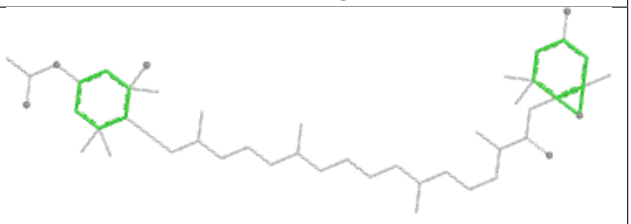
Bond lengths



Bond angles

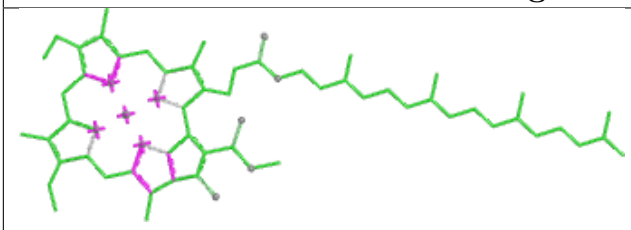


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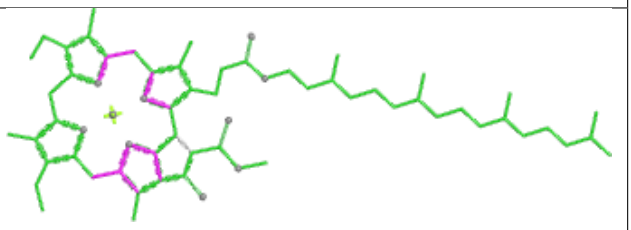


Rings

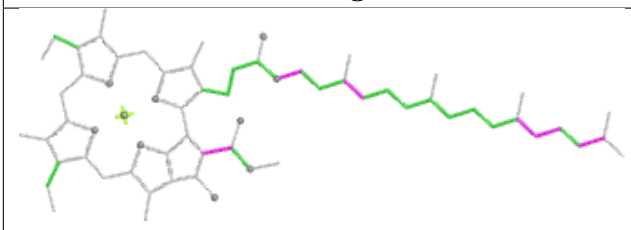
Ligand CLA a 839



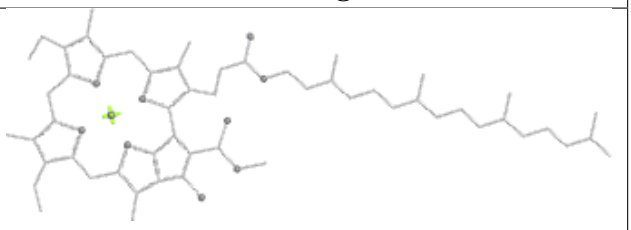
Bond lengths



Bond angles

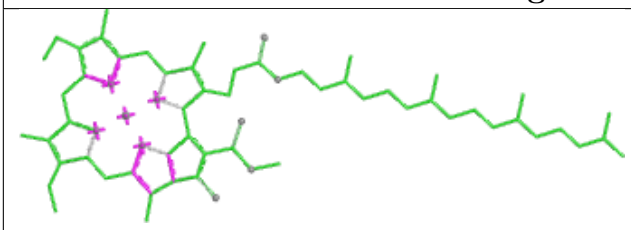


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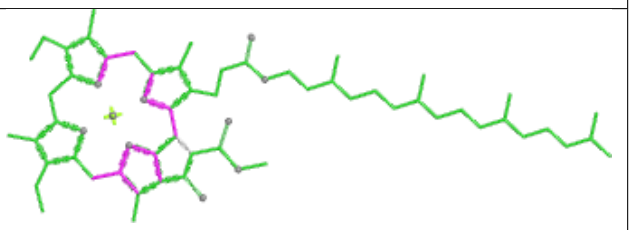


Rings

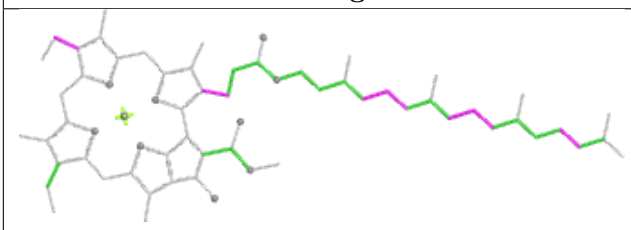
Ligand CLA x 302



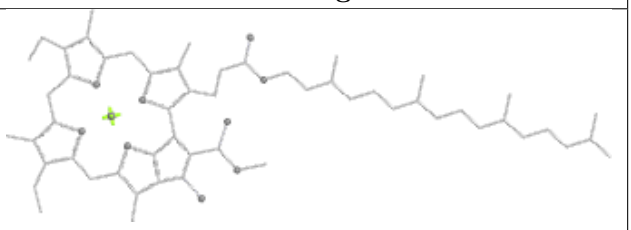
Bond lengths



Bond angles

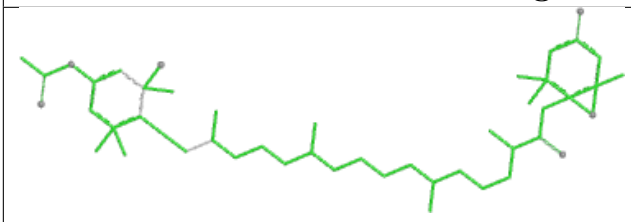


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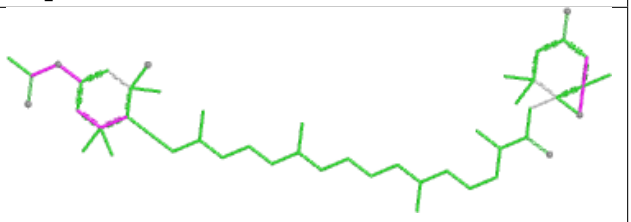


Rings

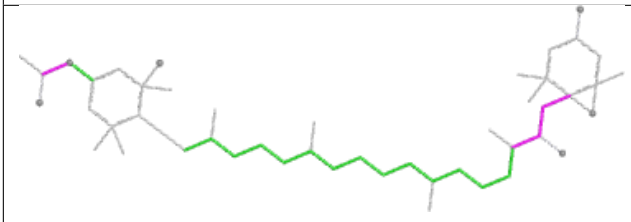
Ligand A86 p 316



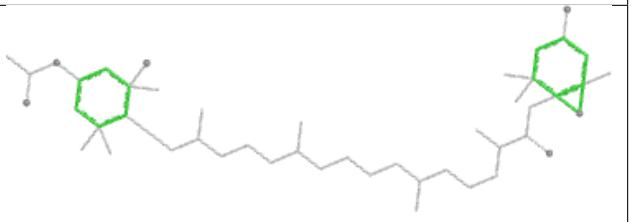
Bond lengths



Bond angles

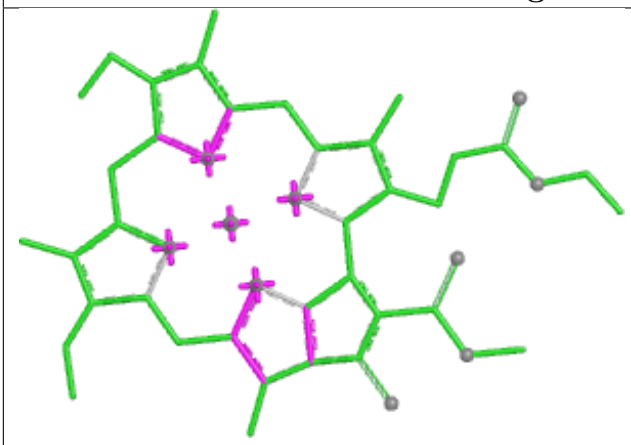


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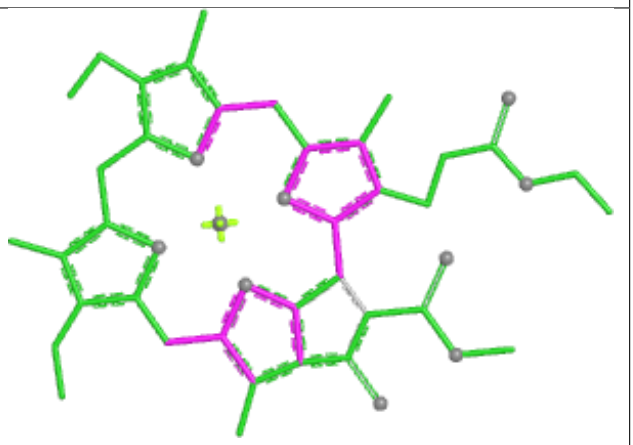


Rings

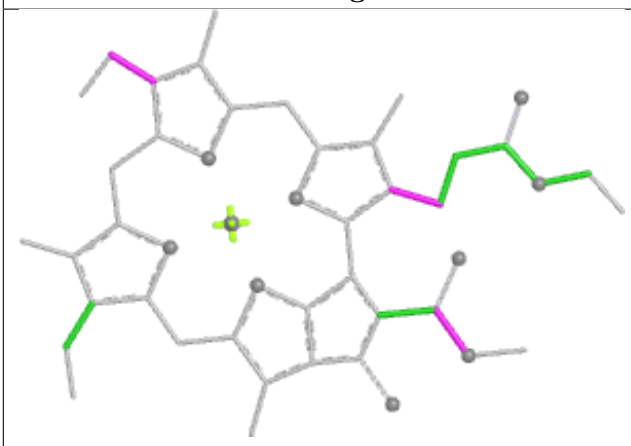
Ligand CLA S 311



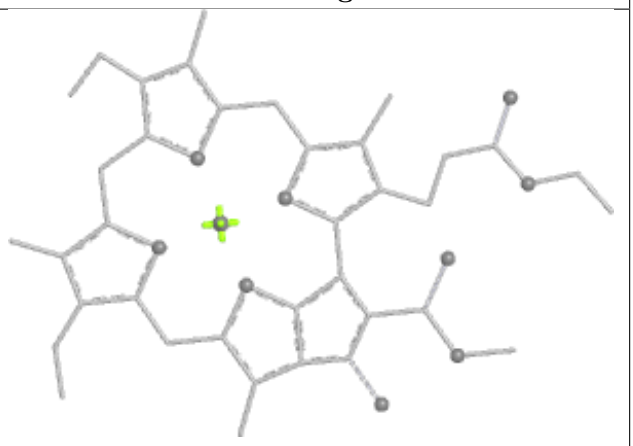
Bond lengths



Bond angles

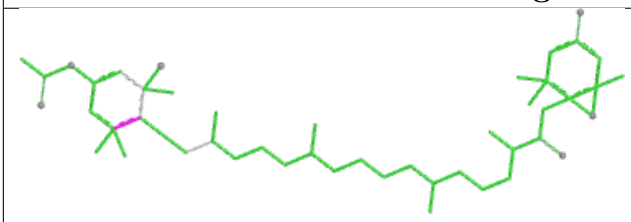


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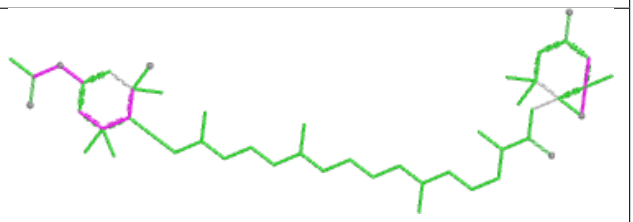


Rings

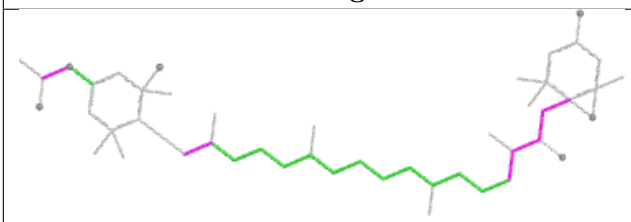
Ligand A86 u 319



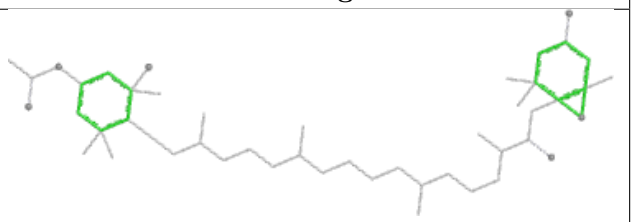
Bond lengths



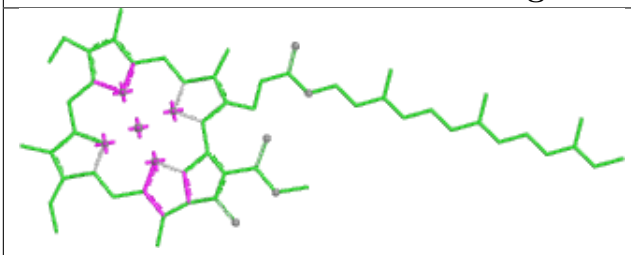
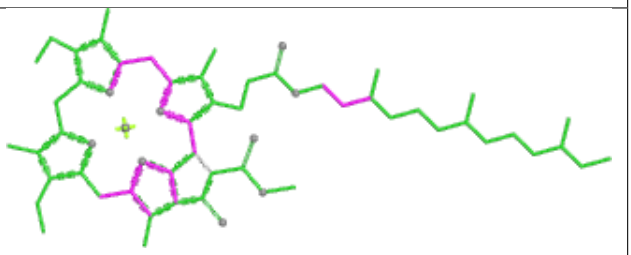
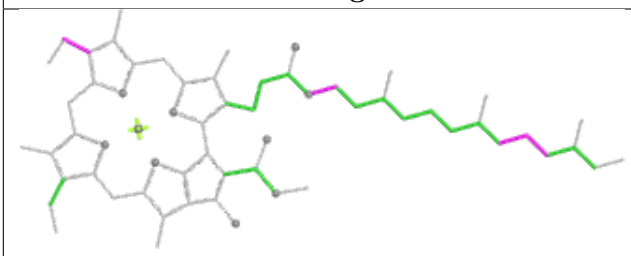
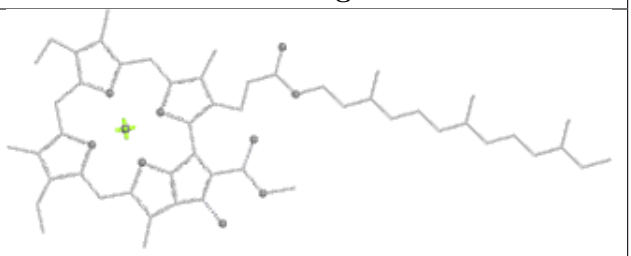
Bond angles

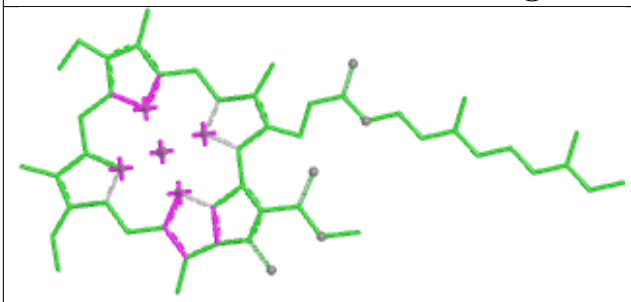
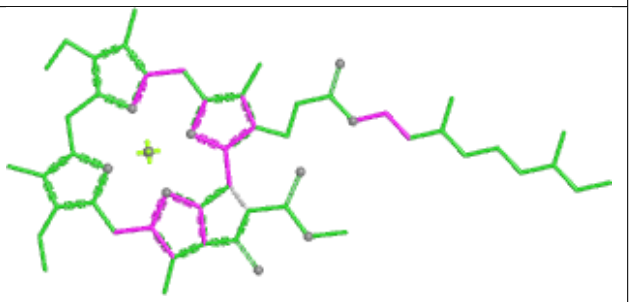
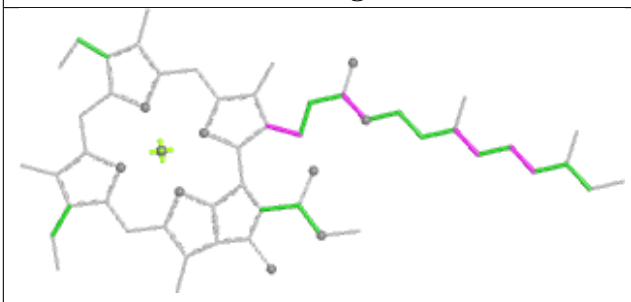
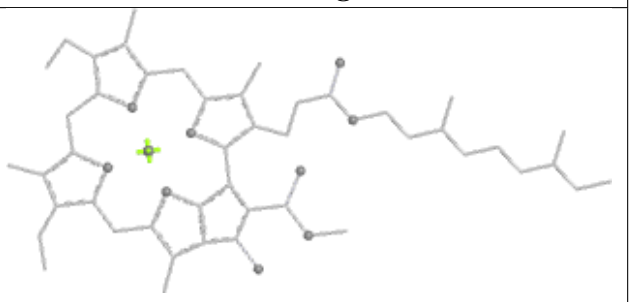


Torsions

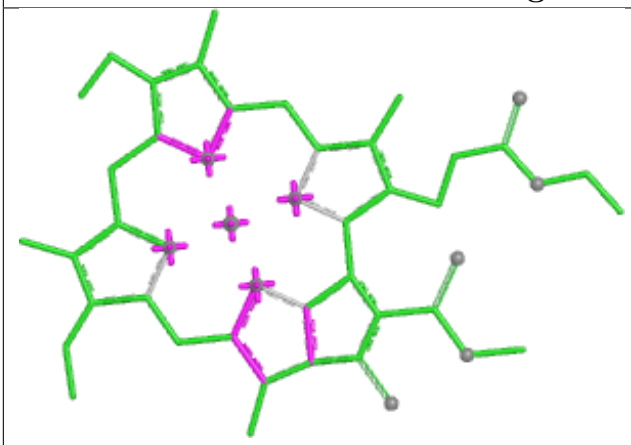


Rings

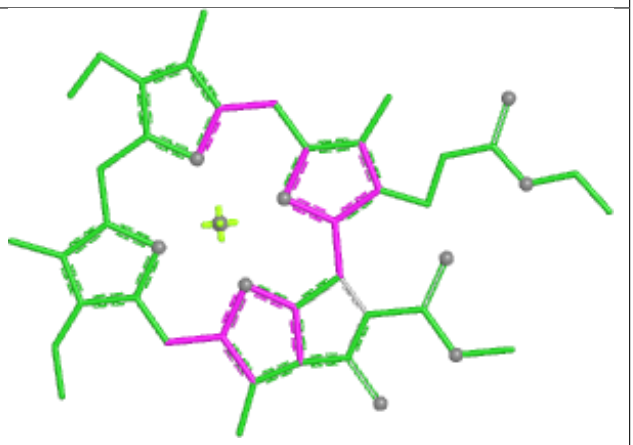
Ligand CLA b 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

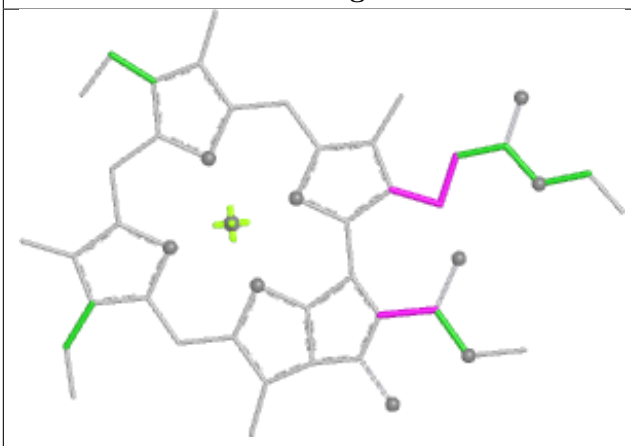
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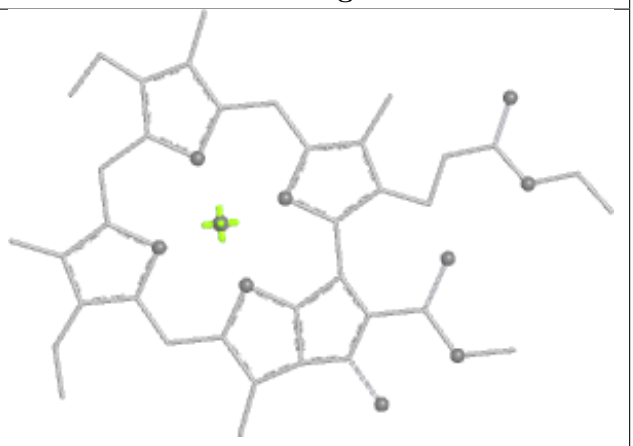
Bond lengths



Bond angles

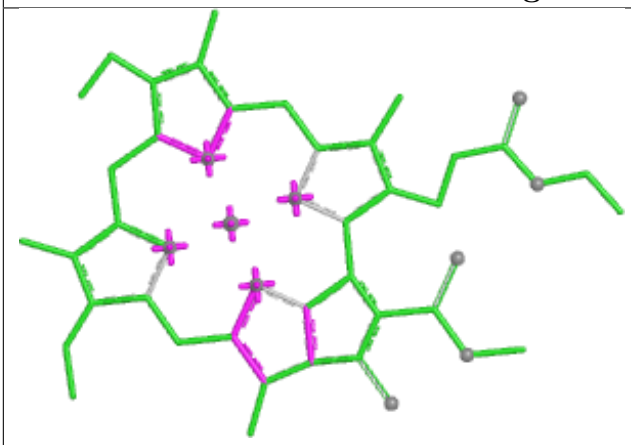


Torsions

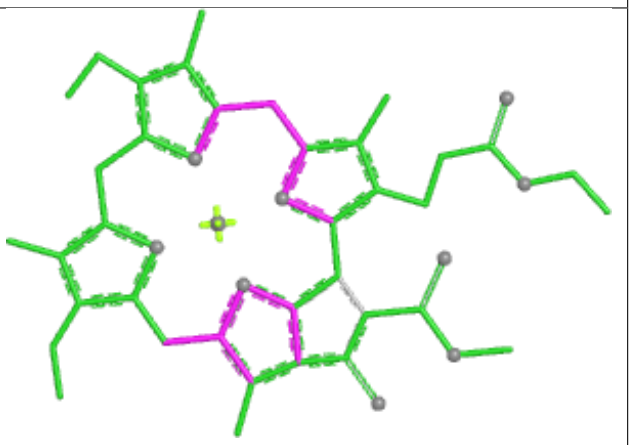


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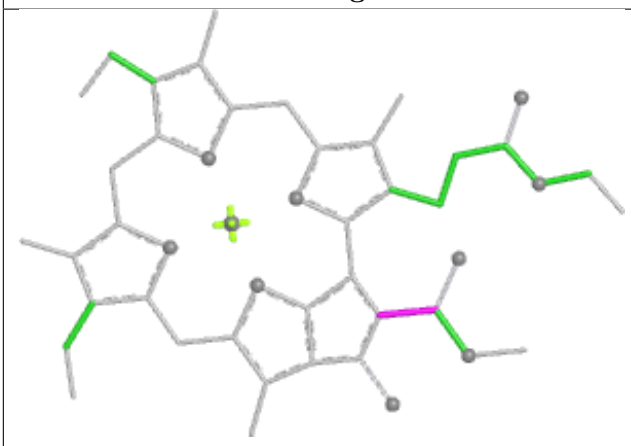
Ligand CLA K 312



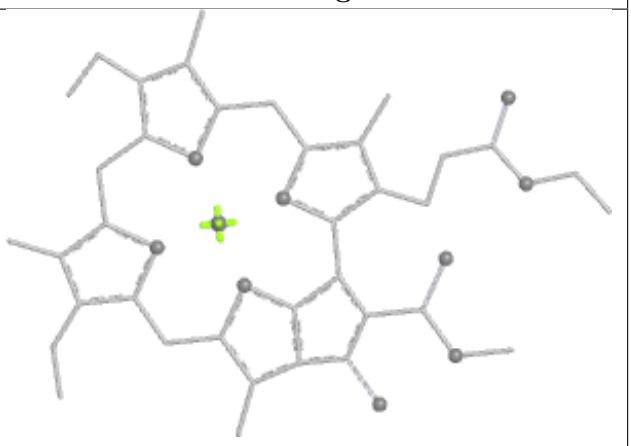
Bond lengths



Bond angles

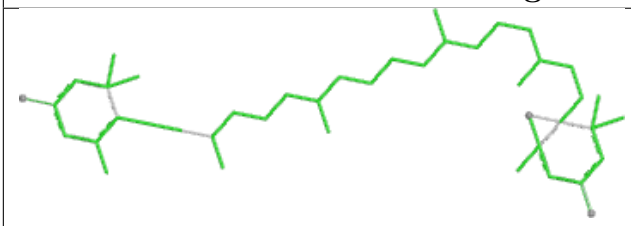


Torsions



Rings

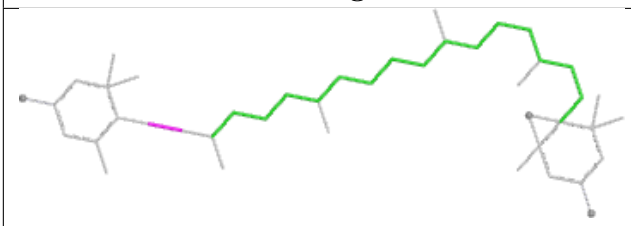
Ligand DD6 G 210



Bond lengths



Bond angles

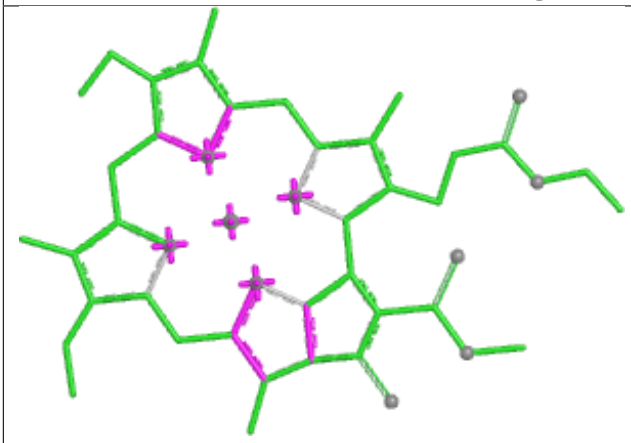


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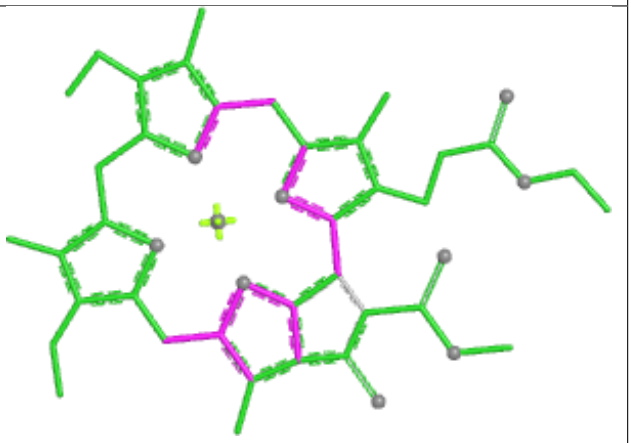


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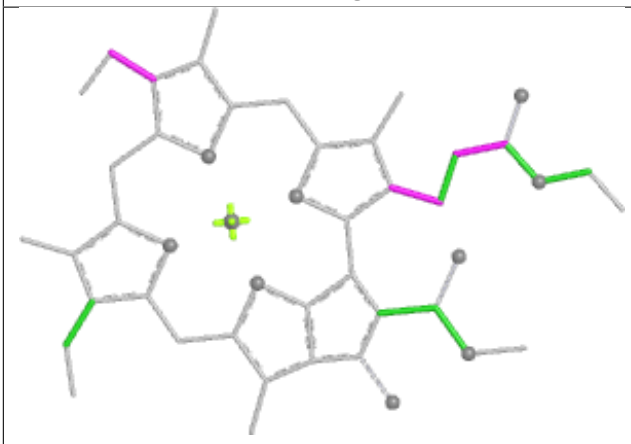
Ligand CLA I 207



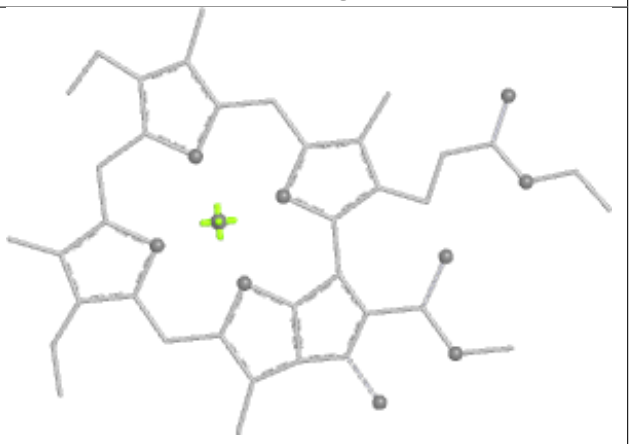
Bond lengths



Bond angles

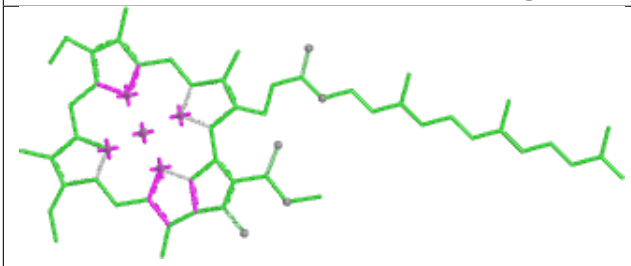


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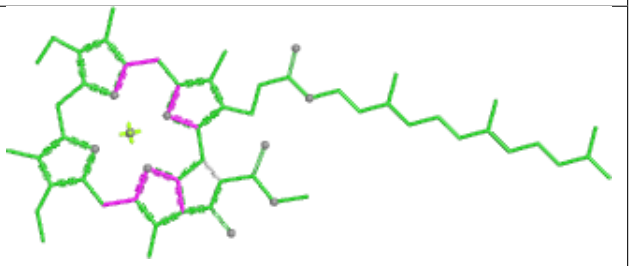


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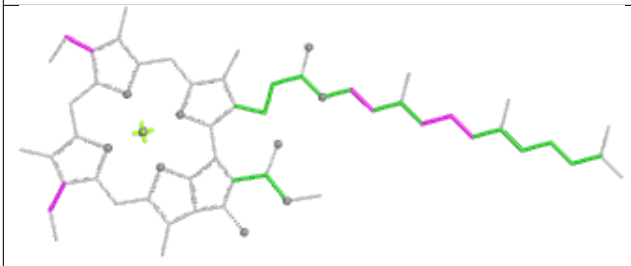
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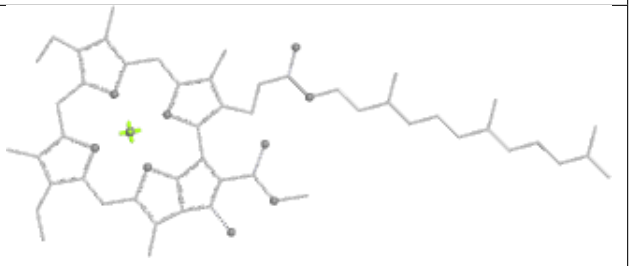
Bond lengths



Bond angles

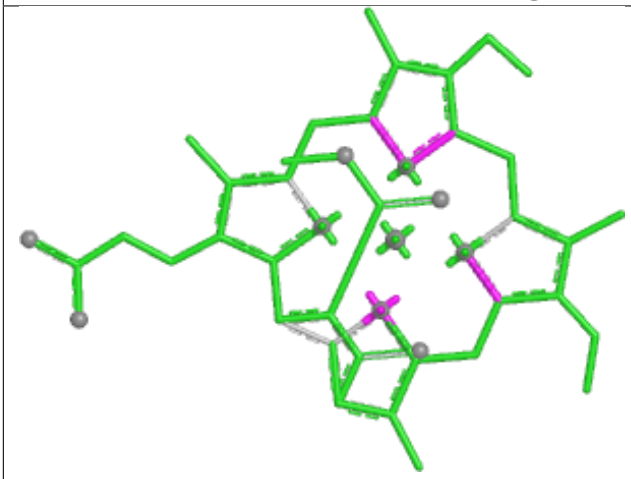


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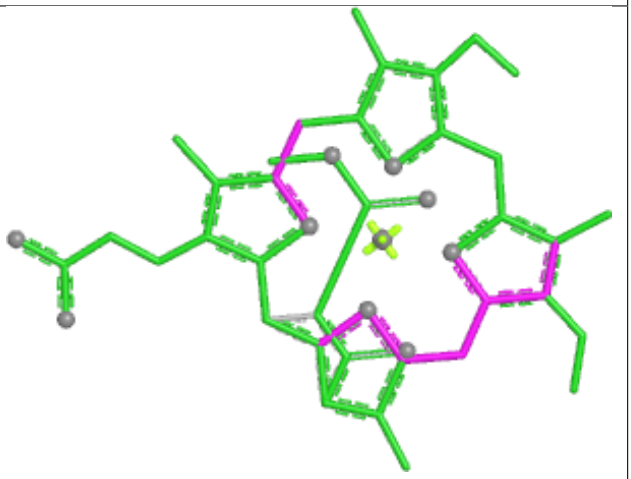


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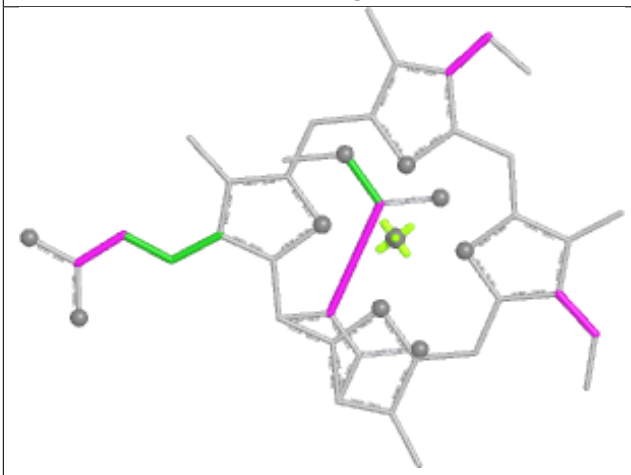
Ligand KC2 Y 308



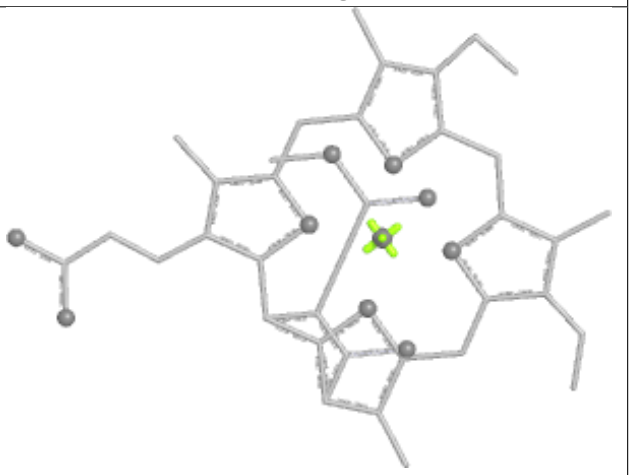
Bond lengths



Bond angles

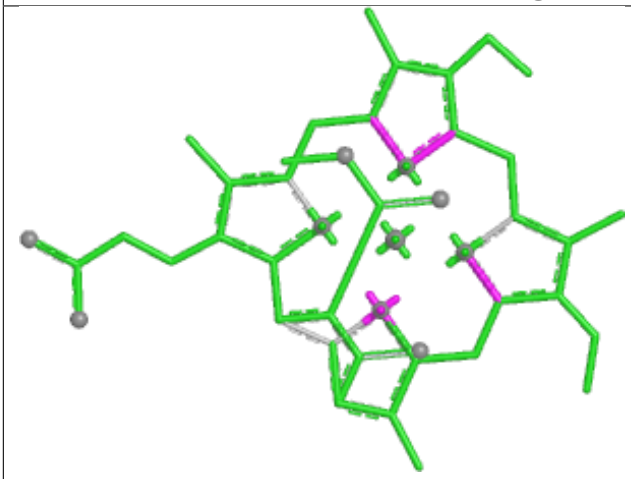


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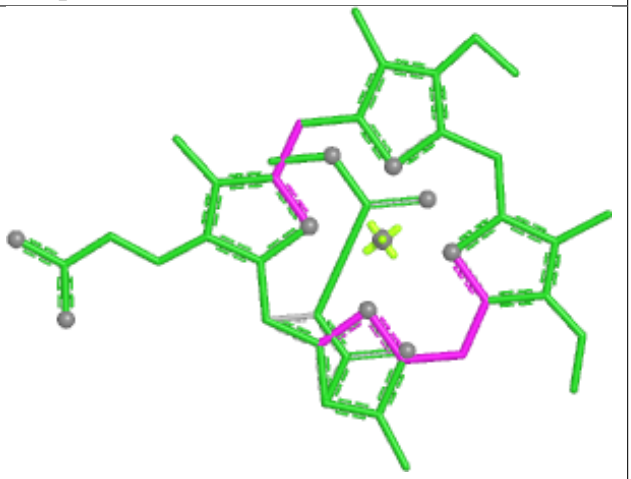


Rings

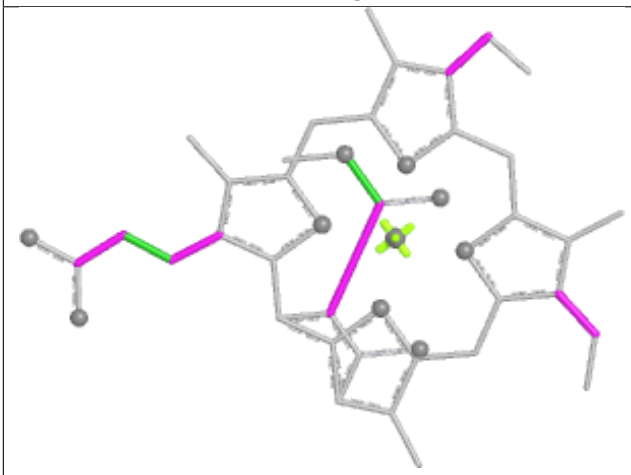
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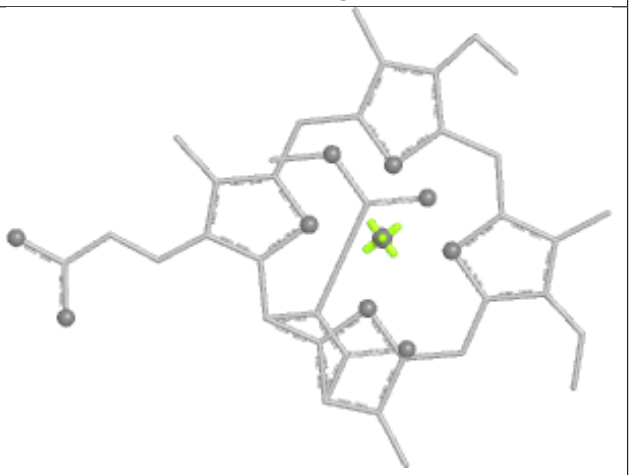
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Bond angles

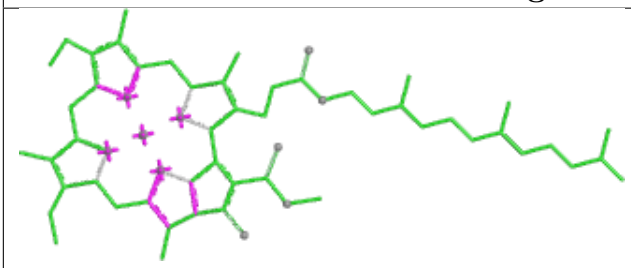


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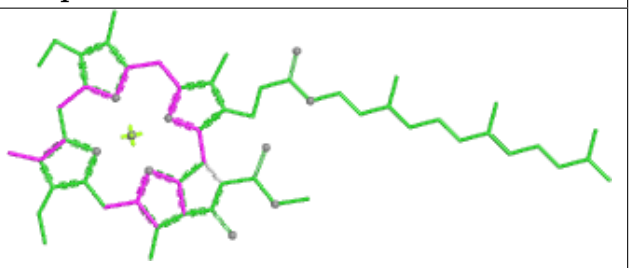


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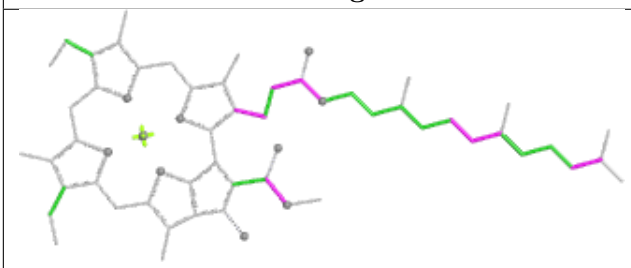
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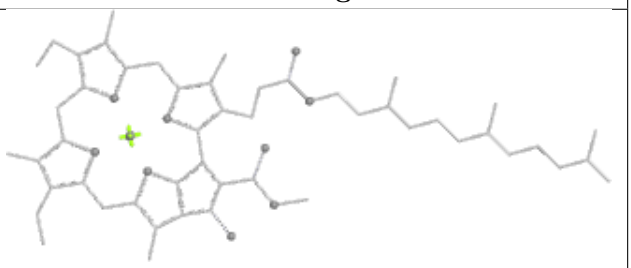
Bond lengths



Bond angles

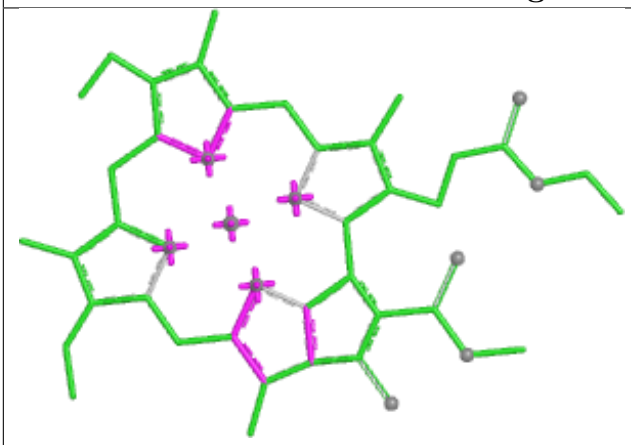


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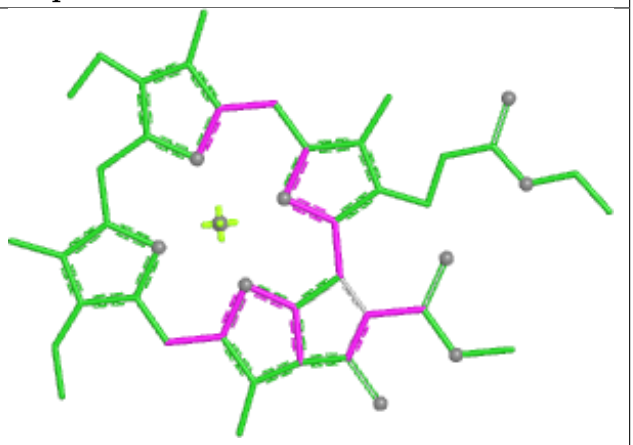


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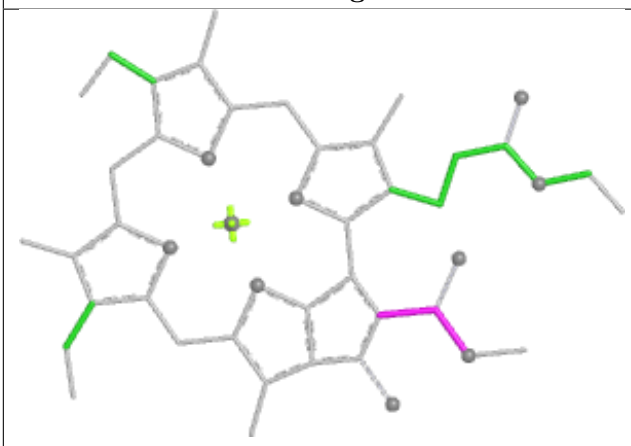
Ligand CLA p 312



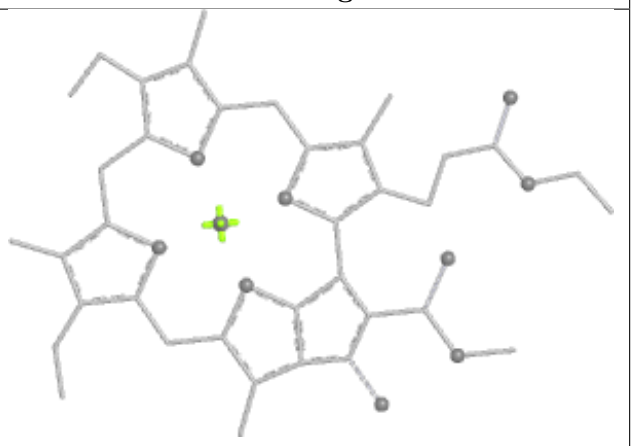
Bond lengths



Bond angles

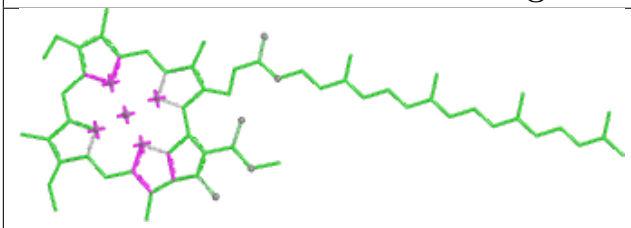


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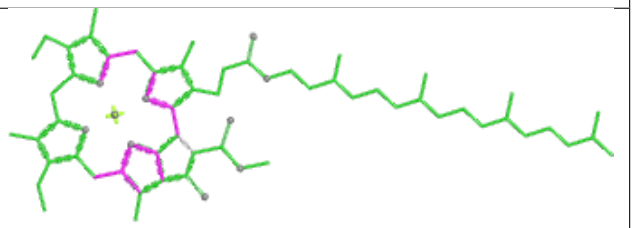


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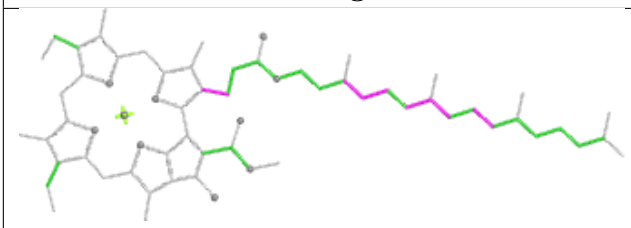
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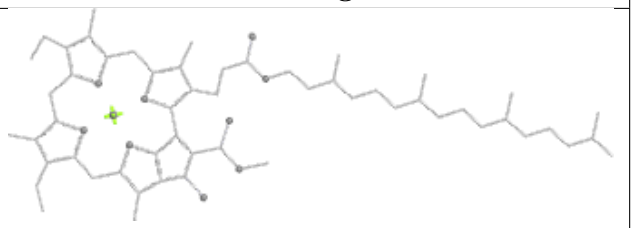
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Bond angles

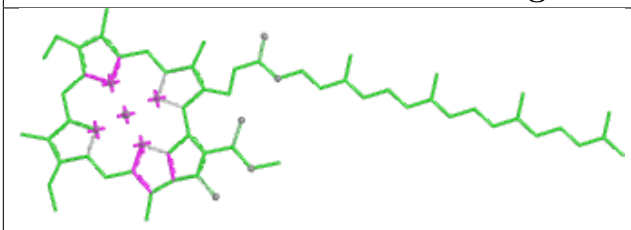


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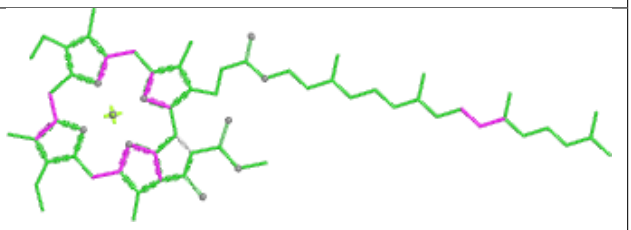


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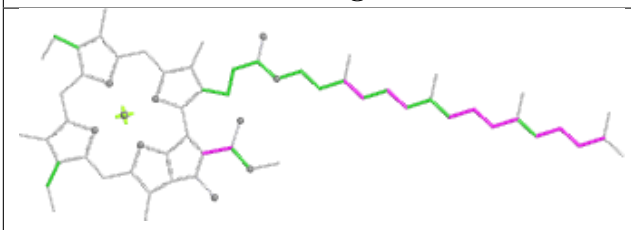
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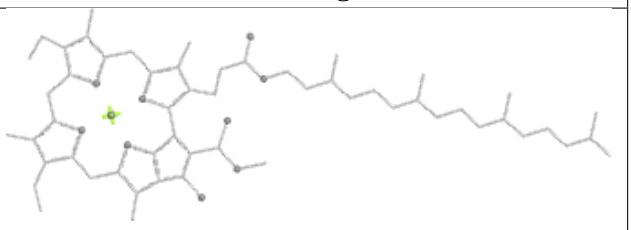
Bond lengths



Bond angles

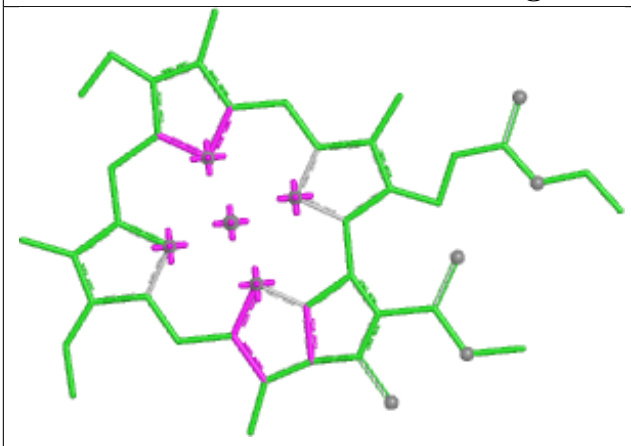


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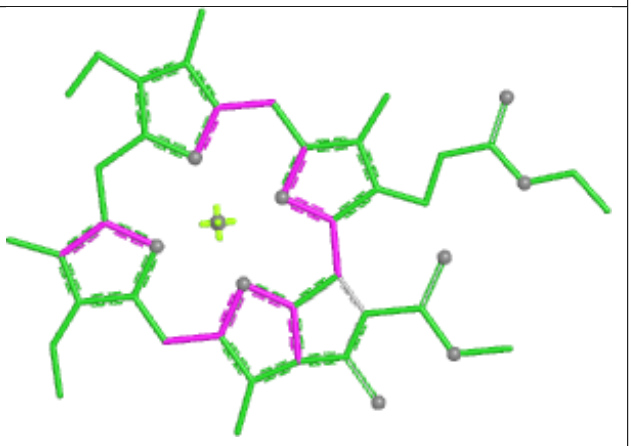


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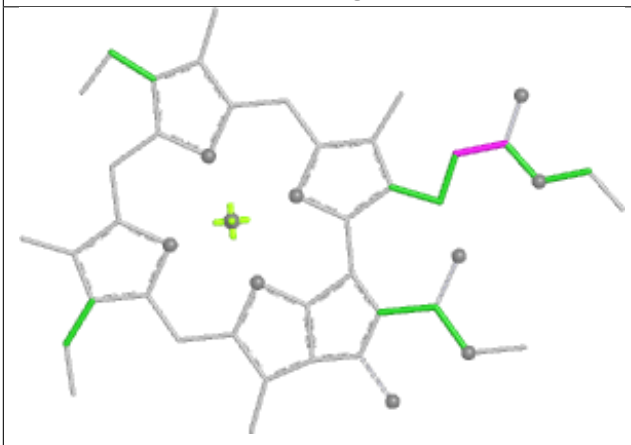
Ligand CLA P 306



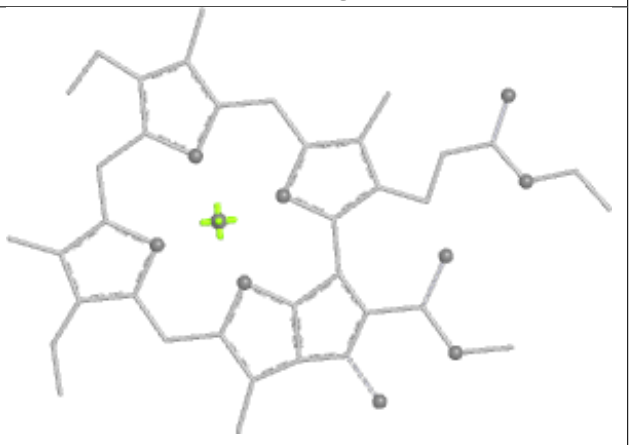
Bond lengths



Bond angles

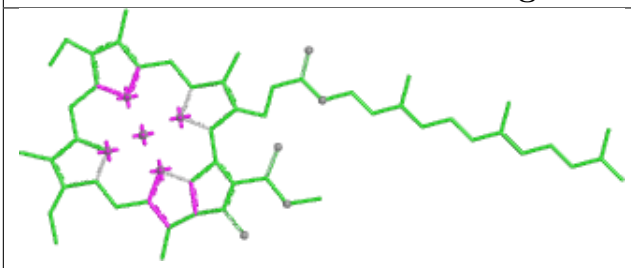


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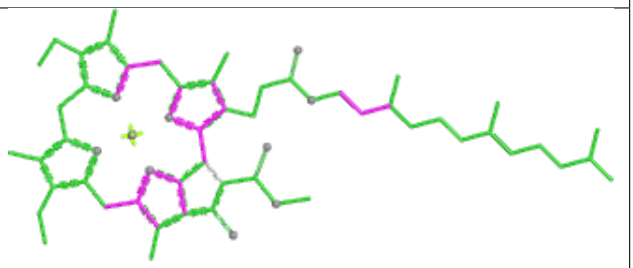


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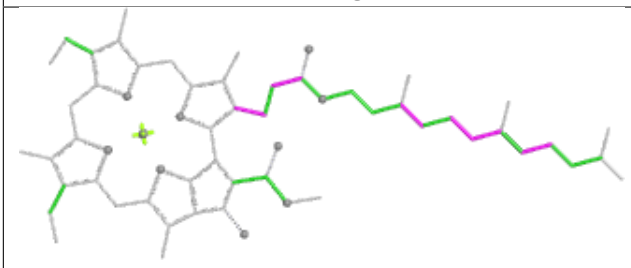
Ligand CLA W 308



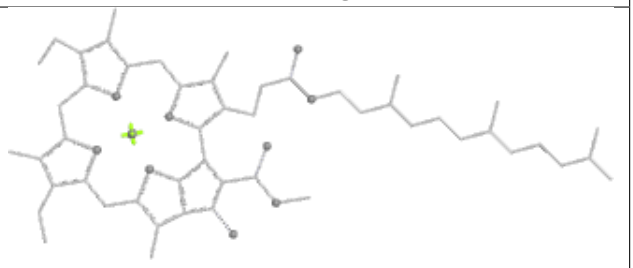
Bond lengths



Bond angles

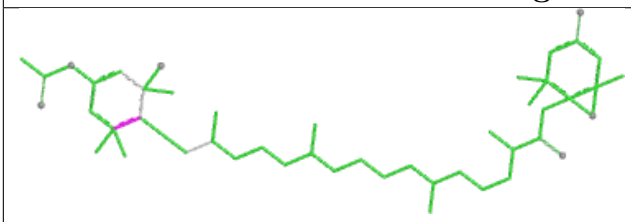


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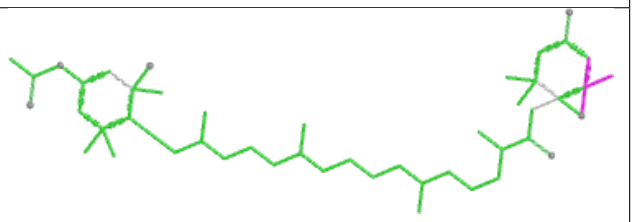


Rings

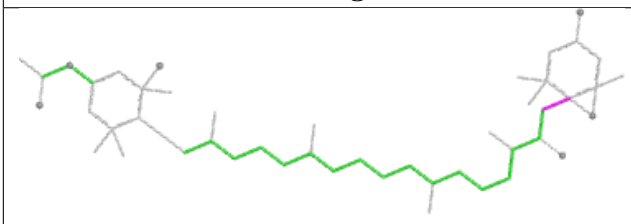
Ligand A86 u 317



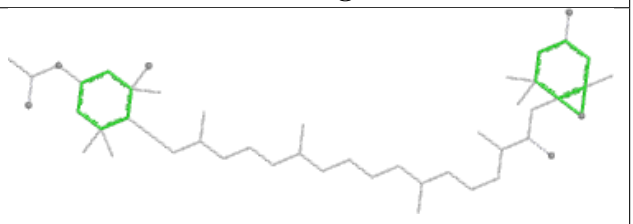
Bond lengths



Bond angles

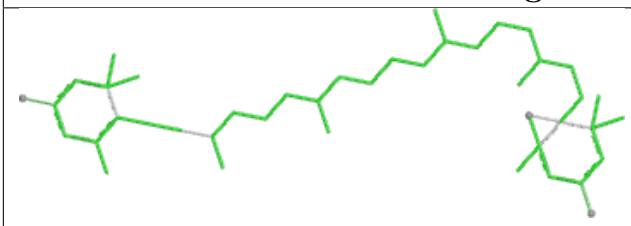


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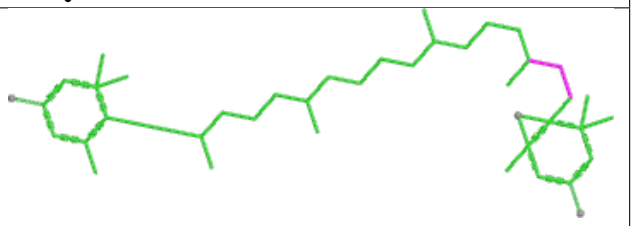


Rings

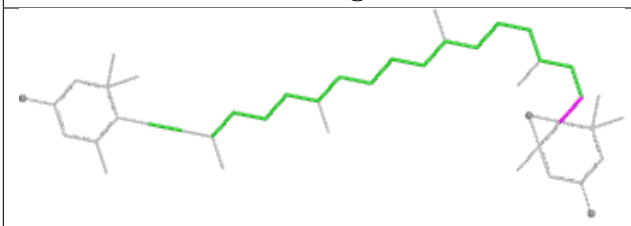
Ligand DD6 Q 214



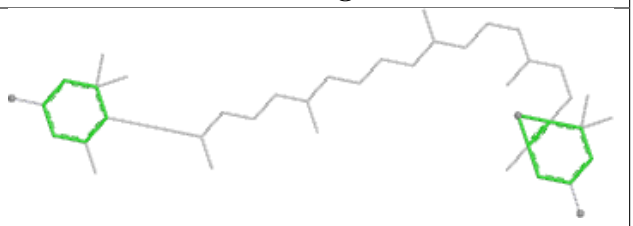
Bond lengths



Bond angles

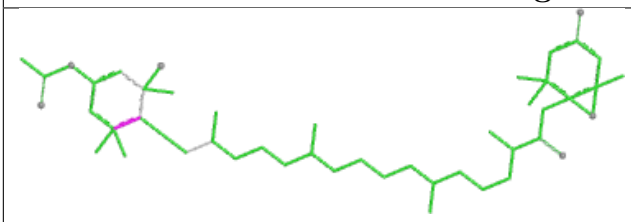


Torsions

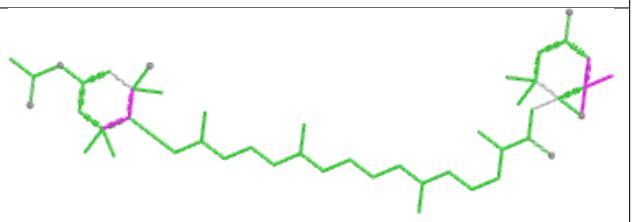


Rings

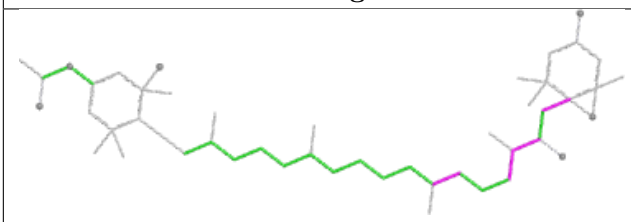
Ligand A86 o 315



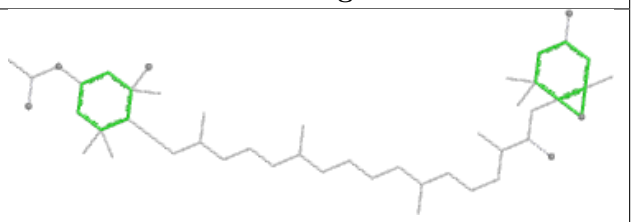
Bond lengths



Bond angles

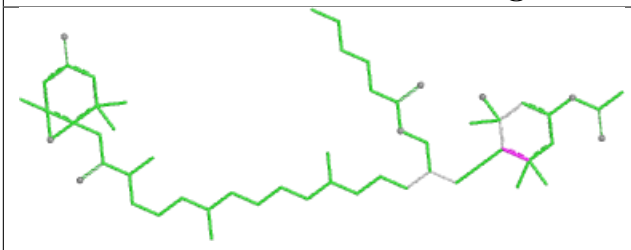


Torsions



Rings

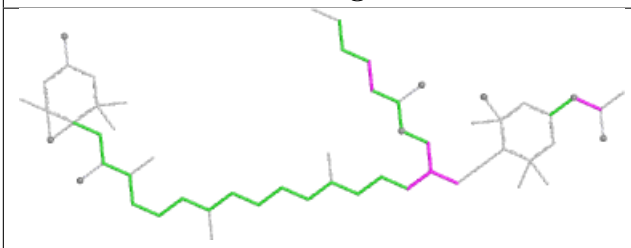
Ligand A1EB1 L 316



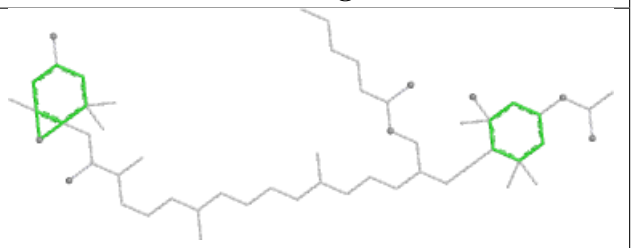
Bond lengths



Bond angles

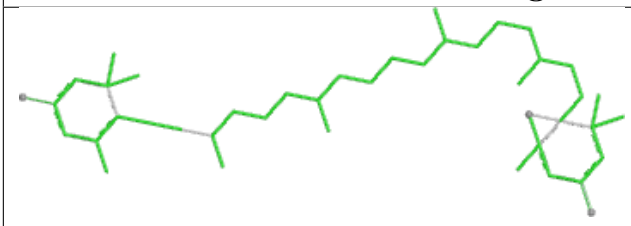


Torsions



Rings

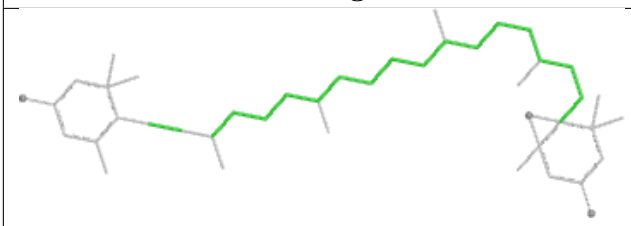
Ligand DD6 L 315



Bond lengths



Bond angles

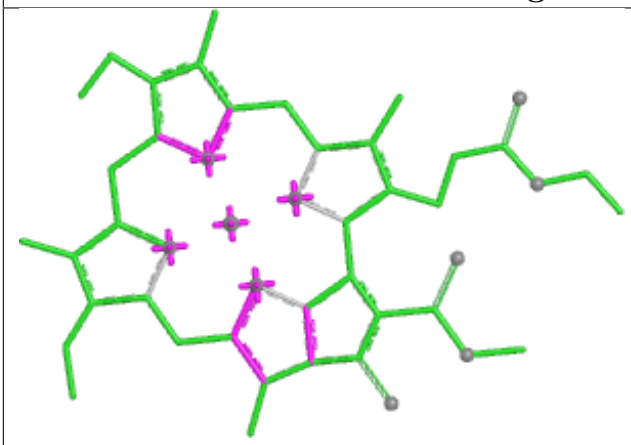


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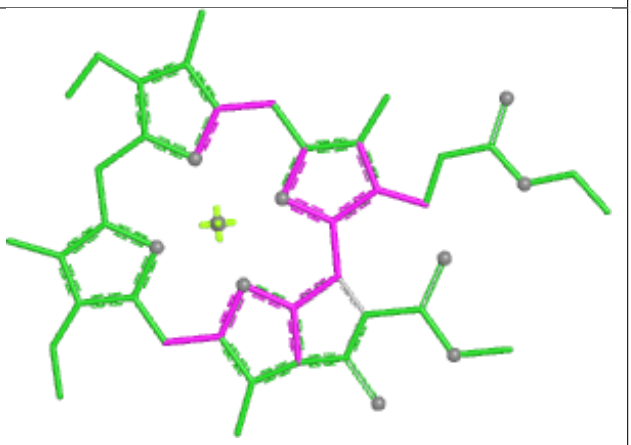


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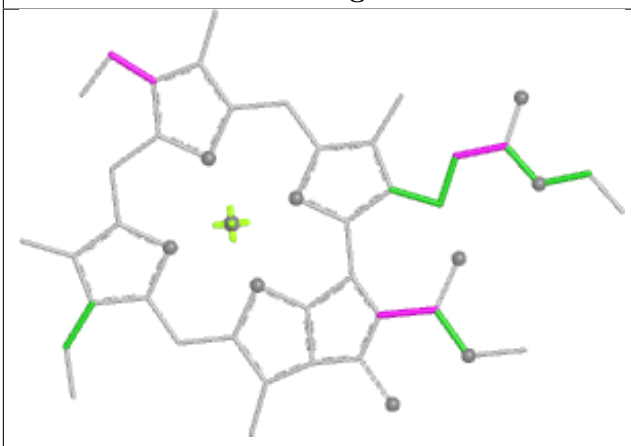
Ligand CLA b 816



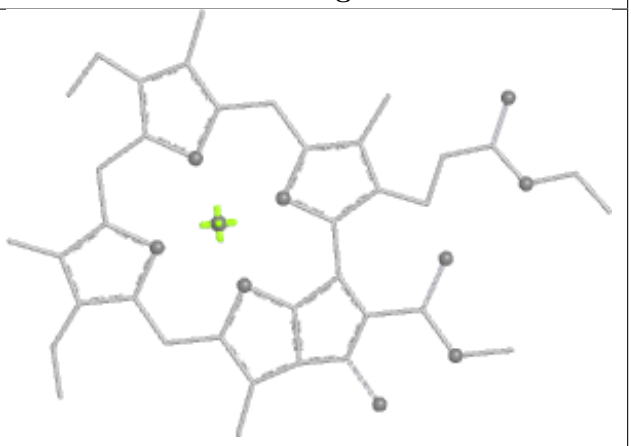
Bond lengths



Bond angles

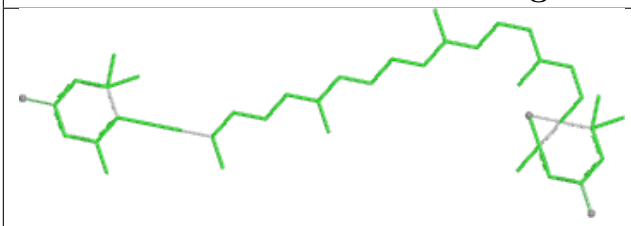


Torsions



Rings

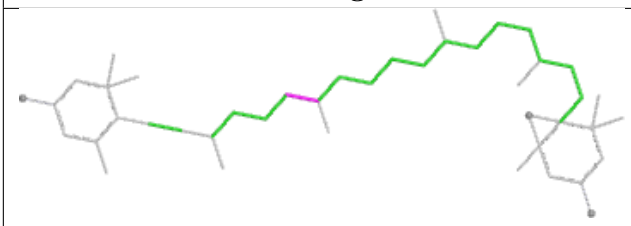
Ligand DD6 z 321



Bond lengths



Bond angles

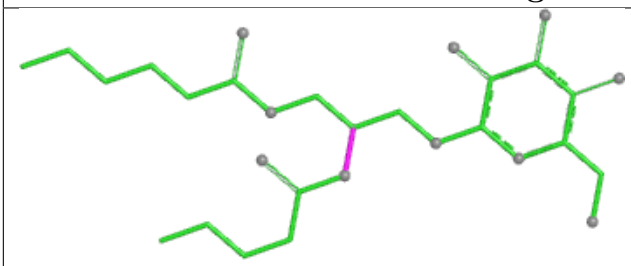


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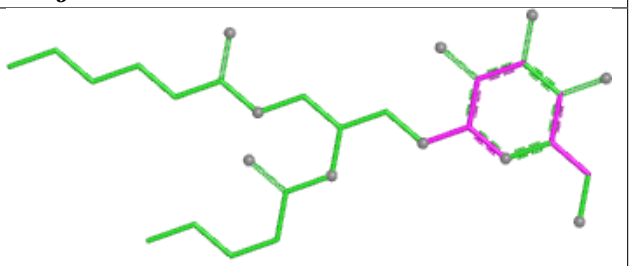


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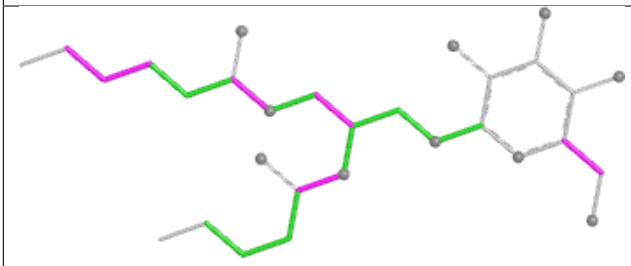
Ligand LMG j 101



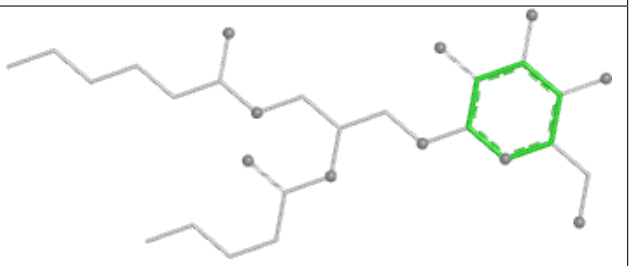
Bond lengths



Bond angles

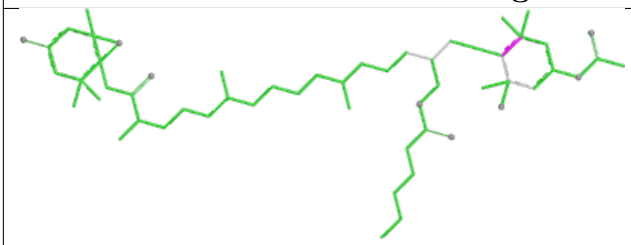


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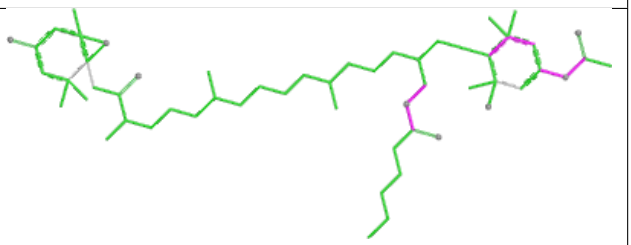


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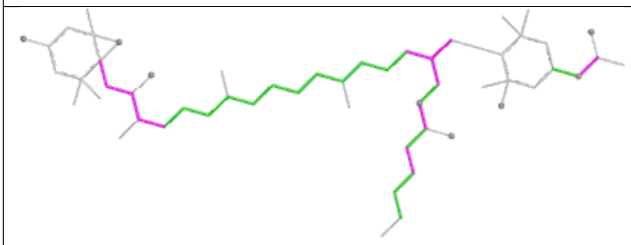
Ligand A1EB1 t 314



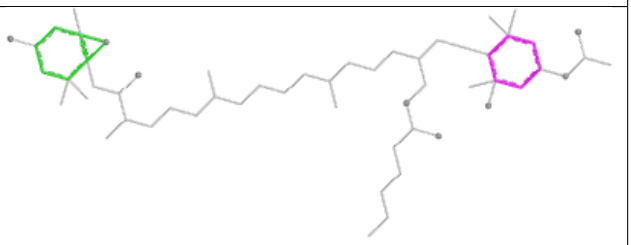
Bond lengths



Bond angles

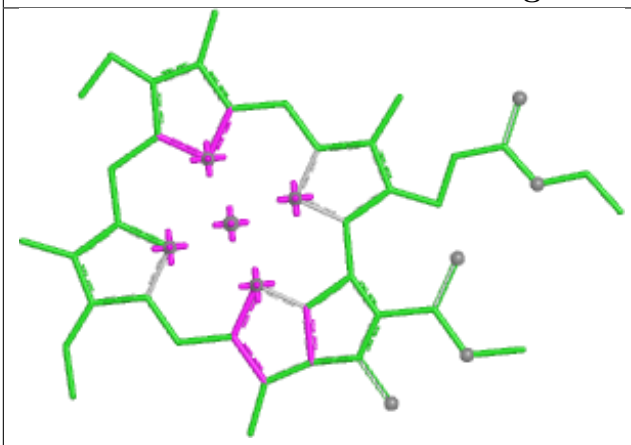


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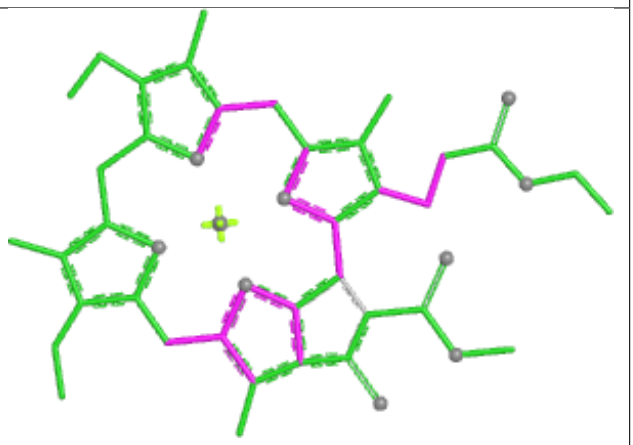


Rings

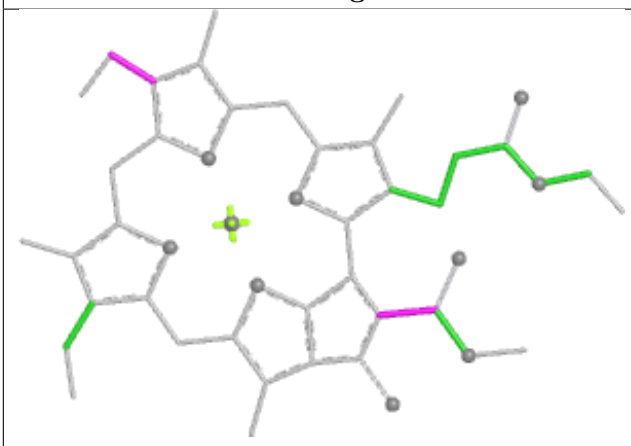
Ligand CLA U 205



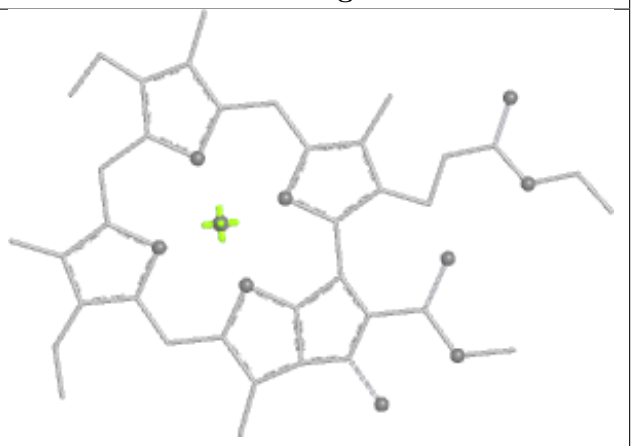
Bond lengths



Bond angles

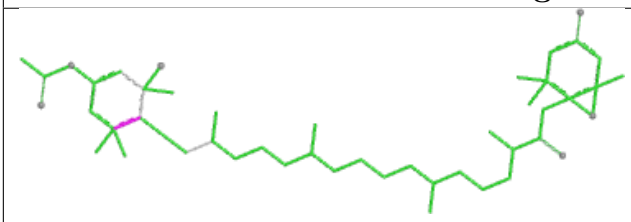


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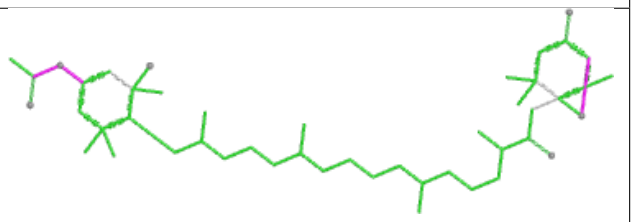


Rings

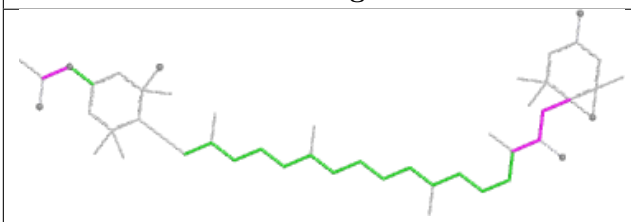
Ligand A86 x 318



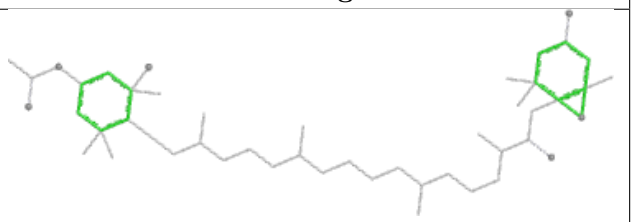
Bond lengths



Bond angles

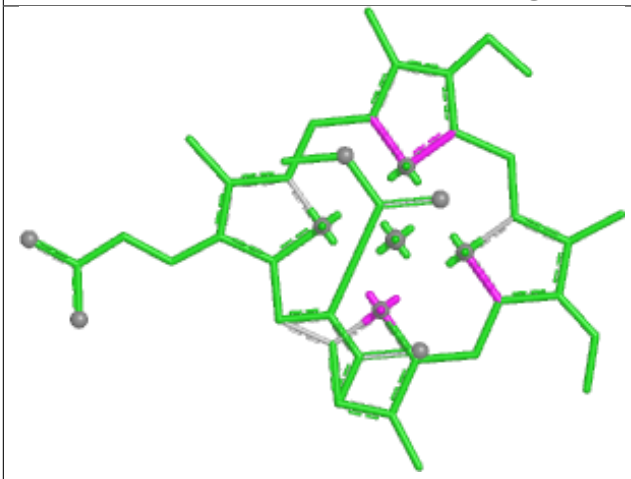


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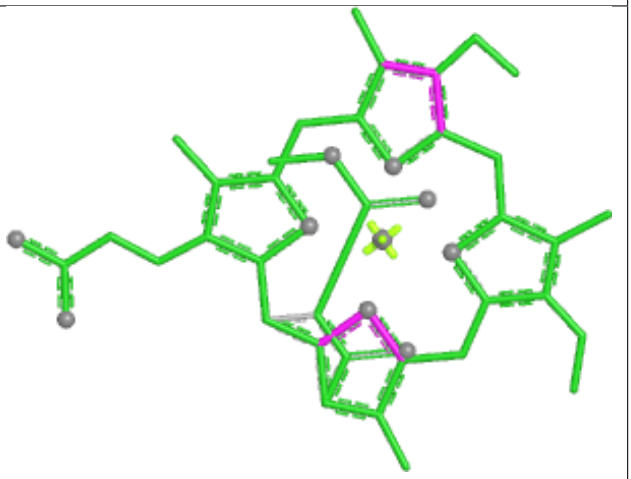


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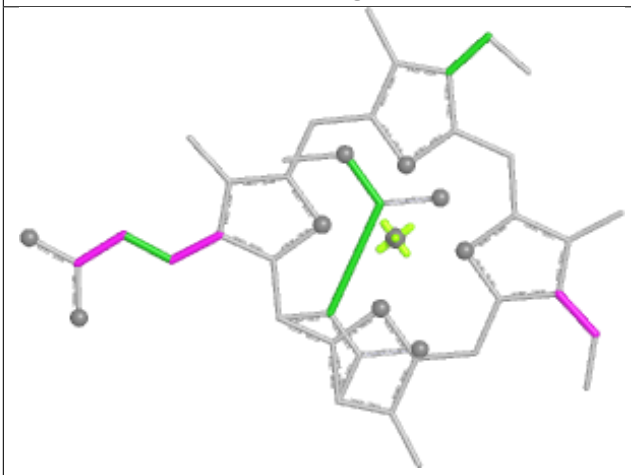
Ligand KC2 X 309



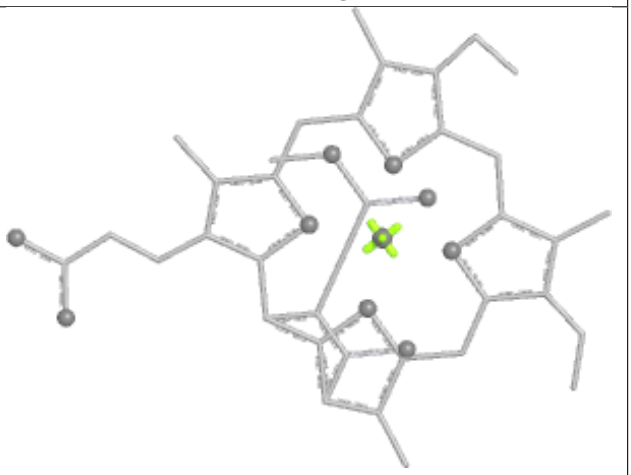
Bond lengths



Bond angles

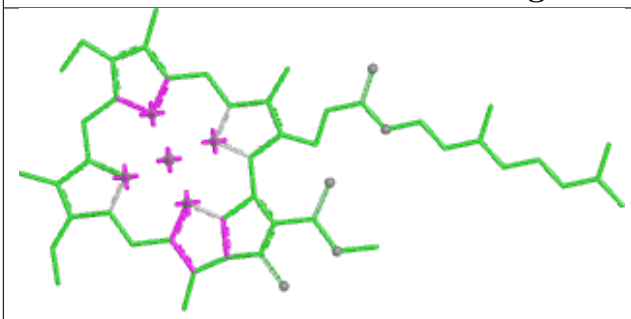


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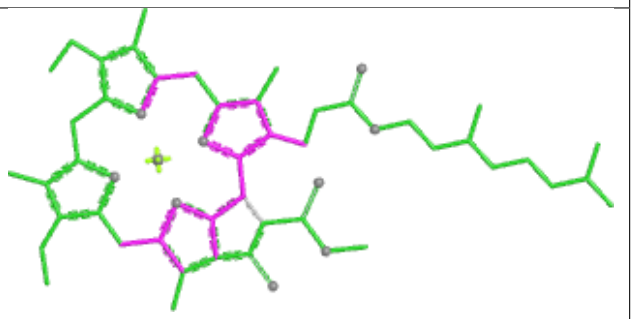


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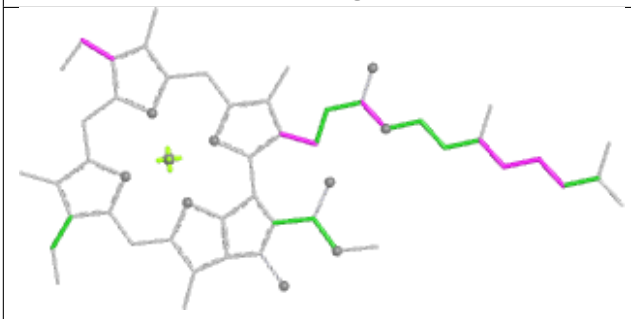
Ligand CLA x 311



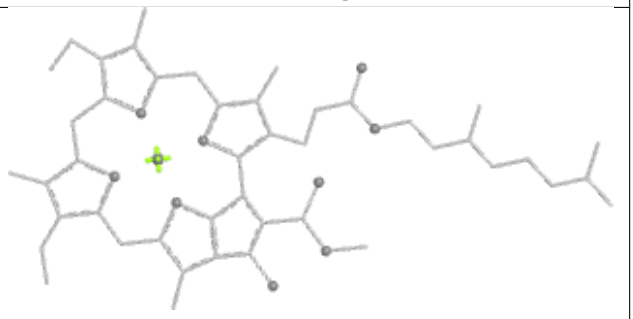
Bond lengths



Bond angles

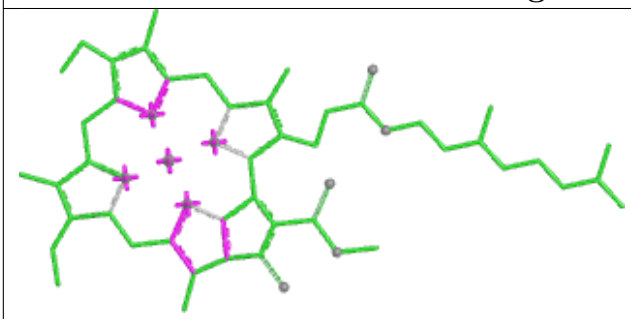


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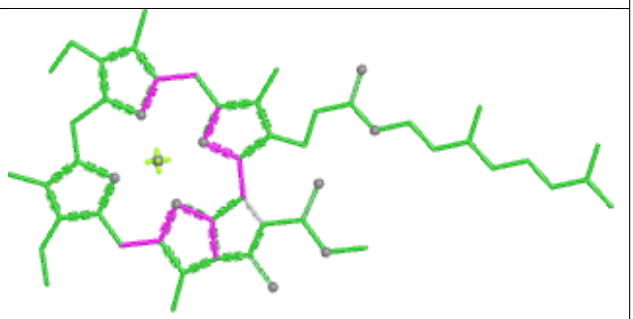


Rings

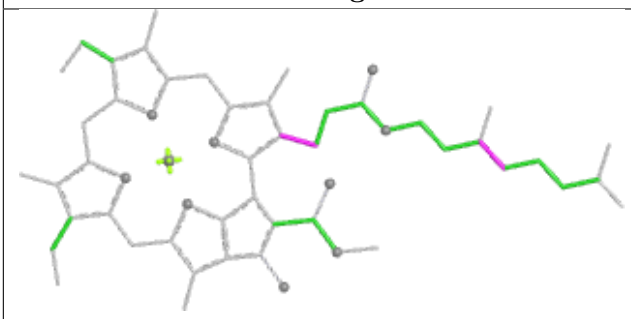
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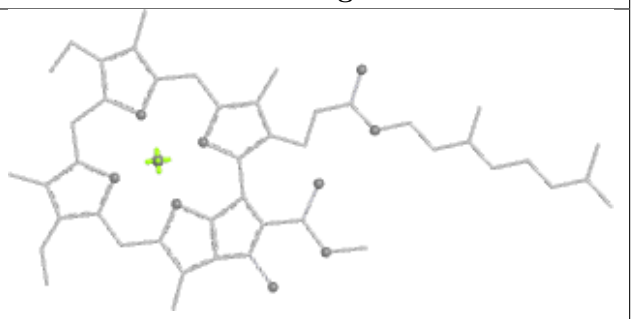
Bond lengths



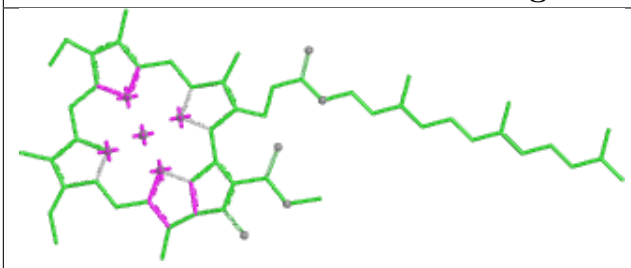
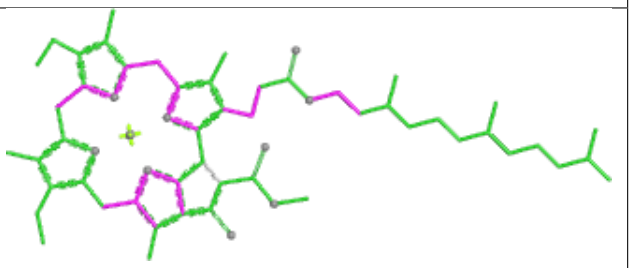
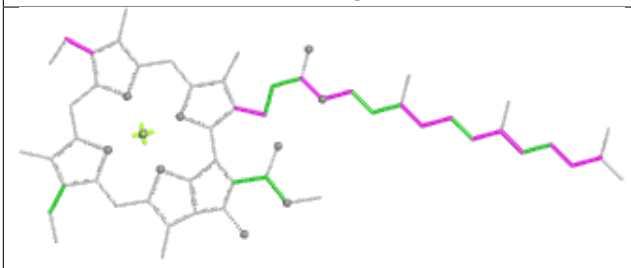
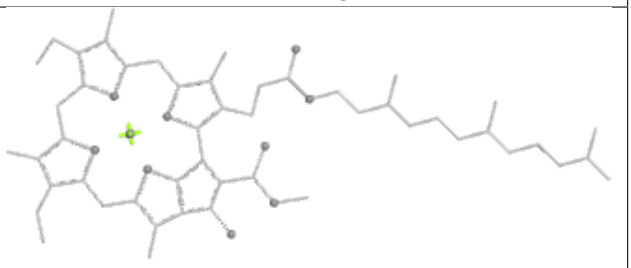
Bond angles

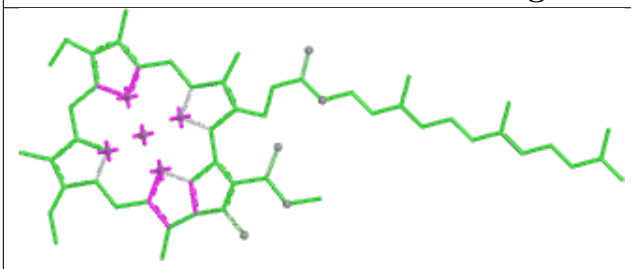
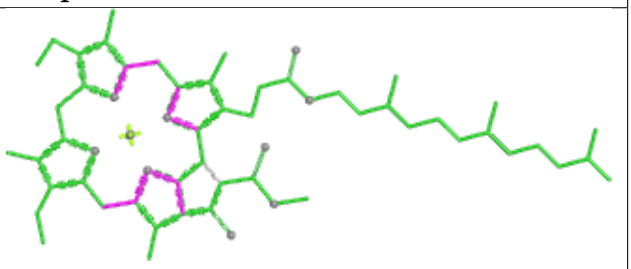
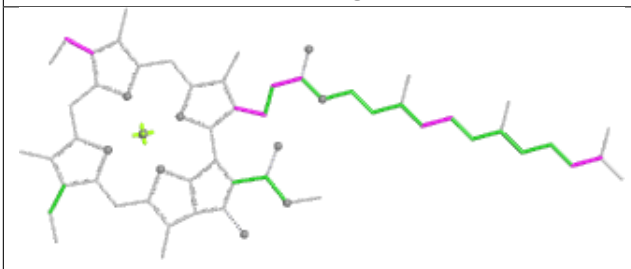
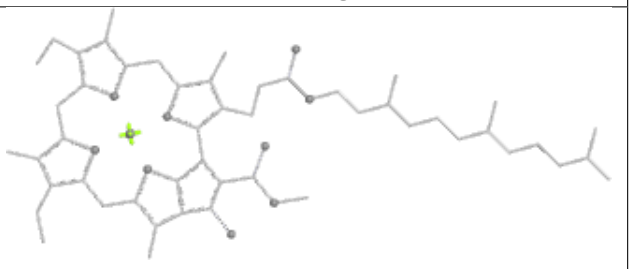


Torsions

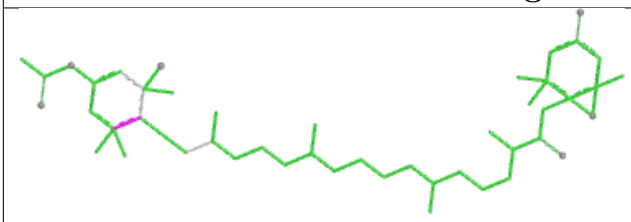


Rings

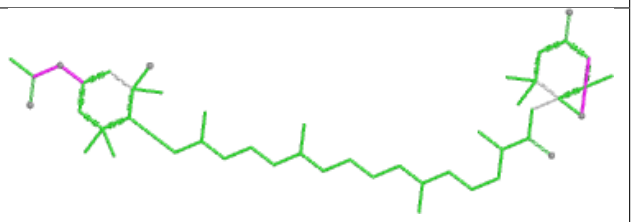
Ligand CLA z 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA q 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

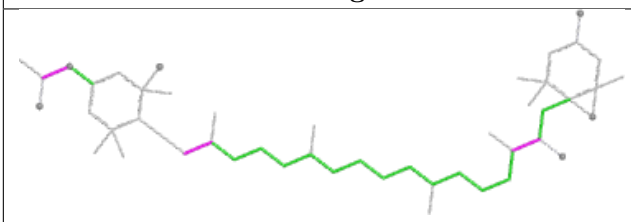
Ligand A86 W 314



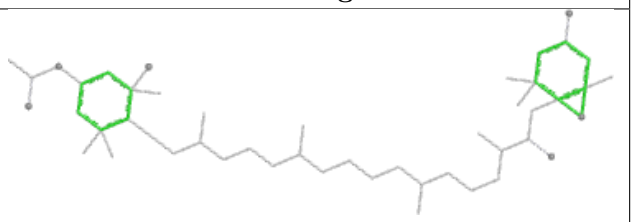
Bond lengths



Bond angles

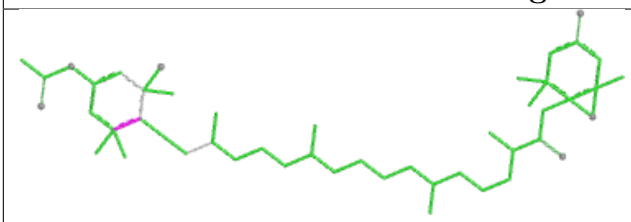


Torsions

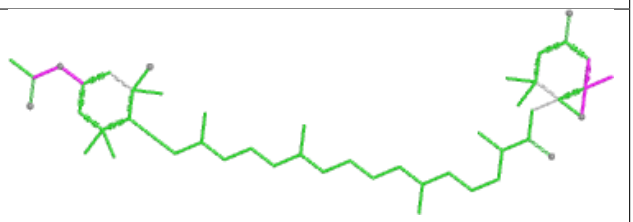


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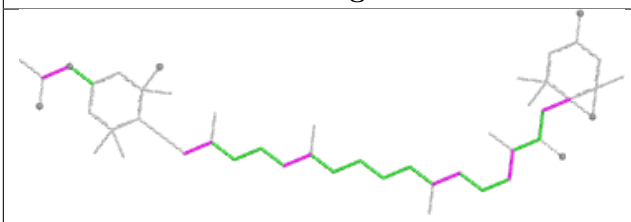
Ligand A86 Y 318



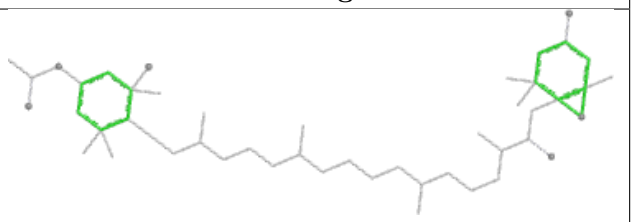
Bond lengths



Bond angles

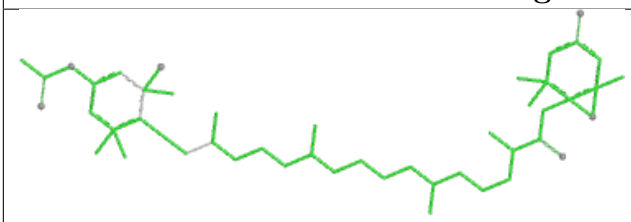


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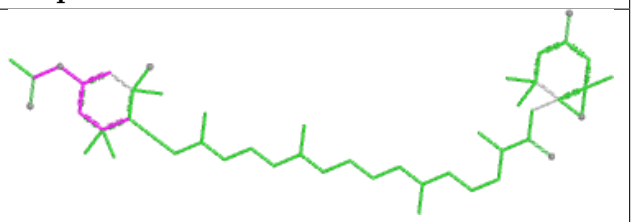


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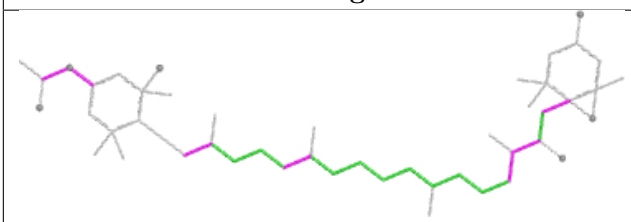
Ligand A86 q 319



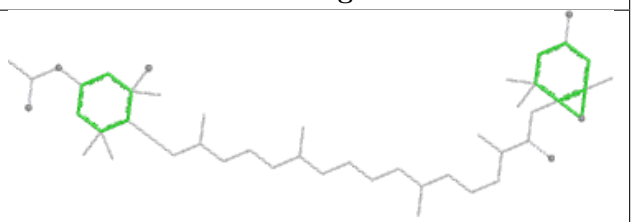
Bond lengths



Bond angles

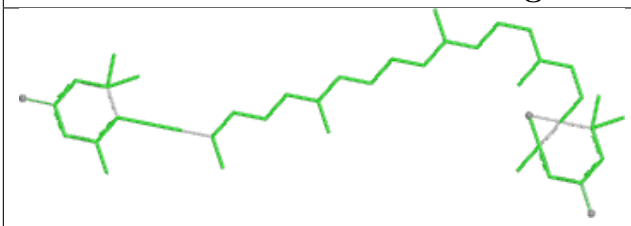


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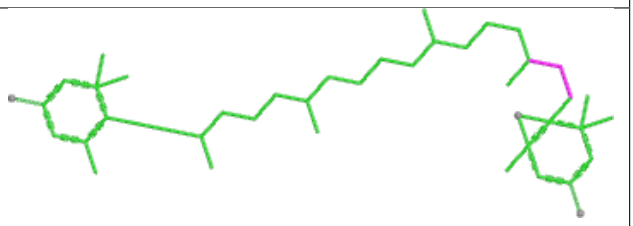


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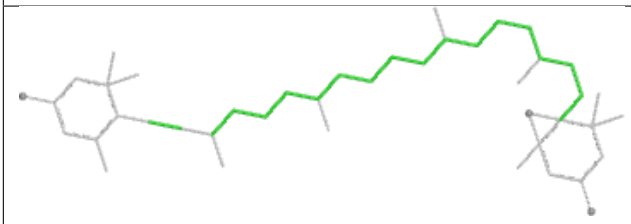
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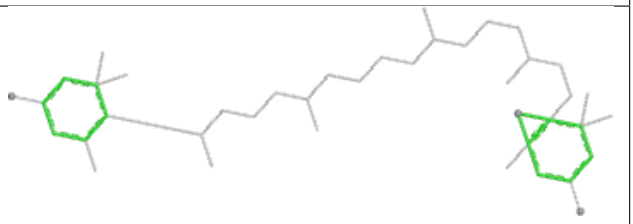
Bond lengths



Bond angles

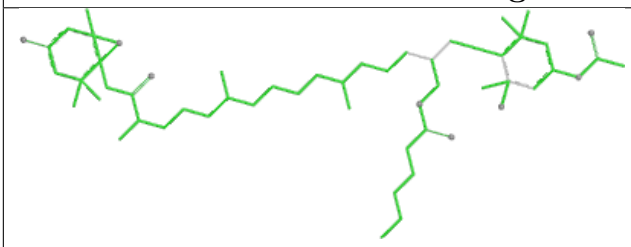


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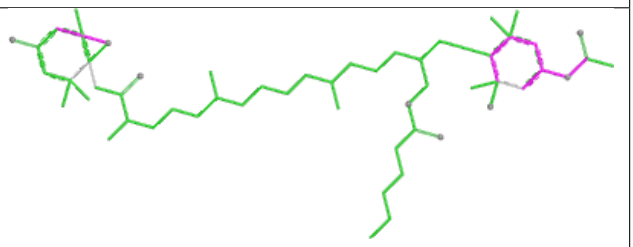


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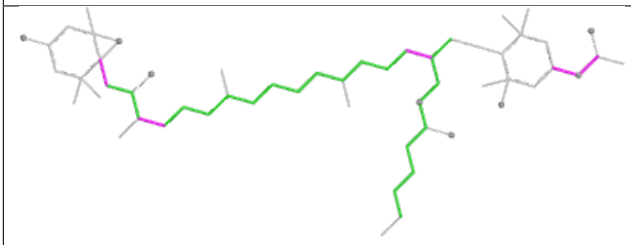
Ligand A1EB1 u 322



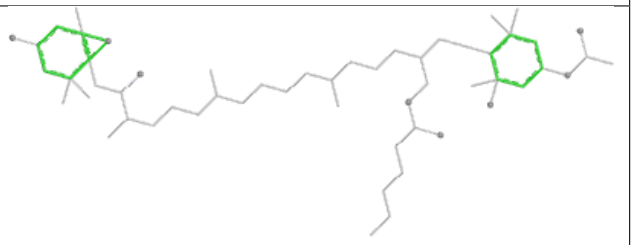
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Bond angles

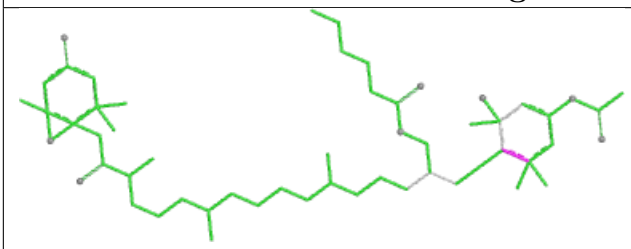


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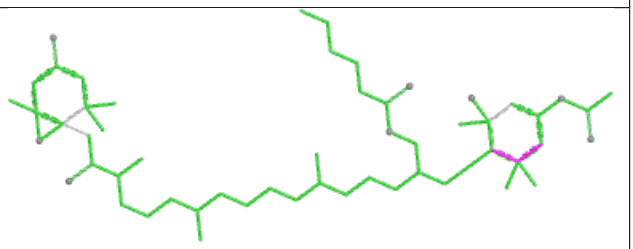


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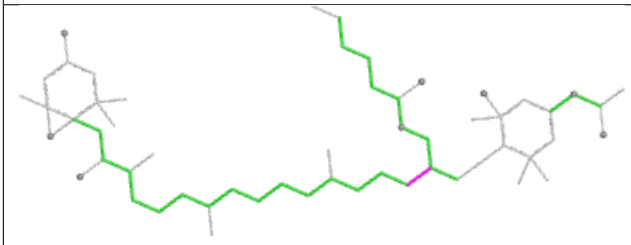
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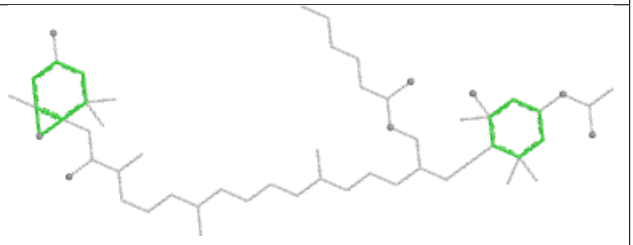
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Bond angles

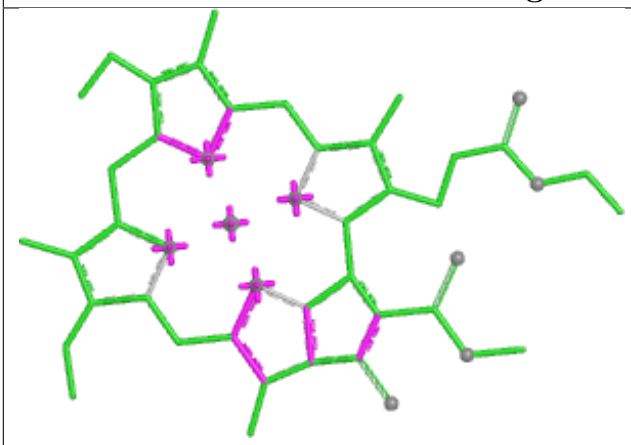


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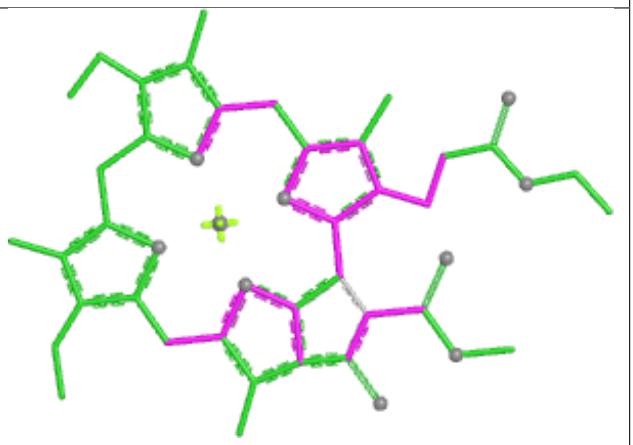


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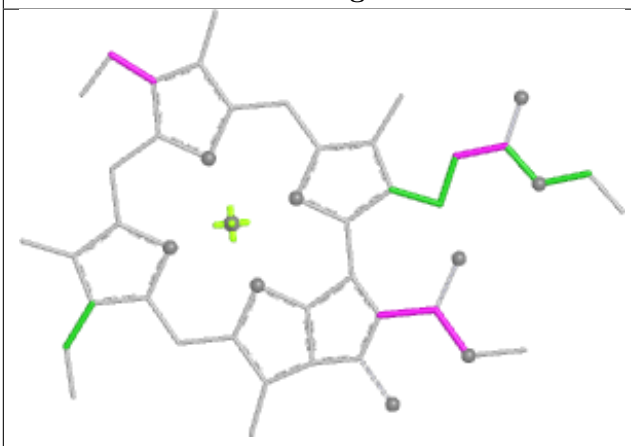
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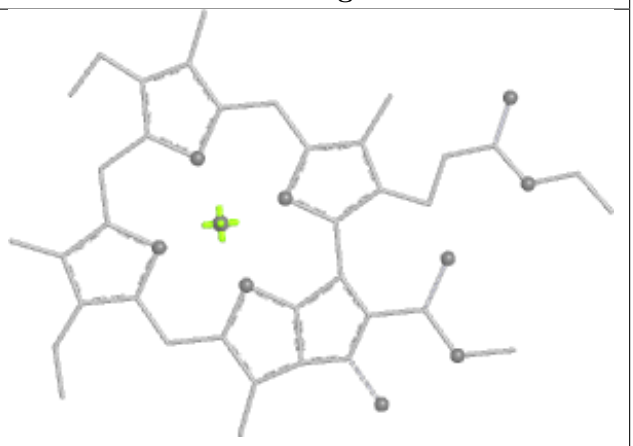
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Bond angles

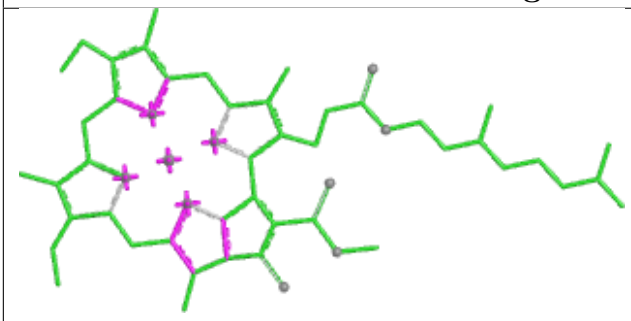


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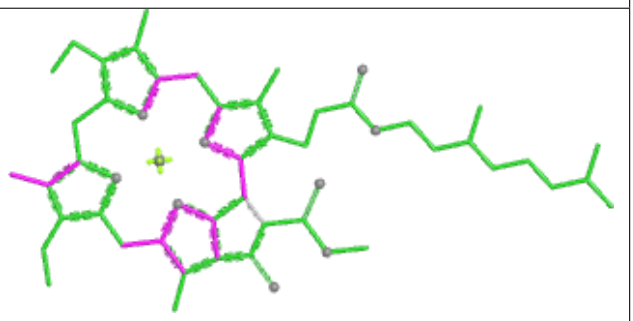


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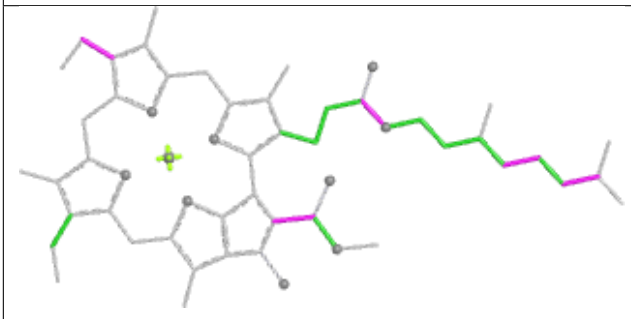
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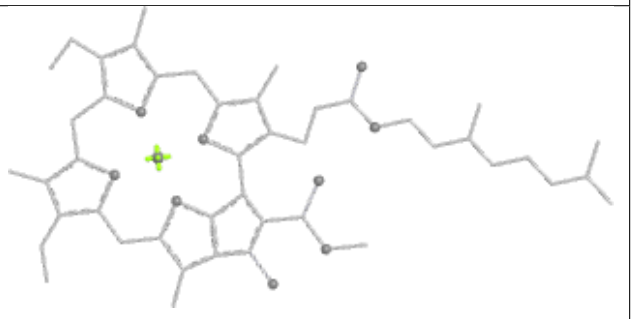
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Bond angles

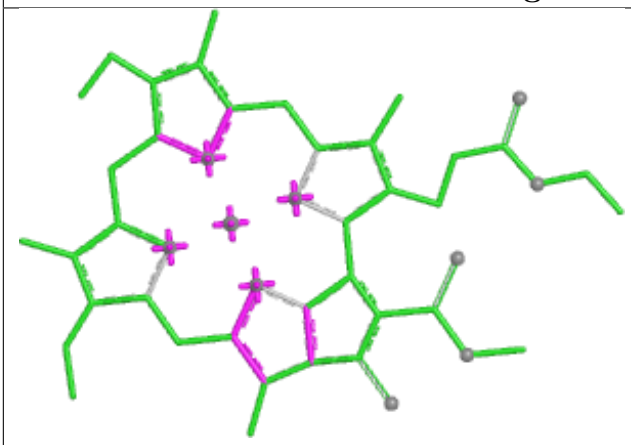


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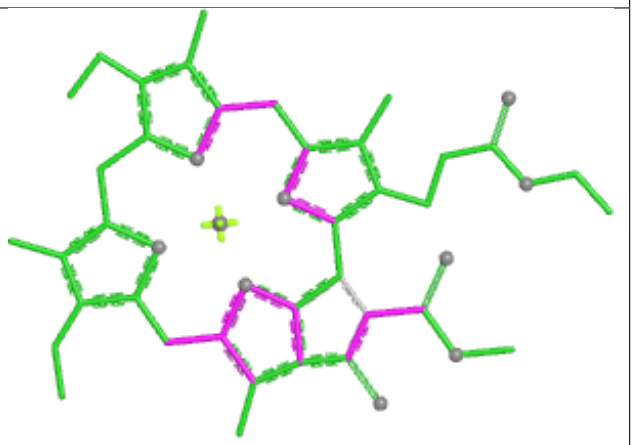


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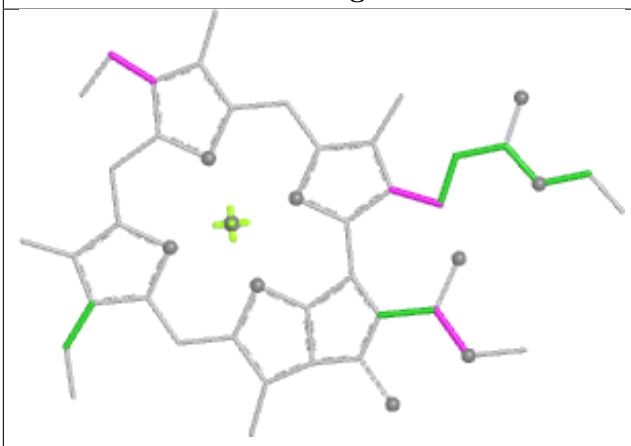
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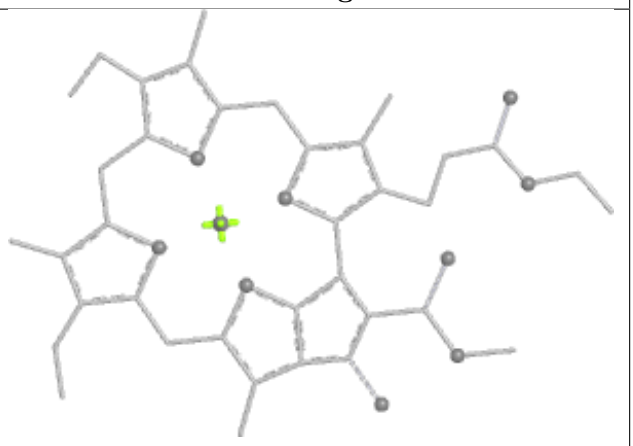
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Bond angles

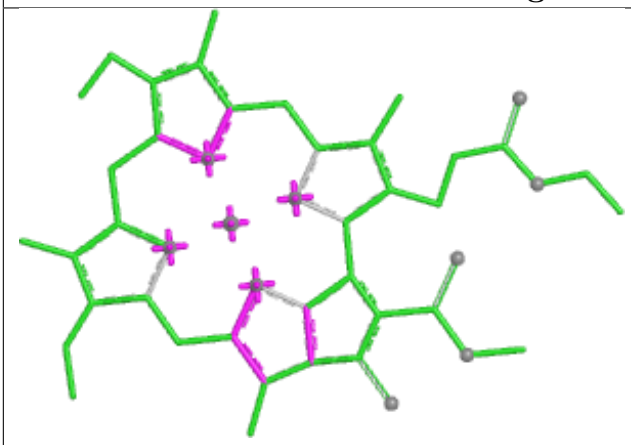


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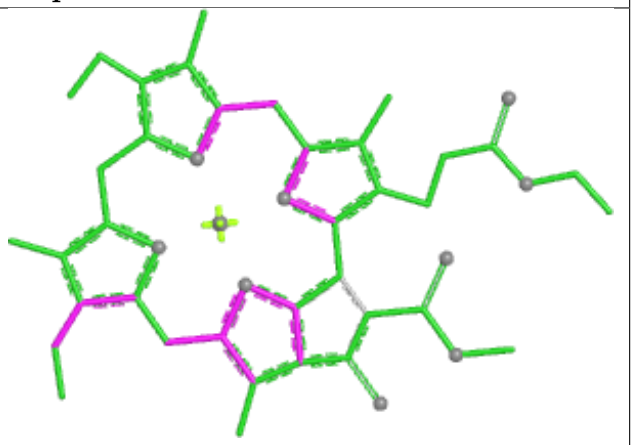


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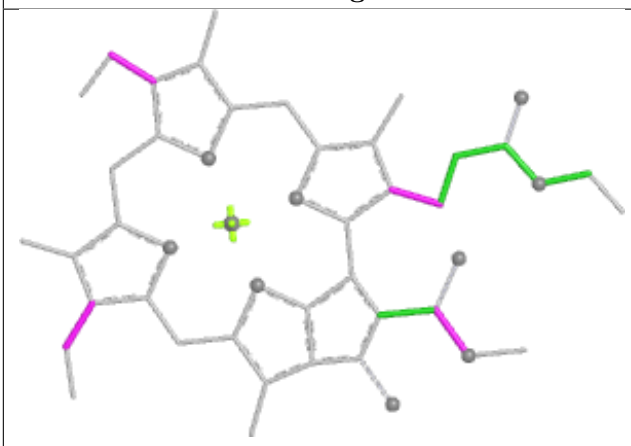
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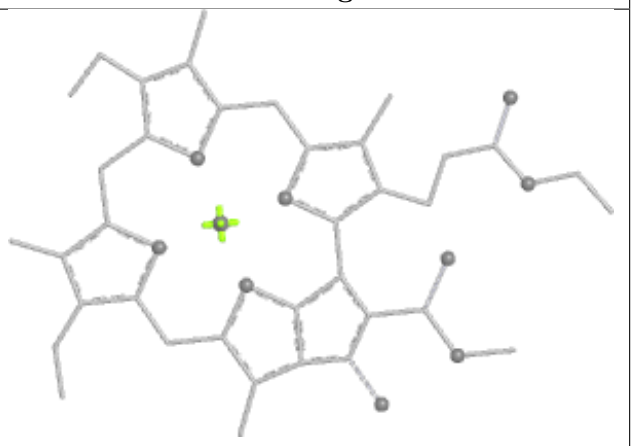
Bond lengths



Bond angles

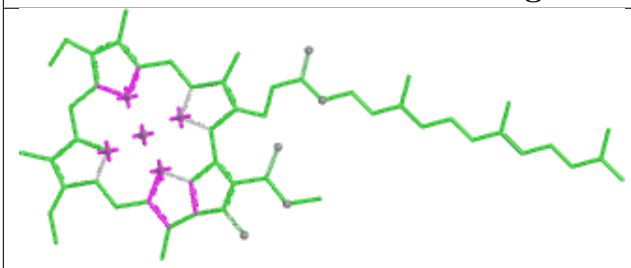


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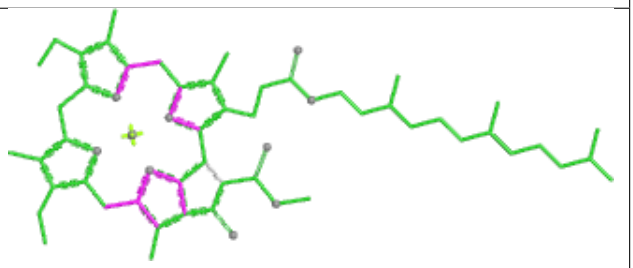


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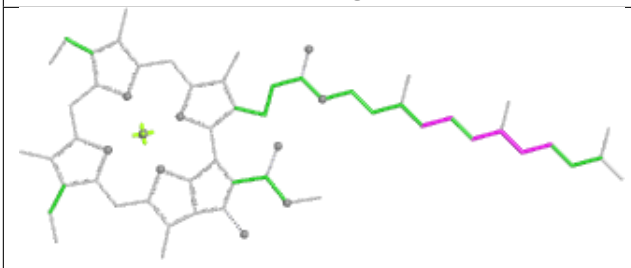
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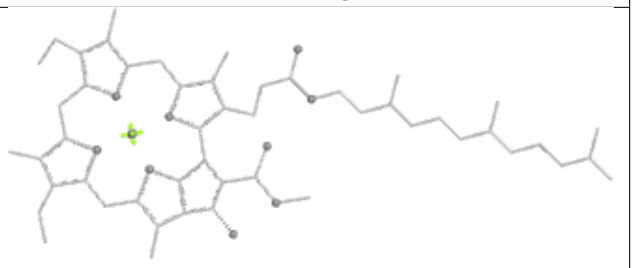
Bond lengths



Bond angles

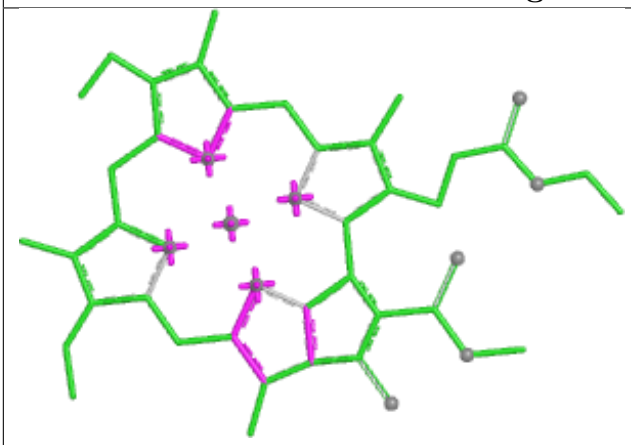


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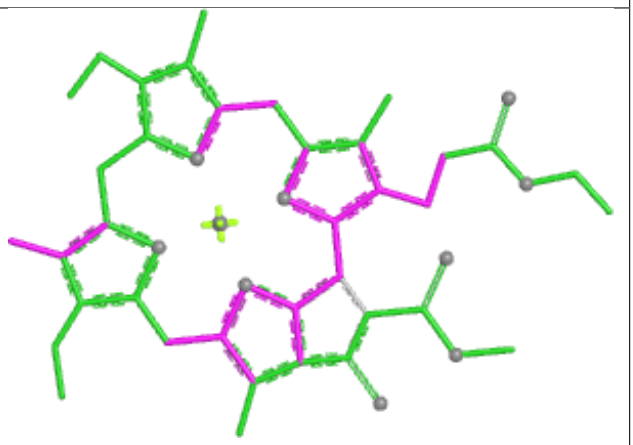


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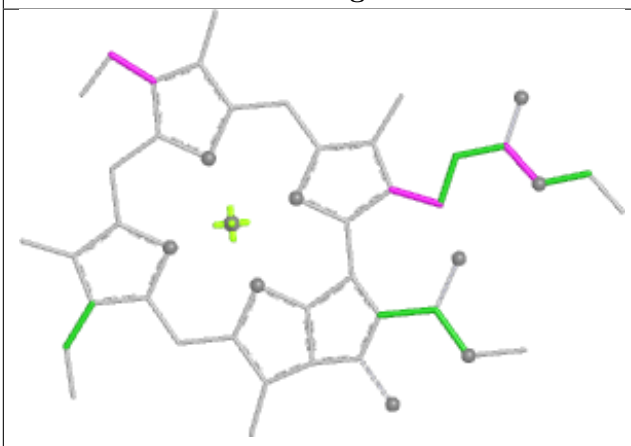
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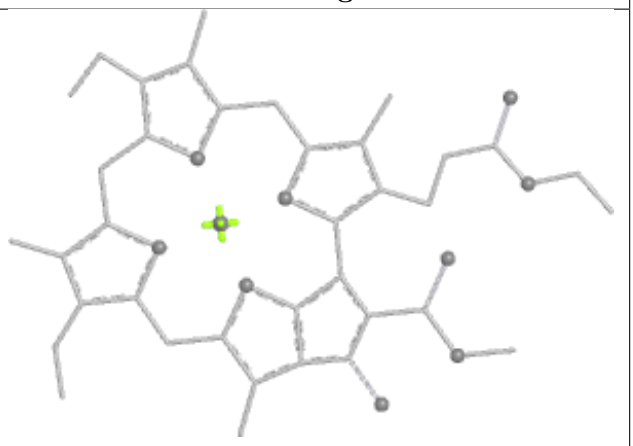
Bond lengths



Bond angles

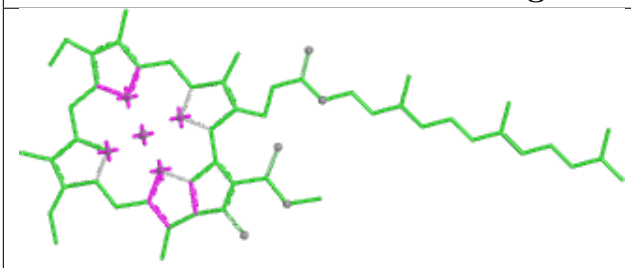


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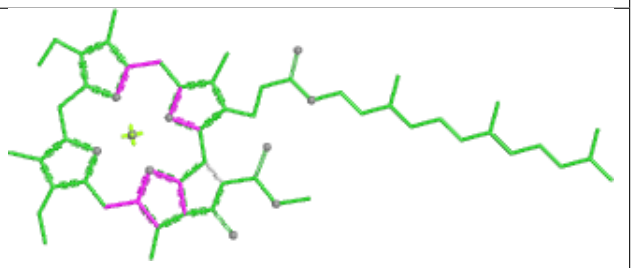


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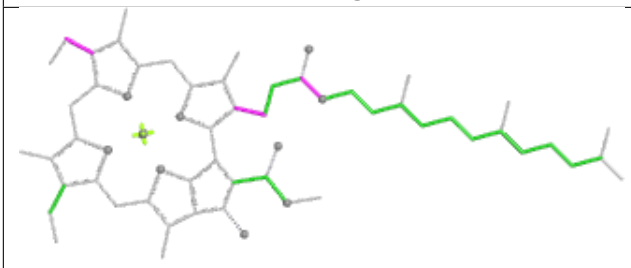
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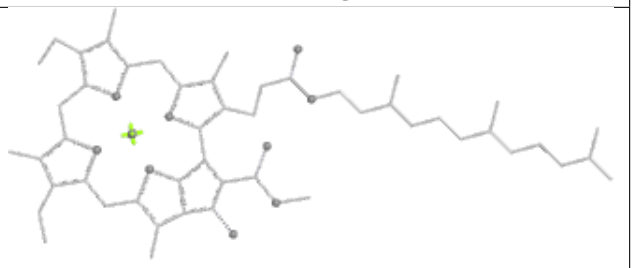
Bond lengths



Bond angles

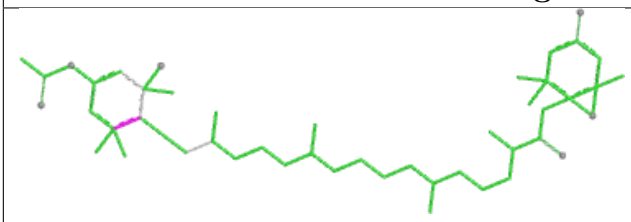


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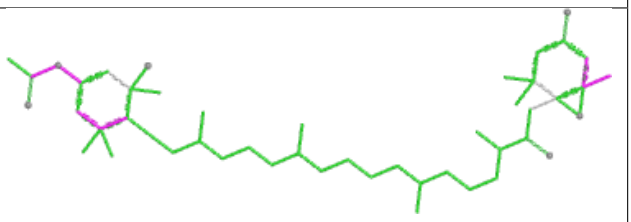


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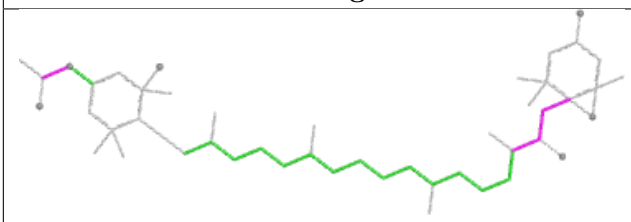
Ligand A86 x 316



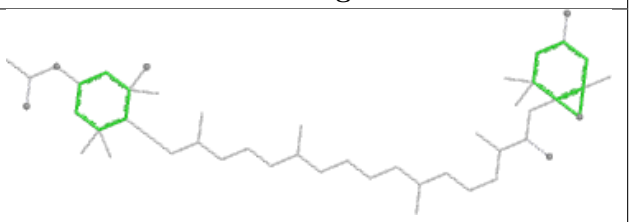
Bond lengths



Bond angles

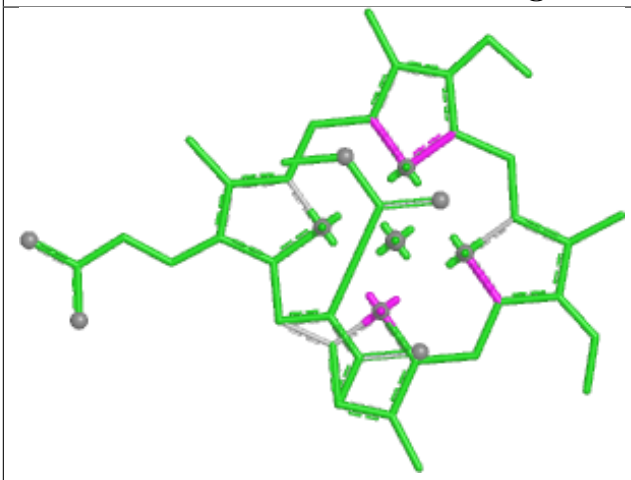


Torsions

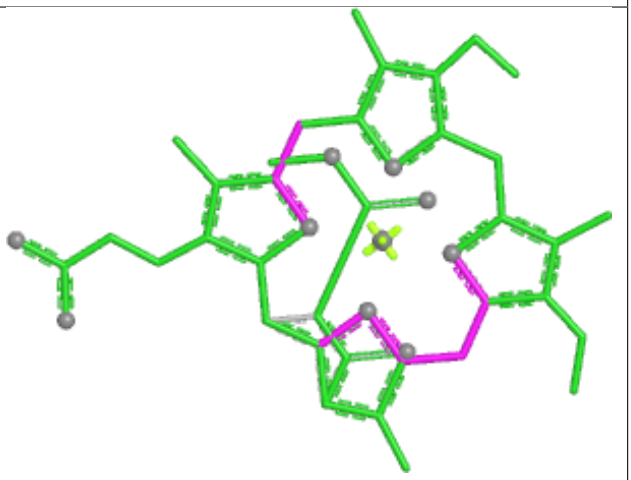


Rings

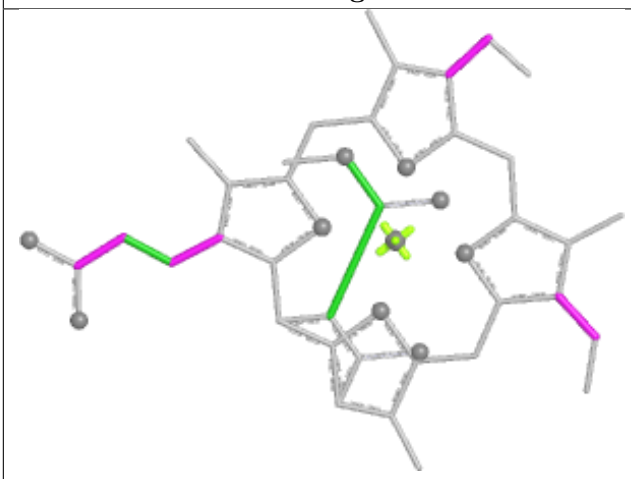
Ligand KC2 F 302



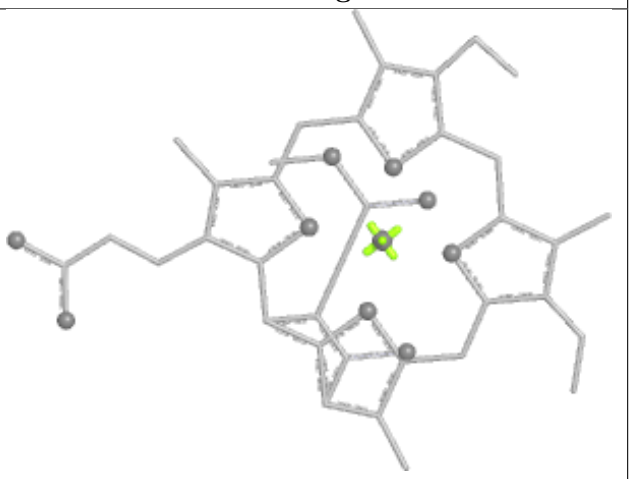
Bond lengths



Bond angles

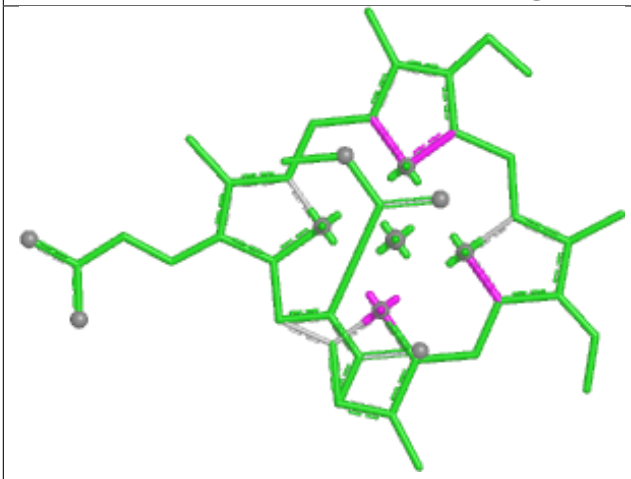


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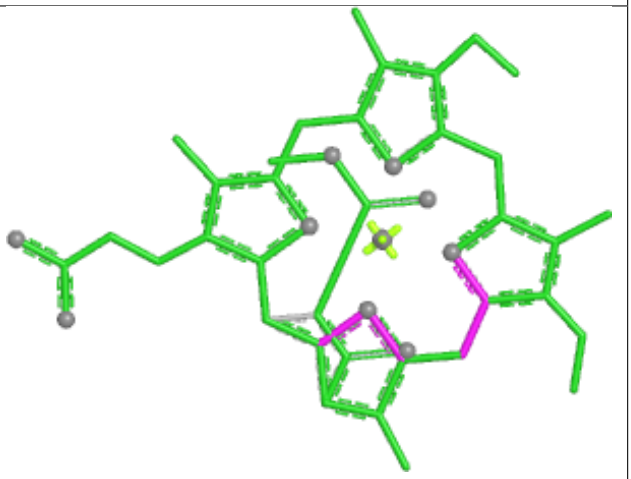


Rings

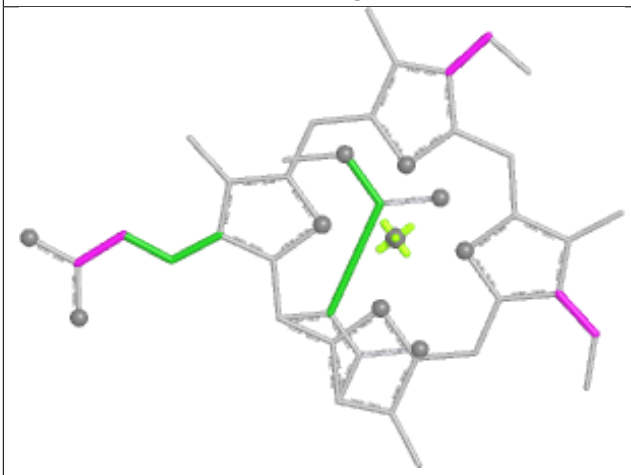
Ligand KC2 Z 309



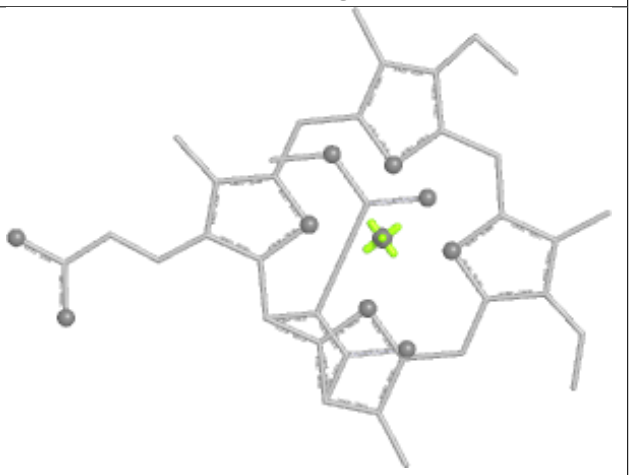
Bond lengths



Bond angles

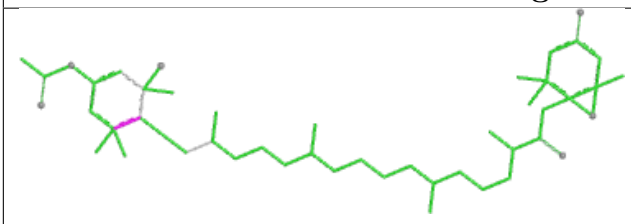


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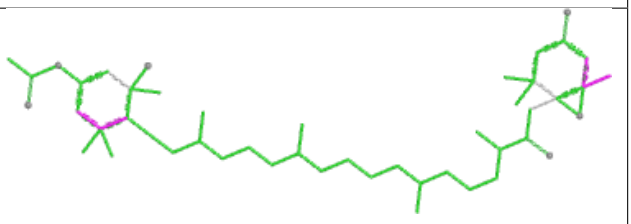


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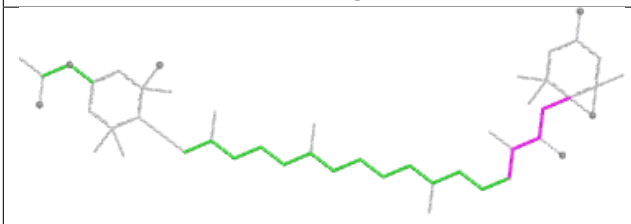
Ligand A86 F 317



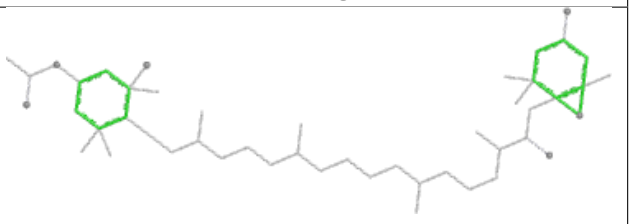
Bond lengths



Bond angles

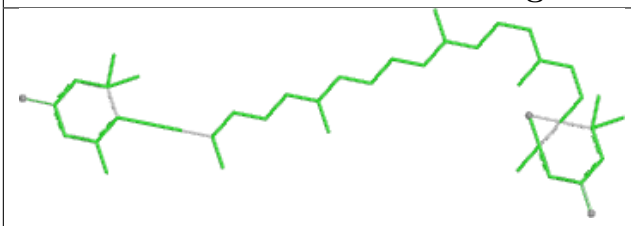


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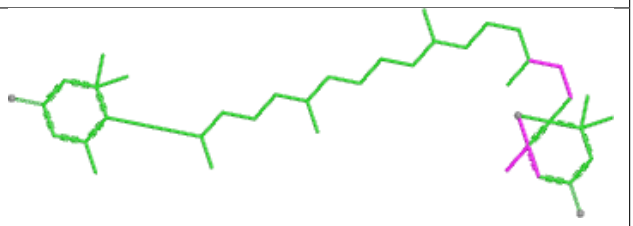


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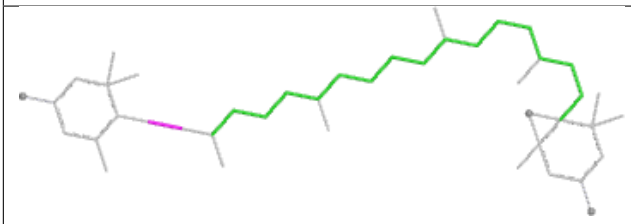
Ligand DD6 E 315



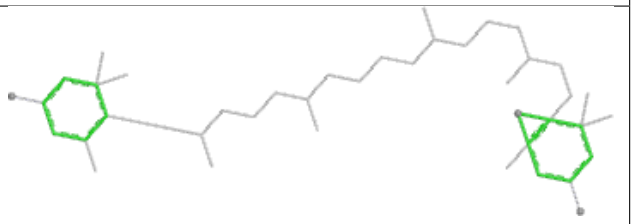
Bond lengths



Bond angles

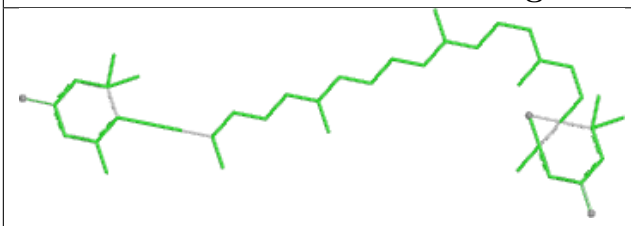


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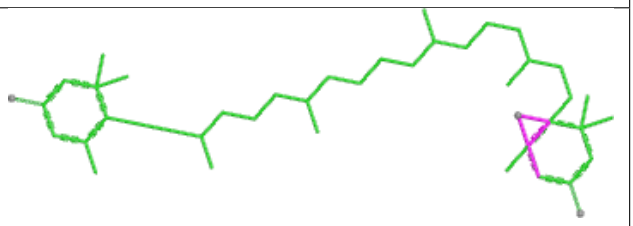


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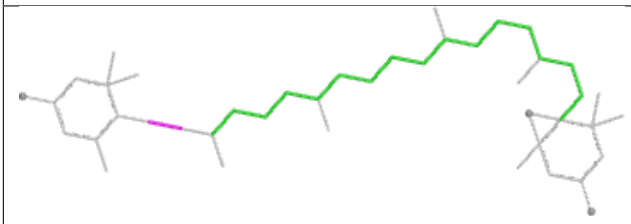
Ligand DD6 P 315



Bond lengths



Bond angles

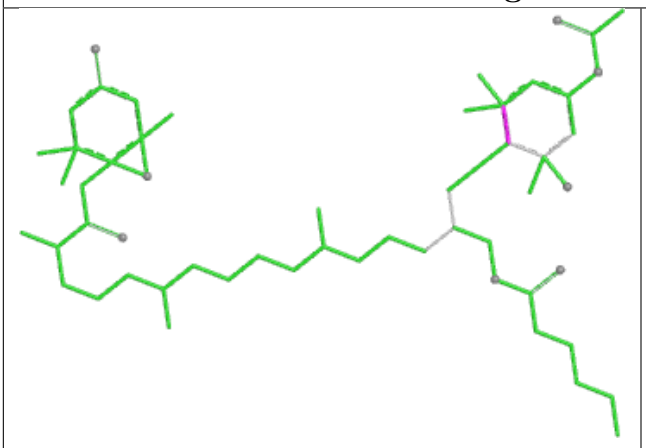


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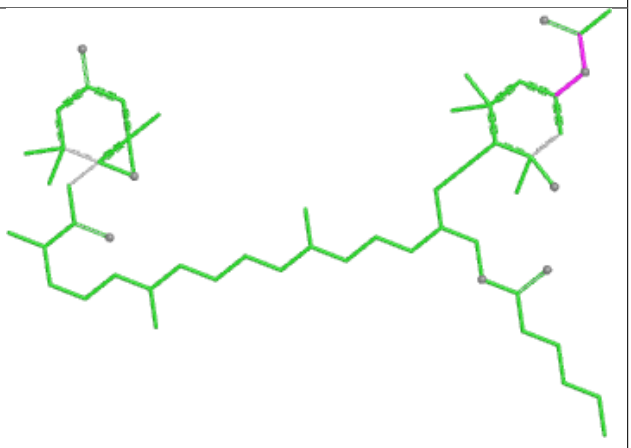


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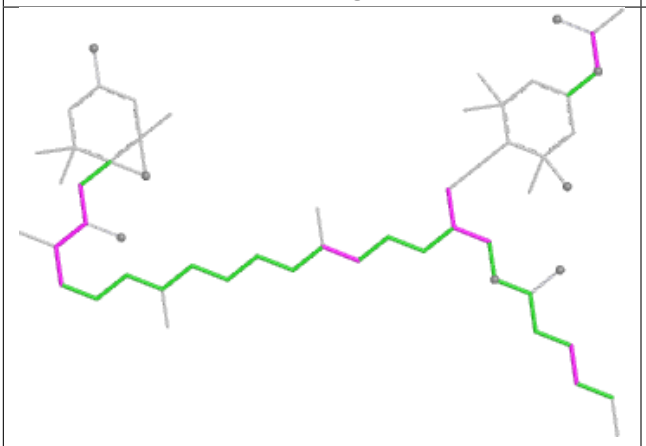
Ligand A1EB1 G 212



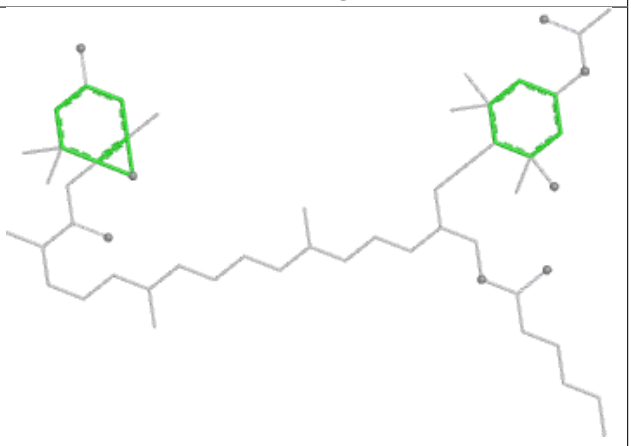
Bond lengths



Bond angles

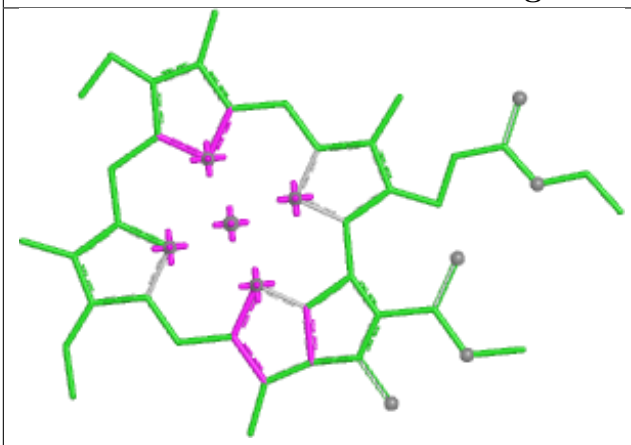


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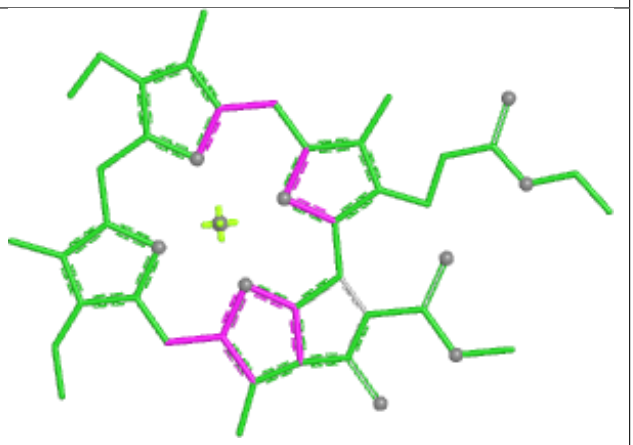


Rings

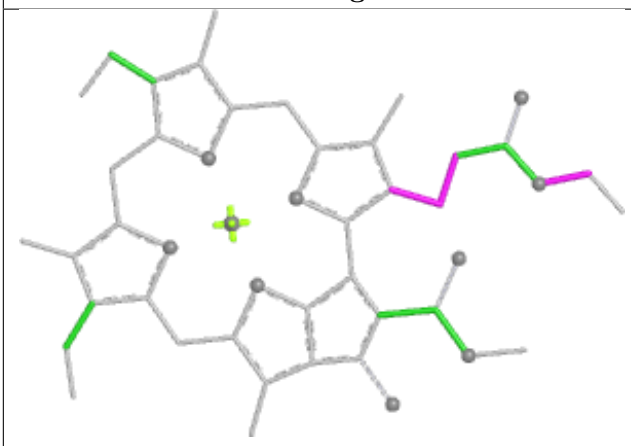
Ligand CLA w 303



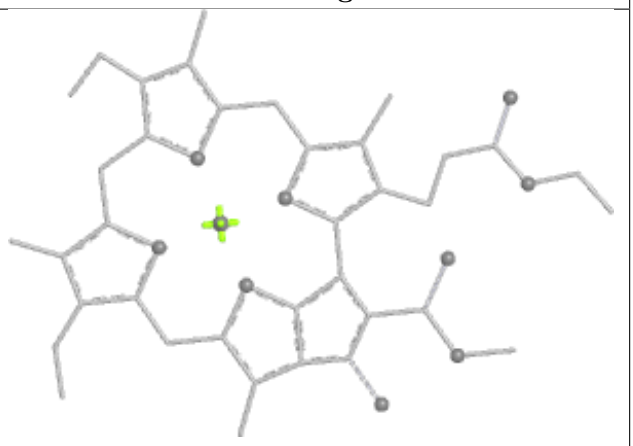
Bond lengths



Bond angles

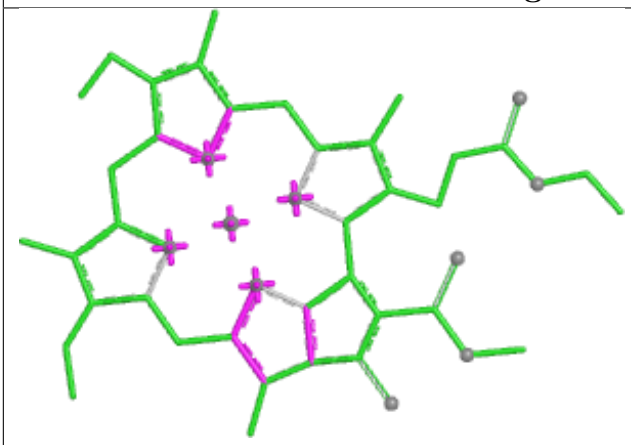


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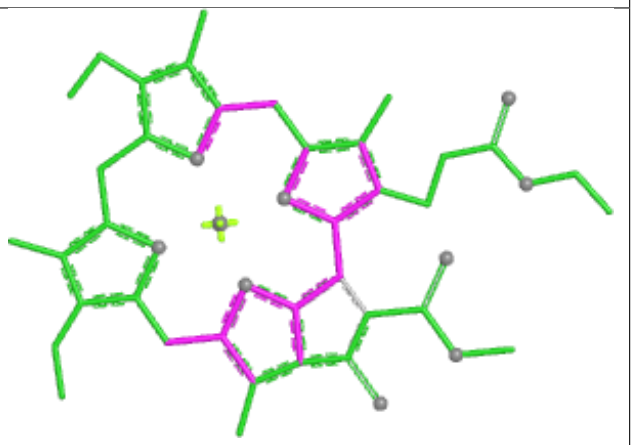


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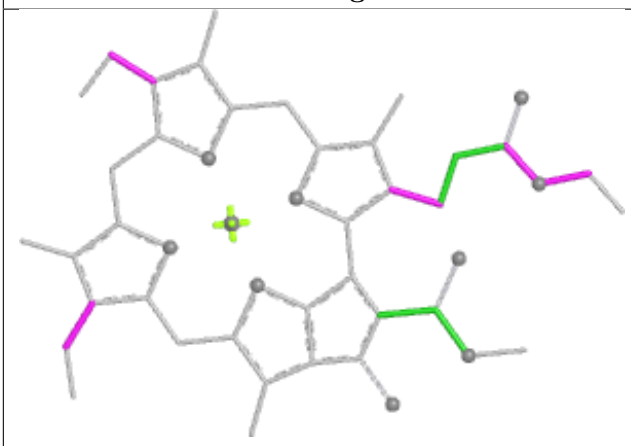
Ligand CLA B 301



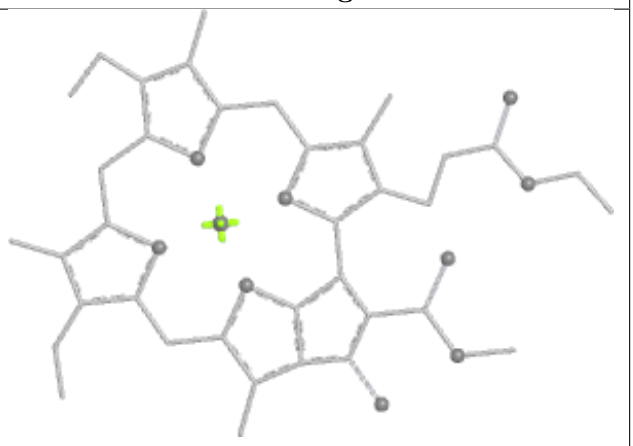
Bond lengths



Bond angles

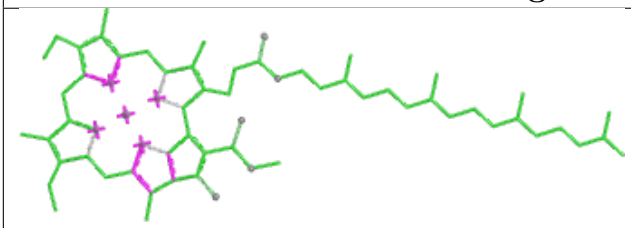


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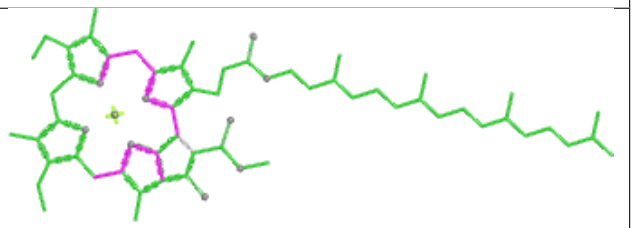


Rings

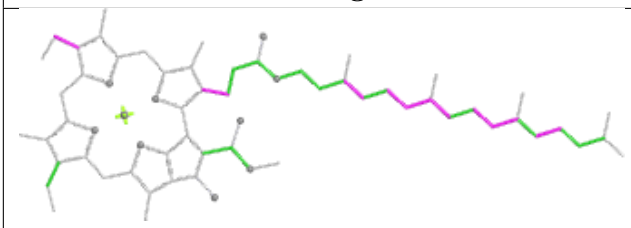
Ligand CLA a 842



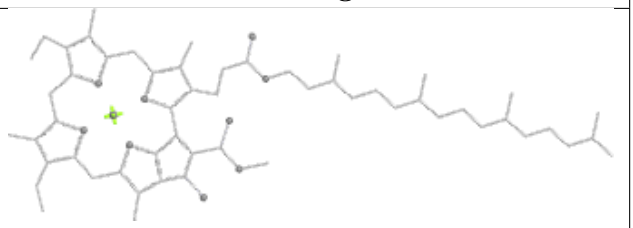
Bond lengths



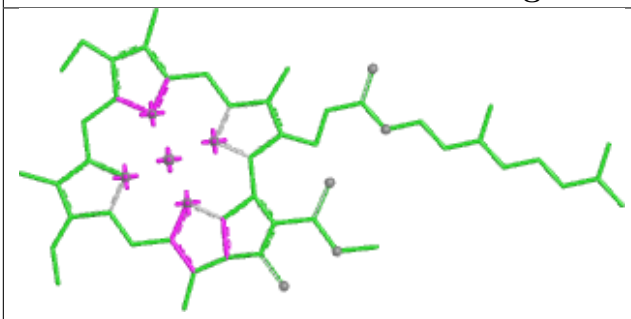
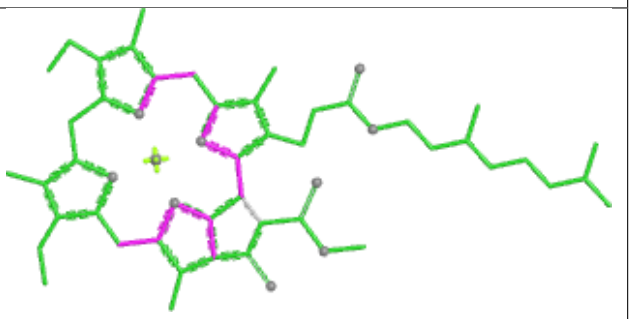
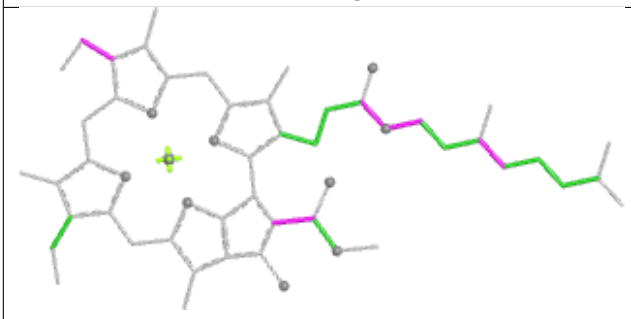
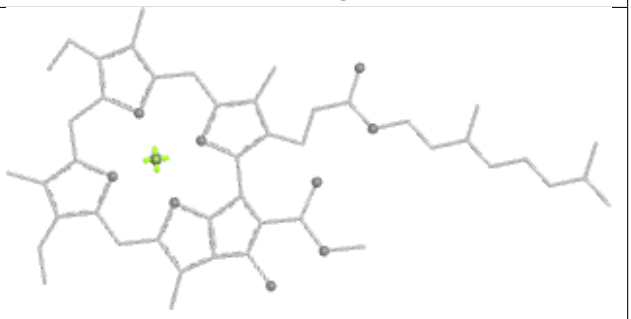
Bond angles

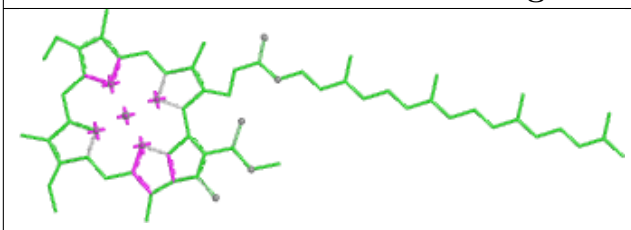
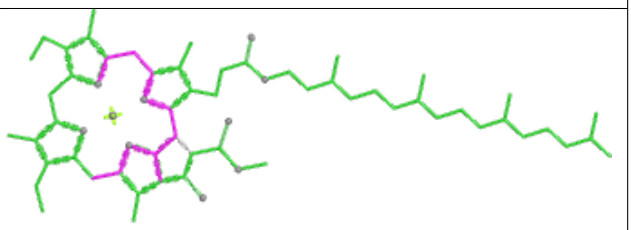
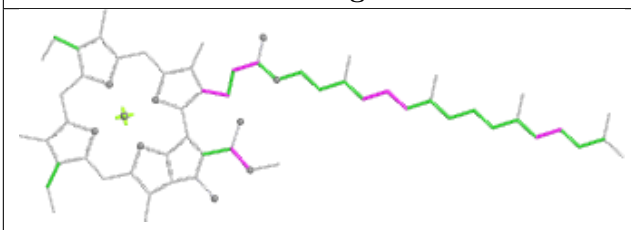
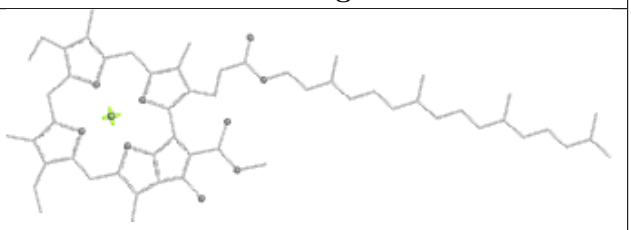


Torsions

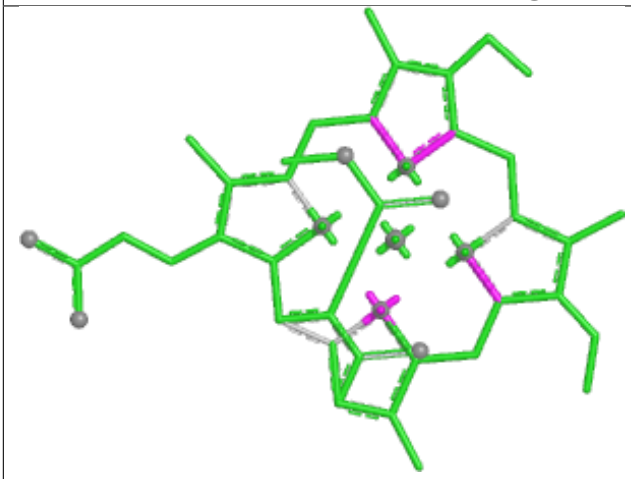


Rings

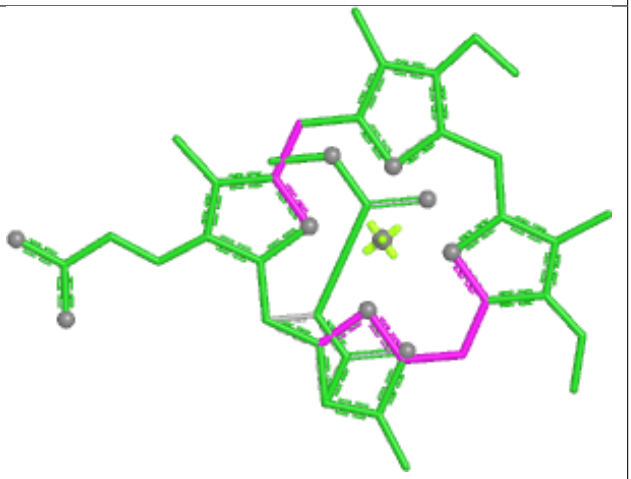
Ligand CLA D 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

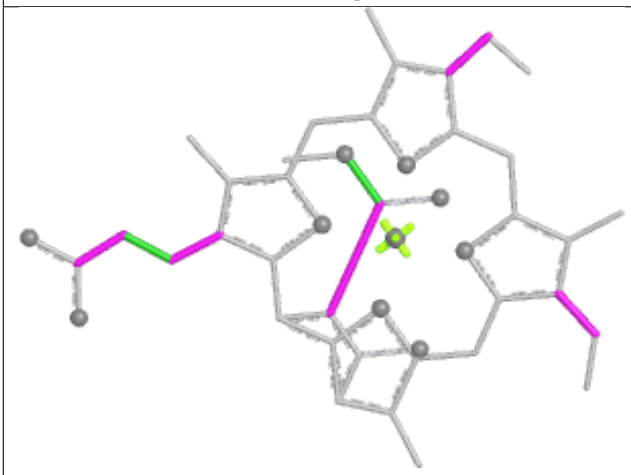
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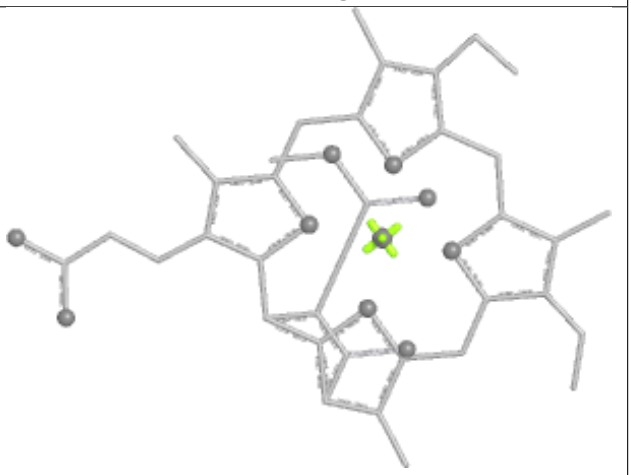
Bond lengths



Bond angles

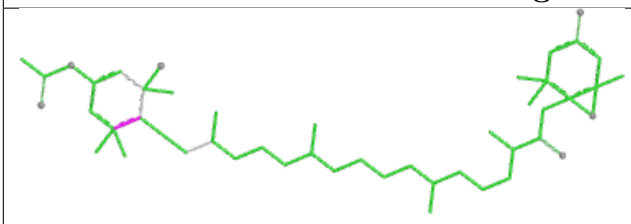


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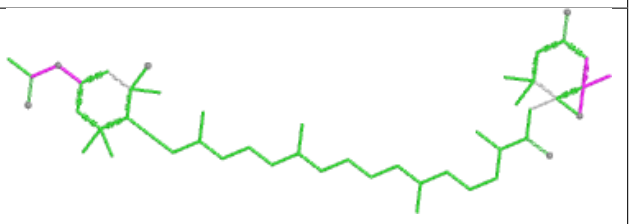


Rings

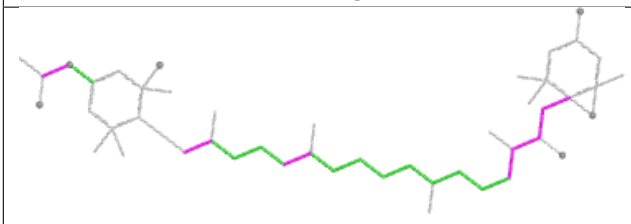
Ligand A86 u 318



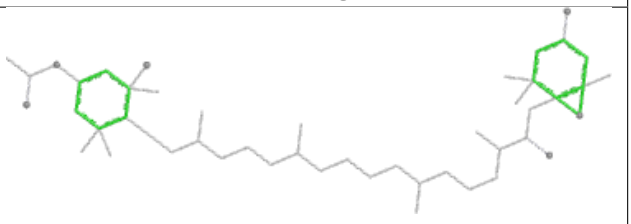
Bond lengths



Bond angles

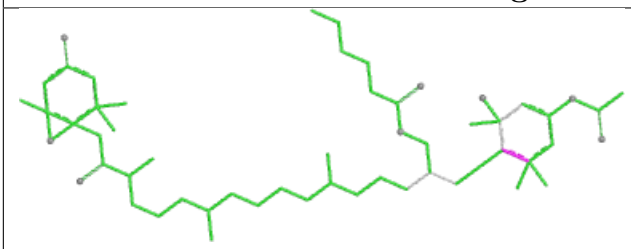


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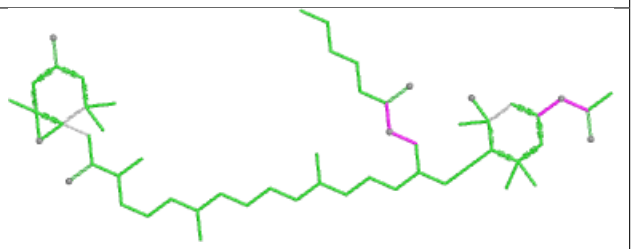


Rings

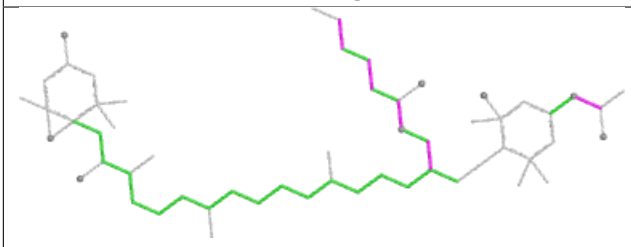
Ligand A1EB1 z 323



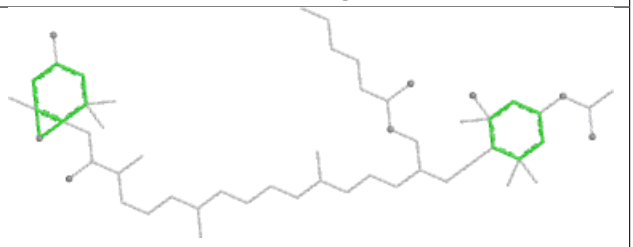
Bond lengths



Bond angles

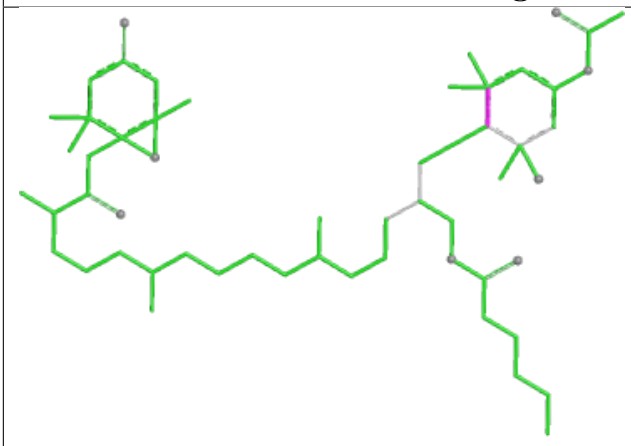


Torsions

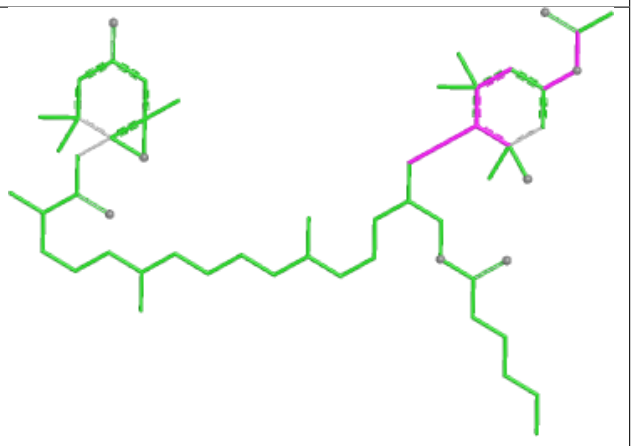


Rings

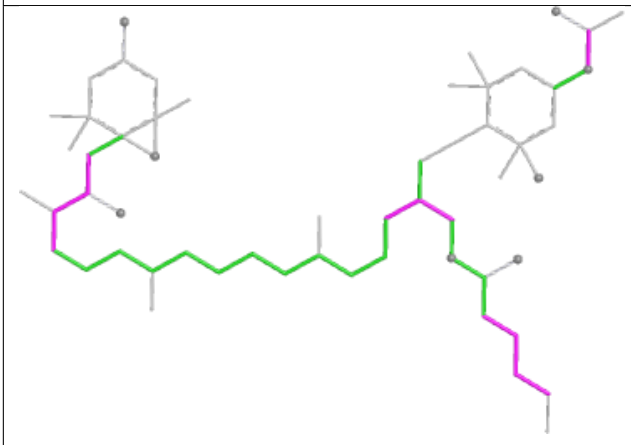
Ligand A1EB1 t 313



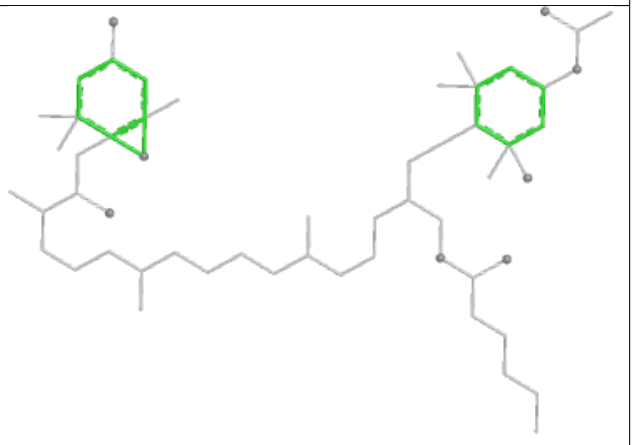
Bond lengths



Bond angles

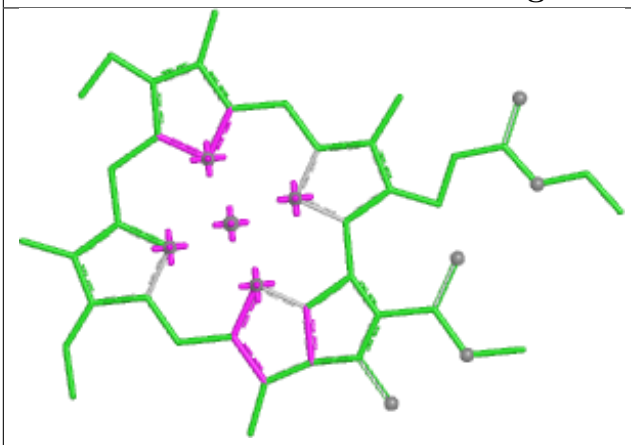


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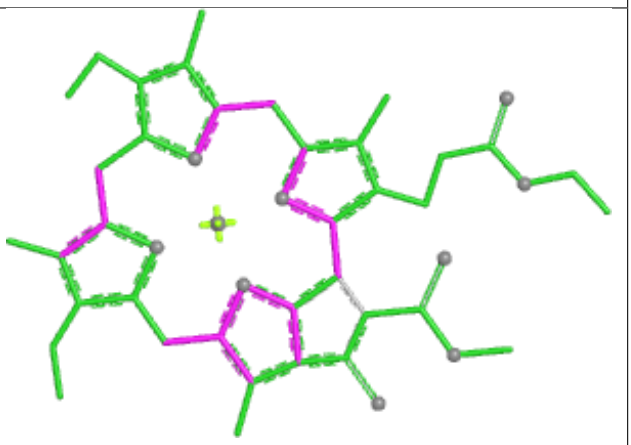


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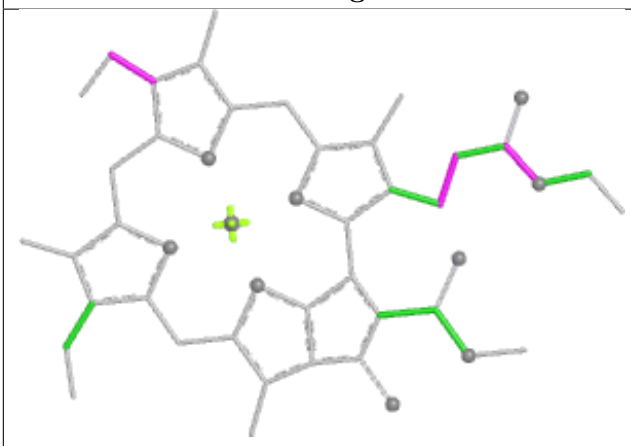
Ligand CLA b 811



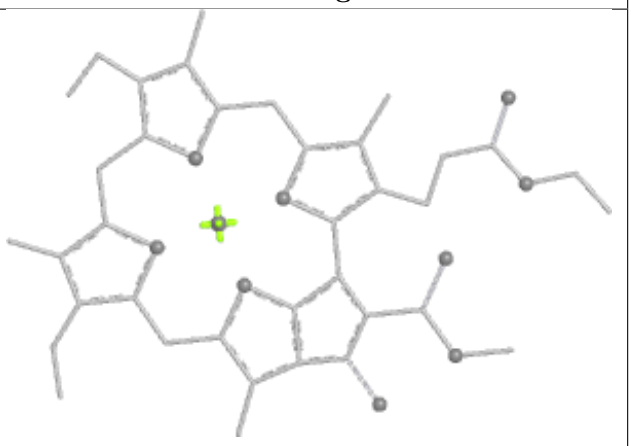
Bond lengths



Bond angles

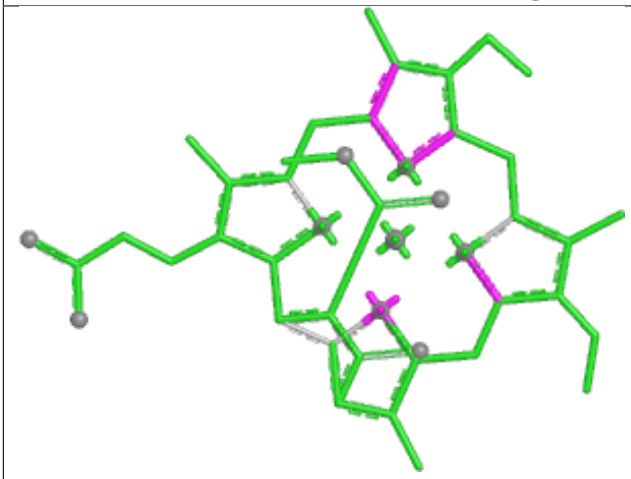


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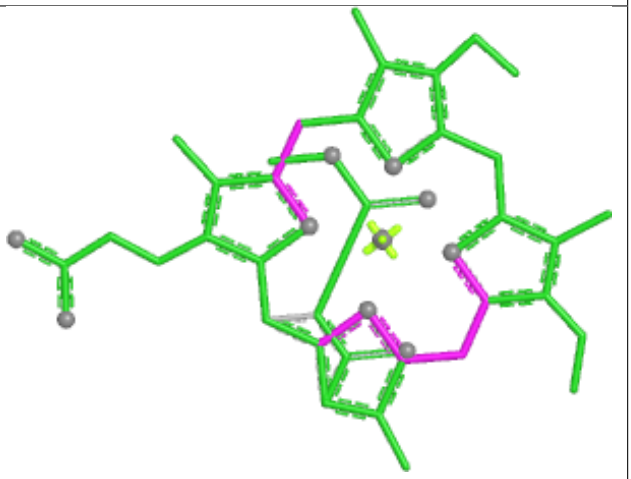


Rings

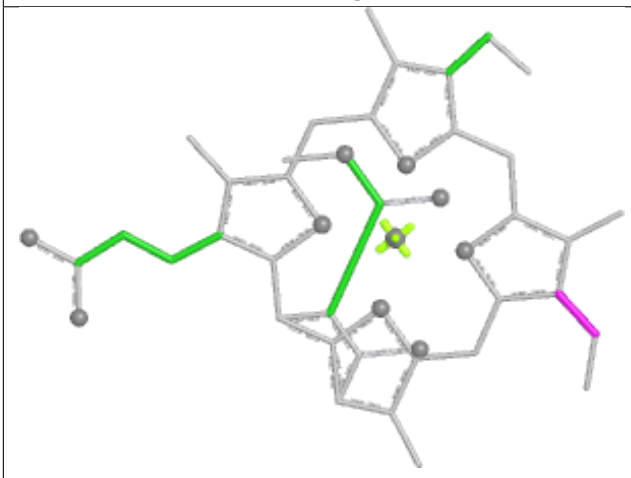
Ligand KC2 T 302



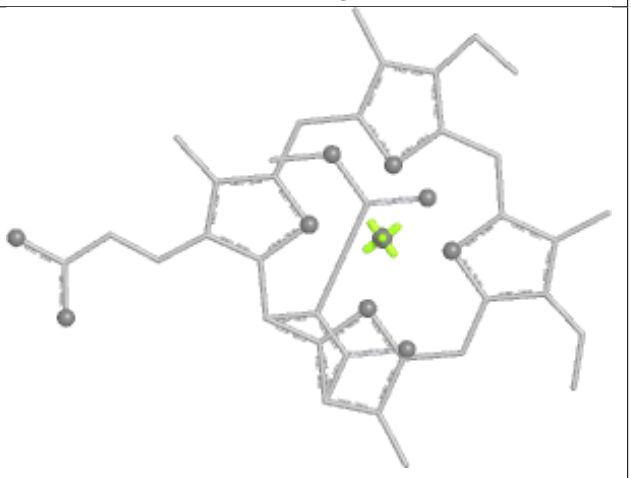
Bond lengths



Bond angles

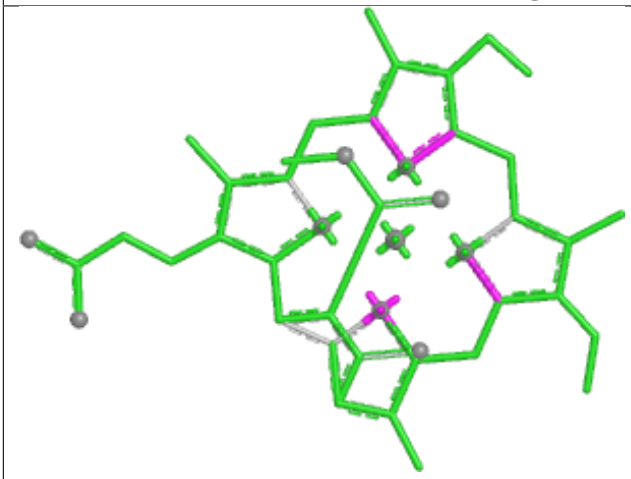


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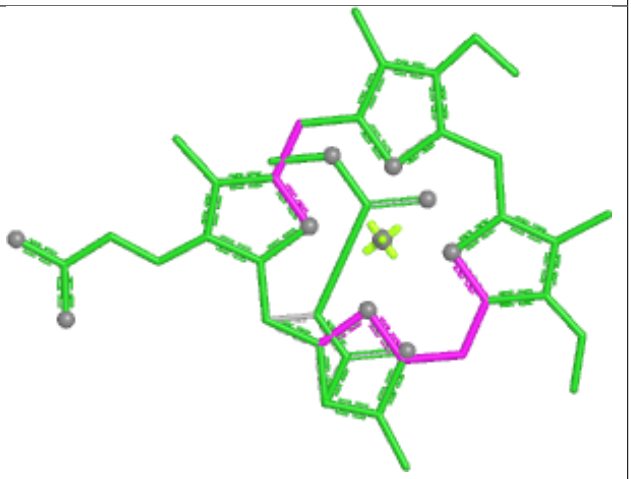


Rings

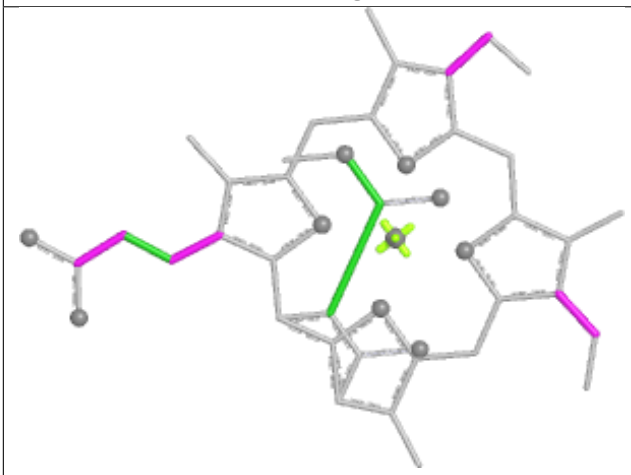
Ligand KC2 C 303



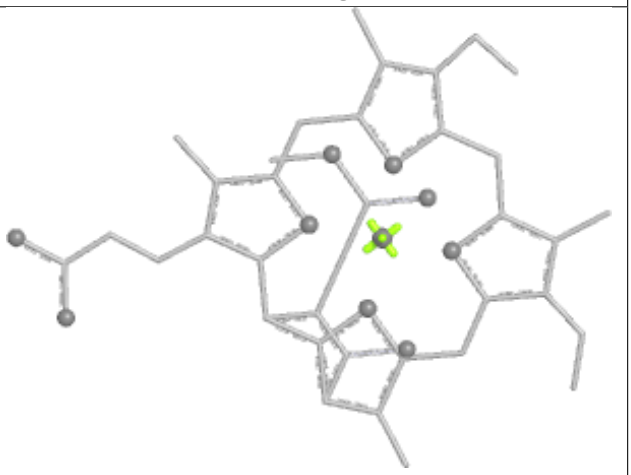
Bond lengths



Bond angles

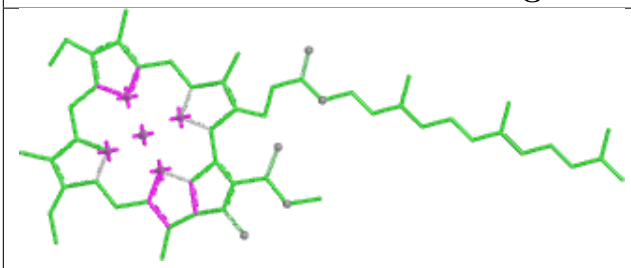


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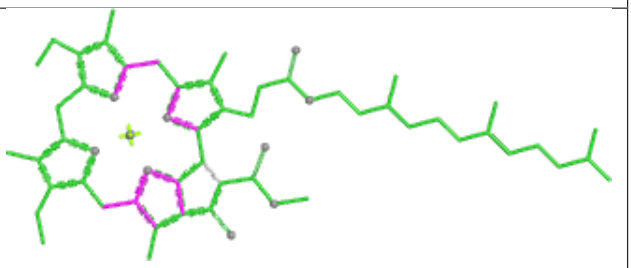


Rings

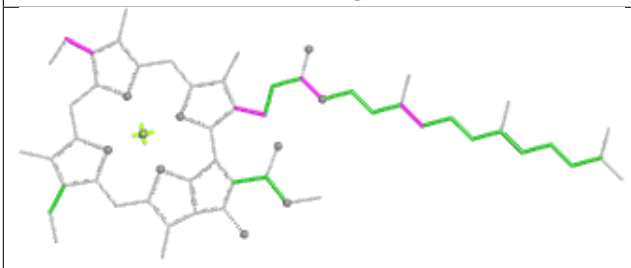
Ligand CLA Y 301



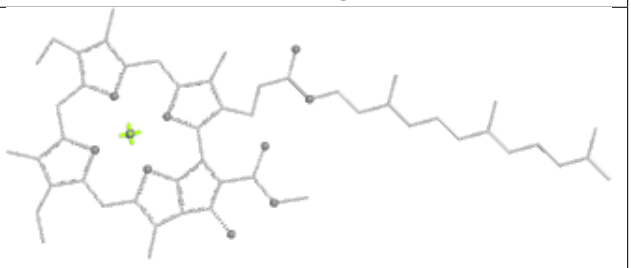
Bond lengths



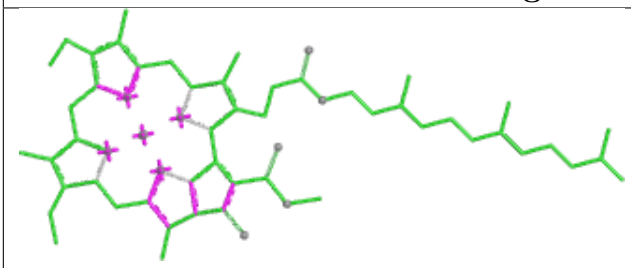
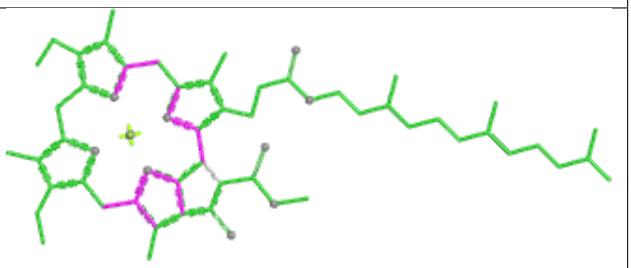
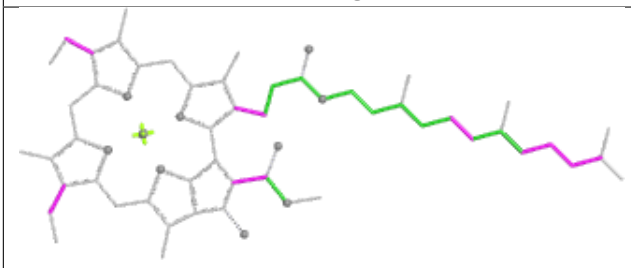
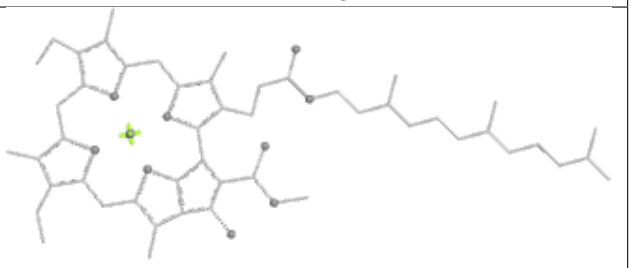
Bond angles

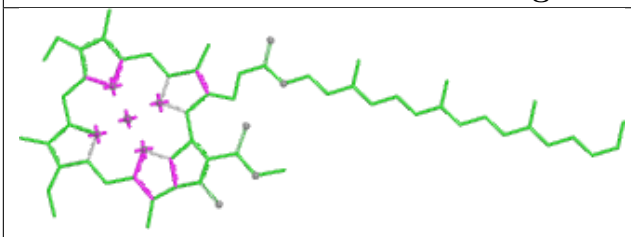
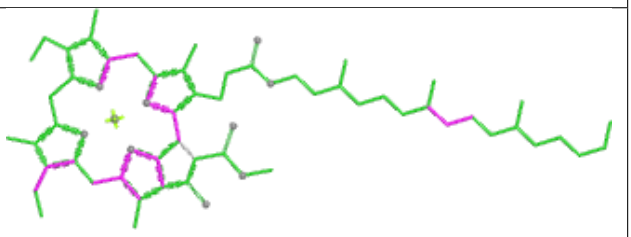
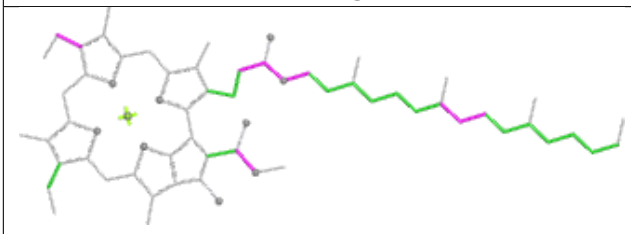
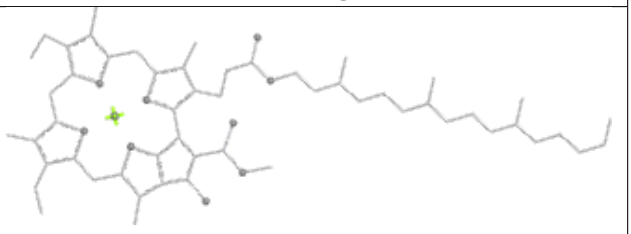


Torsions

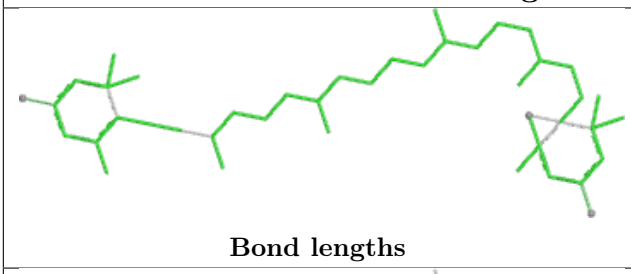


Rings

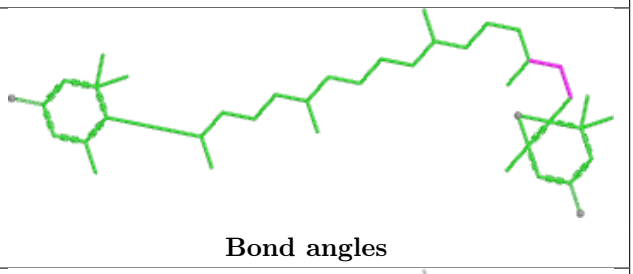
Ligand CLA D 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA l 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

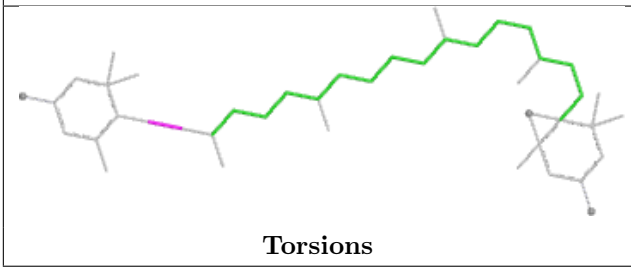
Ligand DD6 M 314



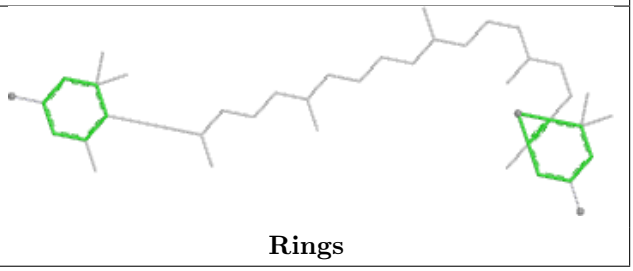
Bond lengths



Bond angles

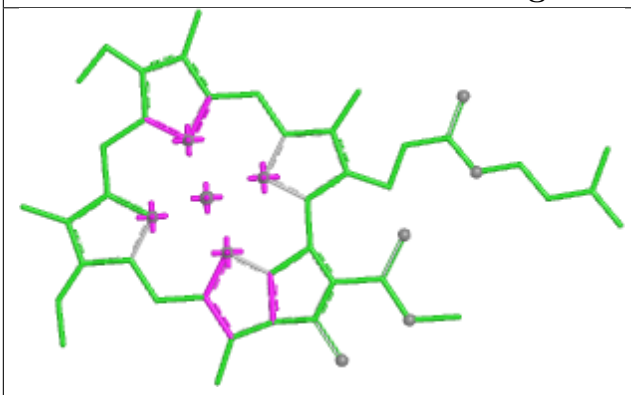


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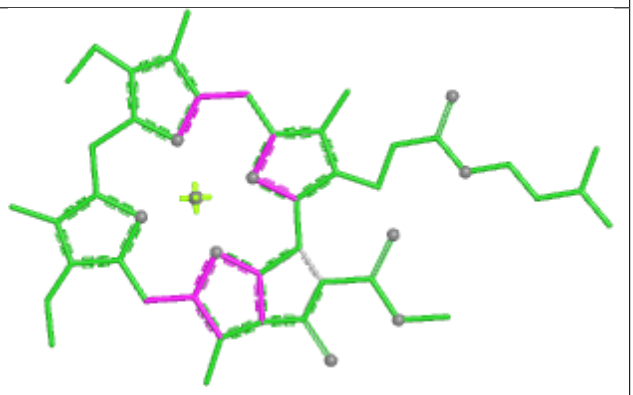


Rings

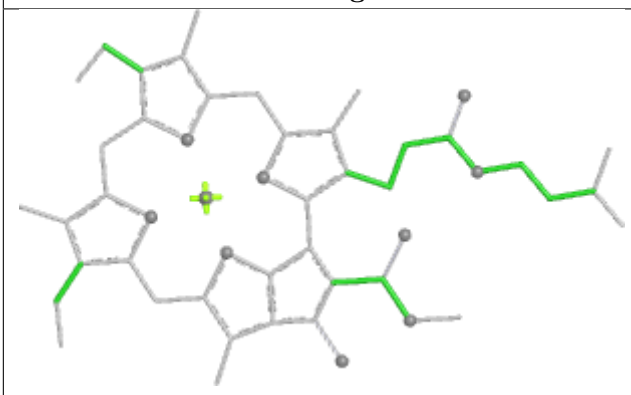
Ligand CLA a 817



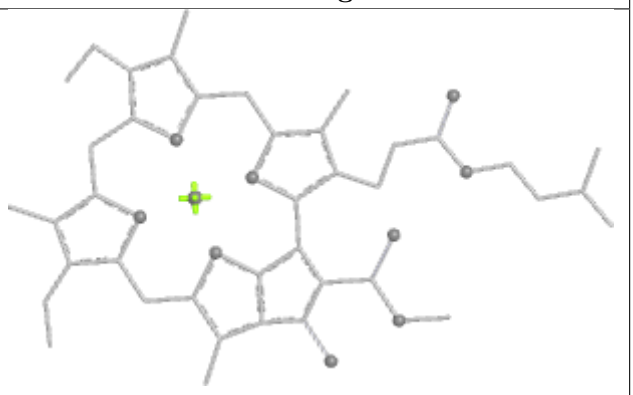
Bond lengths



Bond angles

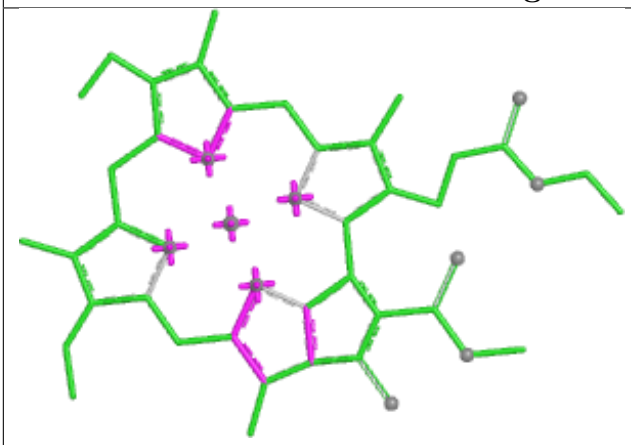


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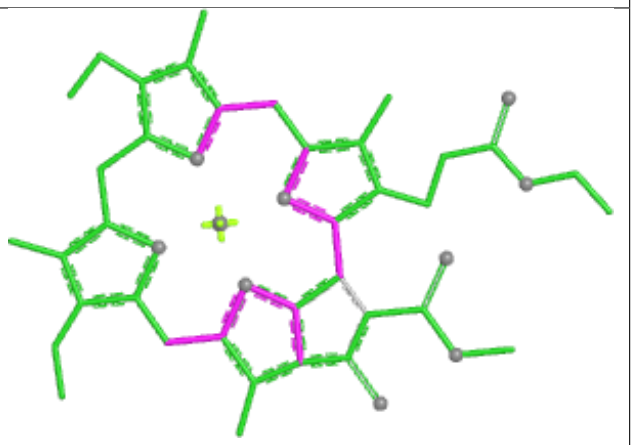


Rings

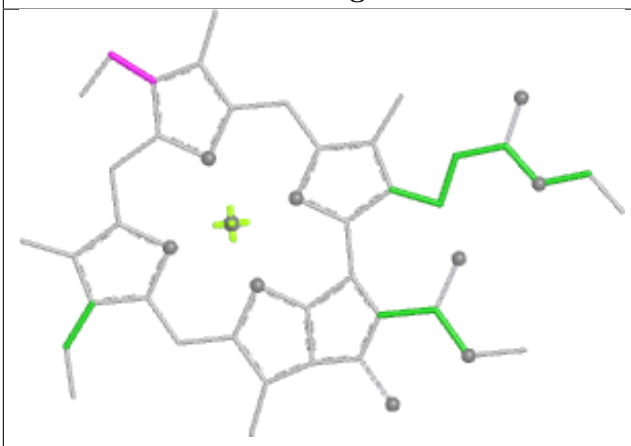
Ligand CLA O 316



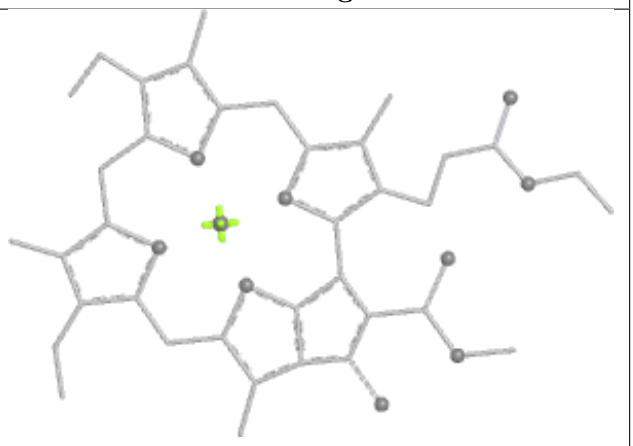
Bond lengths



Bond angles

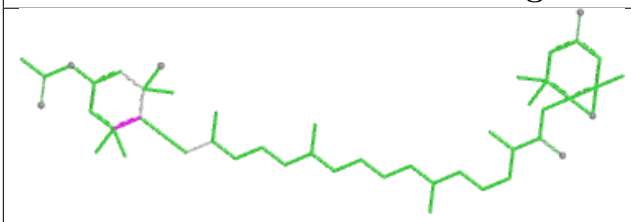


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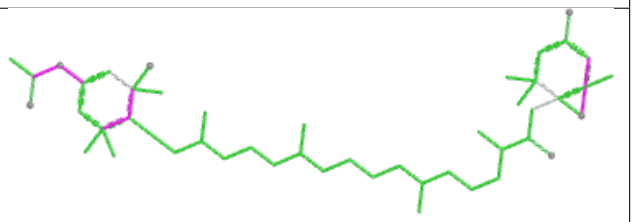


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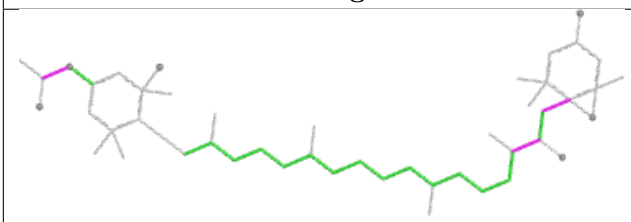
Ligand A86 M 315



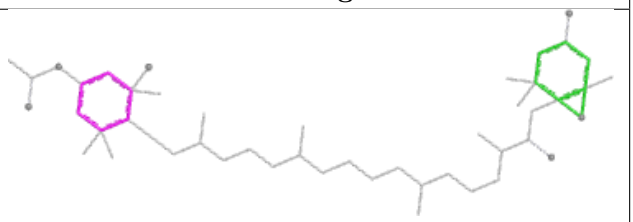
Bond lengths



Bond angles

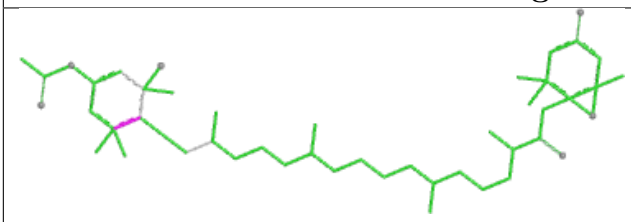


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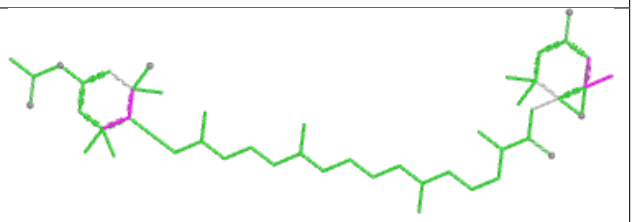


Rings

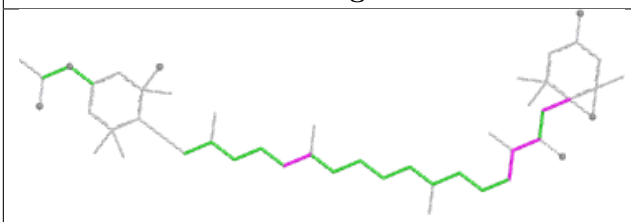
Ligand A86 F 313



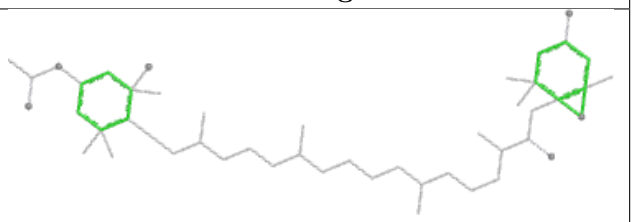
Bond lengths



Bond angles

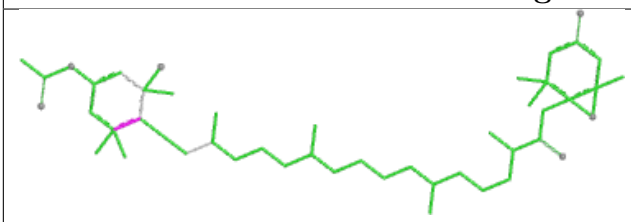


Torsions

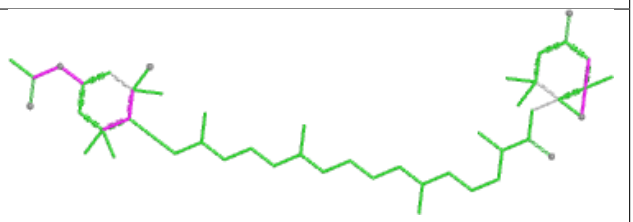


Rings

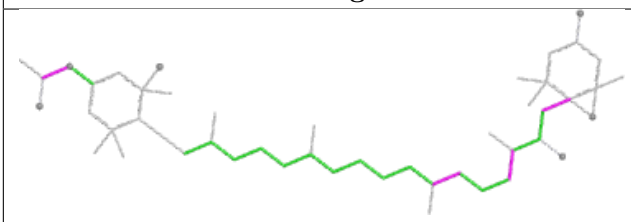
Ligand A86 o 317



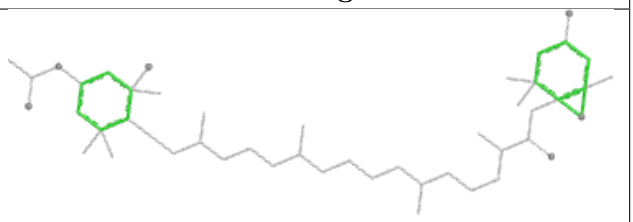
Bond lengths



Bond angles

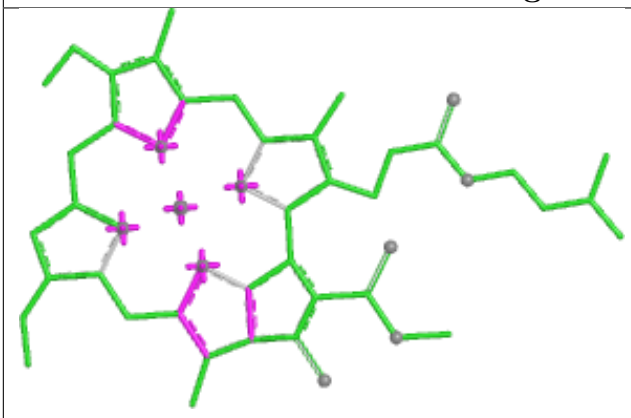


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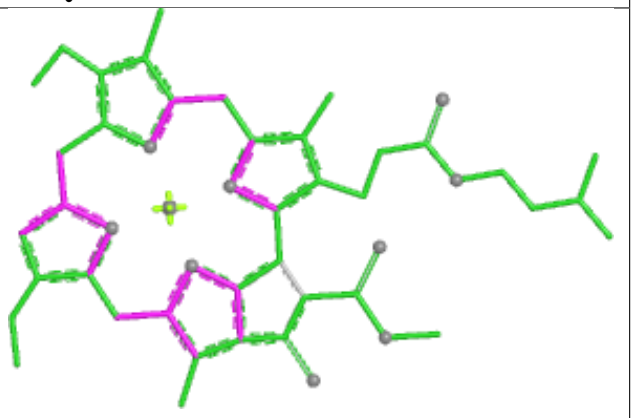


Rings

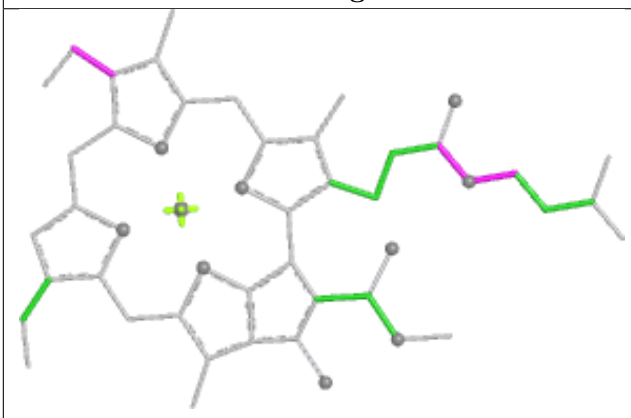
Ligand CLA Q 203



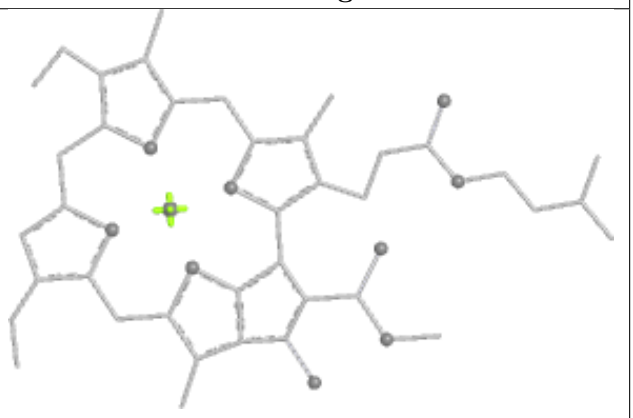
Bond lengths



Bond angles

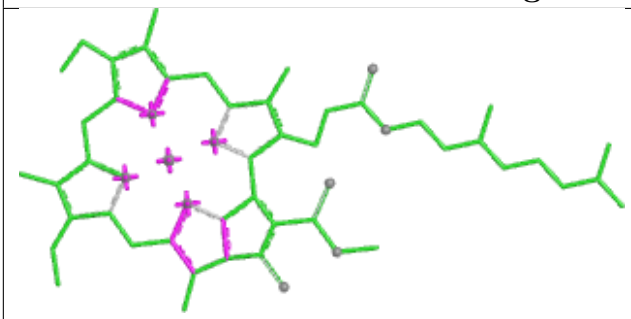


Torsions

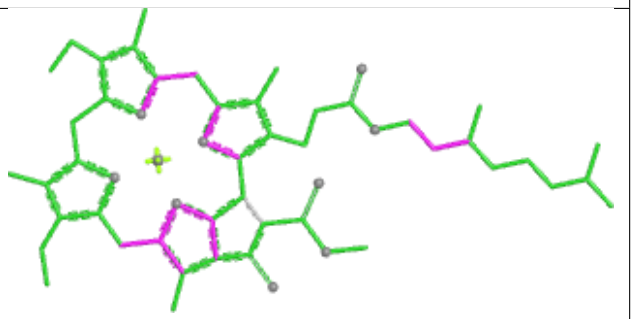


Rings

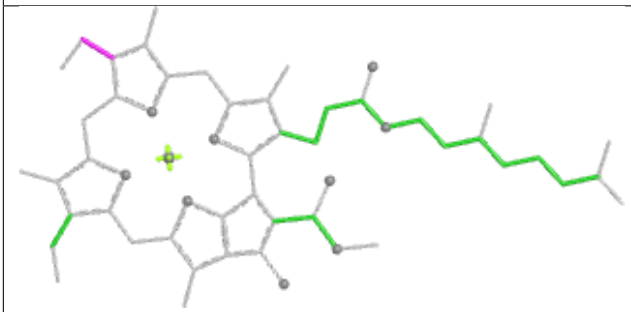
Ligand CLA D 308



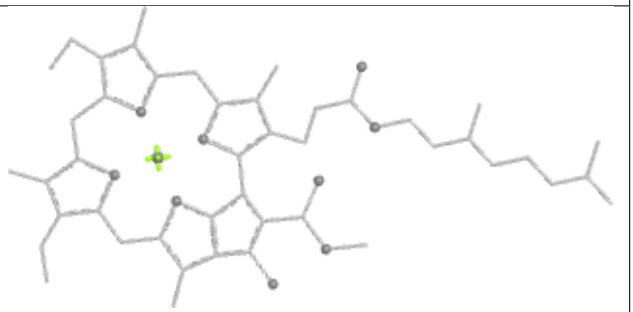
Bond lengths



Bond angles

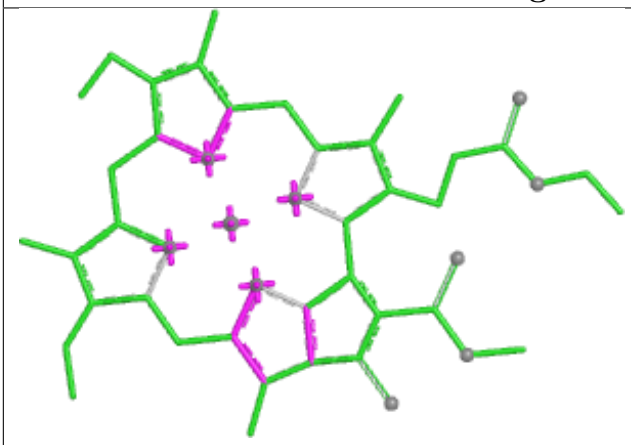


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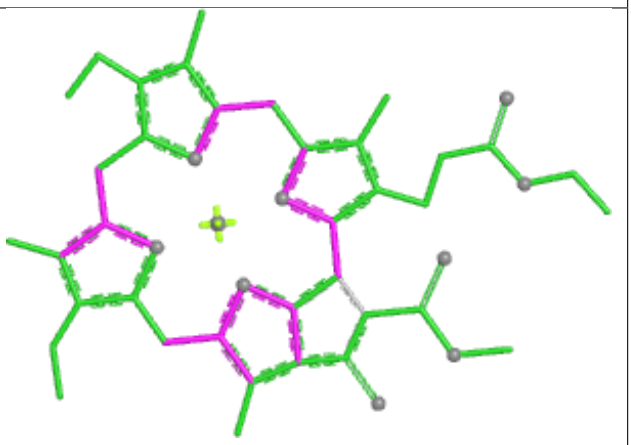


Rings

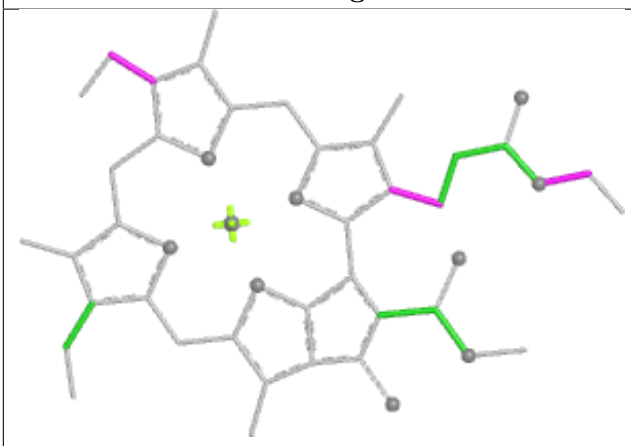
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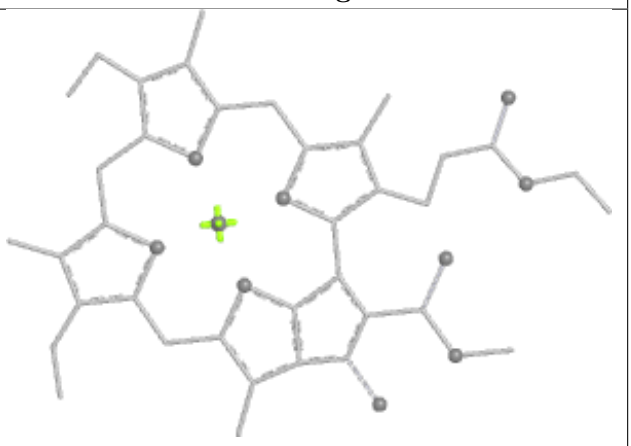
Bond lengths



Bond angles

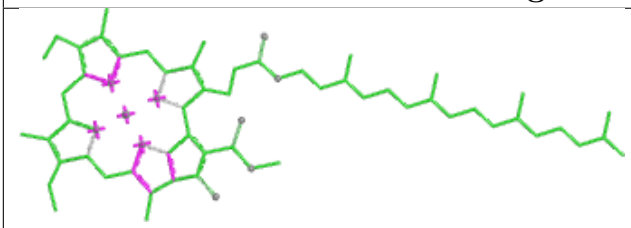


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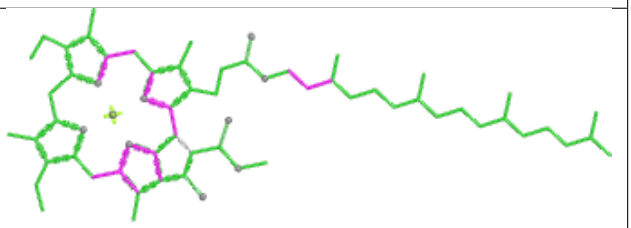


Rings

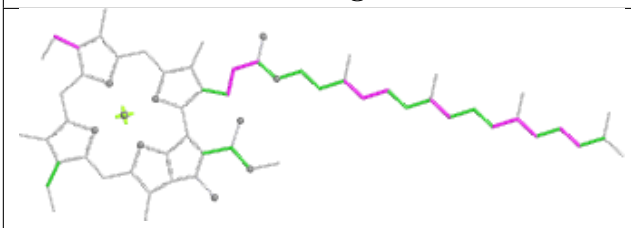
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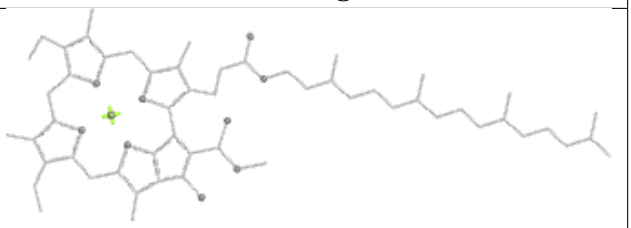
Bond lengths



Bond angles

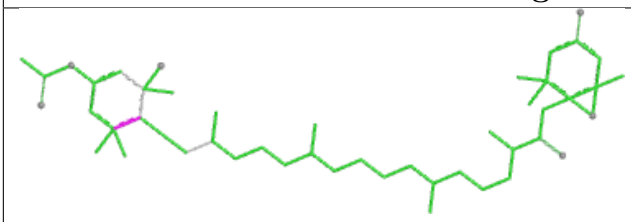


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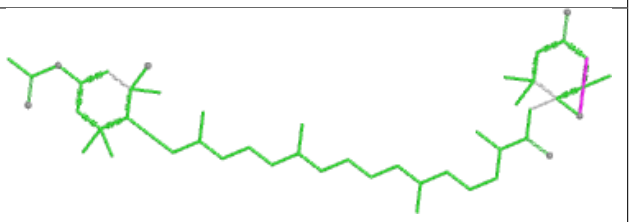


Rings

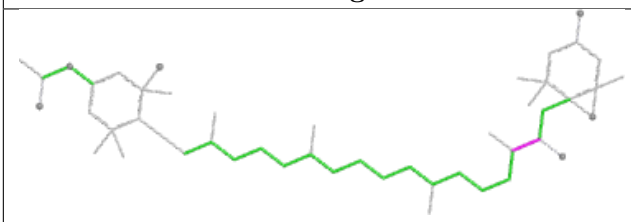
Ligand A86 Z 317



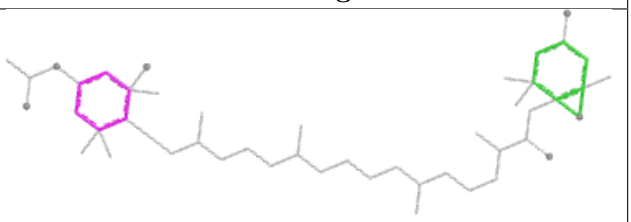
Bond lengths



Bond angles

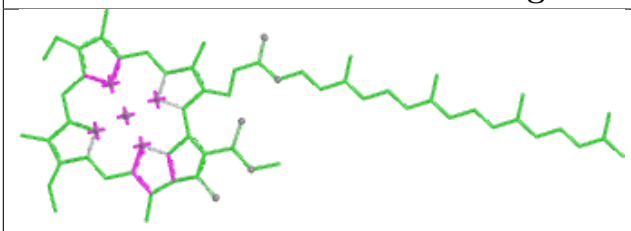


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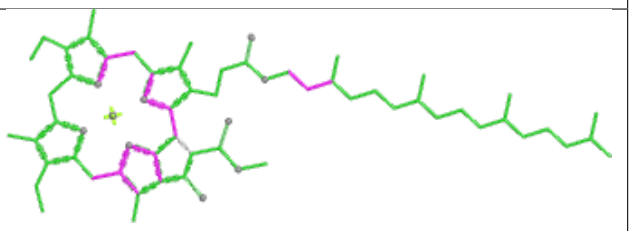


Rings

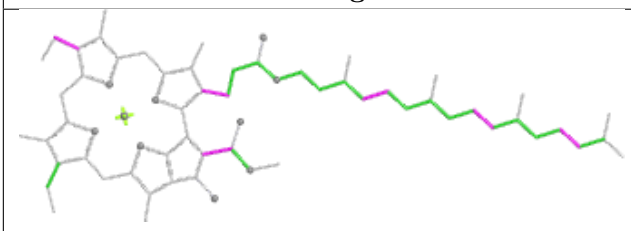
Ligand CLA u 302



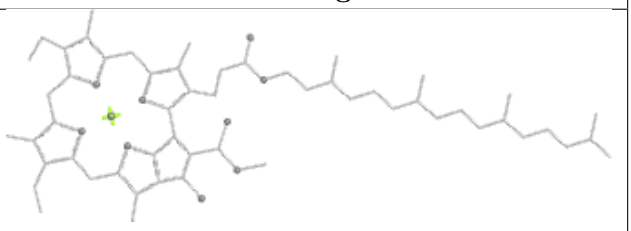
Bond lengths



Bond angles

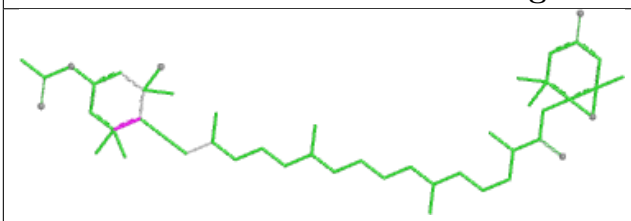


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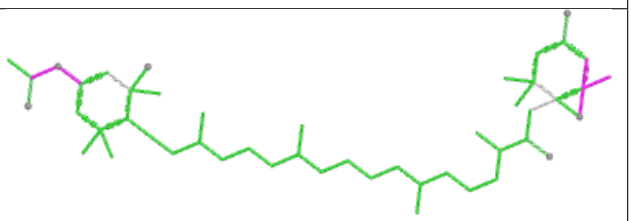


Rings

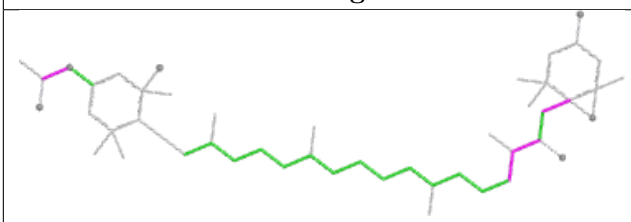
Ligand A86 G 209



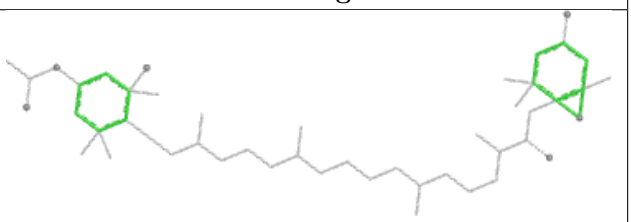
Bond lengths



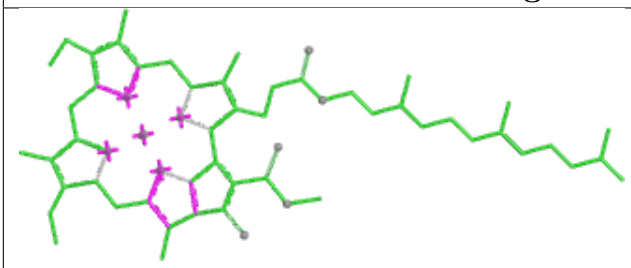
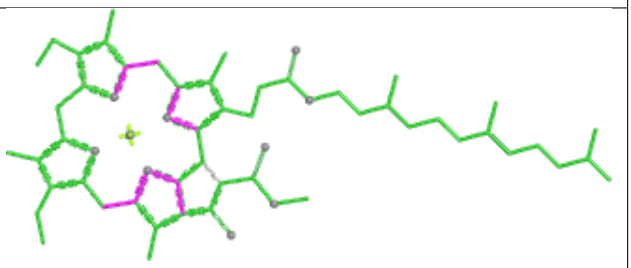
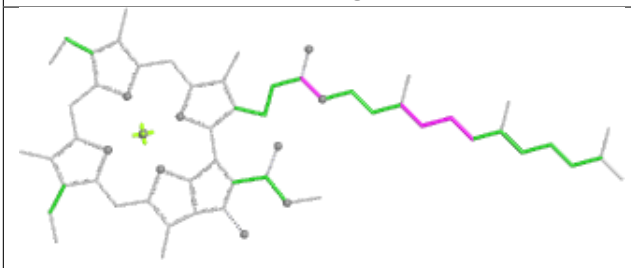
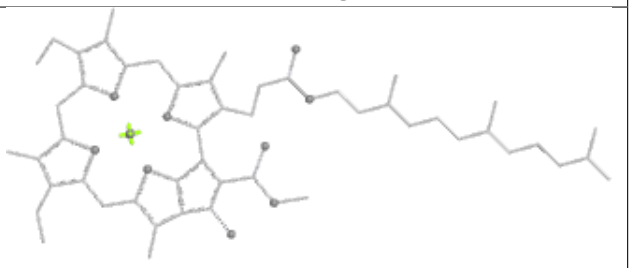
Bond angles

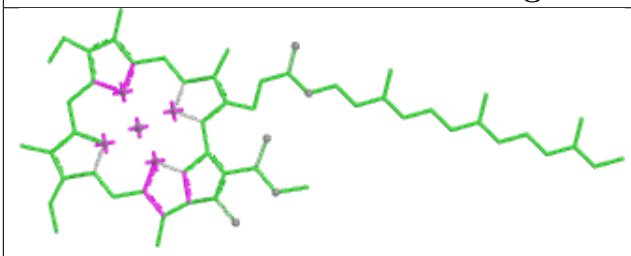
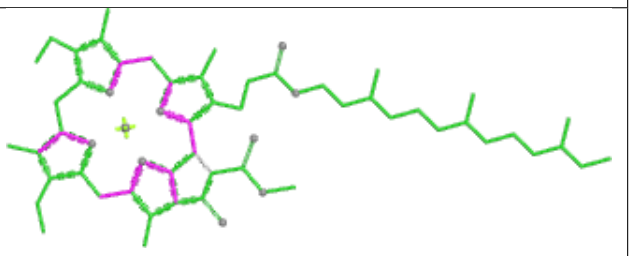
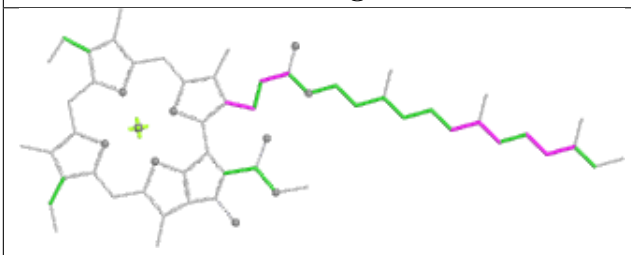
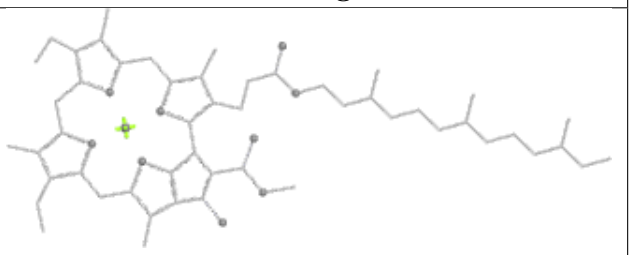


Torsions

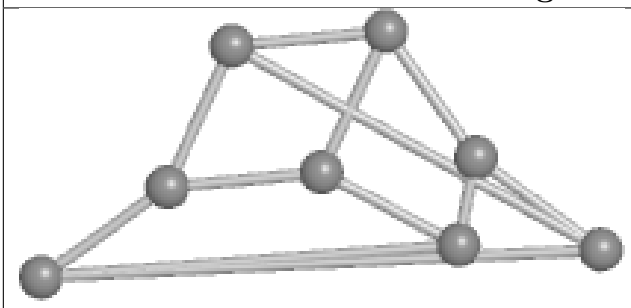


Rings

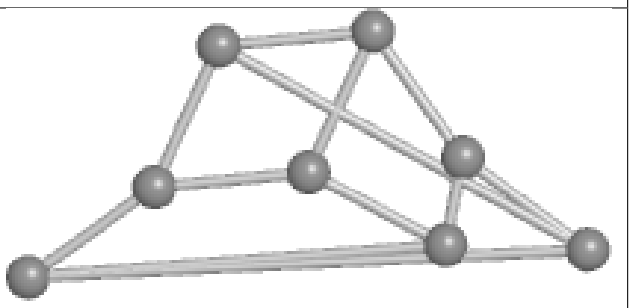
Ligand CLA R 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

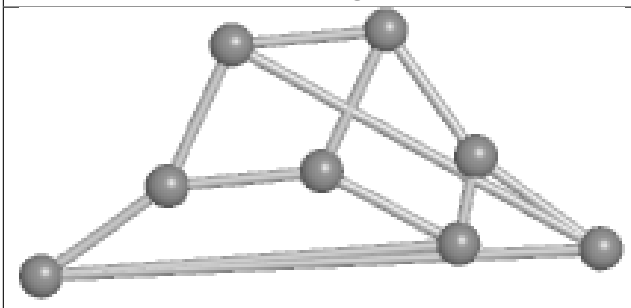
Ligand SF4 c 102



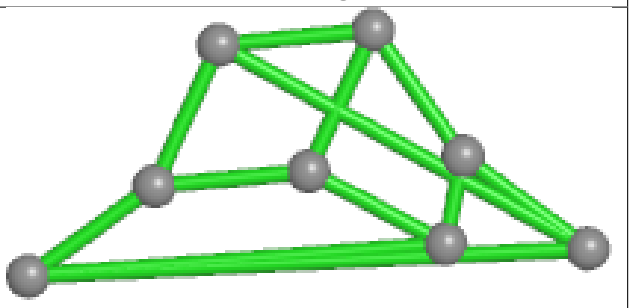
Bond lengths



Bond angles

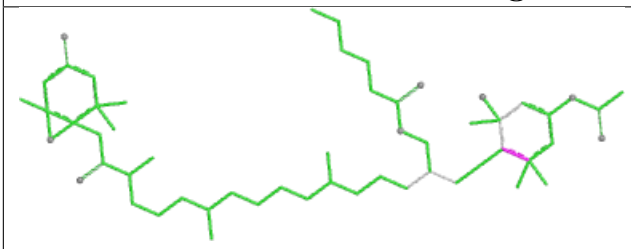


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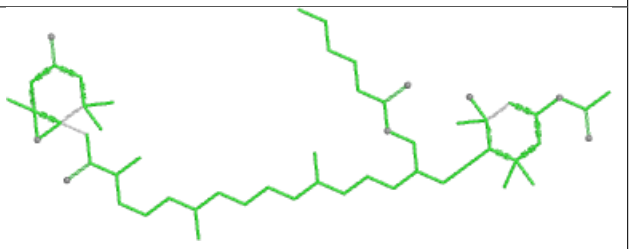


Rings

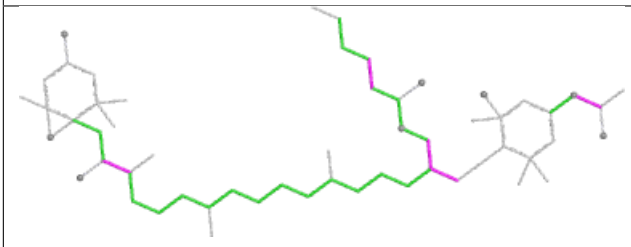
Ligand A1EB1 Z 321



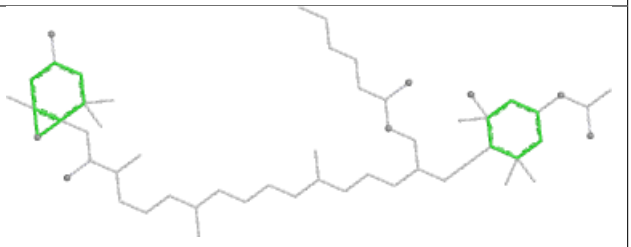
Bond lengths



Bond angles

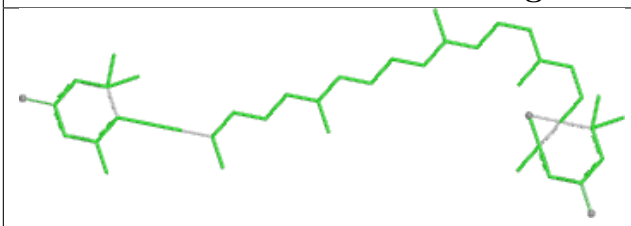


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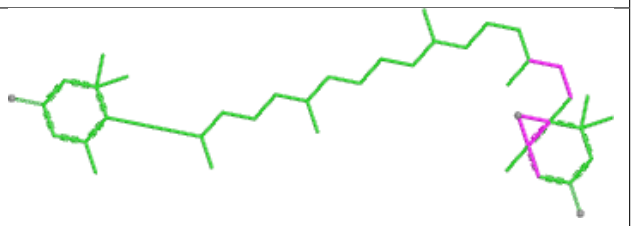


Rings

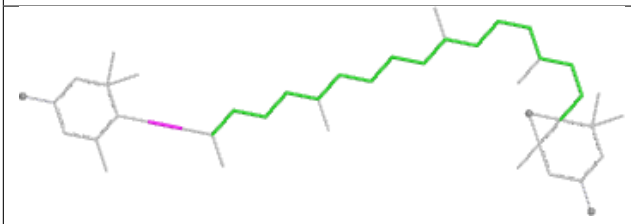
Ligand DD6 w 312



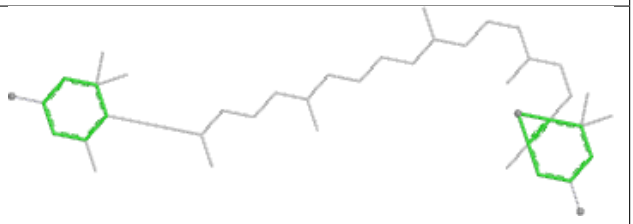
Bond lengths



Bond angles

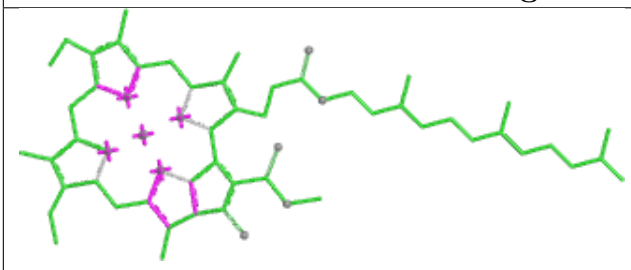


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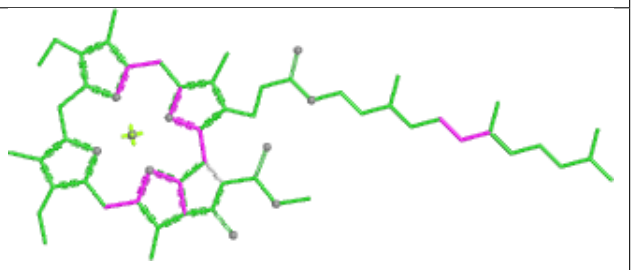


Rings

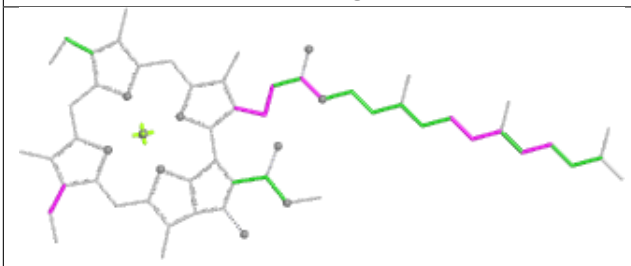
Ligand CLA M 305



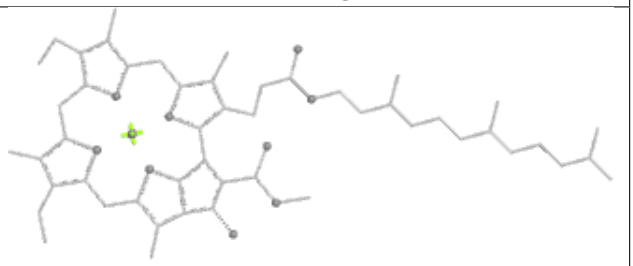
Bond lengths



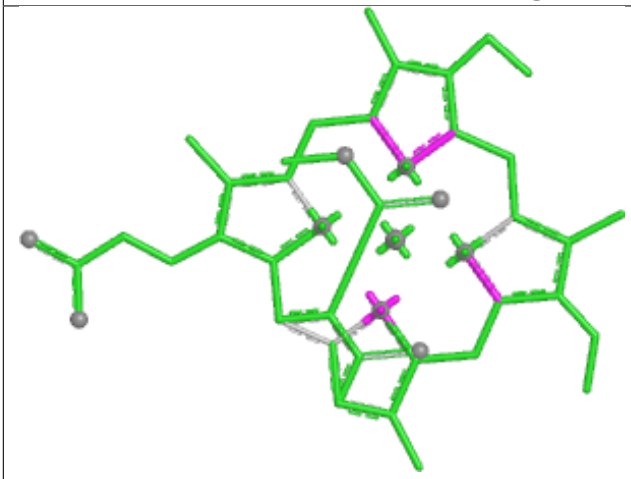
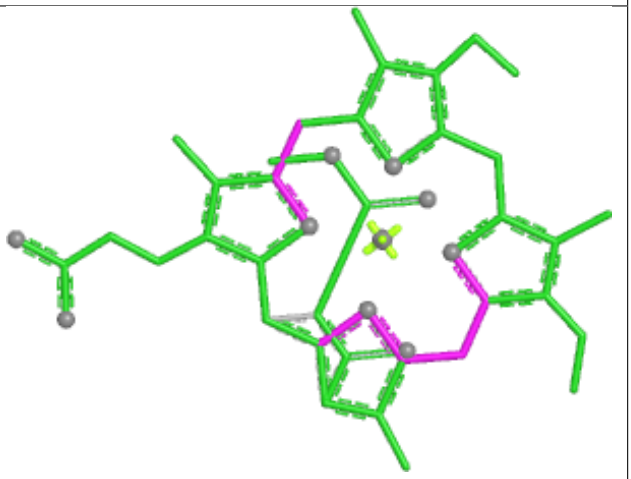
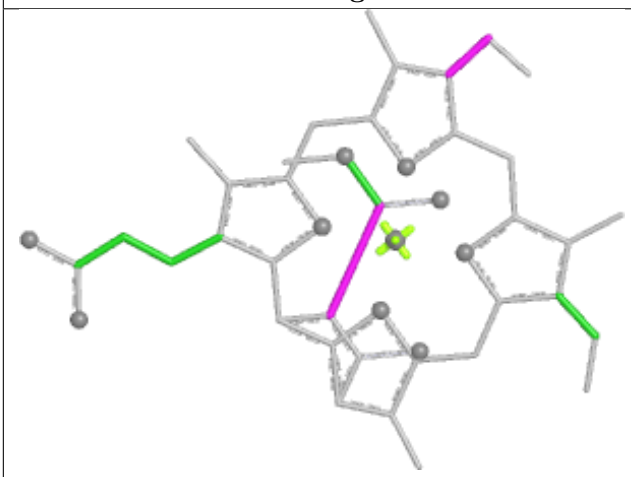
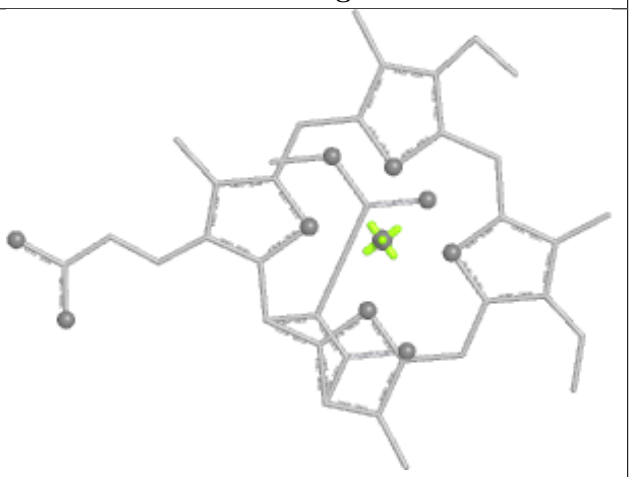
Bond angles

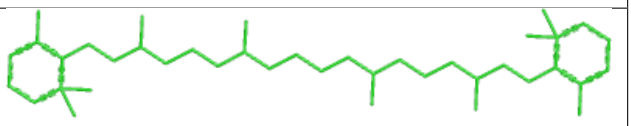
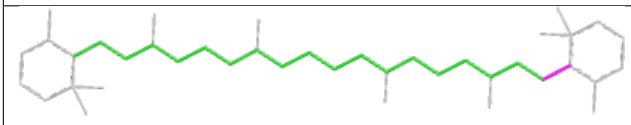
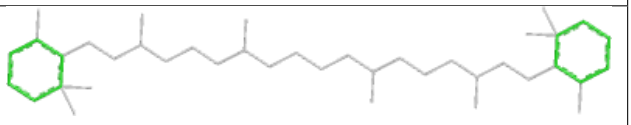


Torsions

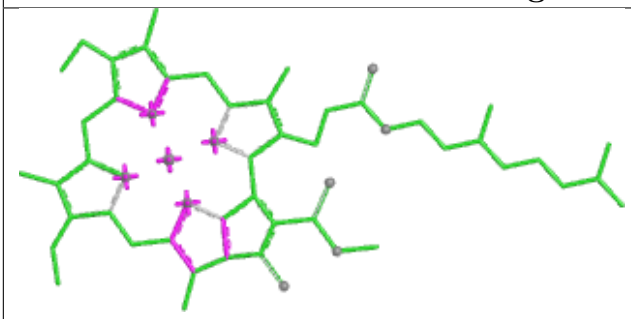


Rings

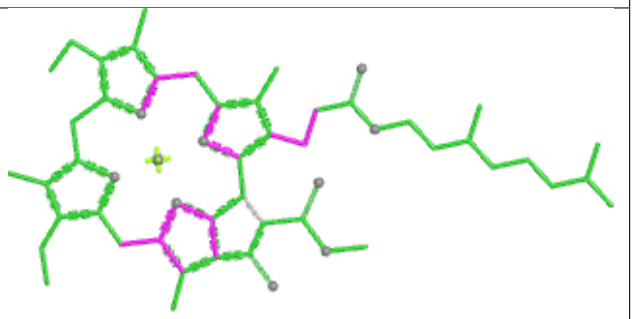
Ligand KC2 Z 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR r 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

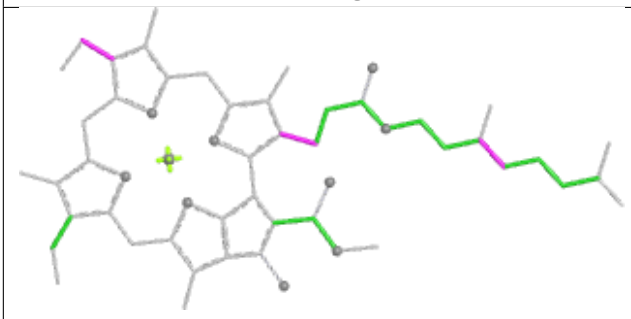
Ligand CLA k 202



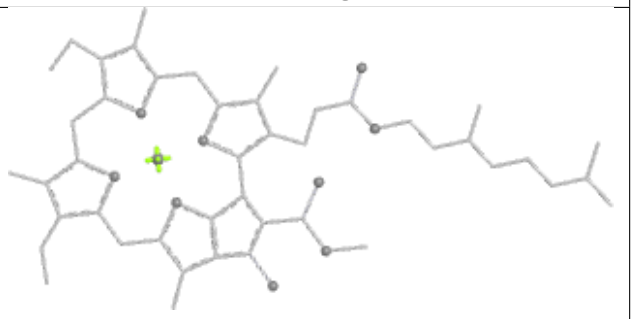
Bond lengths



Bond angles

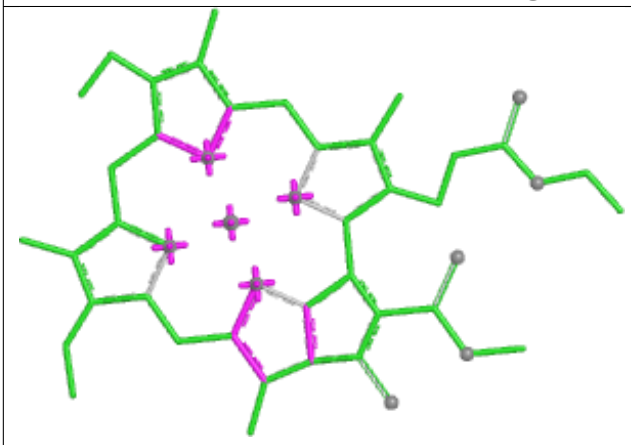


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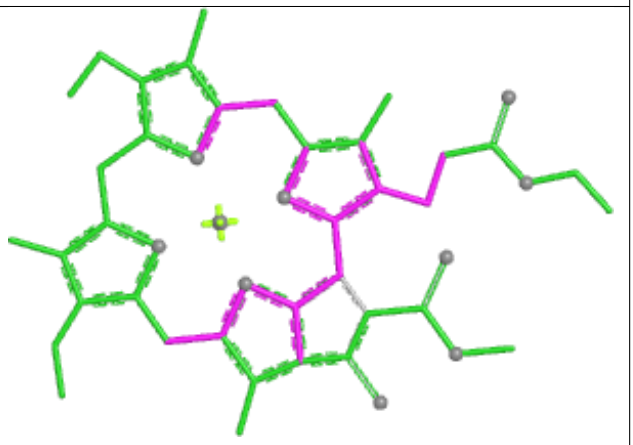


Rings

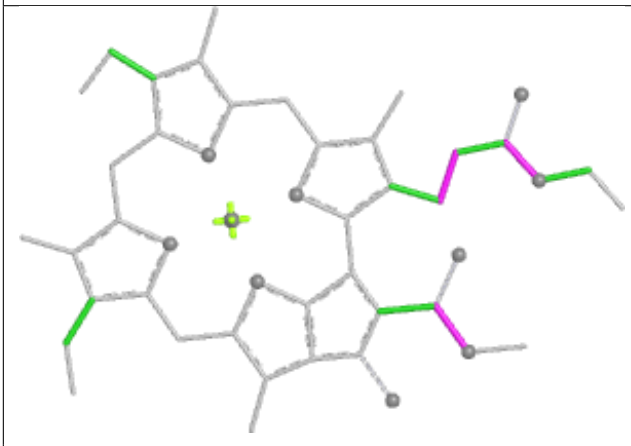
Ligand CLA C 308



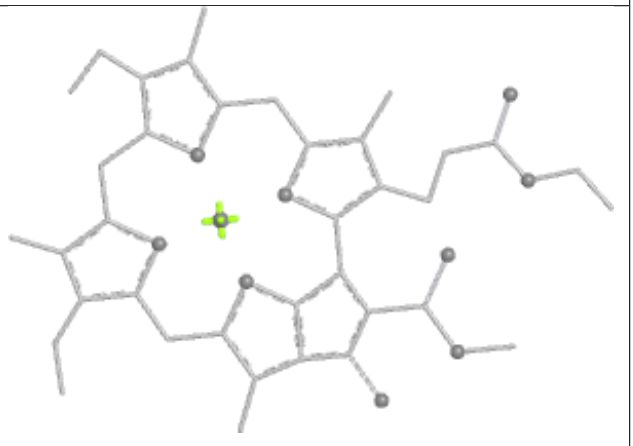
Bond lengths



Bond angles

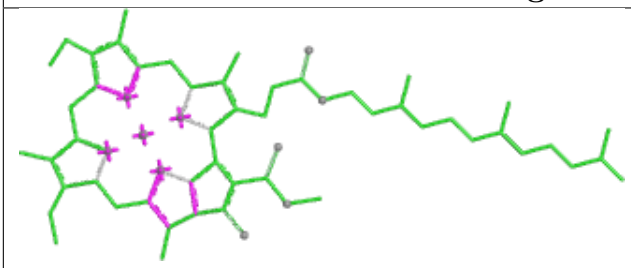


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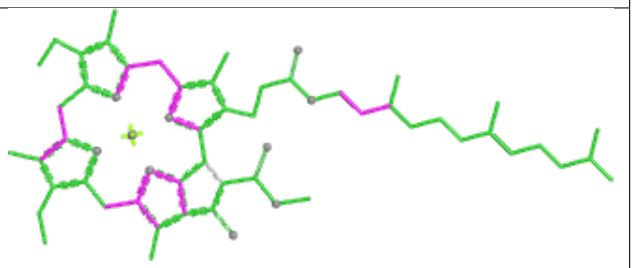


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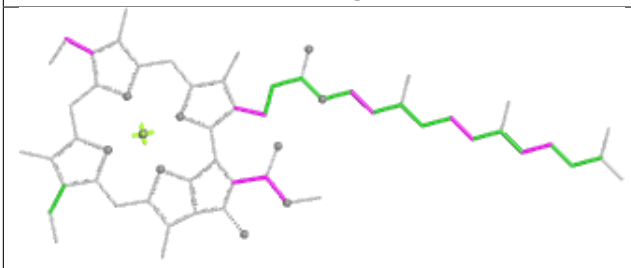
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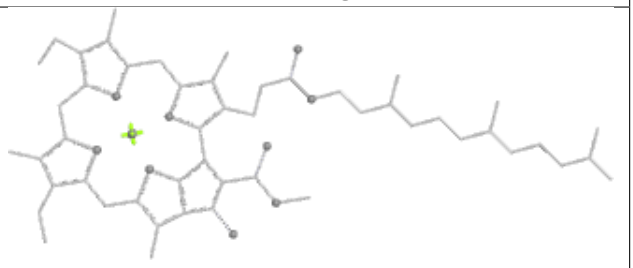
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Bond angles

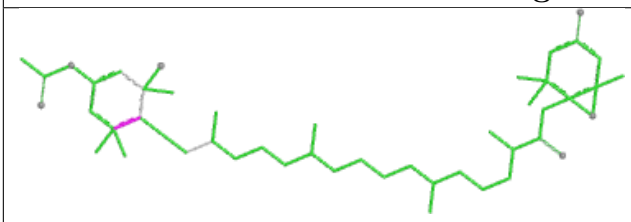


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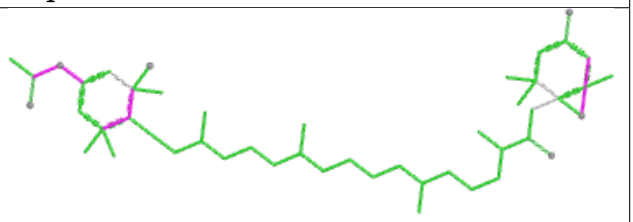


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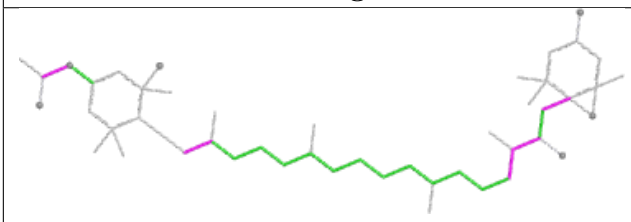
Ligand A86 p 318



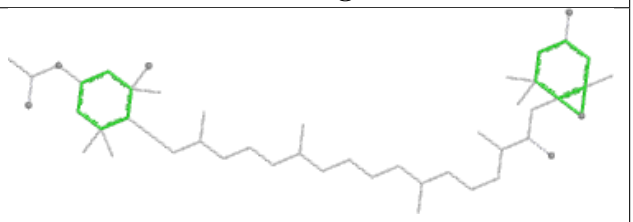
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Bond angles

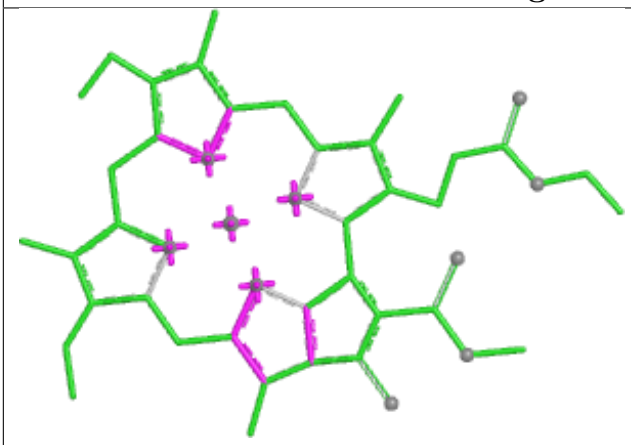


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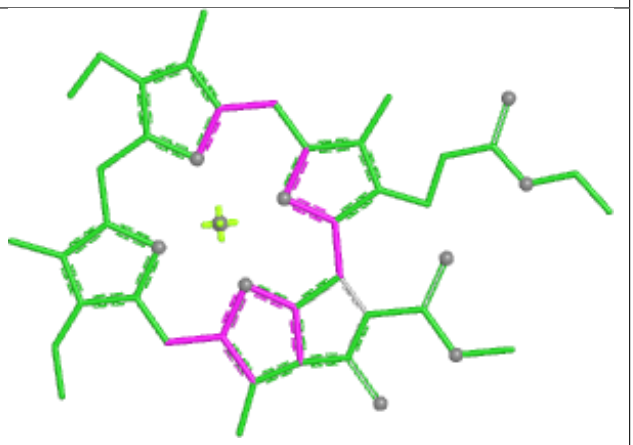


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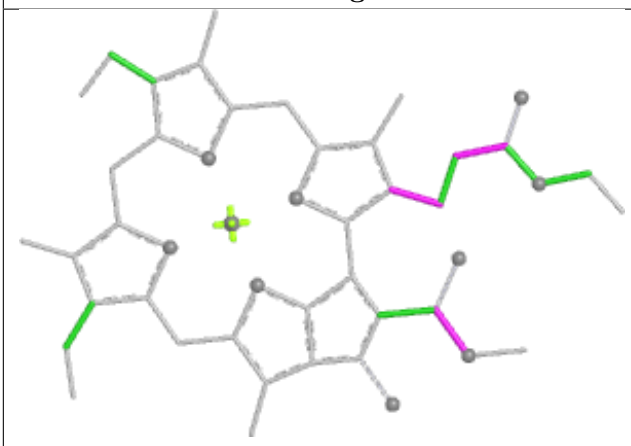
Ligand CLA o 312



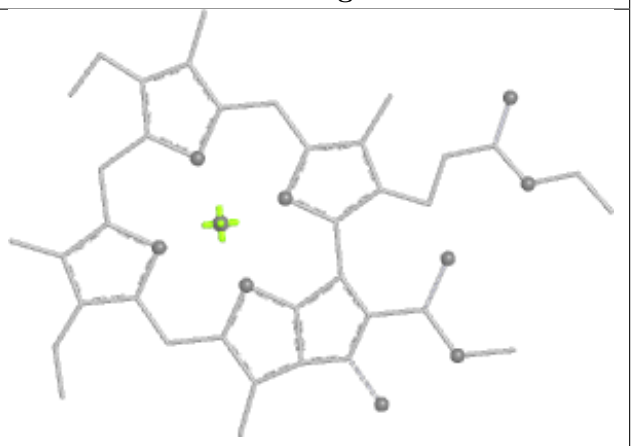
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Bond angles

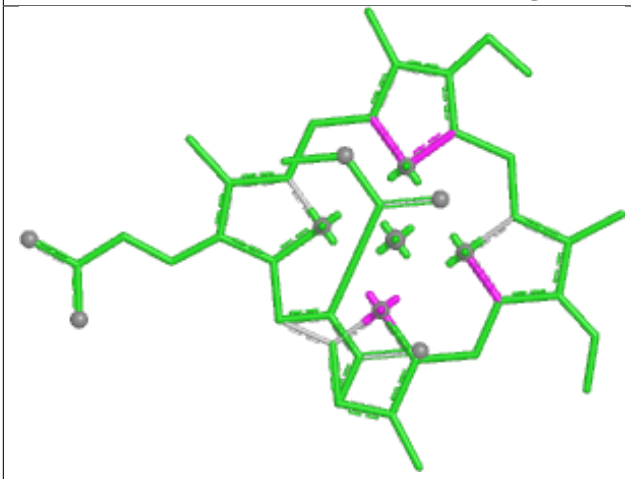


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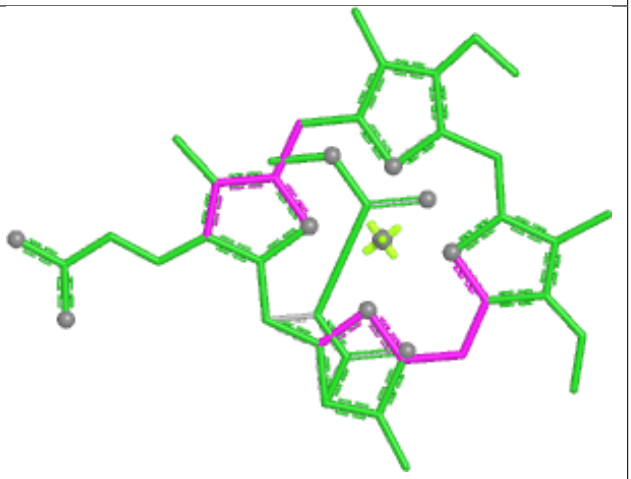


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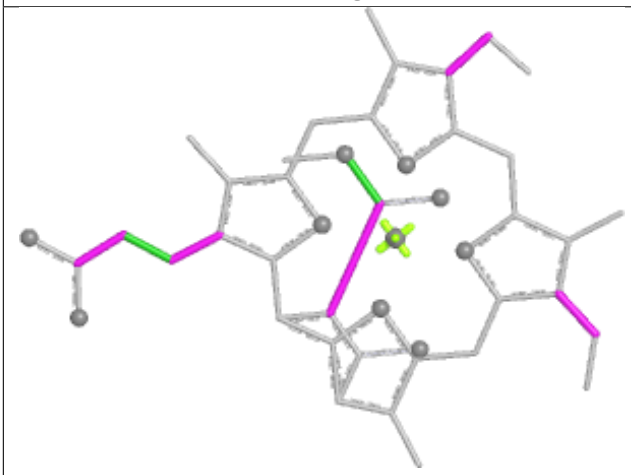
Ligand KC2 O 309



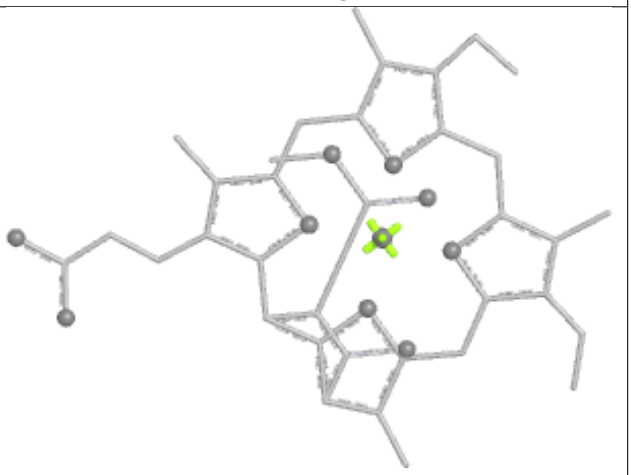
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Bond angles

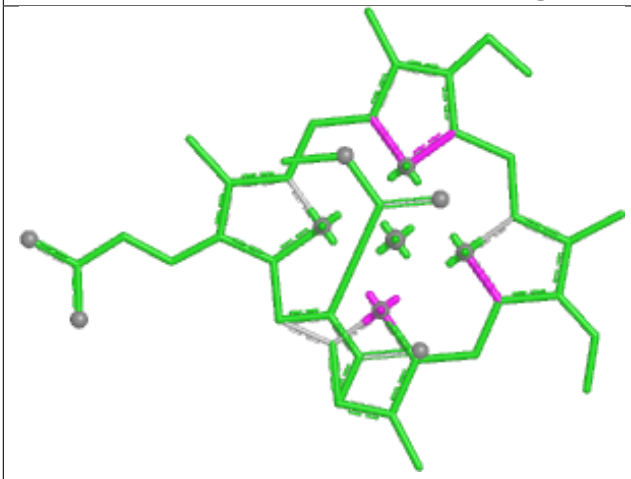


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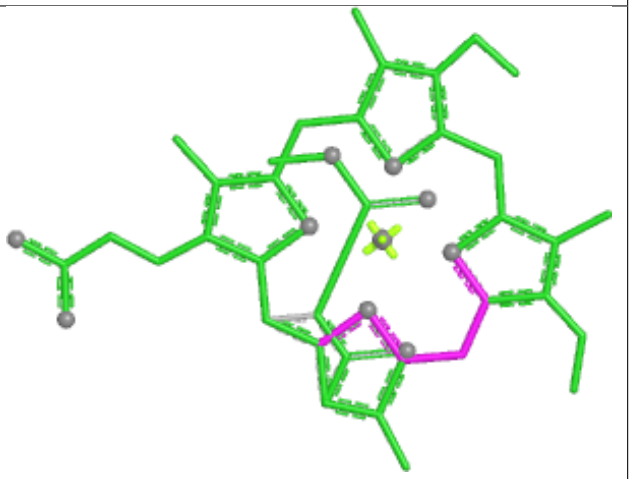


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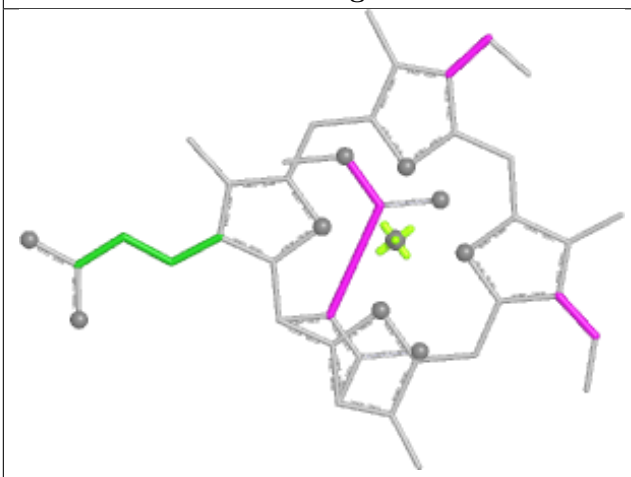
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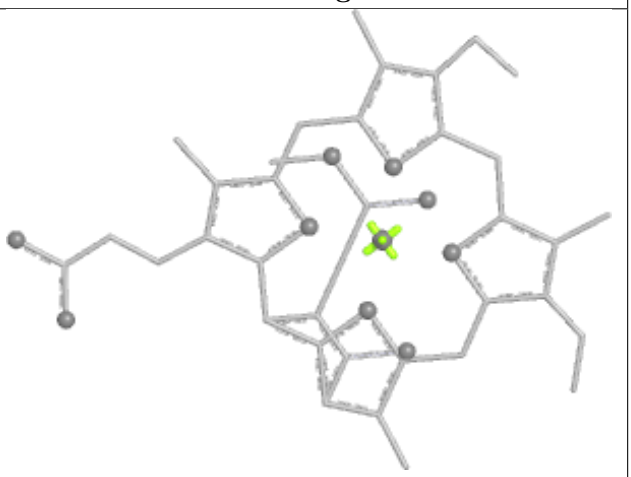
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Bond angles

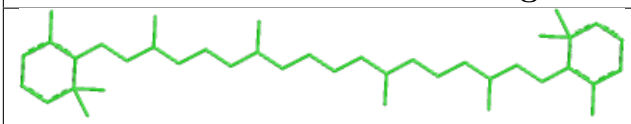


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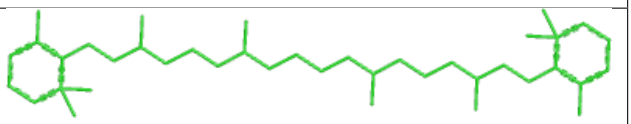


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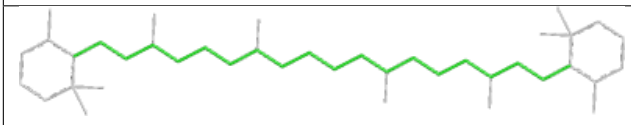
Ligand BCR m 101



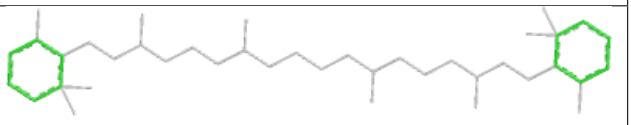
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Bond angles

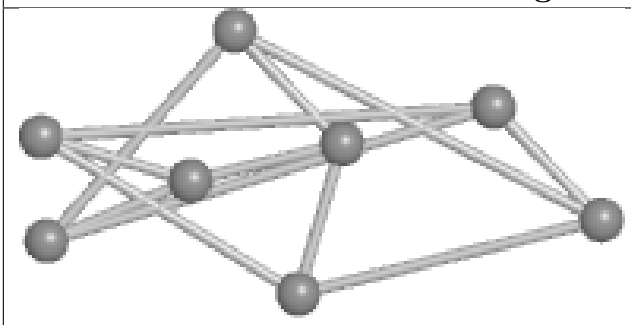


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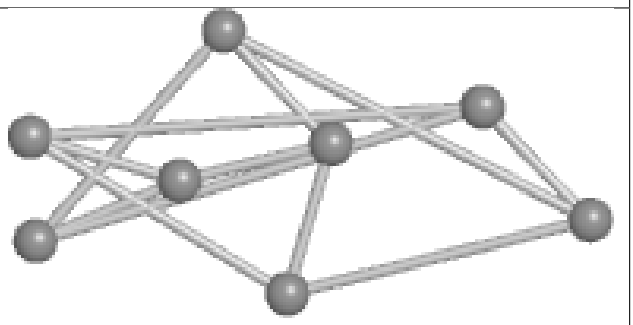


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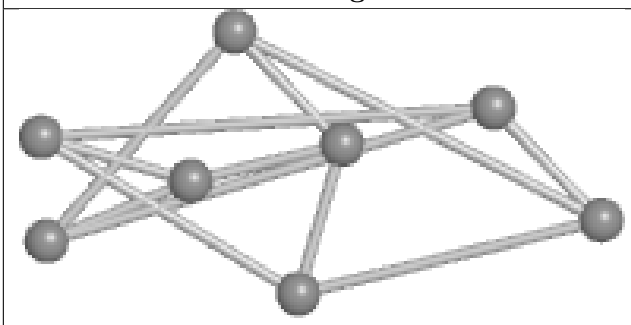
Ligand SF4 b 804



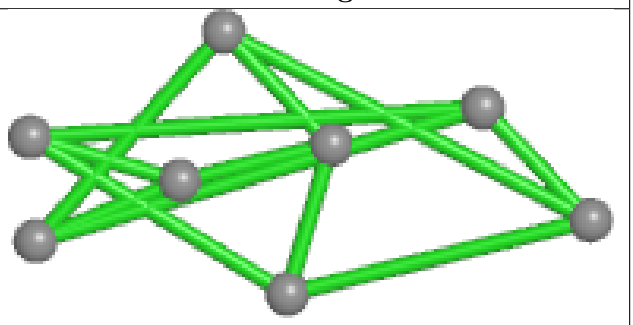
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Bond angles

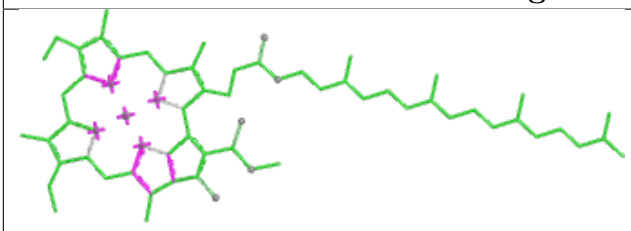


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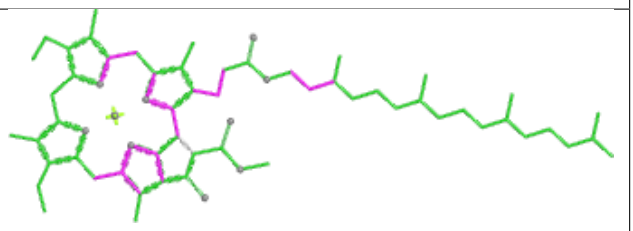


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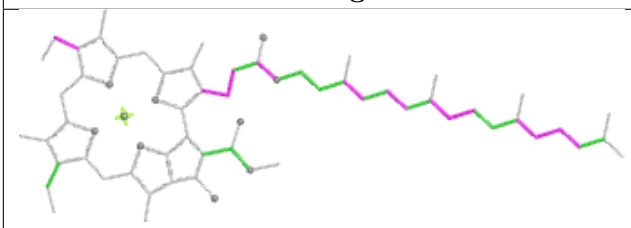
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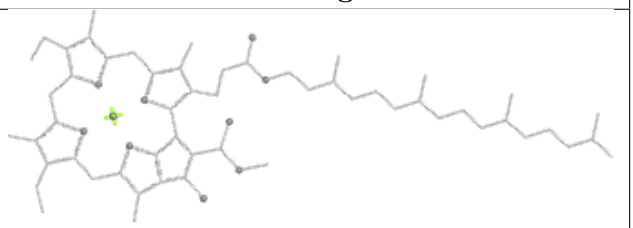
Bond lengths



Bond angles

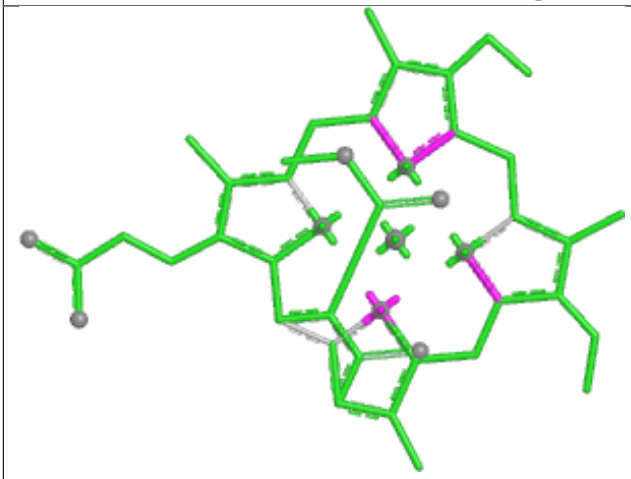


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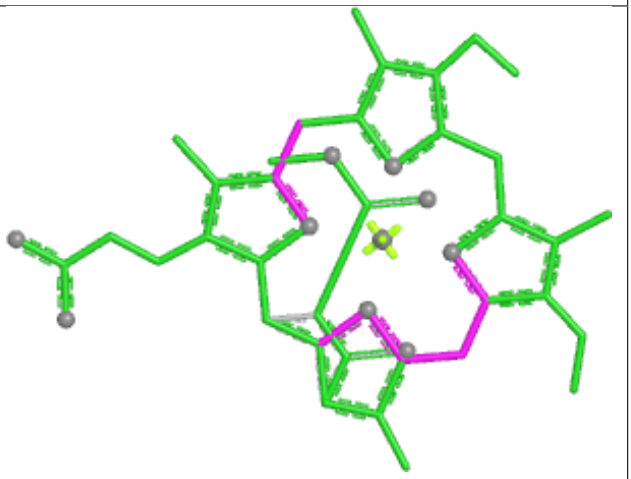


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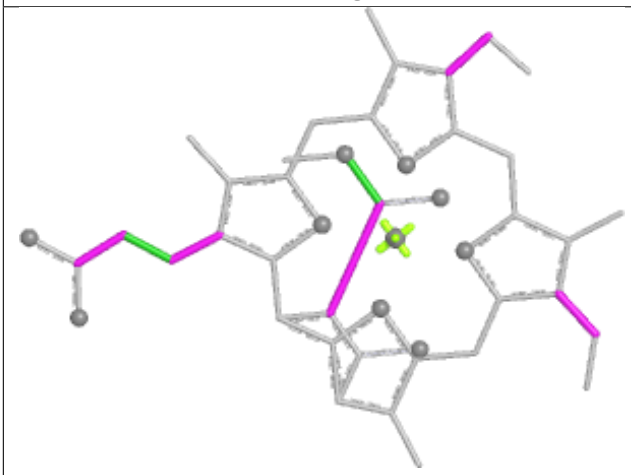
Ligand KC2 o 309



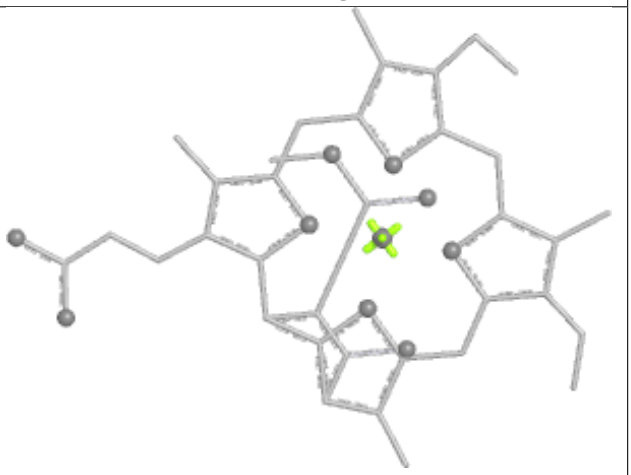
Bond lengths



Bond angles

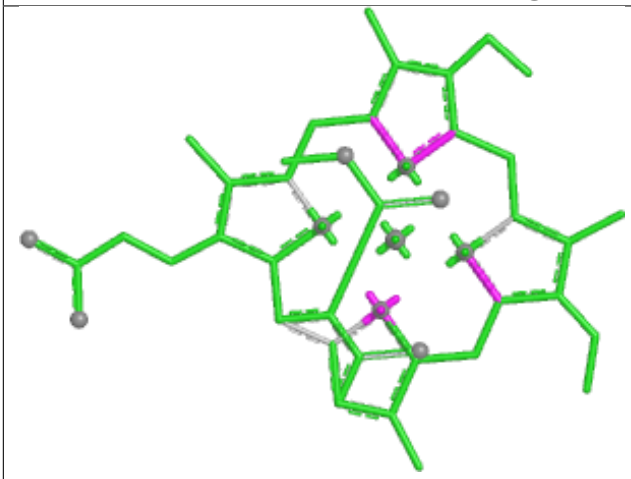


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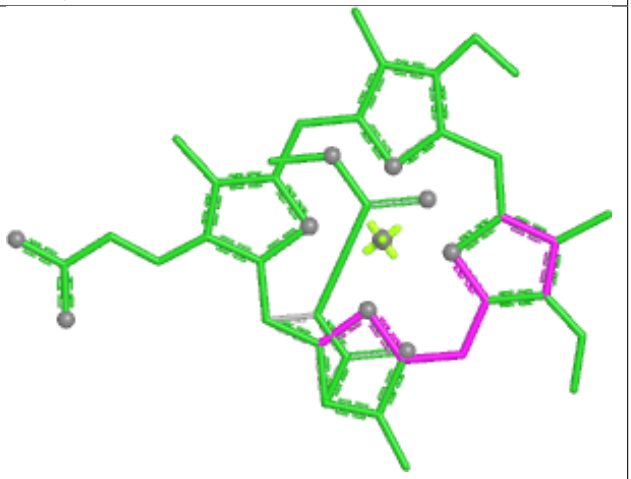


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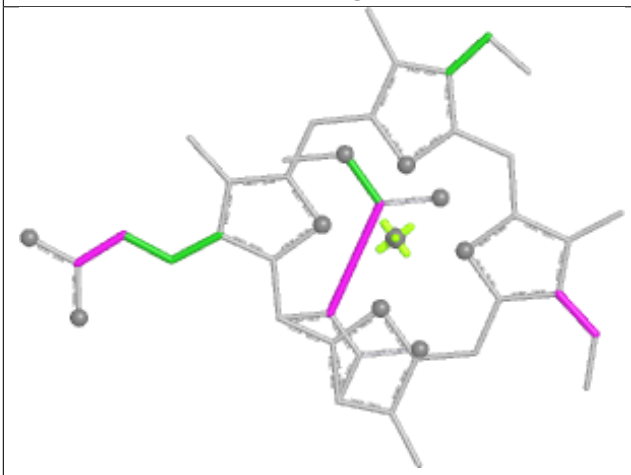
Ligand KC2 Q 201



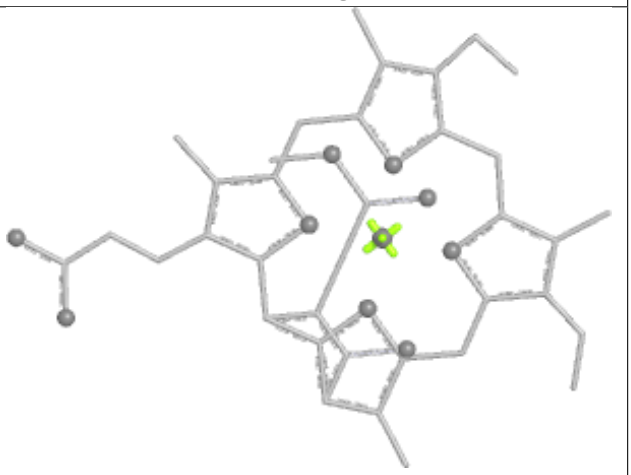
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Bond angles

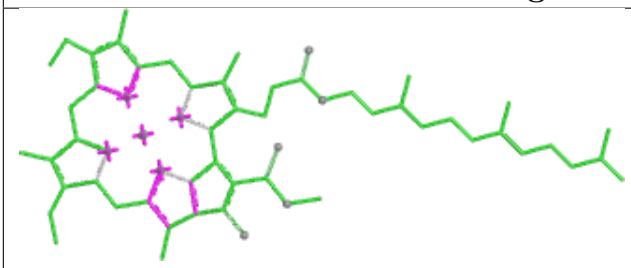


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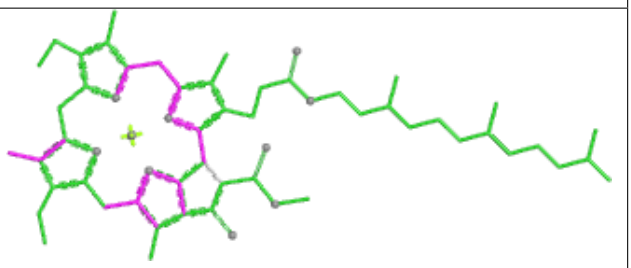


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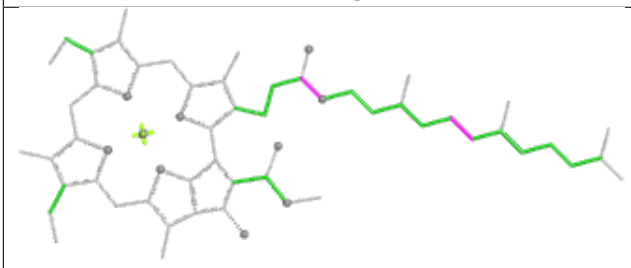
Ligand CLA v 305



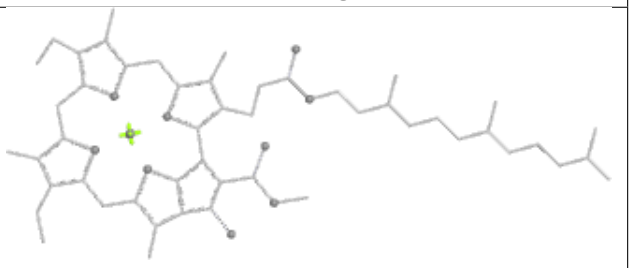
Bond lengths



Bond angles

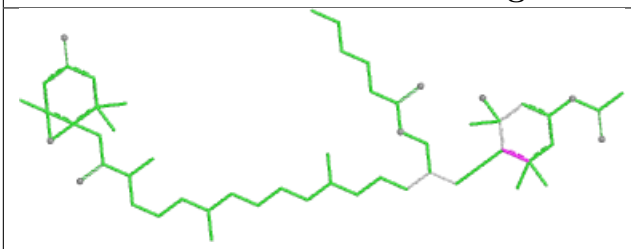


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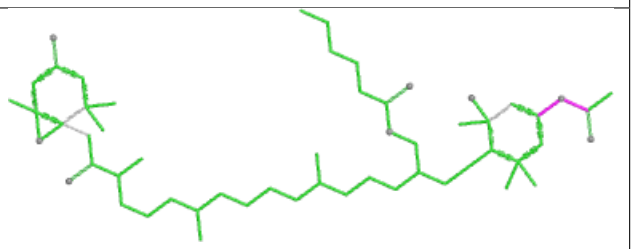


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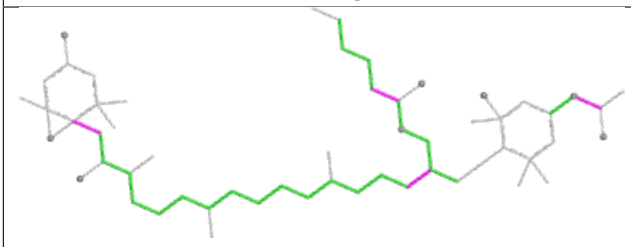
Ligand A1EB1 Z 319



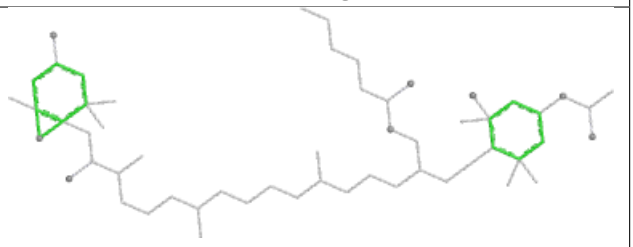
Bond lengths



Bond angles

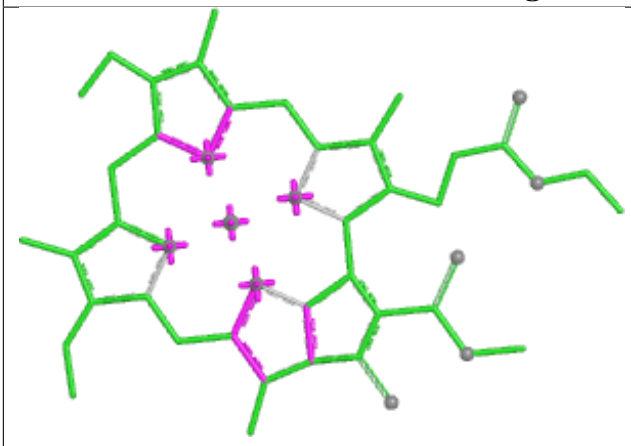


Torsions

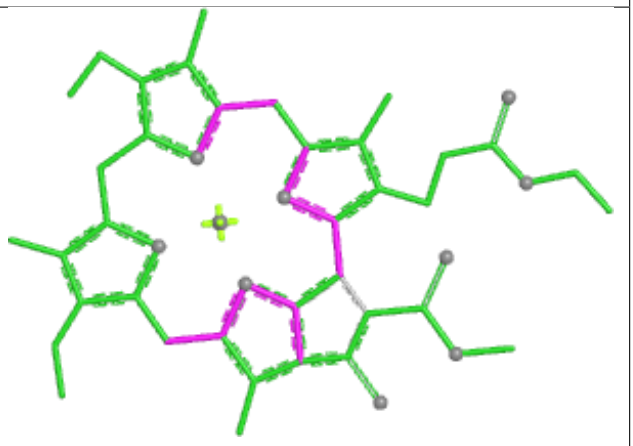


Rings

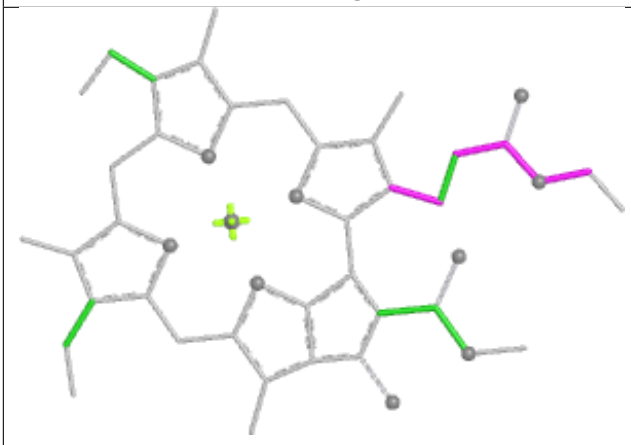
Ligand CLA X 304



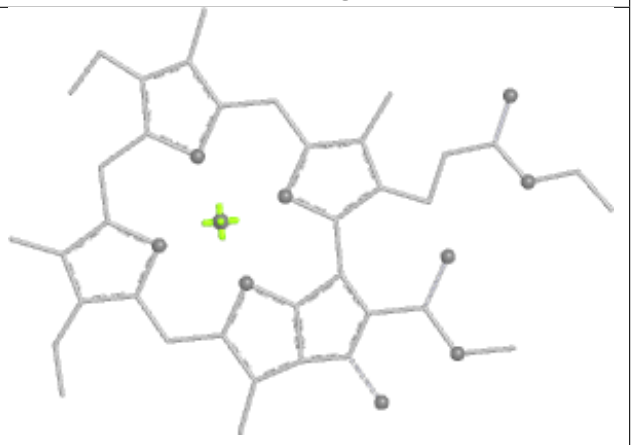
Bond lengths



Bond angles

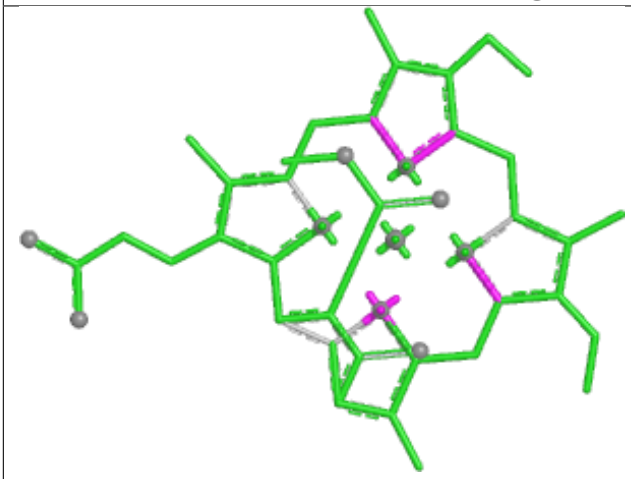


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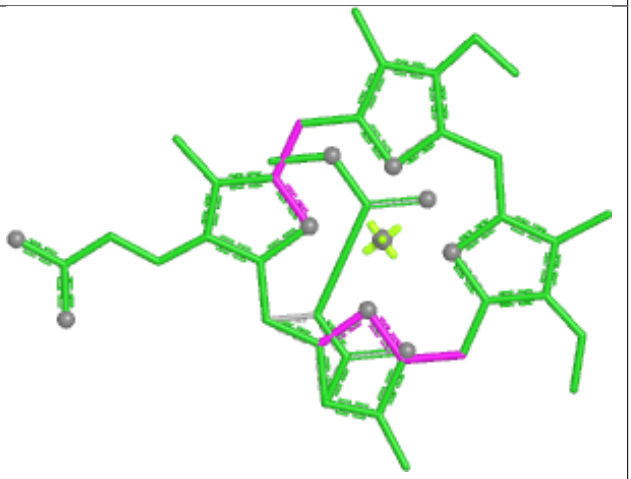


Rings

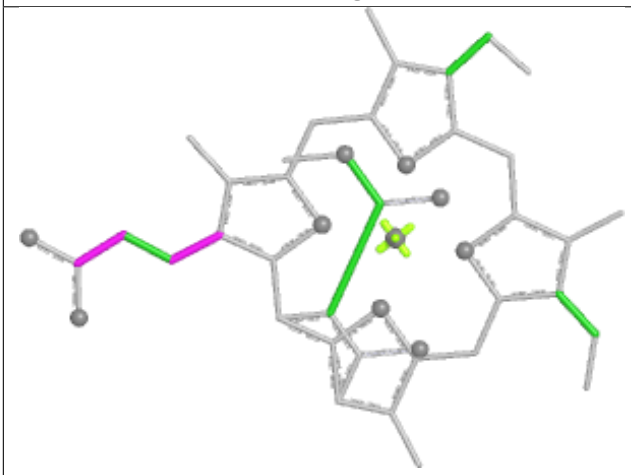
Ligand KC2 L 308



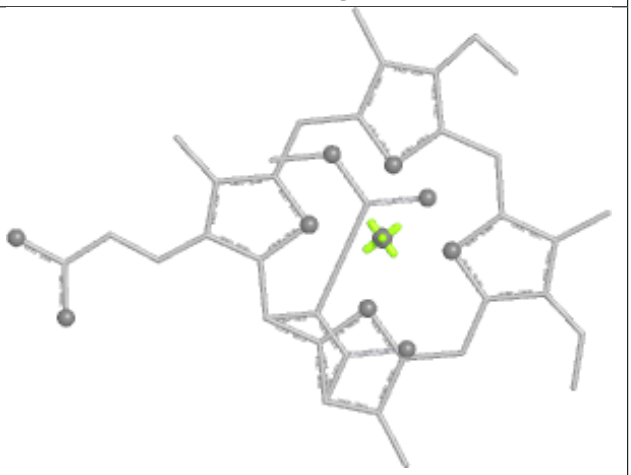
Bond lengths



Bond angles

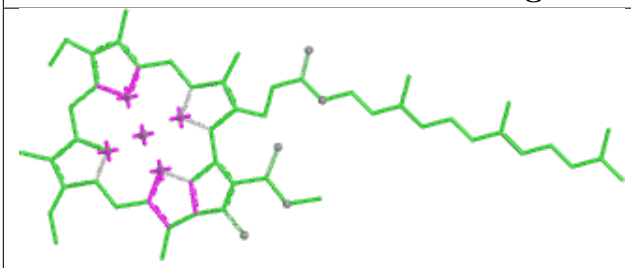


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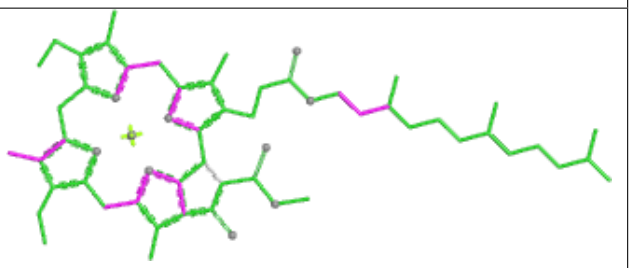


Rings

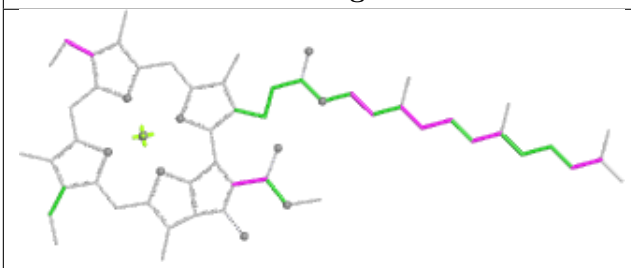
Ligand CLA P 305



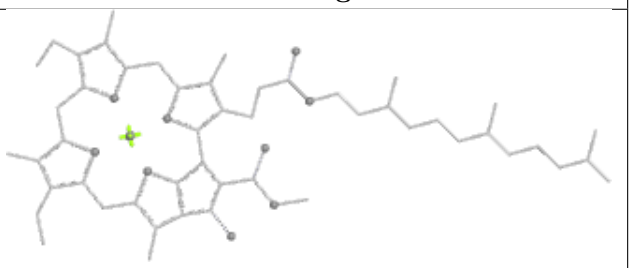
Bond lengths



Bond angles

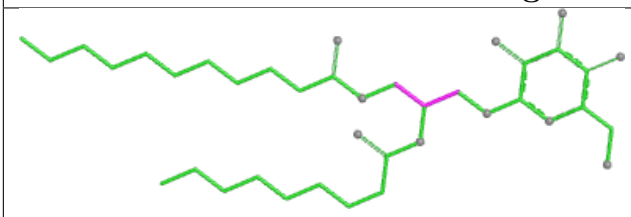


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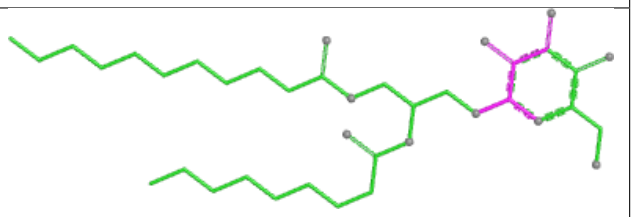


Rings

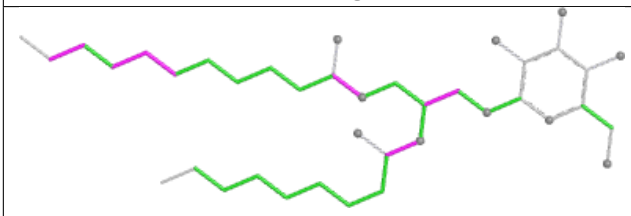
Ligand LMG S 322



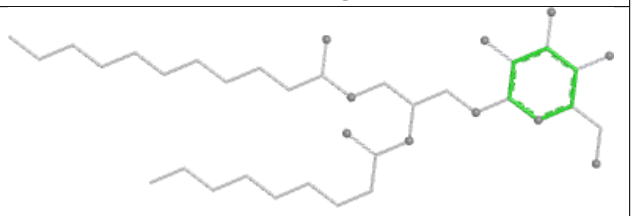
Bond lengths



Bond angles

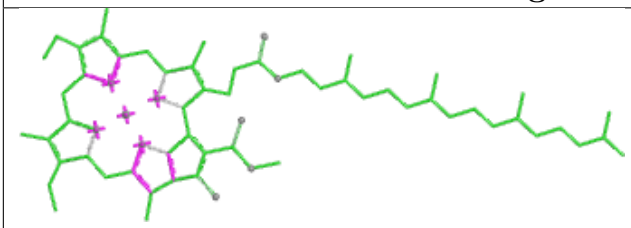


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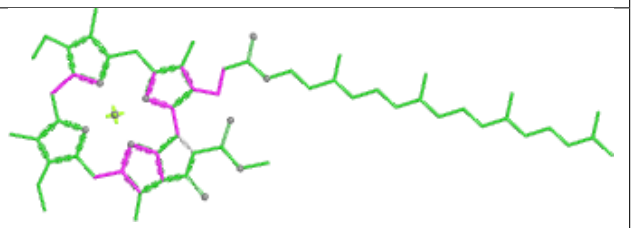


Rings

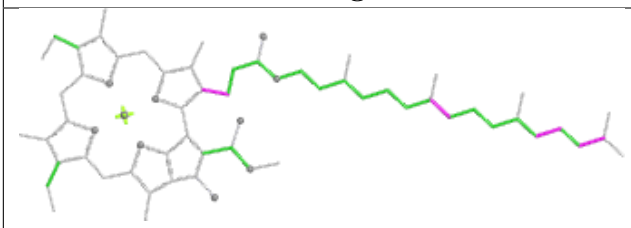
Ligand CLA a 816



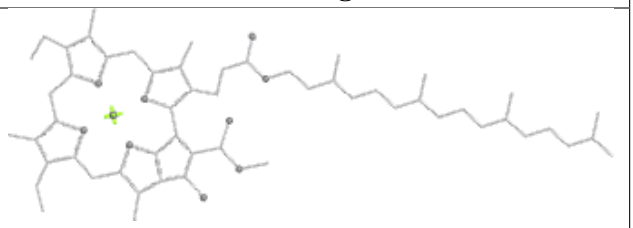
Bond lengths



Bond angles

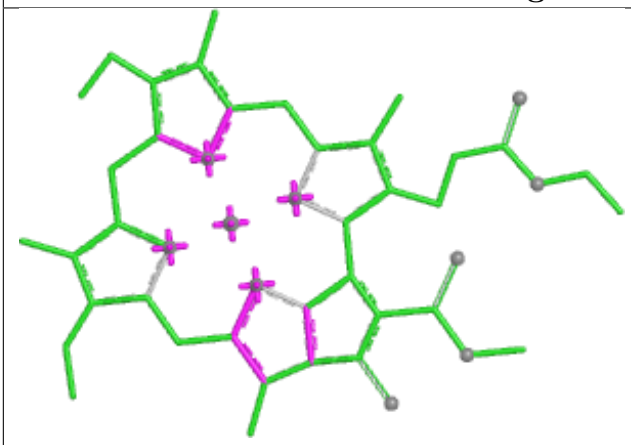


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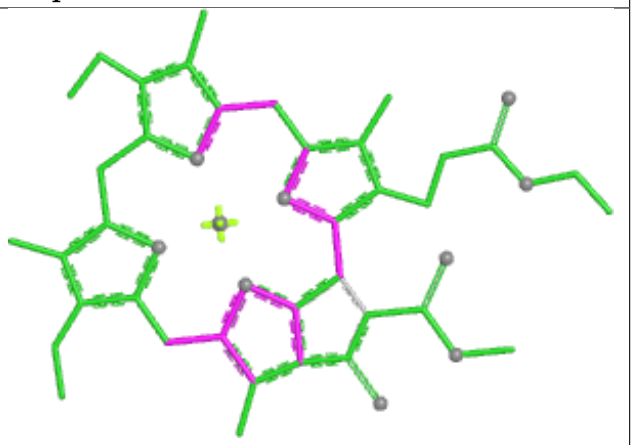


Rings

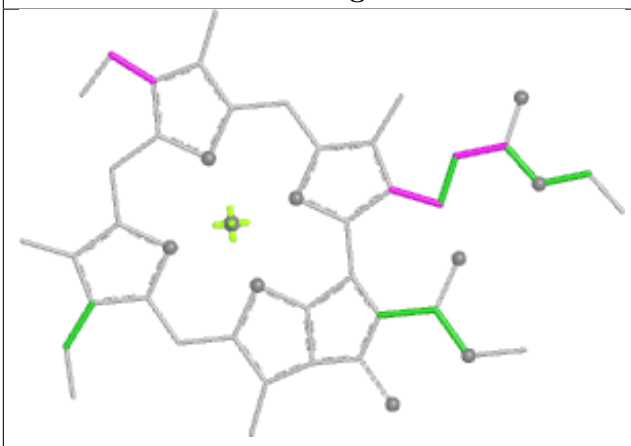
Ligand CLA p 306



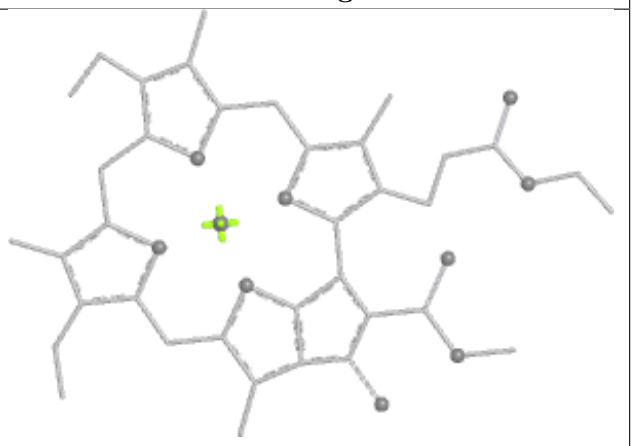
Bond lengths



Bond angles

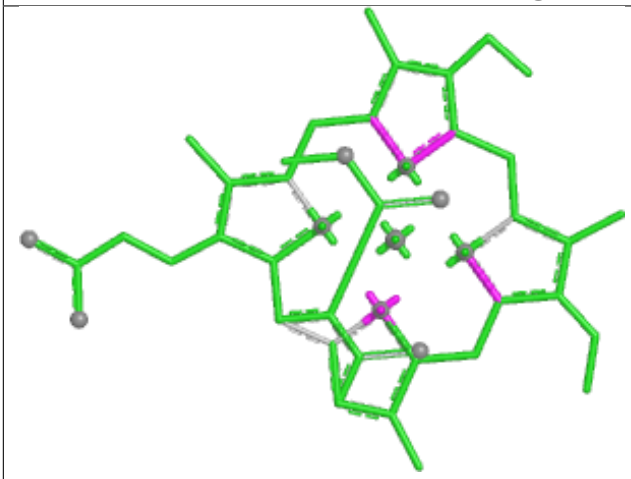


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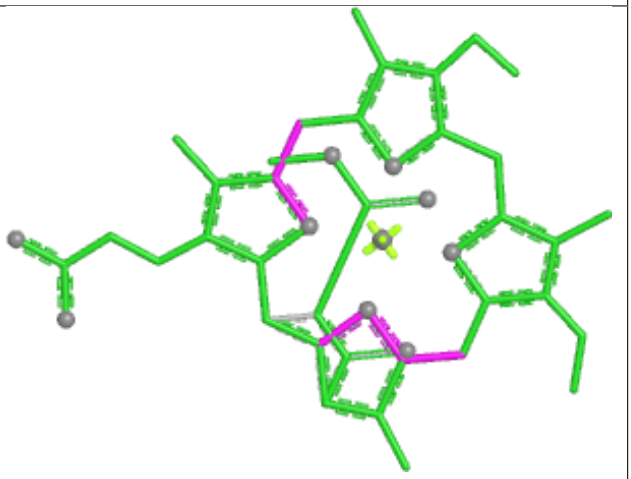


Rings

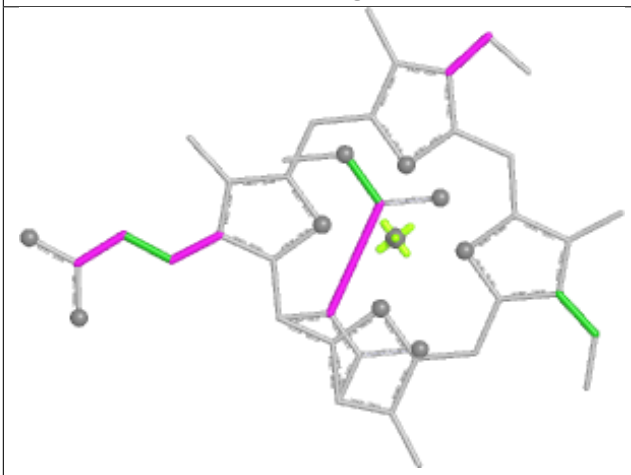
Ligand KC2 x 304



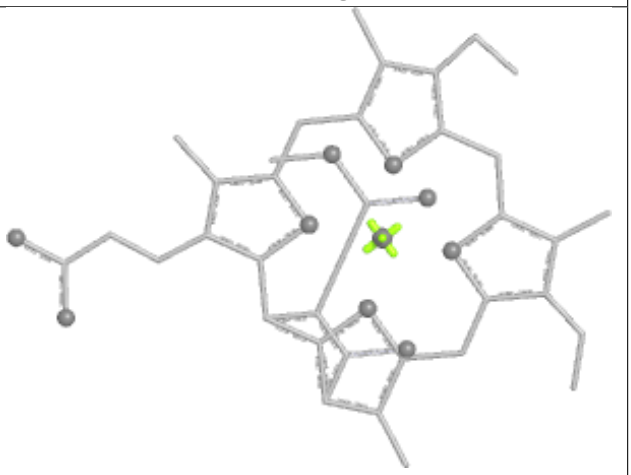
Bond lengths



Bond angles

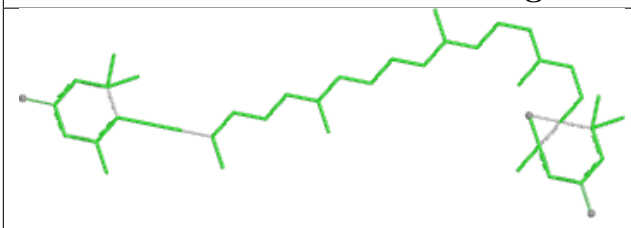


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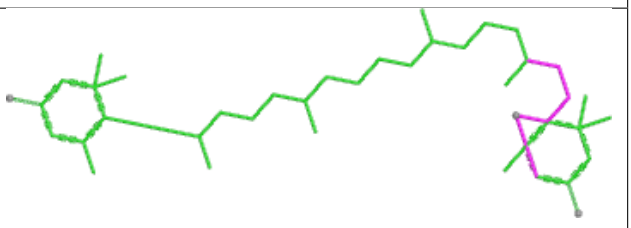


Rings

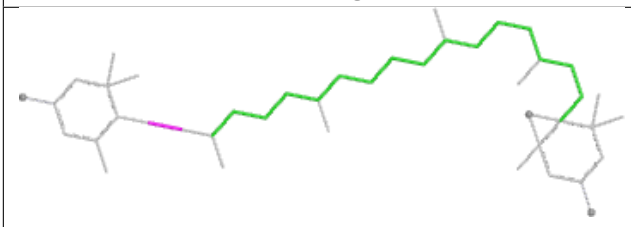
Ligand DD6 C 310



Bond lengths



Bond angles

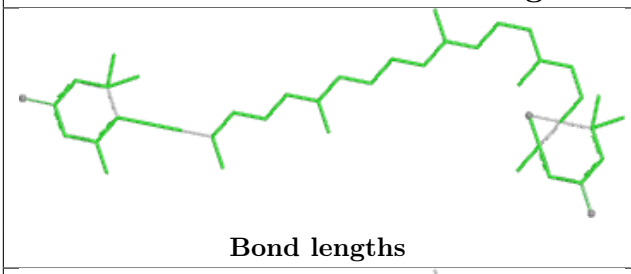


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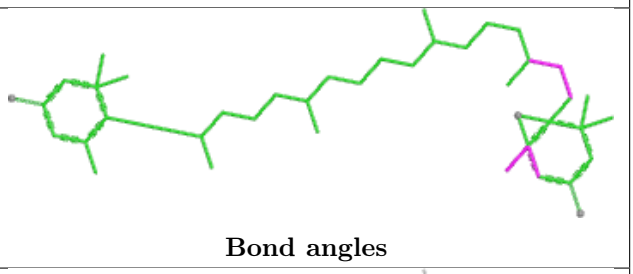


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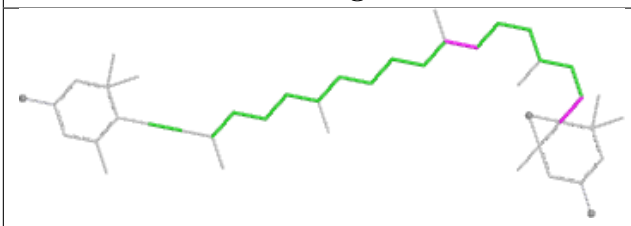
Ligand DD6 B 305



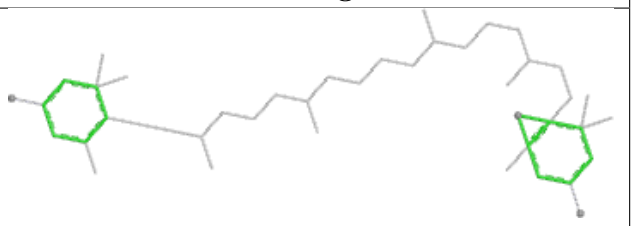
Bond lengths



Bond angles

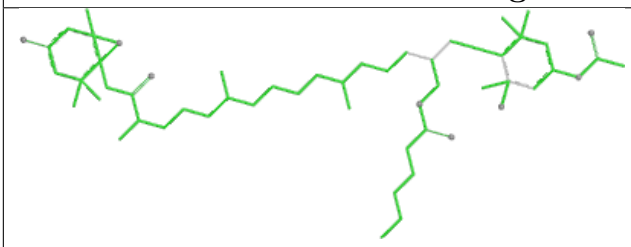


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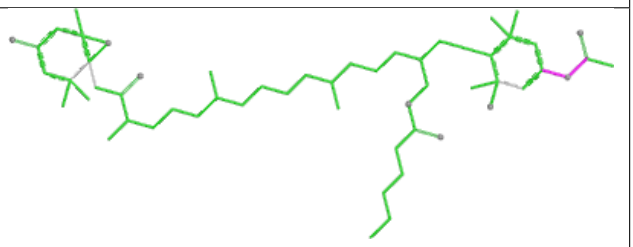


Rings

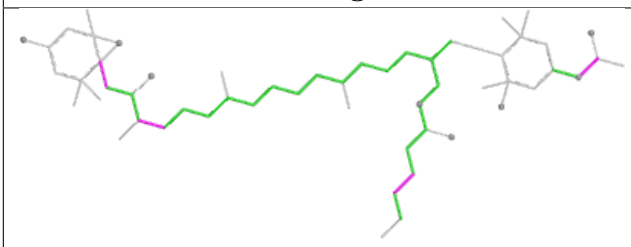
Ligand A1EB1 v 322



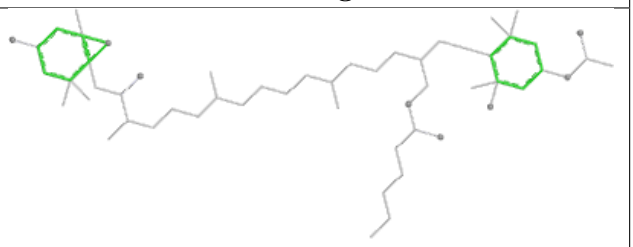
Bond lengths



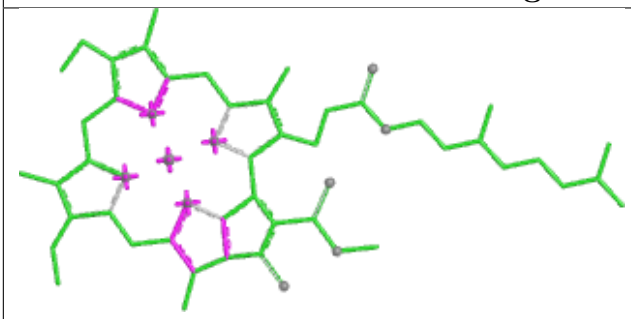
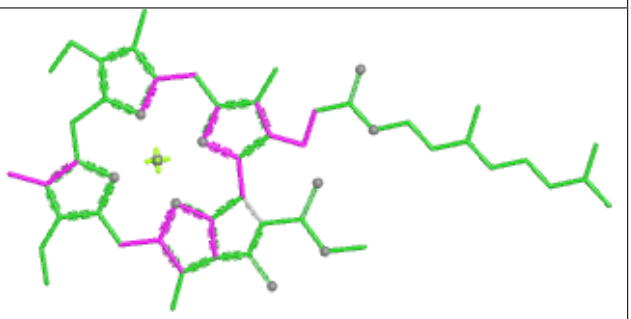
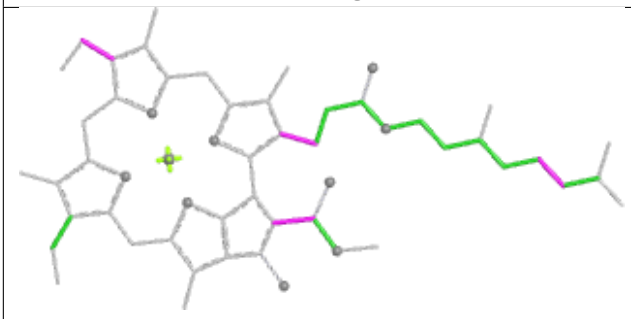
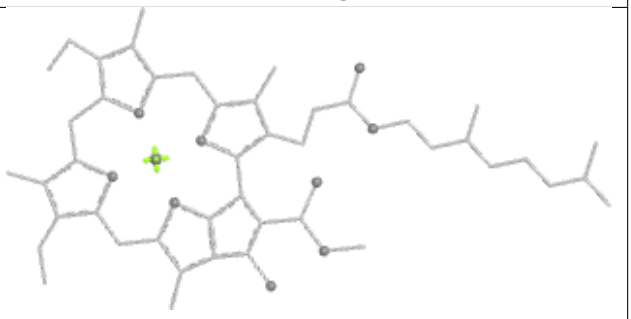
Bond angles

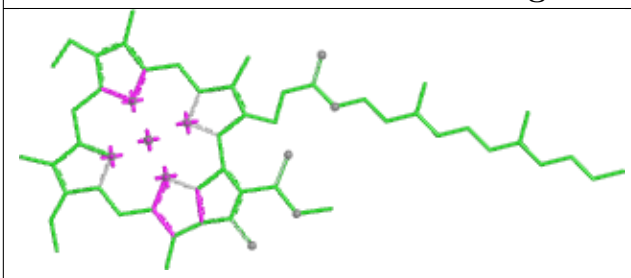
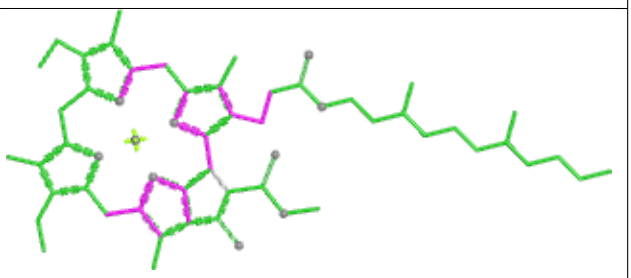
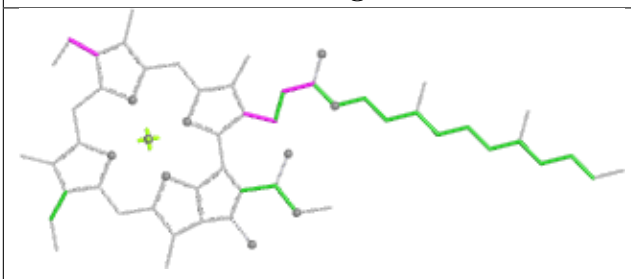
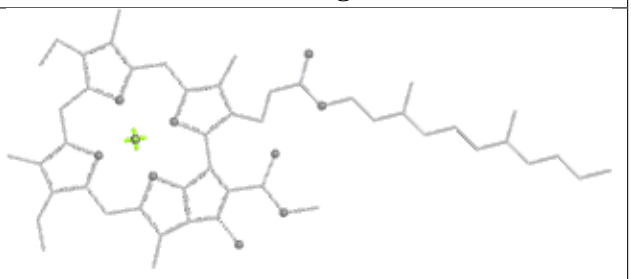


Torsions

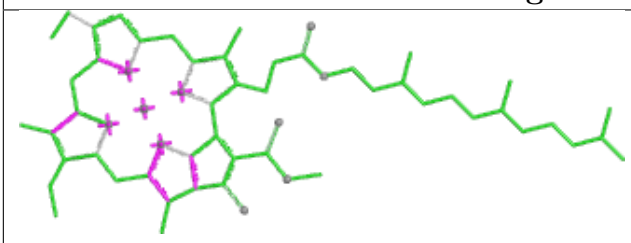


Rings

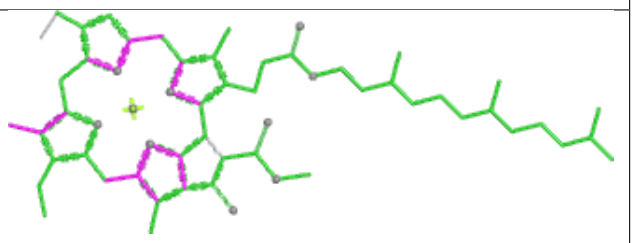
Ligand CLA X 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

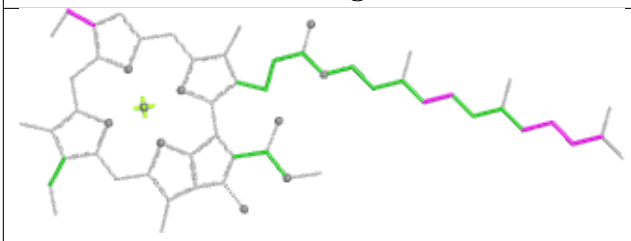
Ligand CLA F 307



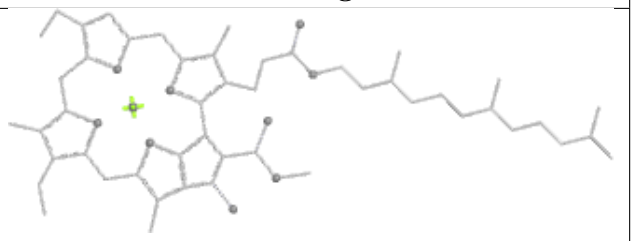
Bond lengths



Bond angles

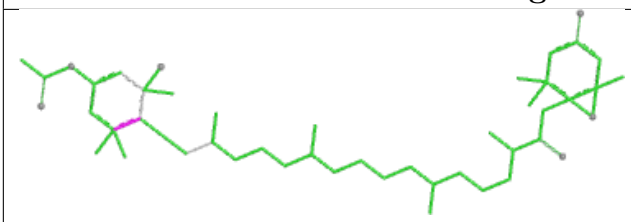


Torsions

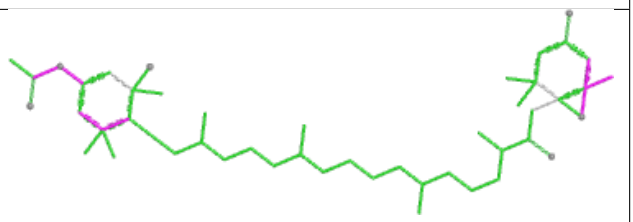


Rings

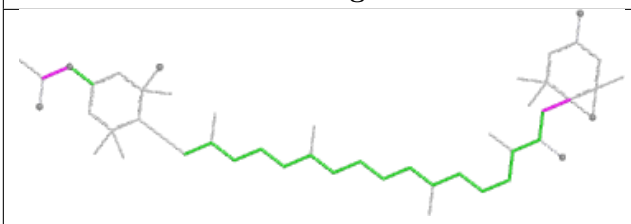
Ligand A86 H 315



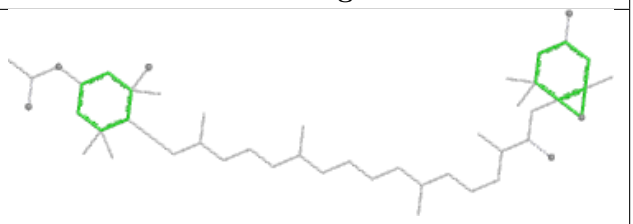
Bond lengths



Bond angles

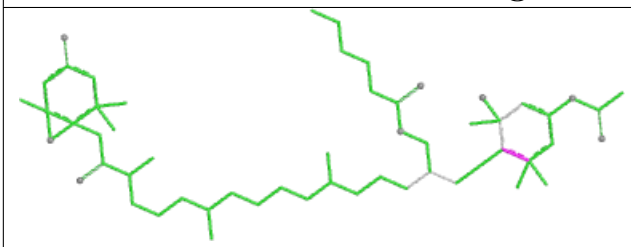


Torsions

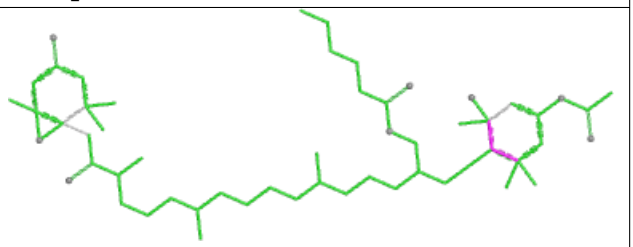


Rings

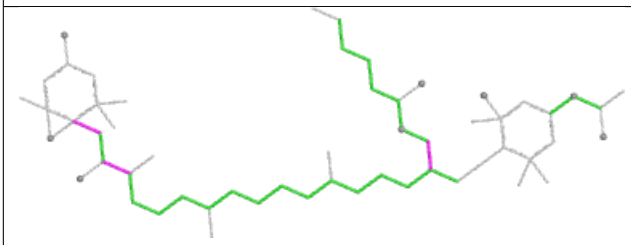
Ligand A1EB1 p 324



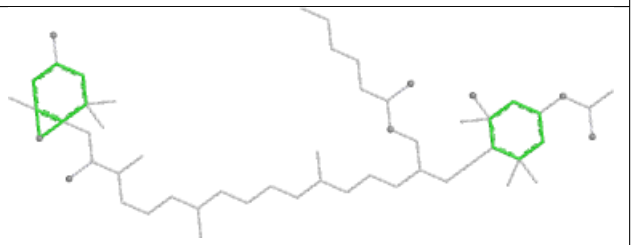
Bond lengths



Bond angles

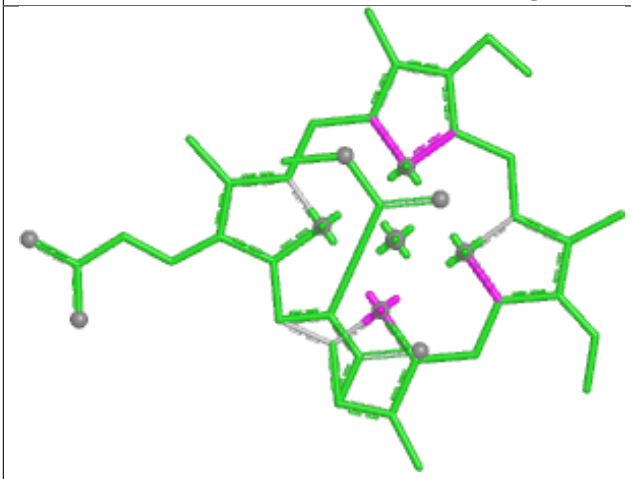


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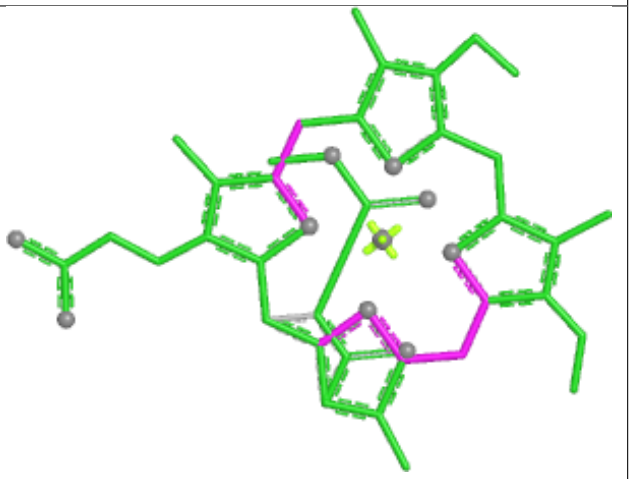


Rings

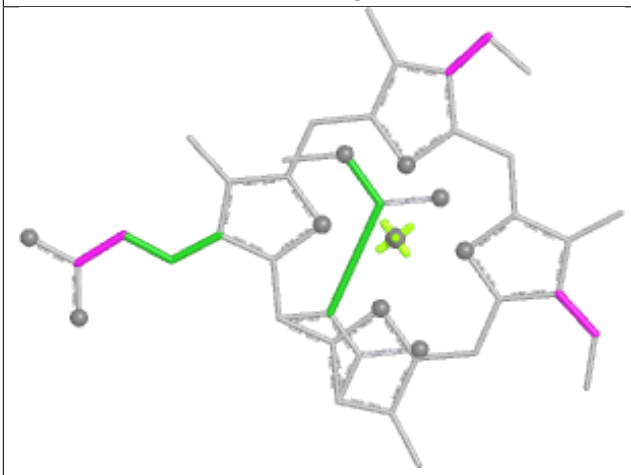
Ligand KC2 A 310



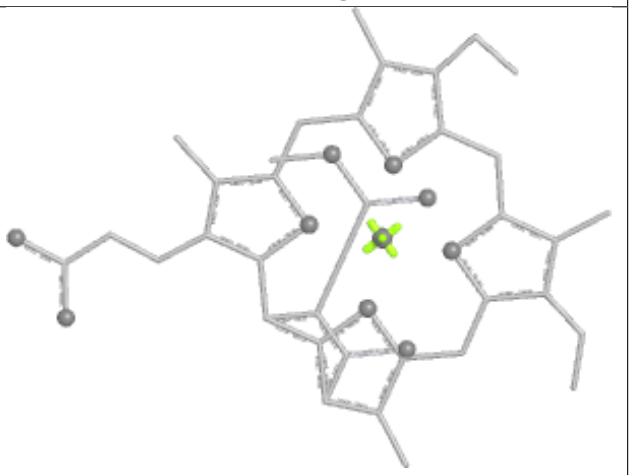
Bond lengths



Bond angles

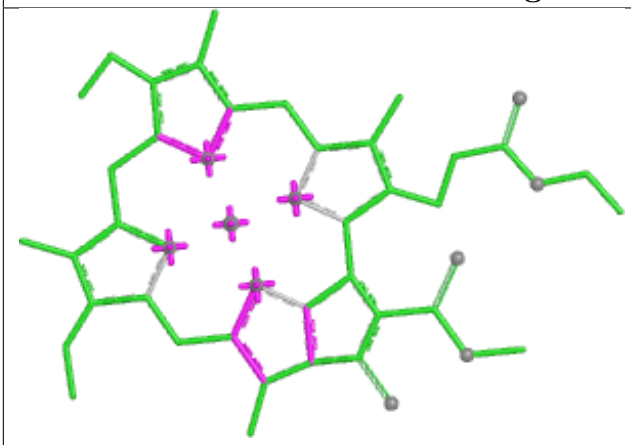


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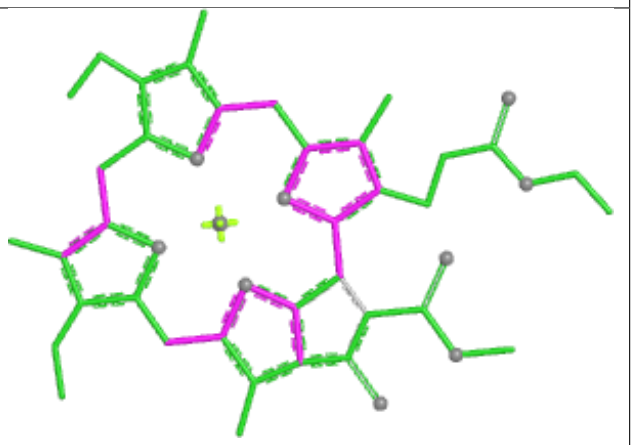


Rings

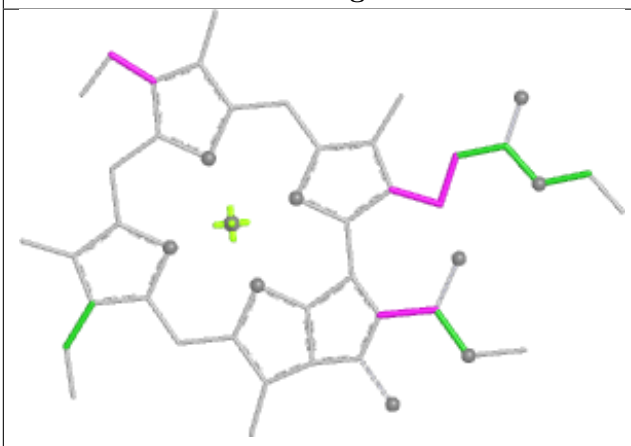
Ligand CLA B 307



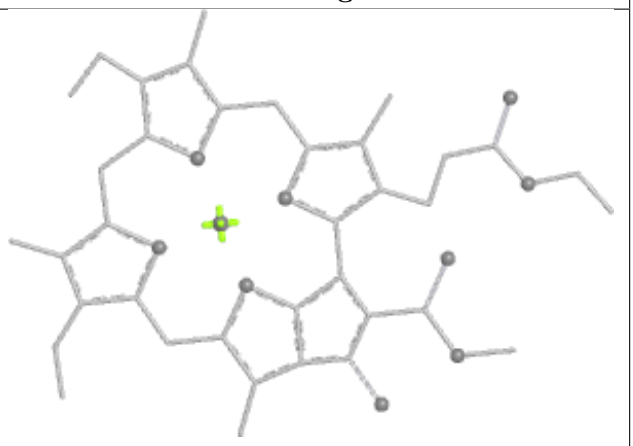
Bond lengths



Bond angles

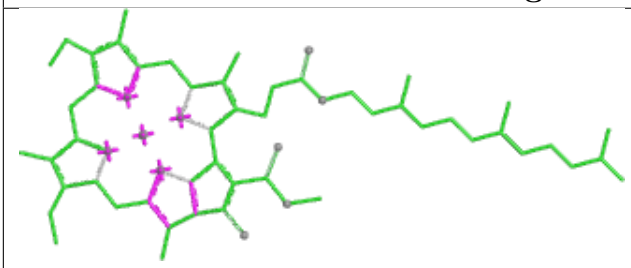


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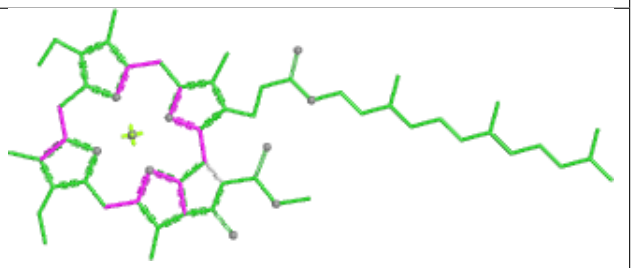


Rings

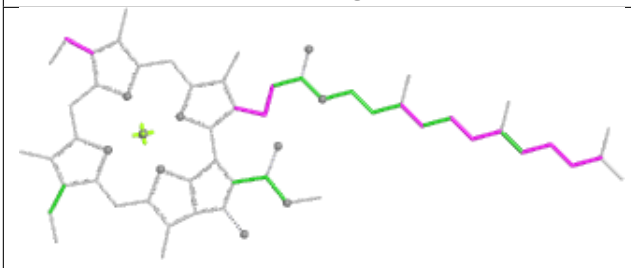
Ligand CLA P 312



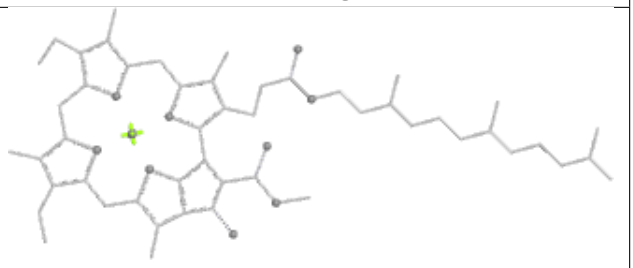
Bond lengths



Bond angles

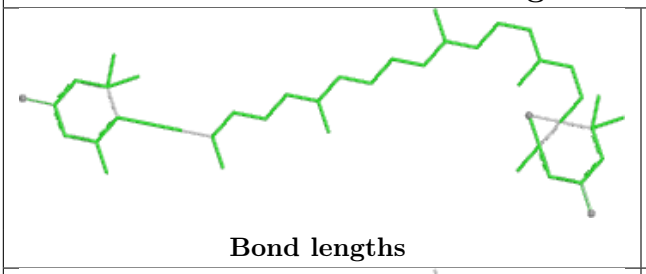


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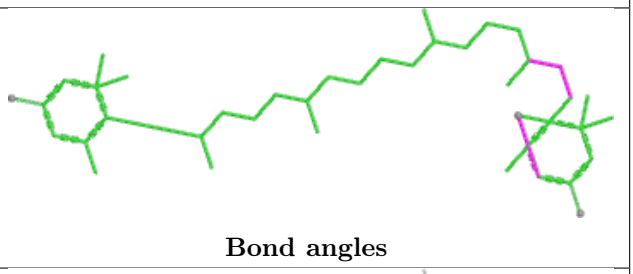


Rings

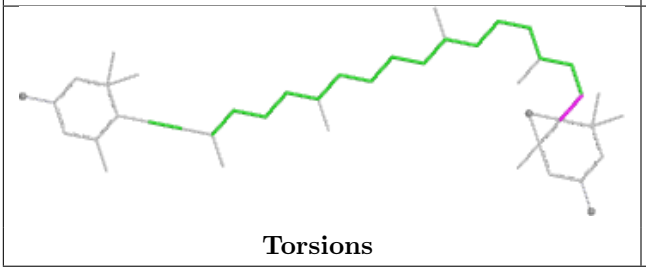
Ligand DD6 Z 318



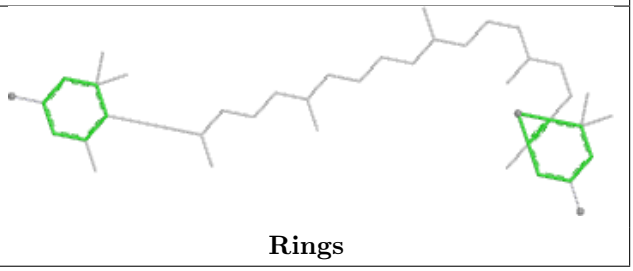
Bond lengths



Bond angles

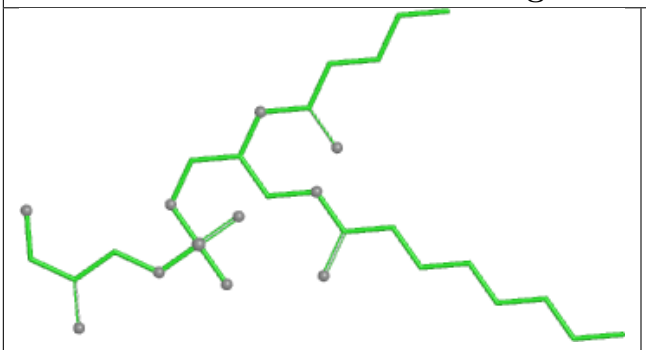


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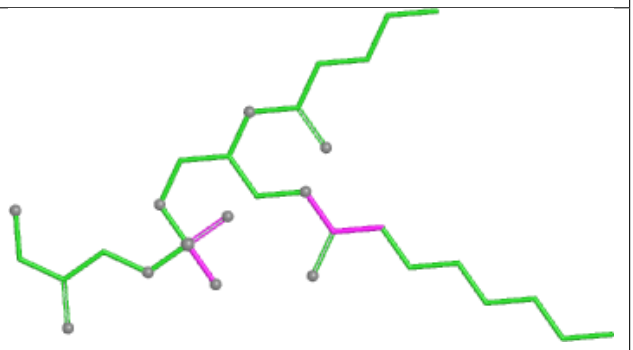


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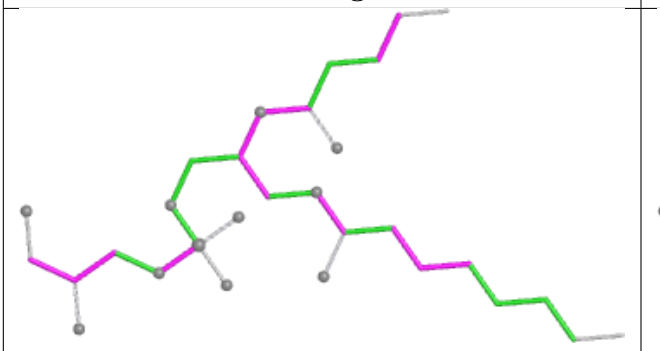
Ligand LHG a 849



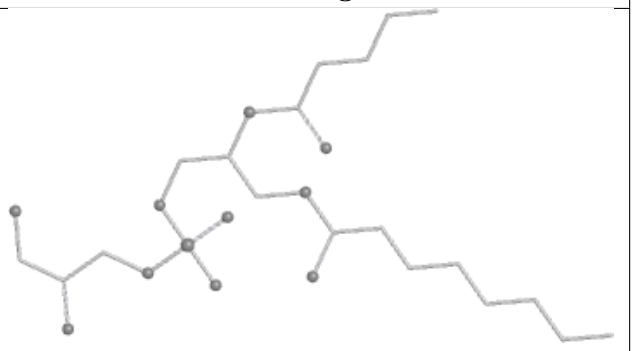
Bond lengths



Bond angles

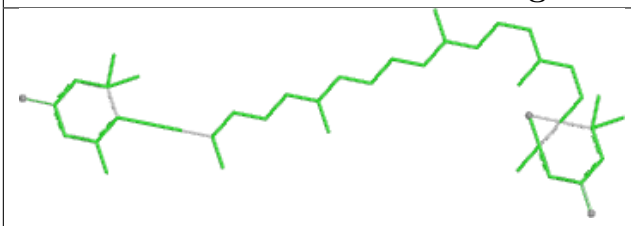


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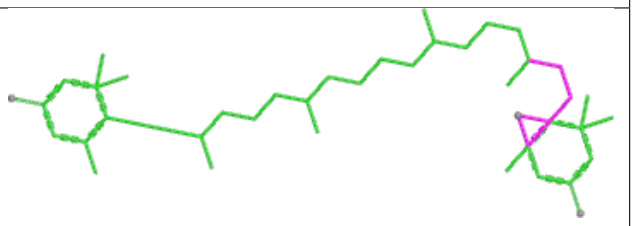


Rings

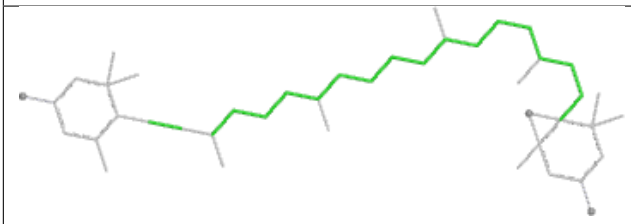
Ligand DD6 J 314



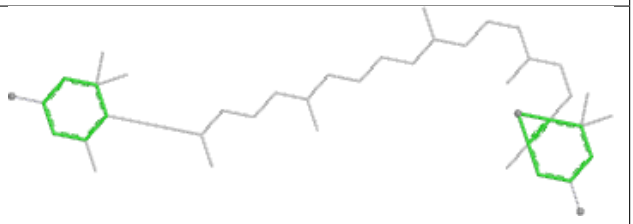
Bond lengths



Bond angles

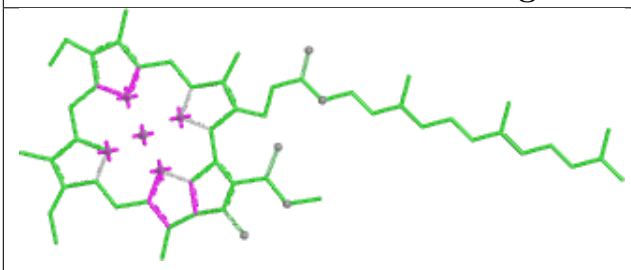


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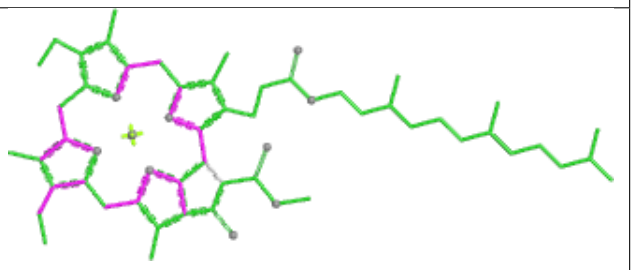


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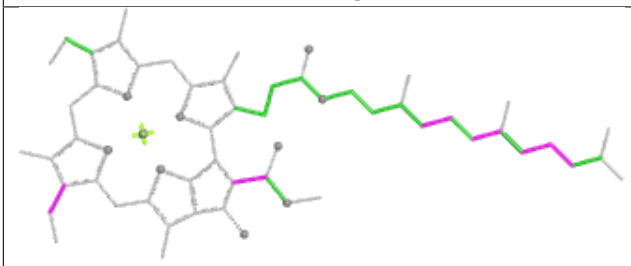
Ligand CLA W 312



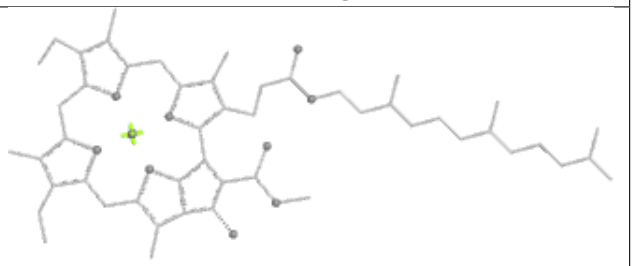
Bond lengths



Bond angles

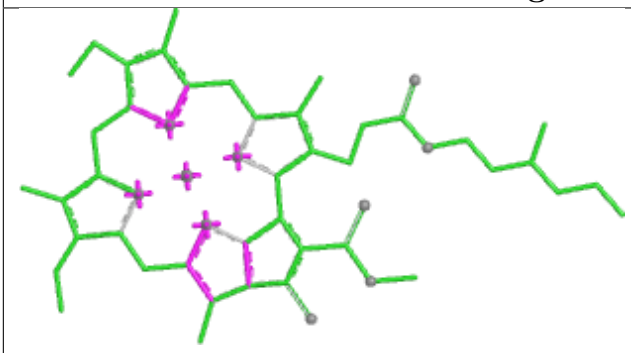


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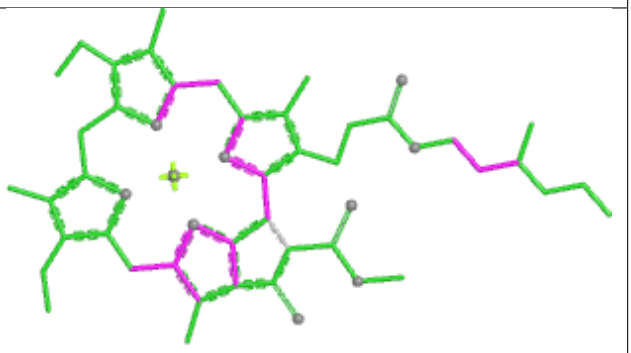


Rings

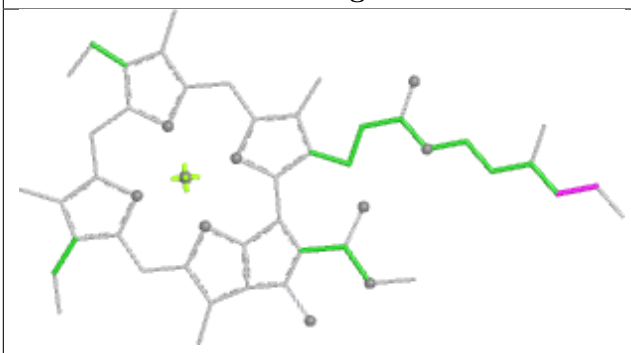
Ligand CLA J 306



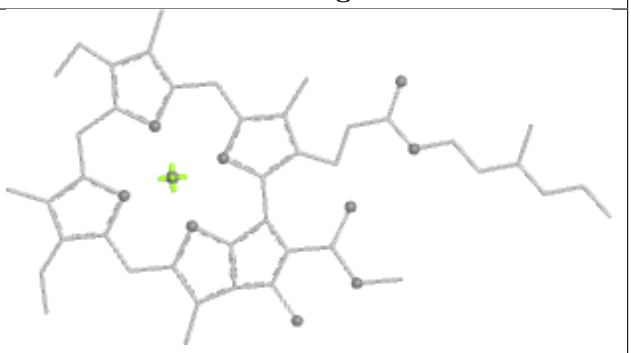
Bond lengths



Bond angles

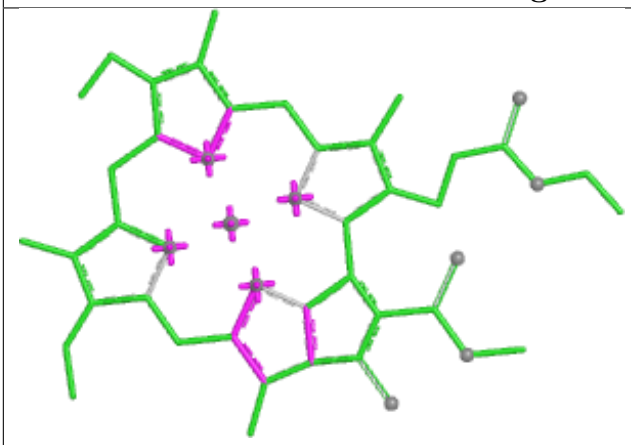


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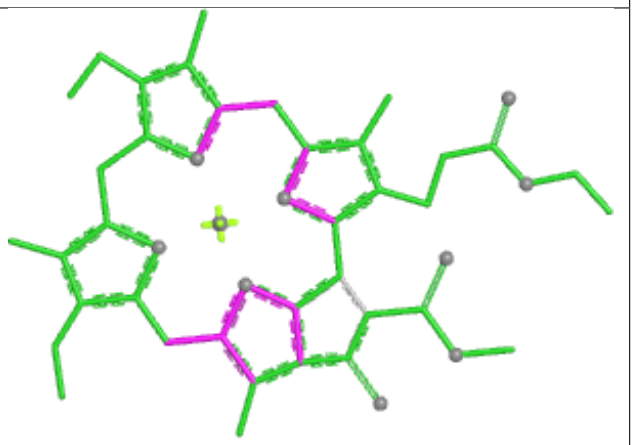


Rings

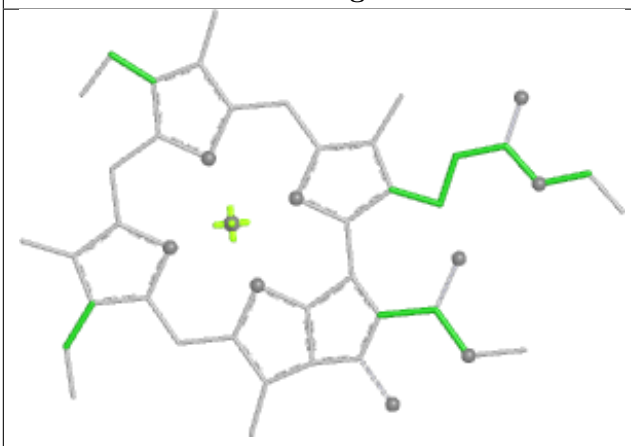
Ligand CLA t 302



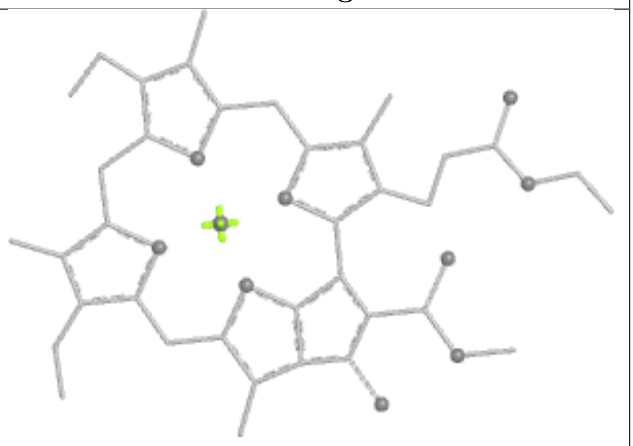
Bond lengths



Bond angles

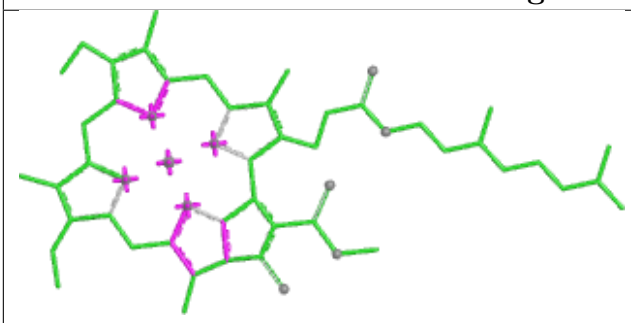


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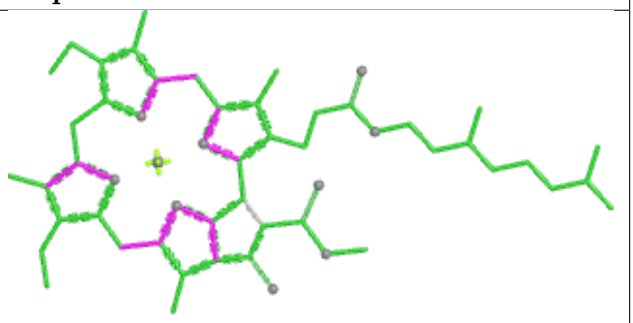


Rings

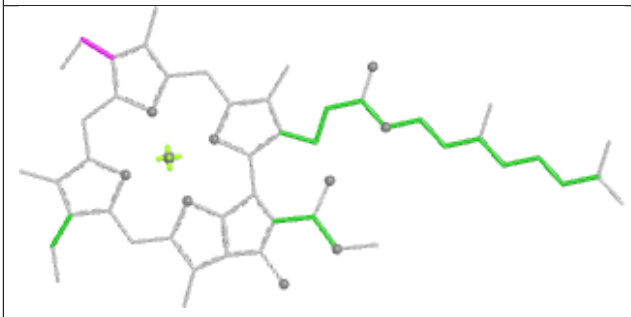
Ligand CLA p 313



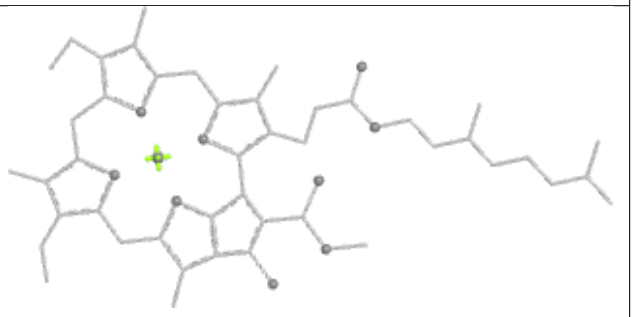
Bond lengths



Bond angles

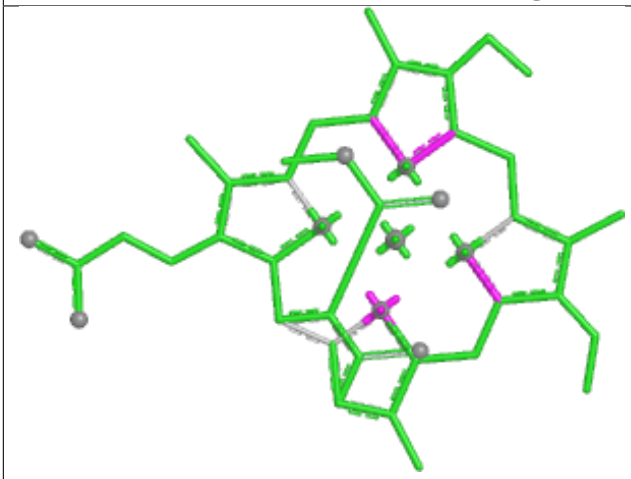


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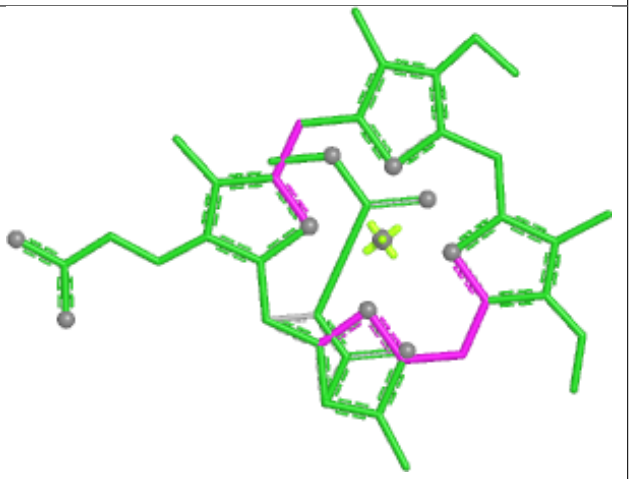


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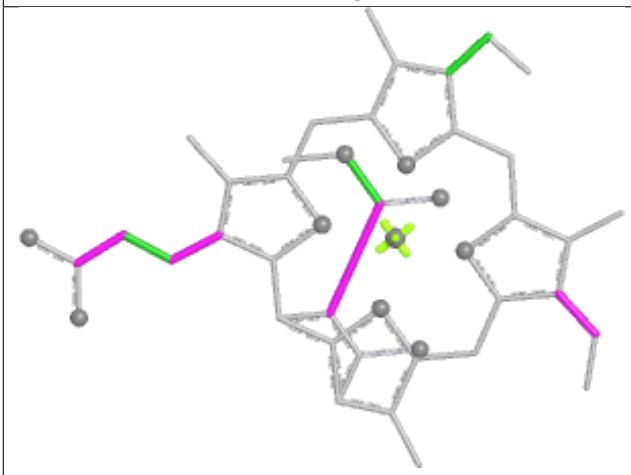
Ligand KC2 Z 302



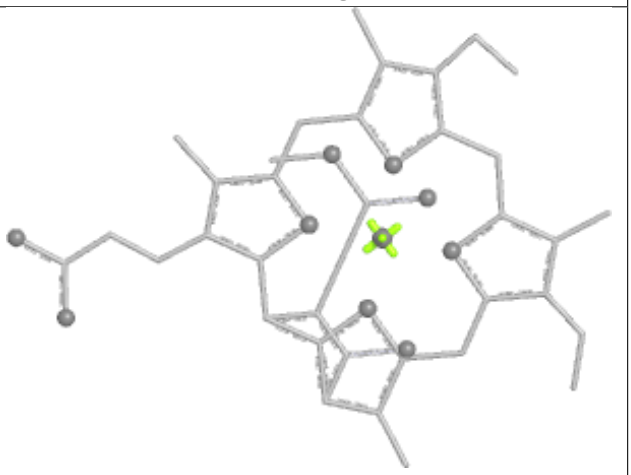
Bond lengths



Bond angles

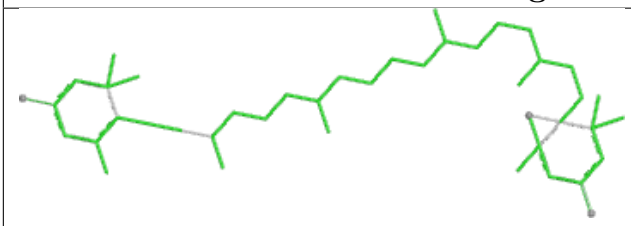


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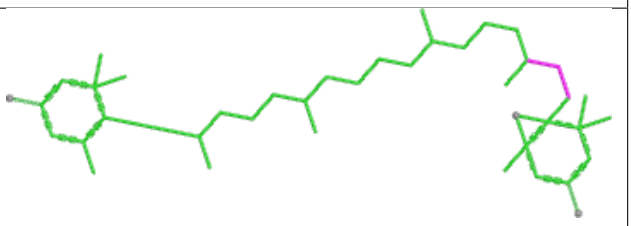


Rings

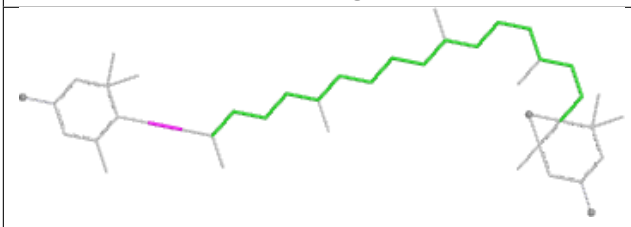
Ligand DD6 J 317



Bond lengths



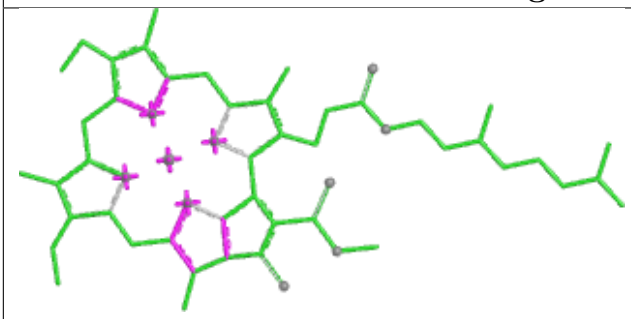
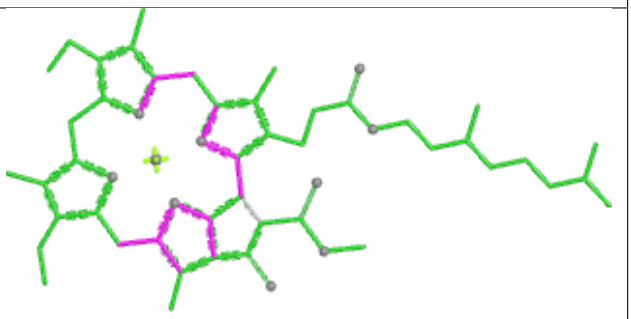
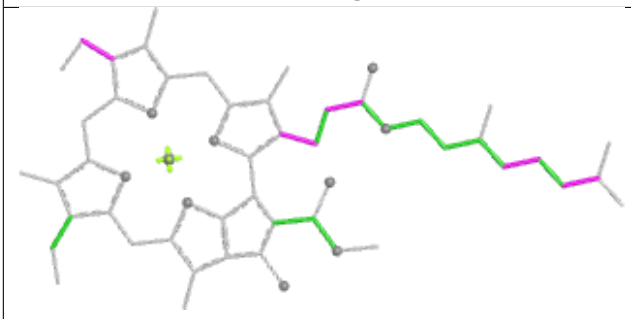
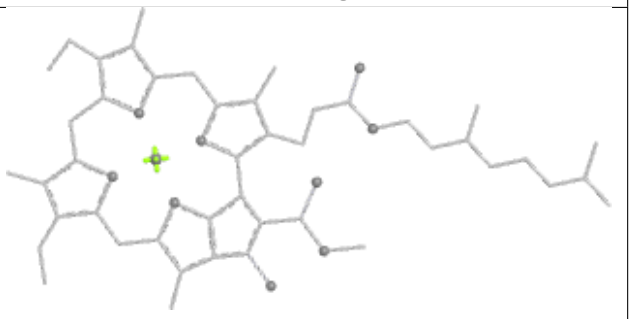
Bond angles

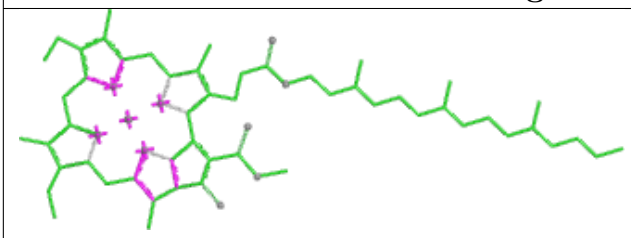
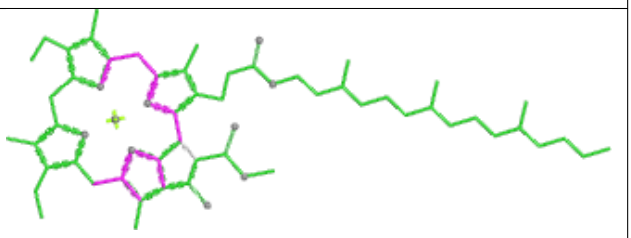
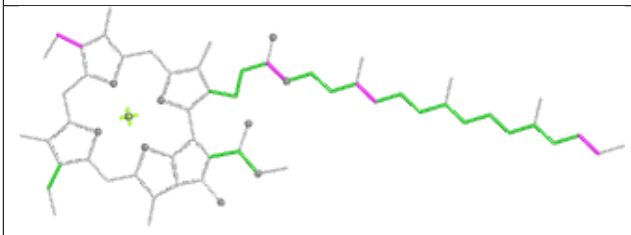
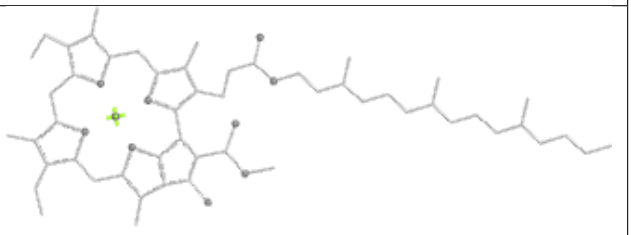


Torsions

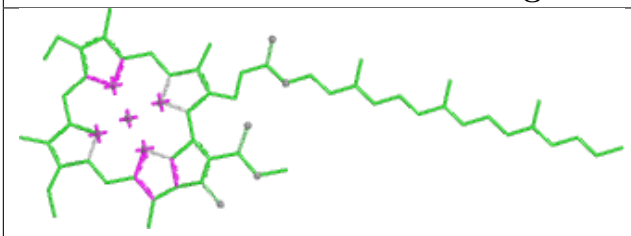


Rings

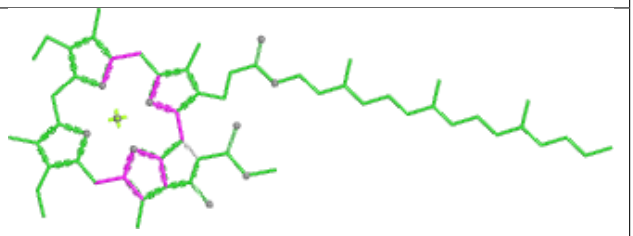
Ligand CLA a 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Z 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

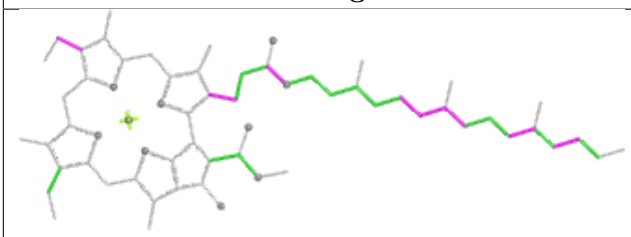
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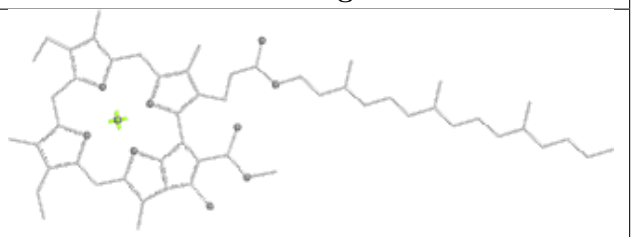
Bond lengths



Bond angles

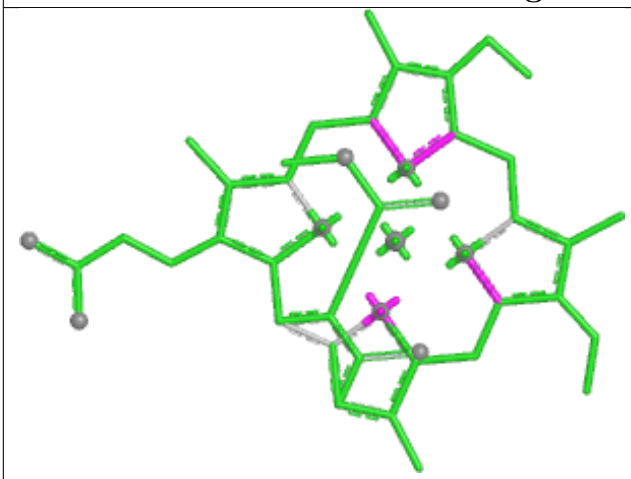


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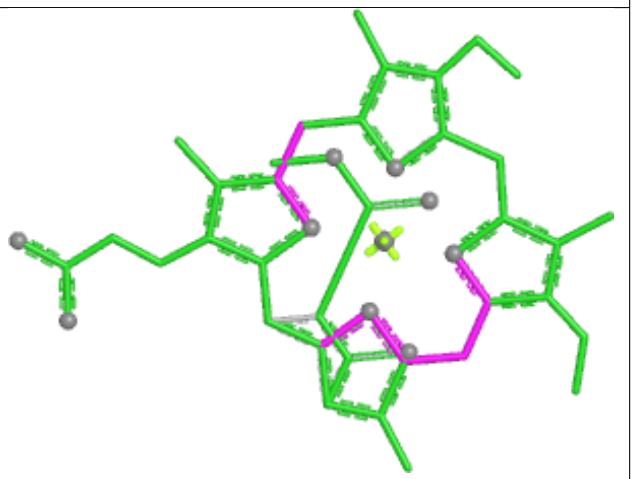


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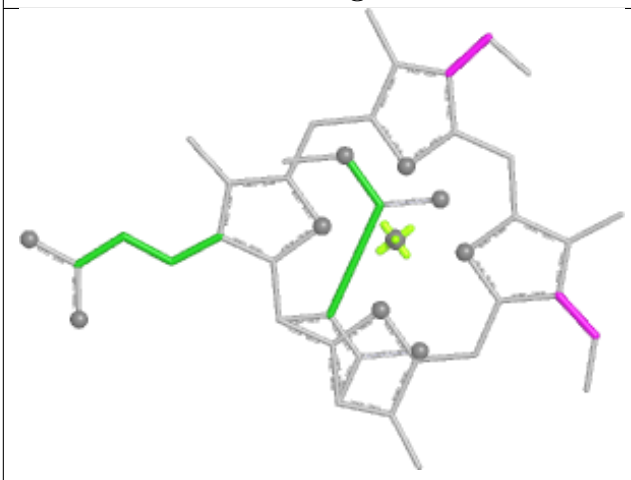
Ligand KC2 H 303



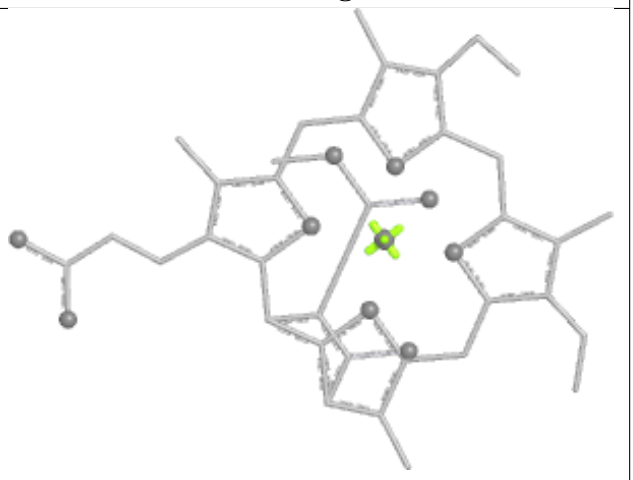
Bond lengths



Bond angles

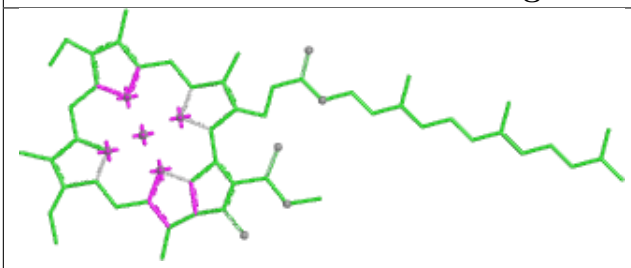


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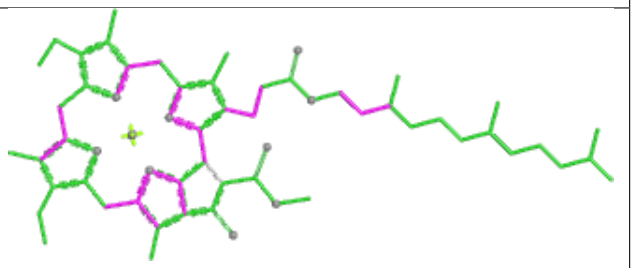


Rings

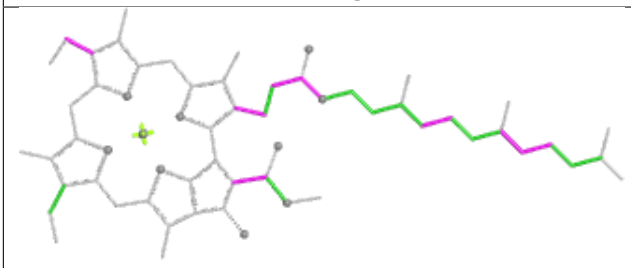
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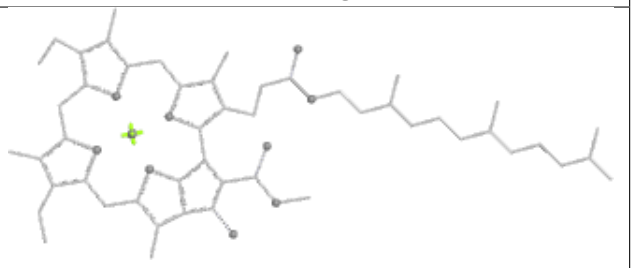
Bond lengths



Bond angles

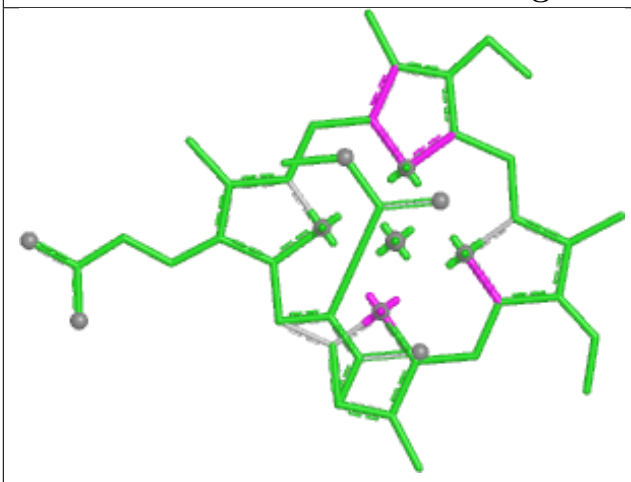


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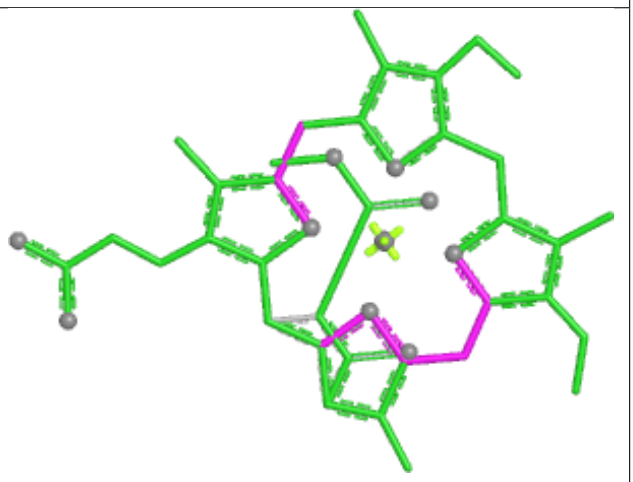


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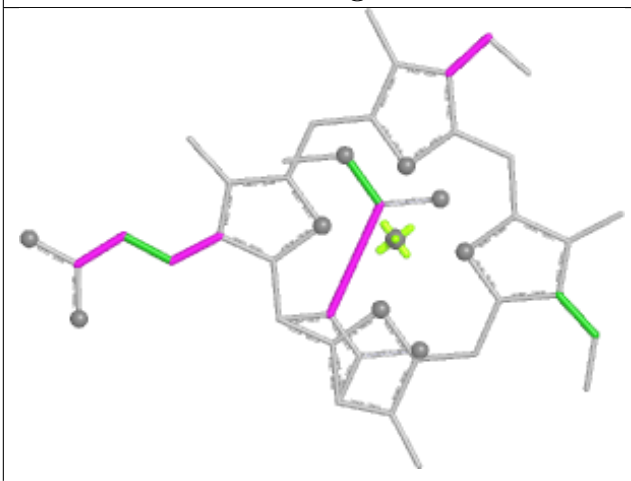
Ligand KC2 t 301



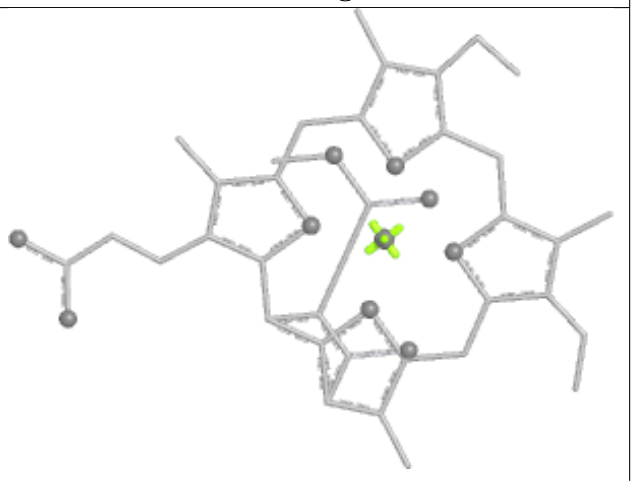
Bond lengths



Bond angles

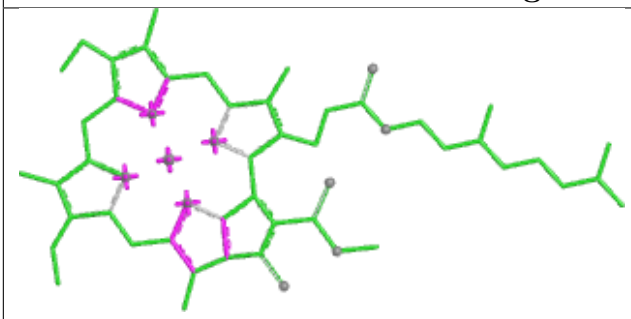


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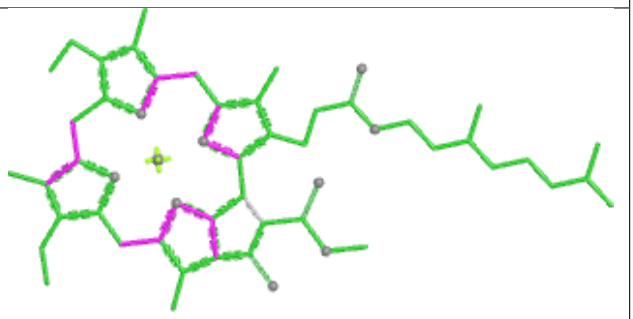


Rings

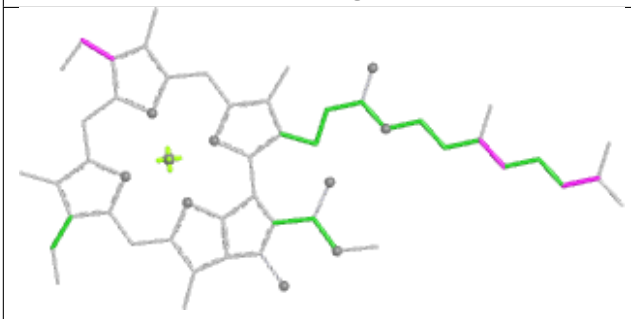
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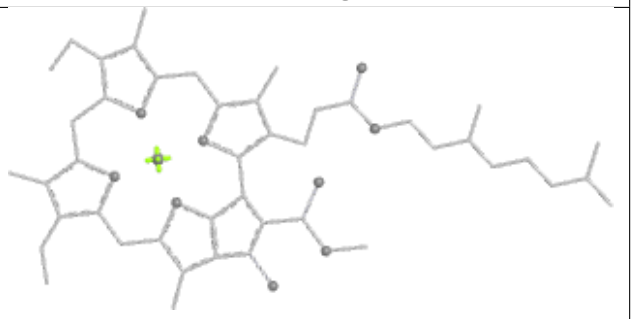
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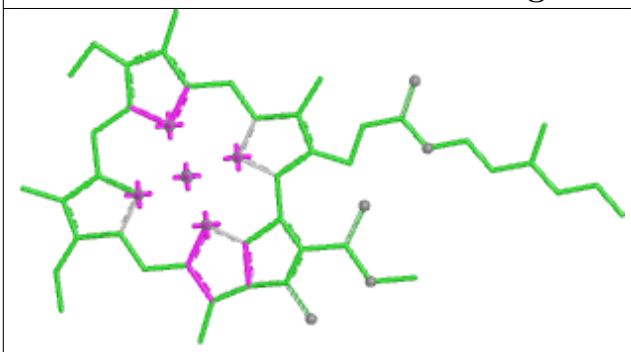


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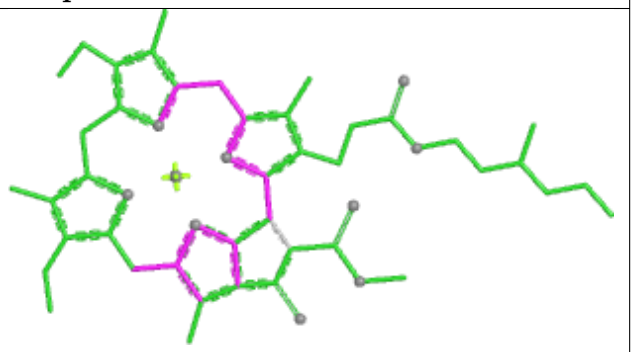


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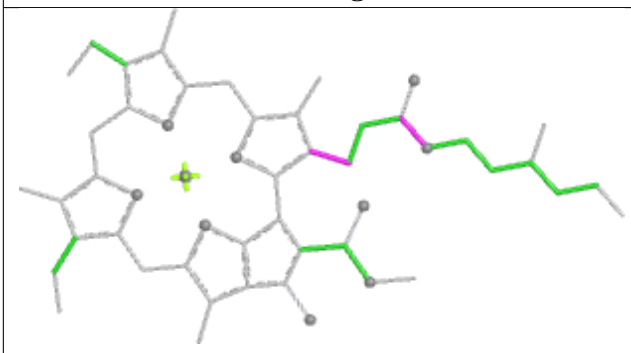
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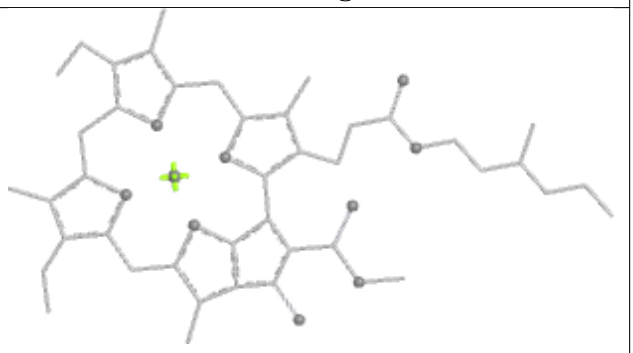
Bond lengths



Bond angles

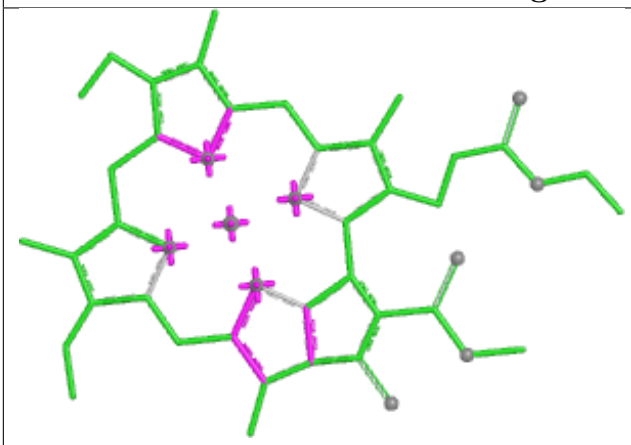


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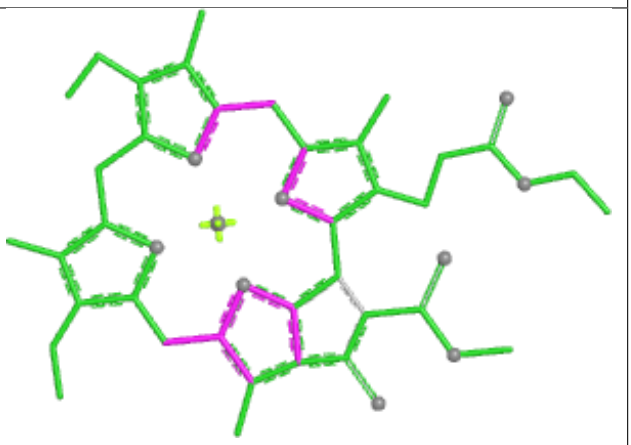


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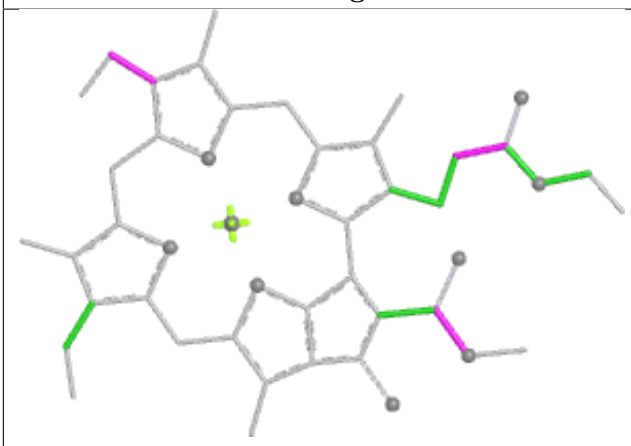
Ligand CLA t 309



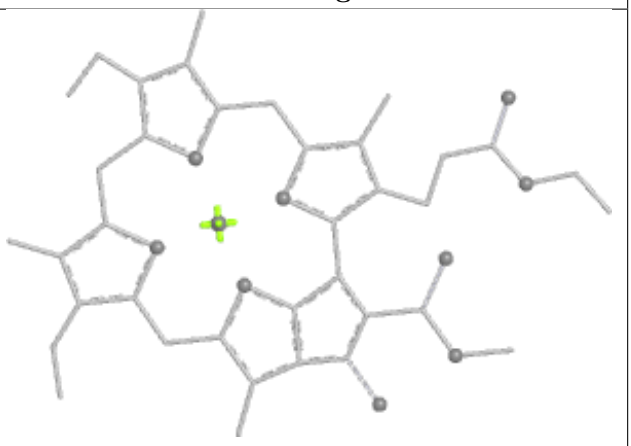
Bond lengths



Bond angles

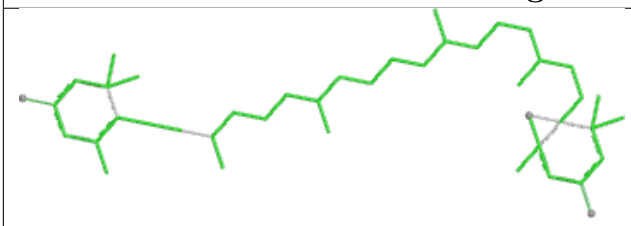


Torsions



Rings

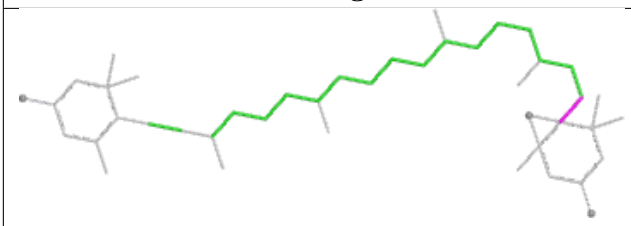
Ligand DD6 F 314



Bond lengths



Bond angles

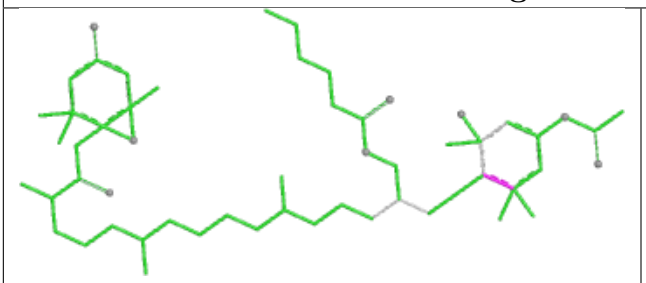


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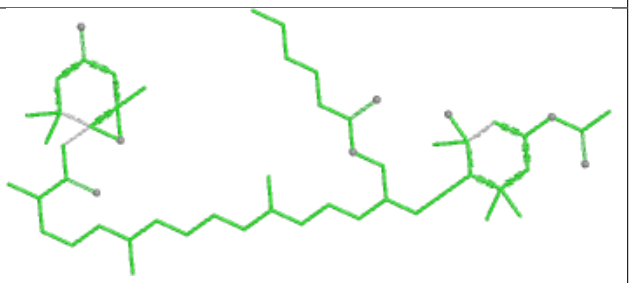


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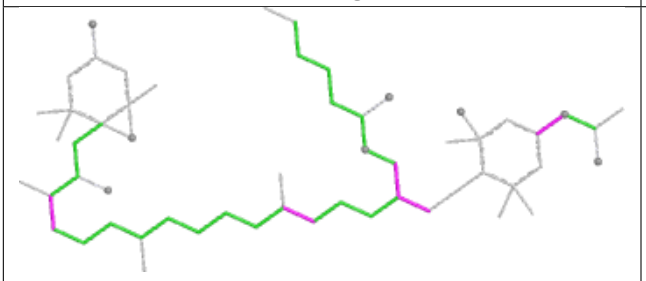
Ligand A1EB1 o 321



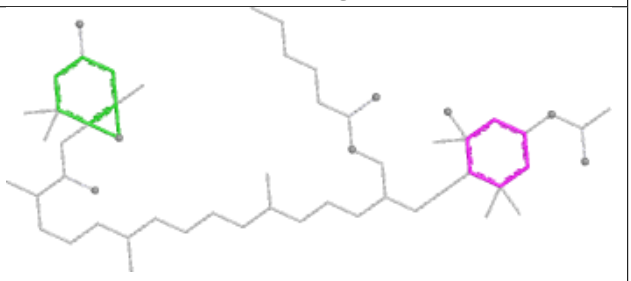
Bond lengths



Bond angles

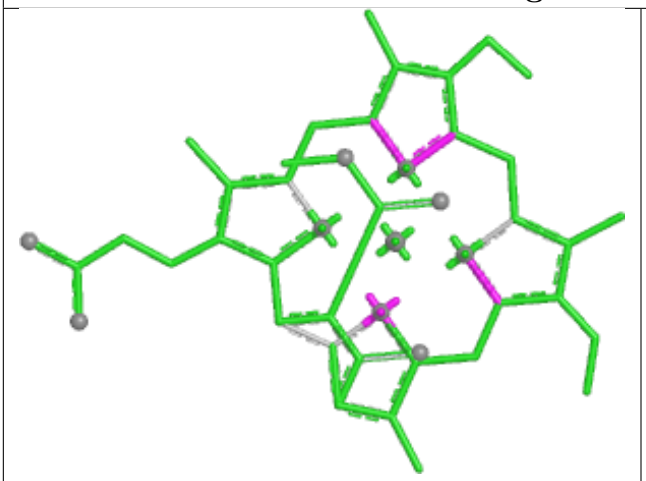


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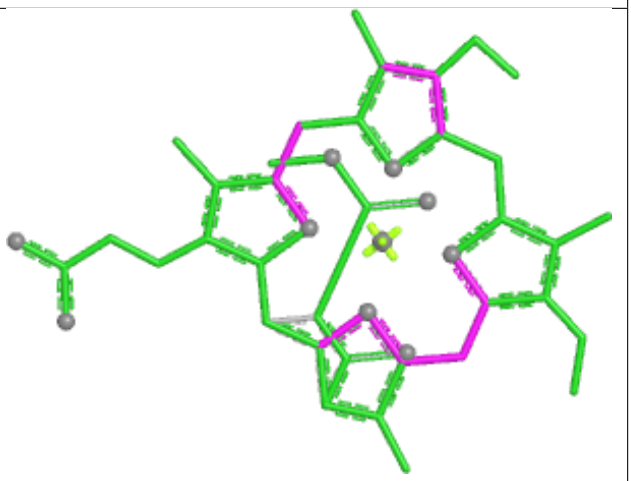


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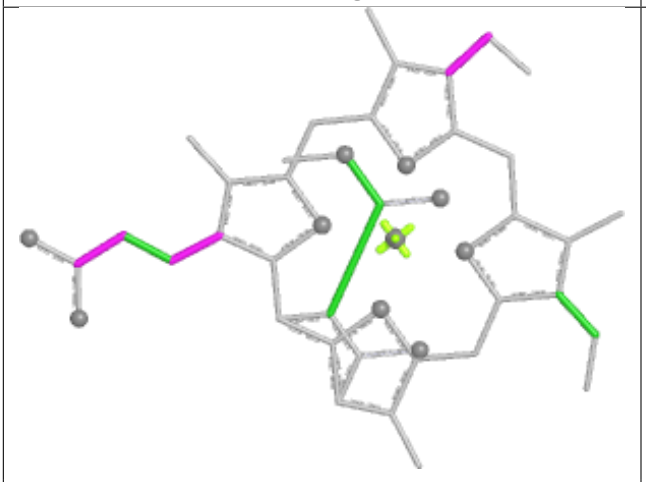
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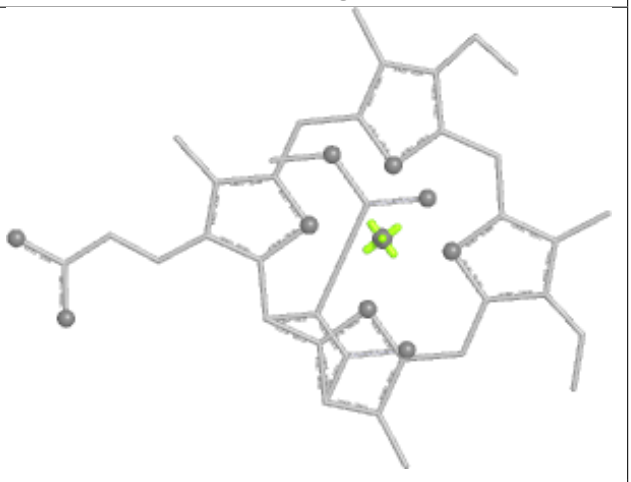
Bond lengths



Bond angles

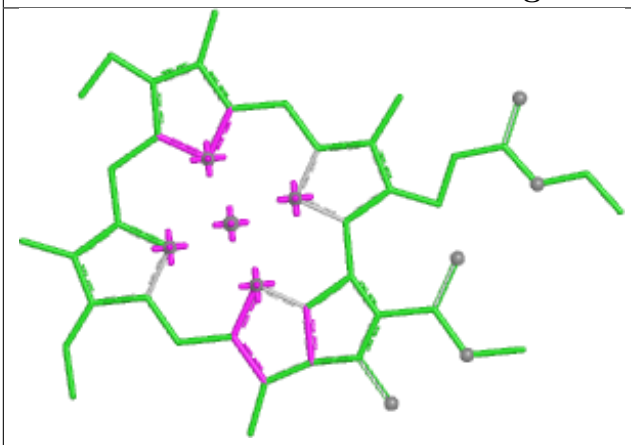


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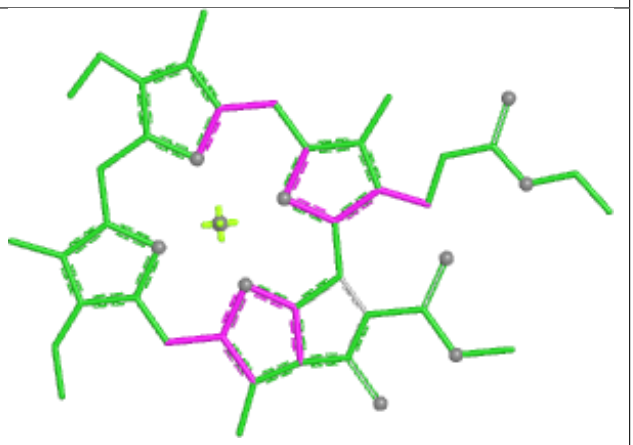


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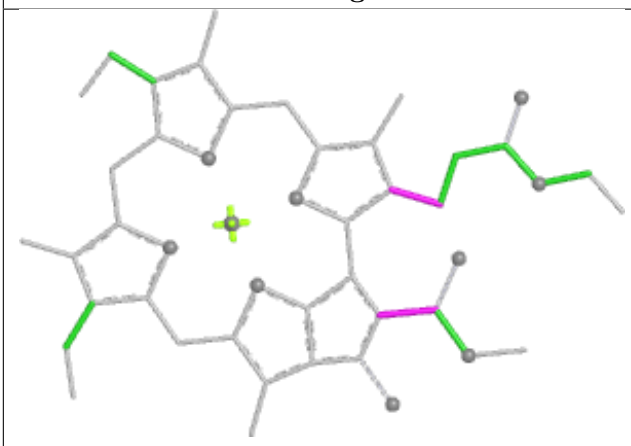
Ligand CLA D 311



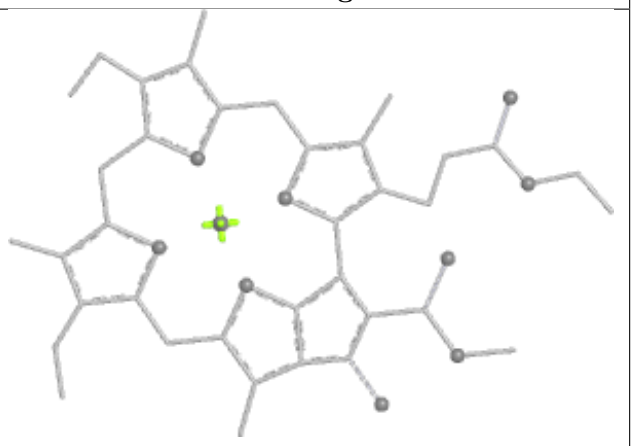
Bond lengths



Bond angles

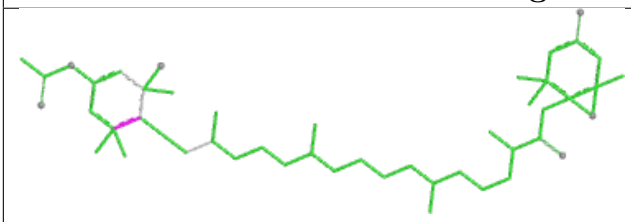


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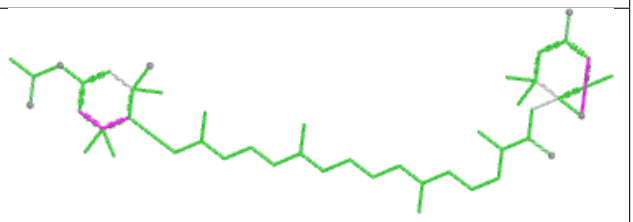


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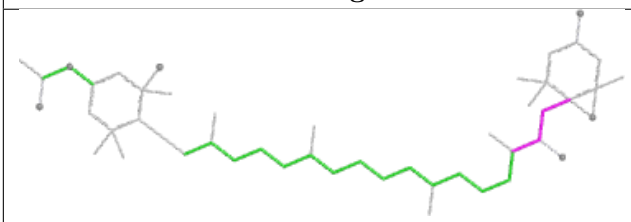
Ligand A86 X 320



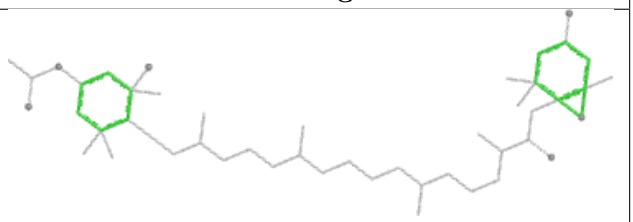
Bond lengths



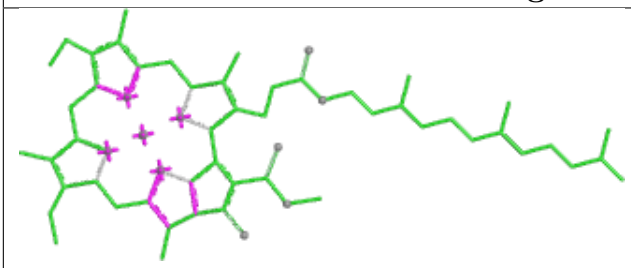
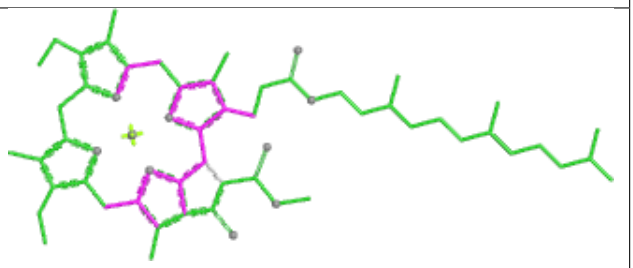
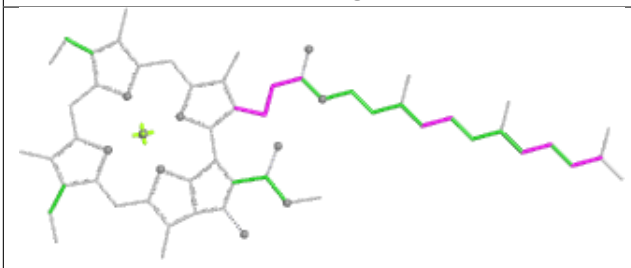
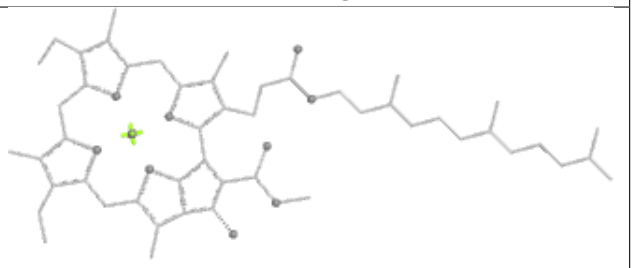
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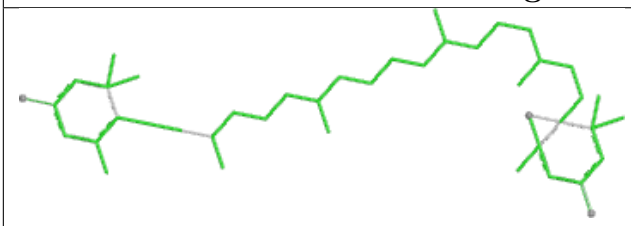
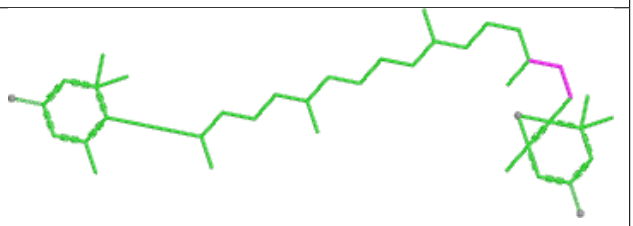
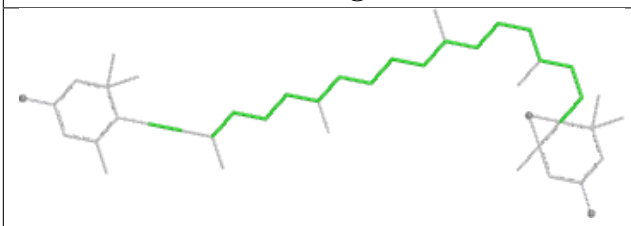
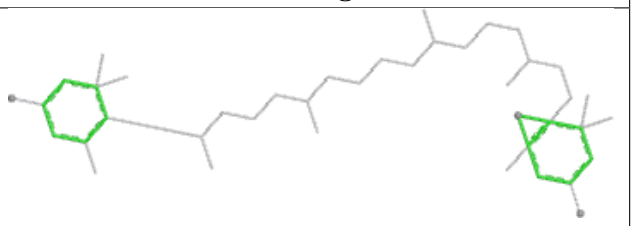


Torsions

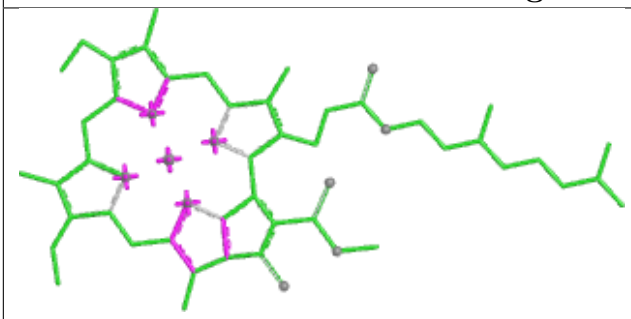


Rings

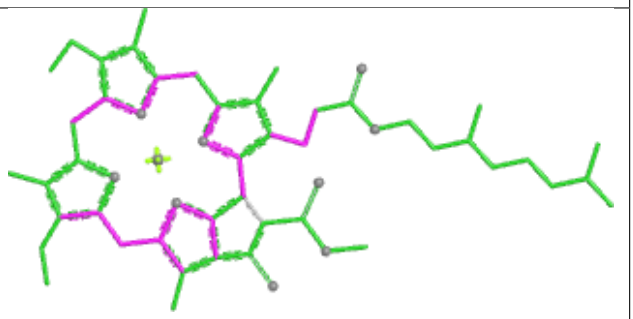
Ligand CLA b 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DD6 K 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

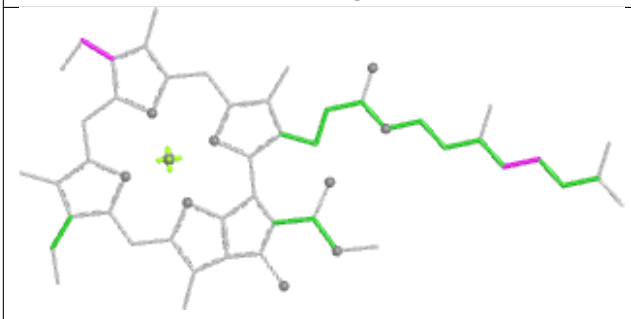
Ligand CLA F 304



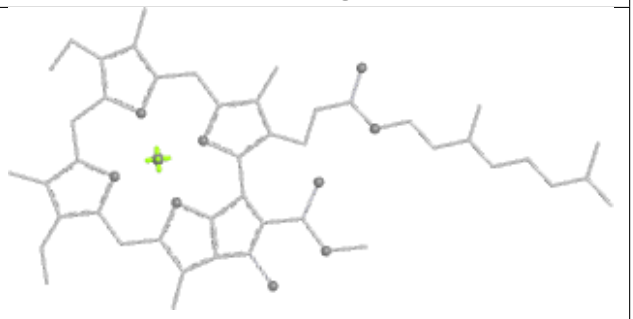
Bond lengths



Bond angles

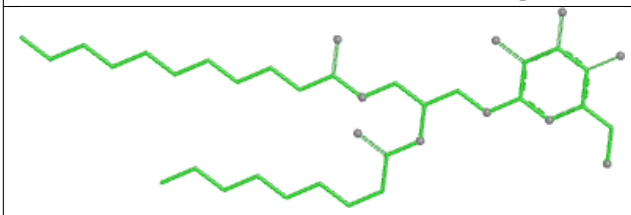


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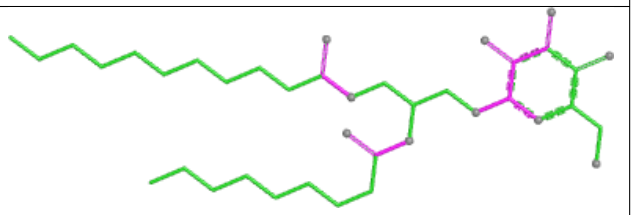


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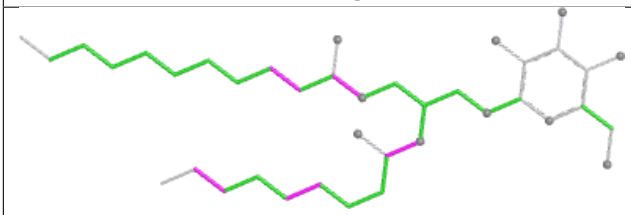
Ligand LMG W 317



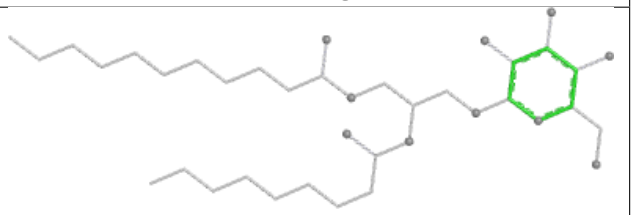
Bond lengths



Bond angles

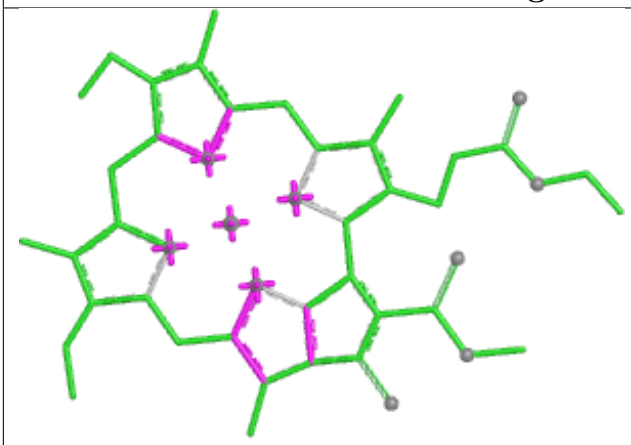


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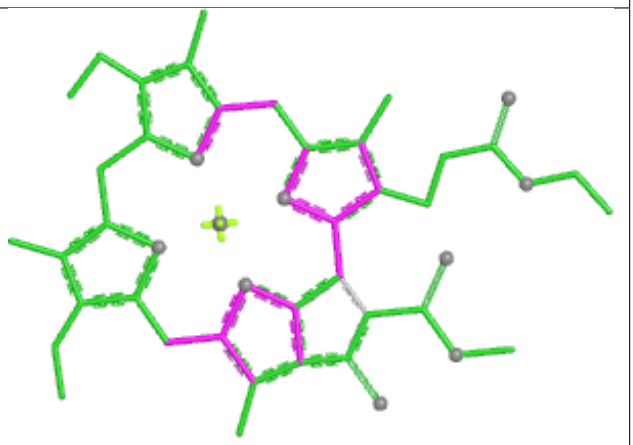


Rings

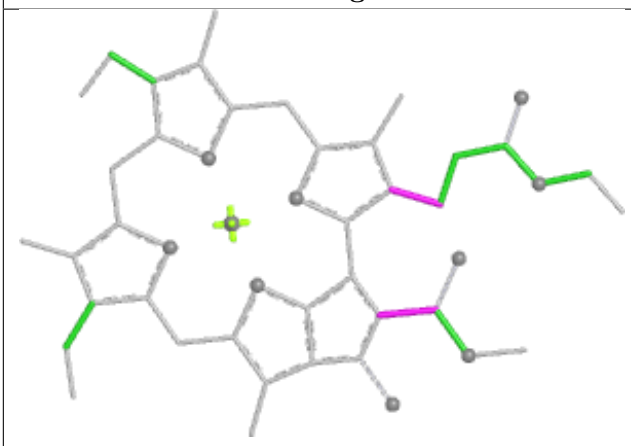
Ligand CLA v 313



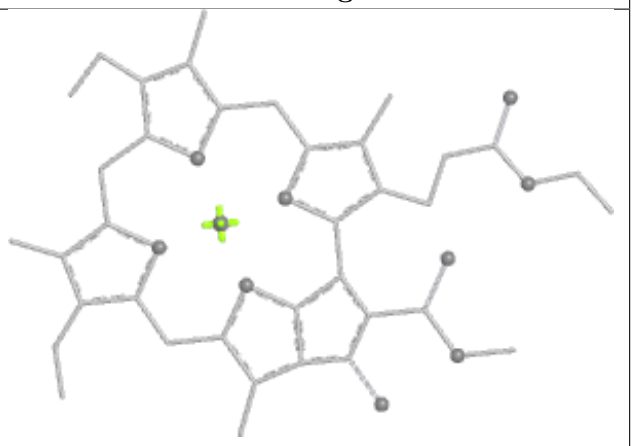
Bond lengths



Bond angles

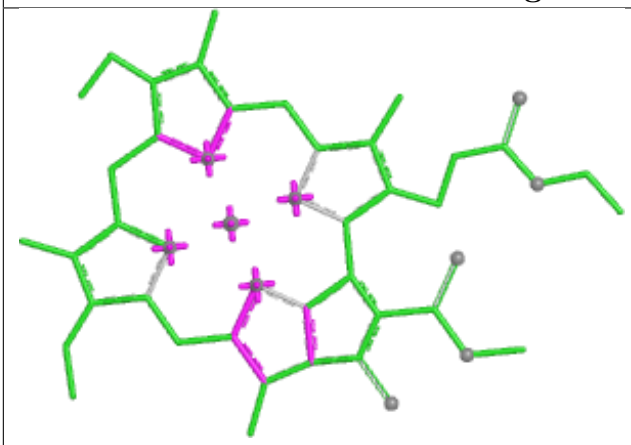


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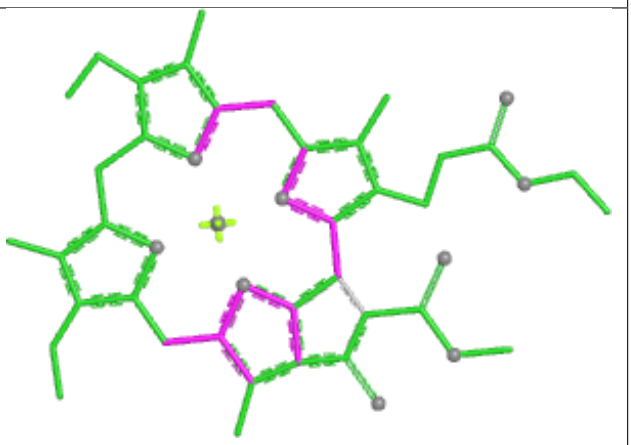


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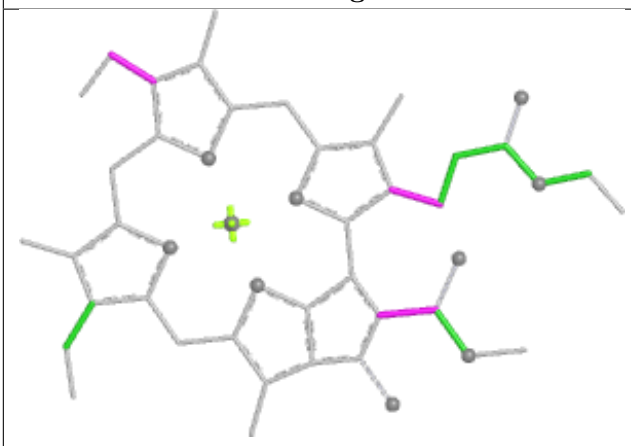
Ligand CLA C 301



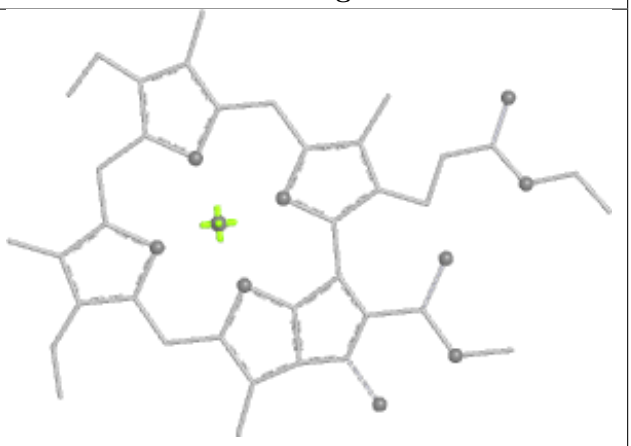
Bond lengths



Bond angles

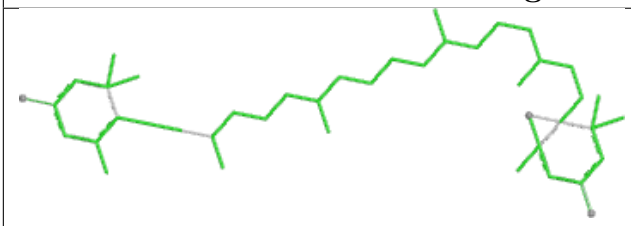


Torsions



Rings

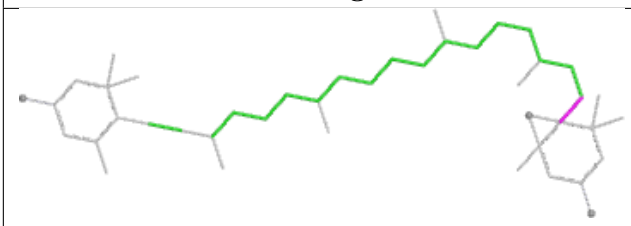
Ligand DD6 D 316



Bond lengths



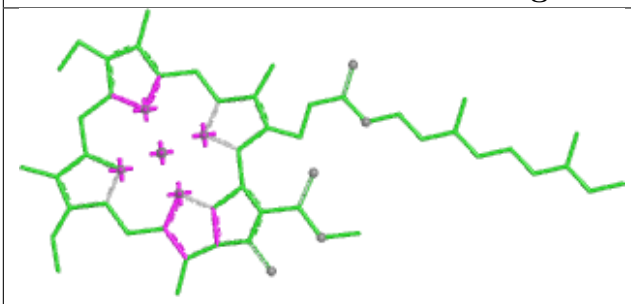
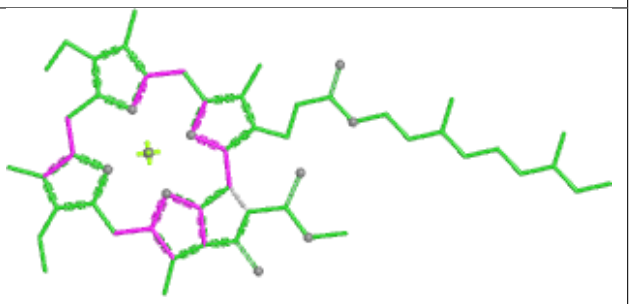
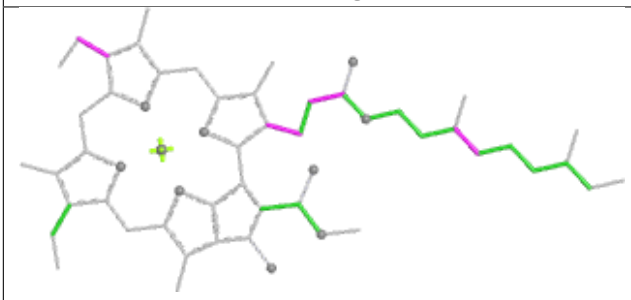
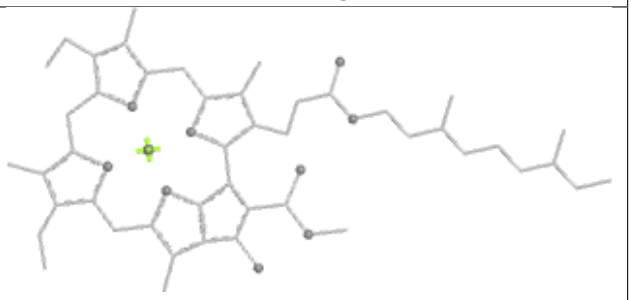
Bond angles

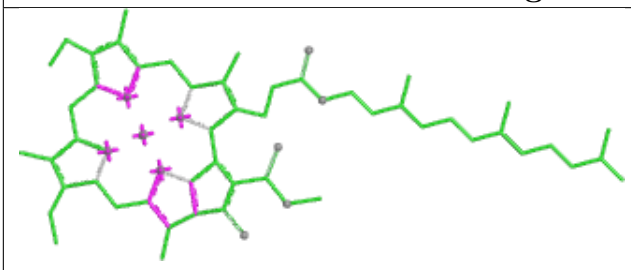
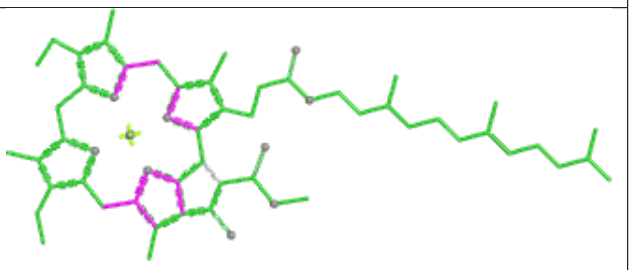
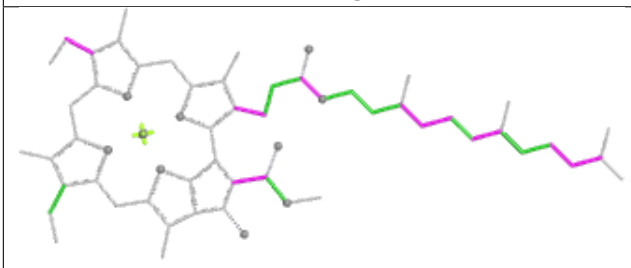
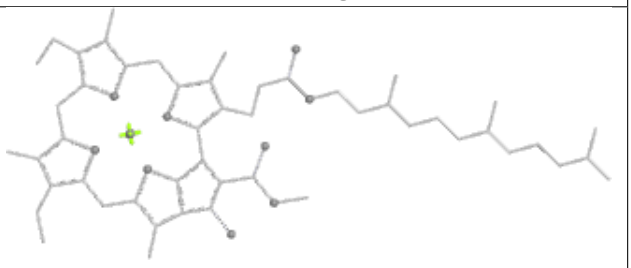


Torsions

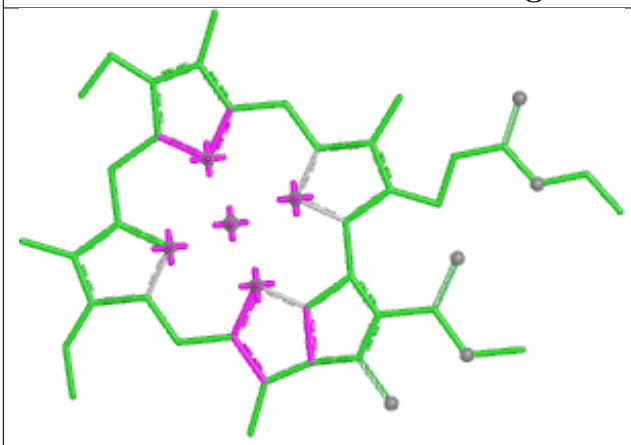


Rings

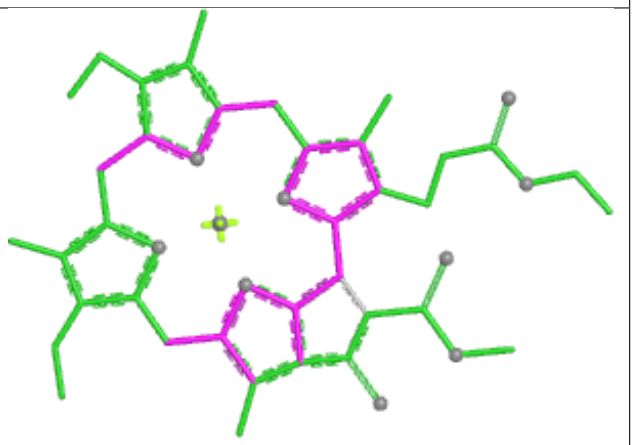
Ligand CLA I 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA P 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

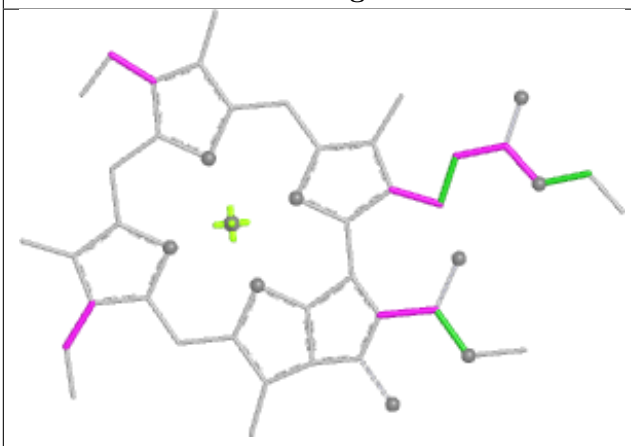
Ligand CLA E 314



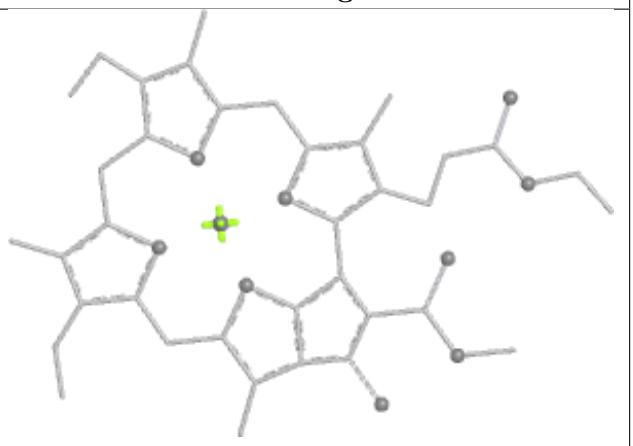
Bond lengths



Bond angles

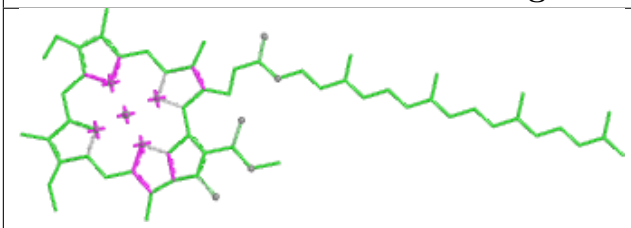


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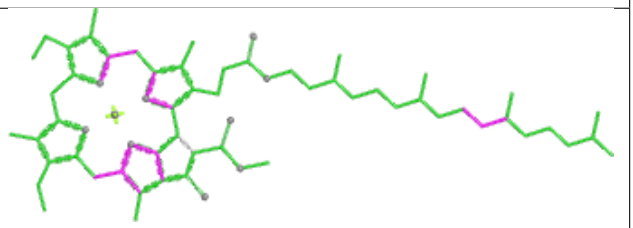


Rings

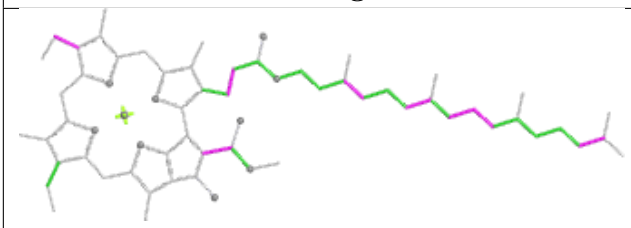
Ligand CLA a 806



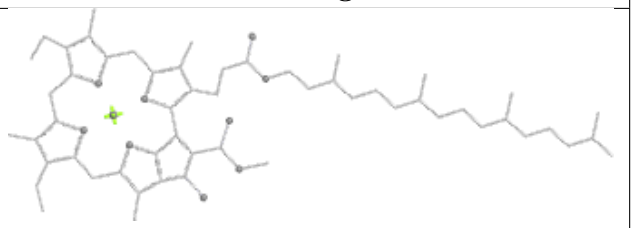
Bond lengths



Bond angles

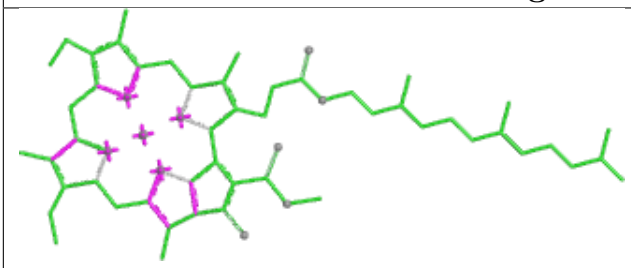


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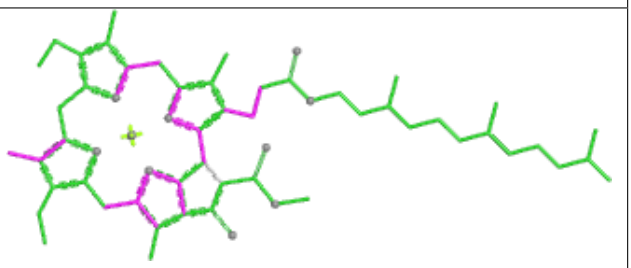


Rings

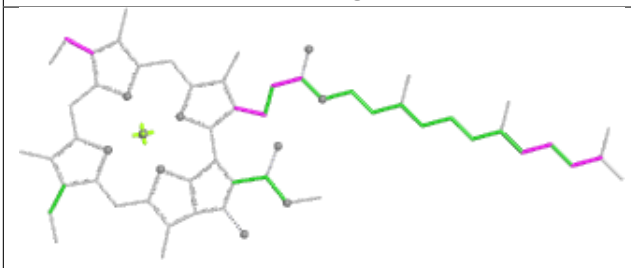
Ligand CLA o 306



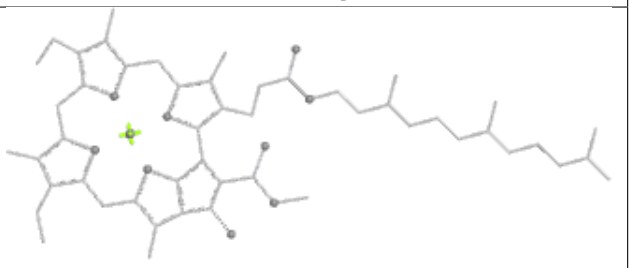
Bond lengths



Bond angles

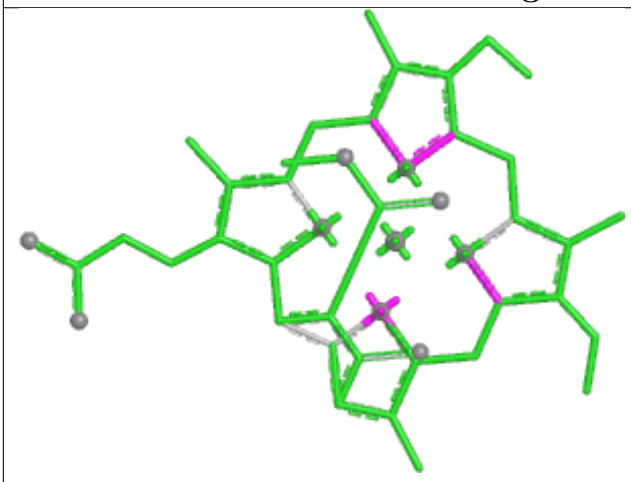


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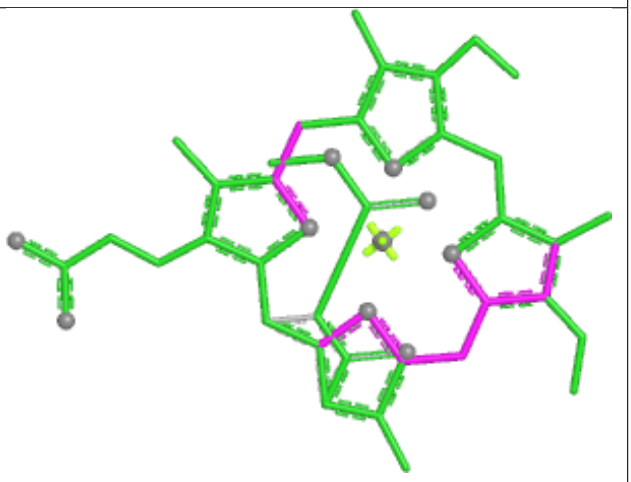


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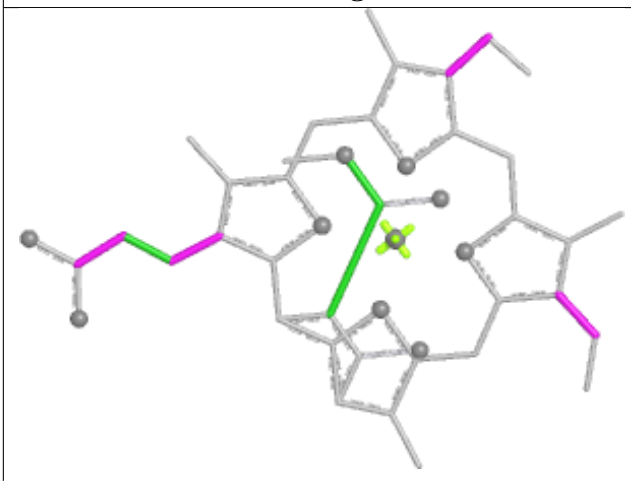
Ligand KC2 M 308



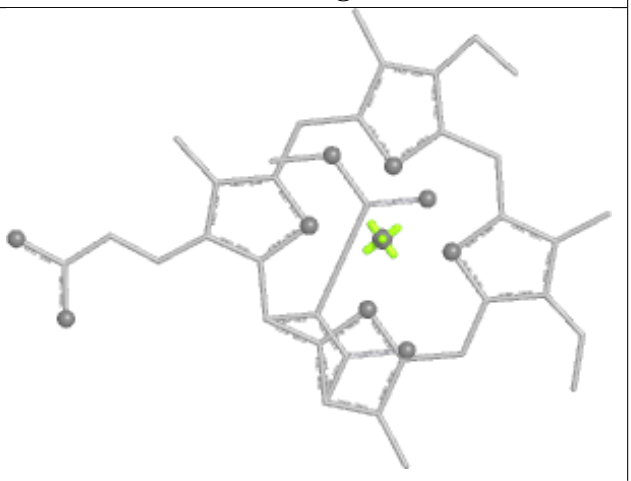
Bond lengths



Bond angles

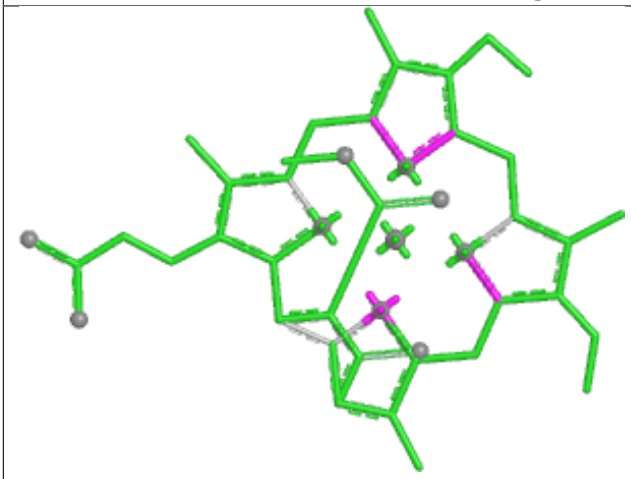


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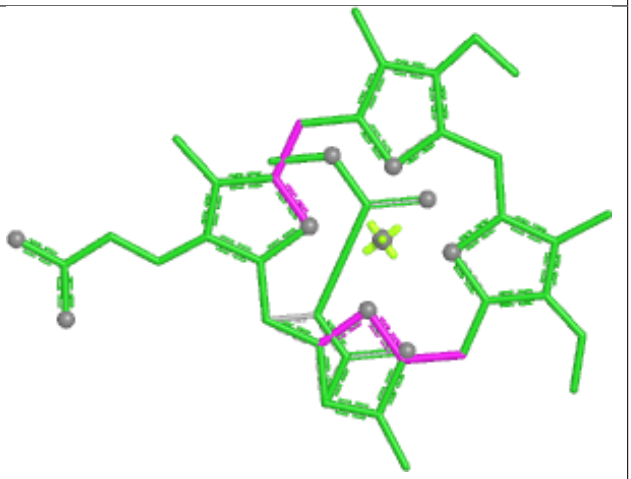


Rings

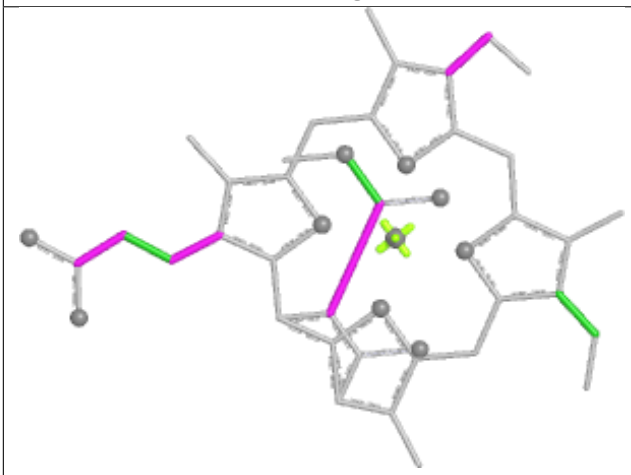
Ligand KC2 u 304



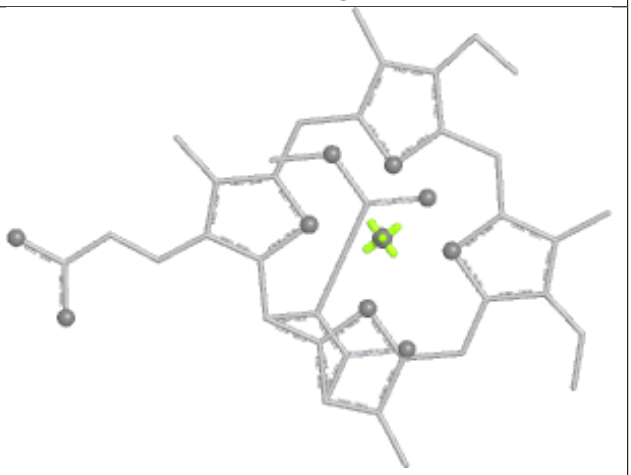
Bond lengths



Bond angles

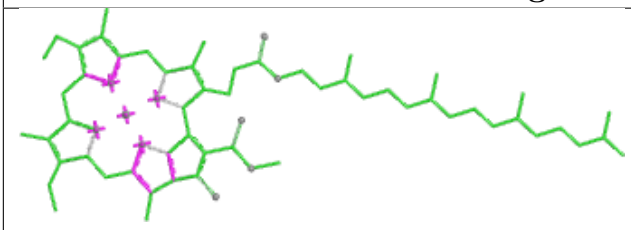


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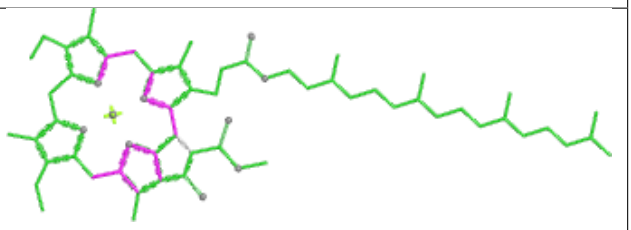


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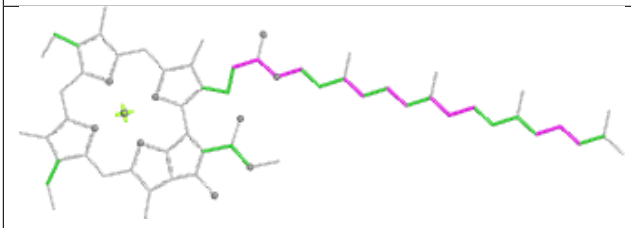
Ligand CLA a 821



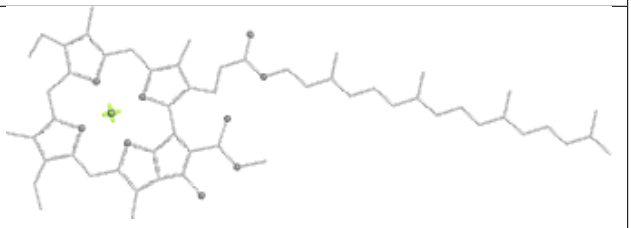
Bond lengths



Bond angles

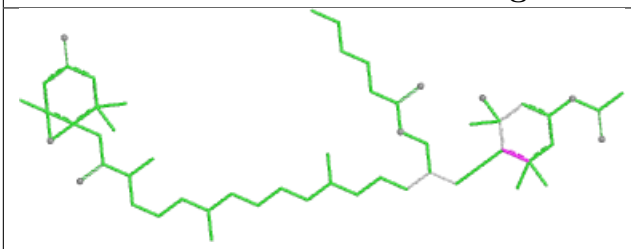


Torsions

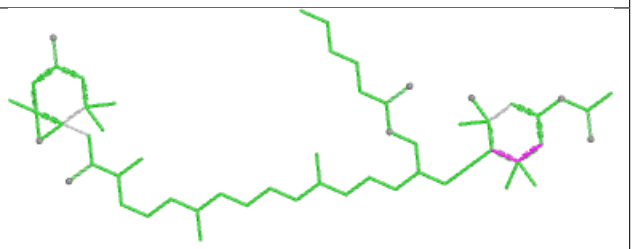


Rings

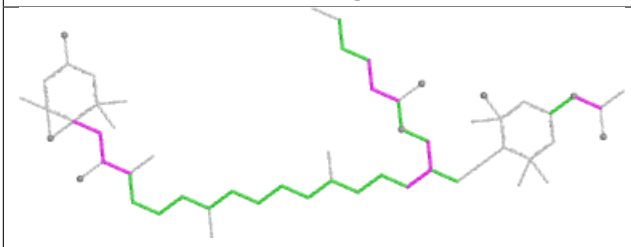
Ligand A1EB1 o 322



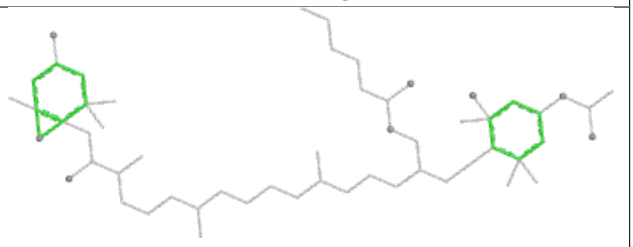
Bond lengths



Bond angles

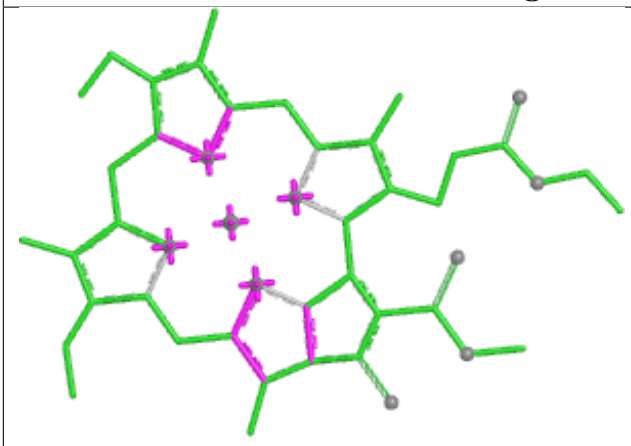


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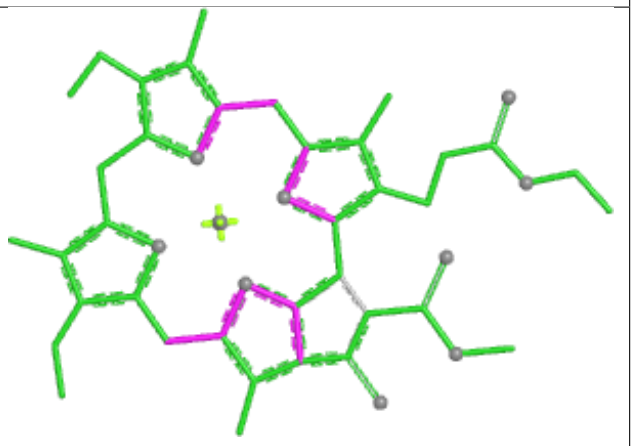


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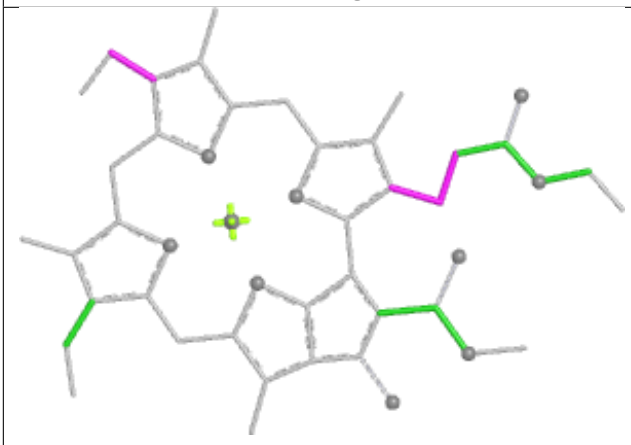
Ligand CLA H 308



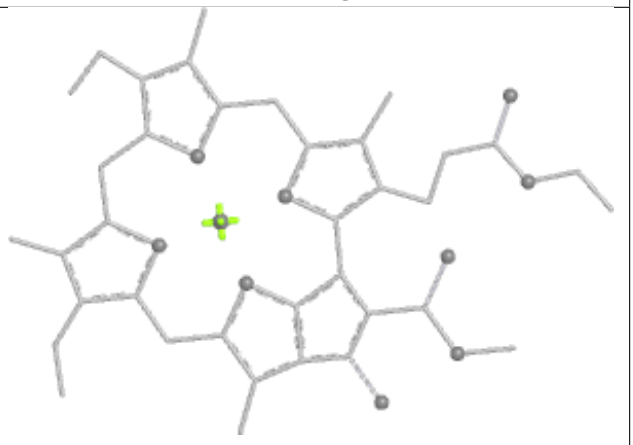
Bond lengths



Bond angles

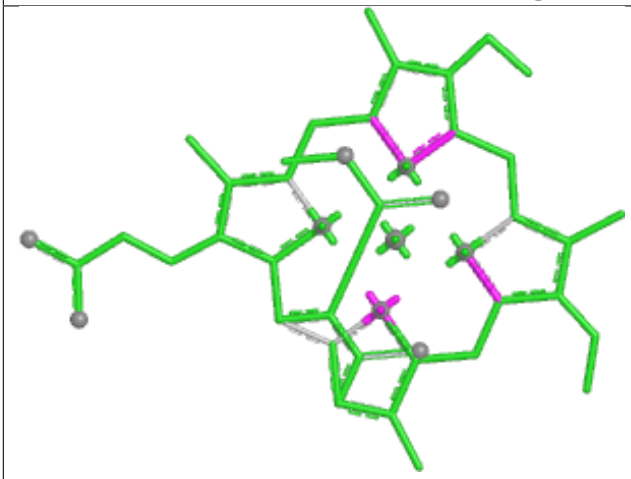


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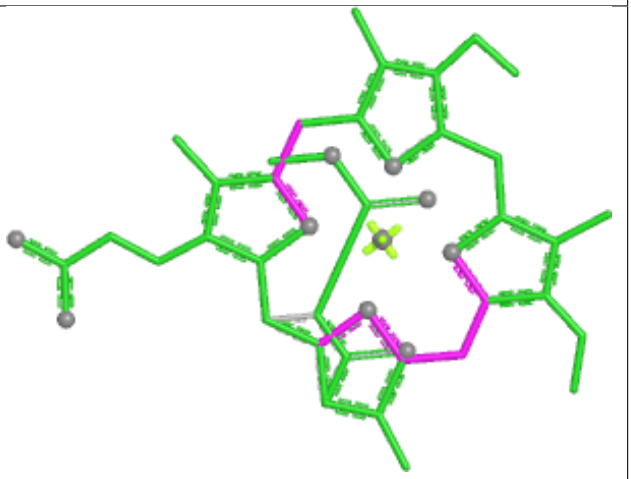


Rings

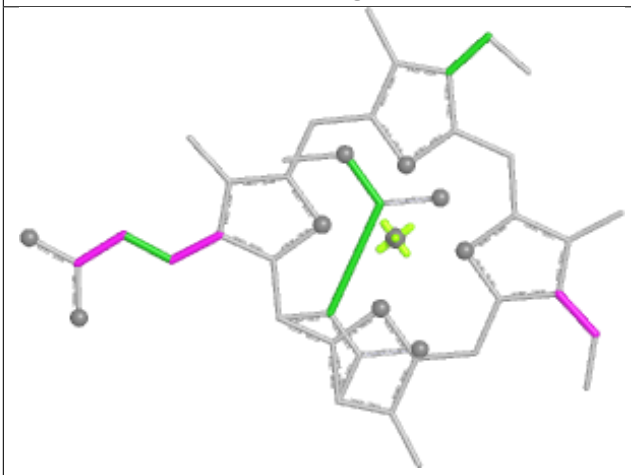
Ligand KC2 v 302



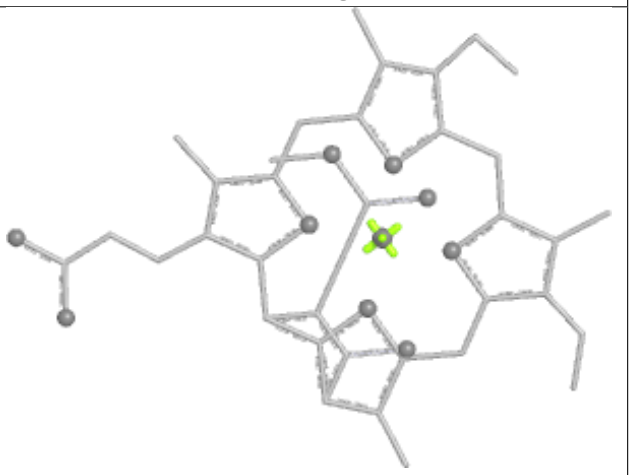
Bond lengths



Bond angles

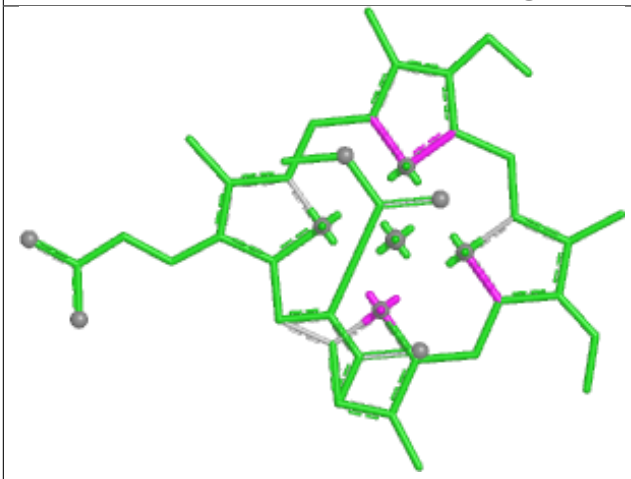


Torsions

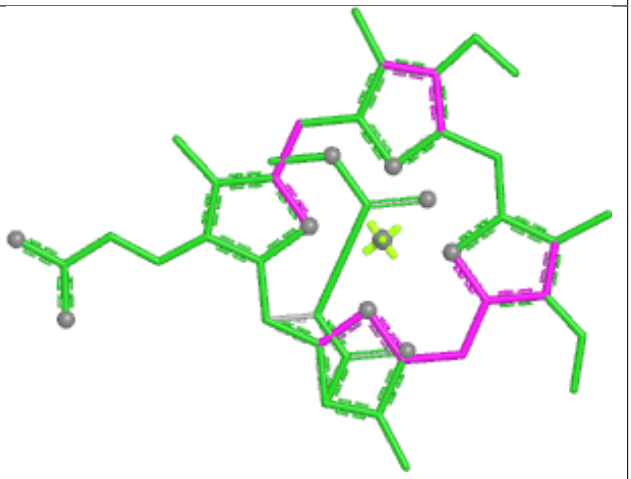


Rings

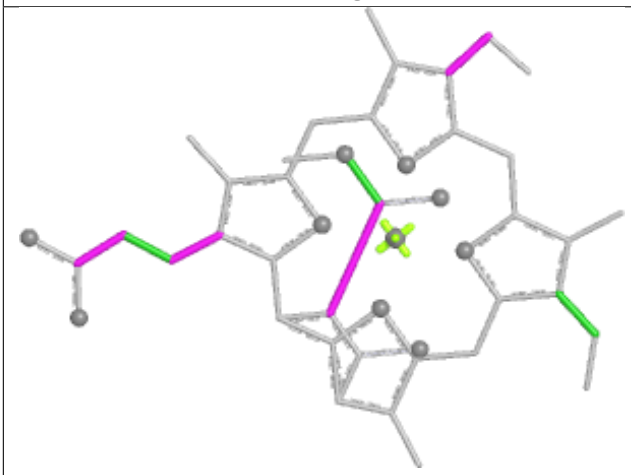
Ligand KC2 W 304



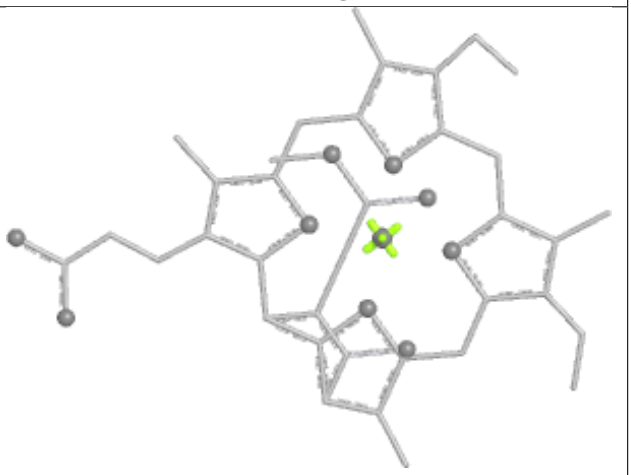
Bond lengths



Bond angles

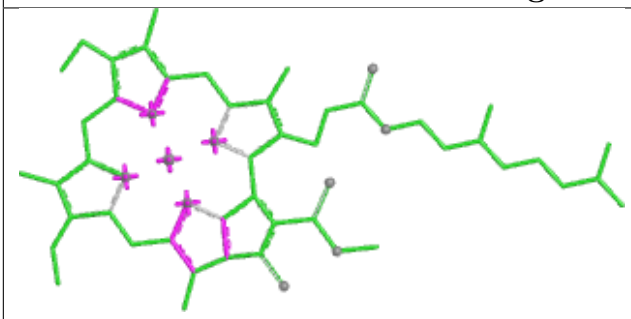


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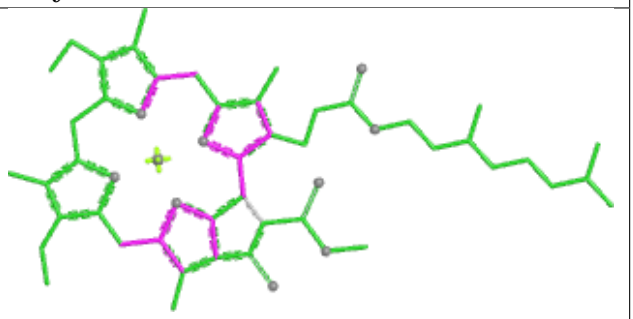


Rings

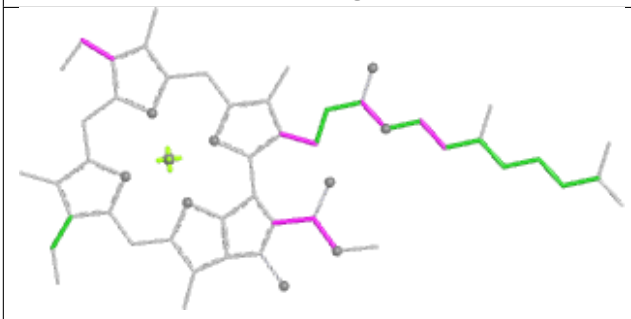
Ligand CLA y 309



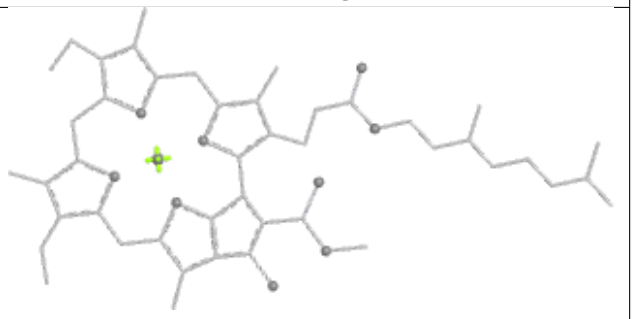
Bond lengths



Bond angles

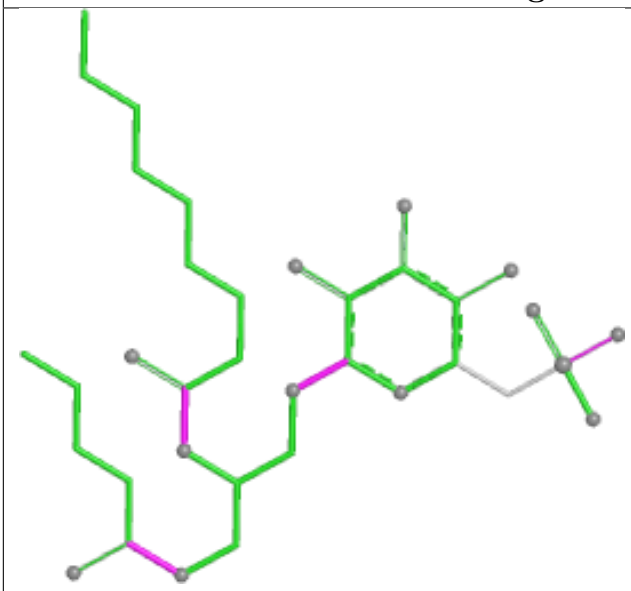


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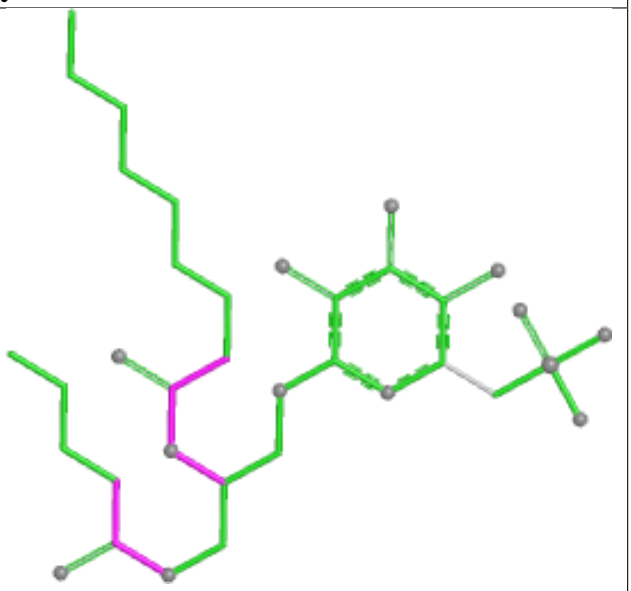


Rings

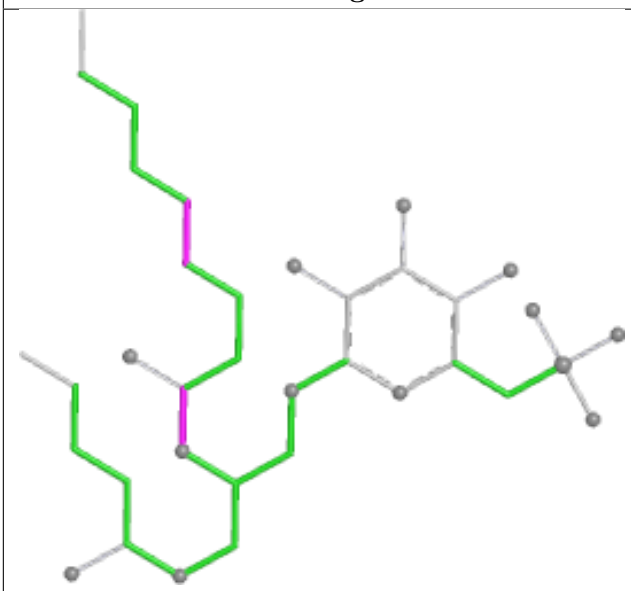
Ligand SQD k 205



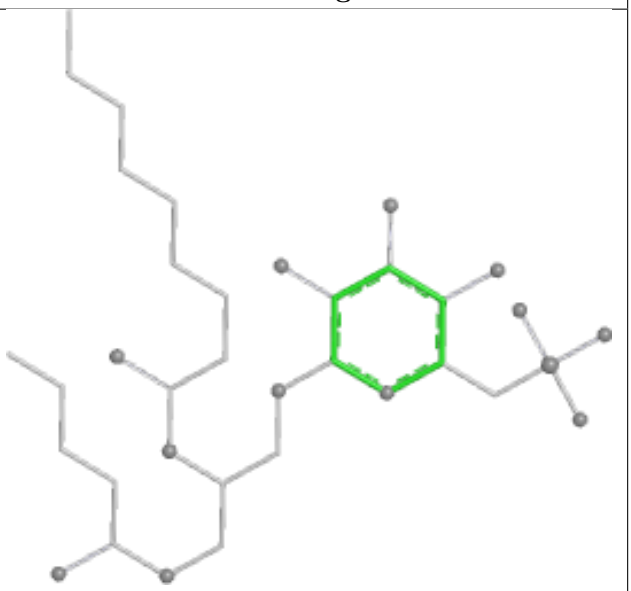
Bond lengths



Bond angles

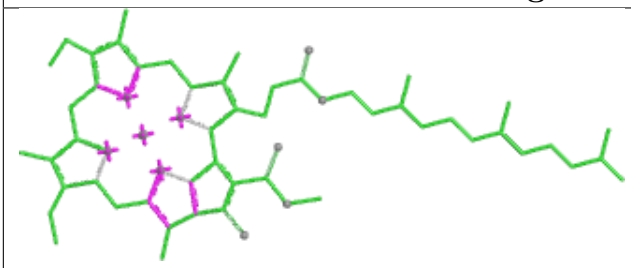


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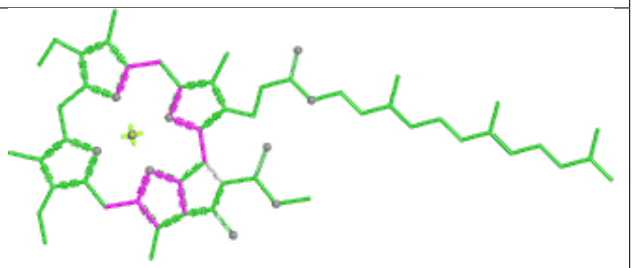


Rings

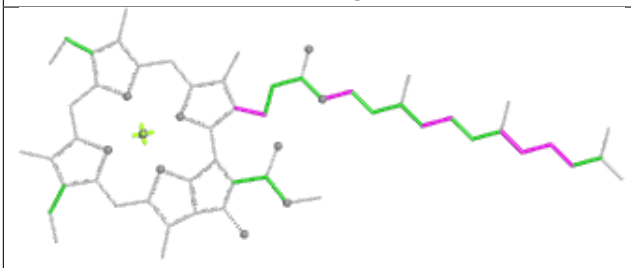
Ligand CLA b 827



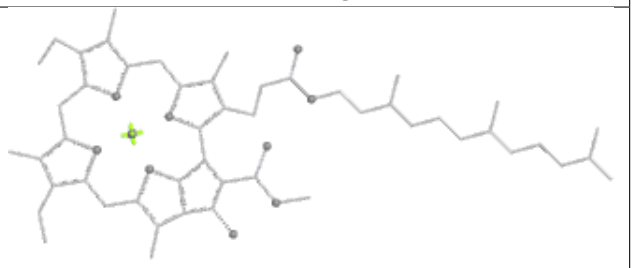
Bond lengths



Bond angles

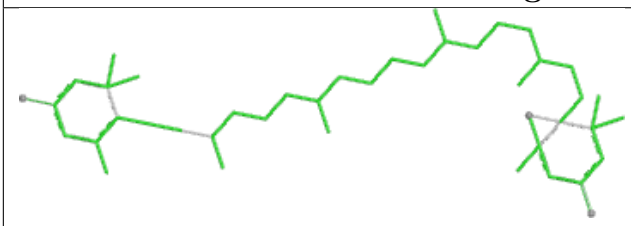


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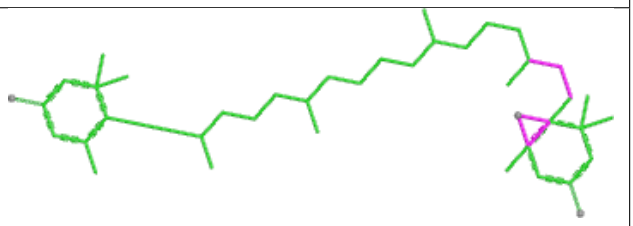


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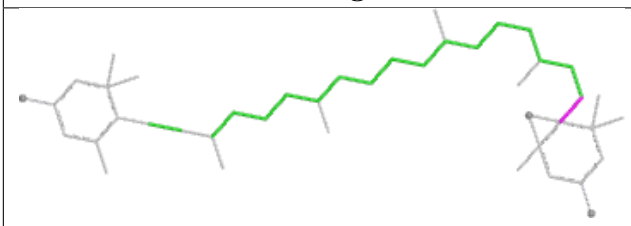
Ligand DD6 K 311



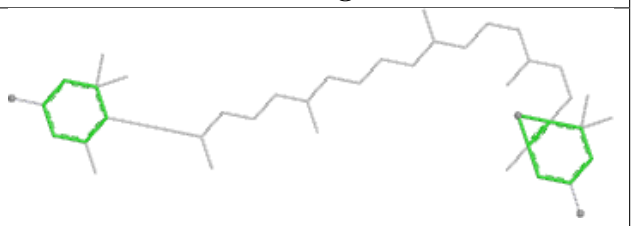
Bond lengths



Bond angles

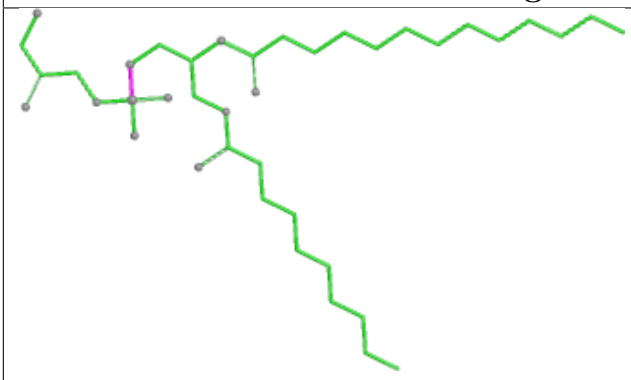


Torsions



Rings

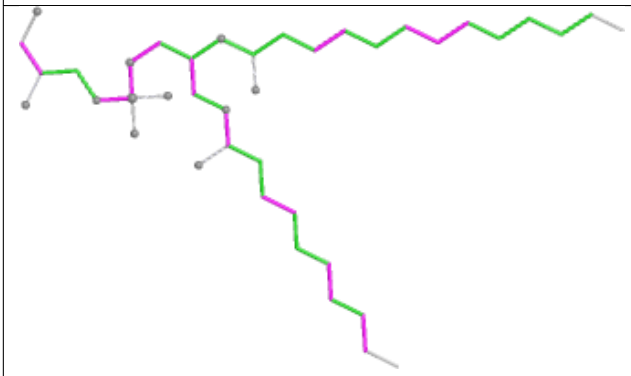
Ligand LHG F 319



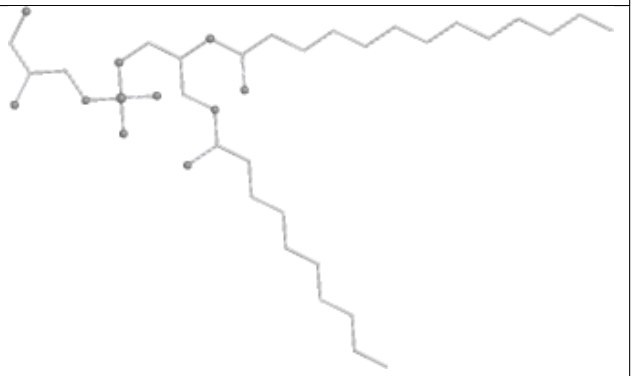
Bond lengths



Bond angles

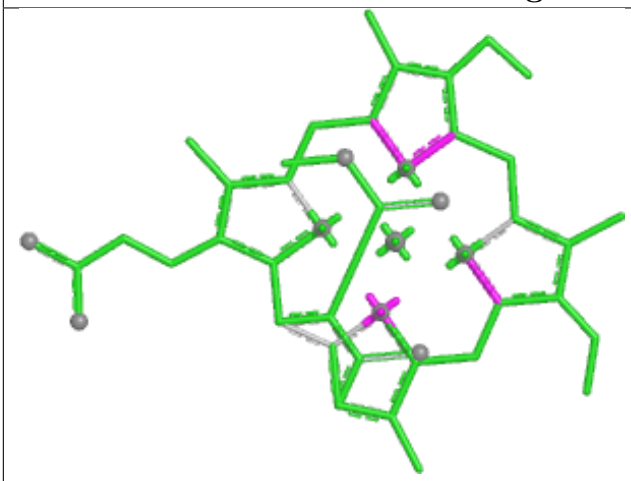


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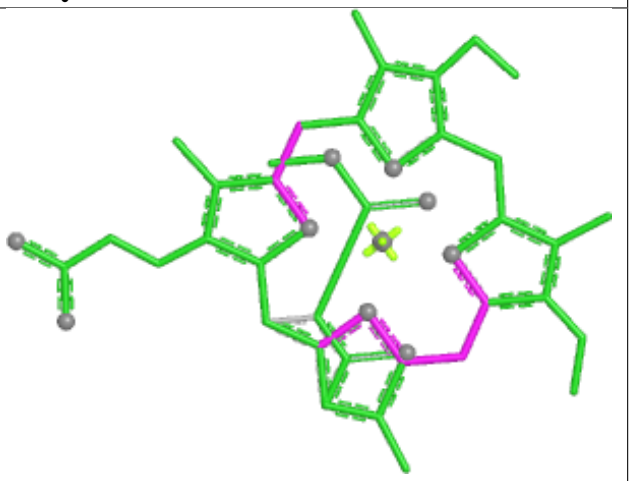


Rings

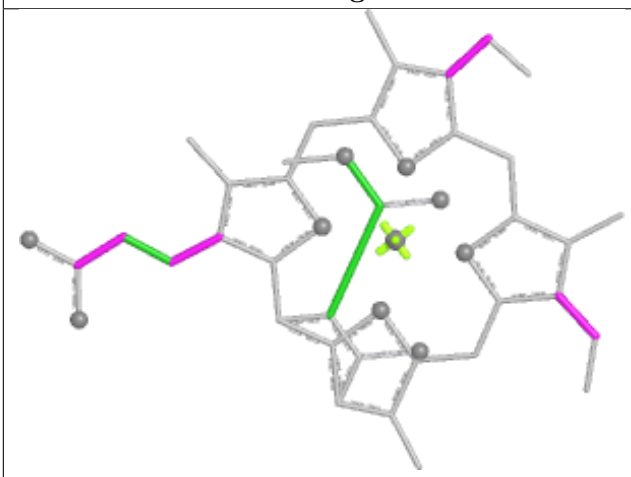
Ligand KC2 Q 216



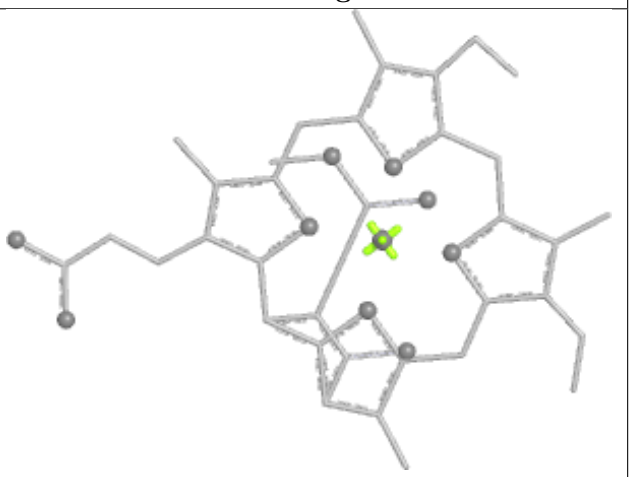
Bond lengths



Bond angles

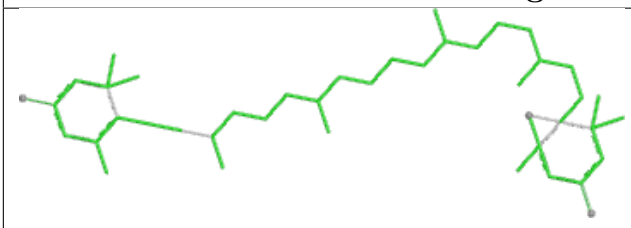


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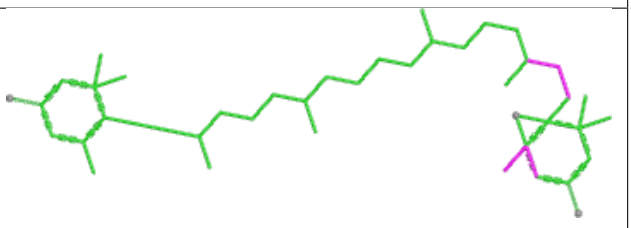


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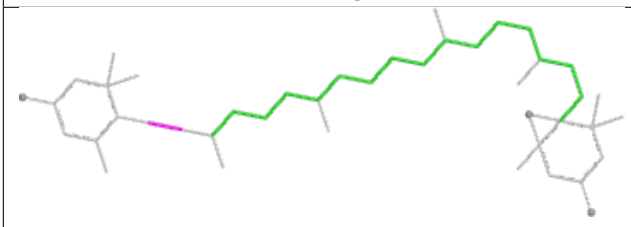
Ligand DD6 E 317



Bond lengths



Bond angles

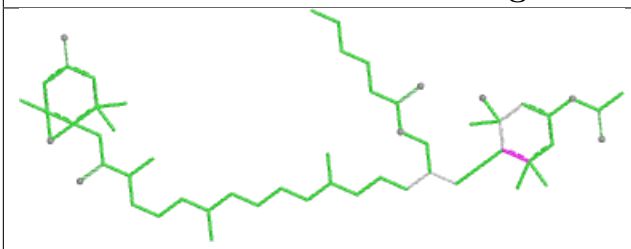


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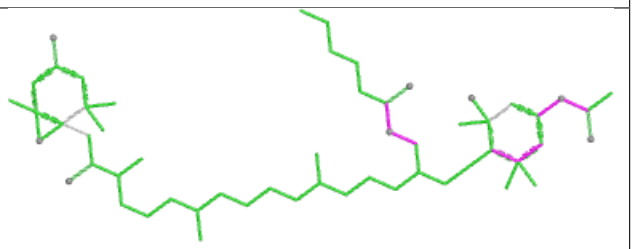


Rings

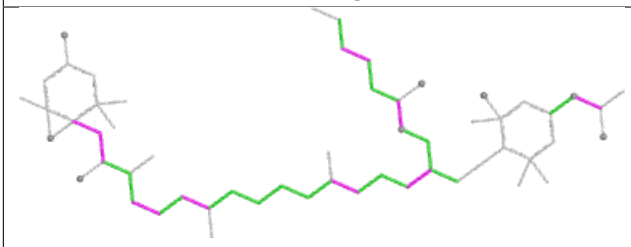
Ligand A1EB1 v 321



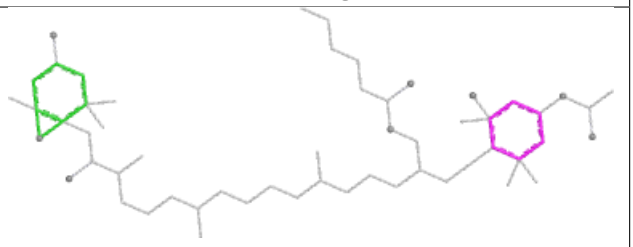
Bond lengths



Bond angles

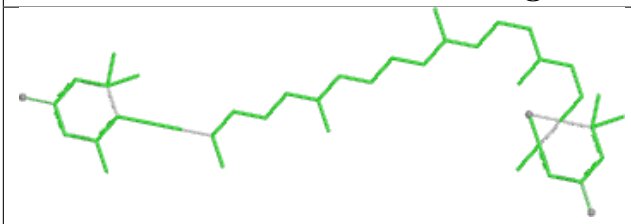


Torsions



Rings

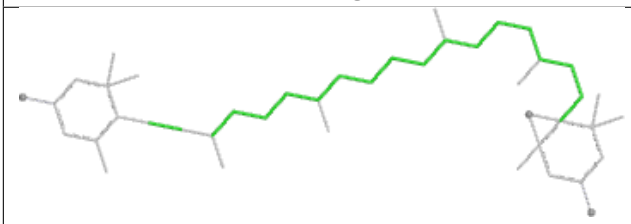
Ligand DD6 A 312



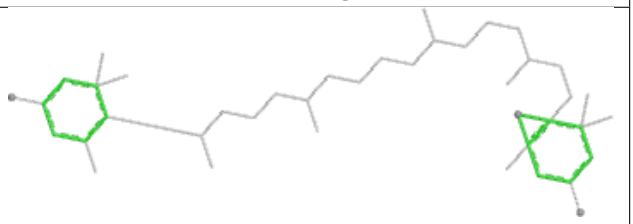
Bond lengths



Bond angles

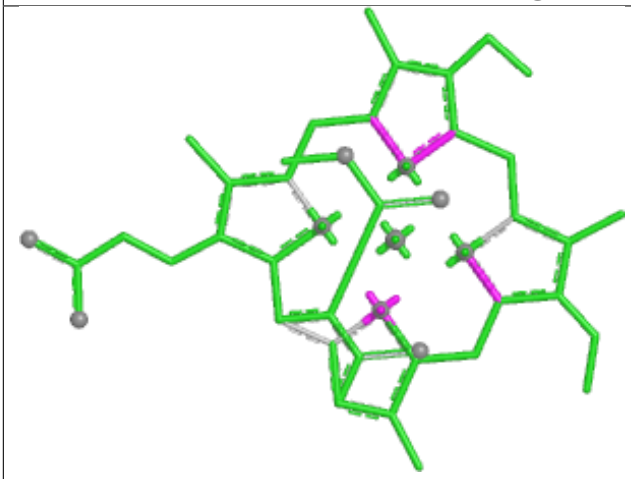


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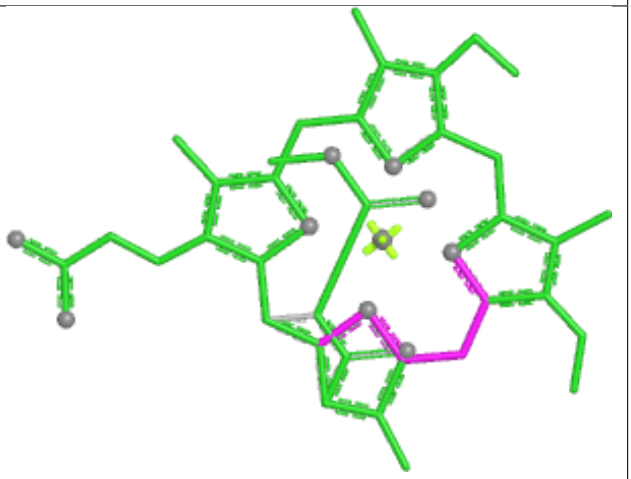


Rings

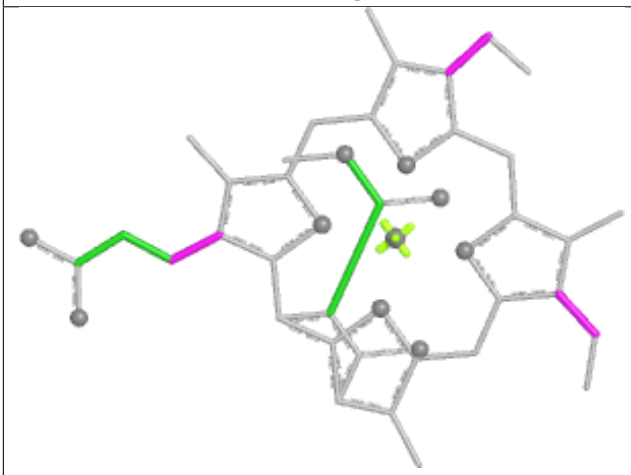
Ligand KC2 u 310



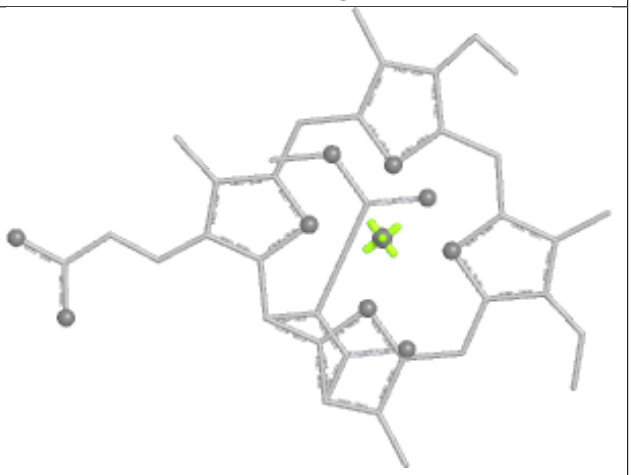
Bond lengths



Bond angles

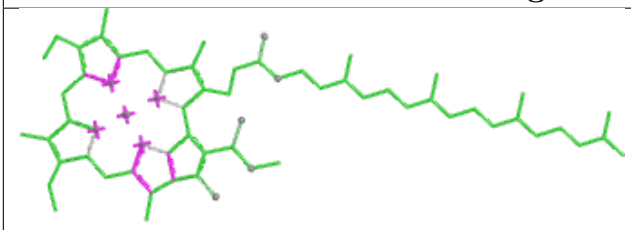


Torsions

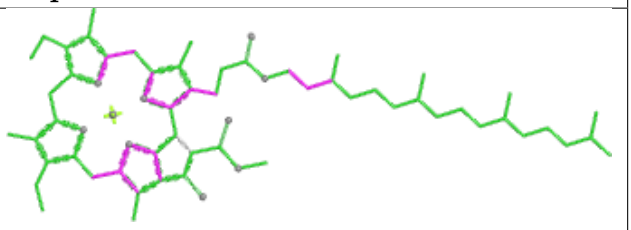


Rings

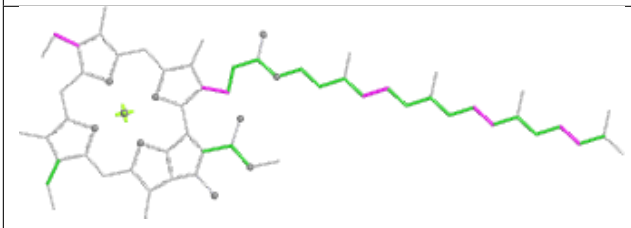
Ligand CLA p 302



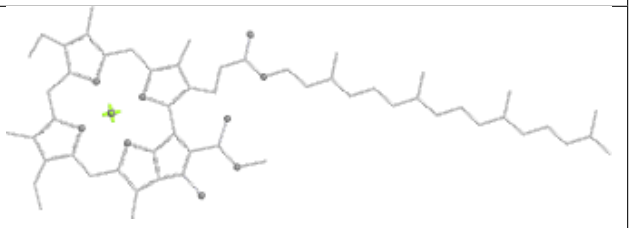
Bond lengths



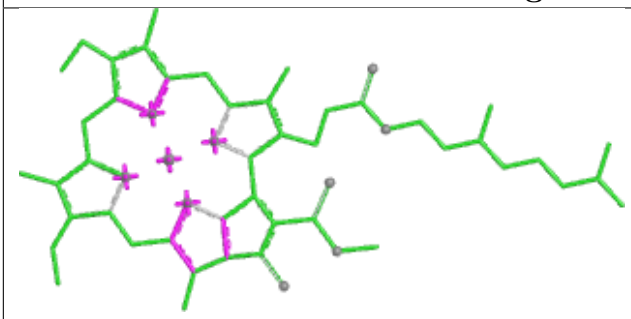
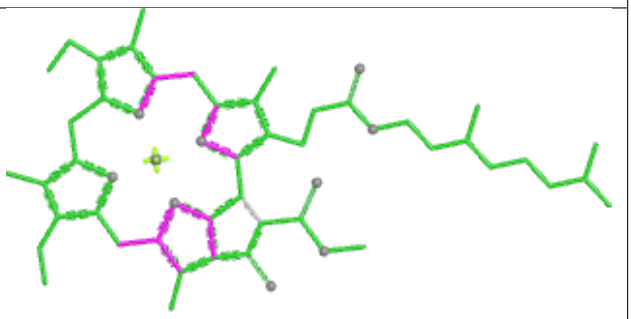
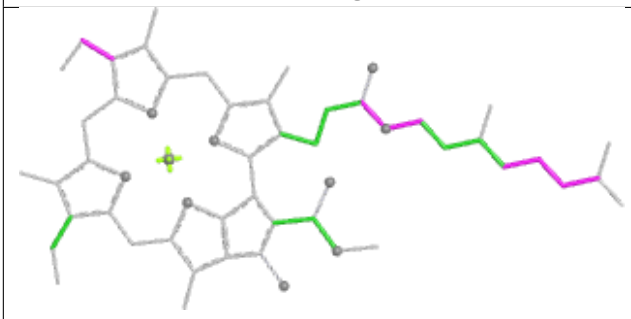
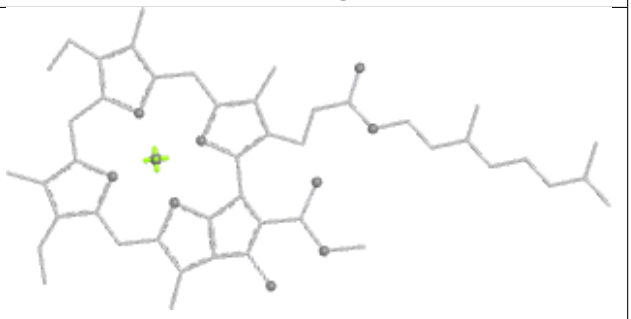
Bond angles

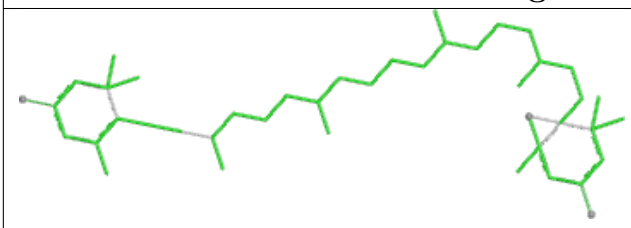
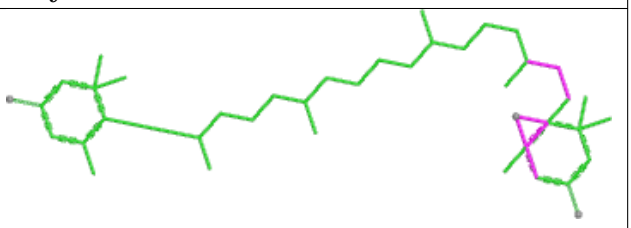
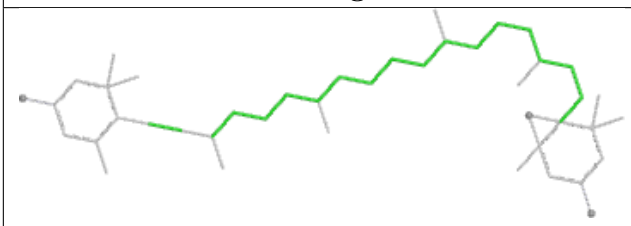
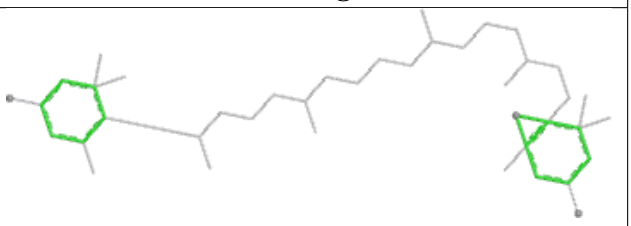


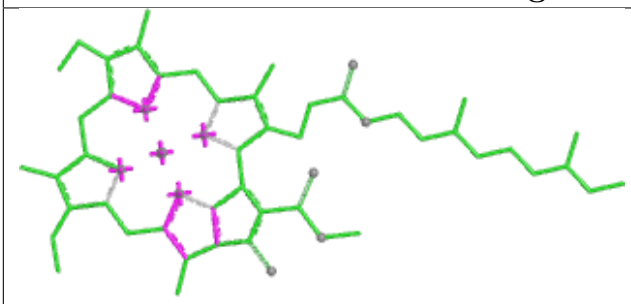
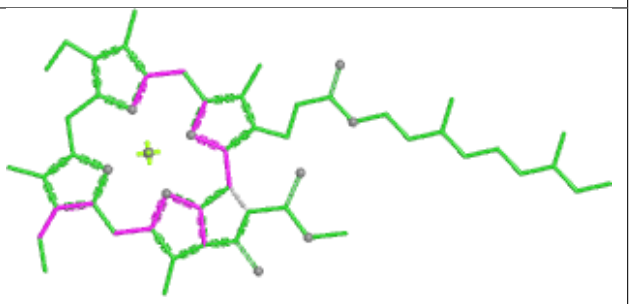
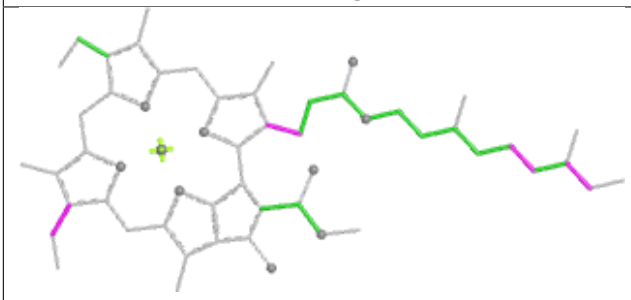
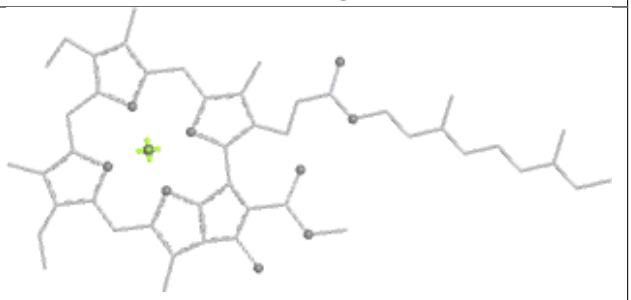
Torsions

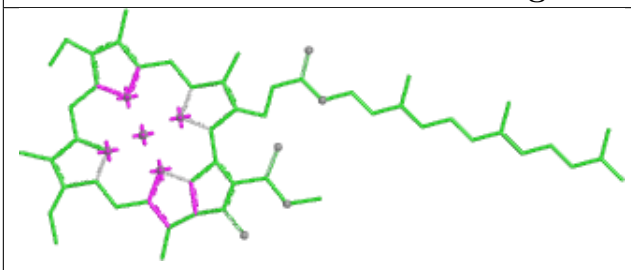
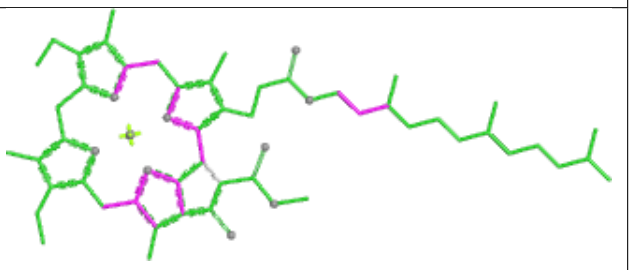
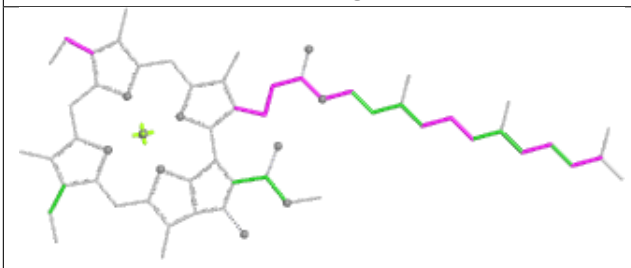
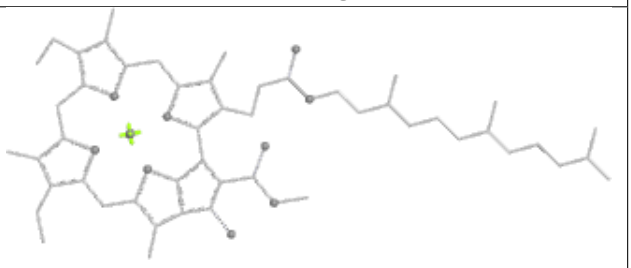


Rings

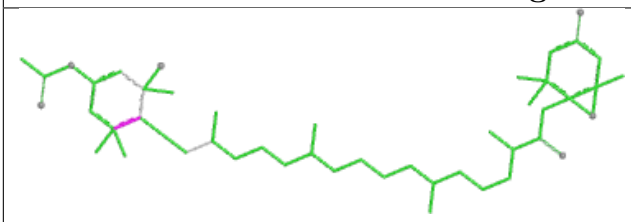
Ligand CLA E 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 y 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

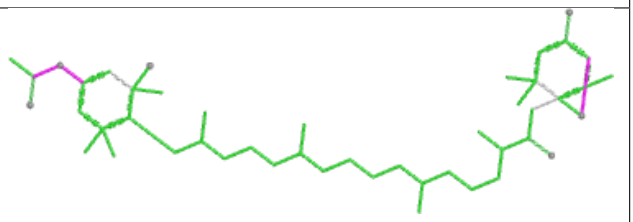
Ligand CLA a 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 820	
	
Bond lengths	Bond angles
	
Torsions	Rings

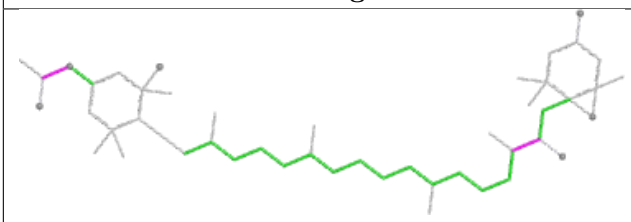
Ligand A86 X 316



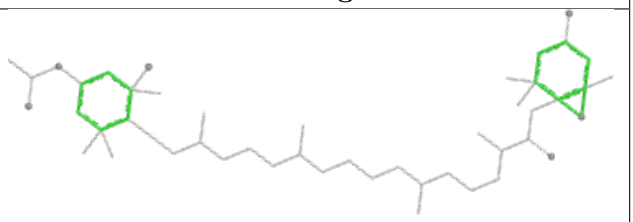
Bond lengths



Bond angles

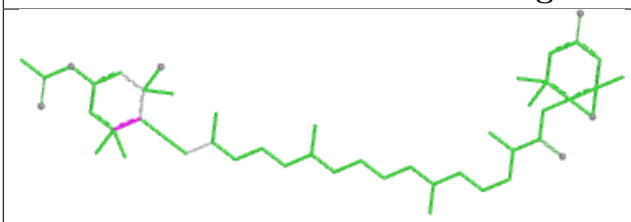


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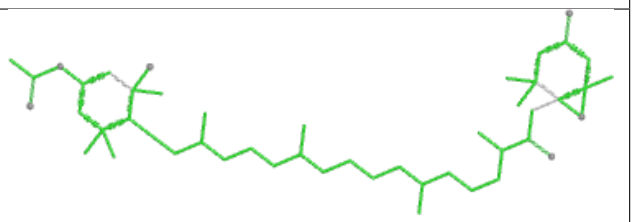


Rings

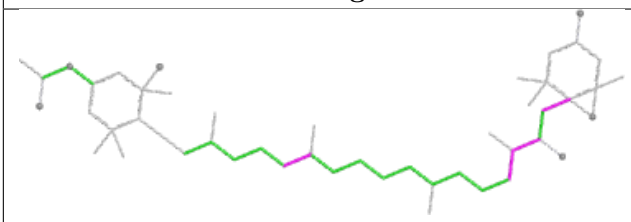
Ligand A86 t 316



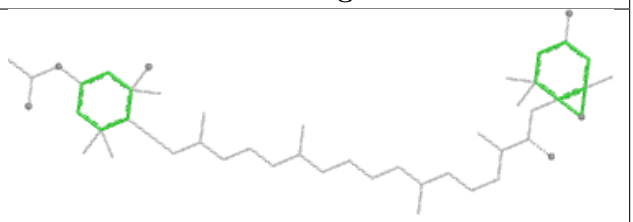
Bond lengths



Bond angles

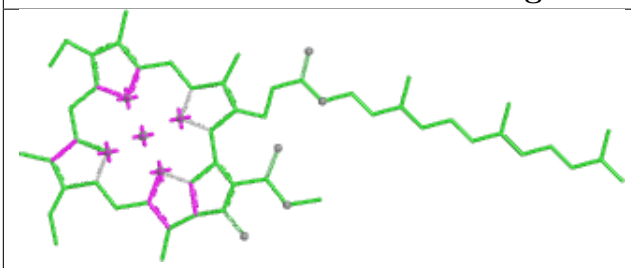


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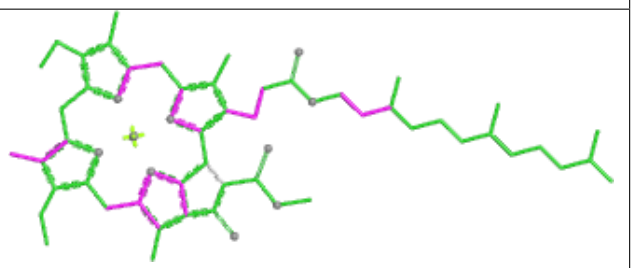


Rings

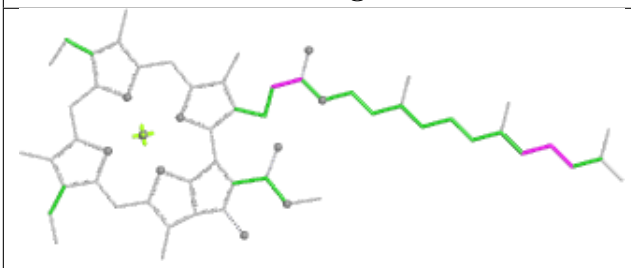
Ligand CLA T 306



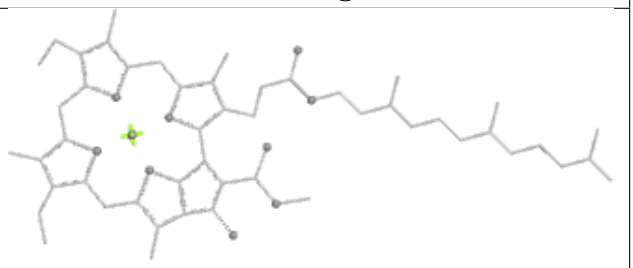
Bond lengths



Bond angles

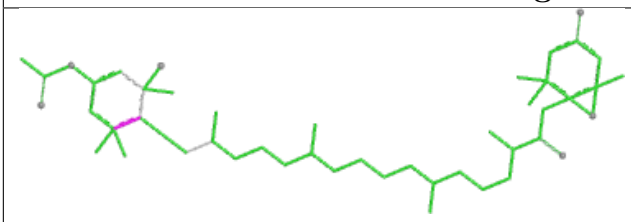


Torsions

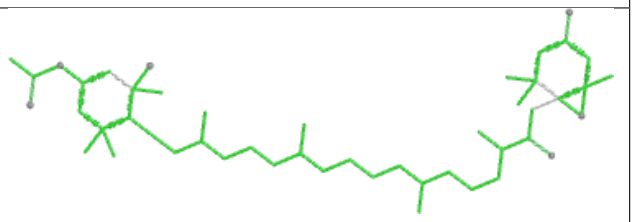


Rings

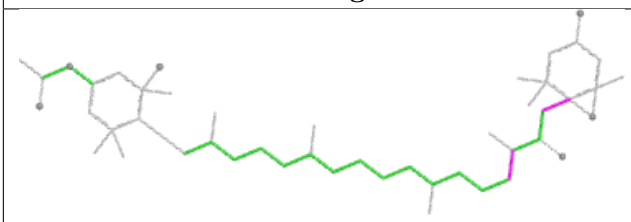
Ligand A86 o 318



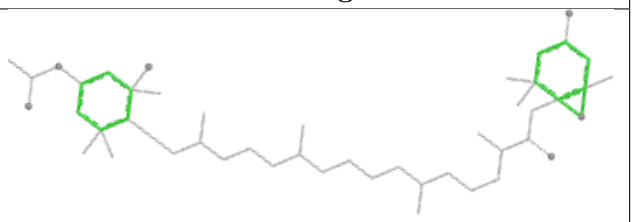
Bond lengths



Bond angles

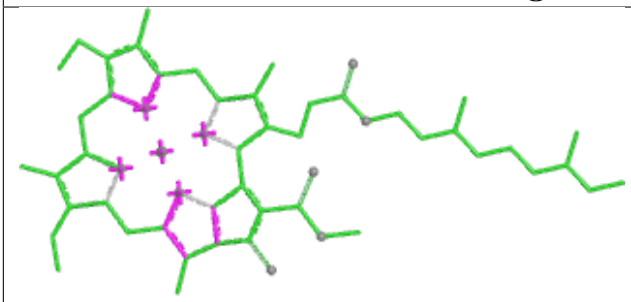


Torsions

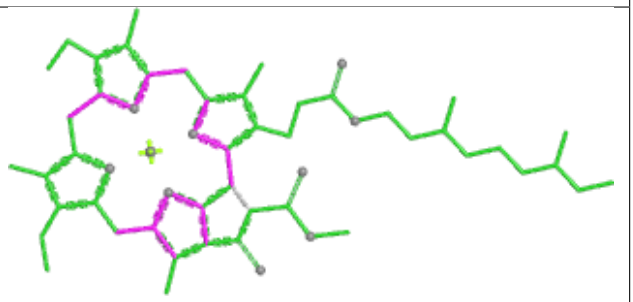


Rings

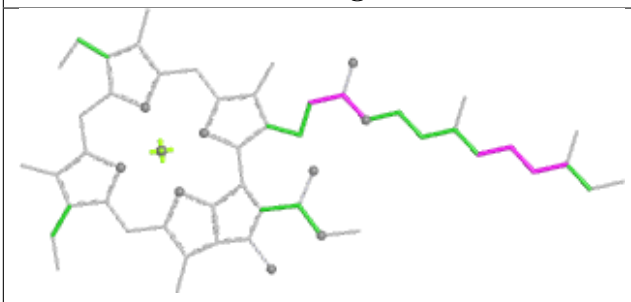
Ligand CLA S 306



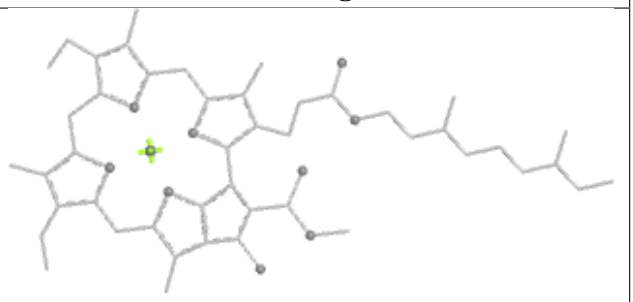
Bond lengths



Bond angles

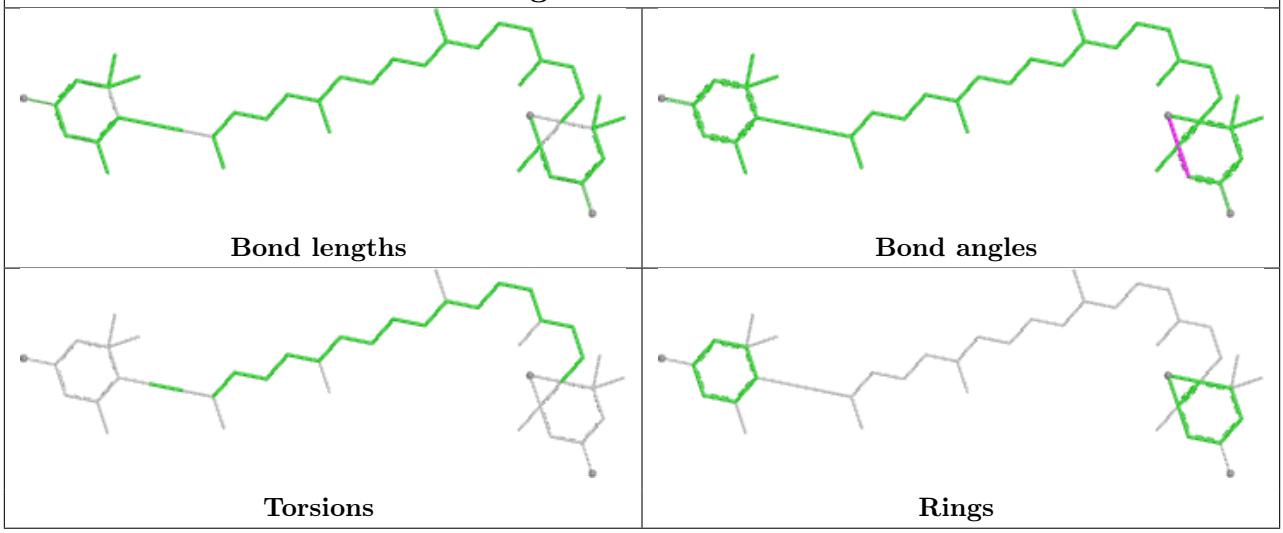


Torsions

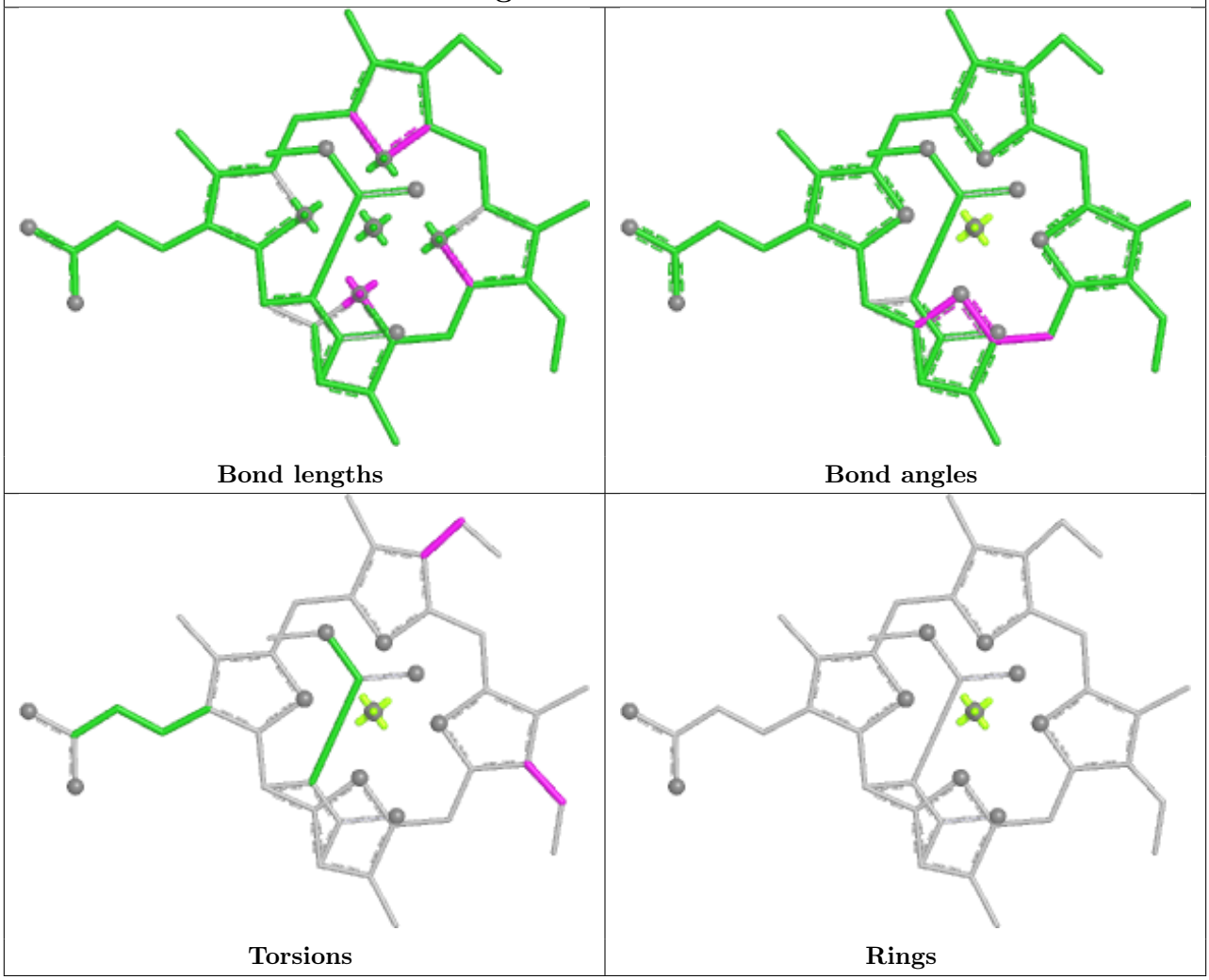


Rings

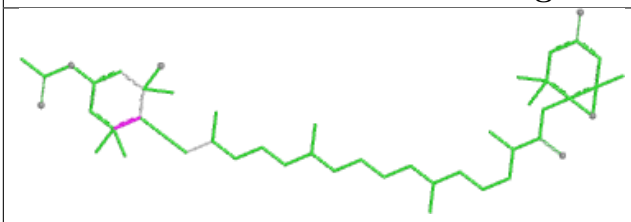
Ligand DD6 o 320



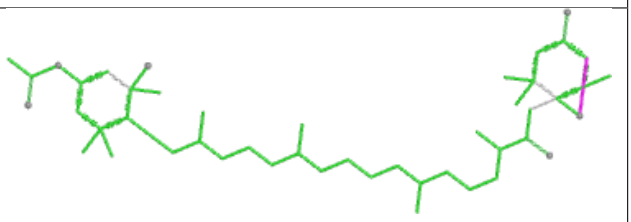
Ligand KC2 N 301



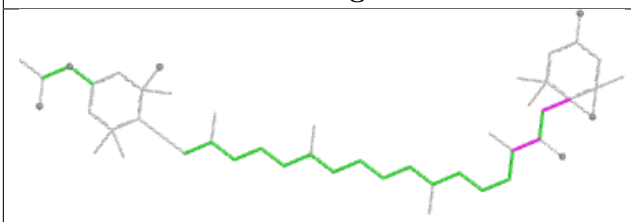
Ligand A86 z 320



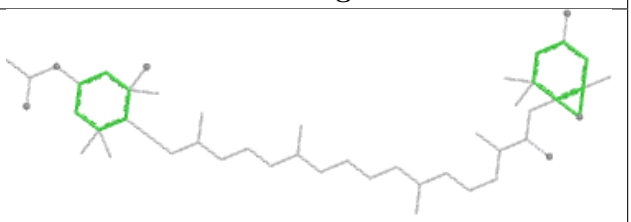
Bond lengths



Bond angles

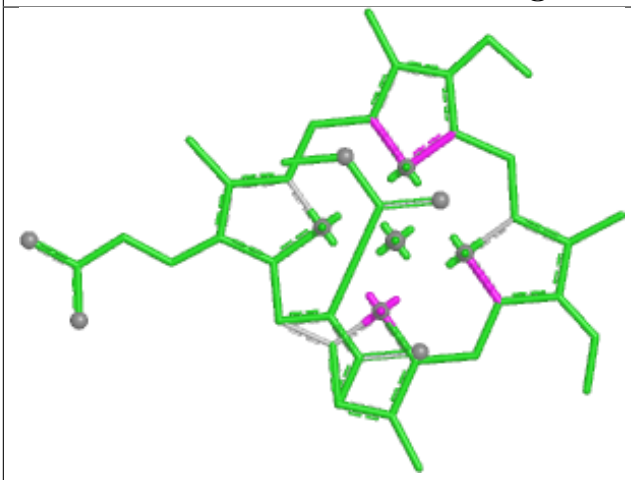


Torsions

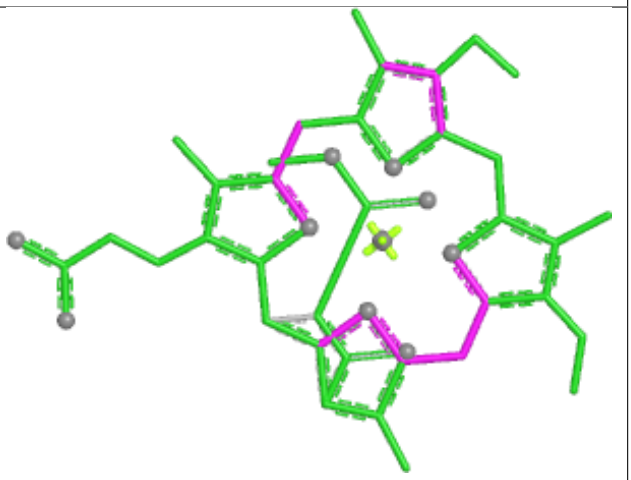


Rings

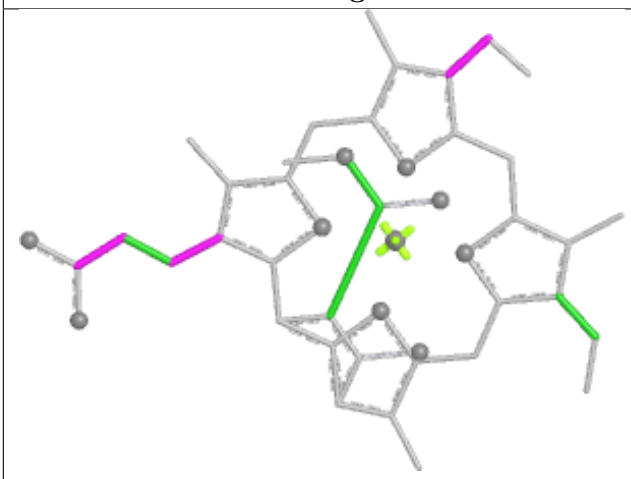
Ligand KC2 S 304



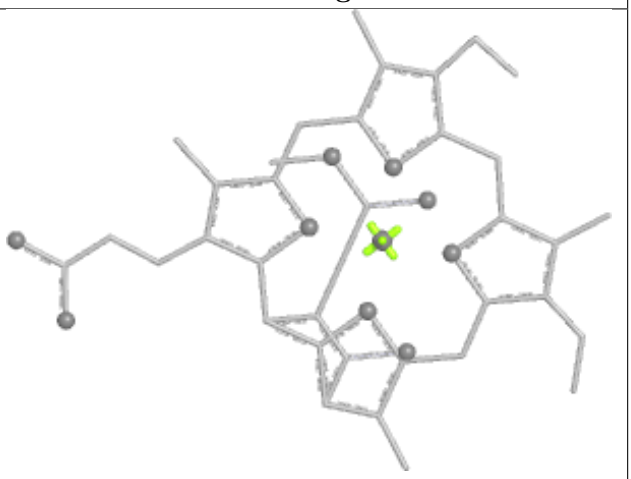
Bond lengths



Bond angles

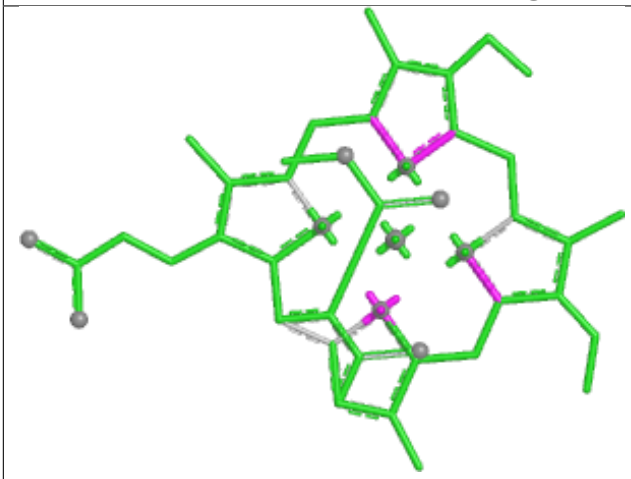


Torsions

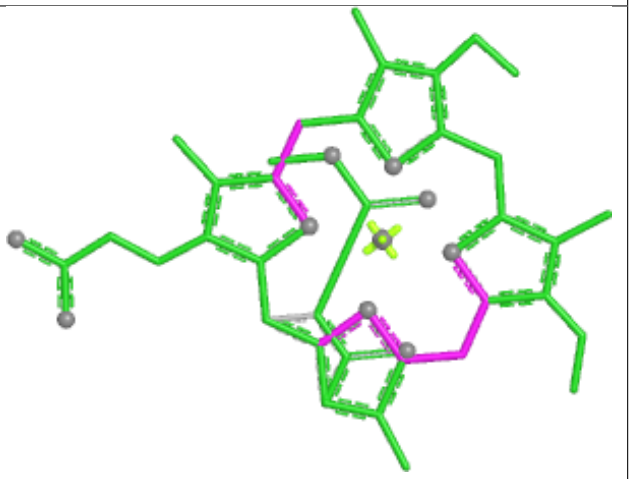


Rings

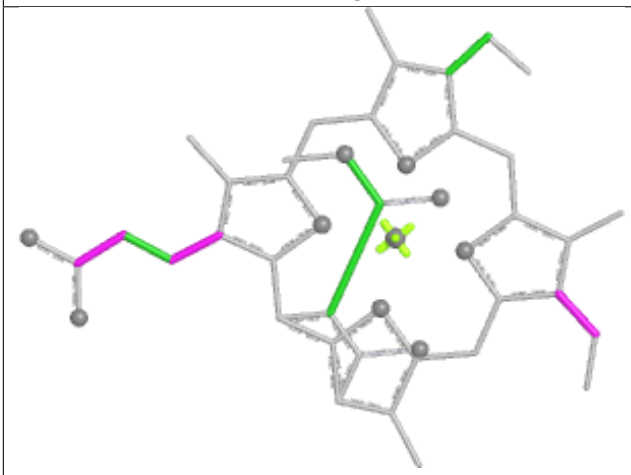
Ligand KC2 K 305



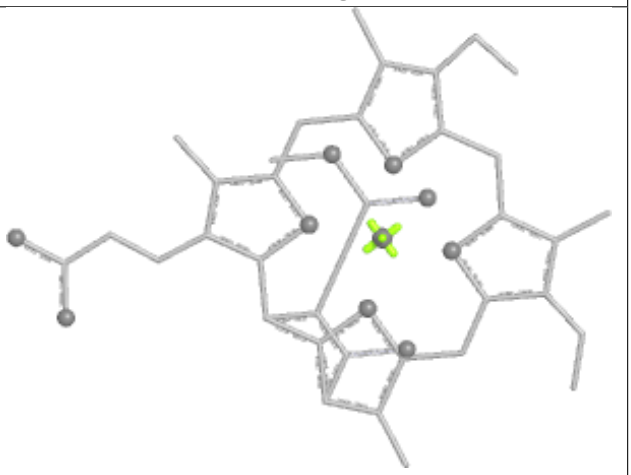
Bond lengths



Bond angles

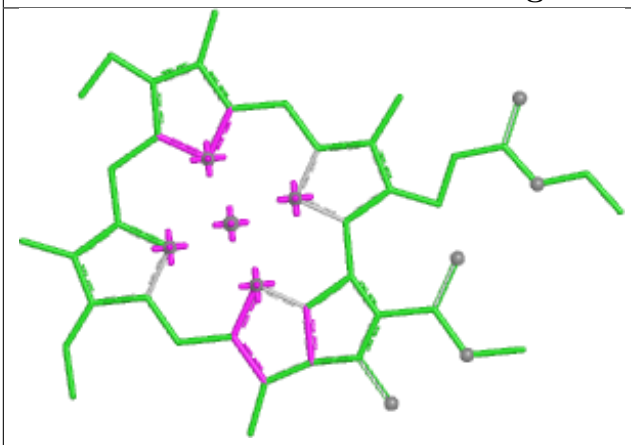


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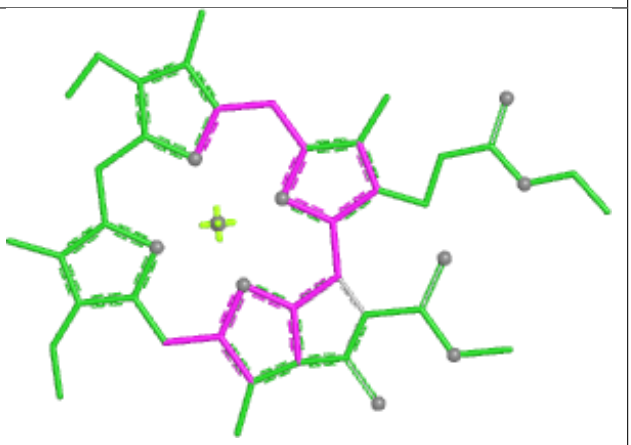


Rings

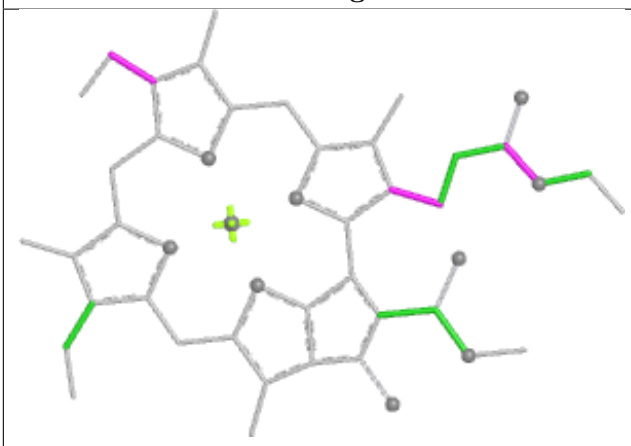
Ligand CLA L 310



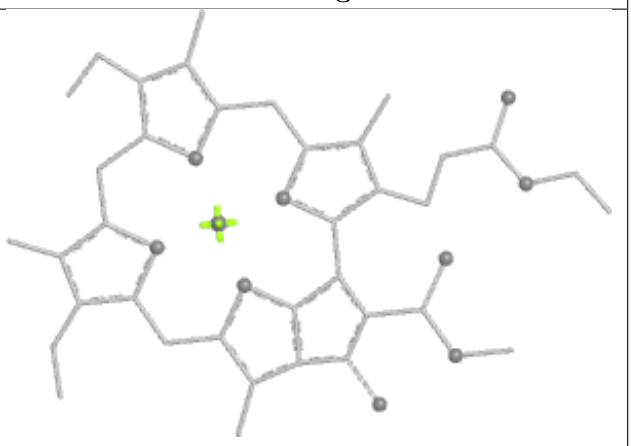
Bond lengths



Bond angles

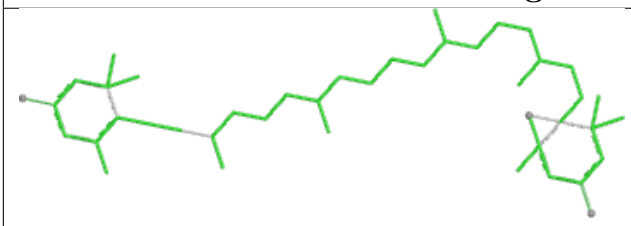


Torsions



Rings

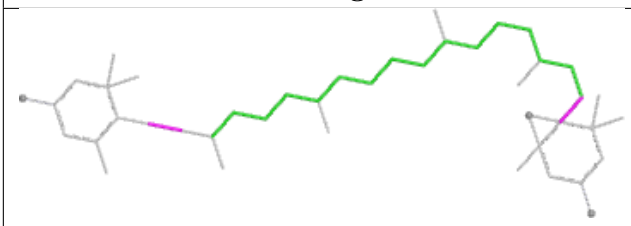
Ligand DD6 C 312



Bond lengths



Bond angles

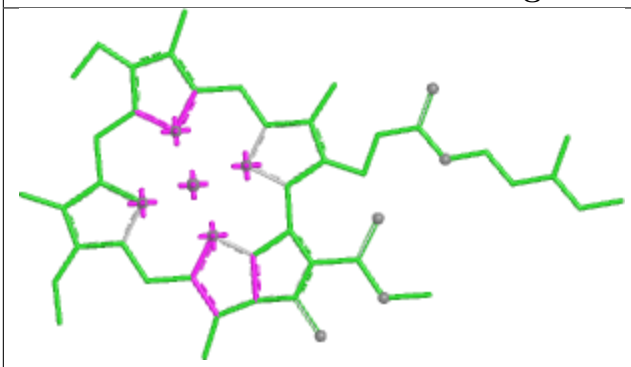


Torsions

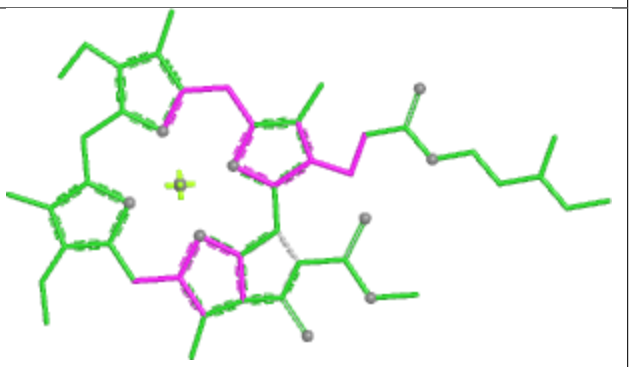


Rings

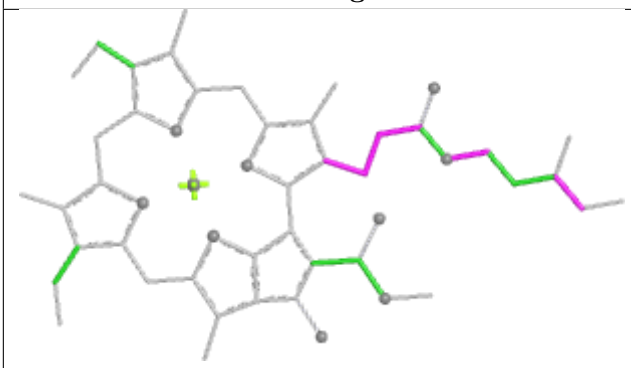
Ligand CLA R 304



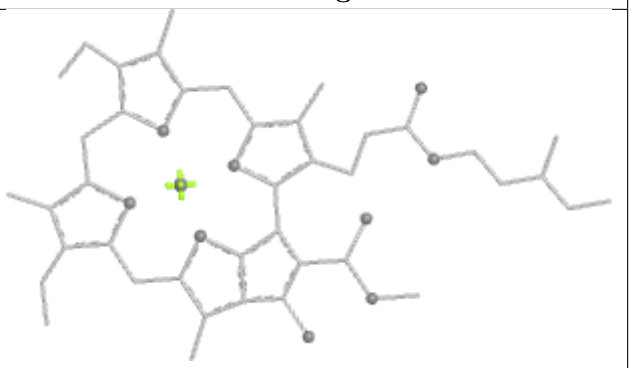
Bond lengths



Bond angles

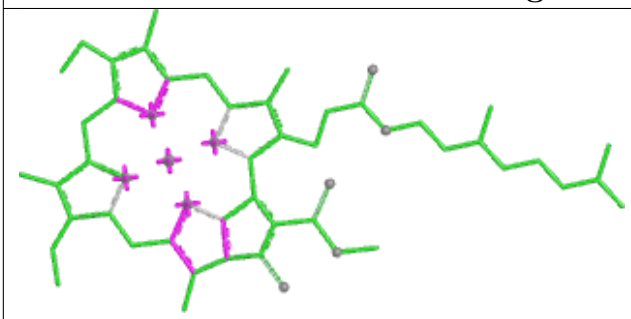


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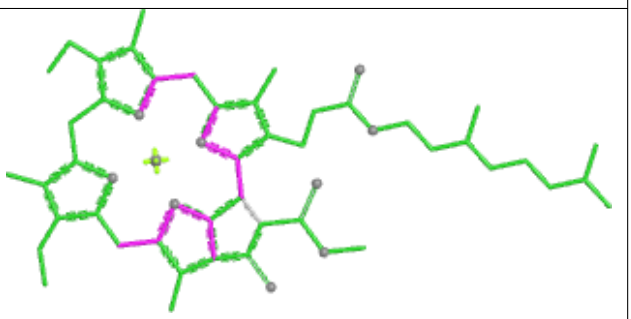


Rings

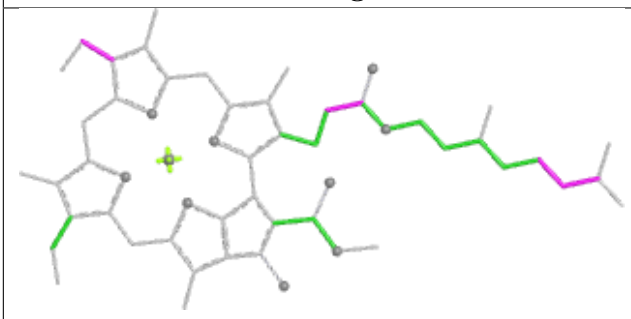
Ligand CLA Z 305



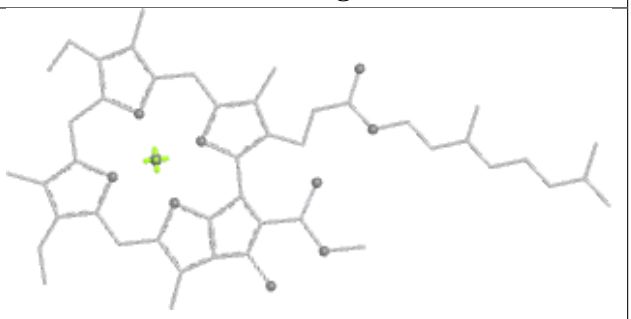
Bond lengths



Bond angles

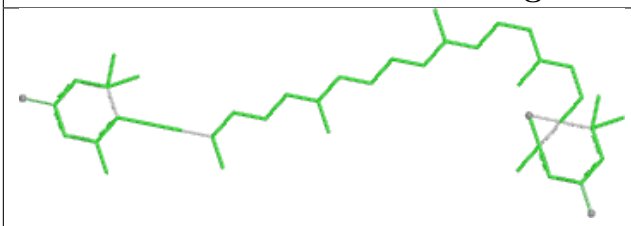


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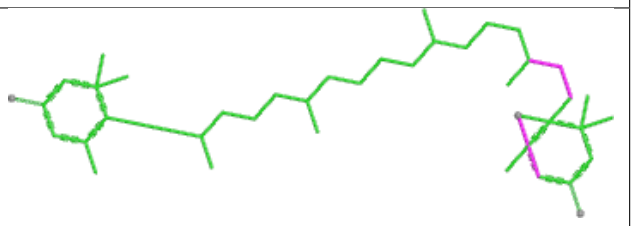


Rings

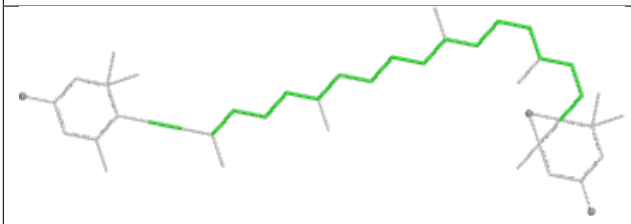
Ligand DD6 D 313



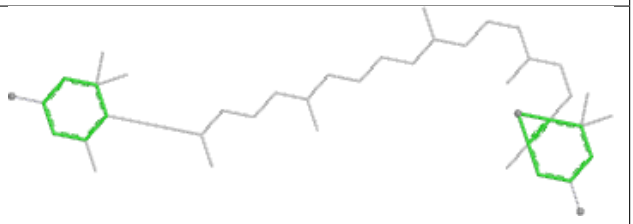
Bond lengths



Bond angles

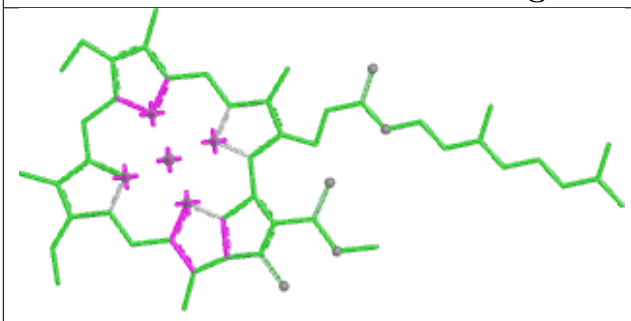


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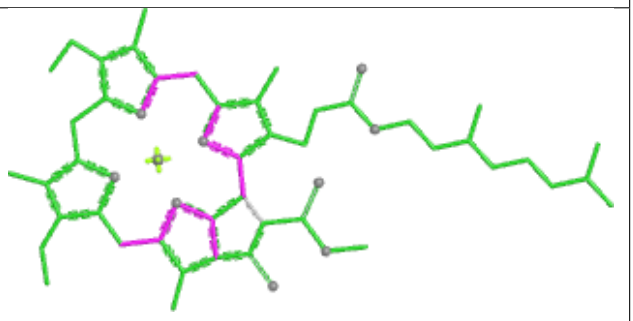


Rings

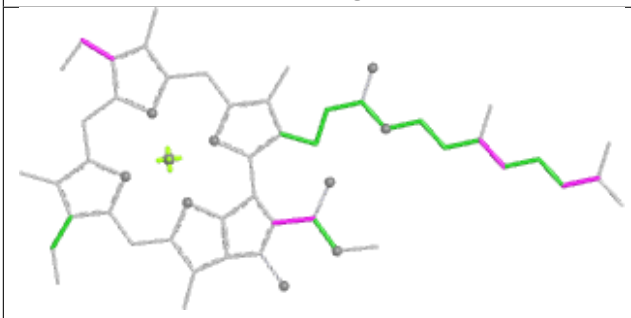
Ligand CLA a 837



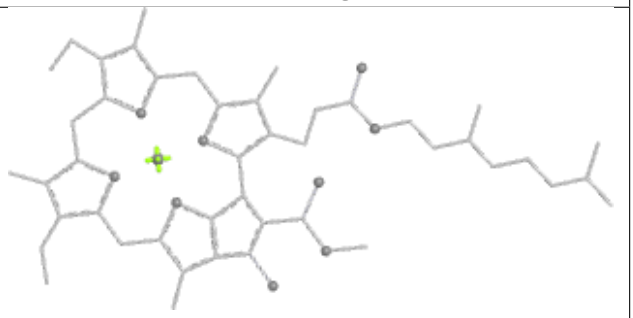
Bond lengths



Bond angles

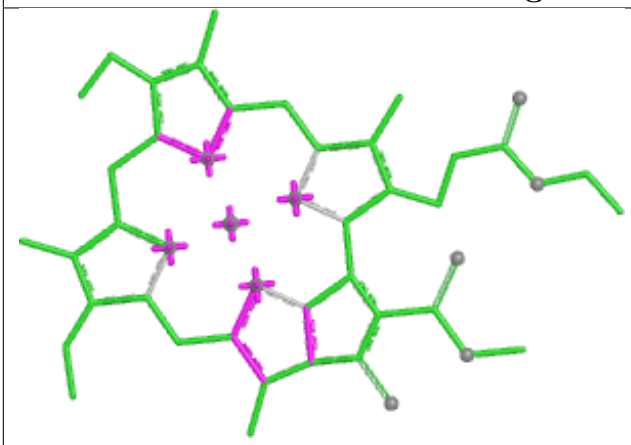


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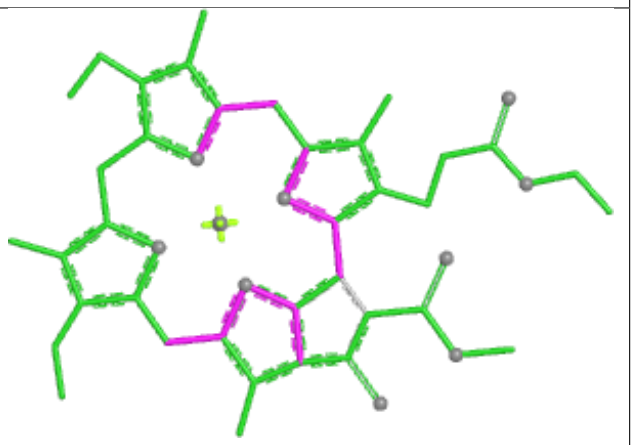


Rings

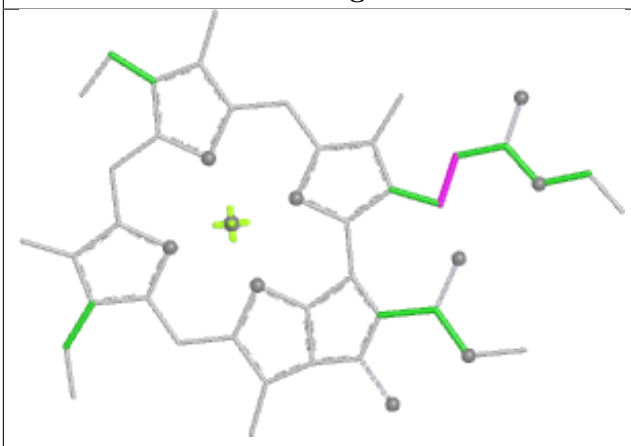
Ligand CLA E 313



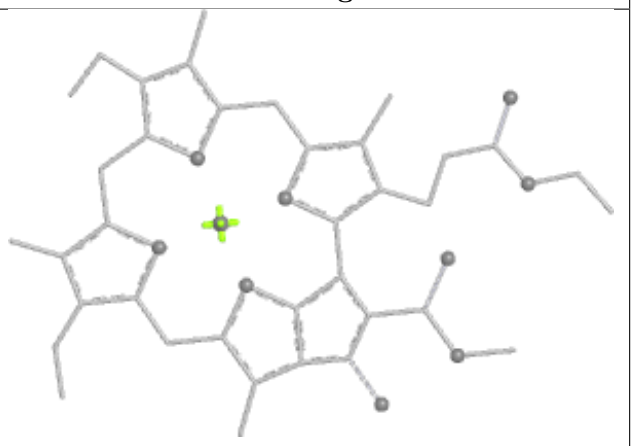
Bond lengths



Bond angles

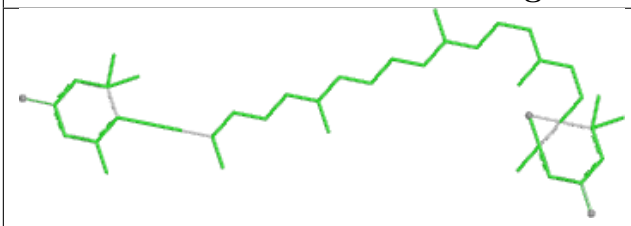


Torsions



Rings

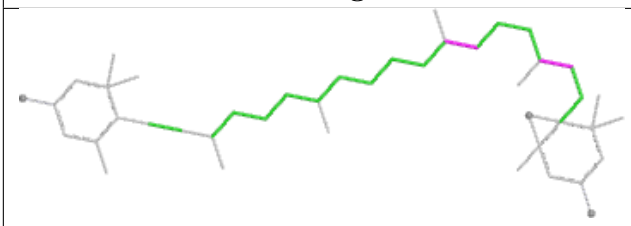
Ligand DD6 D 314



Bond lengths



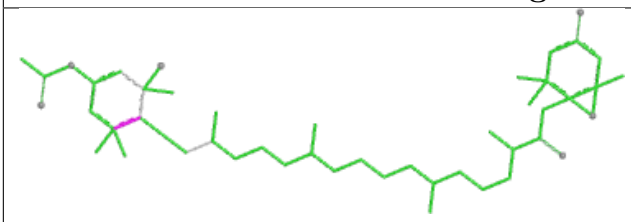
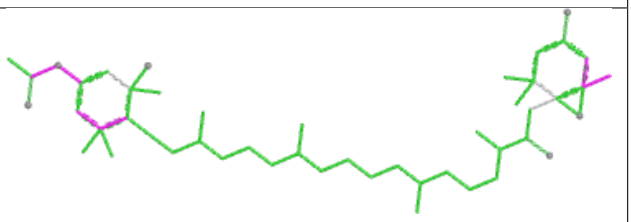
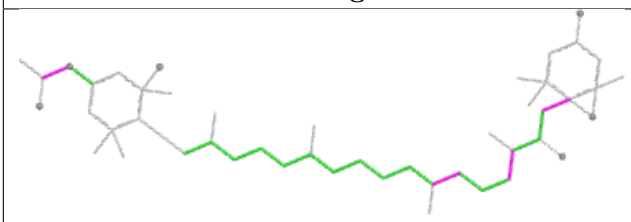
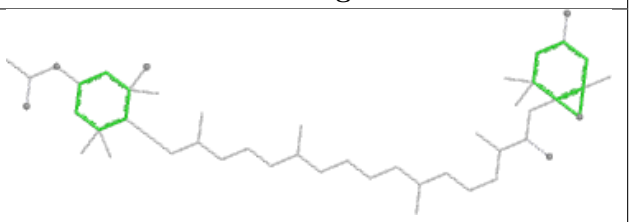
Bond angles

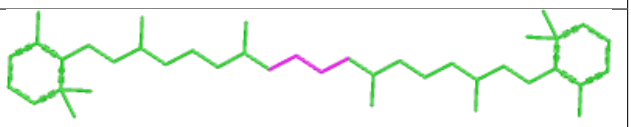
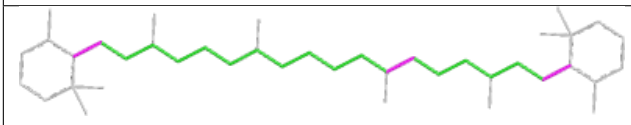
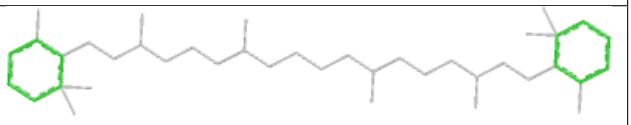


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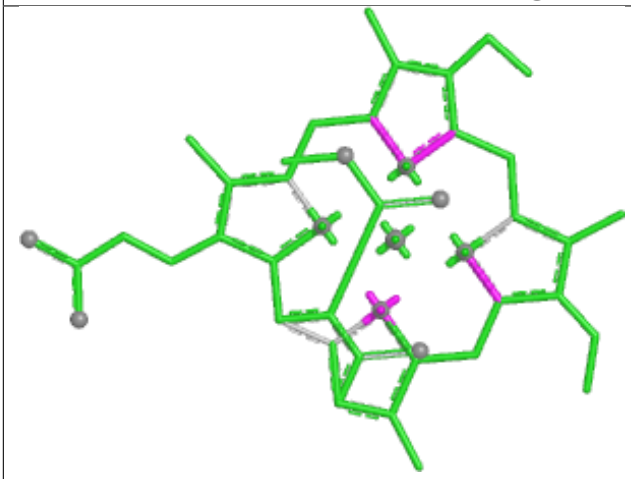


Rings

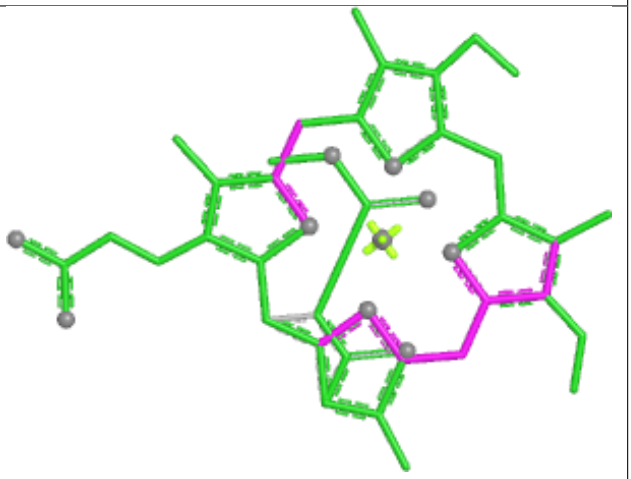
Ligand A86 Y 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR l 208	
 Bond lengths	 Bond angles
 Torsions	 Rings

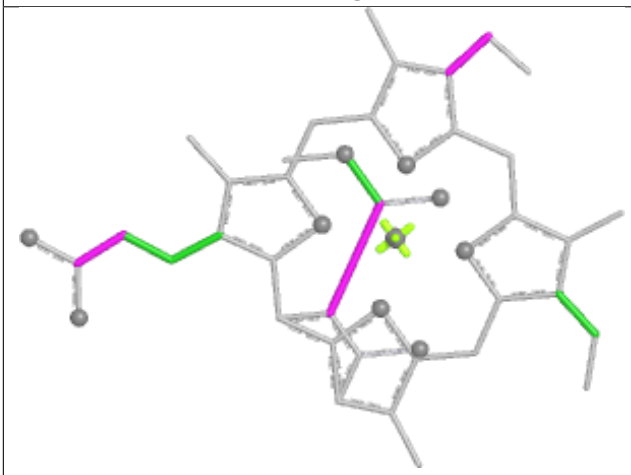
Ligand KC2 L 303



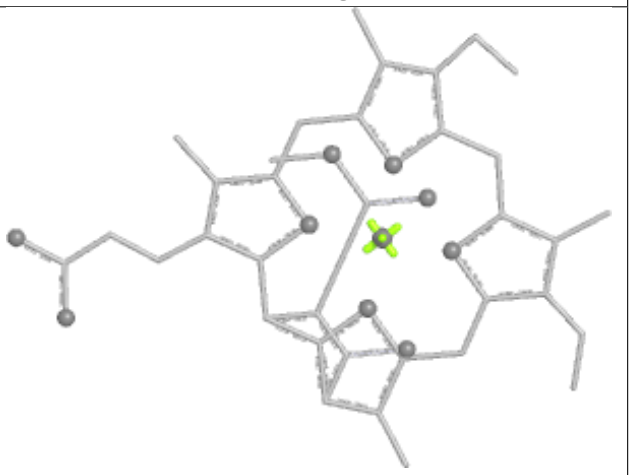
Bond lengths



Bond angles

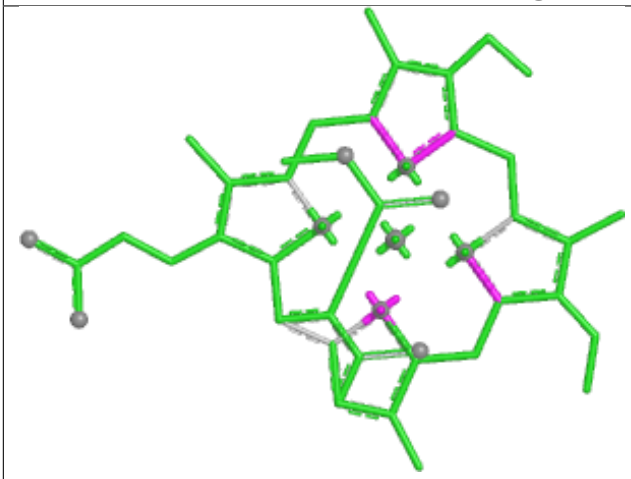


Torsions

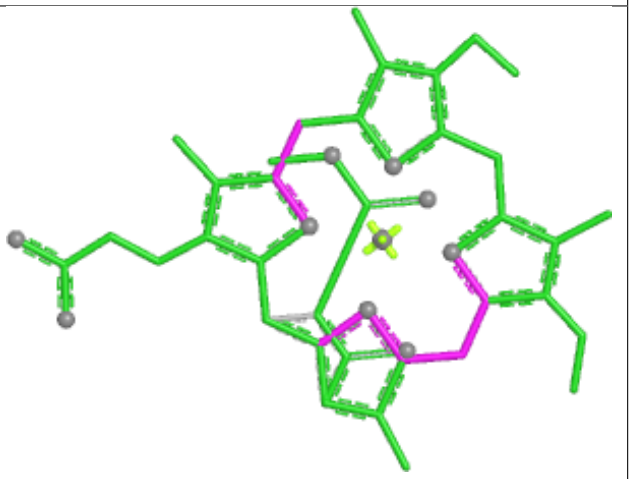


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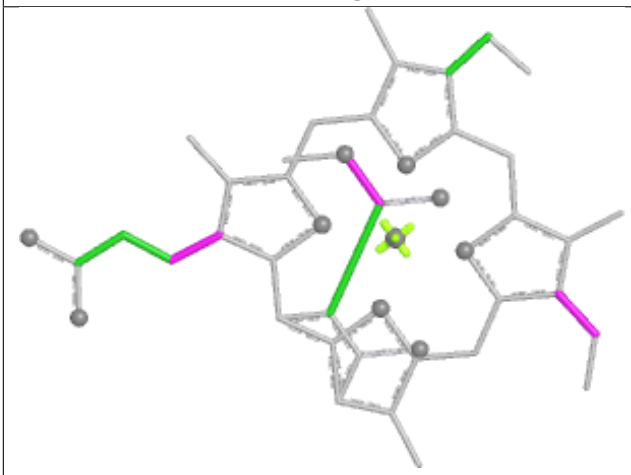
Ligand KC2 o 302



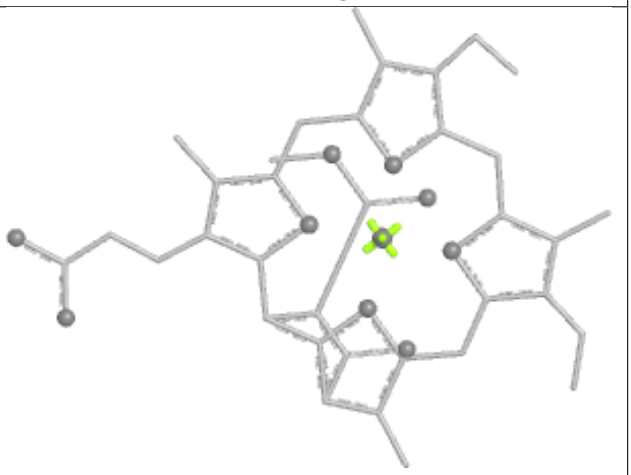
Bond lengths



Bond angles

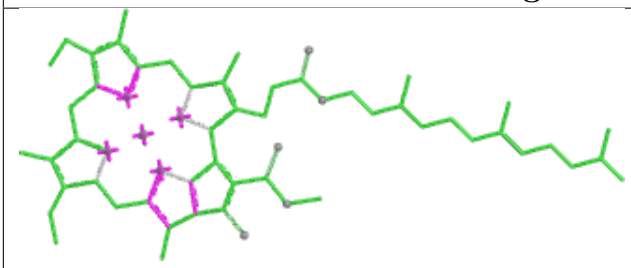


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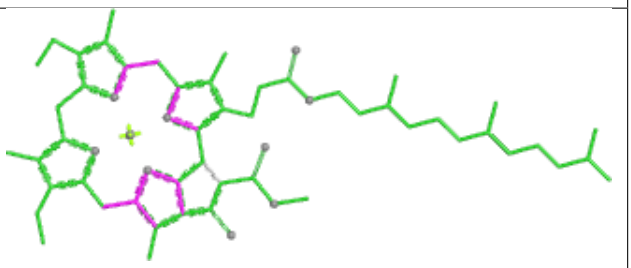


Rings

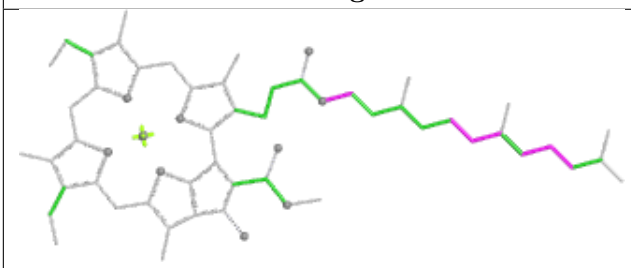
Ligand CLA K 304



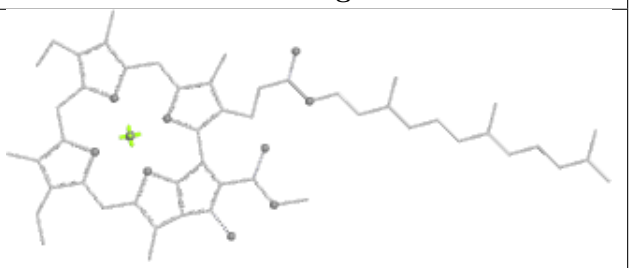
Bond lengths



Bond angles

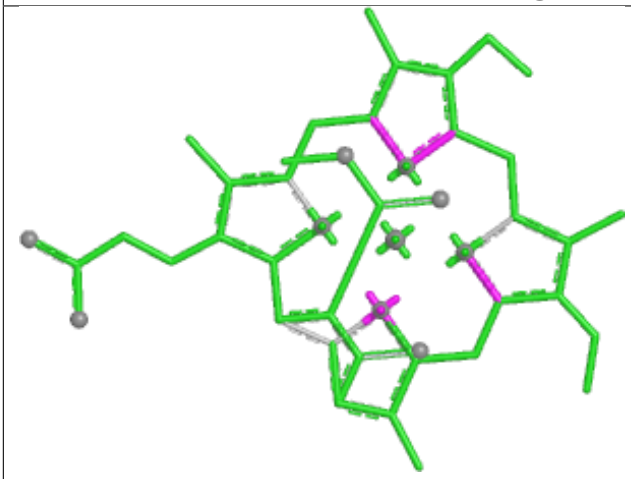


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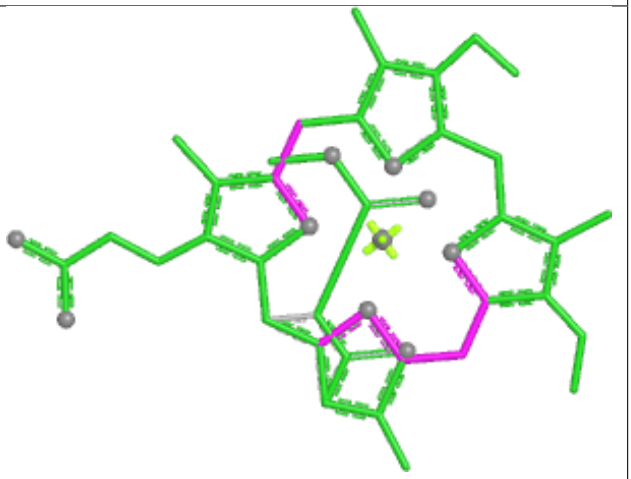


Rings

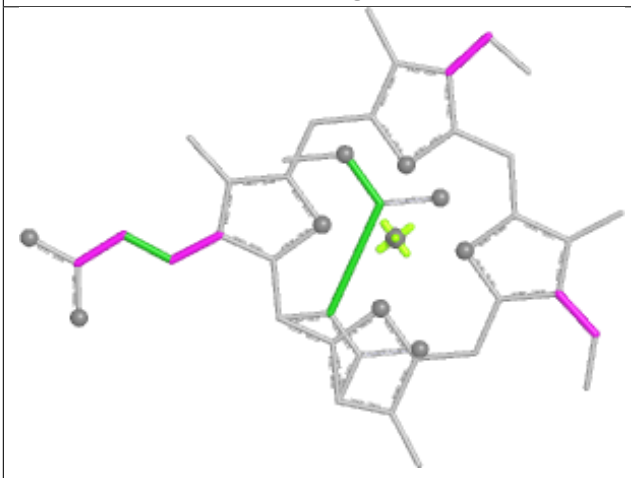
Ligand KC2 z 309



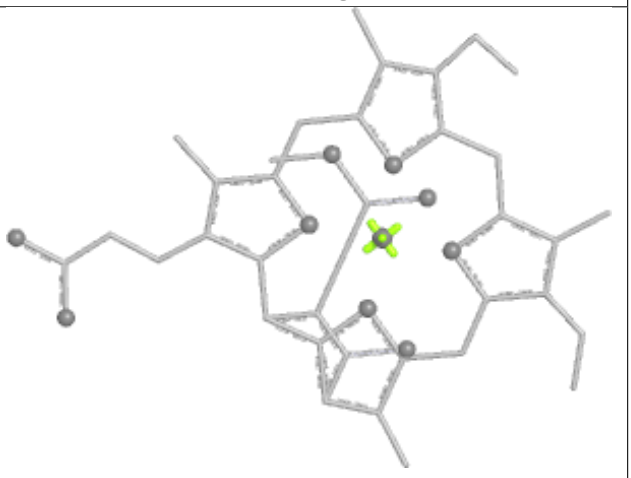
Bond lengths



Bond angles

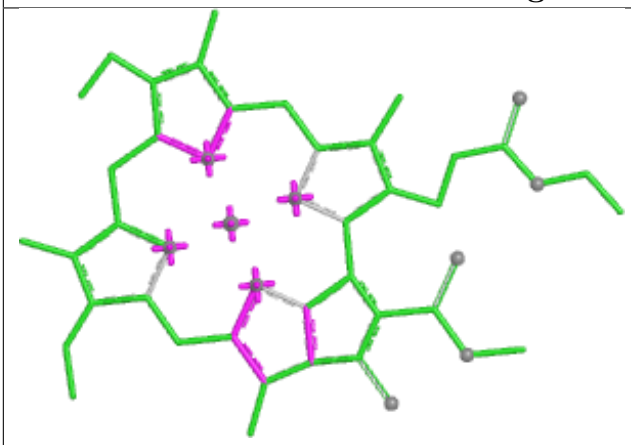


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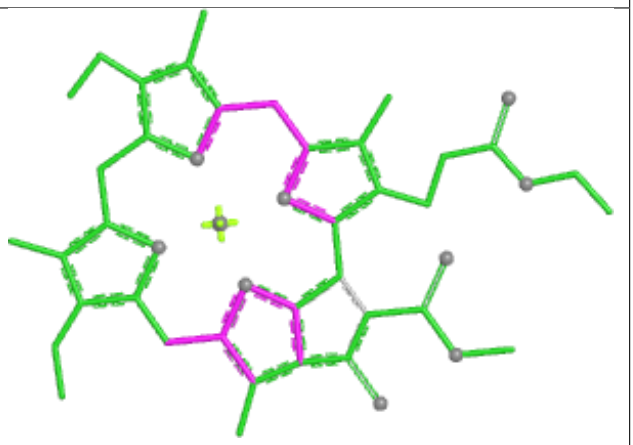


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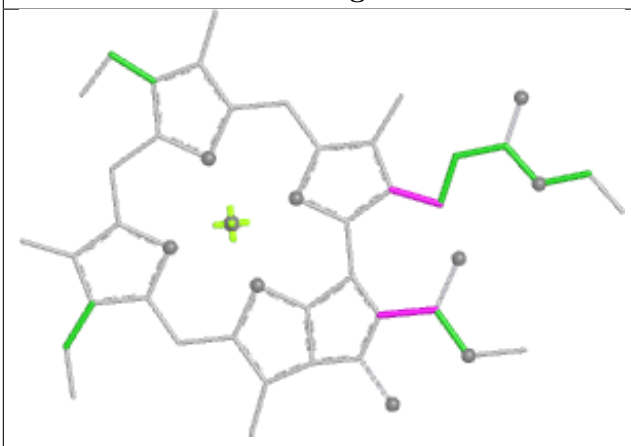
Ligand CLA S 313



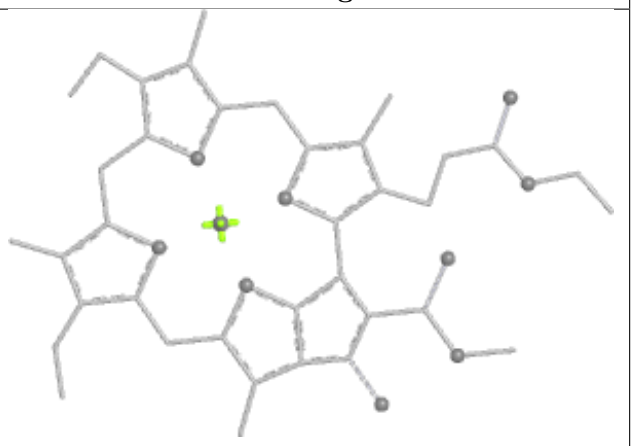
Bond lengths



Bond angles

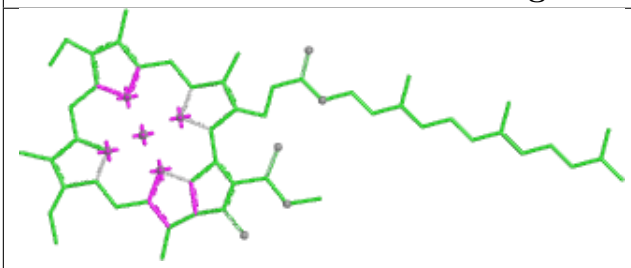


Torsions

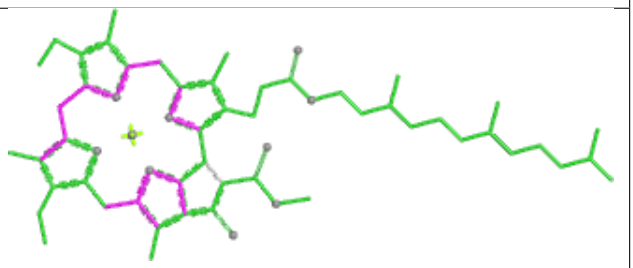


Rings

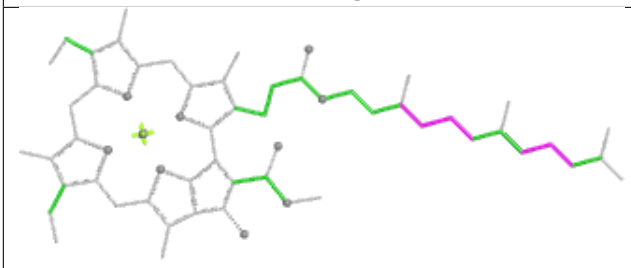
Ligand CLA a 810



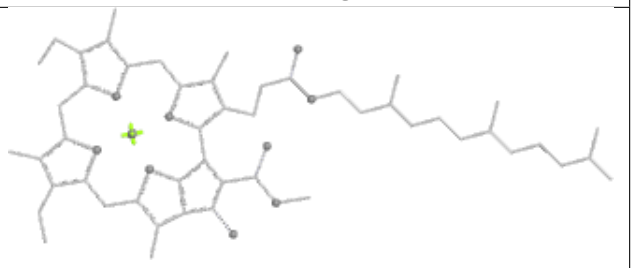
Bond lengths



Bond angles

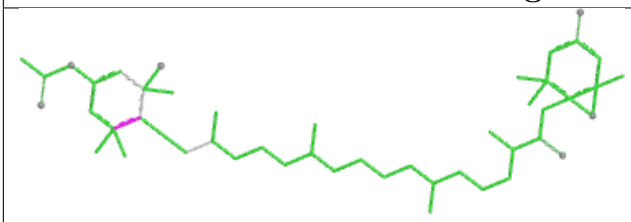


Torsions

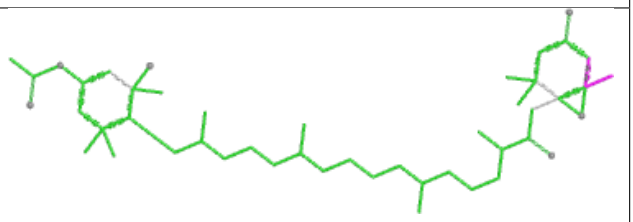


Rings

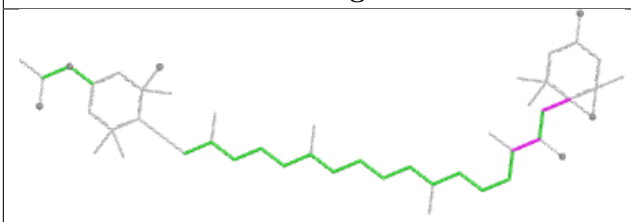
Ligand A86 W 316



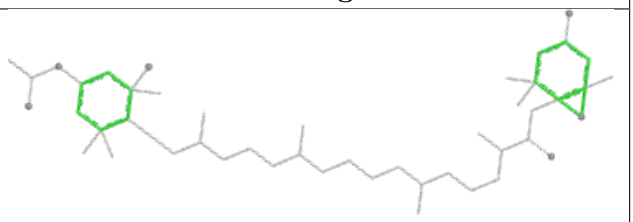
Bond lengths



Bond angles

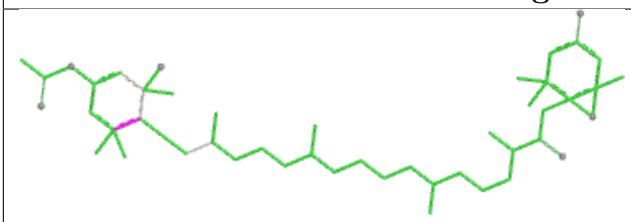


Torsions

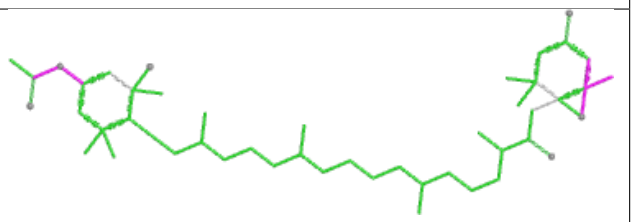


Rings

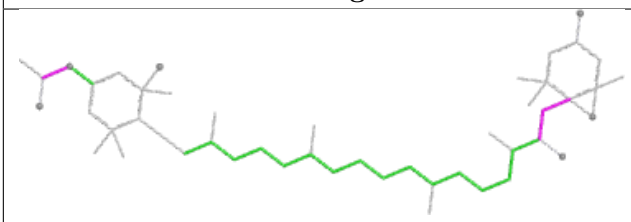
Ligand A86 Z 316



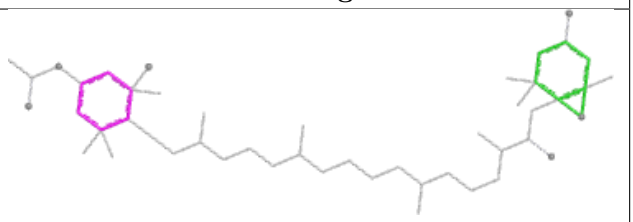
Bond lengths



Bond angles

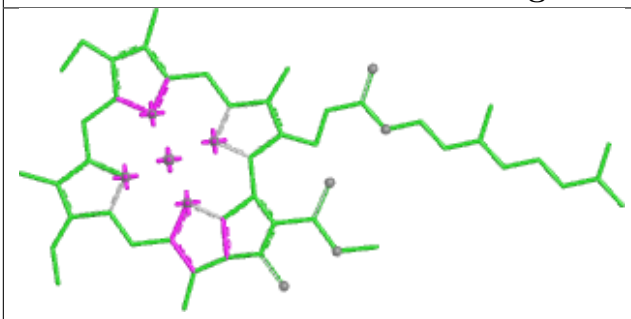


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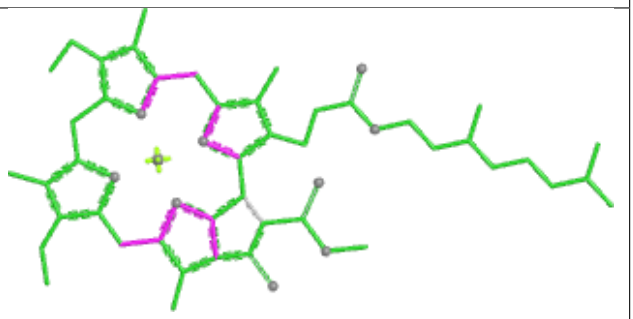


Rings

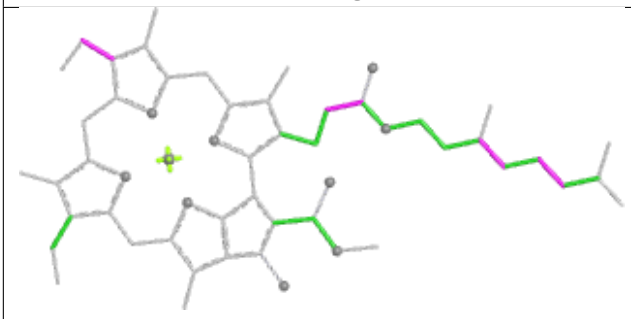
Ligand CLA a 852



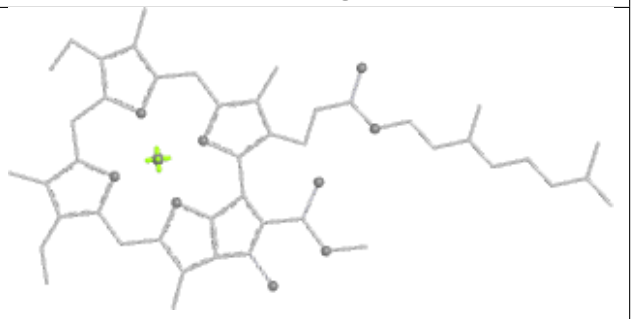
Bond lengths



Bond angles

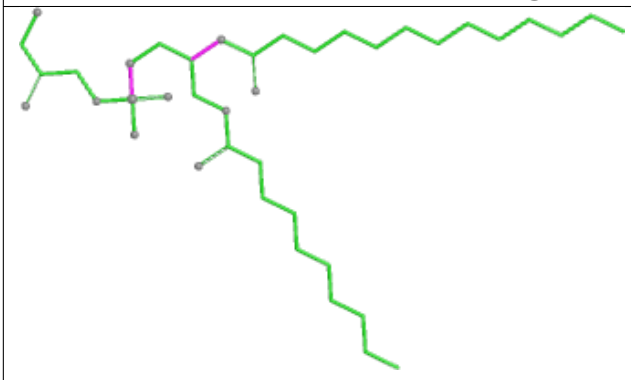


Torsions

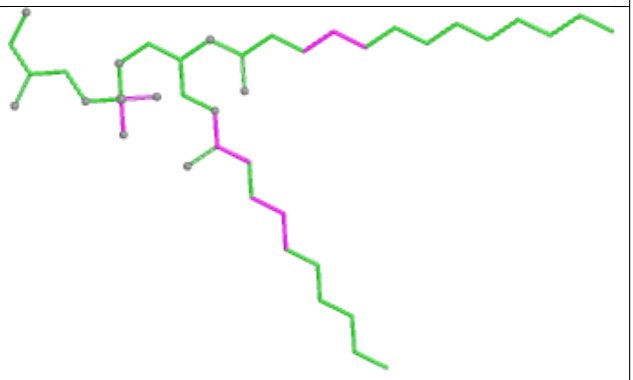


Rings

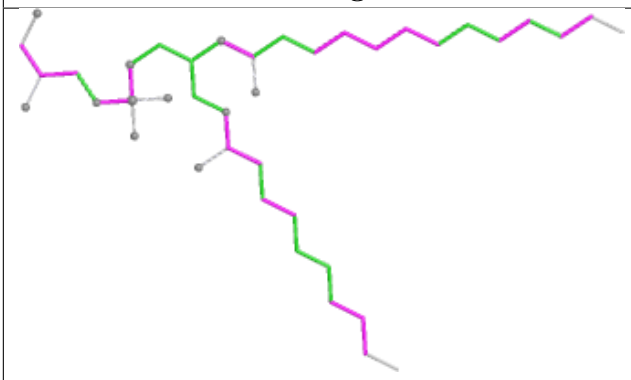
Ligand LHG S 323



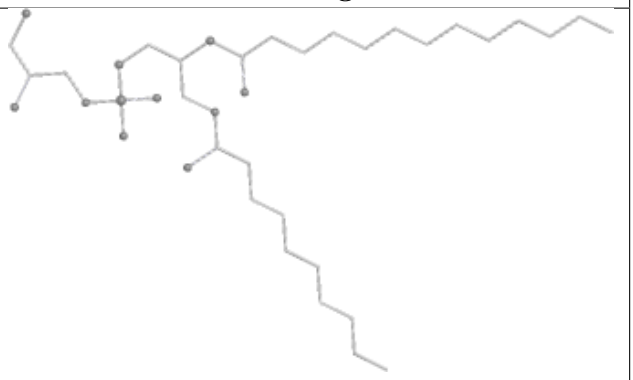
Bond lengths



Bond angles

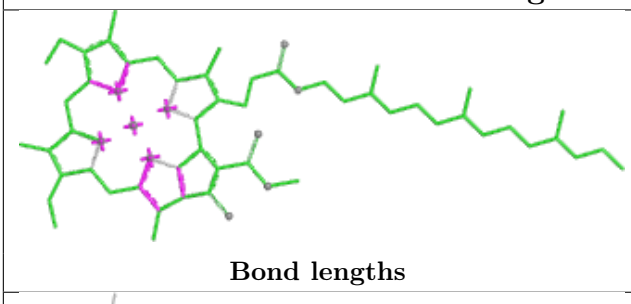


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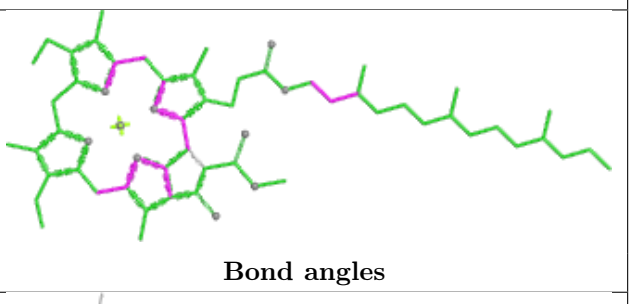


Rings

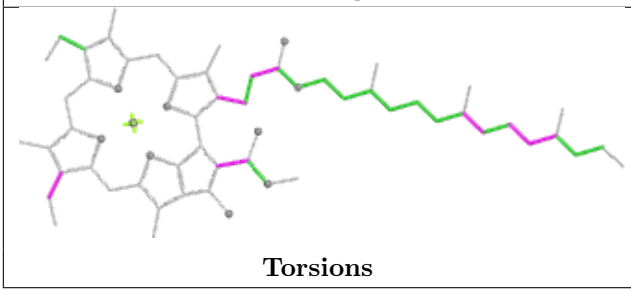
Ligand CLA b 818



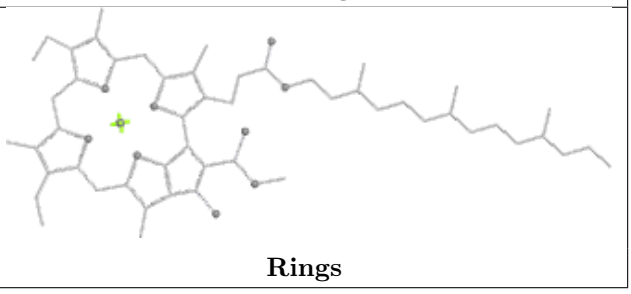
Bond lengths



Bond angles

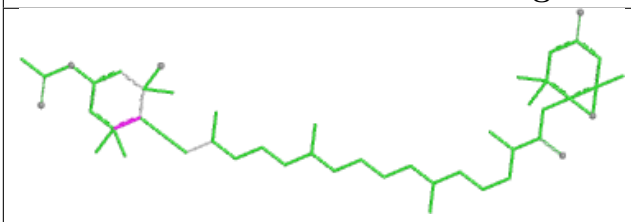


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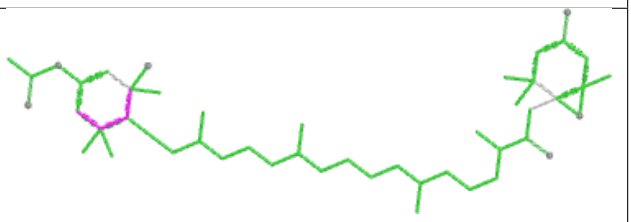


Rings

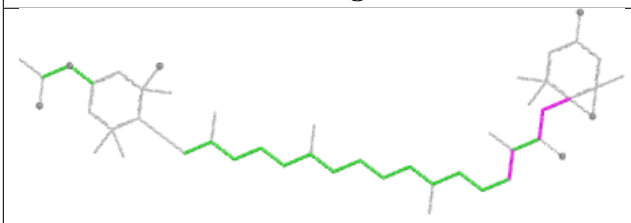
Ligand A86 S 317



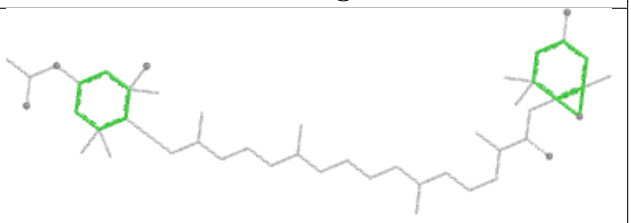
Bond lengths



Bond angles

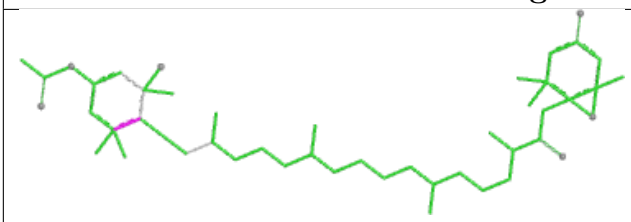


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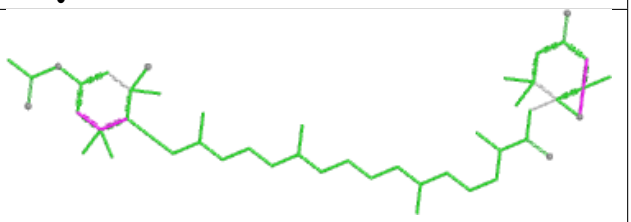


Rings

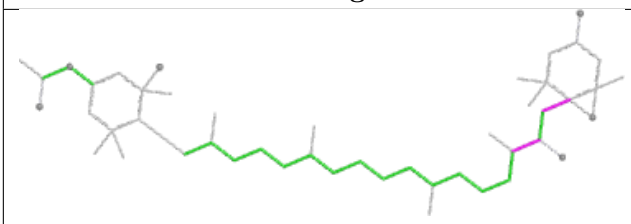
Ligand A86 Q 215



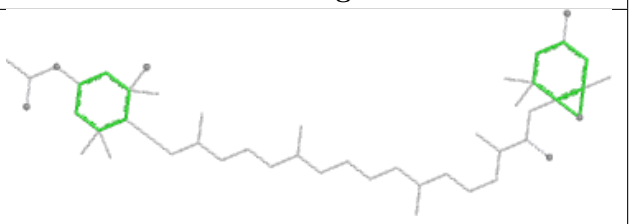
Bond lengths



Bond angles

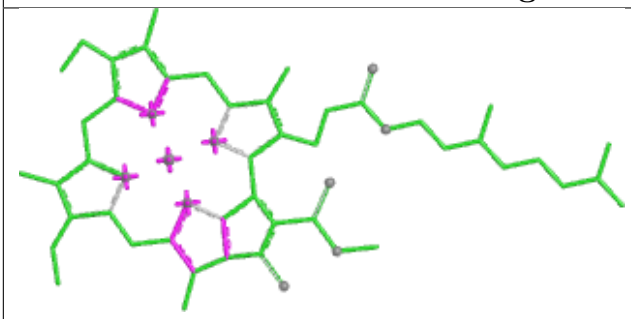


Torsions

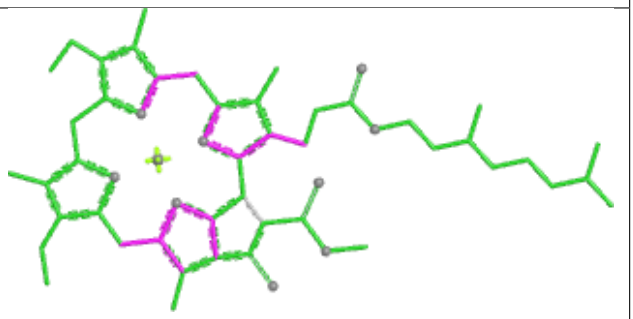


Rings

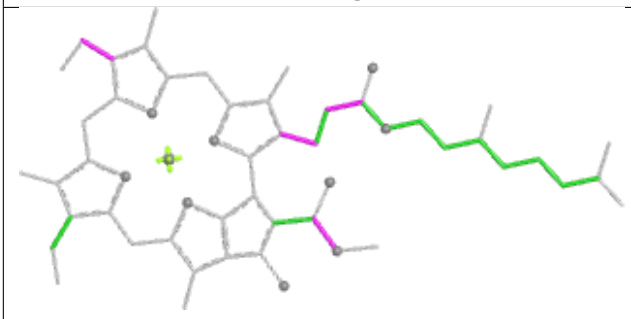
Ligand CLA W 311



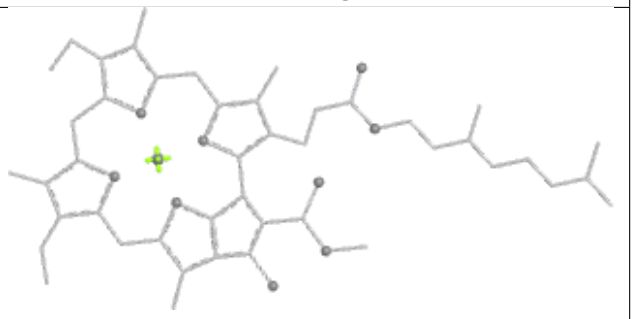
Bond lengths



Bond angles

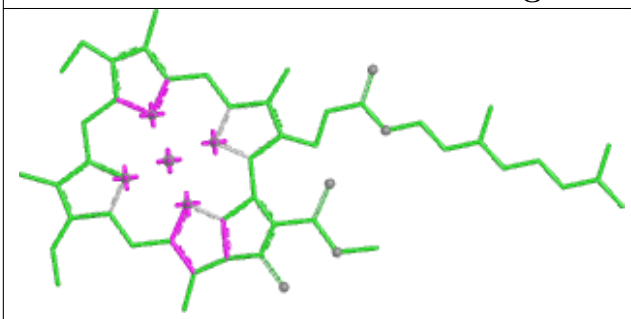


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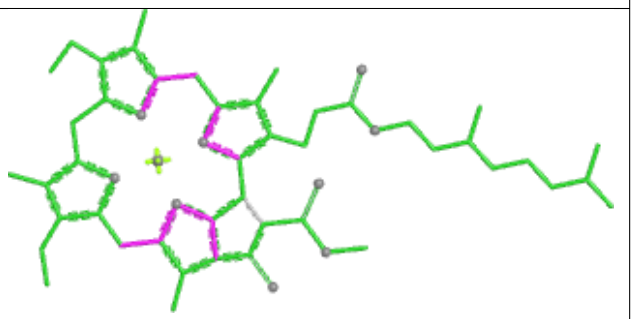


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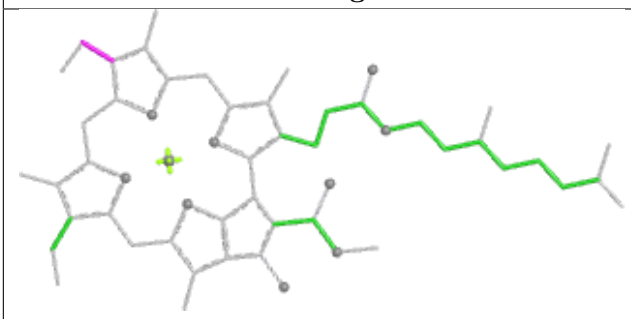
Ligand CLA A 308



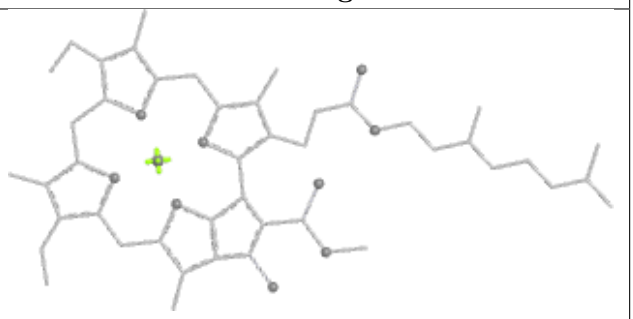
Bond lengths



Bond angles

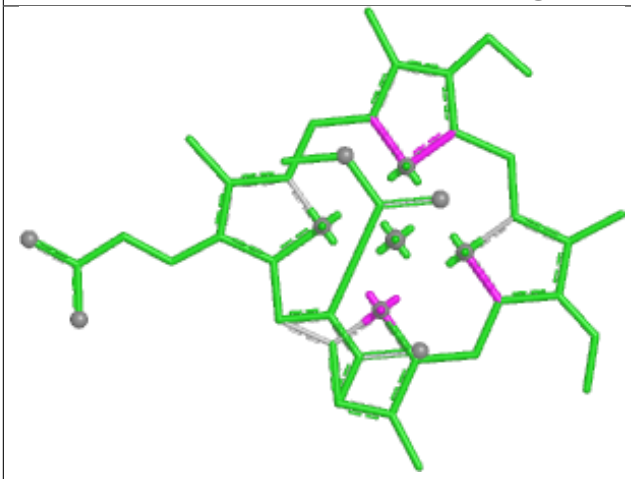


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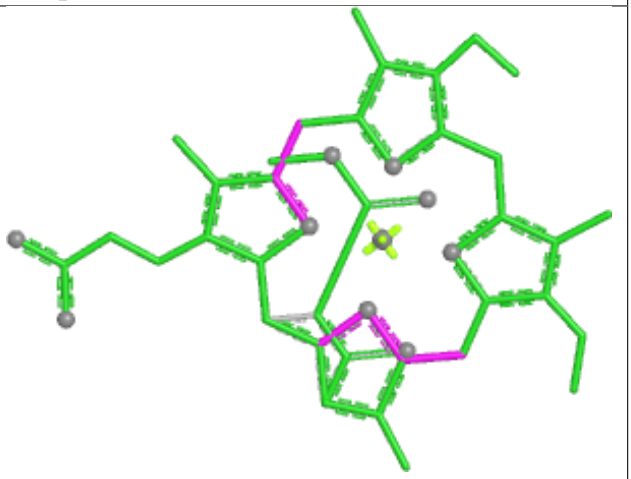


Rings

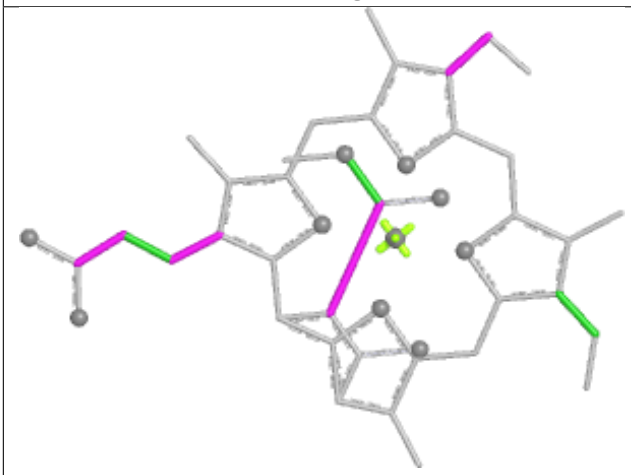
Ligand KC2 q 303



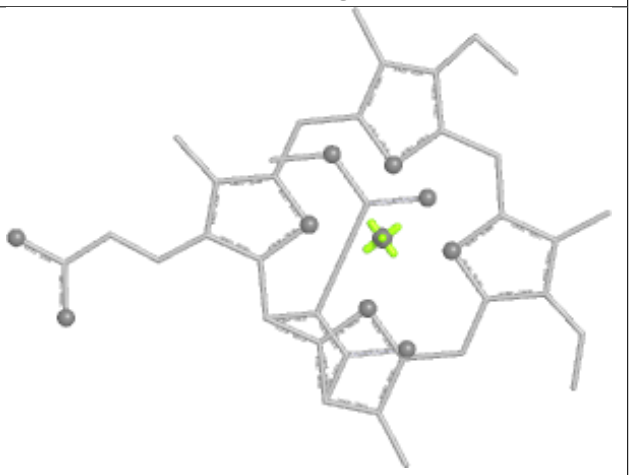
Bond lengths



Bond angles

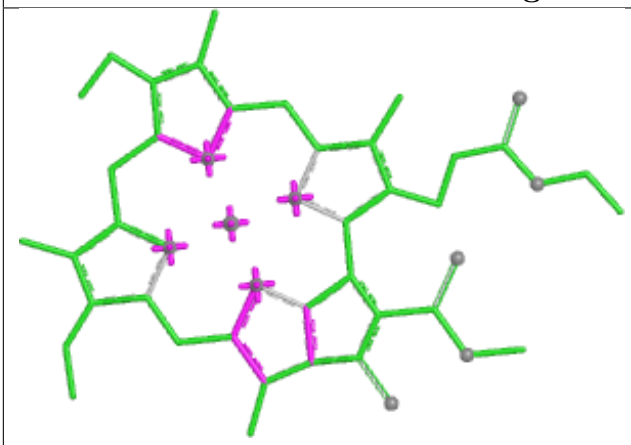


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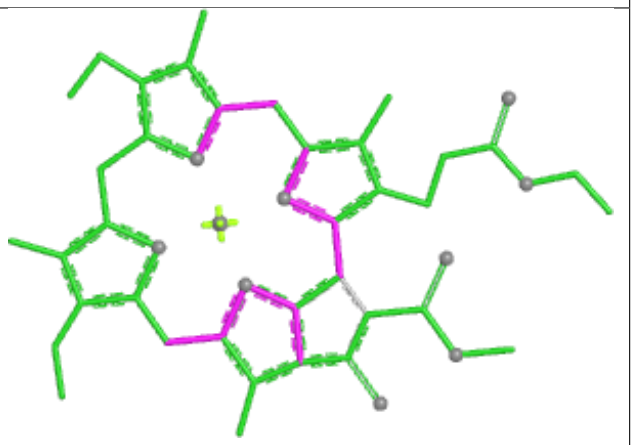


Rings

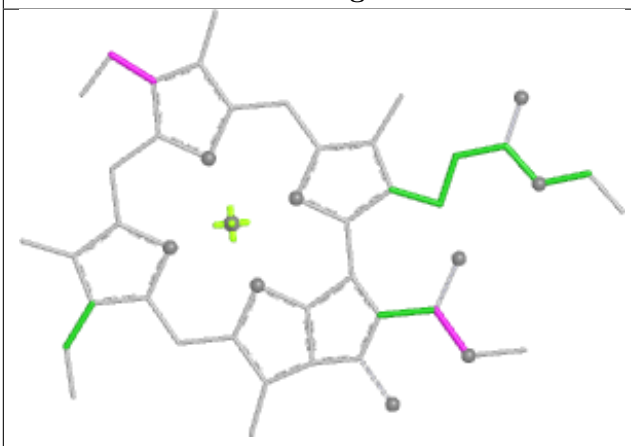
Ligand CLA G 201



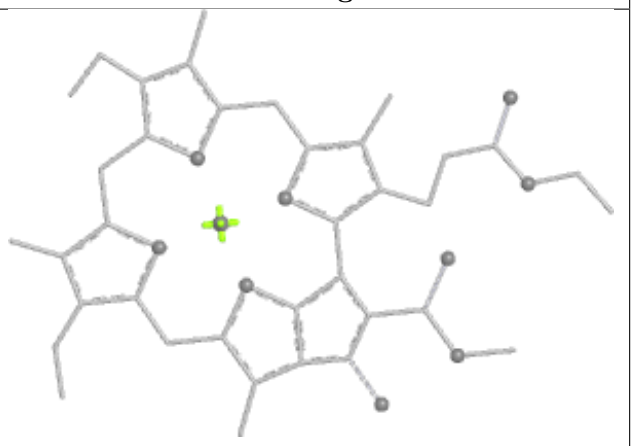
Bond lengths



Bond angles

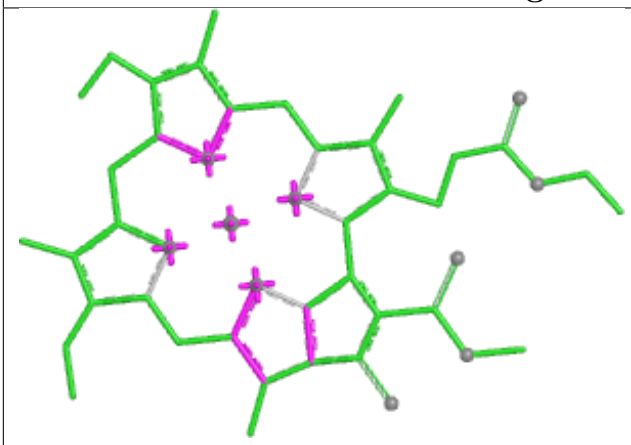


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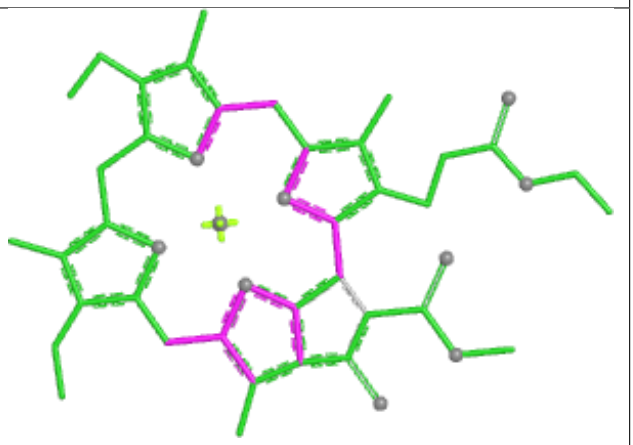


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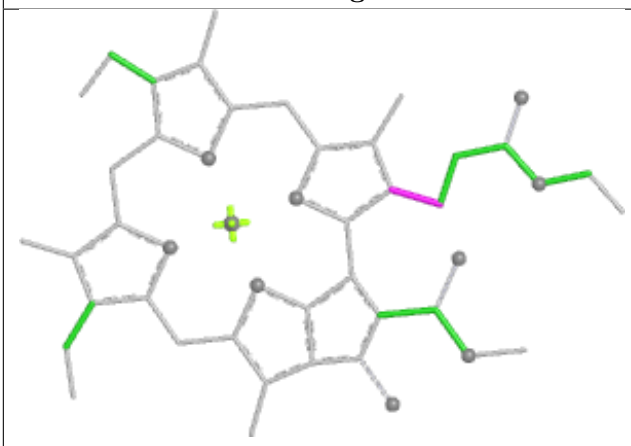
Ligand CLA L 312



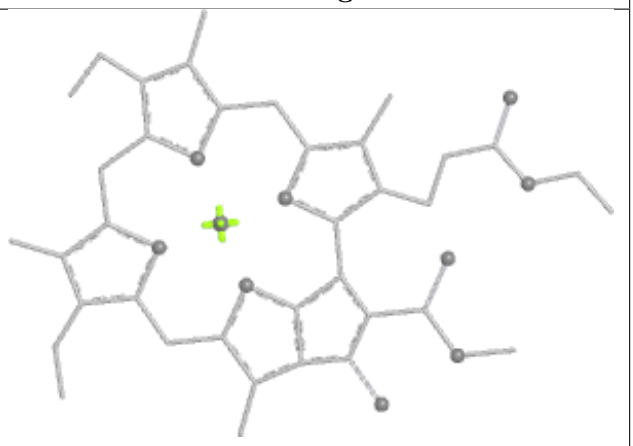
Bond lengths



Bond angles

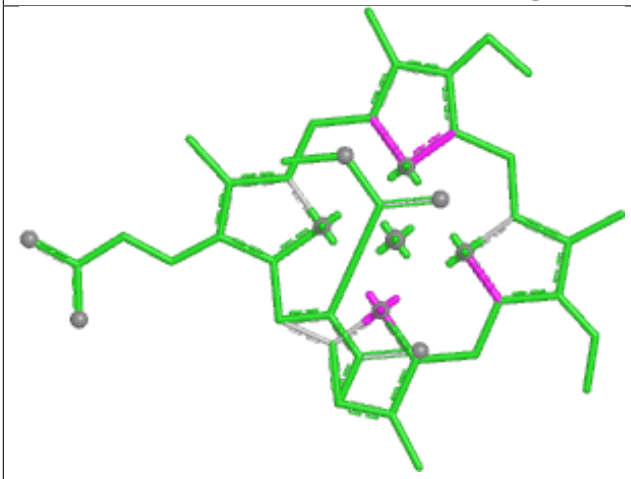


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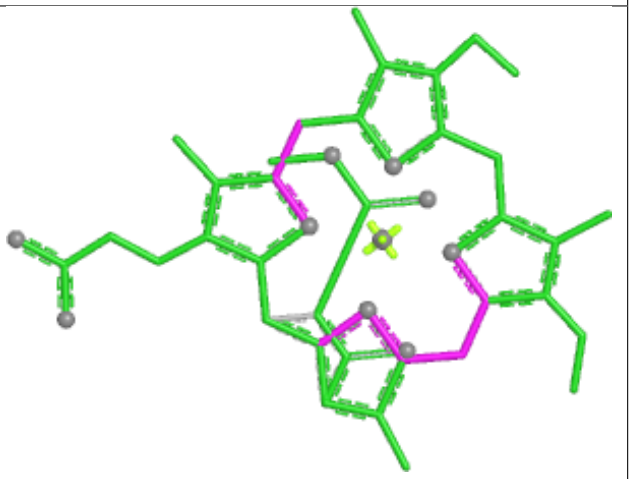


Rings

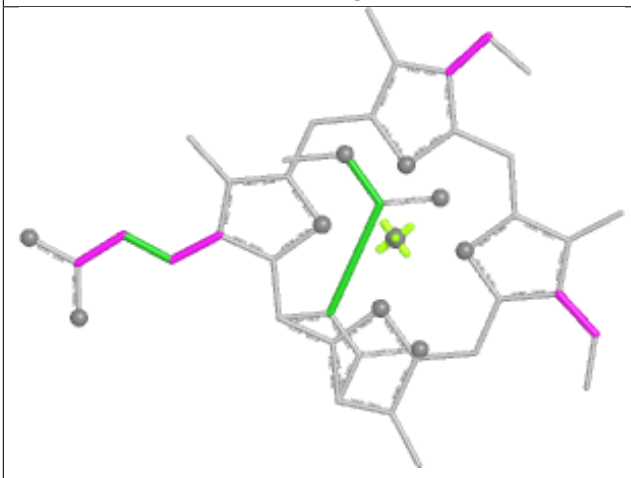
Ligand KC2 P 310



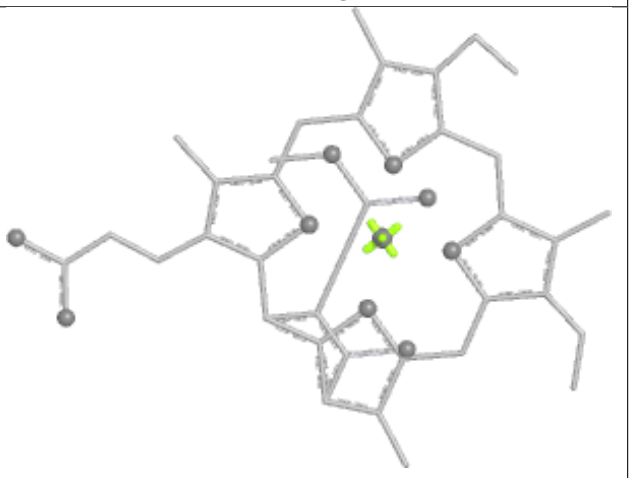
Bond lengths



Bond angles

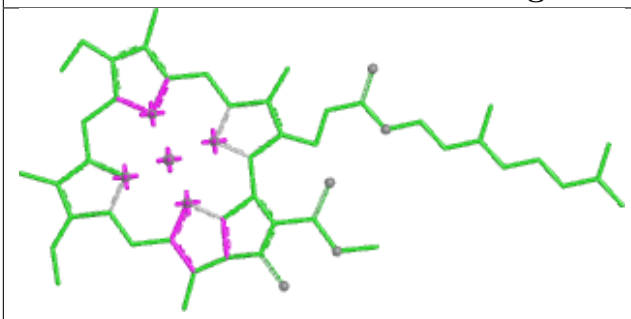


Torsions

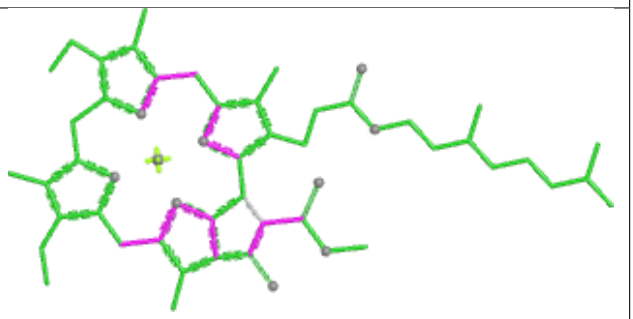


Rings

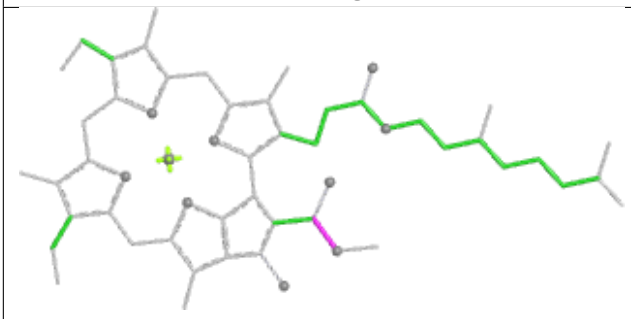
Ligand CLA u 313



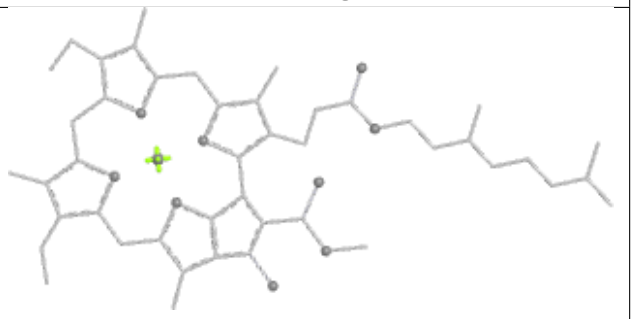
Bond lengths



Bond angles

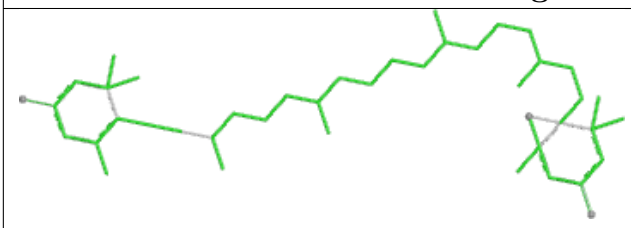


Torsions

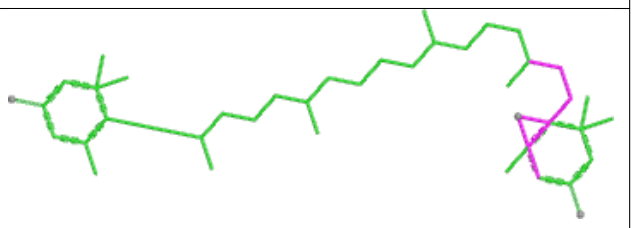


Rings

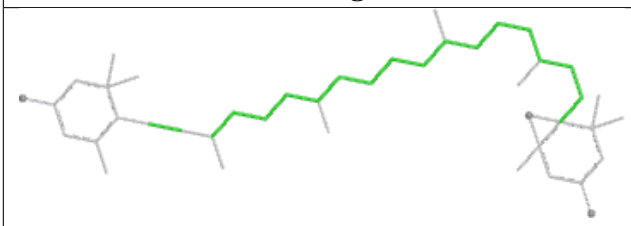
Ligand DD6 t 312



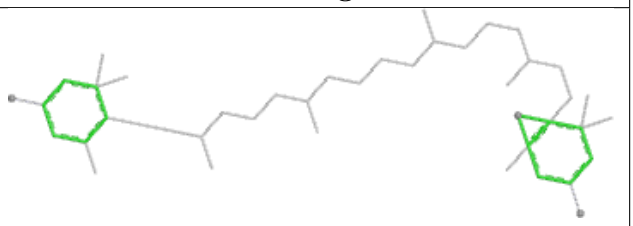
Bond lengths



Bond angles

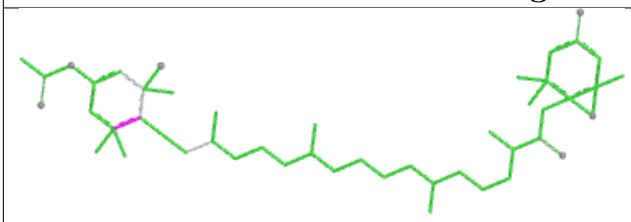


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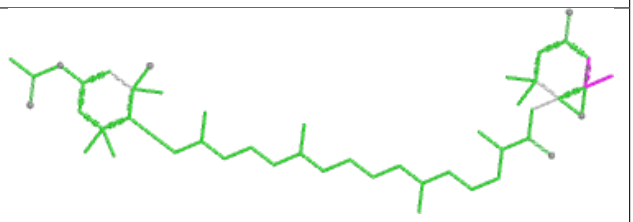


Rings

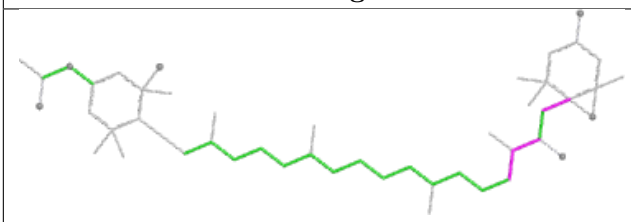
Ligand A86 O 315



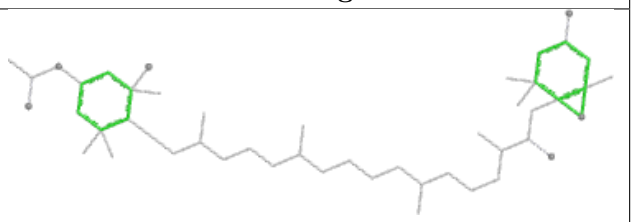
Bond lengths



Bond angles

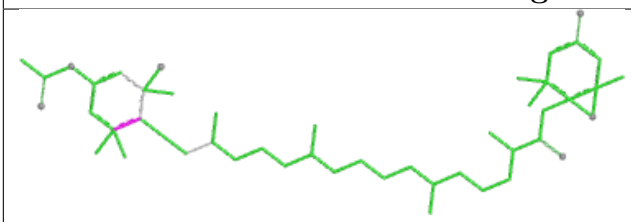


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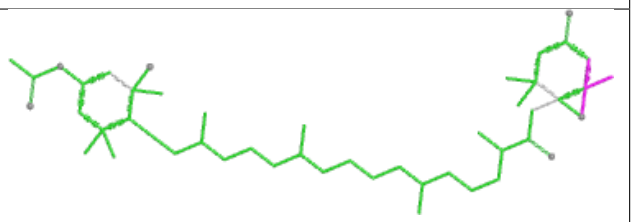


Rings

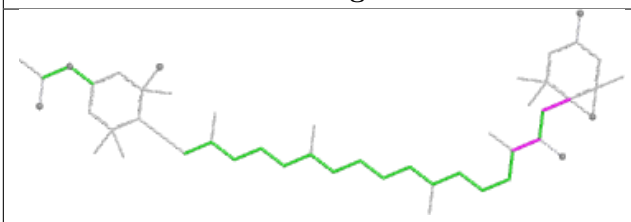
Ligand A86 T 319



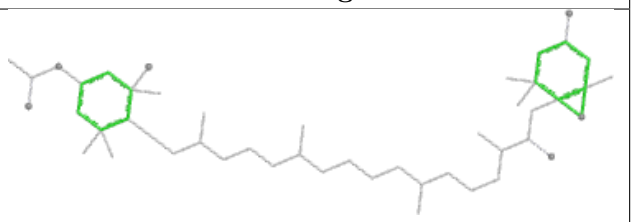
Bond lengths



Bond angles

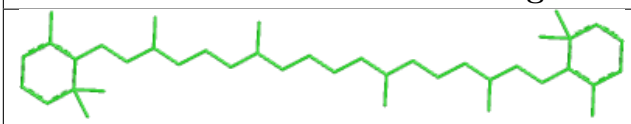


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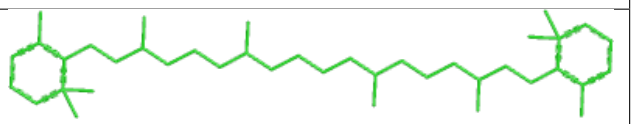


Rings

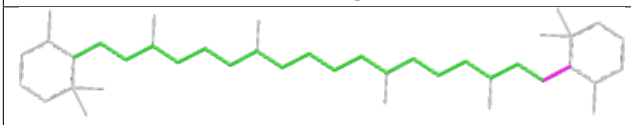
Ligand BCR a 845



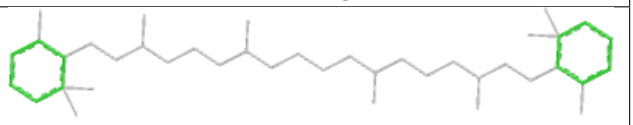
Bond lengths



Bond angles

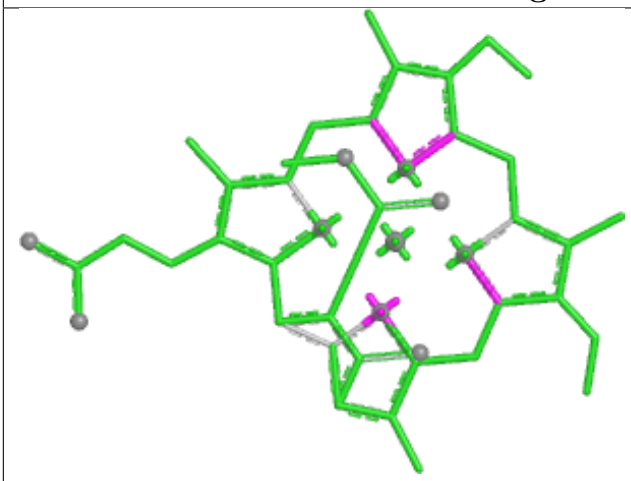


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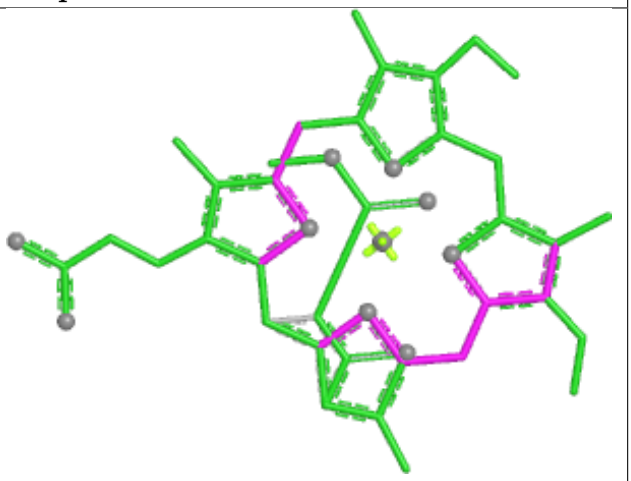


Rings

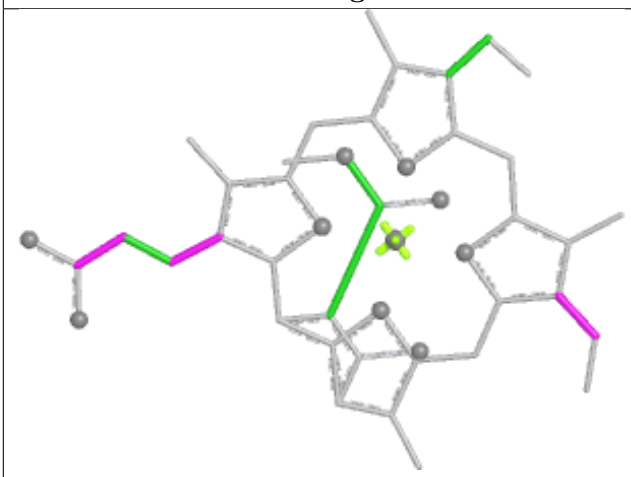
Ligand KC2 q 302



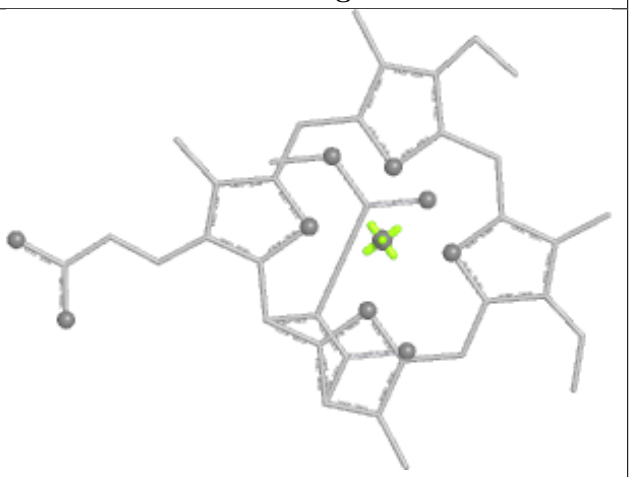
Bond lengths



Bond angles

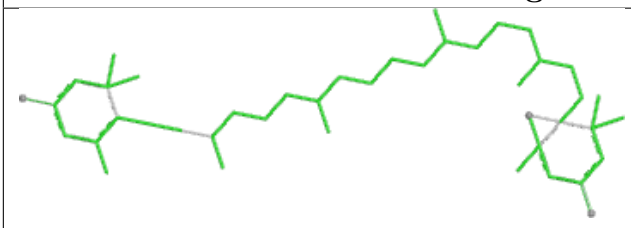


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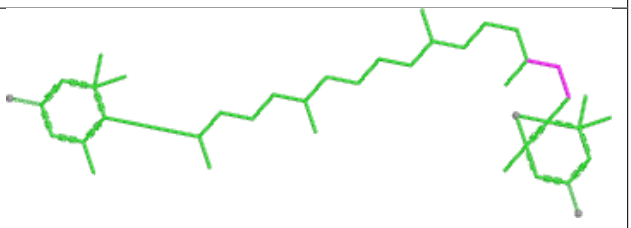


Rings

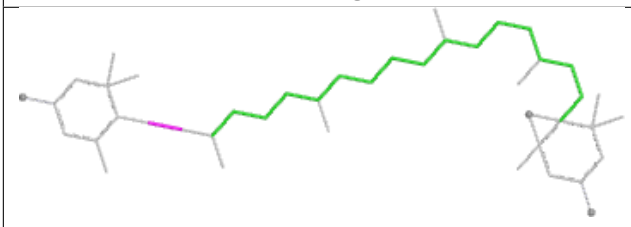
Ligand DD6 T 314



Bond lengths



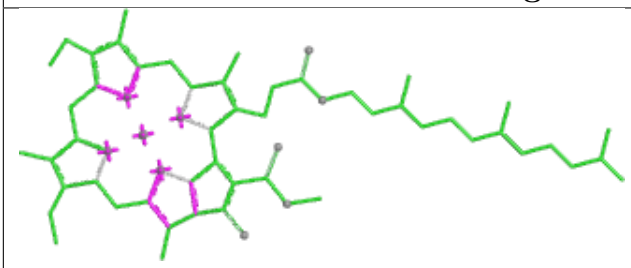
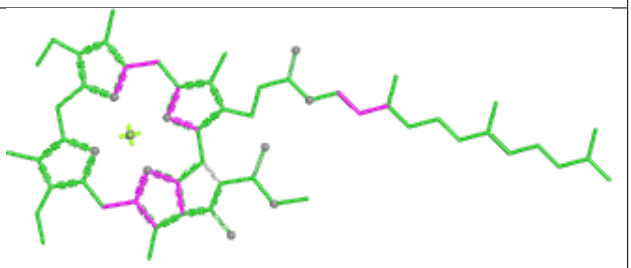
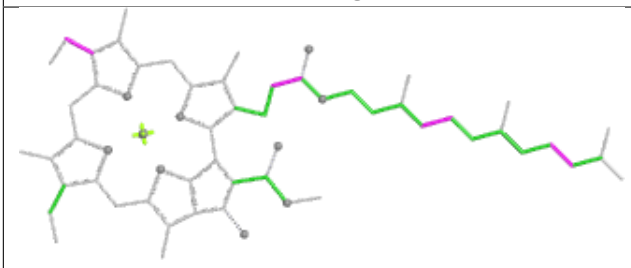
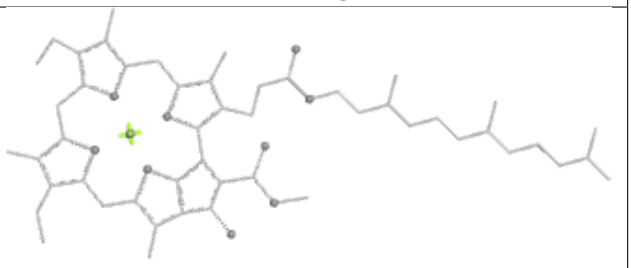
Bond angles

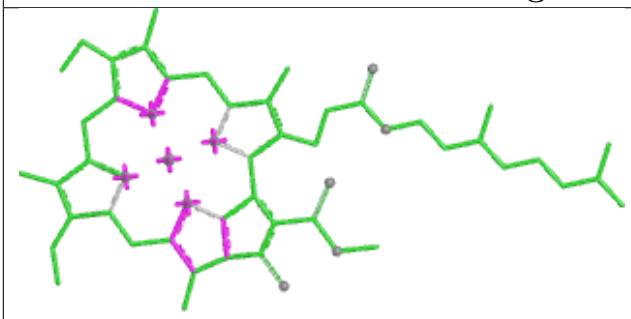
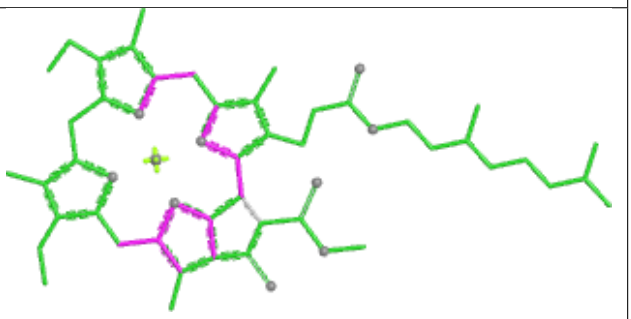
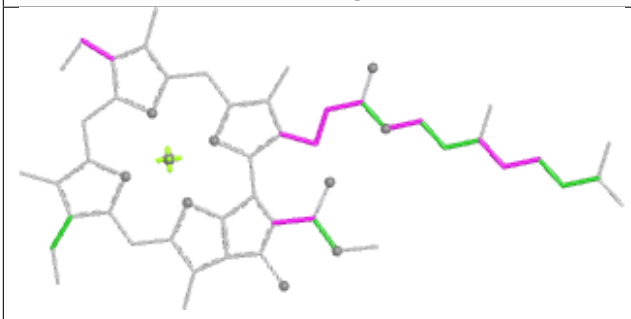
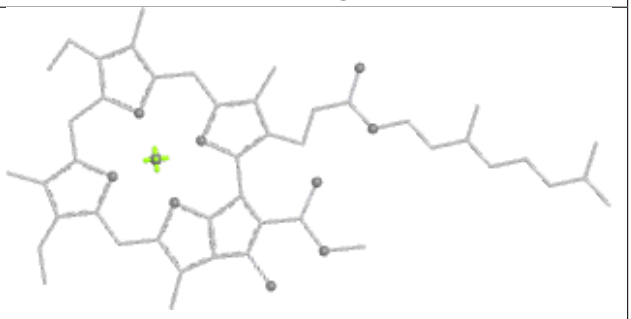


Torsions

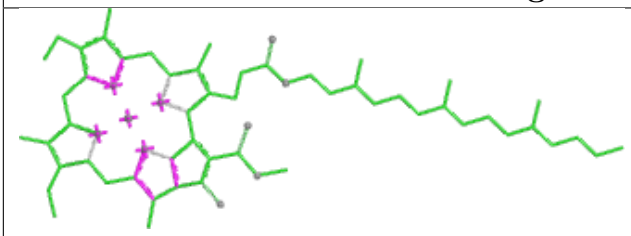


Rings

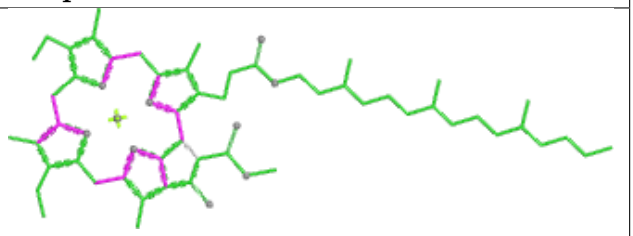
Ligand CLA R 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA S 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

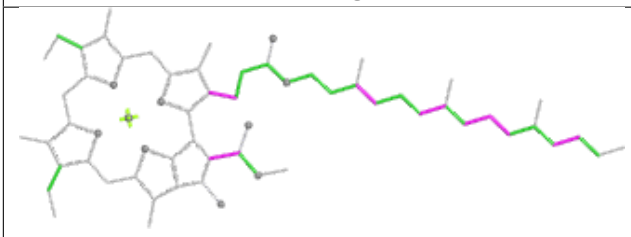
Ligand CLA q 311



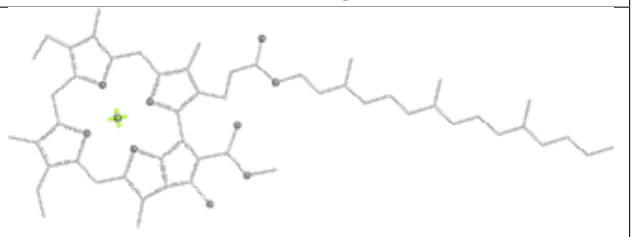
Bond lengths



Bond angles

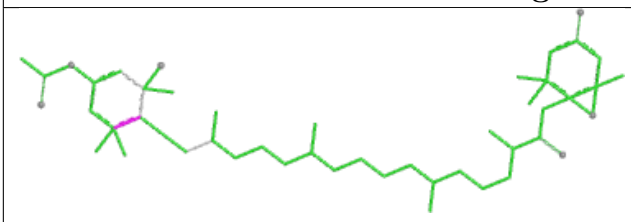


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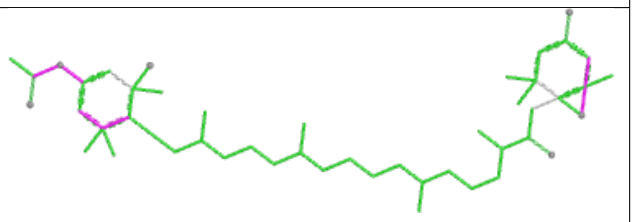


Rings

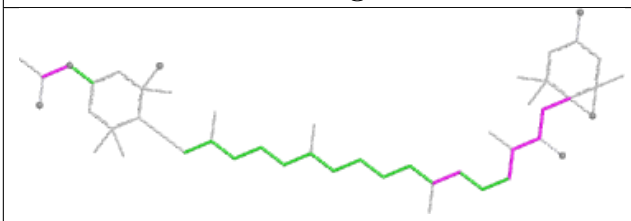
Ligand A86 Z 315



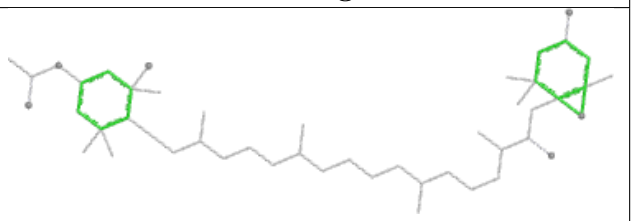
Bond lengths



Bond angles

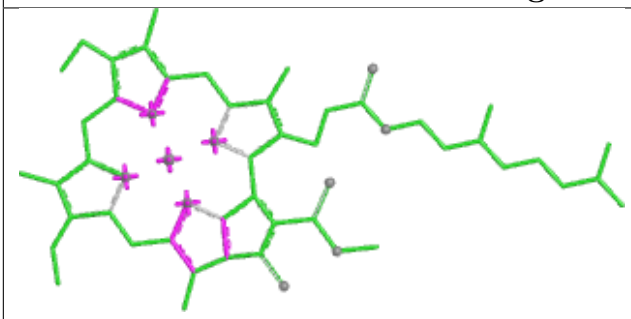


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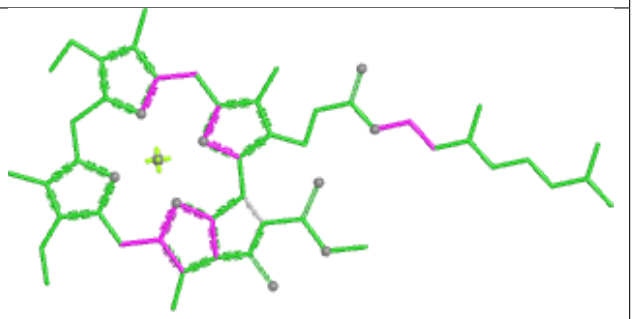


Rings

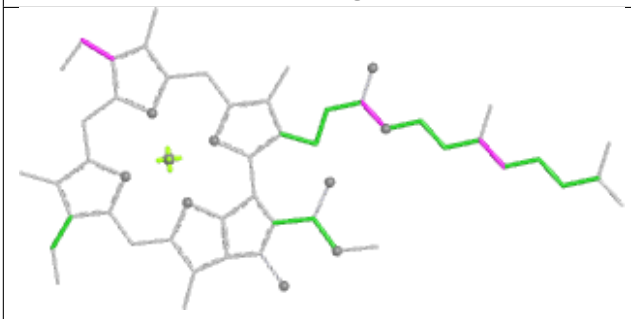
Ligand CLA k 201



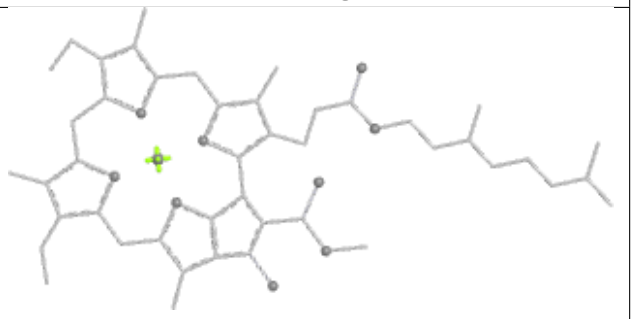
Bond lengths



Bond angles

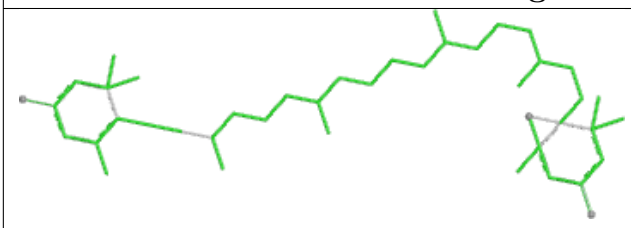


Torsions

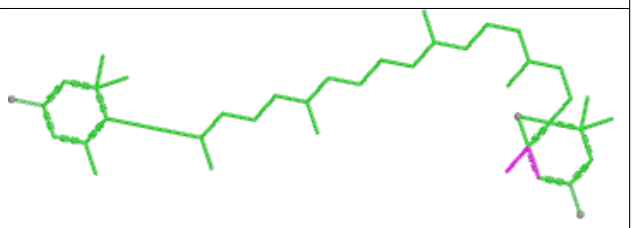


Rings

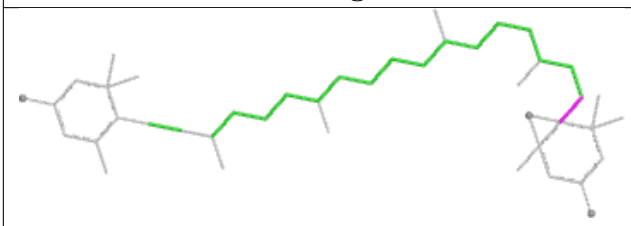
Ligand DD6 J 301



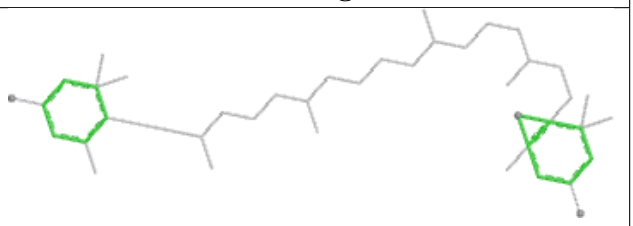
Bond lengths



Bond angles

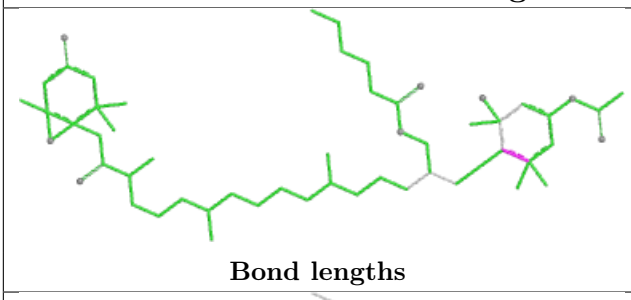


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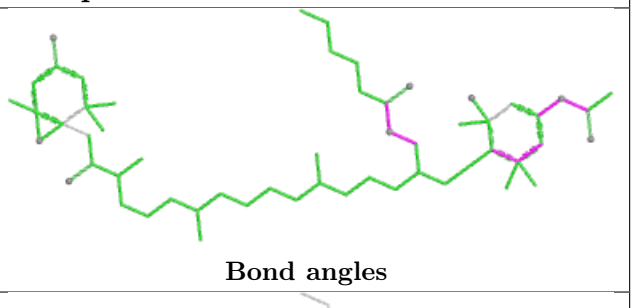


Rings

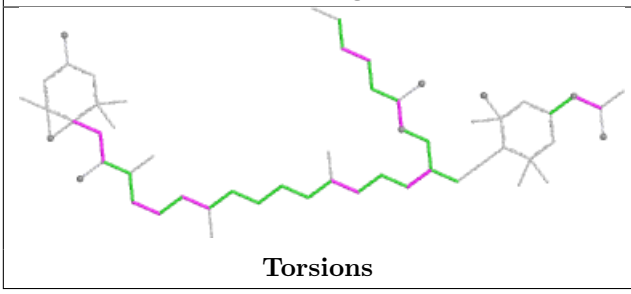
Ligand A1EB1 q 321



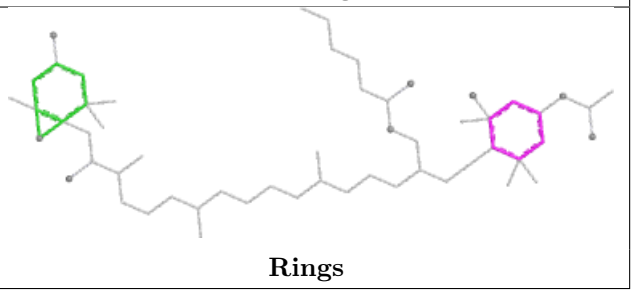
Bond lengths



Bond angles

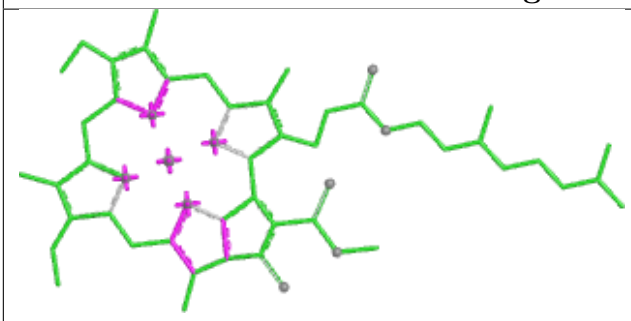


Torsions

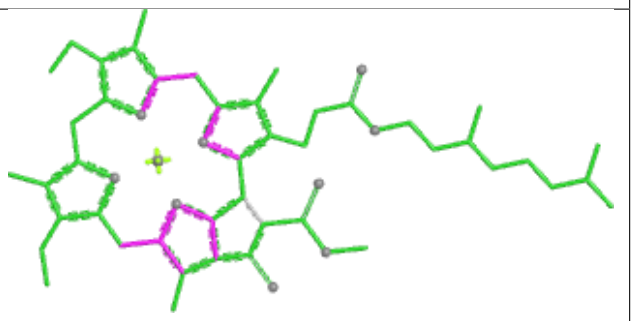


Rings

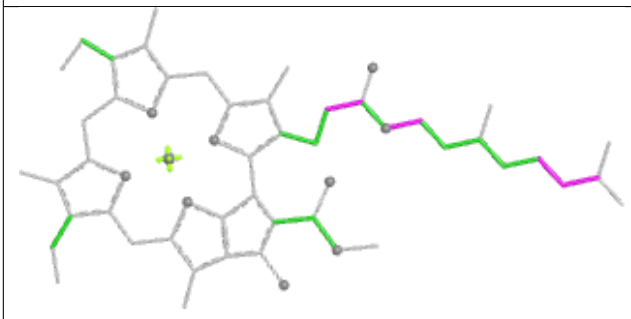
Ligand CLA N 305



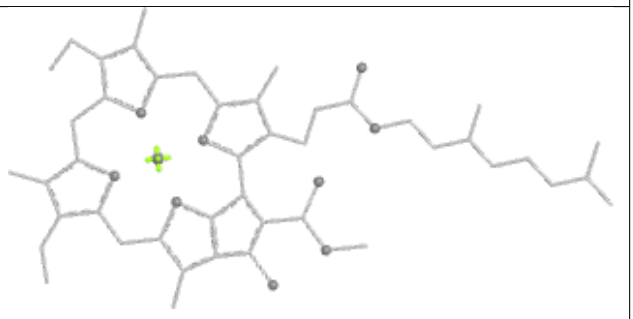
Bond lengths



Bond angles

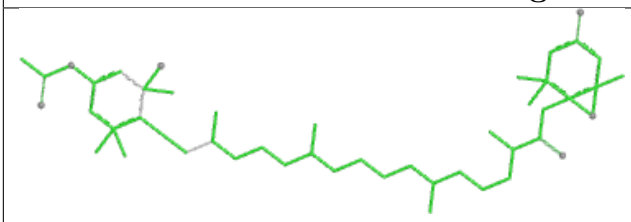


Torsions

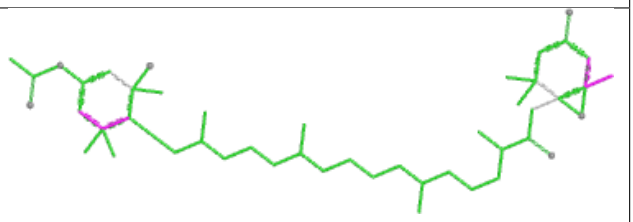


Rings

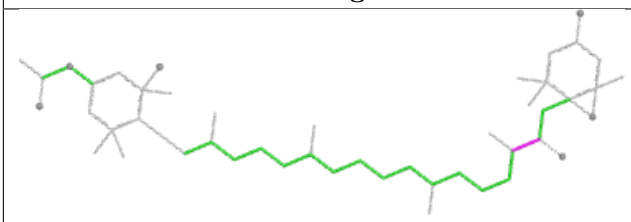
Ligand A86 O 313



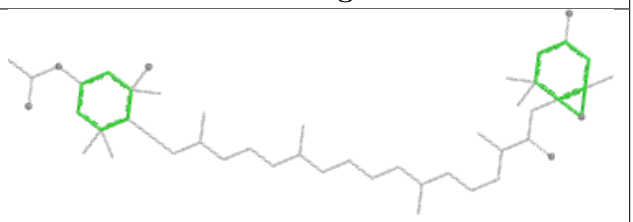
Bond lengths



Bond angles

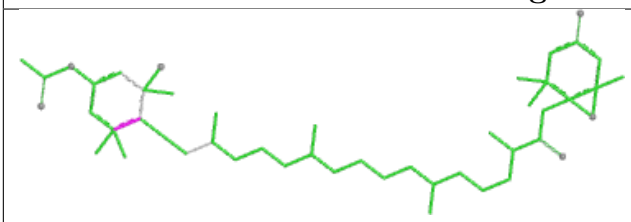


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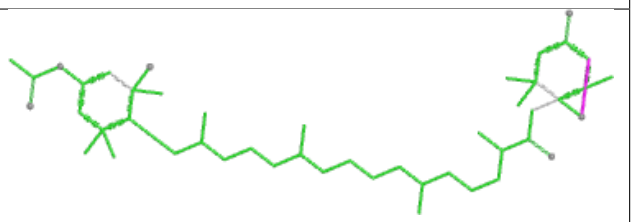


Rings

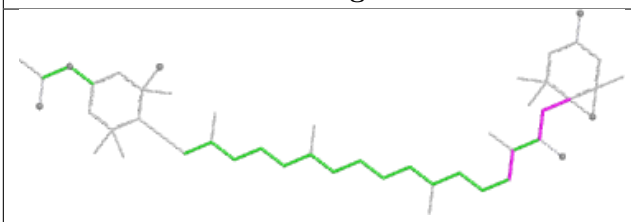
Ligand A86 Y 321



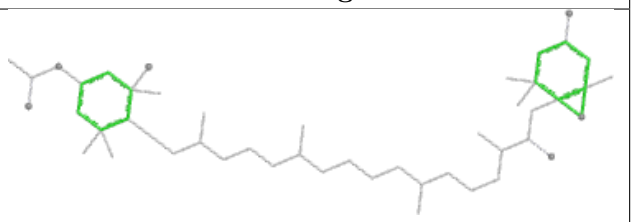
Bond lengths



Bond angles

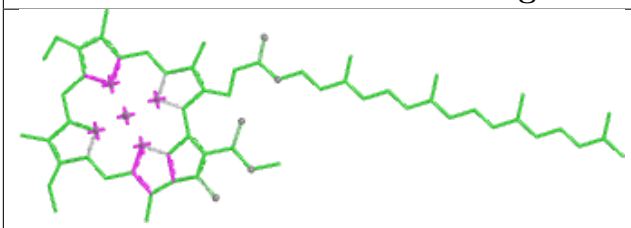


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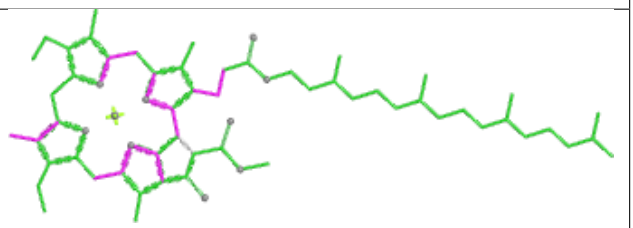


Rings

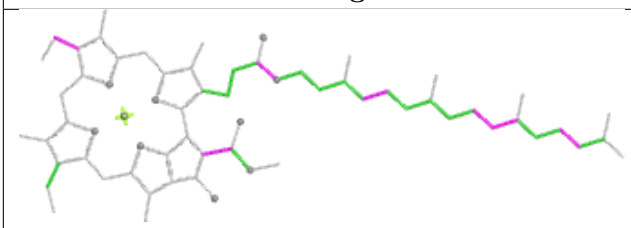
Ligand CLA W 307



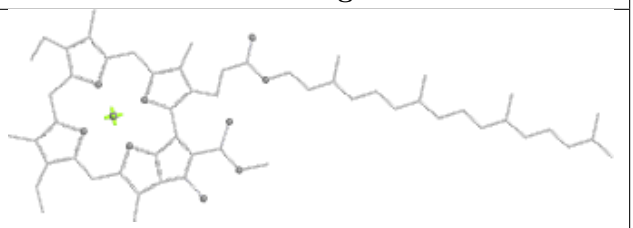
Bond lengths



Bond angles

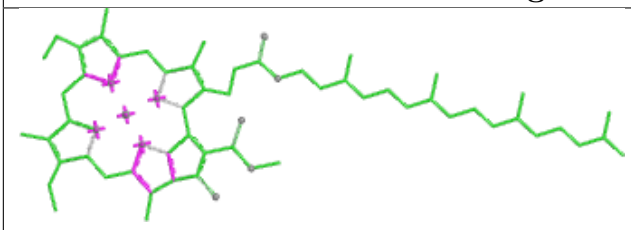


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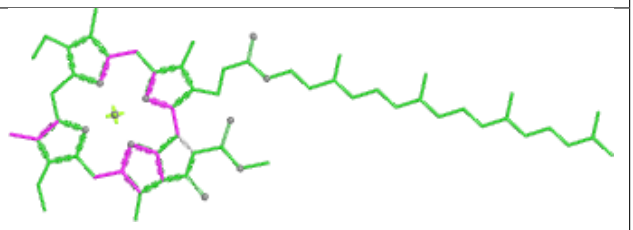


Rings

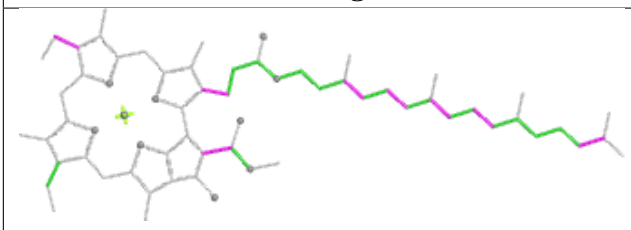
Ligand CLA b 840



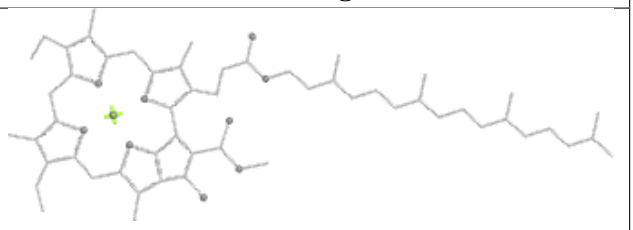
Bond lengths



Bond angles

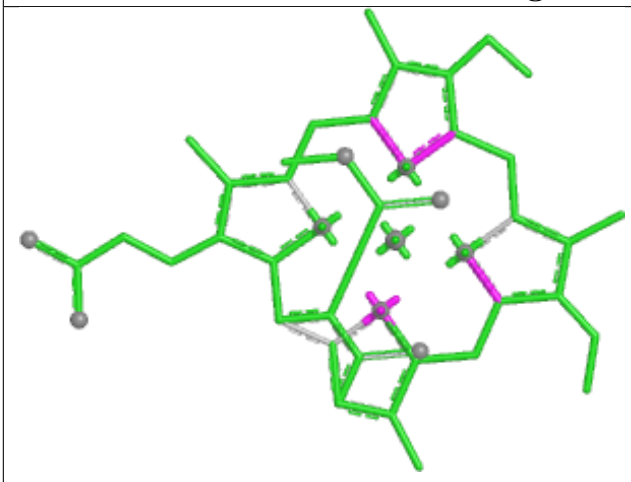


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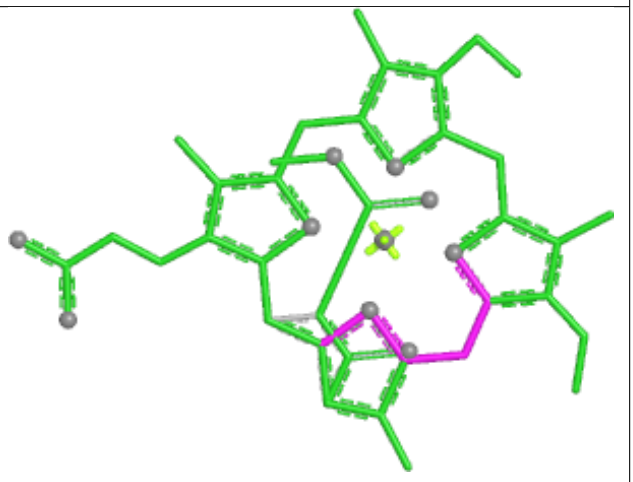


Rings

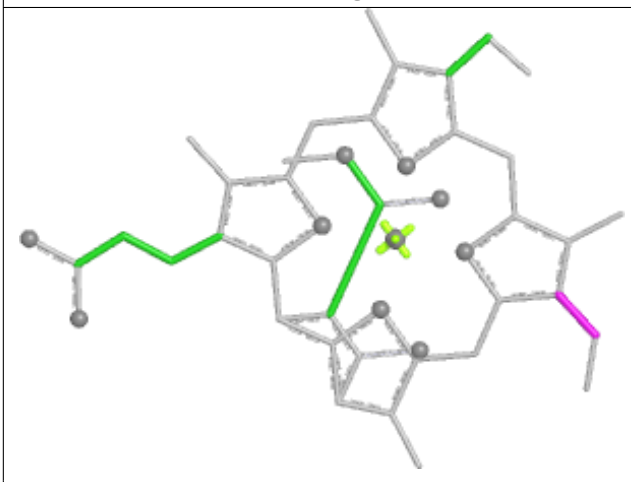
Ligand KC2 P 303



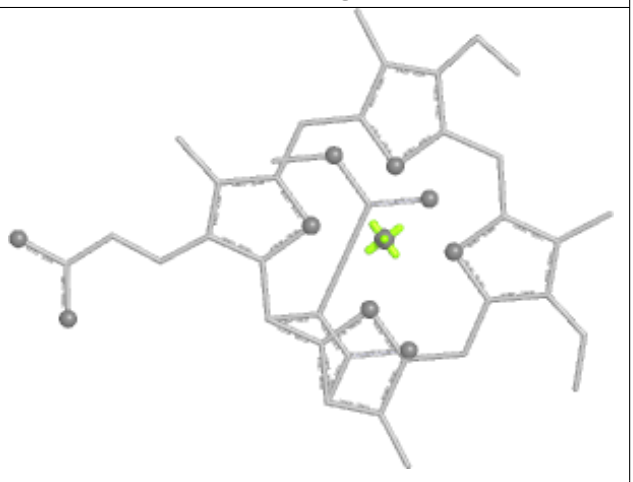
Bond lengths



Bond angles

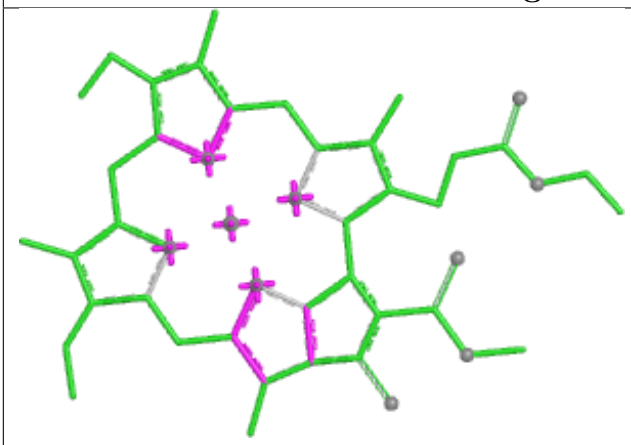


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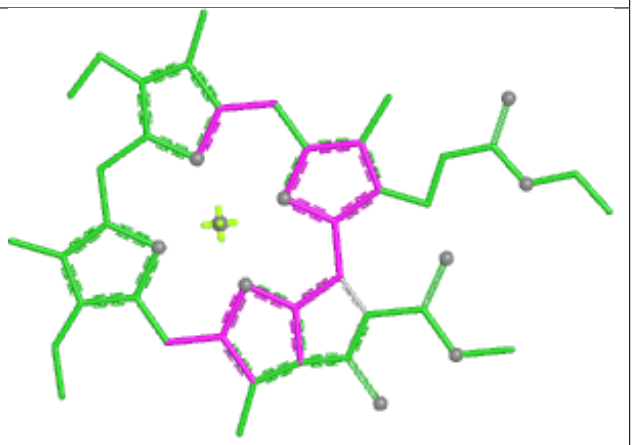


Rings

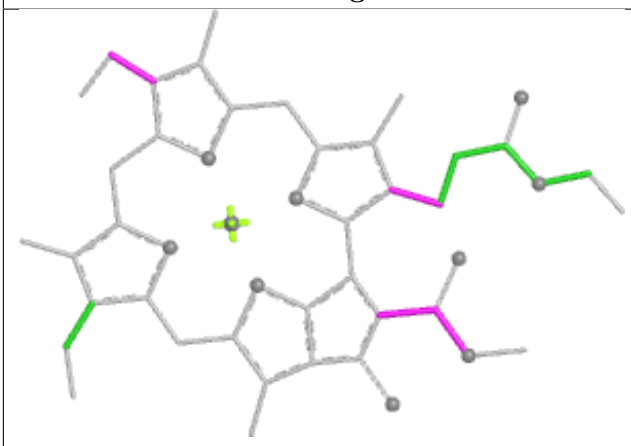
Ligand CLA O 310



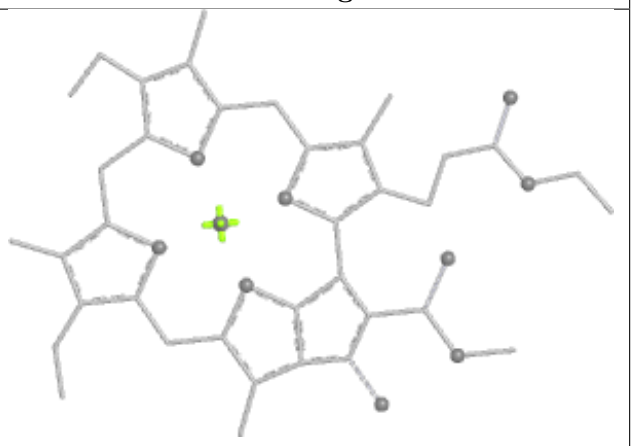
Bond lengths



Bond angles

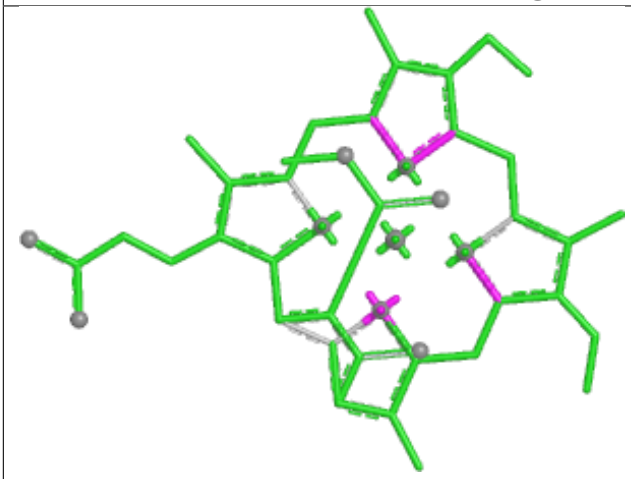


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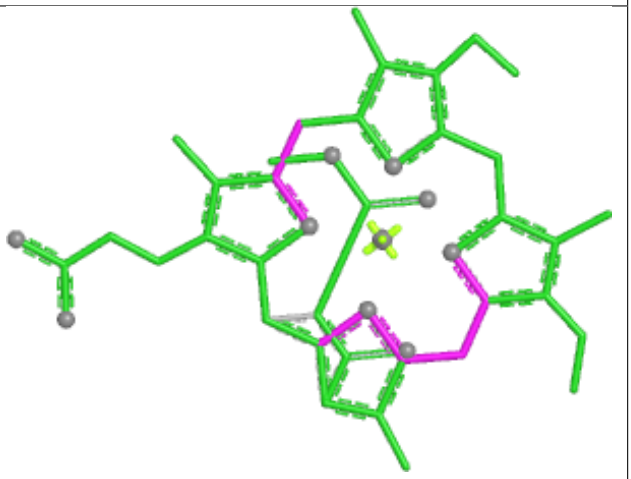


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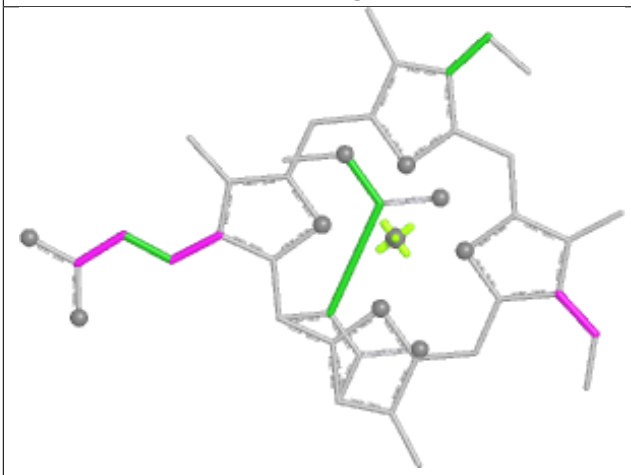
Ligand KC2 u 303



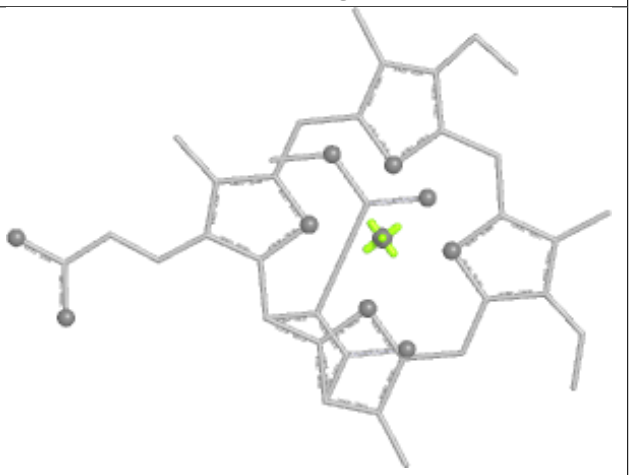
Bond lengths



Bond angles

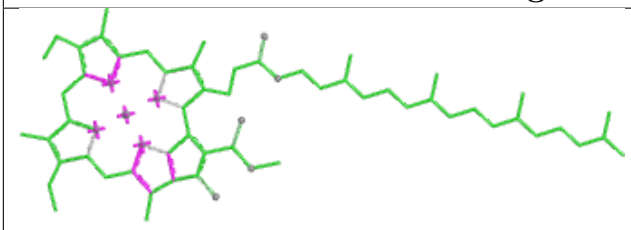


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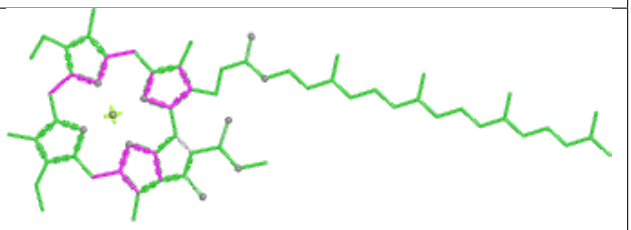


Rings

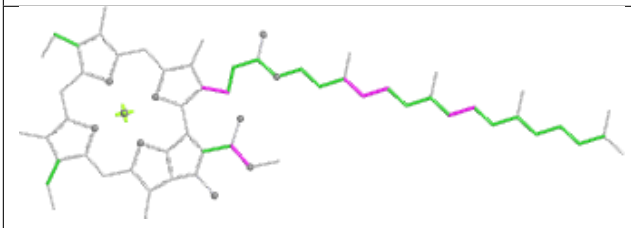
Ligand CLA b 832



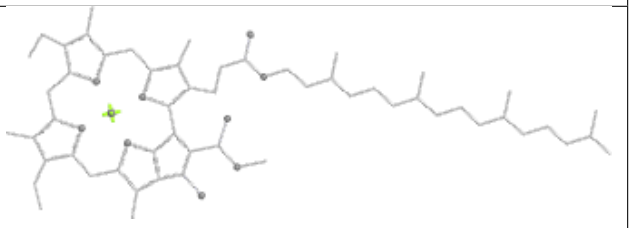
Bond lengths



Bond angles

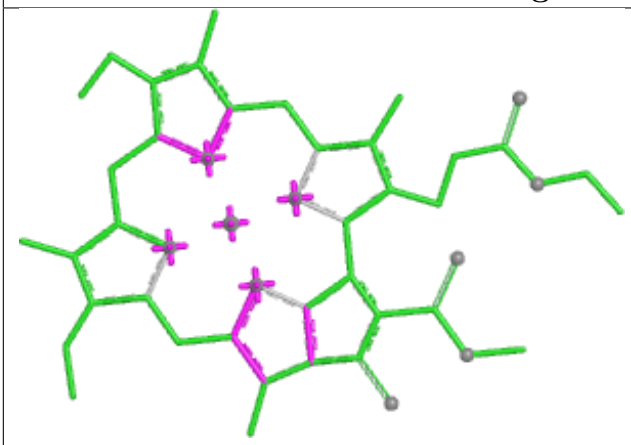


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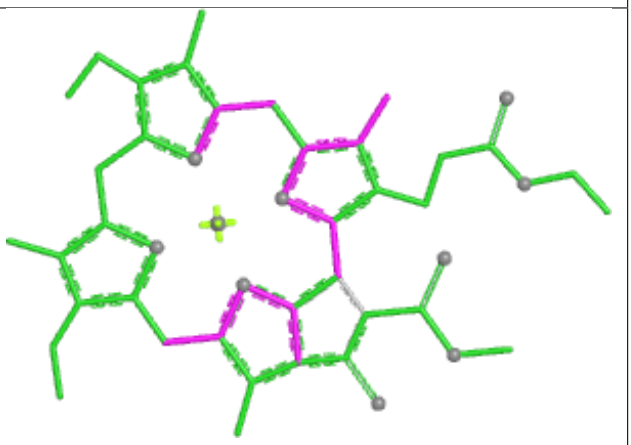


Rings

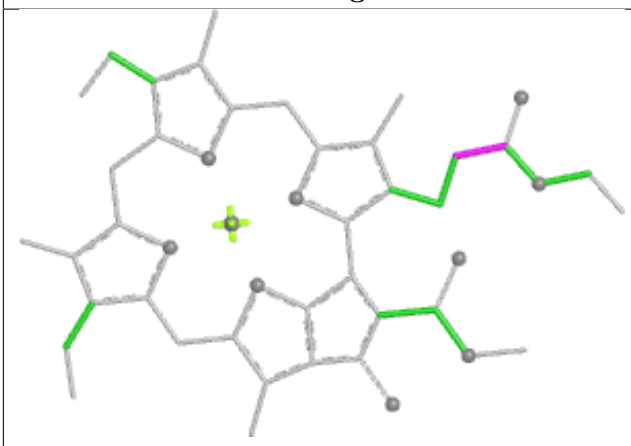
Ligand CLA f 205



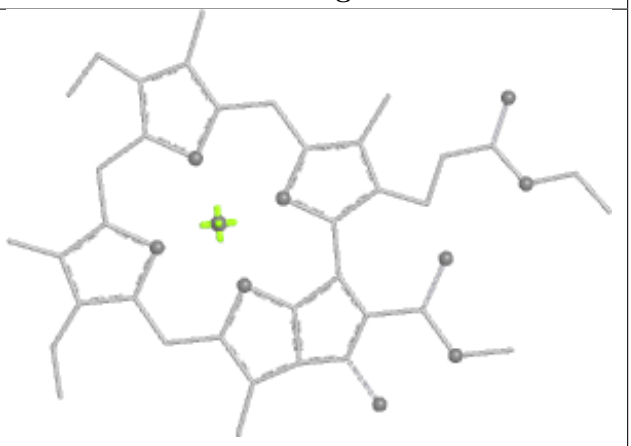
Bond lengths



Bond angles

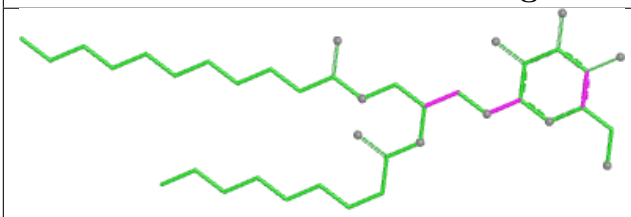


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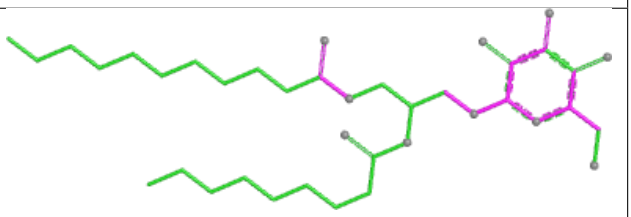


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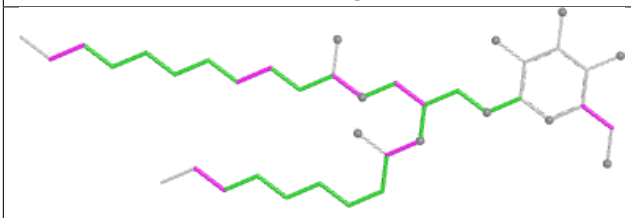
Ligand LMG P 318



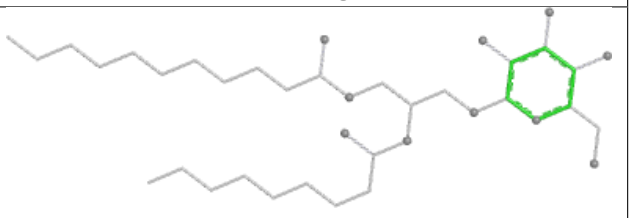
Bond lengths



Bond angles

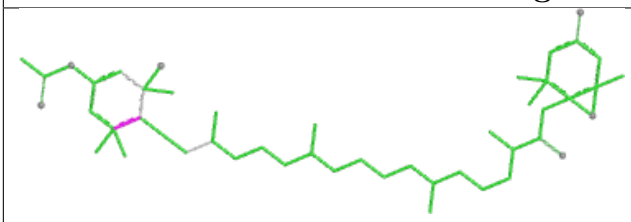


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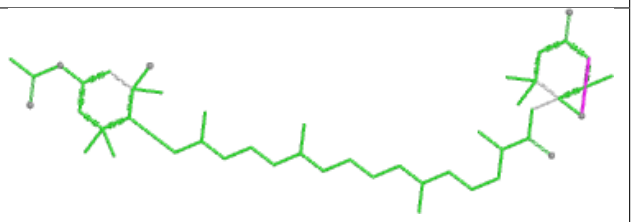


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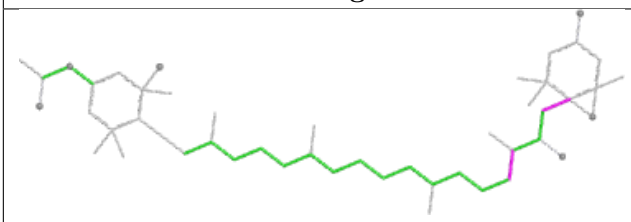
Ligand A86 v 316



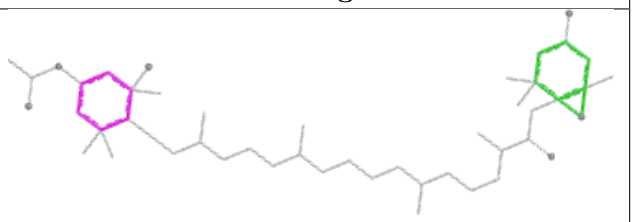
Bond lengths



Bond angles

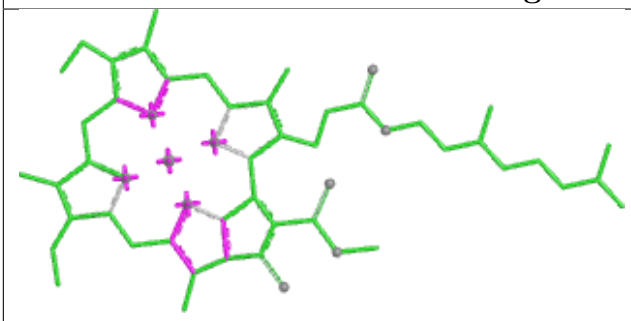


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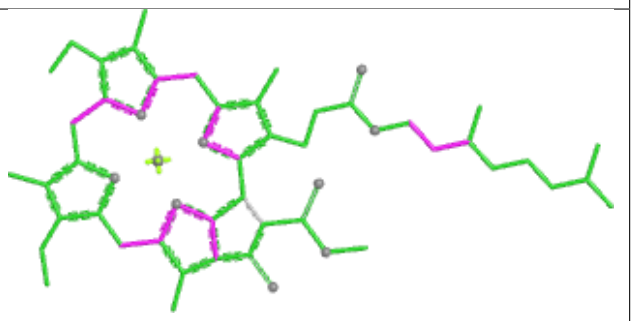


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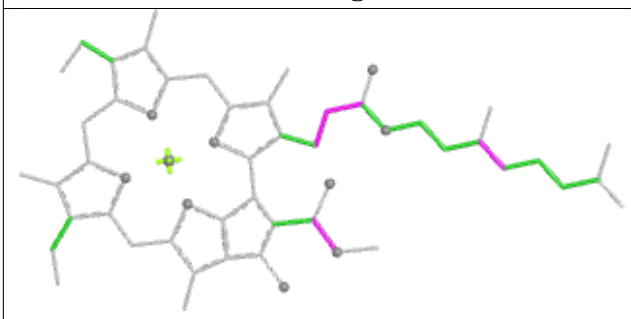
Ligand CLA Y 305



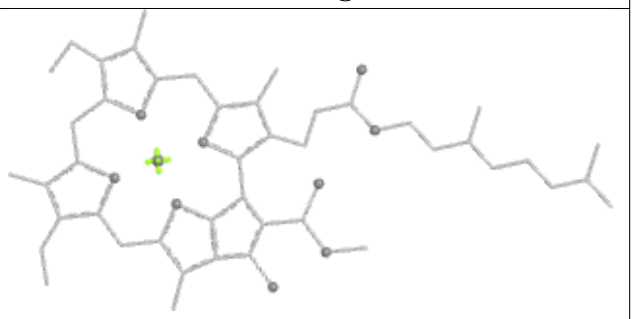
Bond lengths



Bond angles

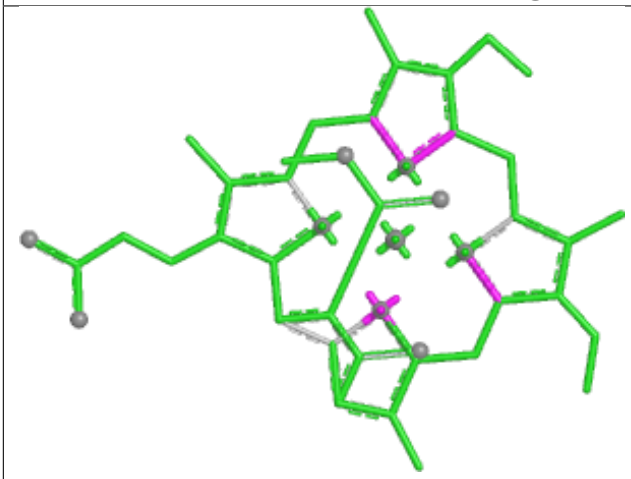


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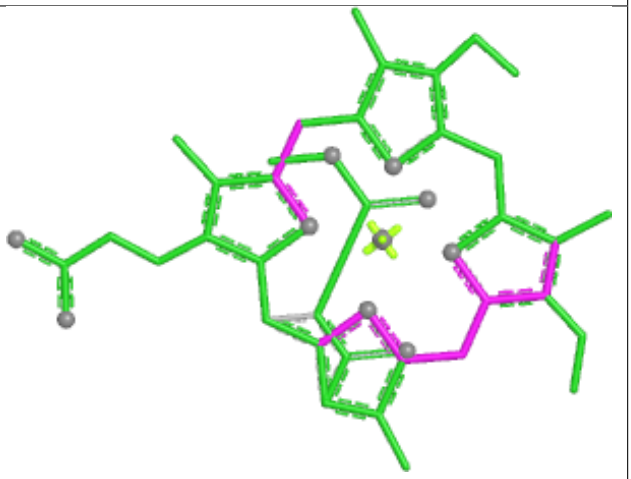


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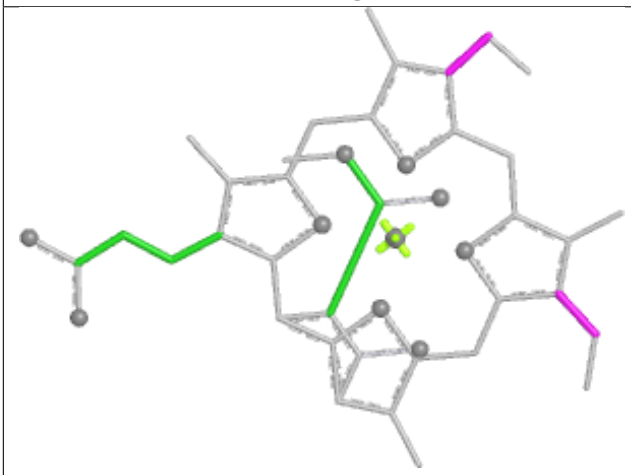
Ligand KC2 P 302



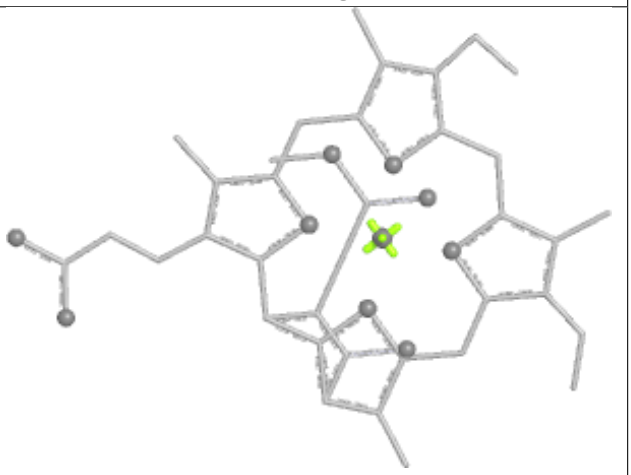
Bond lengths



Bond angles

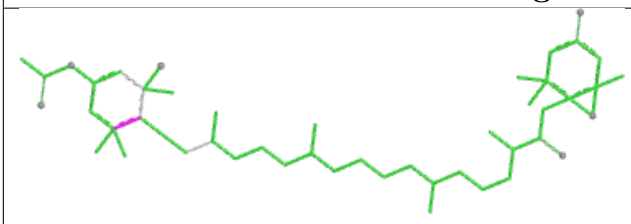


Torsions

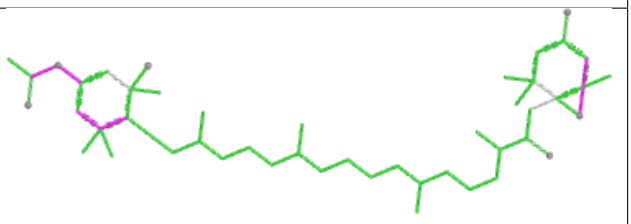


Rings

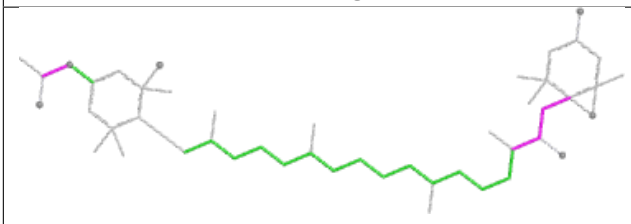
Ligand A86 u 316



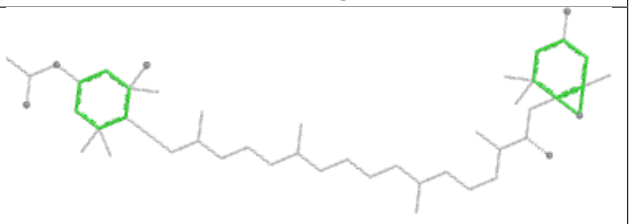
Bond lengths



Bond angles

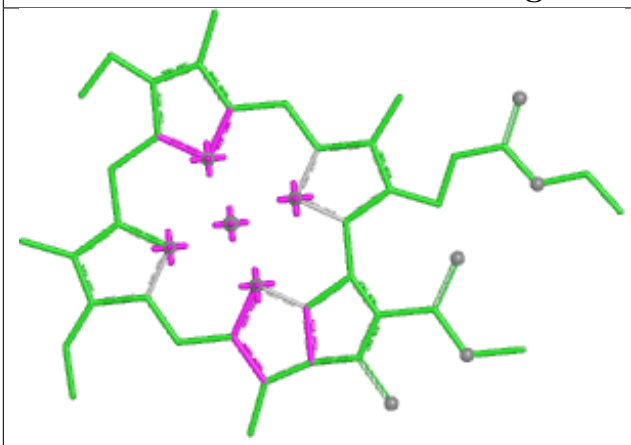


Torsions

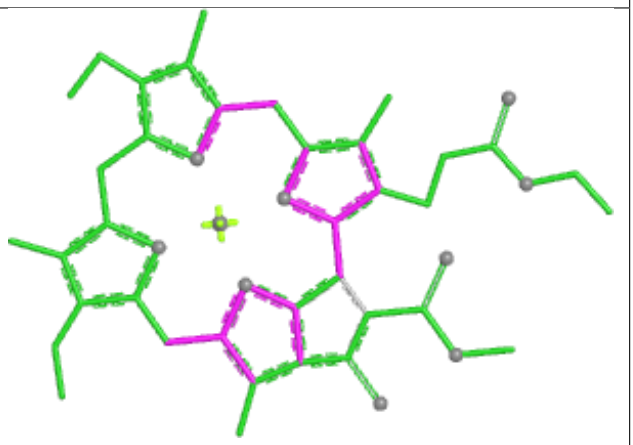


Rings

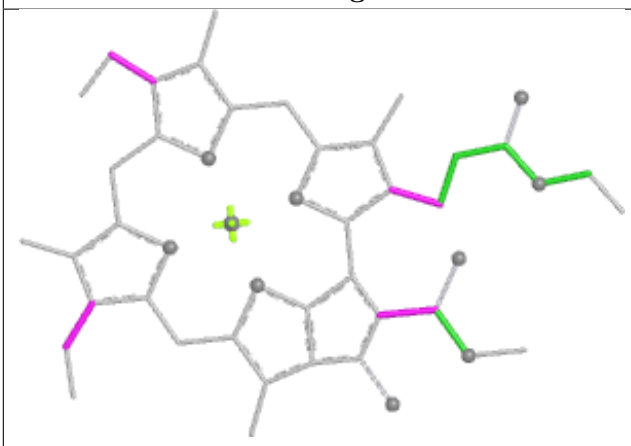
Ligand CLA E 302



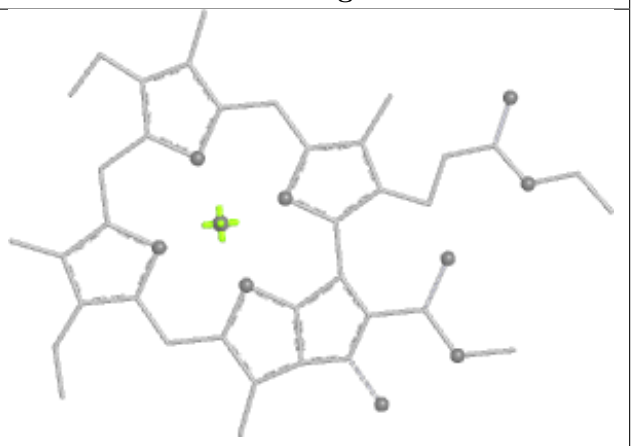
Bond lengths



Bond angles

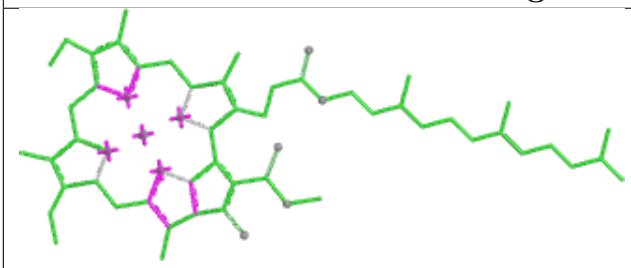


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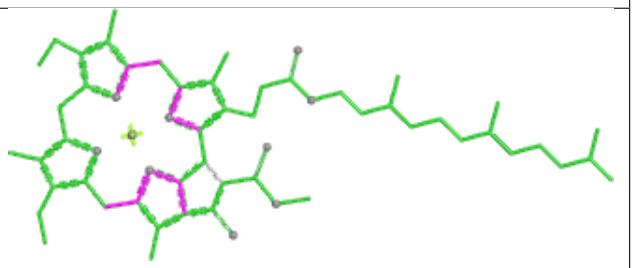


Rings

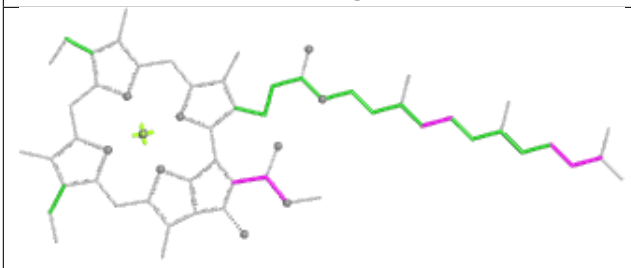
Ligand CLA u 312



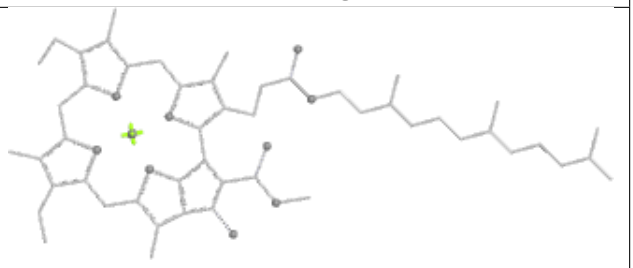
Bond lengths



Bond angles

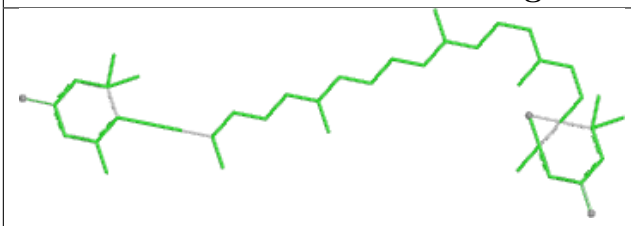


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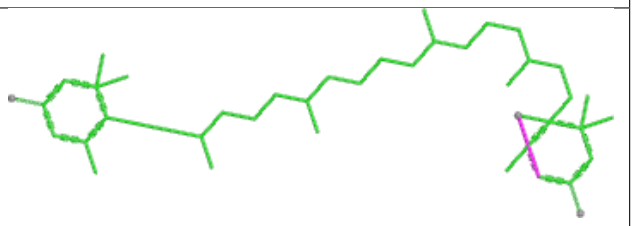


Rings

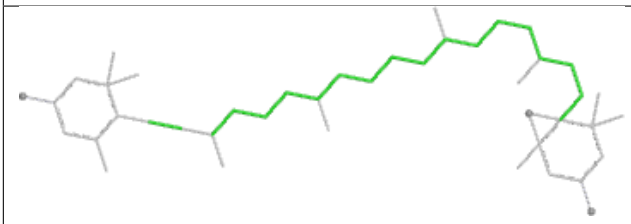
Ligand DD6 X 322



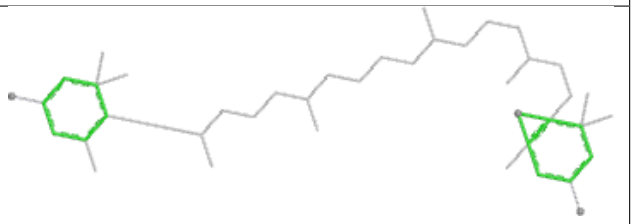
Bond lengths



Bond angles

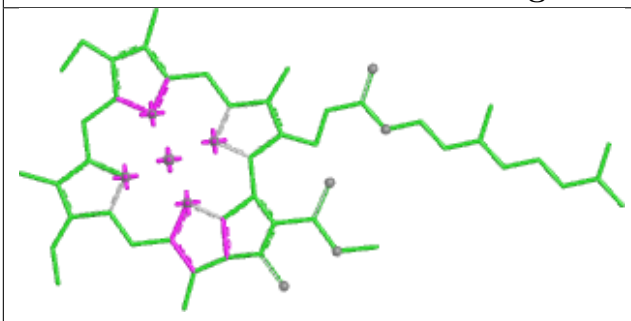


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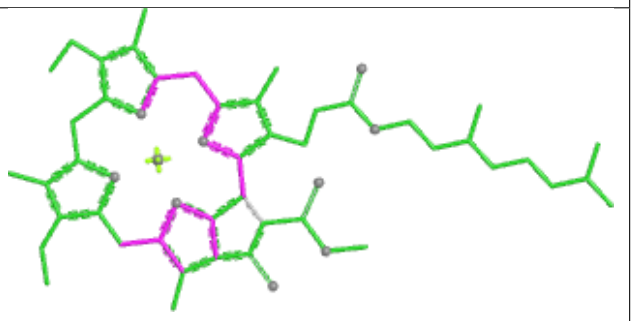


Rings

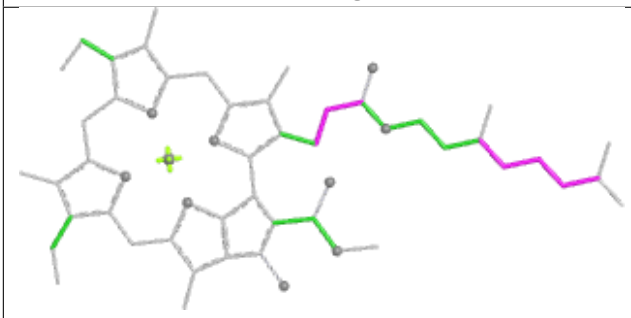
Ligand CLA o 305



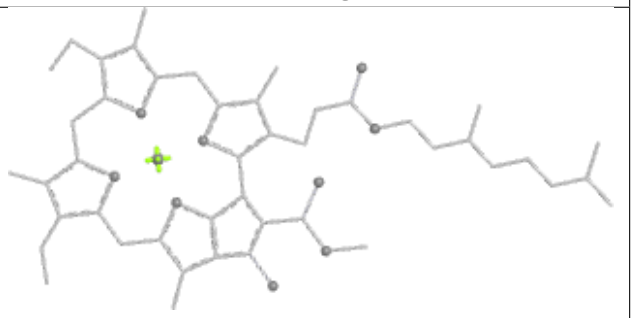
Bond lengths



Bond angles

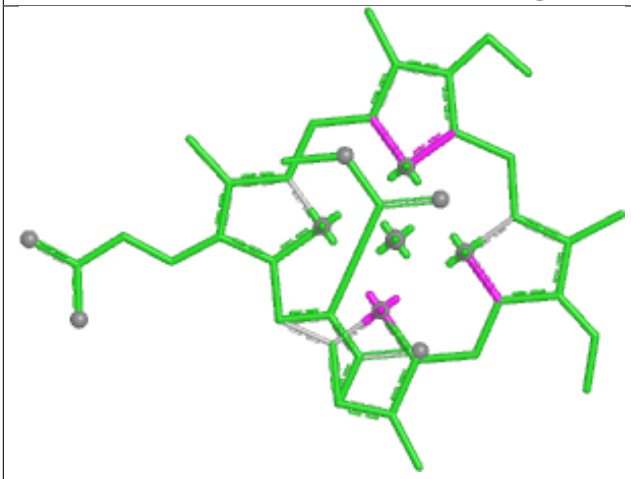


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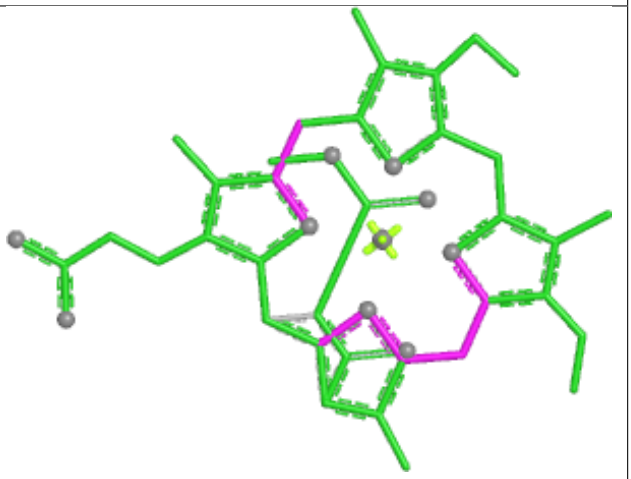


Rings

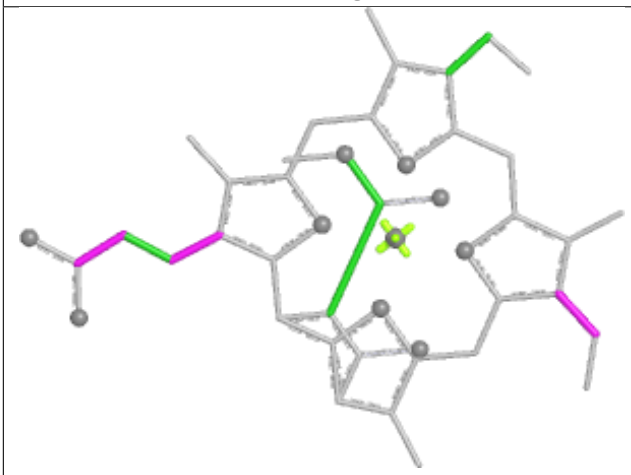
Ligand KC2 z 303



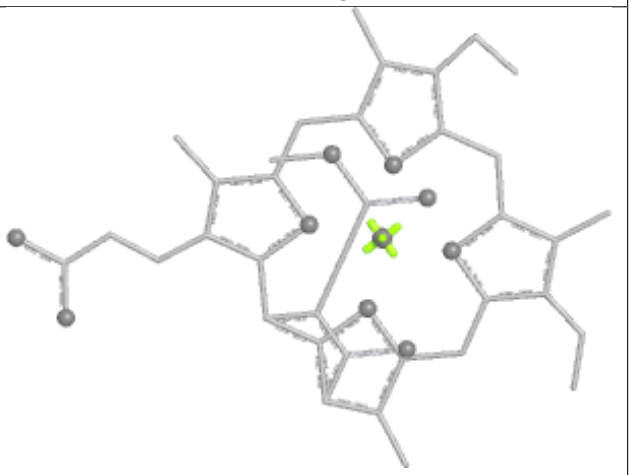
Bond lengths



Bond angles

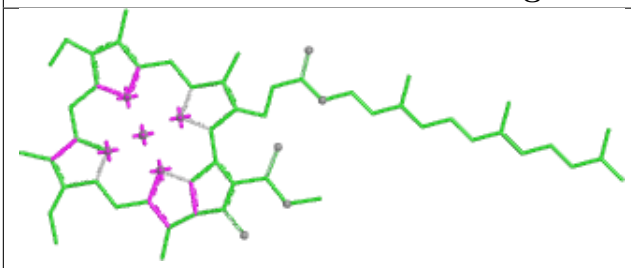


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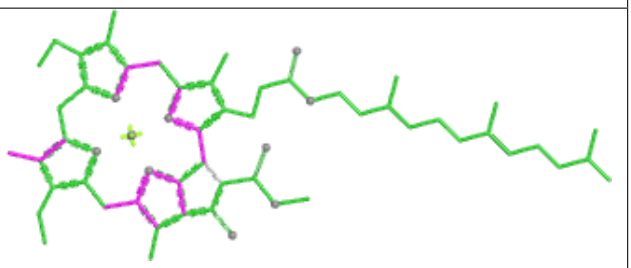


Rings

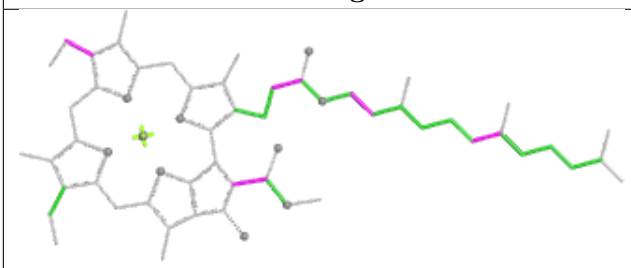
Ligand CLA A 307



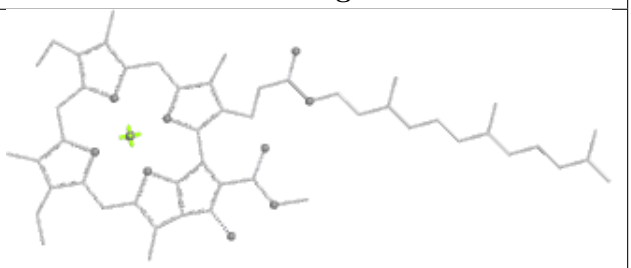
Bond lengths



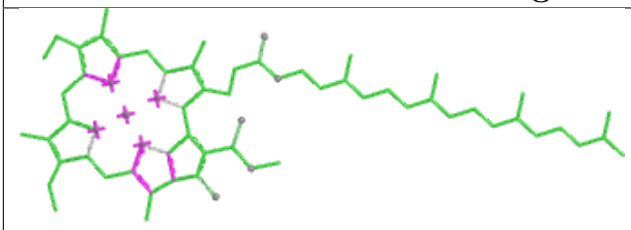
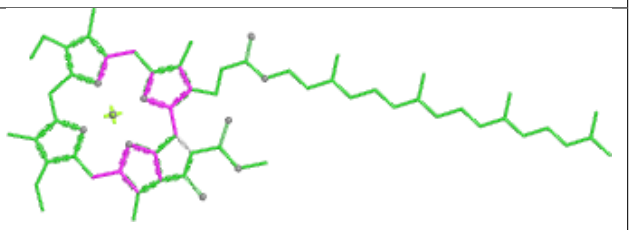
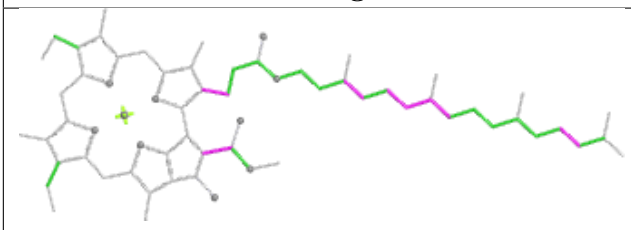
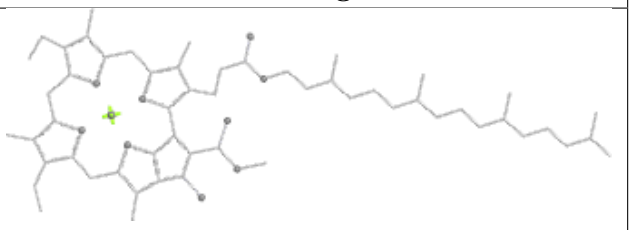
Bond angles

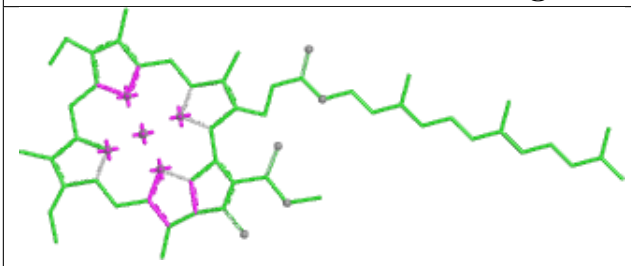
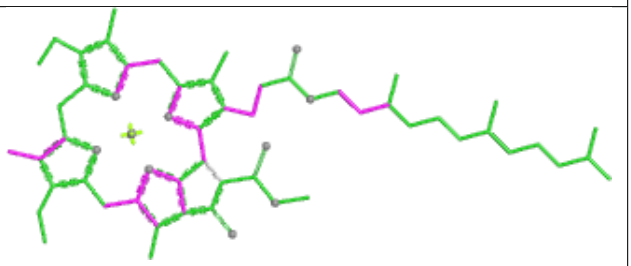
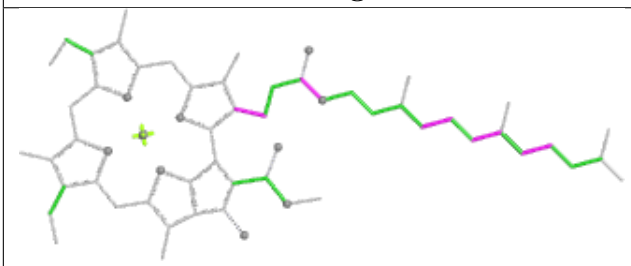
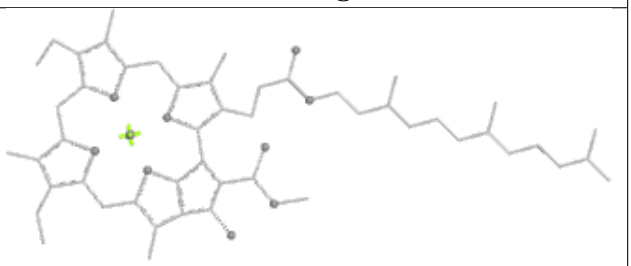


Torsions

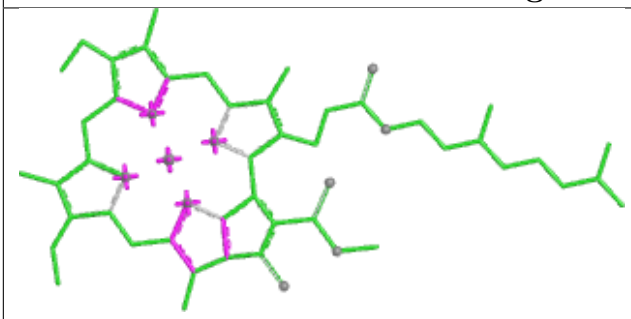


Rings

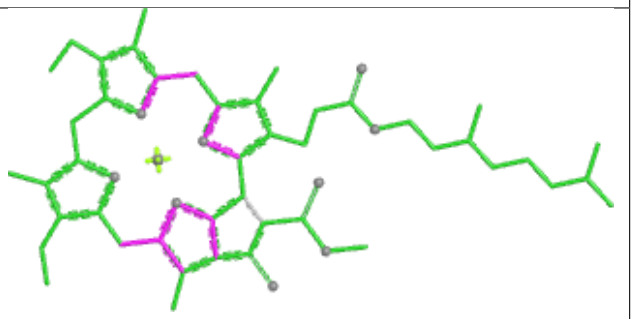
Ligand CLA l 205	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA z 307	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

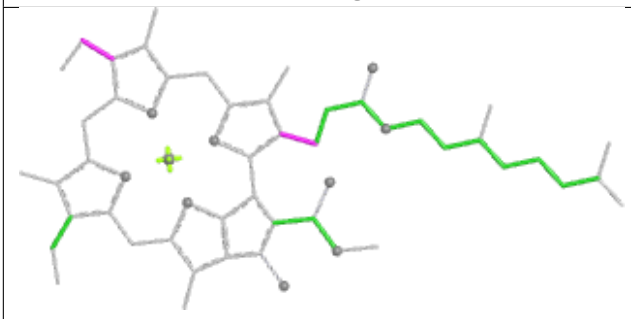
Ligand CLA F 308



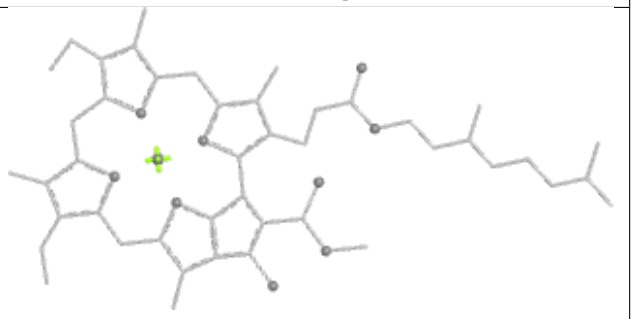
Bond lengths



Bond angles

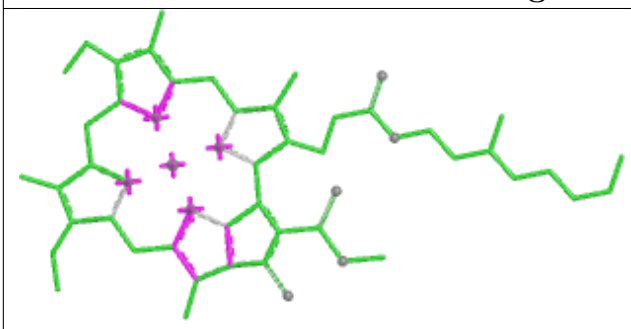


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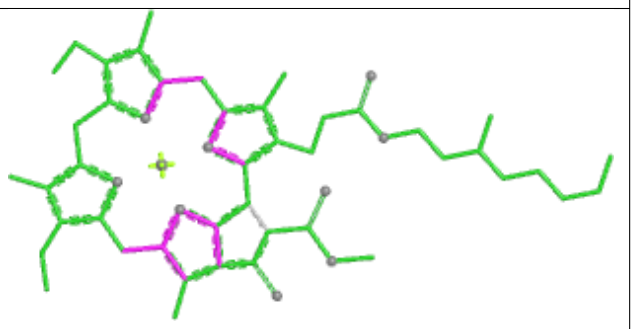


Rings

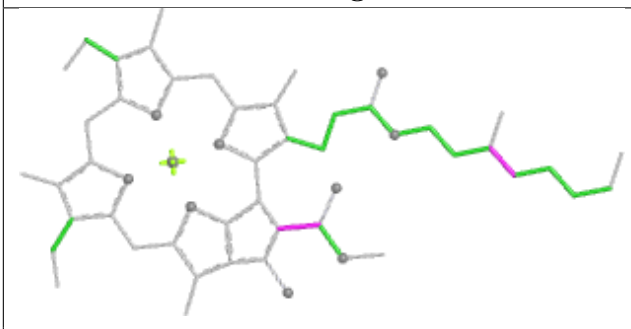
Ligand CLA a 805



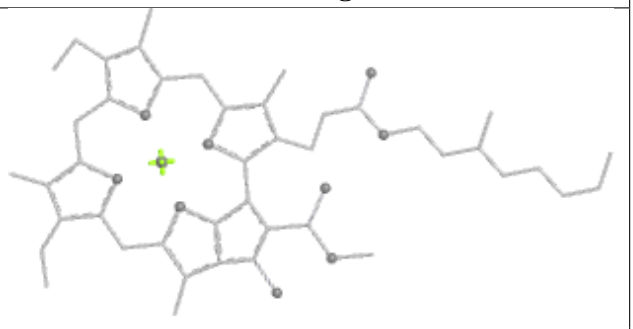
Bond lengths



Bond angles

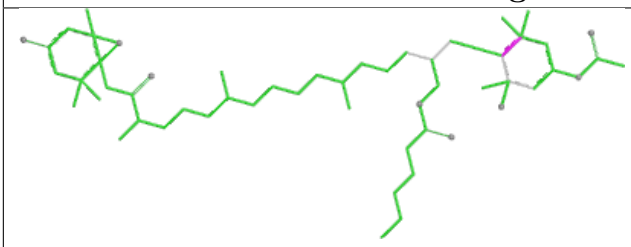


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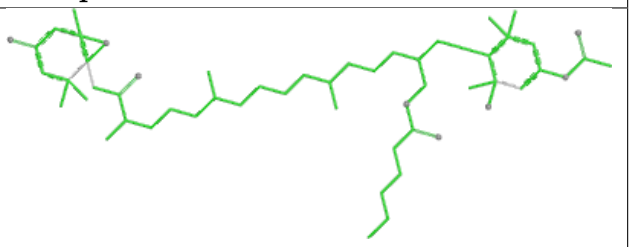


Rings

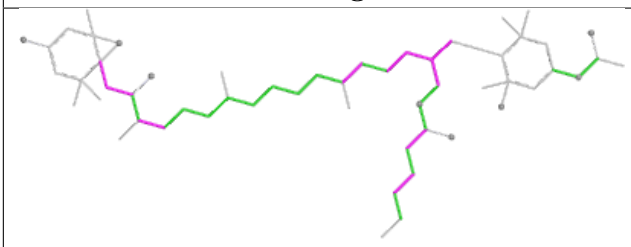
Ligand A1EB1 q 323



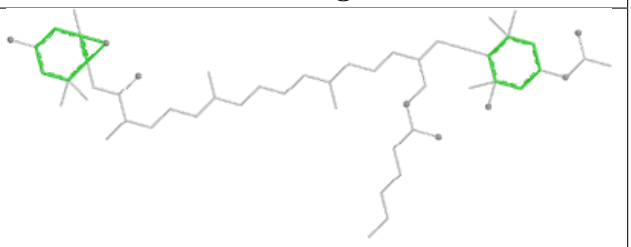
Bond lengths



Bond angles

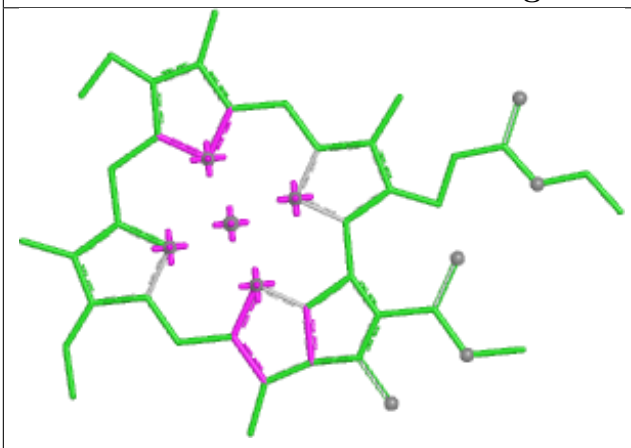


Torsions

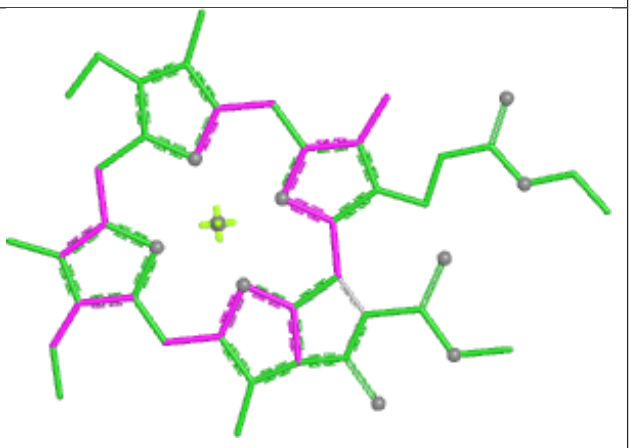


Rings

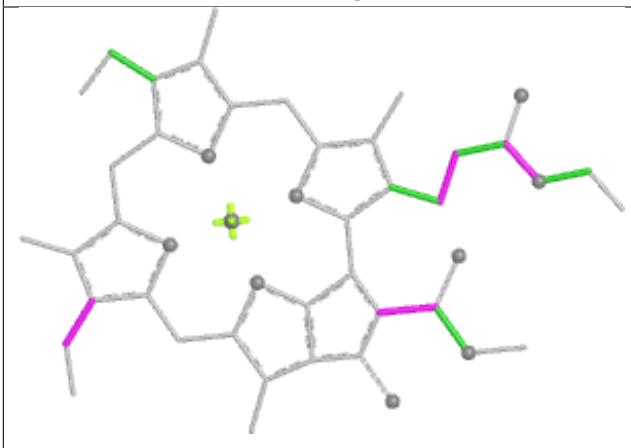
Ligand CLA U 208



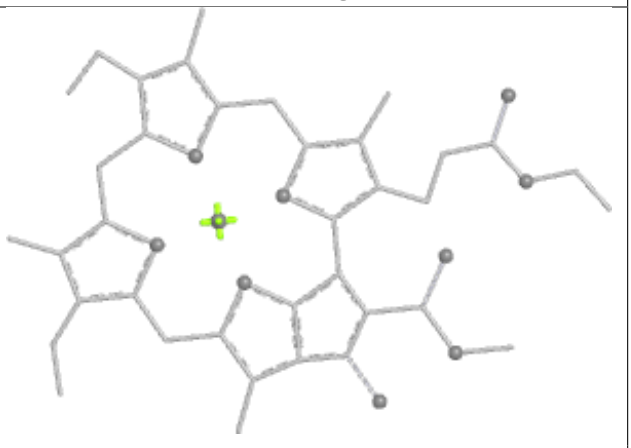
Bond lengths



Bond angles

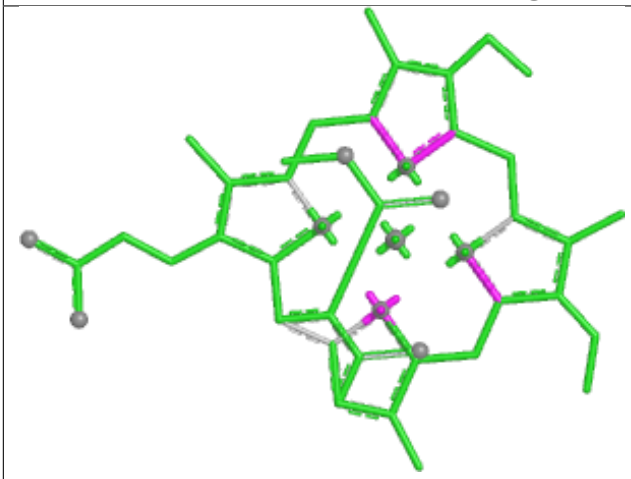


Torsions

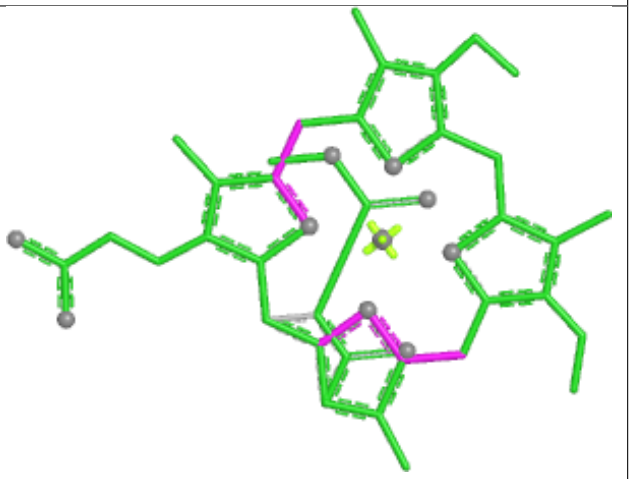


Rings

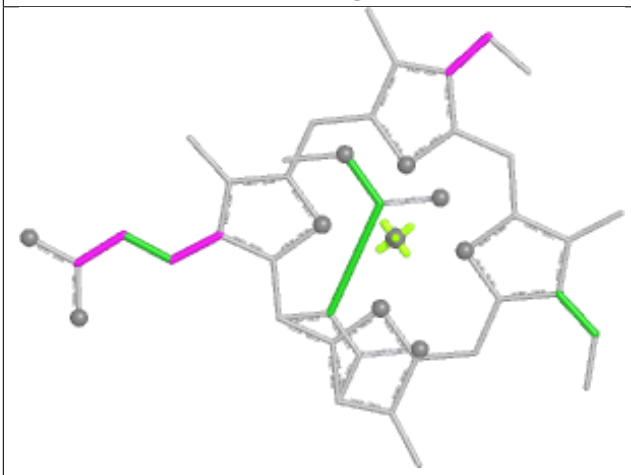
Ligand KC2 X 308



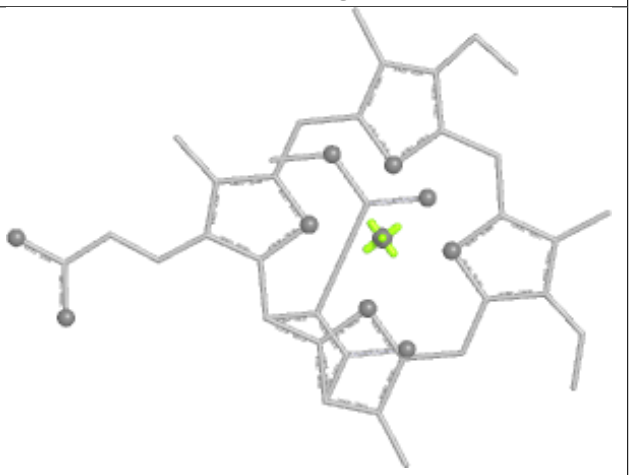
Bond lengths



Bond angles

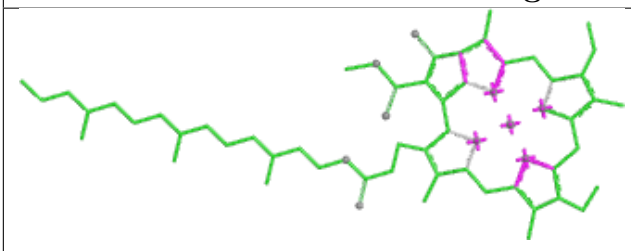


Torsions

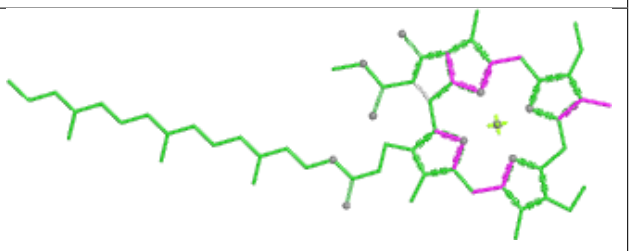


Rings

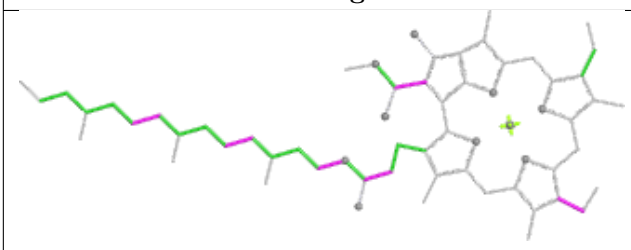
Ligand CLA O 307



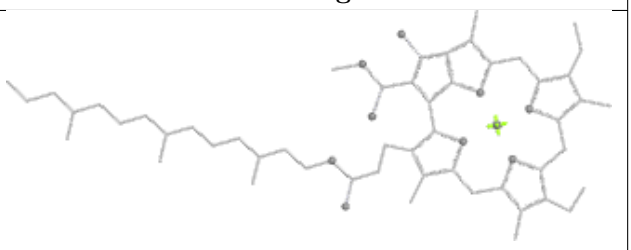
Bond lengths



Bond angles

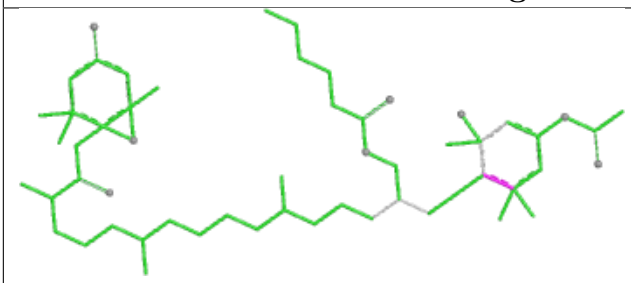


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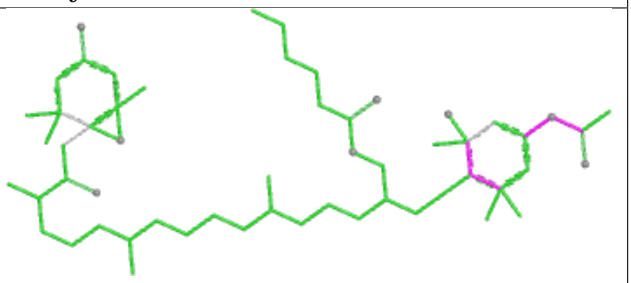


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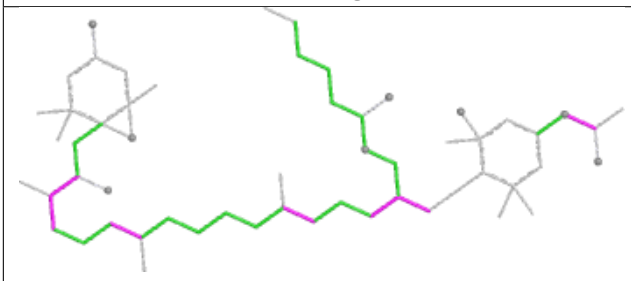
Ligand A1EB1 y 313



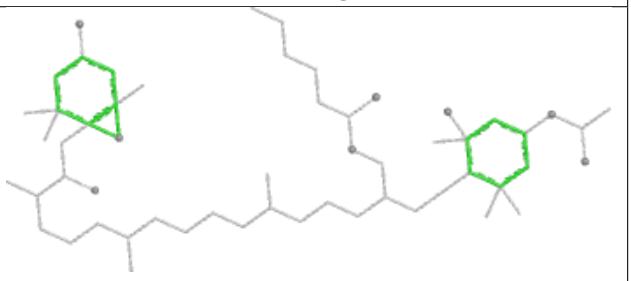
Bond lengths



Bond angles

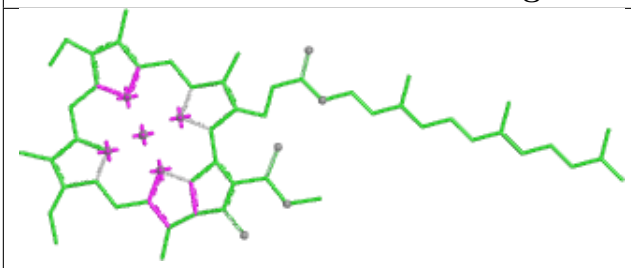


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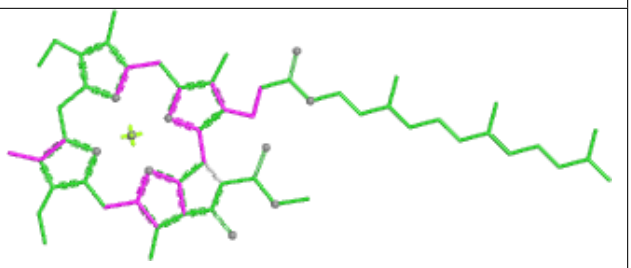


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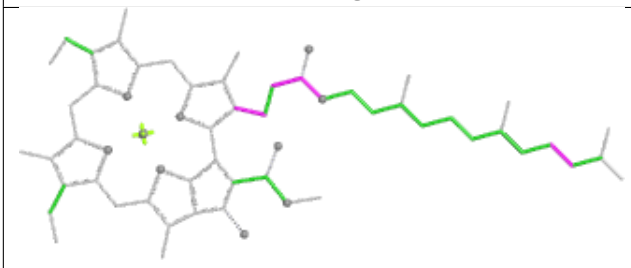
Ligand CLA K 306



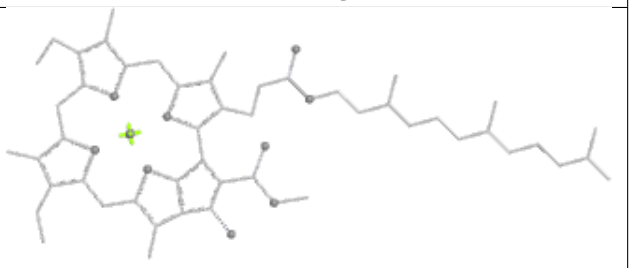
Bond lengths



Bond angles



Torsions



Rings

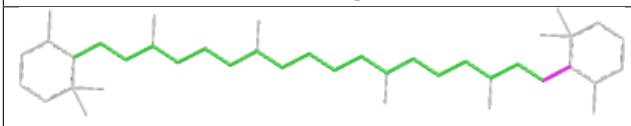
Ligand BCR a 844



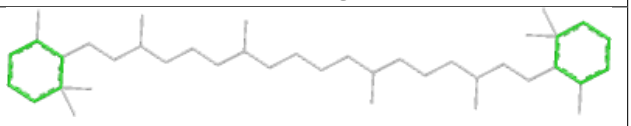
Bond lengths



Bond angles

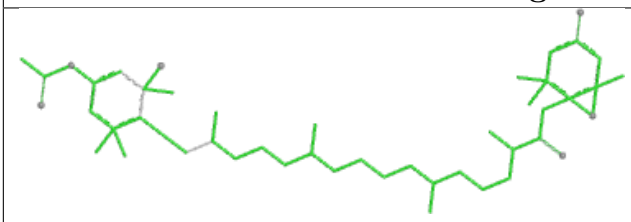


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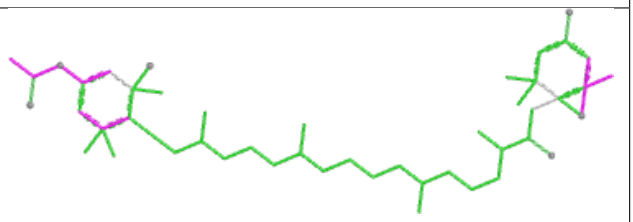


Rings

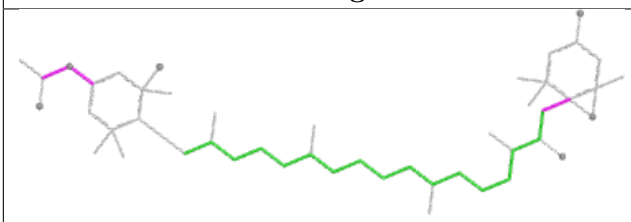
Ligand A86 X 315



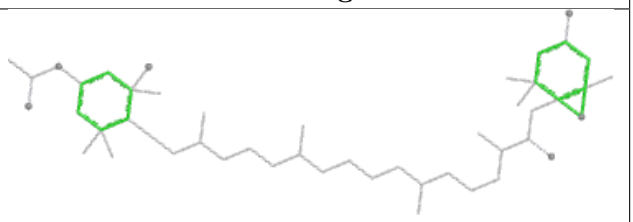
Bond lengths



Bond angles

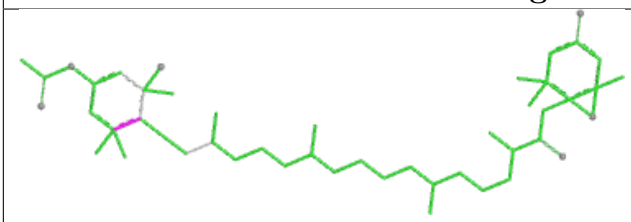


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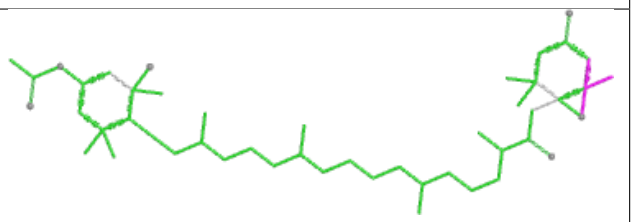


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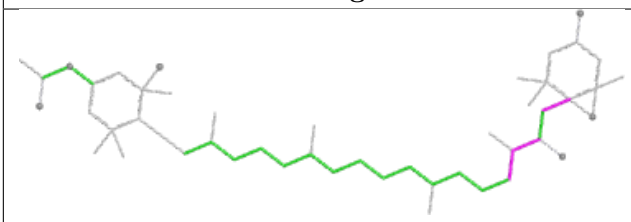
Ligand A86 O 312



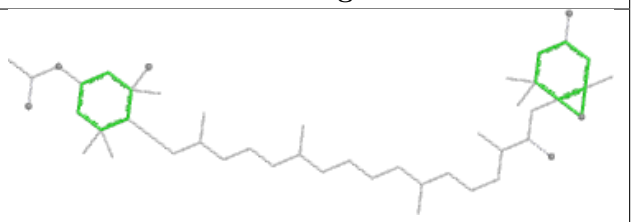
Bond lengths



Bond angles

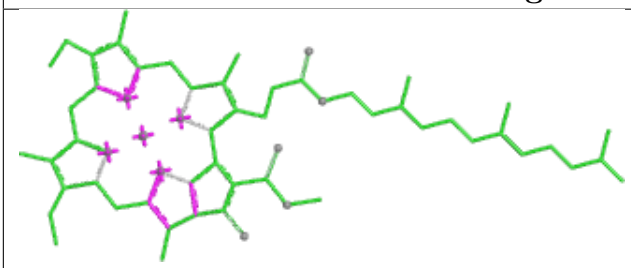


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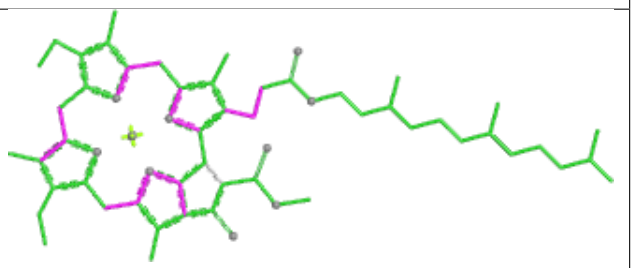


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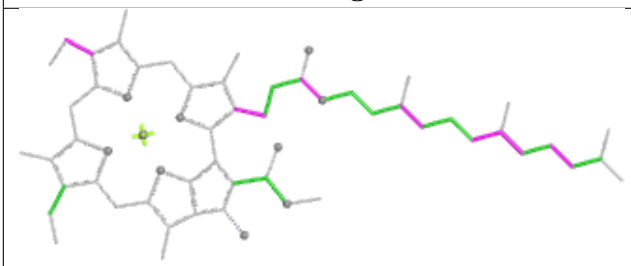
Ligand CLA E 309



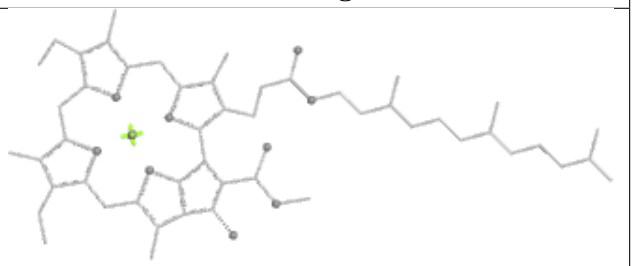
Bond lengths



Bond angles

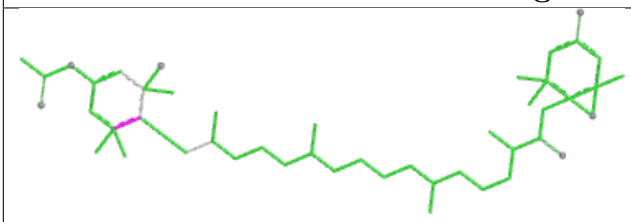


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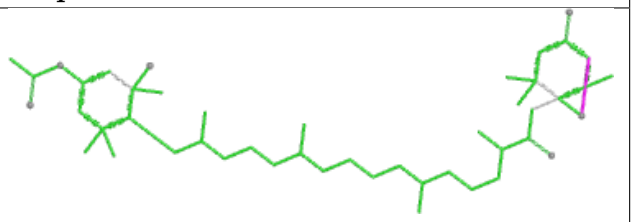


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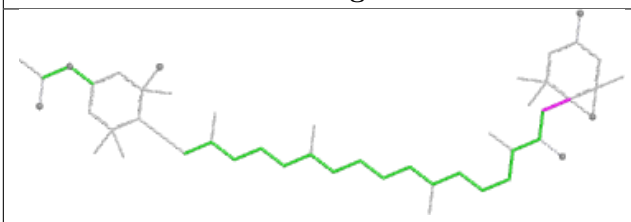
Ligand A86 q 317



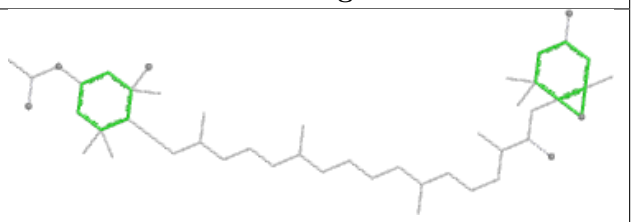
Bond lengths



Bond angles

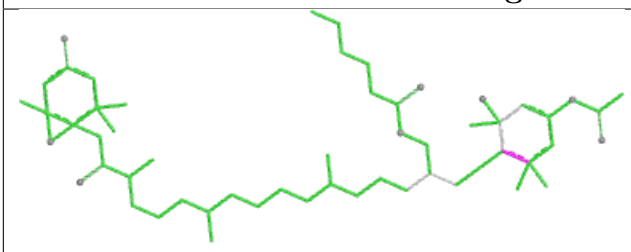


Torsions



Rings

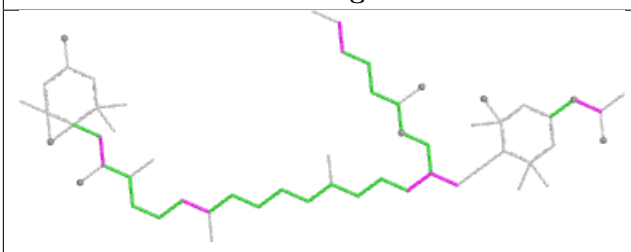
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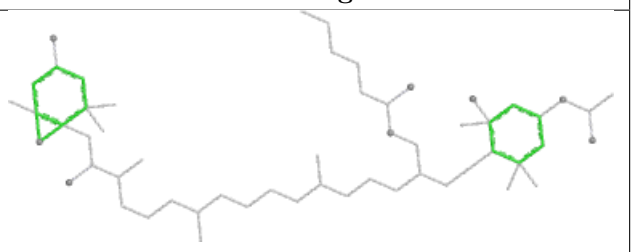
Bond lengths



Bond angles

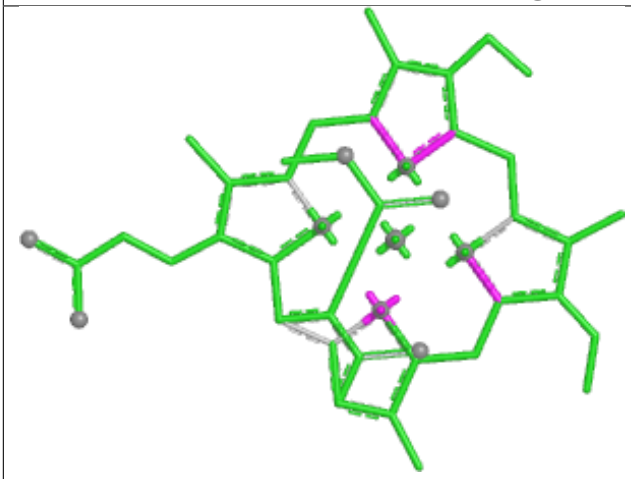


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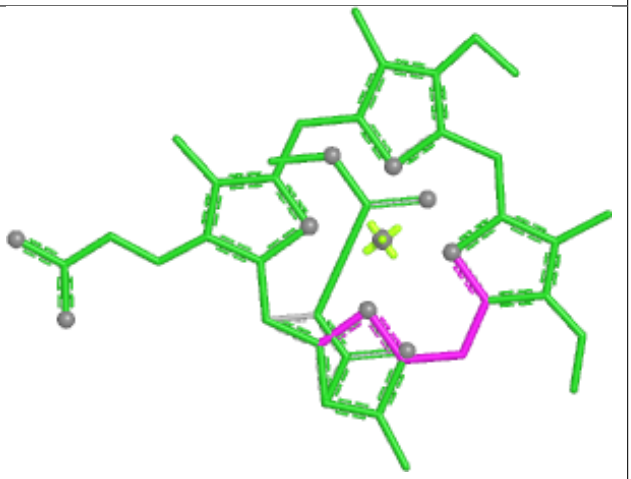


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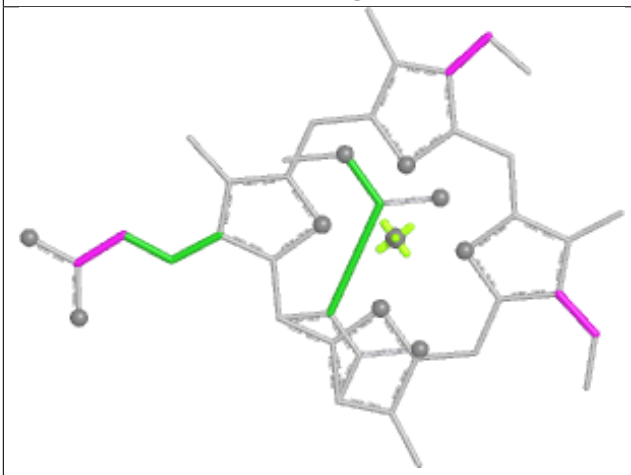
Ligand KC2 S 310



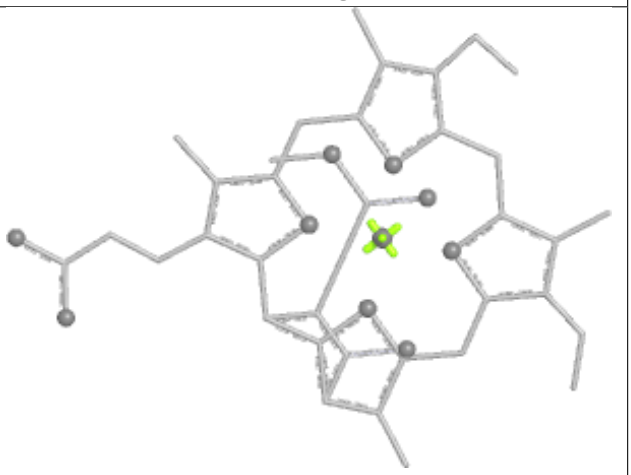
Bond lengths



Bond angles

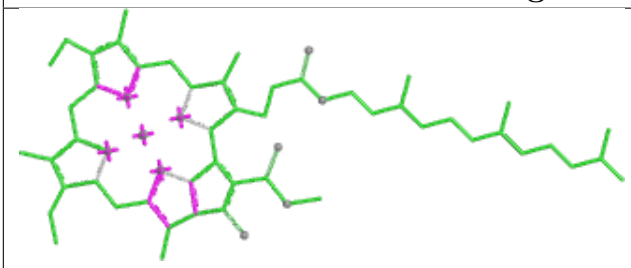


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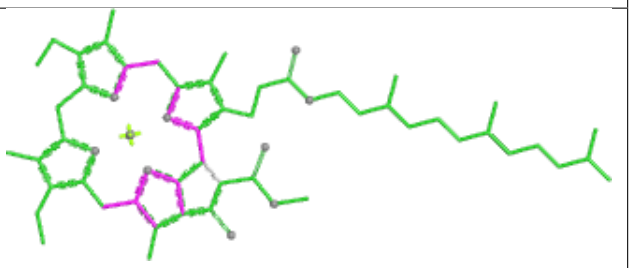


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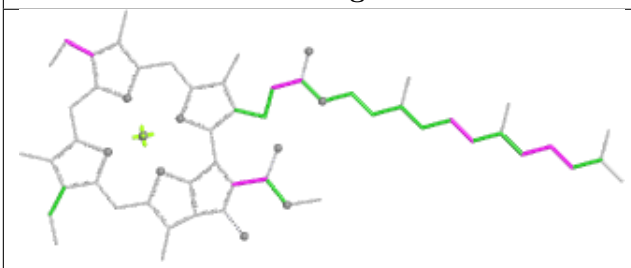
Ligand CLA u 308



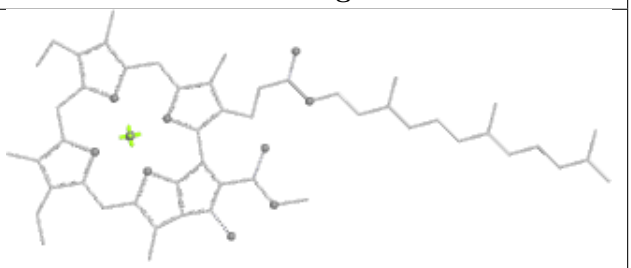
Bond lengths



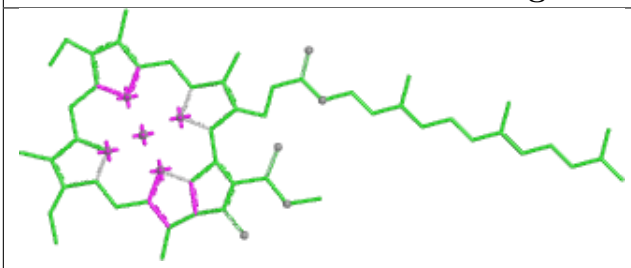
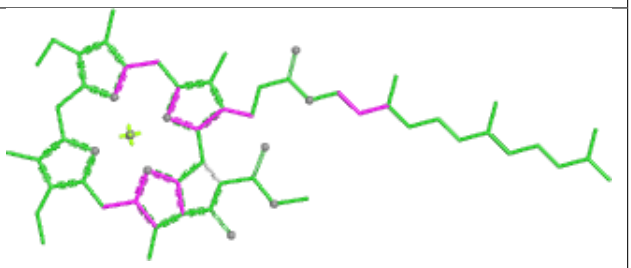
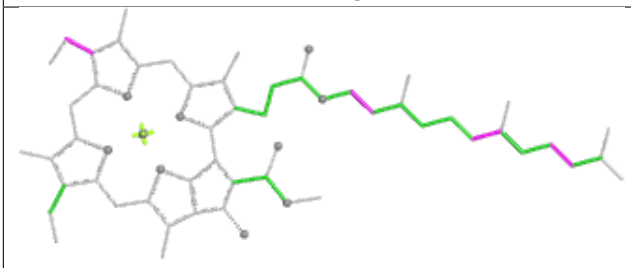
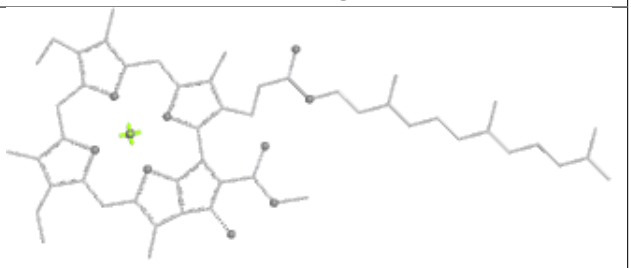
Bond angles

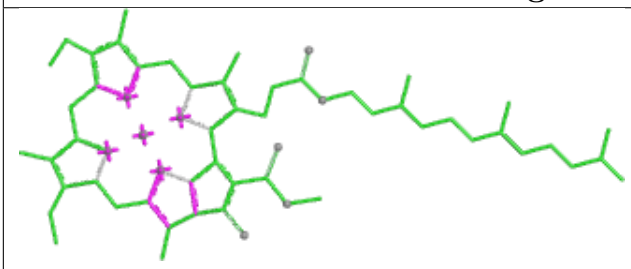
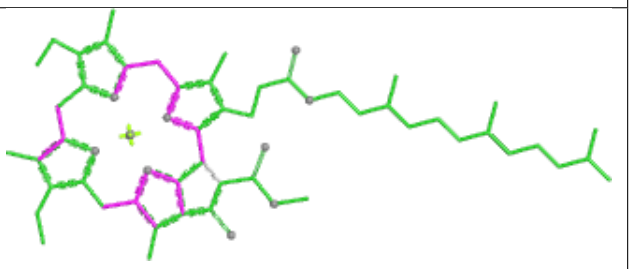
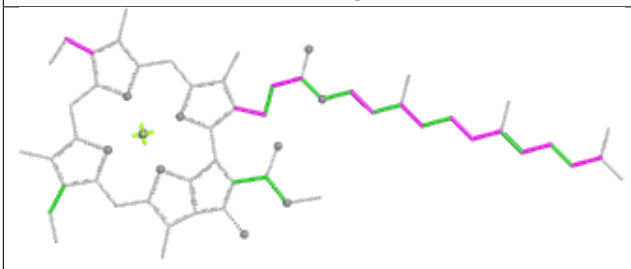
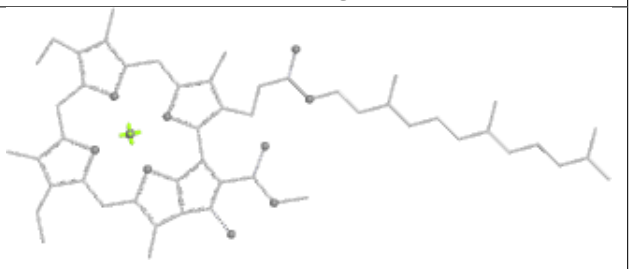


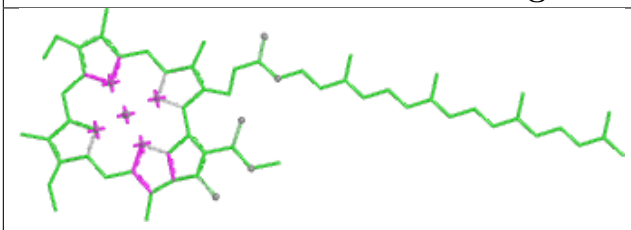
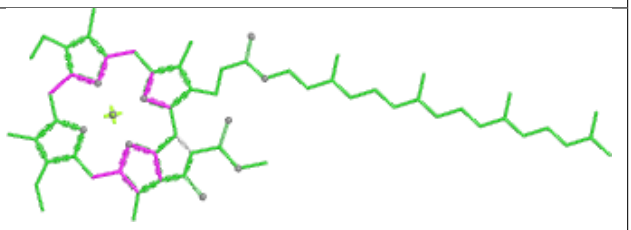
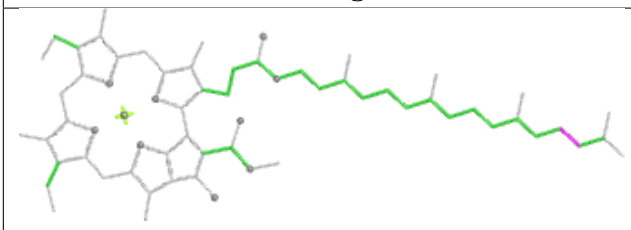
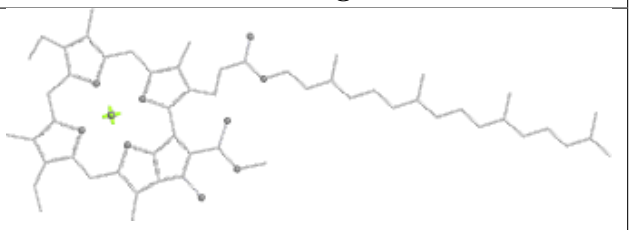
Torsions

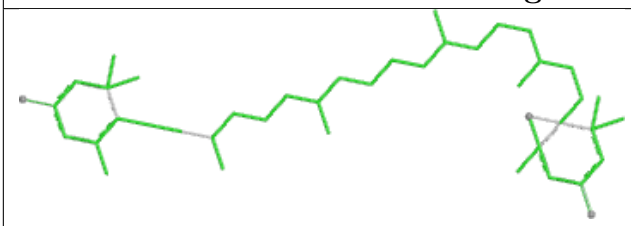
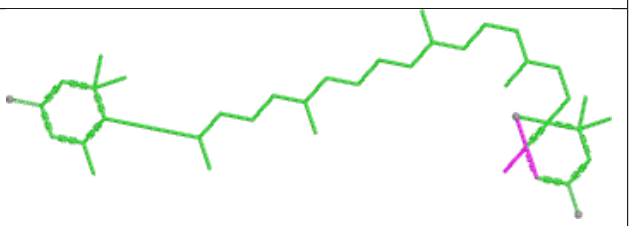
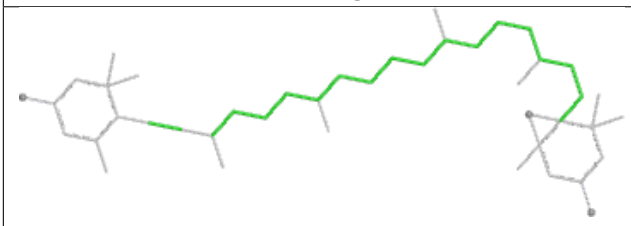
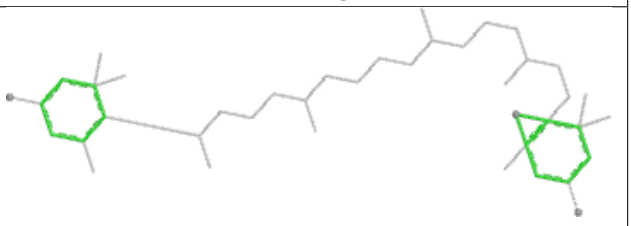


Rings

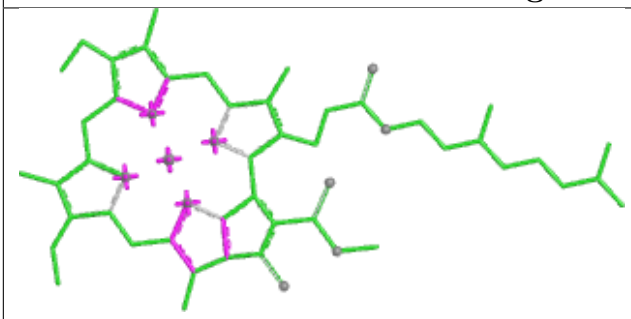
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA x 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

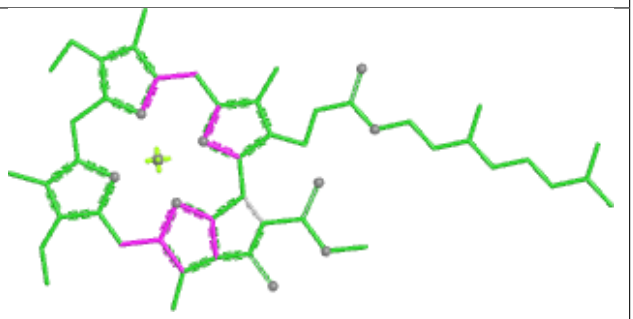
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand DD6 U 209	
	
Bond lengths	Bond angles
	
Torsions	Rings

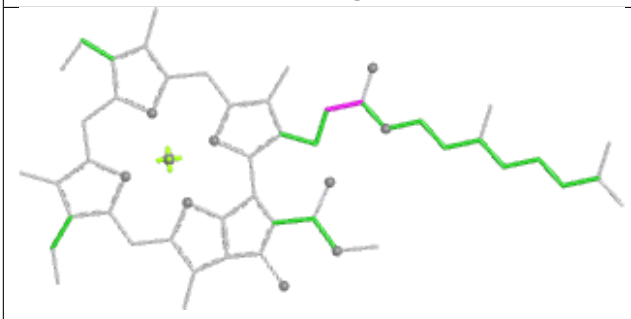
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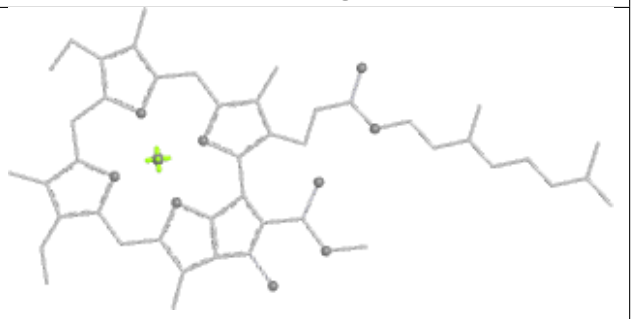
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Bond angles

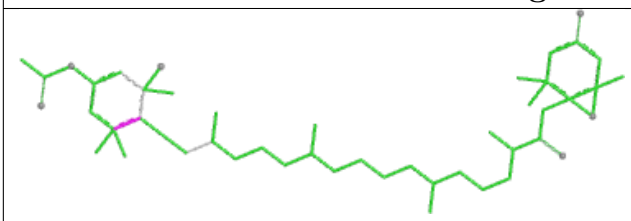


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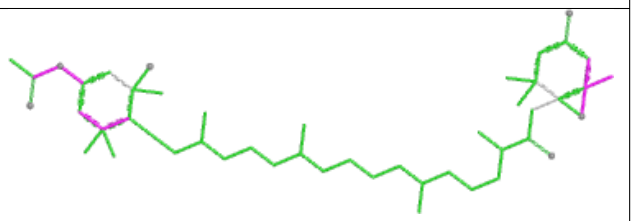


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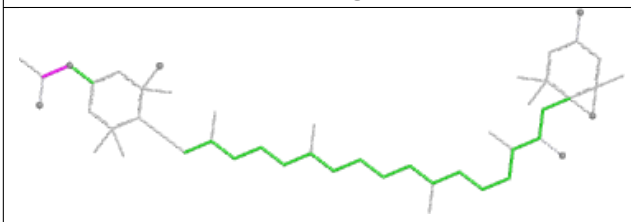
Ligand A86 N 314



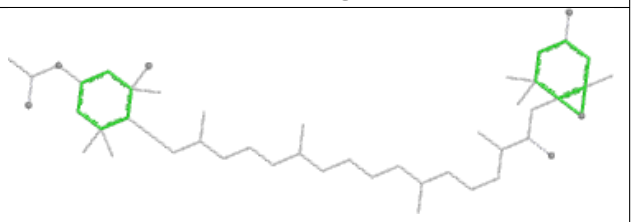
Bond lengths



Bond angles

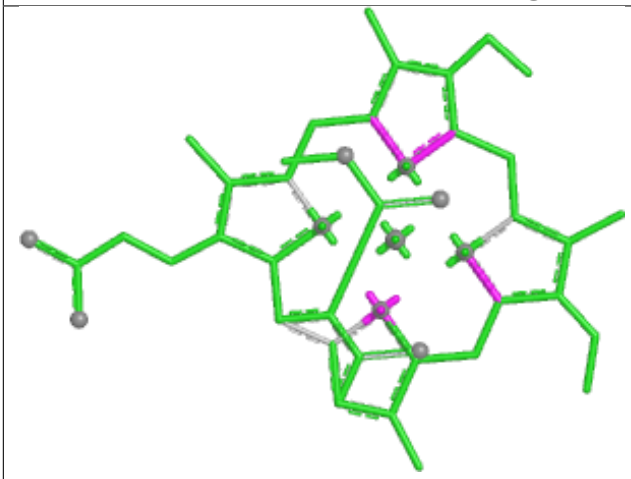


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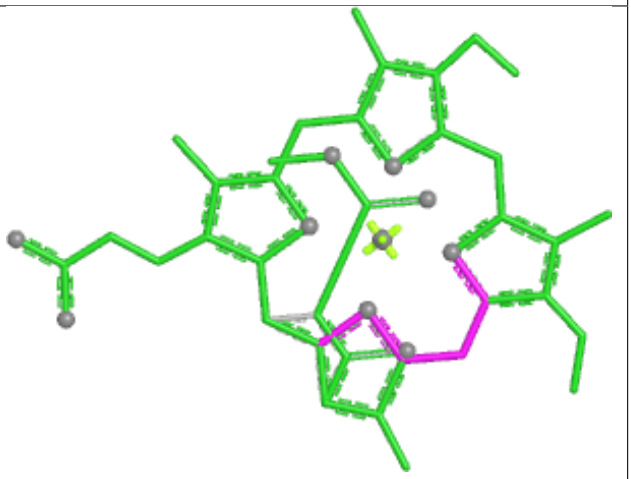


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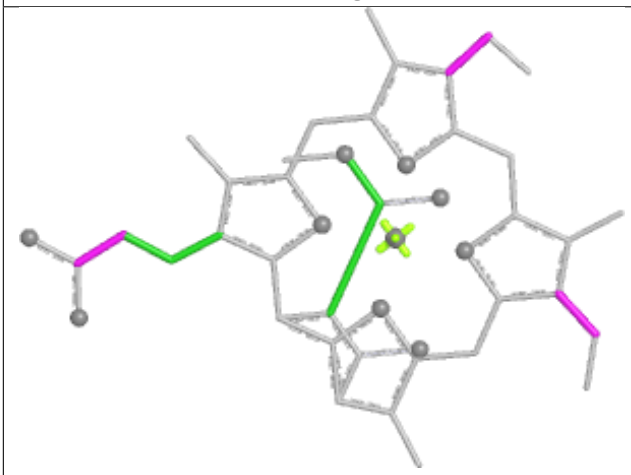
Ligand KC2 K 302



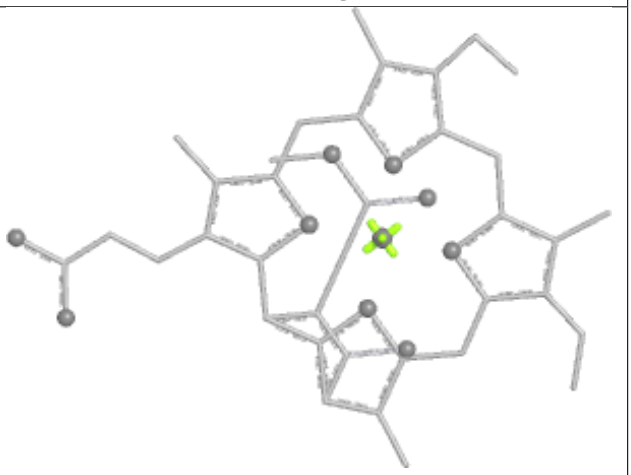
Bond lengths



Bond angles

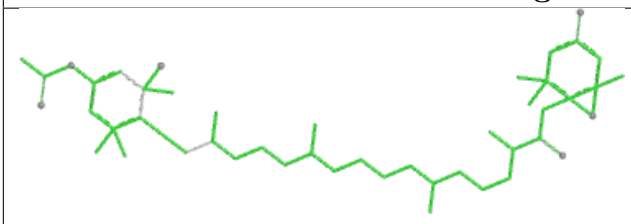


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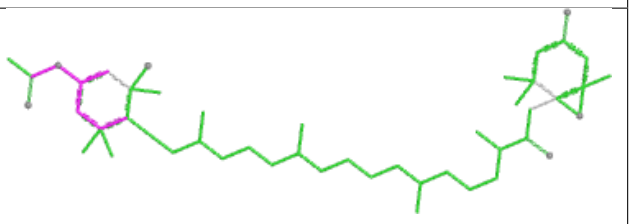


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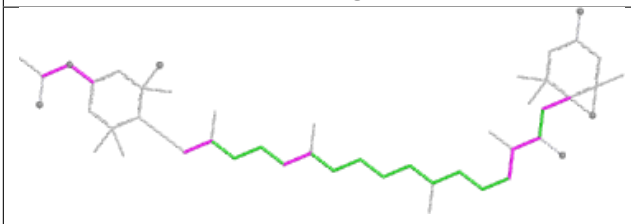
Ligand A86 v 319



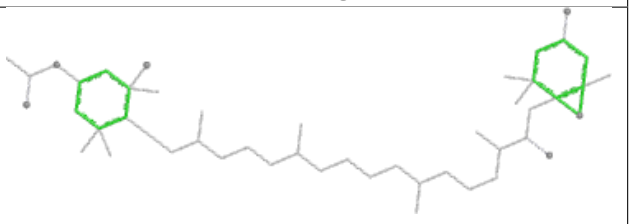
Bond lengths



Bond angles

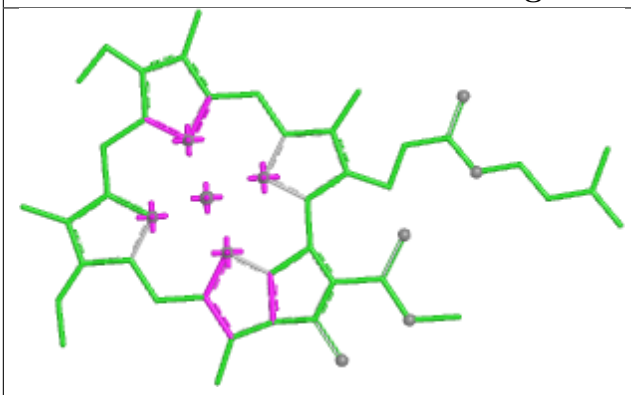


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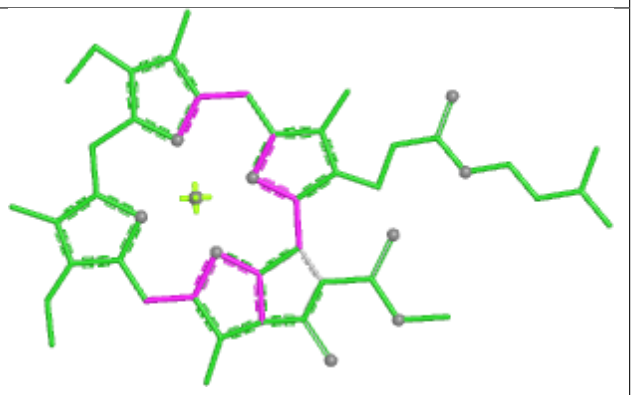


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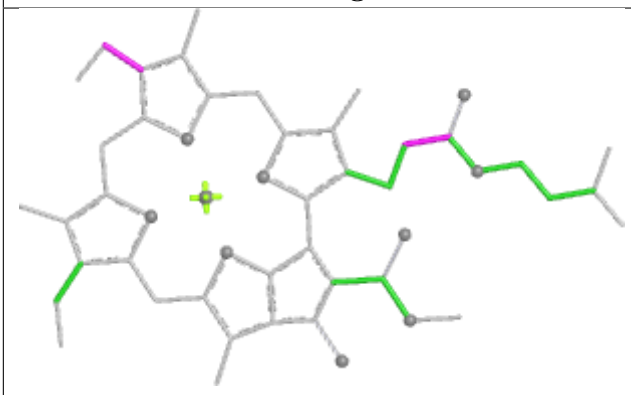
Ligand CLA T 305



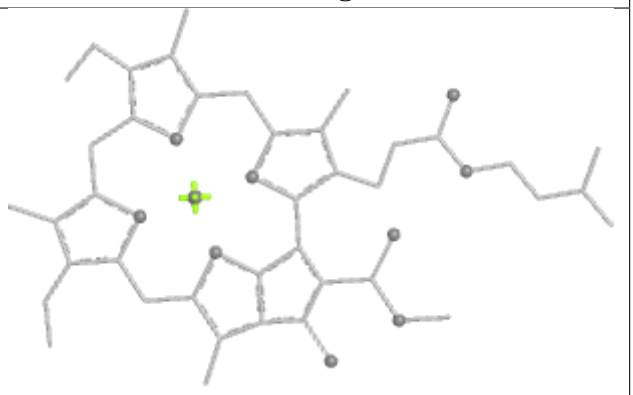
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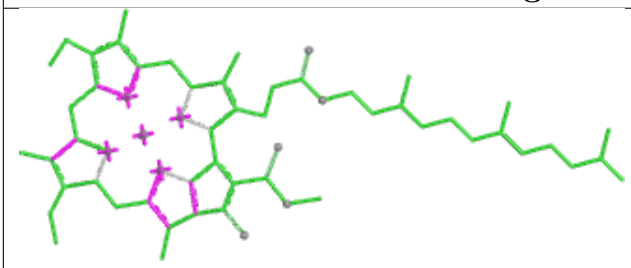


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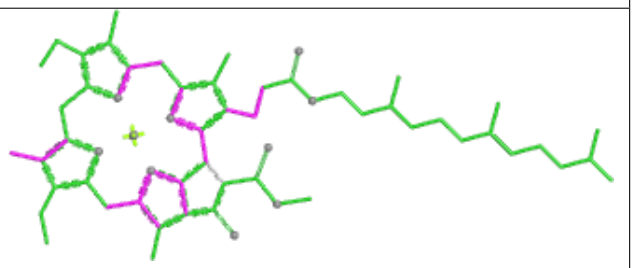


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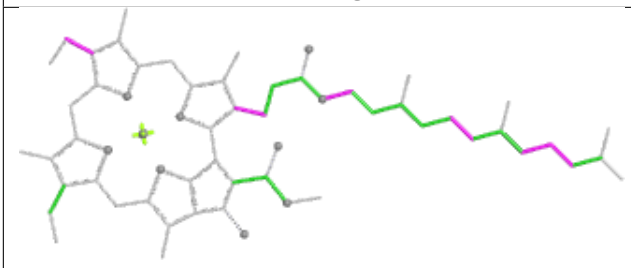
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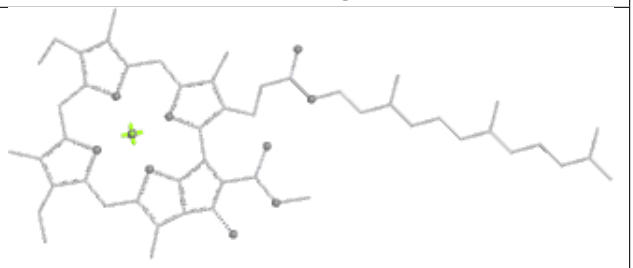
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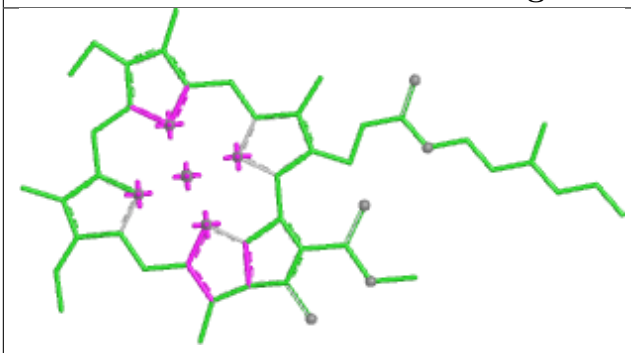


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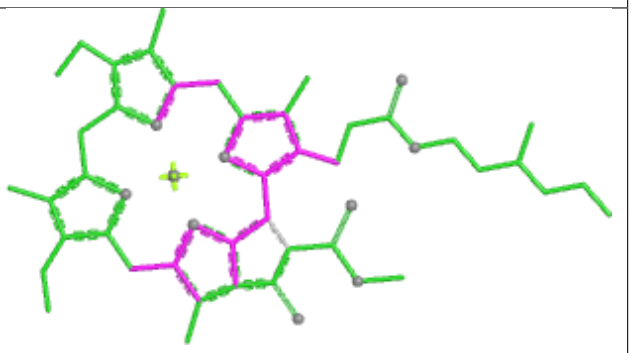


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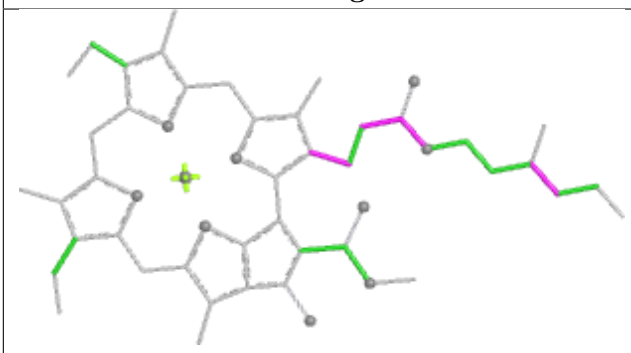
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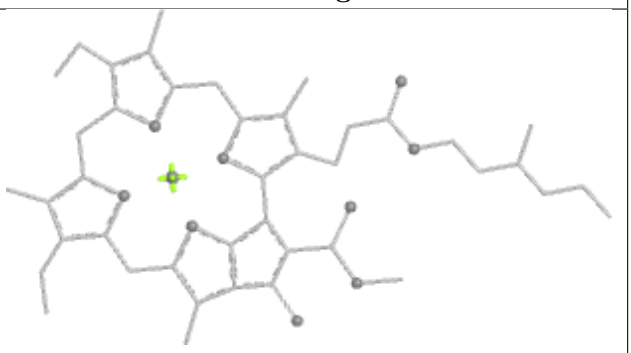
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Bond angles

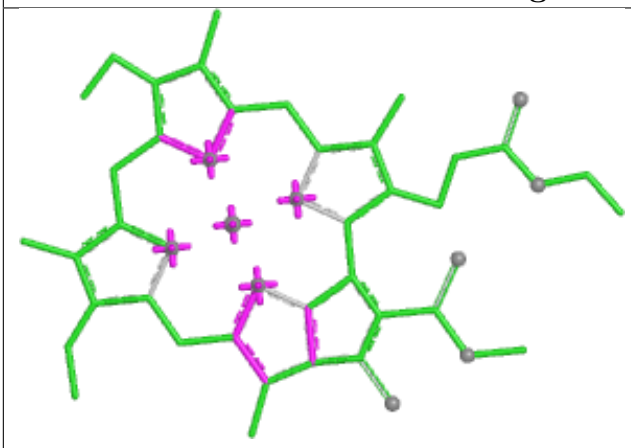


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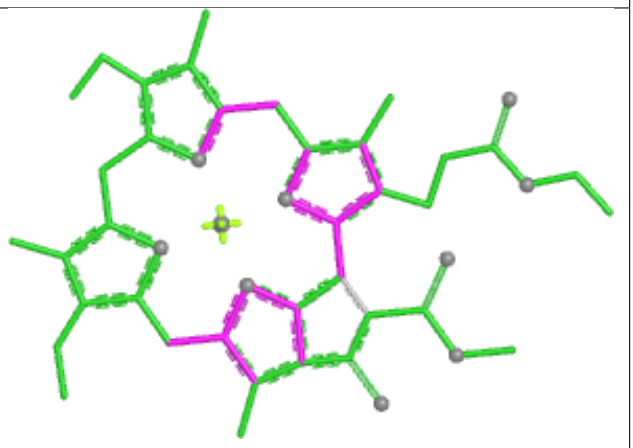


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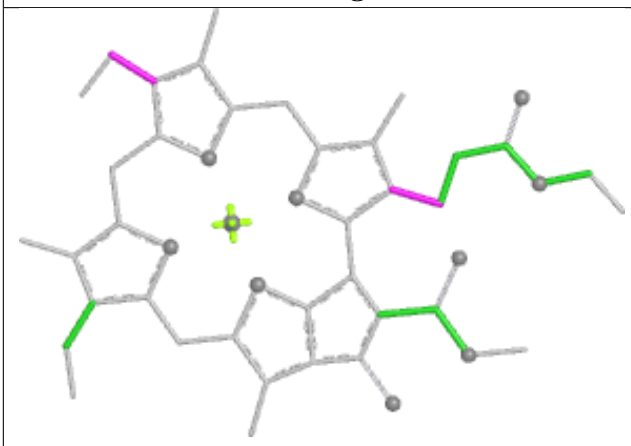
Ligand CLA z 313



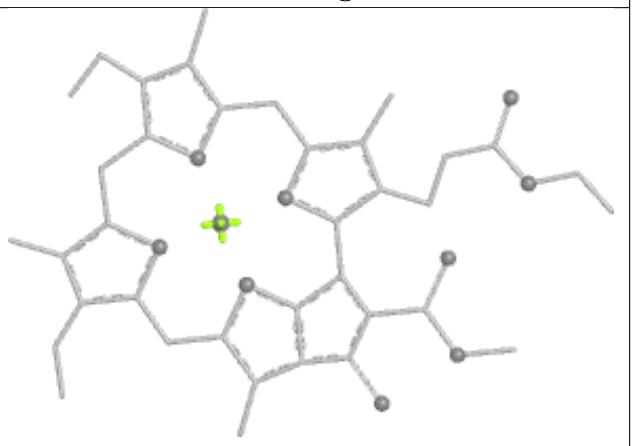
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Bond angles

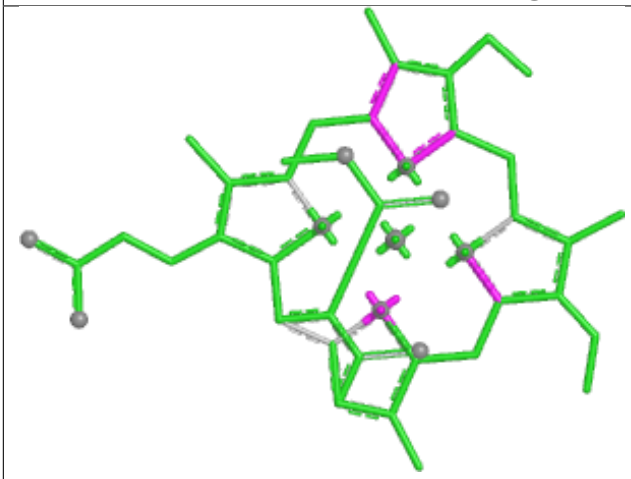


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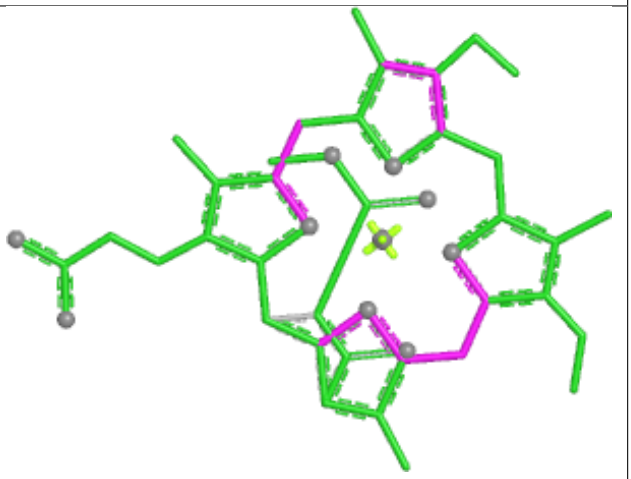


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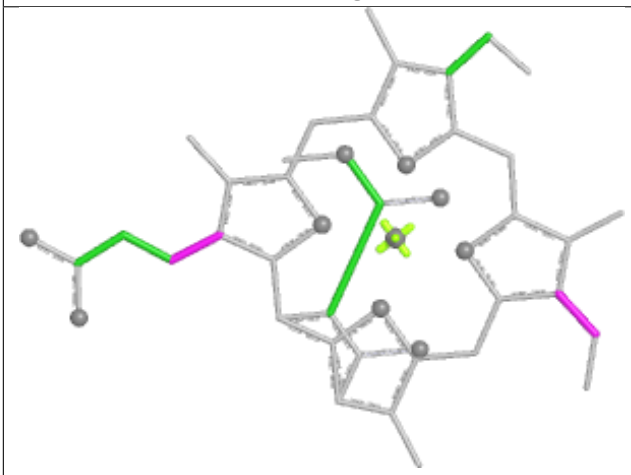
Ligand KC2 R 302



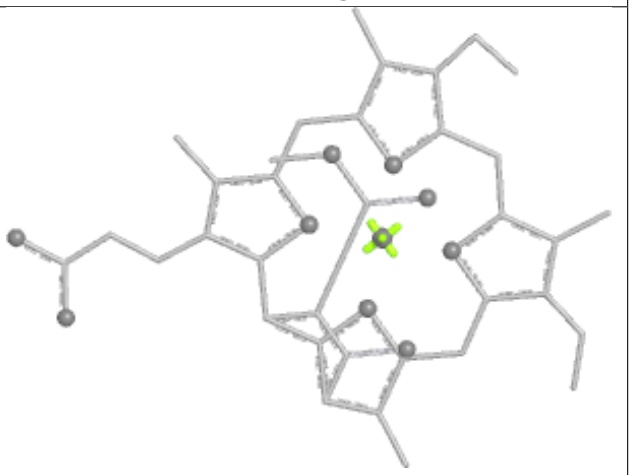
Bond lengths



Bond angles

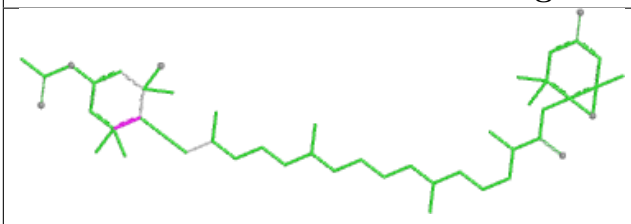


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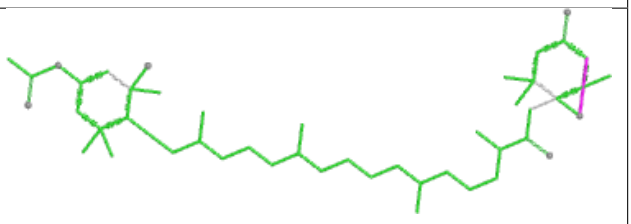


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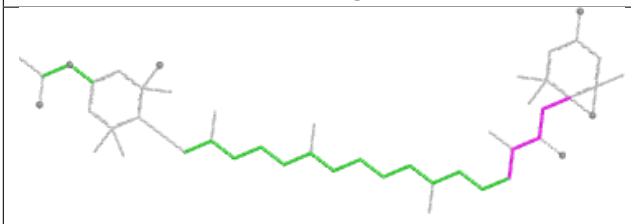
Ligand A86 z 319



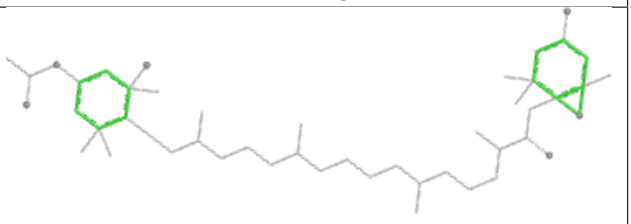
Bond lengths



Bond angles

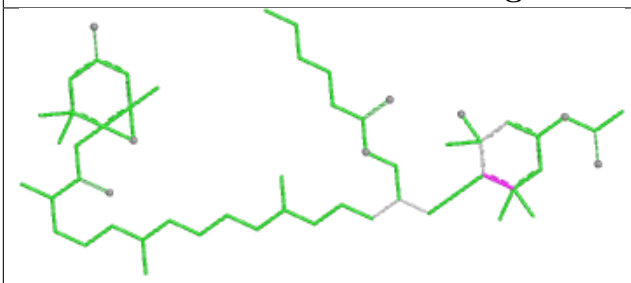


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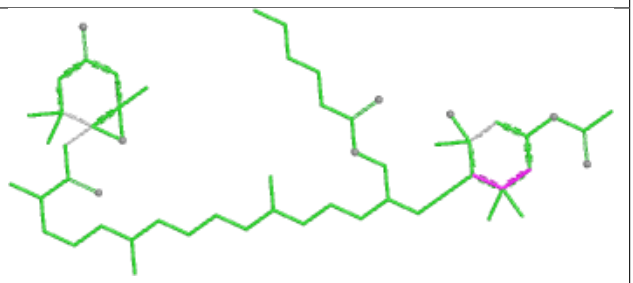


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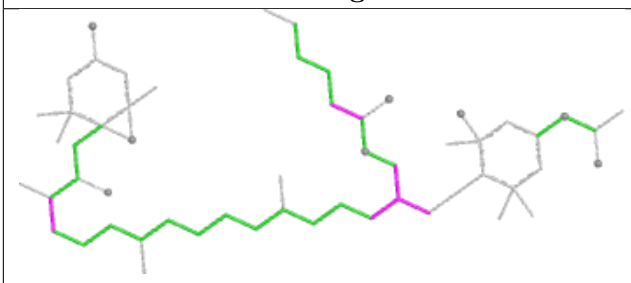
Ligand A1EB1 O 317



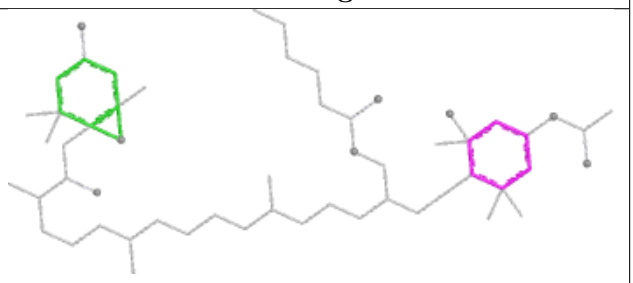
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Bond angles

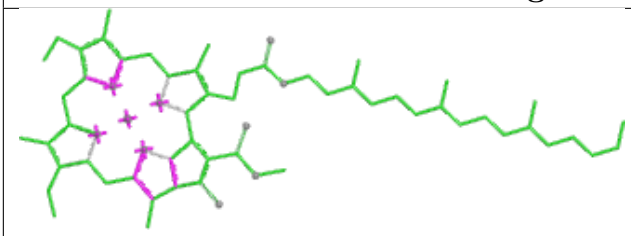


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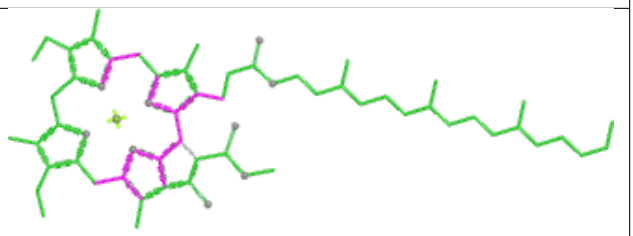


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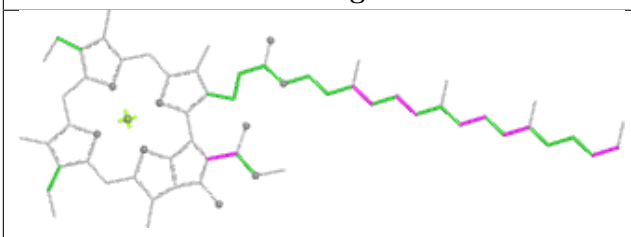
Ligand CLA b 822



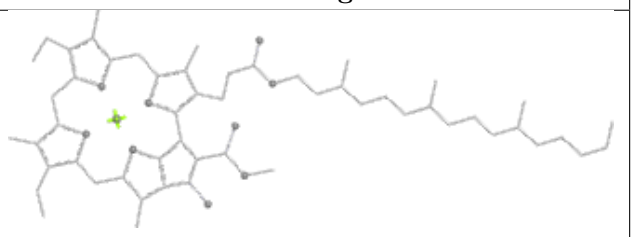
Bond lengths



Bond angles

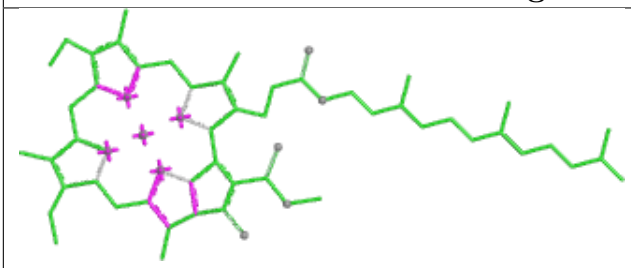


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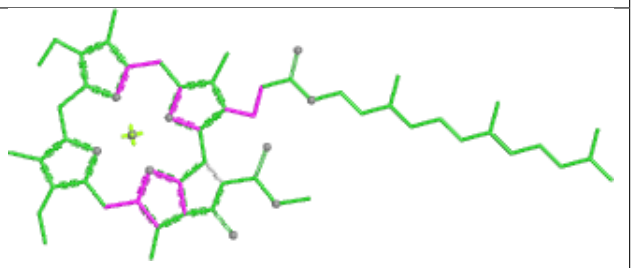


Rings

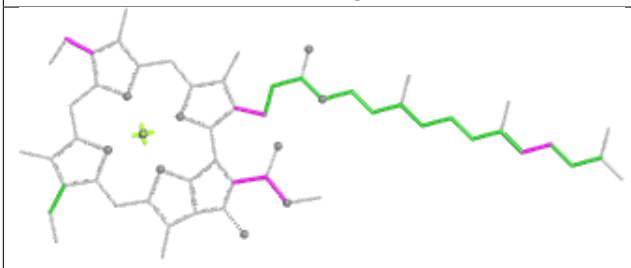
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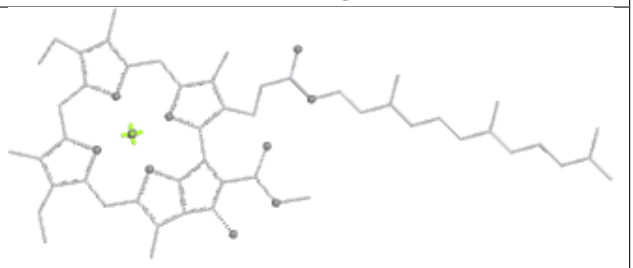
Bond lengths



Bond angles

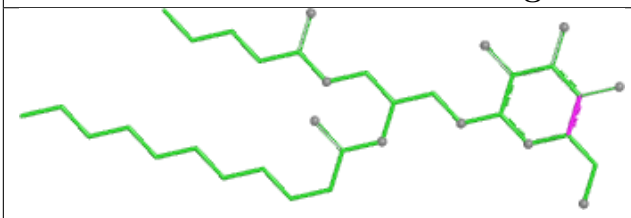


Torsions

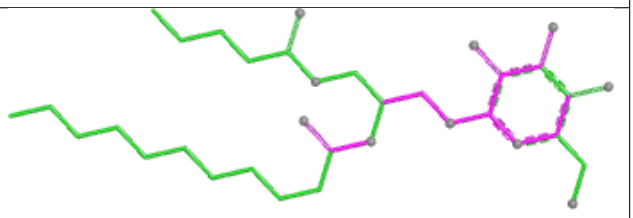


Rings

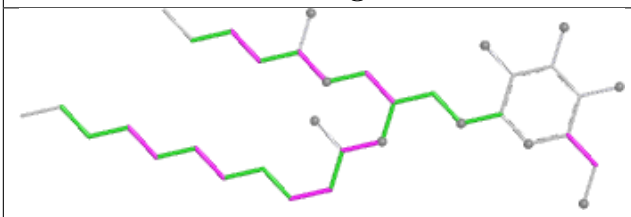
Ligand LMG a 802



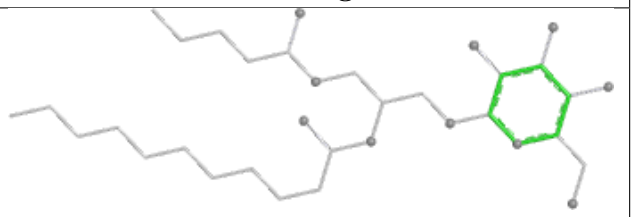
Bond lengths



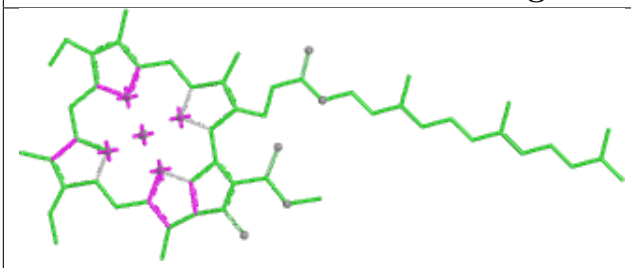
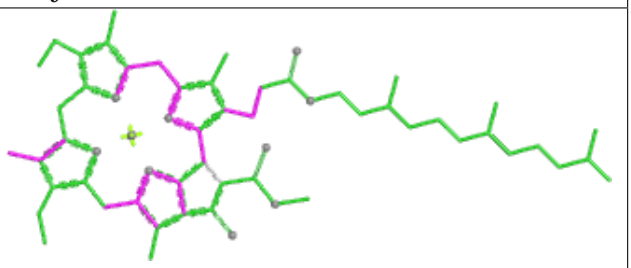
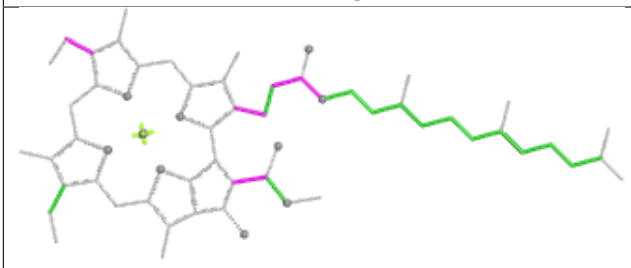
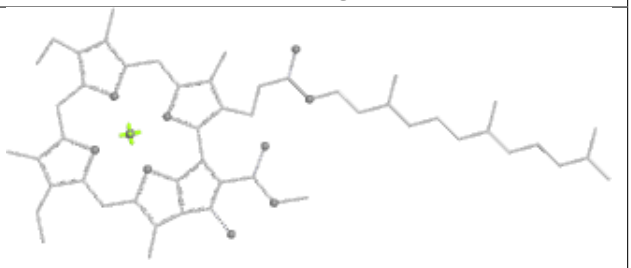
Bond angles

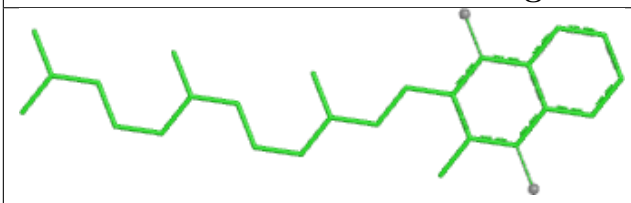
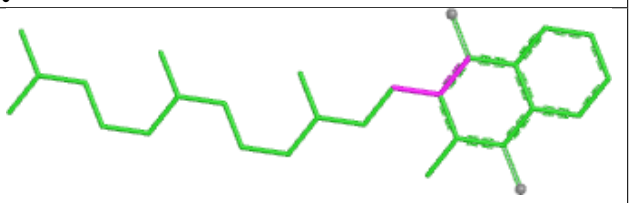
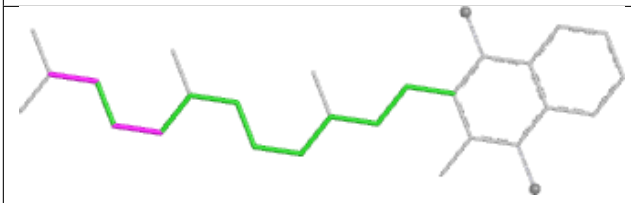
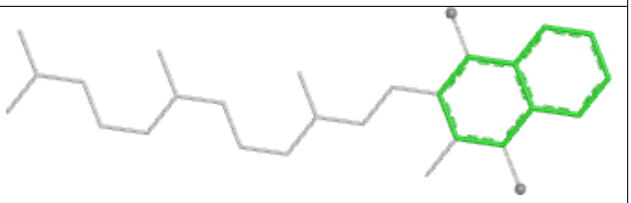


Torsions

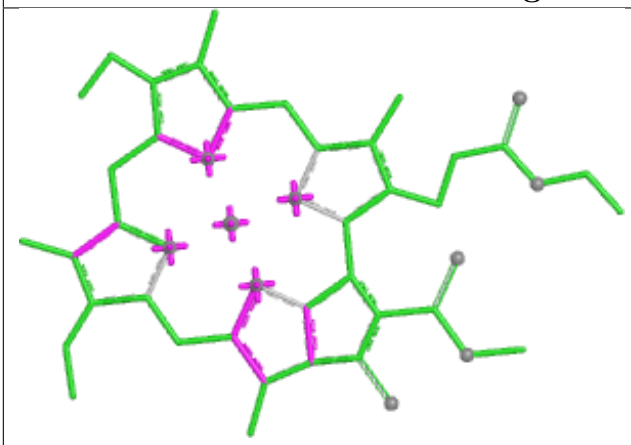


Rings

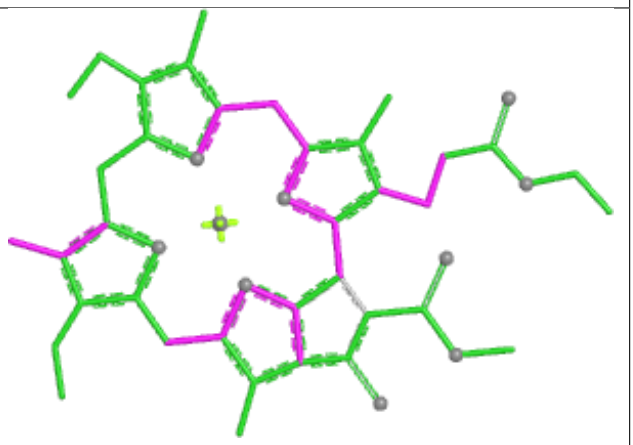
Ligand CLA y 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PQN b 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

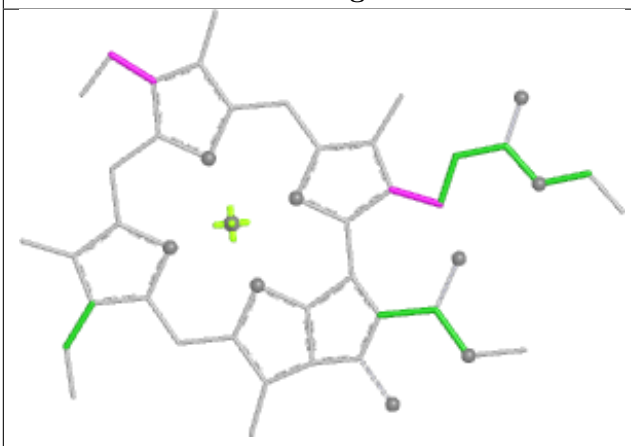
Ligand CLA H 304



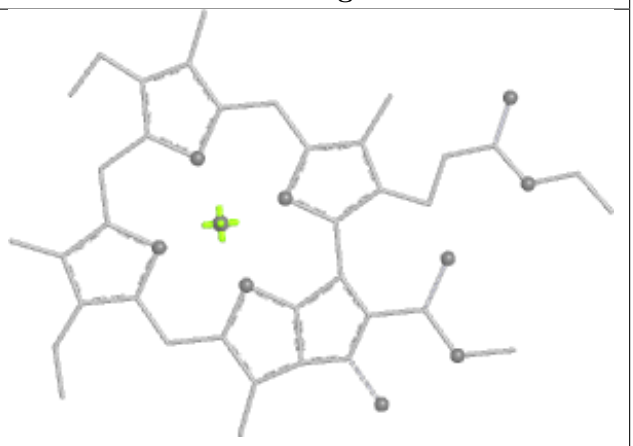
Bond lengths



Bond angles

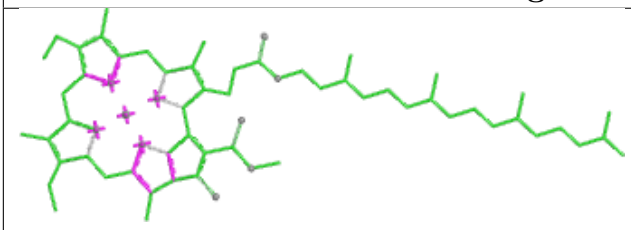


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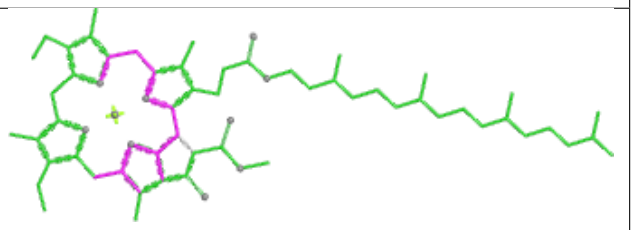


Rings

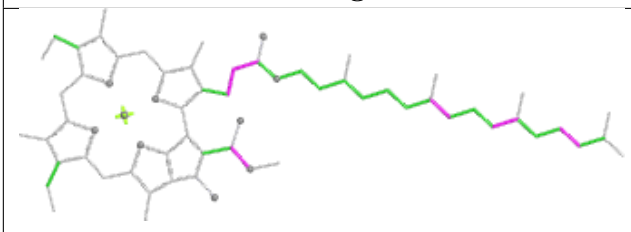
Ligand CLA b 808



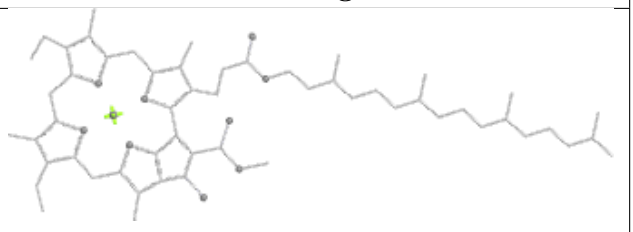
Bond lengths



Bond angles

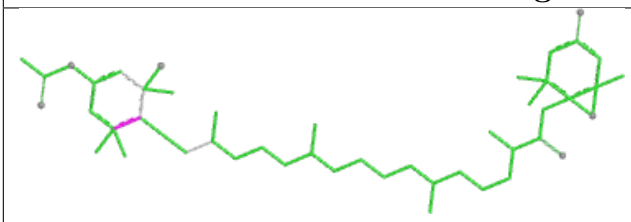


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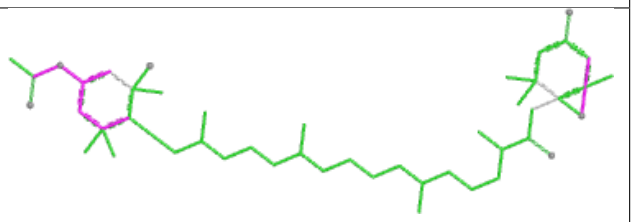


Rings

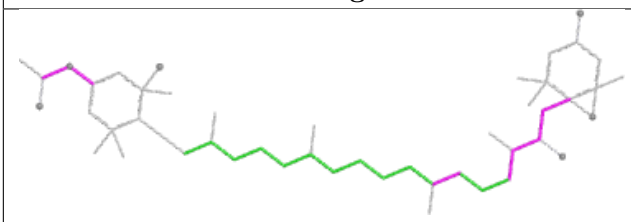
Ligand A86 o 314



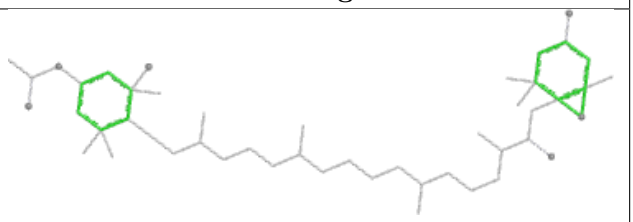
Bond lengths



Bond angles

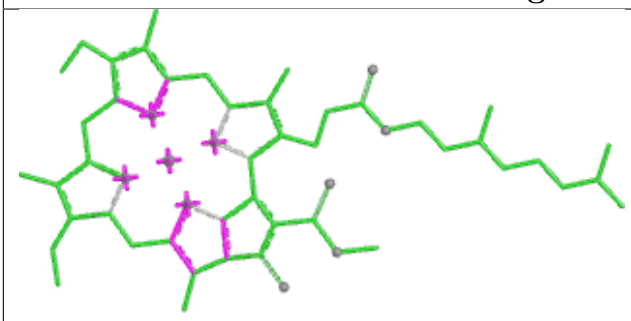


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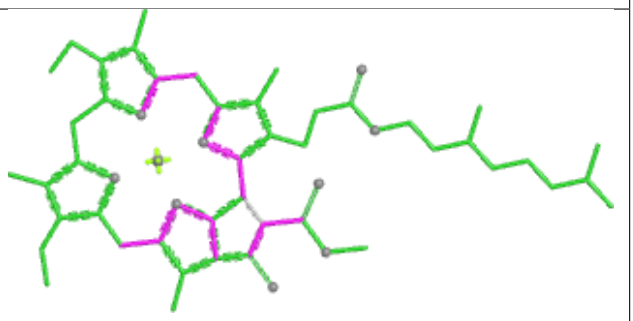


Rings

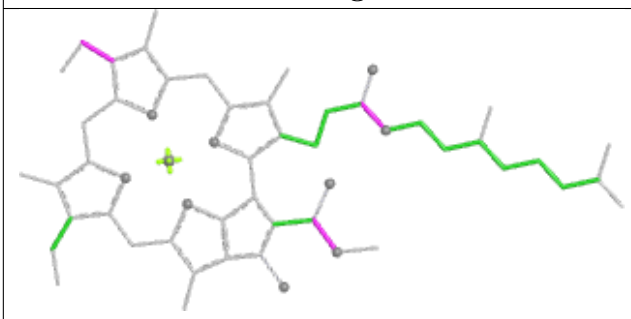
Ligand CLA x 313



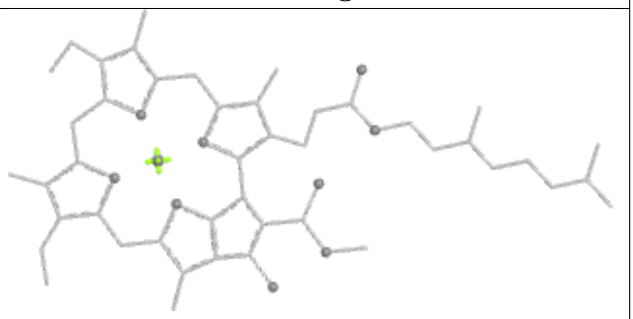
Bond lengths



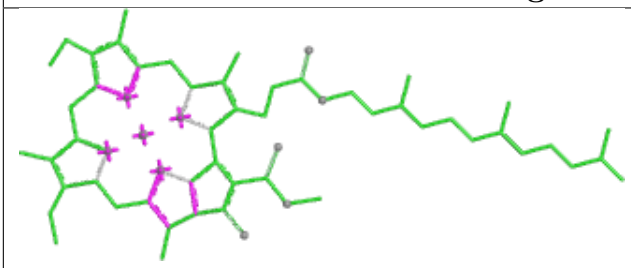
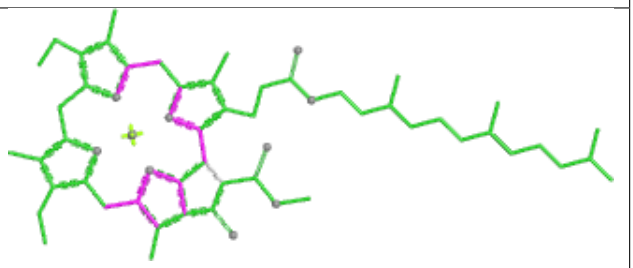
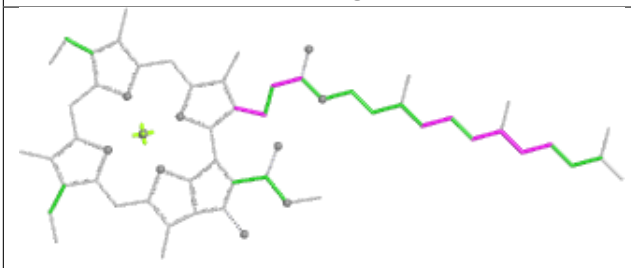
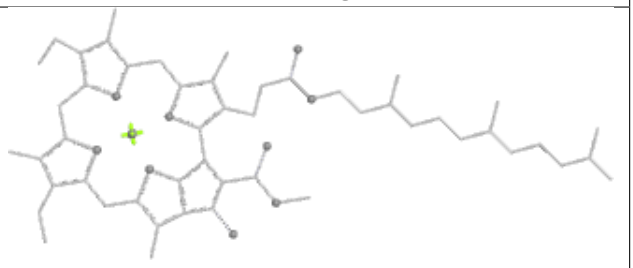
Bond angles

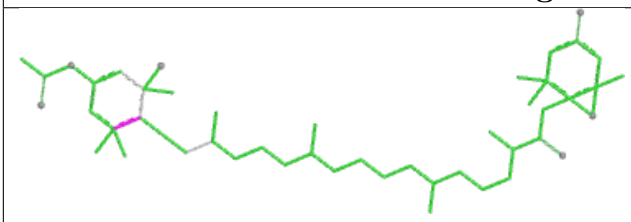
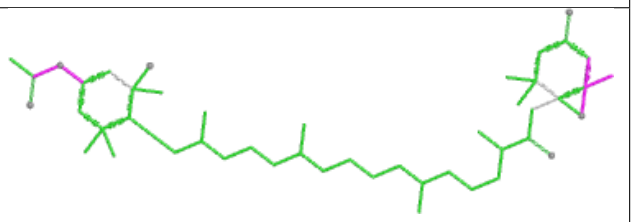
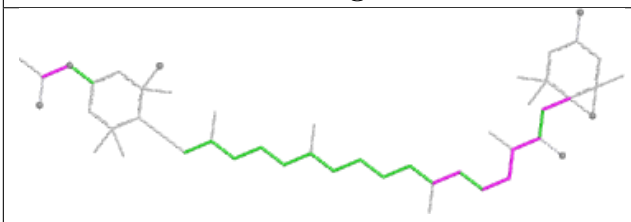
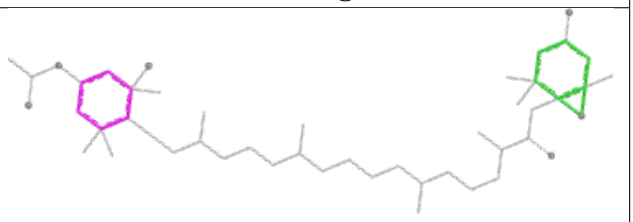


Torsions

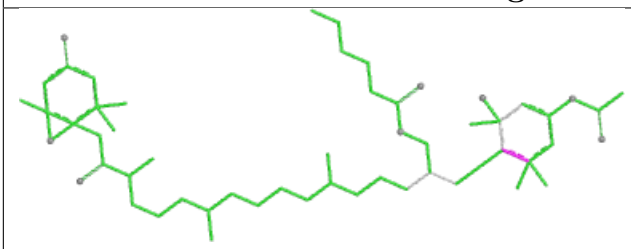


Rings

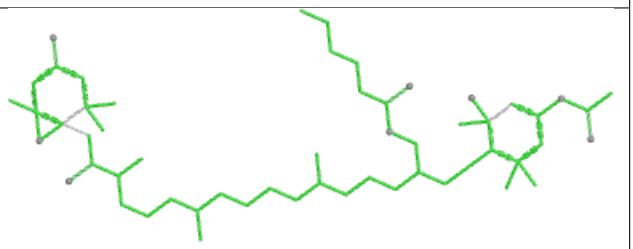
Ligand CLA b 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A86 t 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

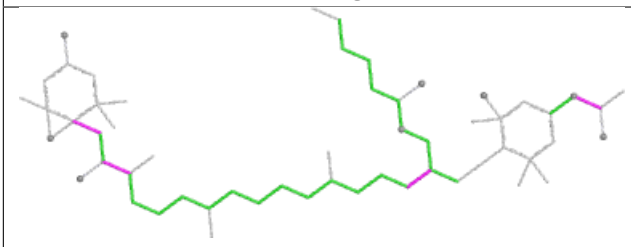
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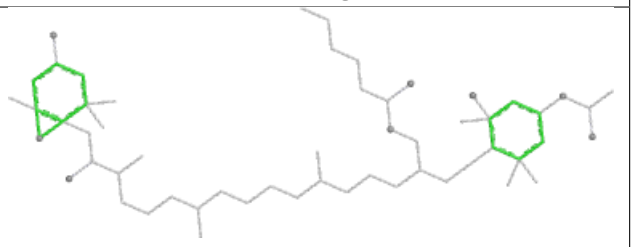
Bond lengths



Bond angles

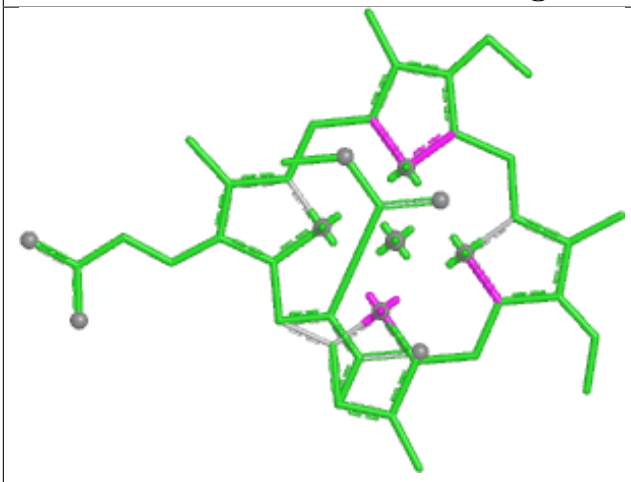


Torsions

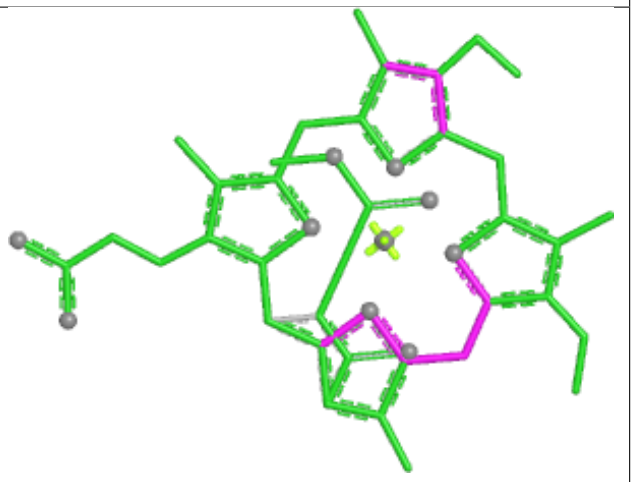


Rings

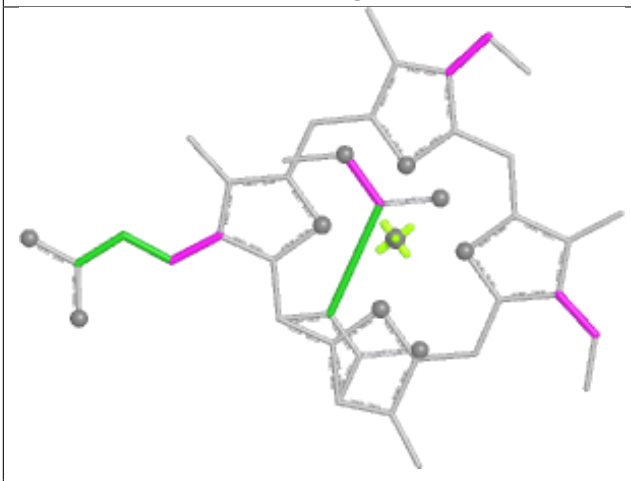
Ligand KC2 x 310



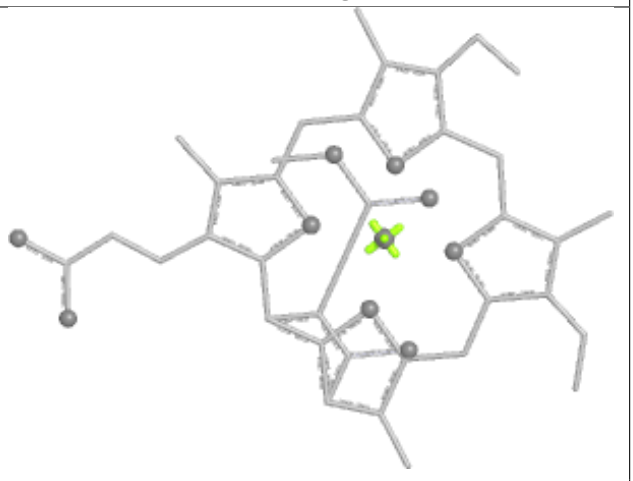
Bond lengths



Bond angles

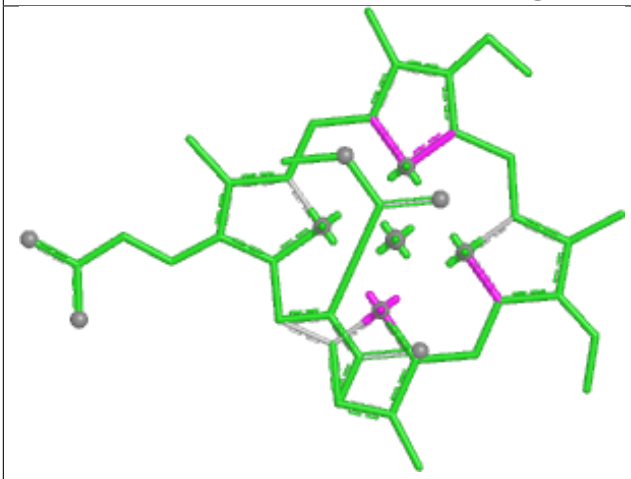


Torsions

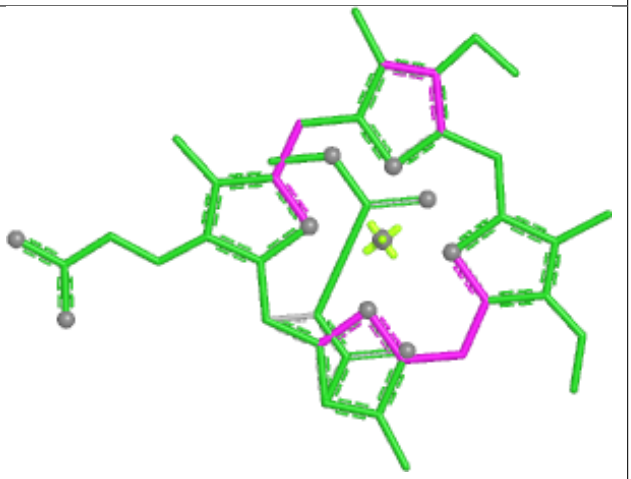


Rings

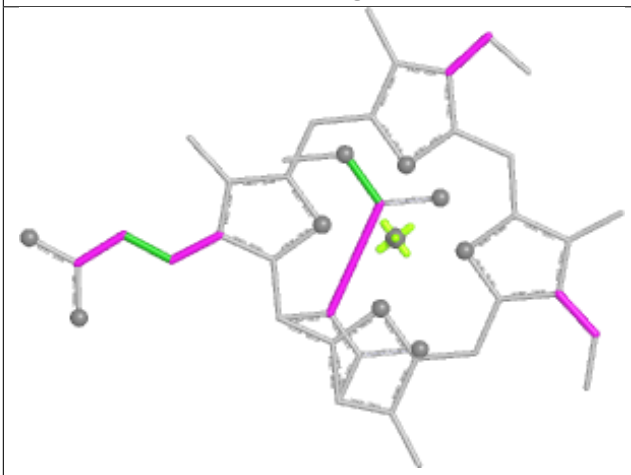
Ligand KC2 S 309



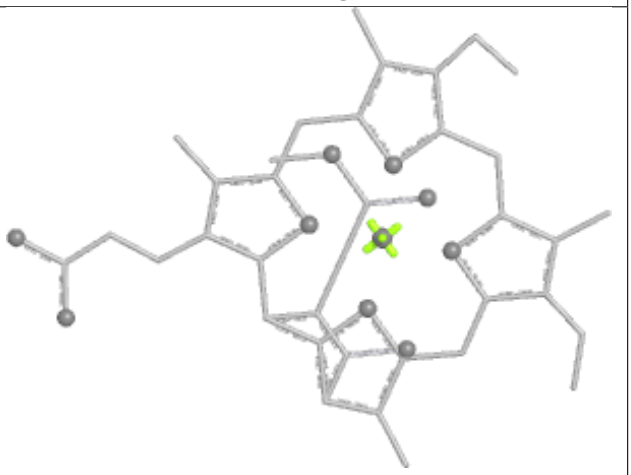
Bond lengths



Bond angles

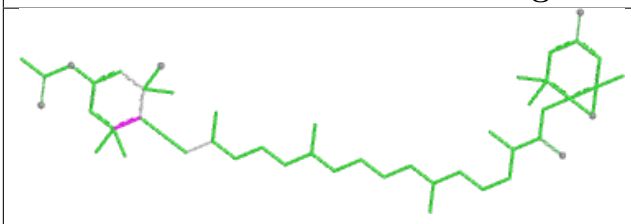


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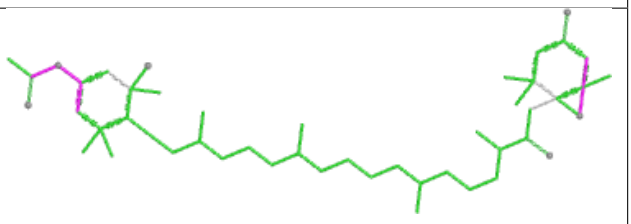


Rings

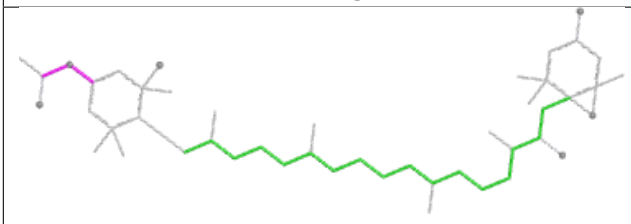
Ligand A86 Z 314



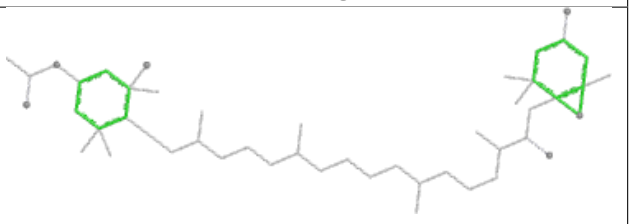
Bond lengths



Bond angles

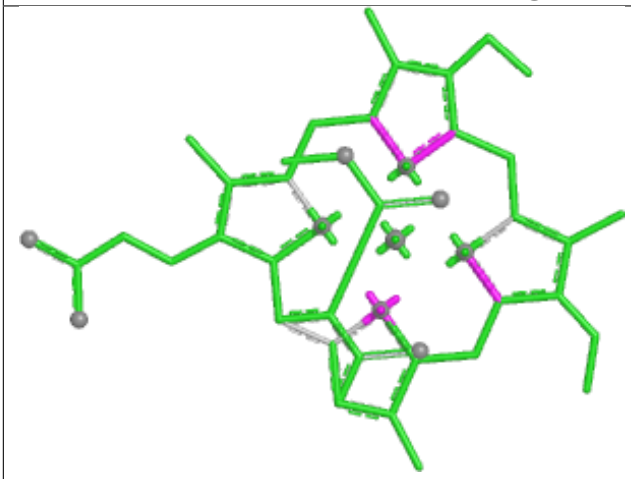


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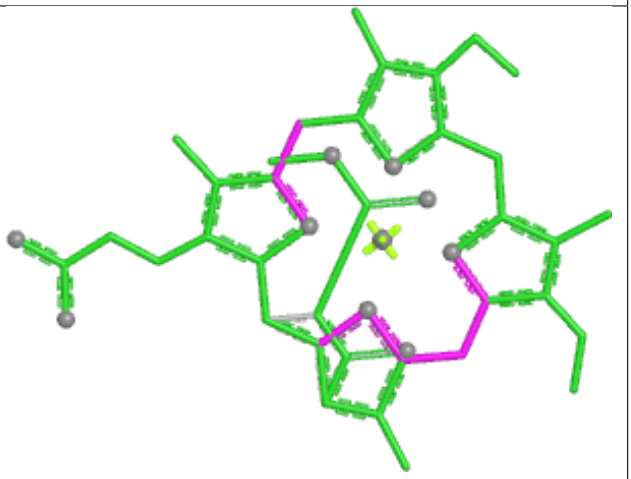


Rings

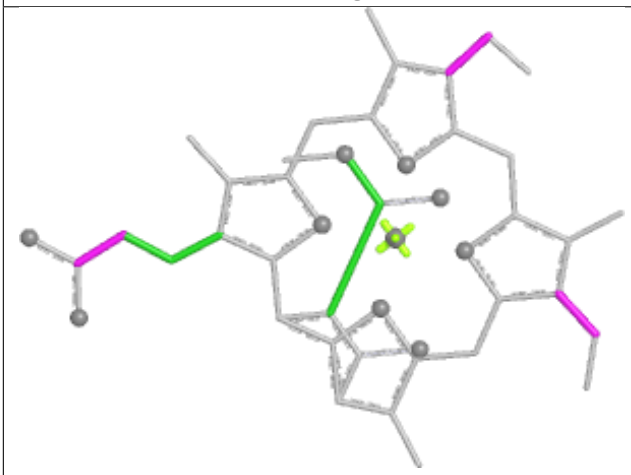
Ligand KC2 O 311



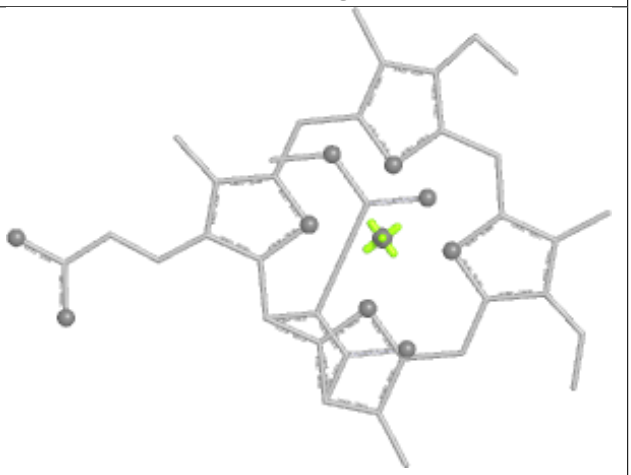
Bond lengths



Bond angles

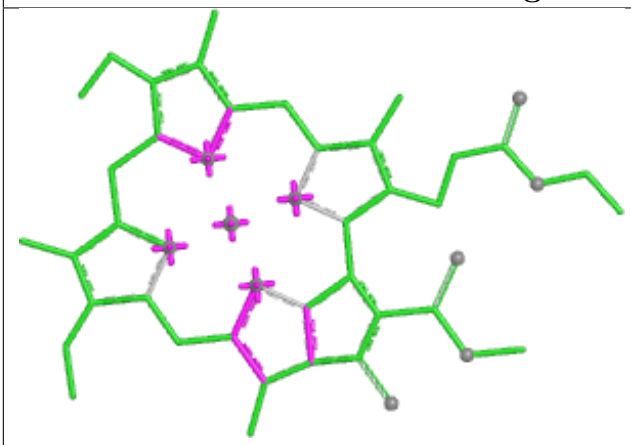


Torsions

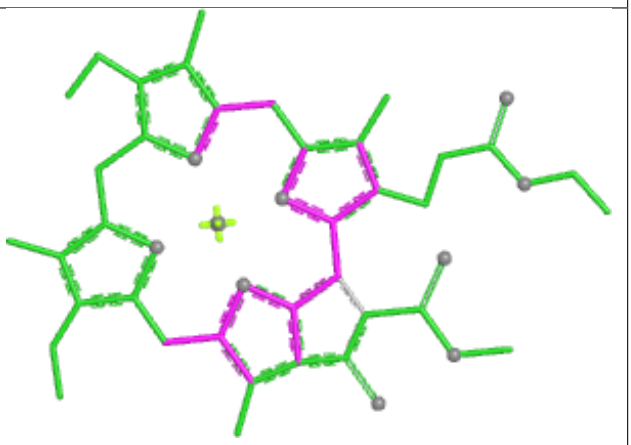


Rings

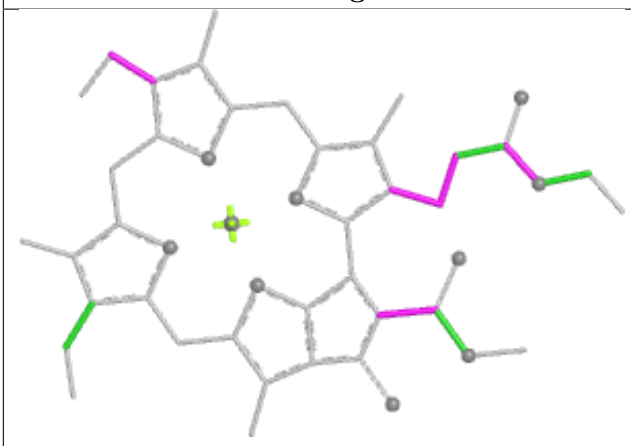
Ligand CLA Y 313



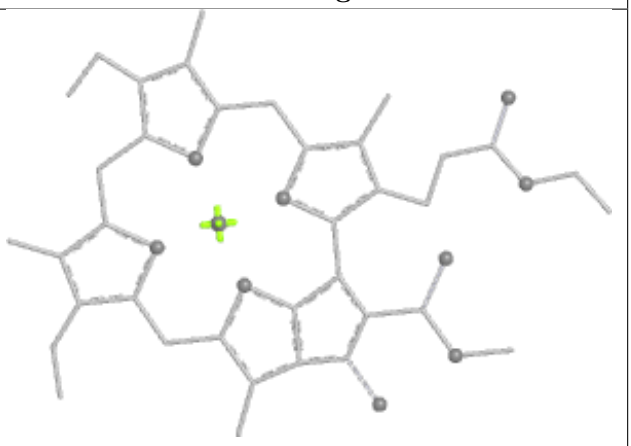
Bond lengths



Bond angles

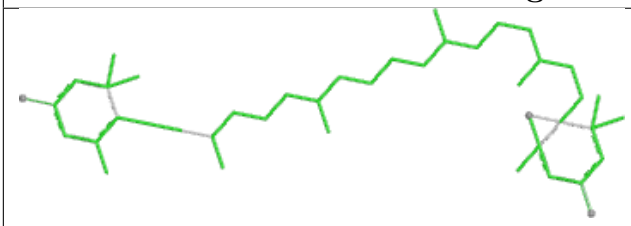


Torsions



Rings

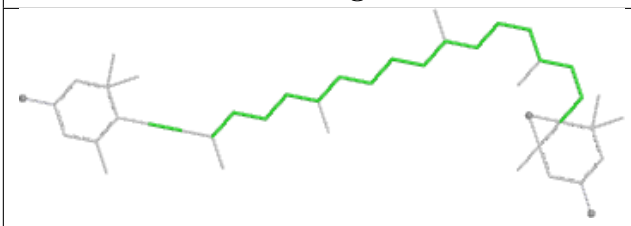
Ligand DD6 E 316



Bond lengths



Bond angles

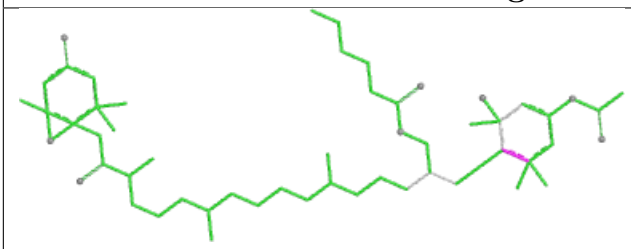


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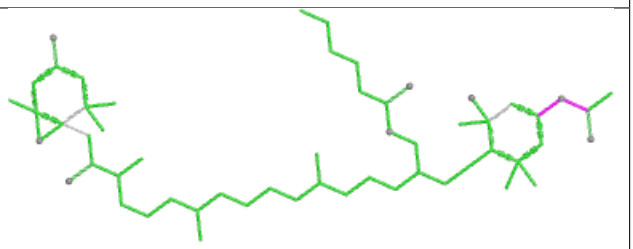


Rings

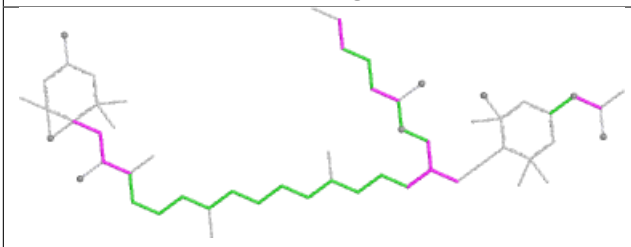
Ligand A1EB1 L 318



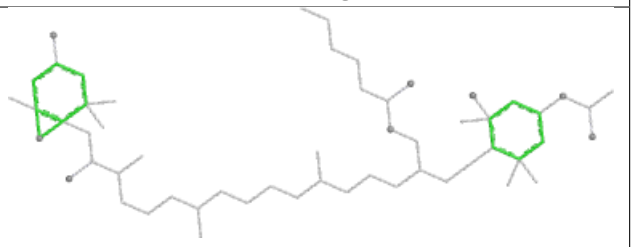
Bond lengths



Bond angles

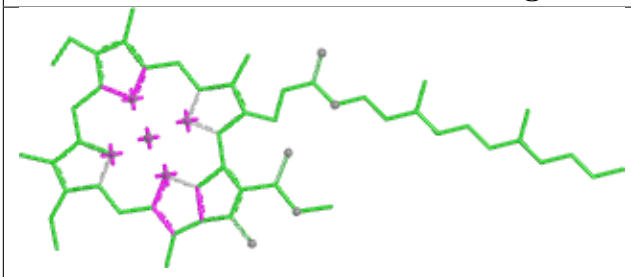


Torsions

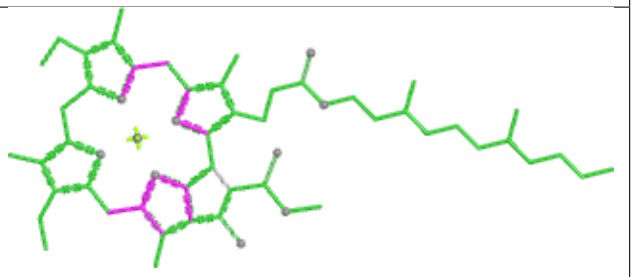


Rings

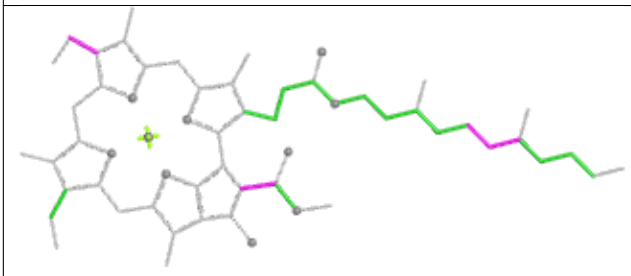
Ligand CLA D 309



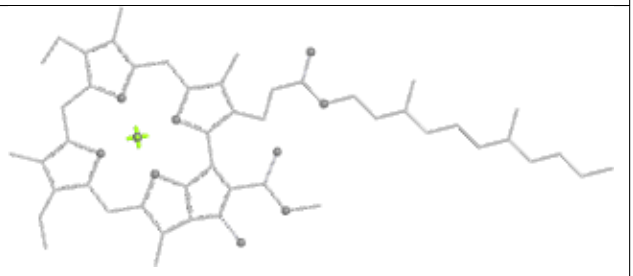
Bond lengths



Bond angles

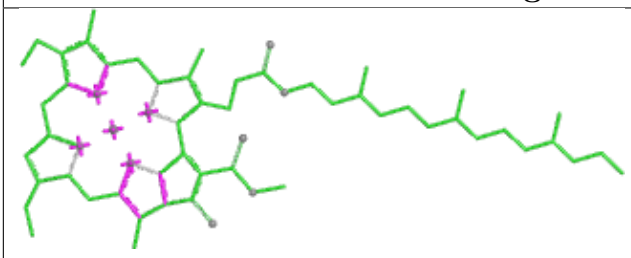


Torsions

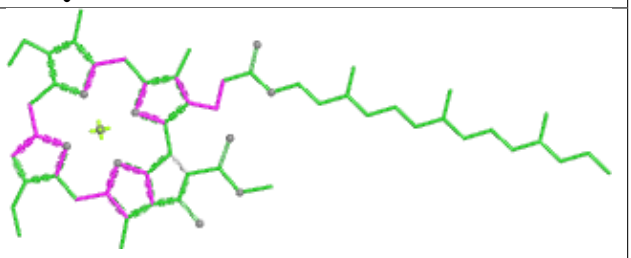


Rings

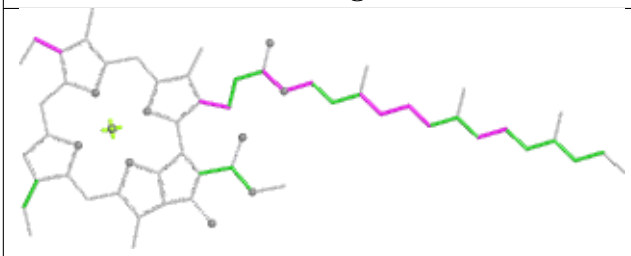
Ligand CLA Q 205



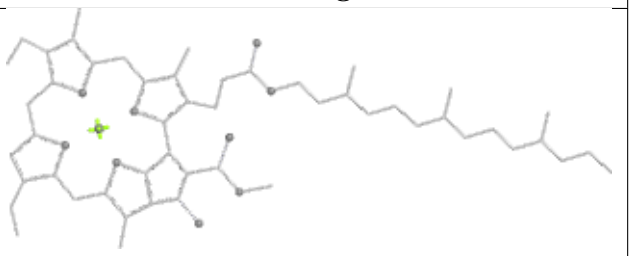
Bond lengths



Bond angles

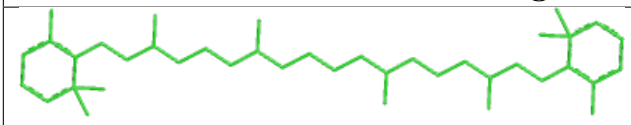


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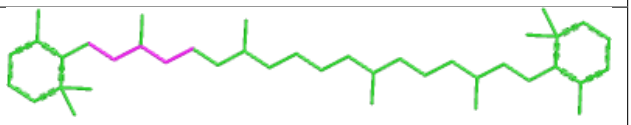


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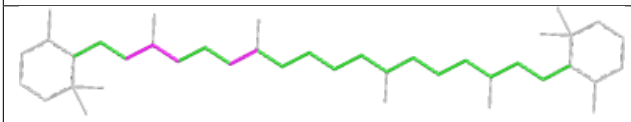
Ligand BCR l 207



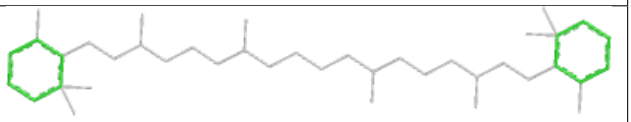
Bond lengths



Bond angles

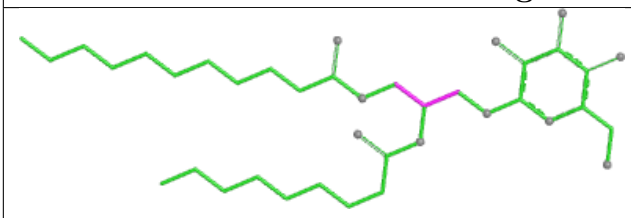


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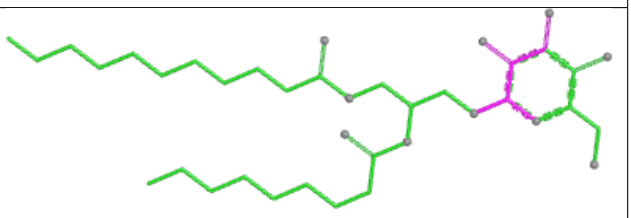


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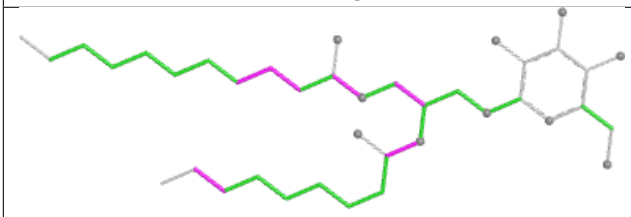
Ligand LMG M 317



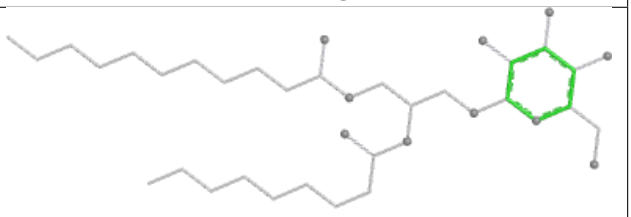
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Bond angles

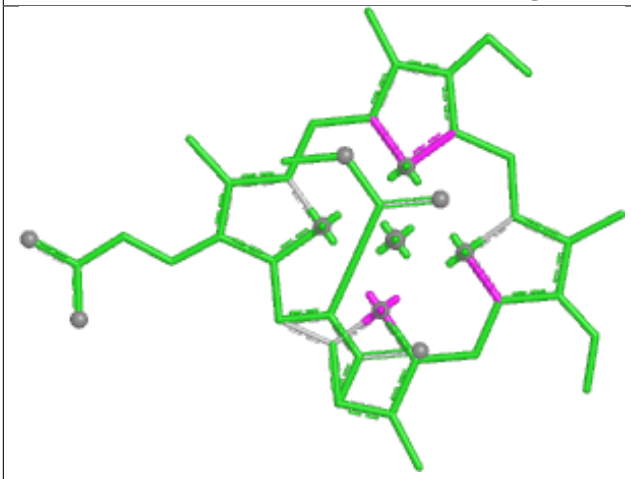


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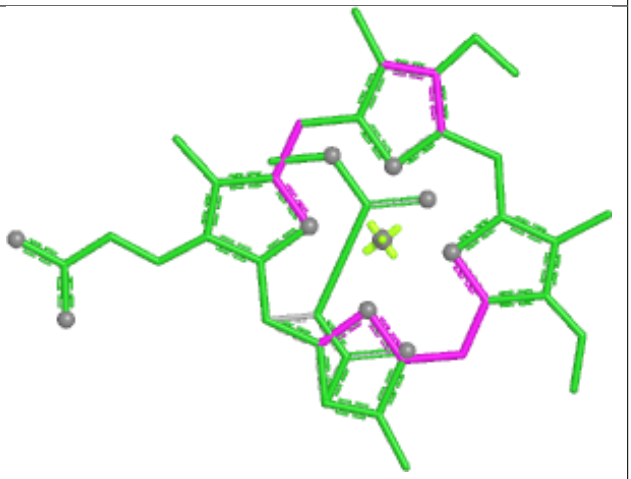


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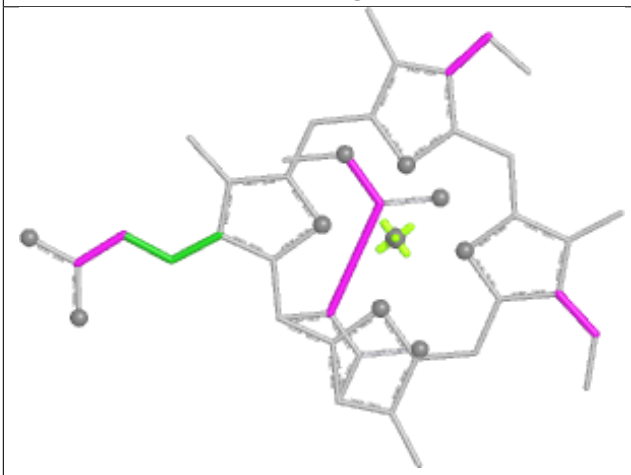
Ligand KC2 w 306



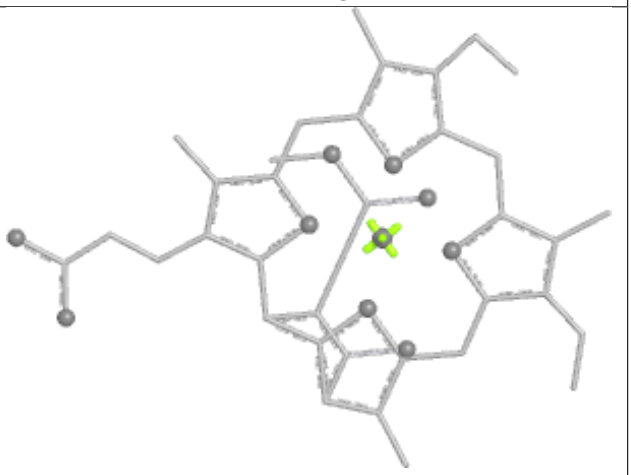
Bond lengths



Bond angles

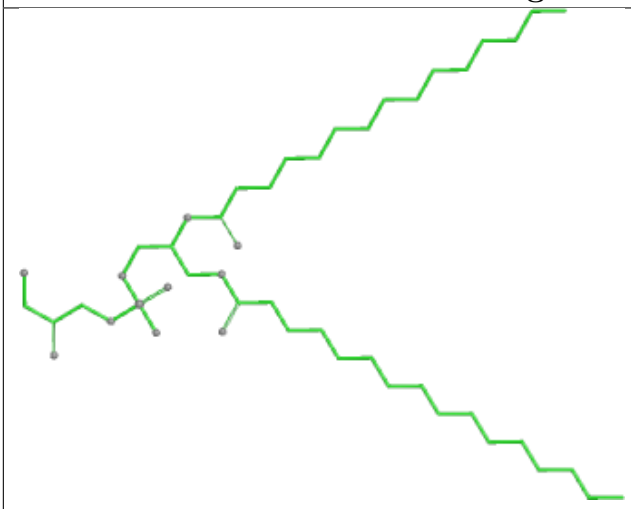


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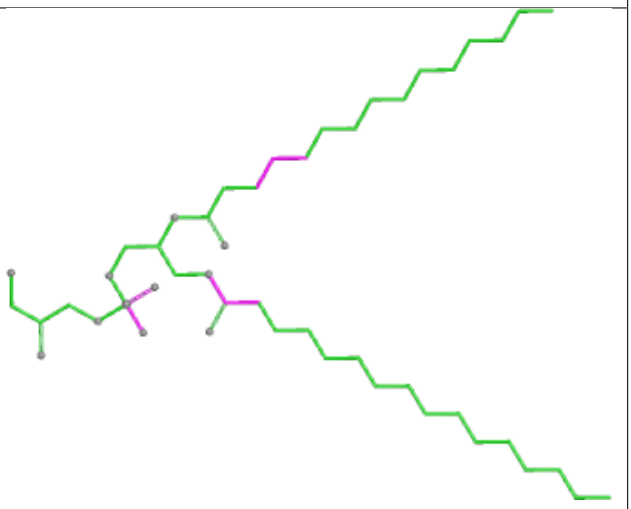


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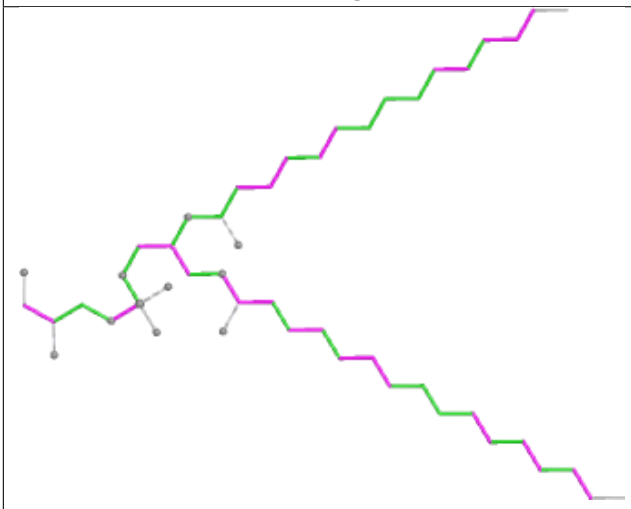
Ligand LHG a 848



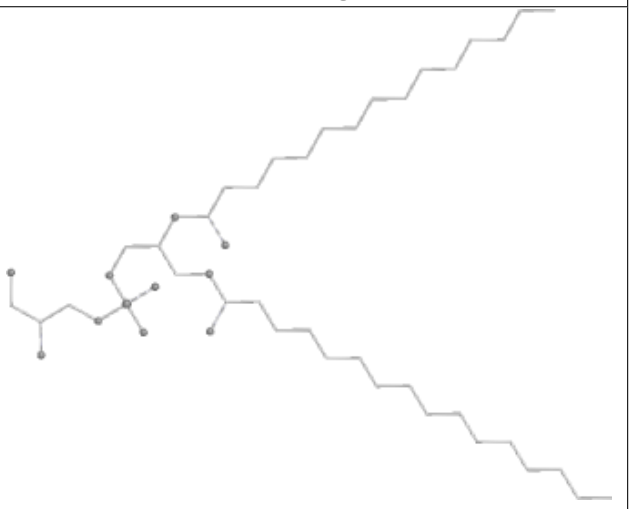
Bond lengths



Bond angles

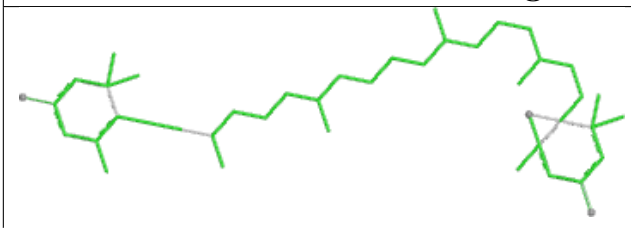


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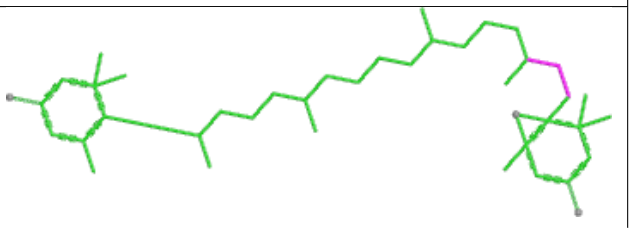


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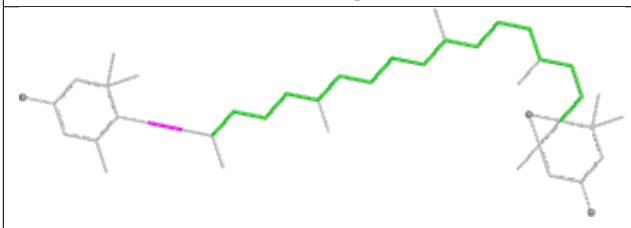
Ligand DD6 A 314



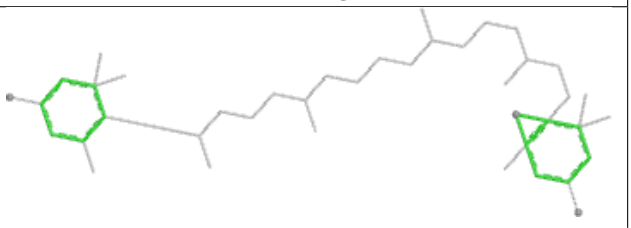
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Bond angles

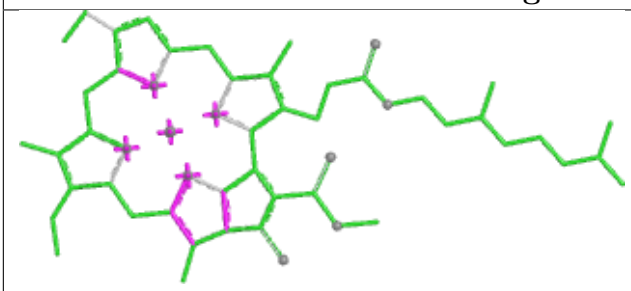


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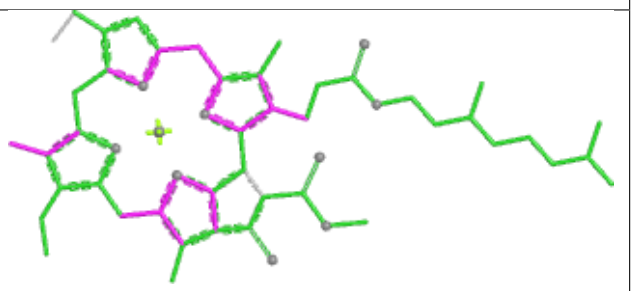


Rings

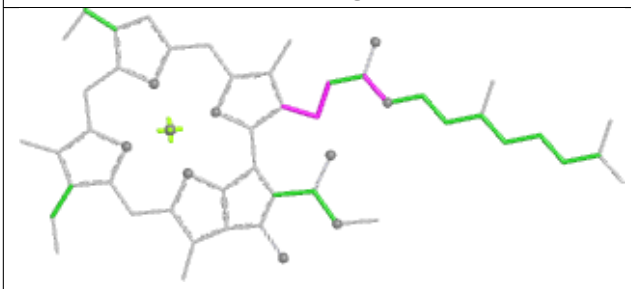
Ligand CLA G 203



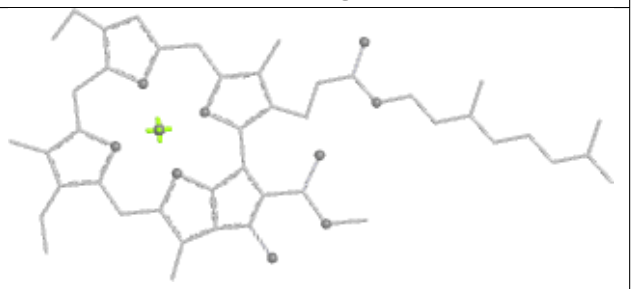
Bond lengths



Bond angles

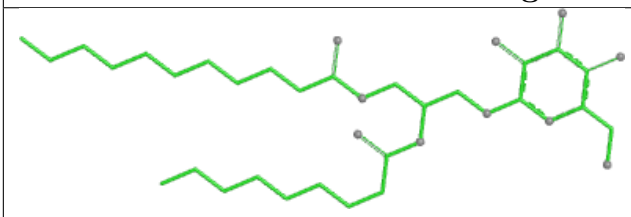


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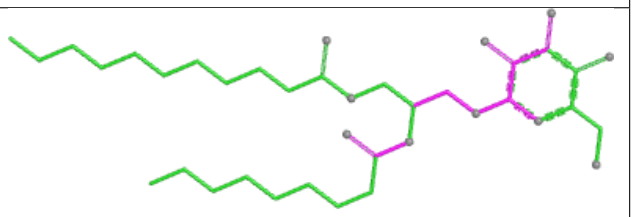


Rings

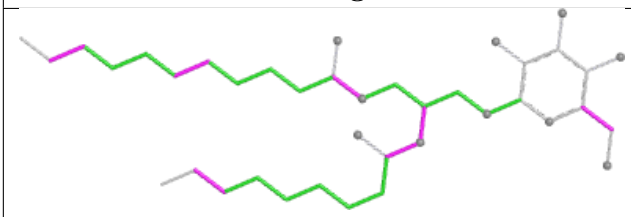
Ligand LMG F 318



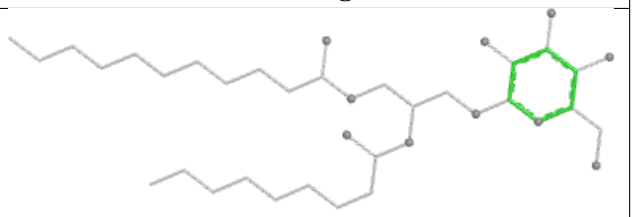
Bond lengths



Bond angles

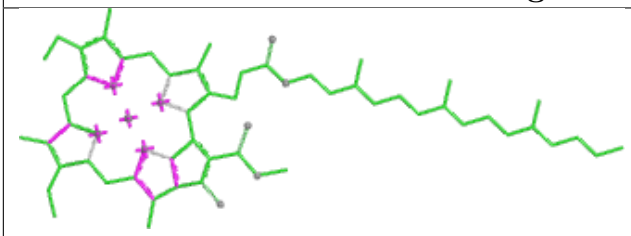


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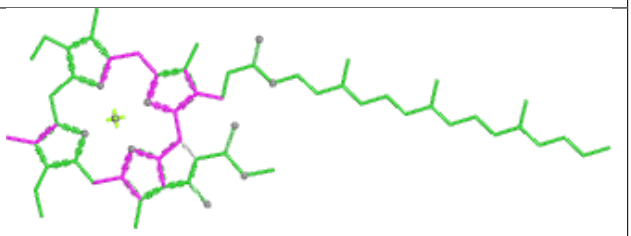


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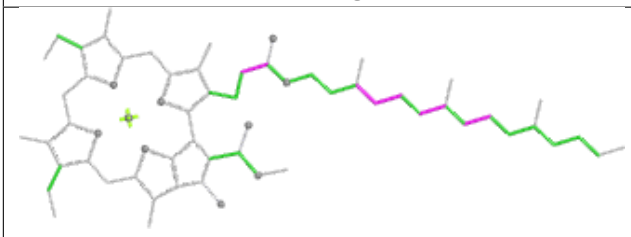
Ligand CLA b 801



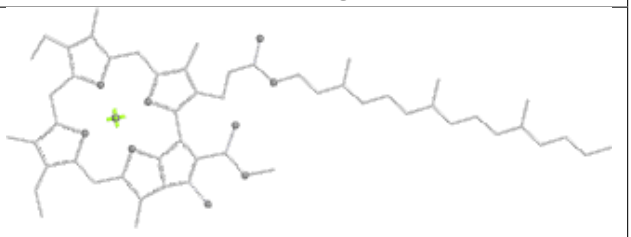
Bond lengths



Bond angles

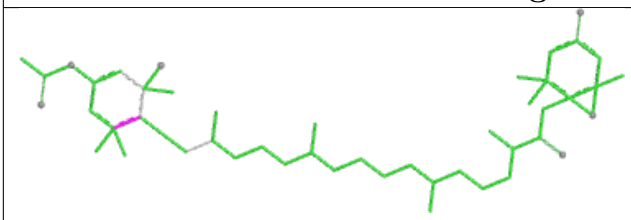


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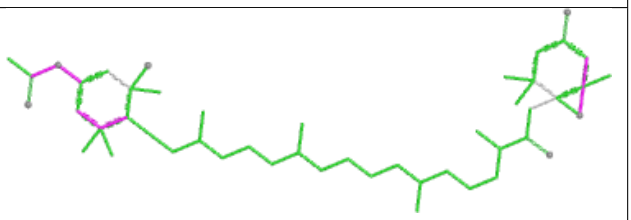


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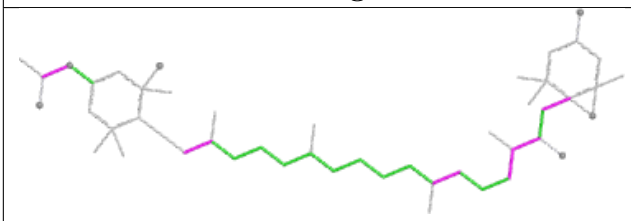
Ligand A86 Y 320



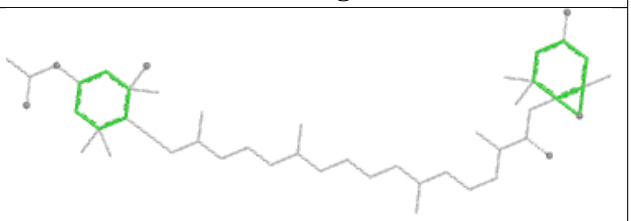
Bond lengths



Bond angles

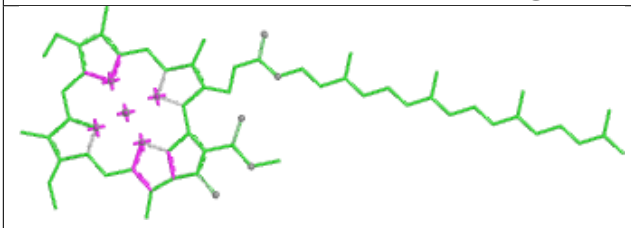


Torsions

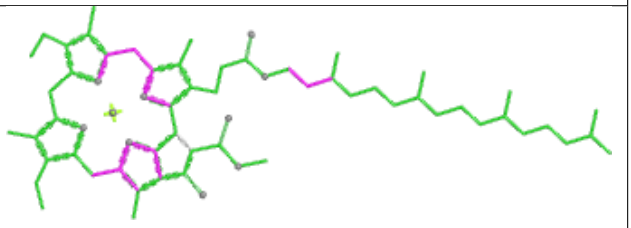


Rings

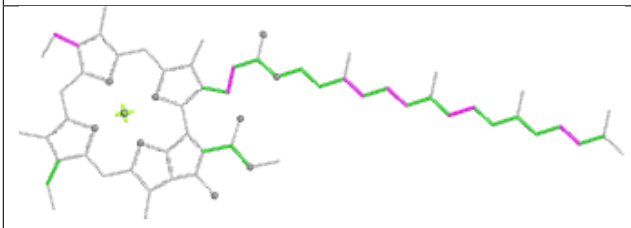
Ligand CLA b 802



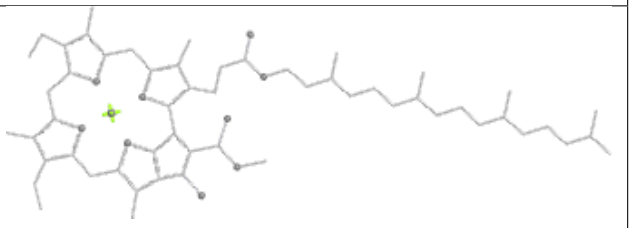
Bond lengths



Bond angles

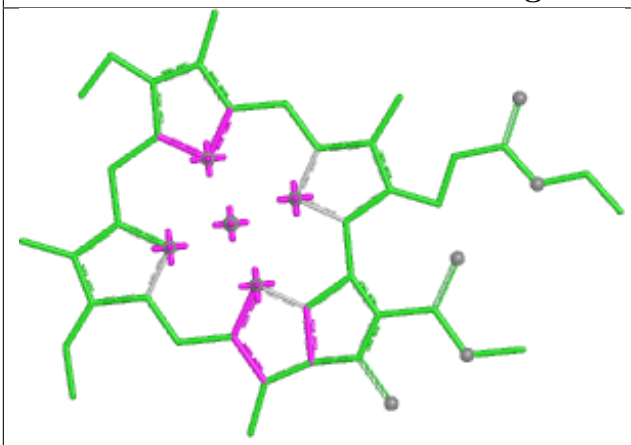


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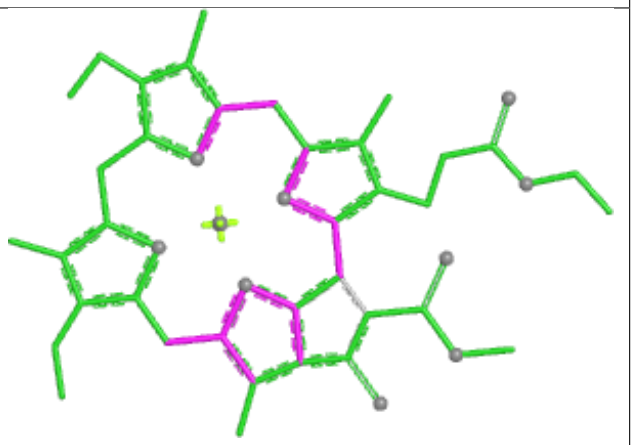


Rings

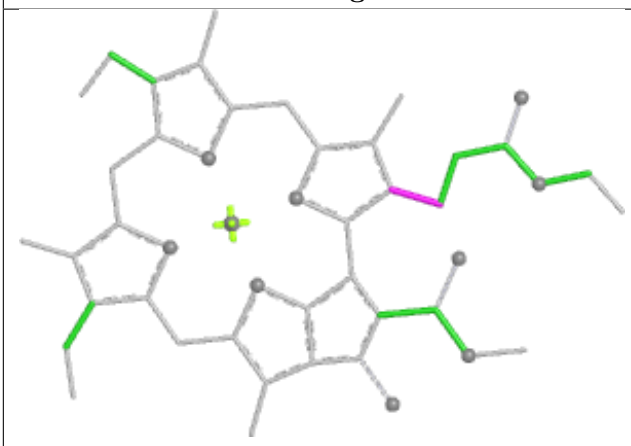
Ligand CLA C 309



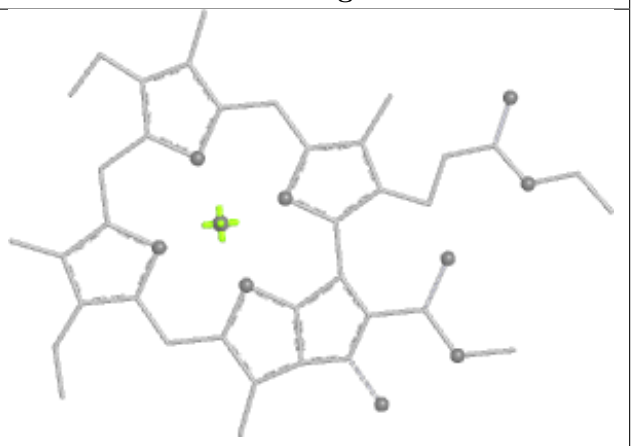
Bond lengths



Bond angles

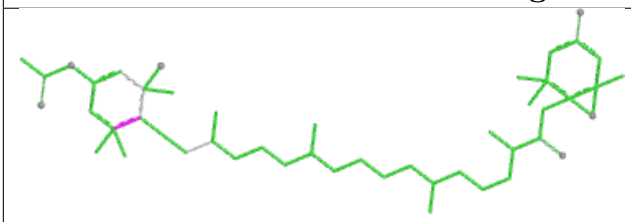


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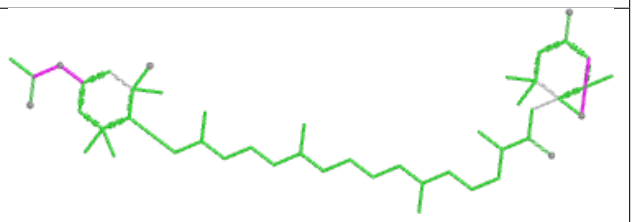


Rings

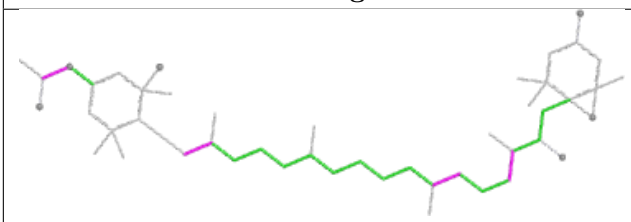
Ligand A86 N 321



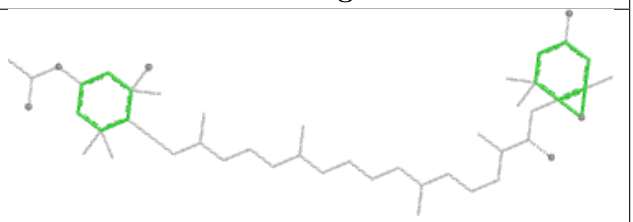
Bond lengths



Bond angles

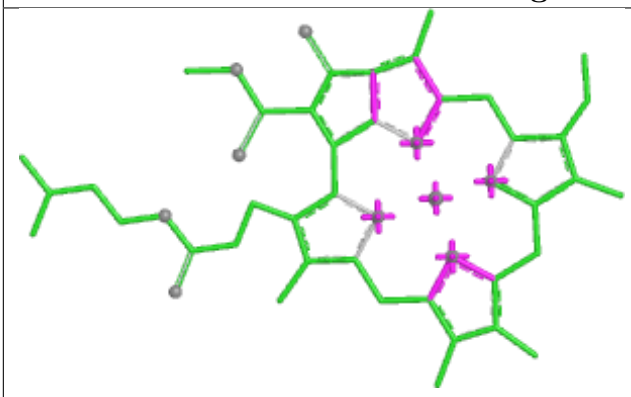


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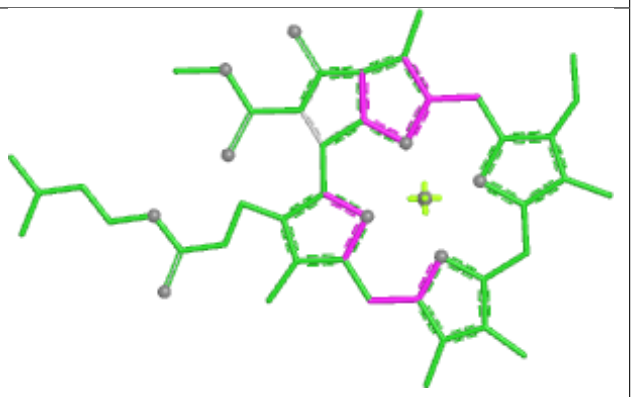


Rings

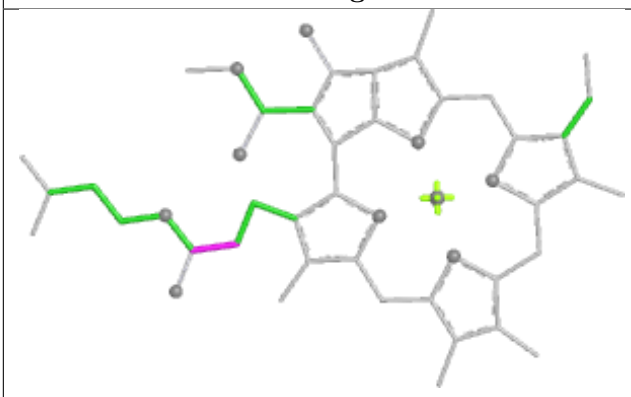
Ligand CLA t 305



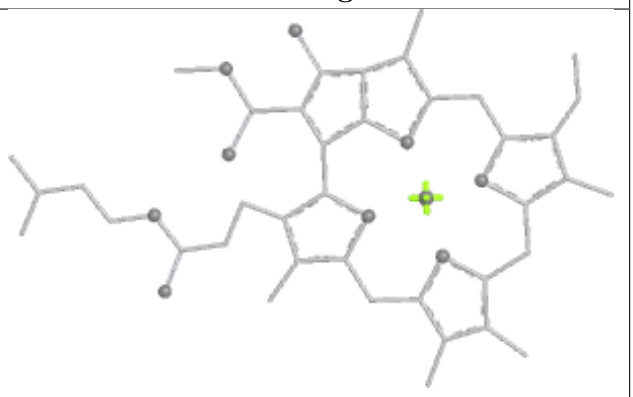
Bond lengths



Bond angles

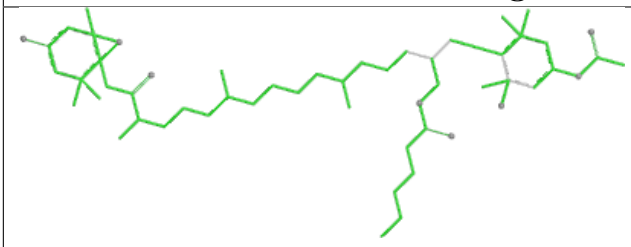


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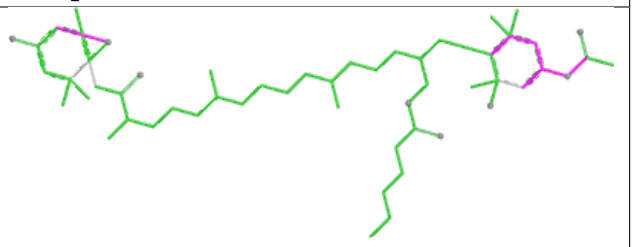


Rings

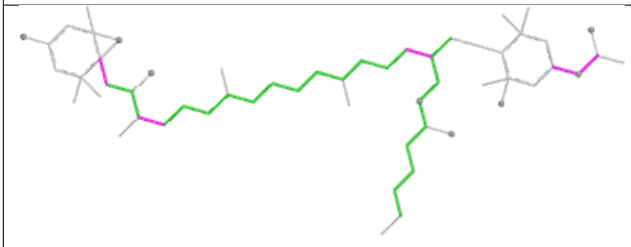
Ligand A1EB1 p 323



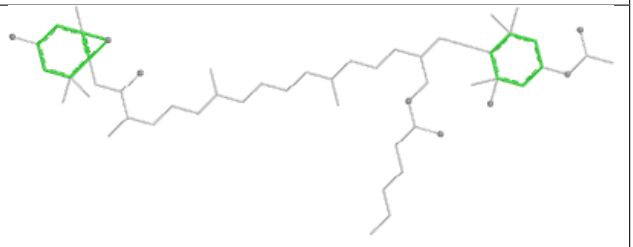
Bond lengths



Bond angles

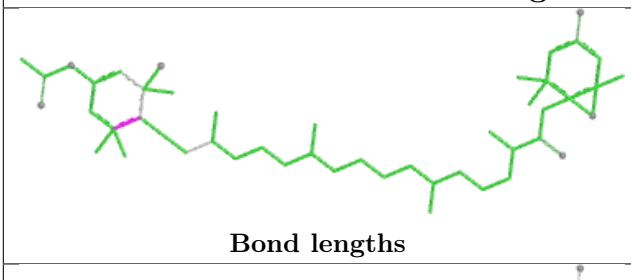


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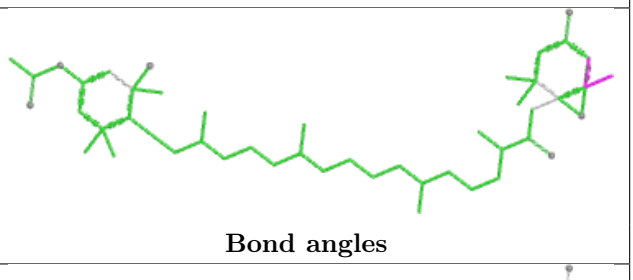


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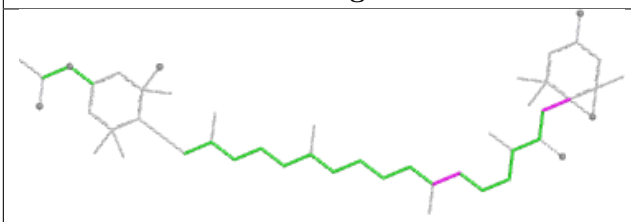
Ligand A86 Y 316



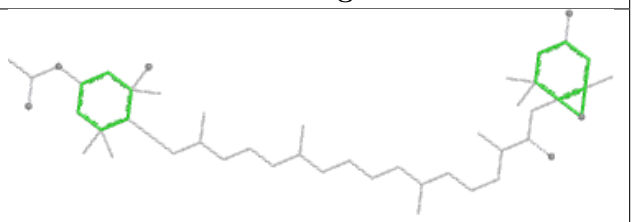
Bond lengths



Bond angles

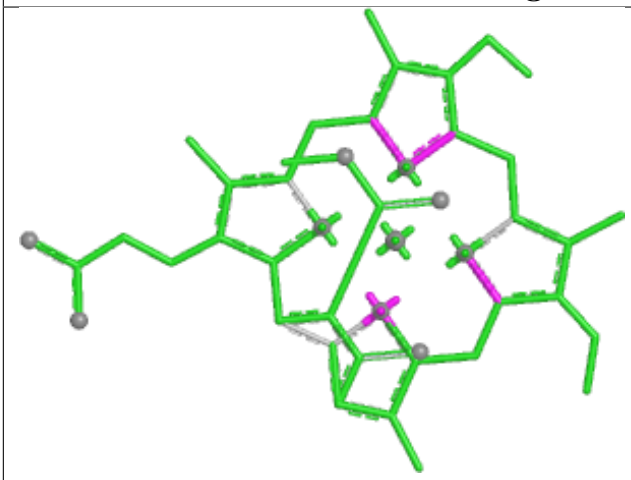


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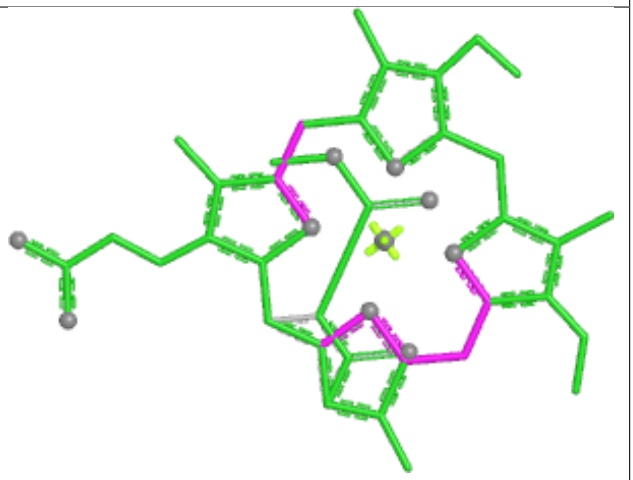


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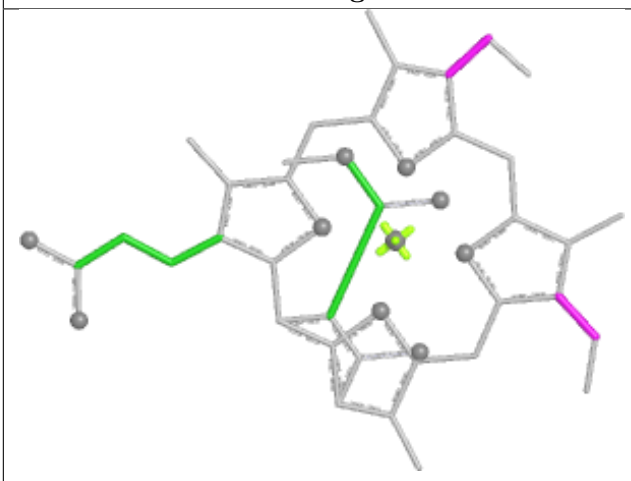
Ligand KC2 N 313



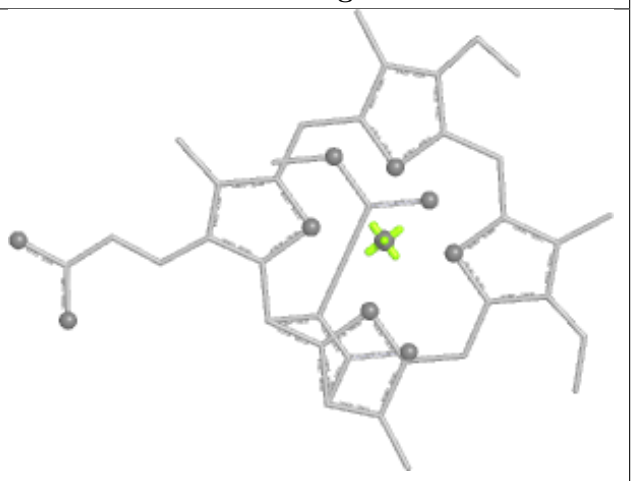
Bond lengths



Bond angles

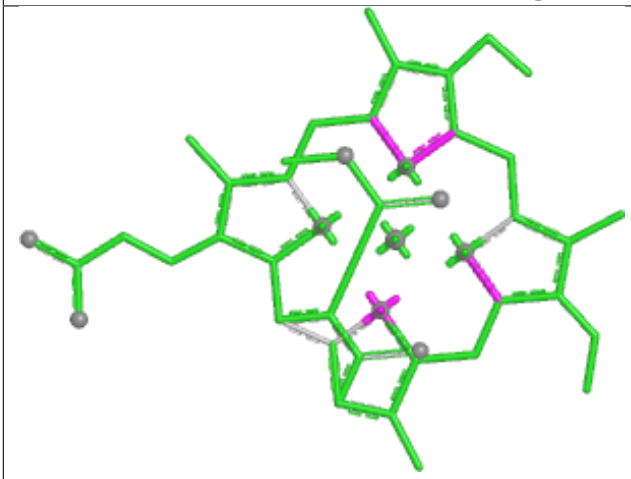


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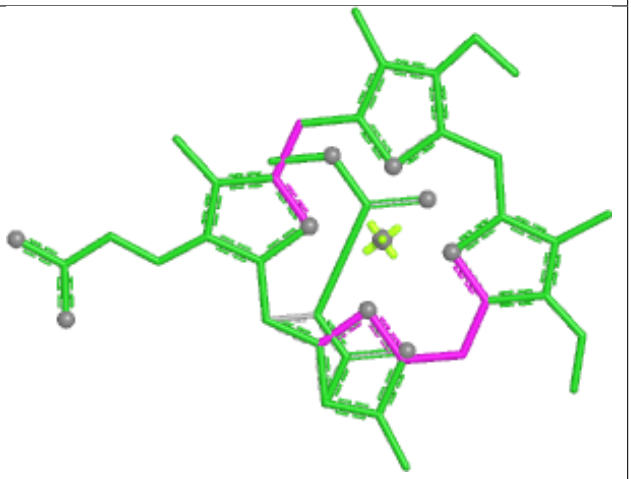


Rings

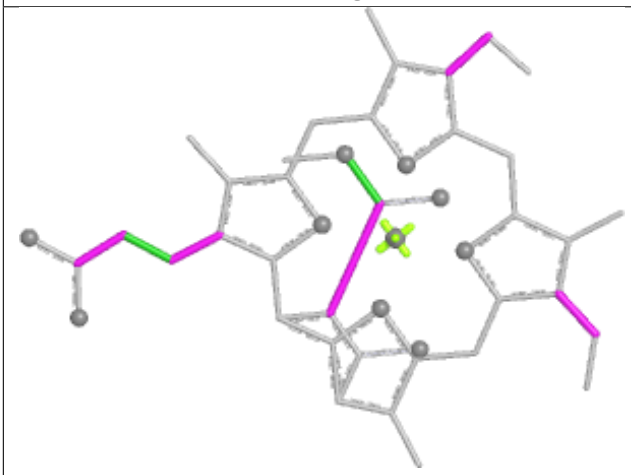
Ligand KC2 J 304



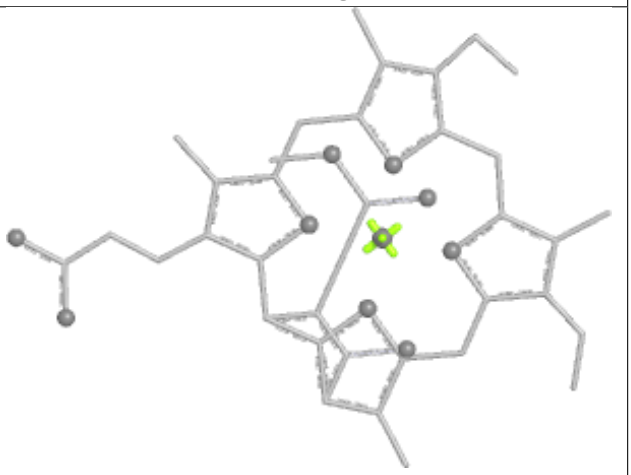
Bond lengths



Bond angles

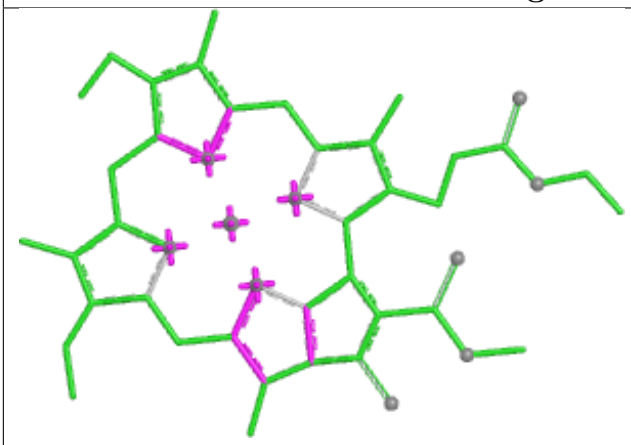


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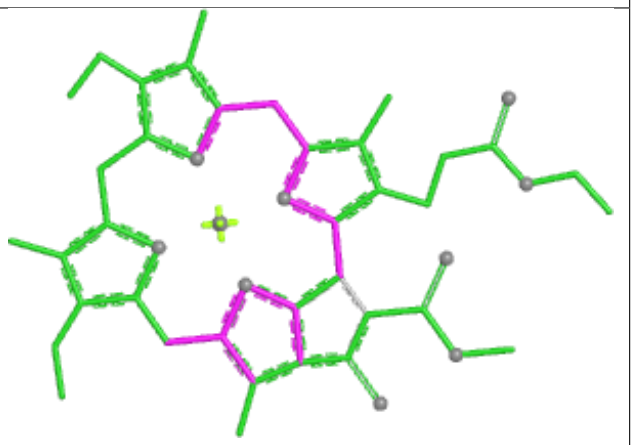


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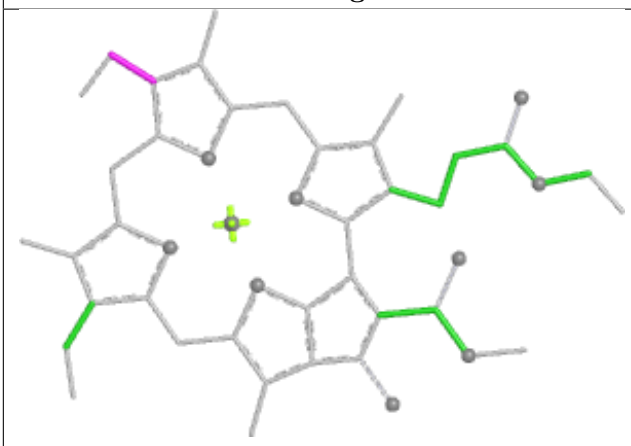
Ligand CLA b 829



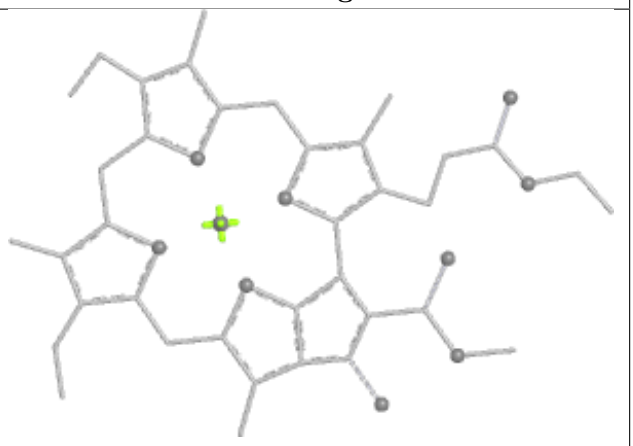
Bond lengths



Bond angles

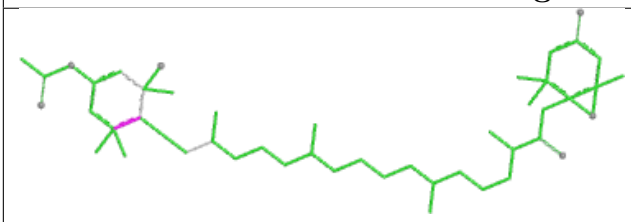


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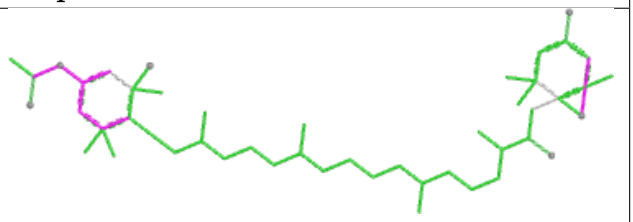


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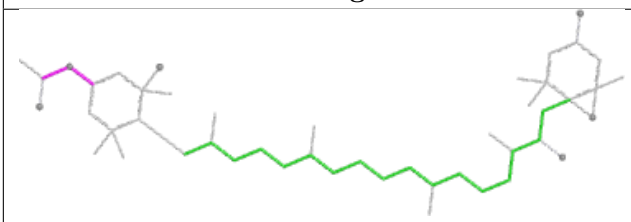
Ligand A86 q 314



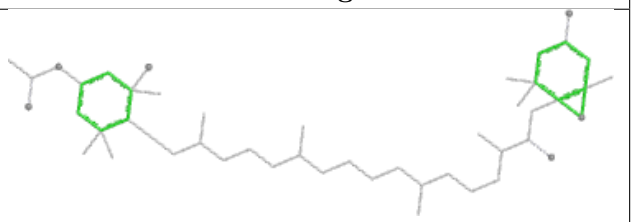
Bond lengths



Bond angles

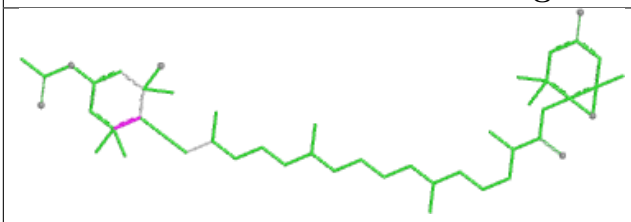


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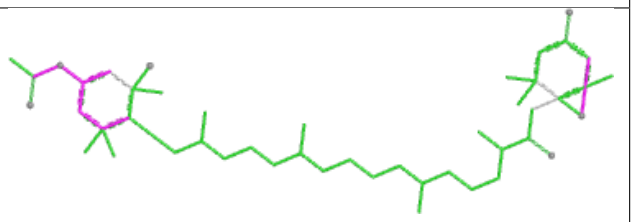


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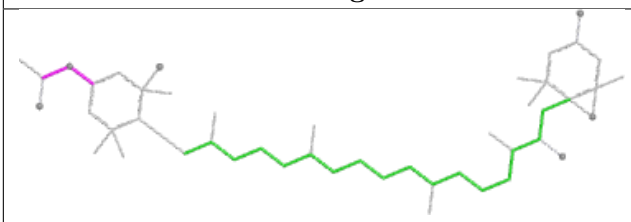
Ligand A86 v 314



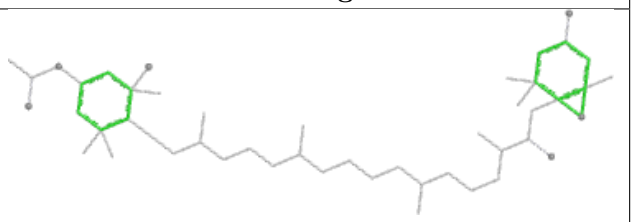
Bond lengths



Bond angles

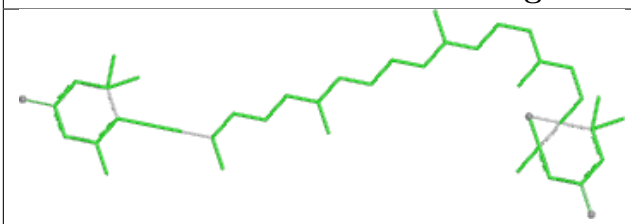


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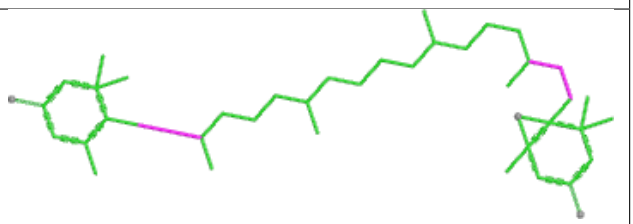


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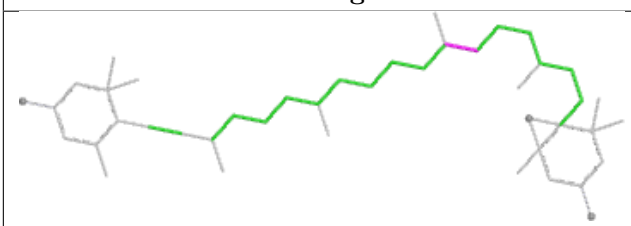
Ligand DD6 D 317



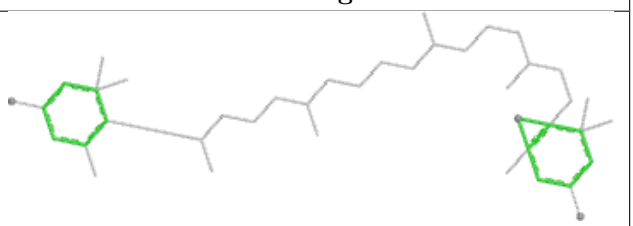
Bond lengths



Bond angles

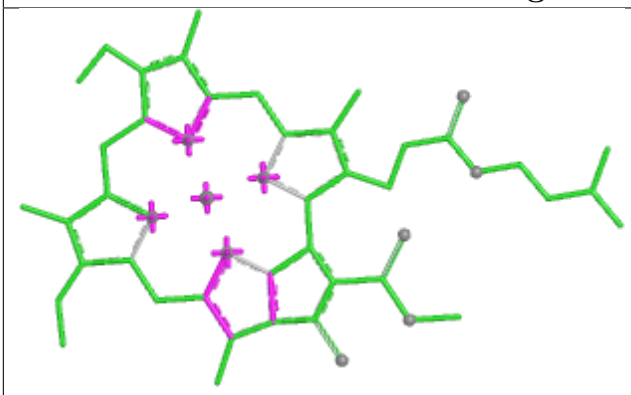


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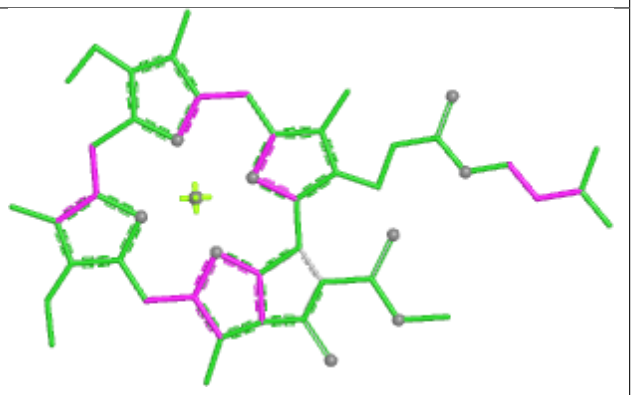


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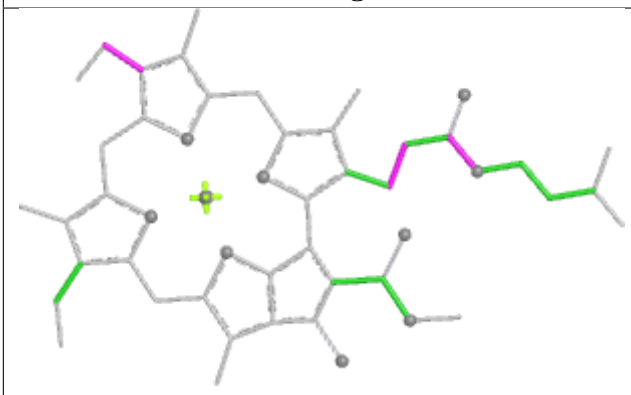
Ligand CLA b 813



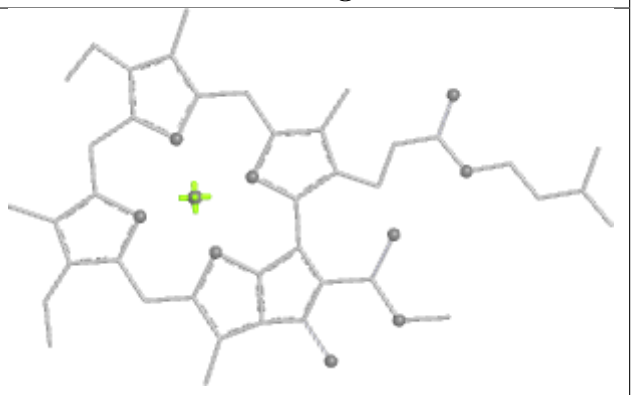
Bond lengths



Bond angles

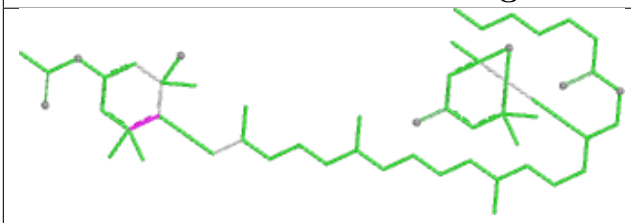


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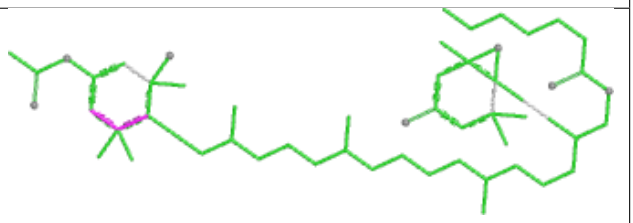


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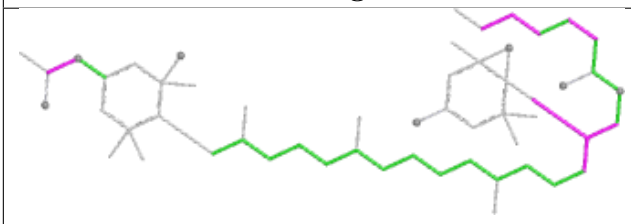
Ligand A1EB4 W 319



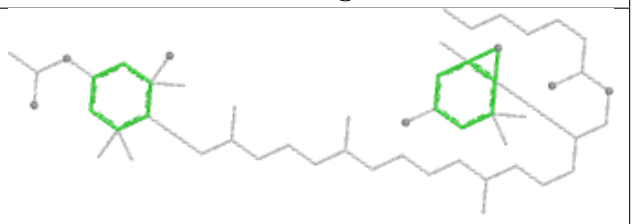
Bond lengths



Bond angles

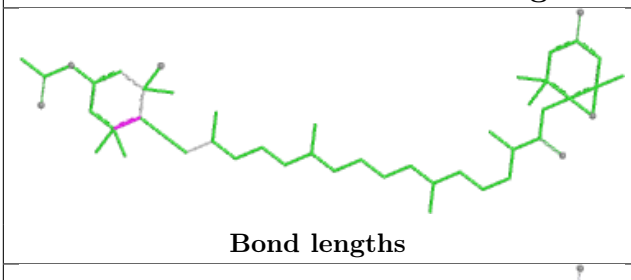


Torsions

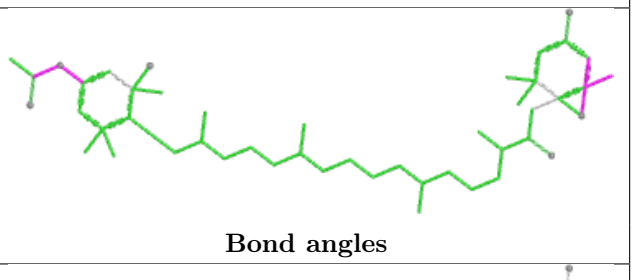


Rings

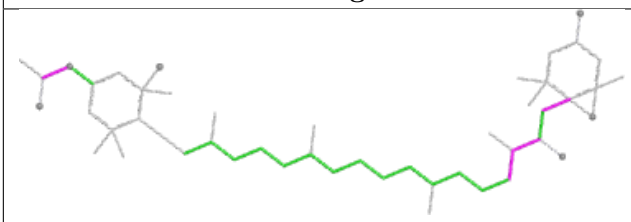
Ligand A86 C 311



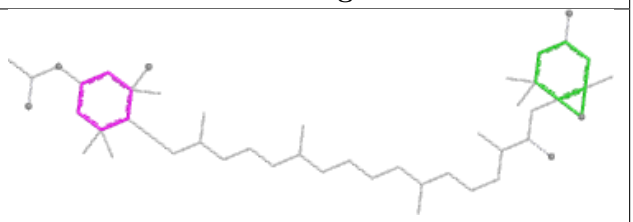
Bond lengths



Bond angles

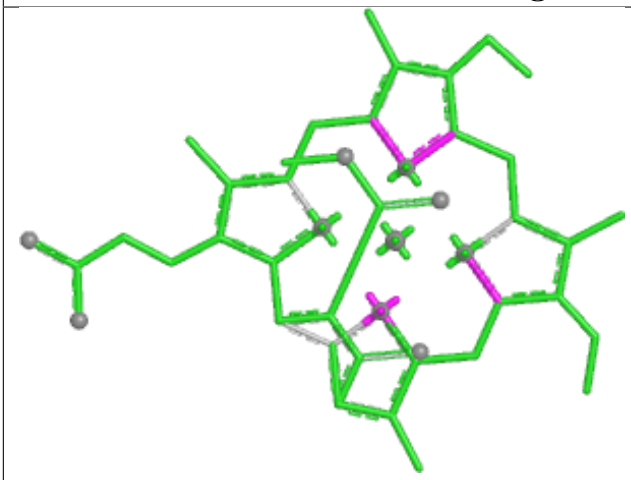


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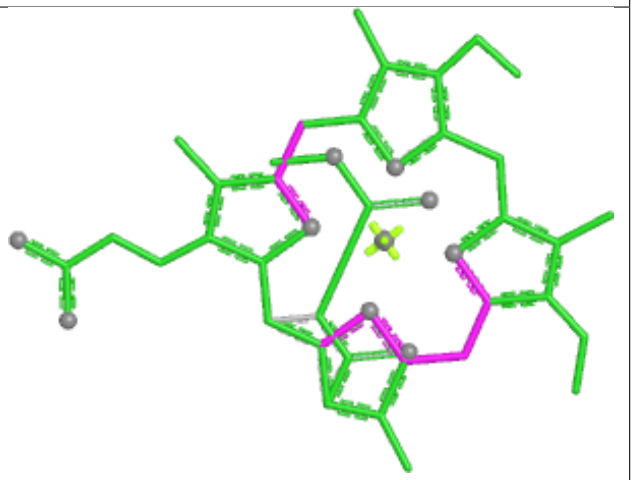


Rings

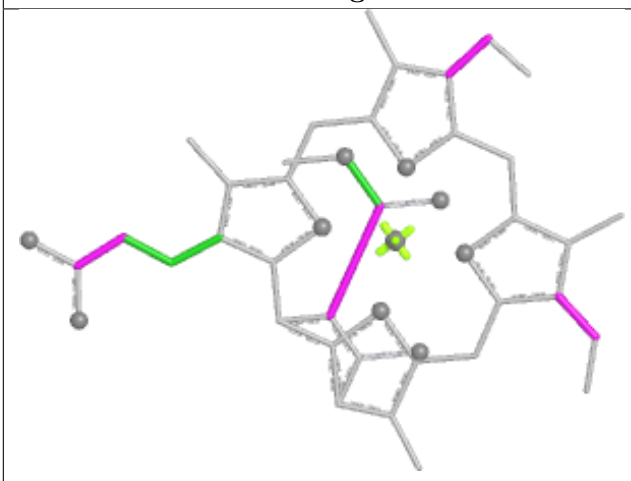
Ligand KC2 u 315



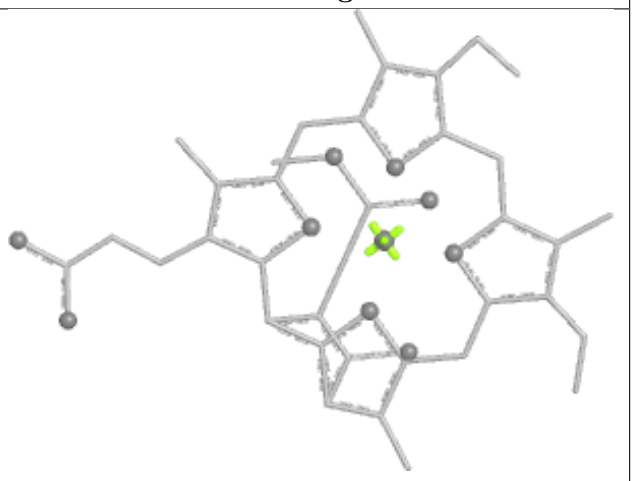
Bond lengths



Bond angles

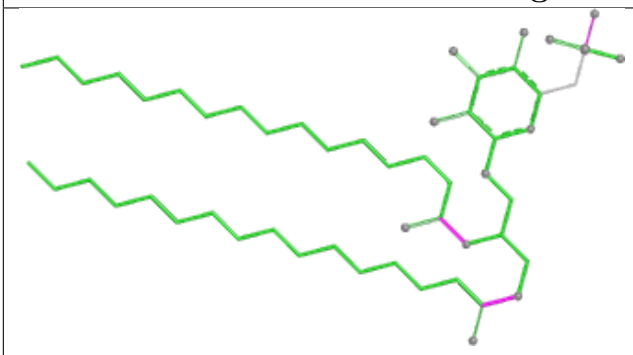


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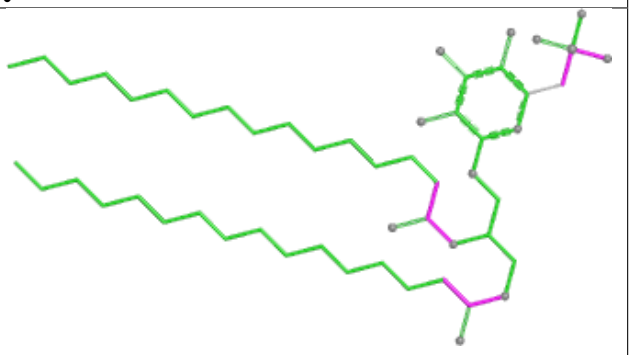


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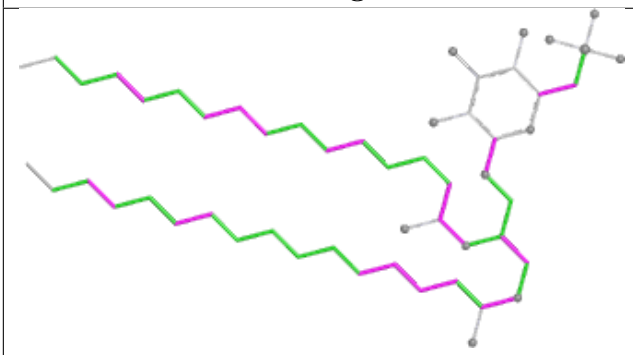
Ligand SQD I 215



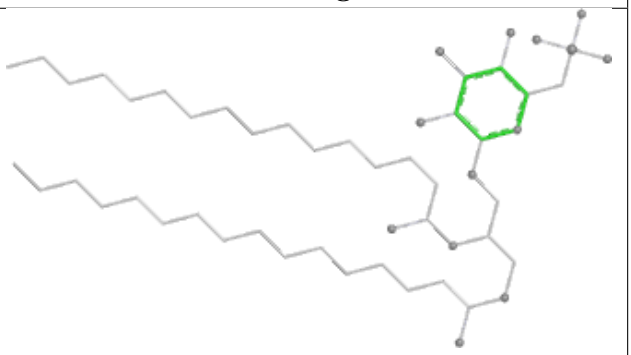
Bond lengths



Bond angles

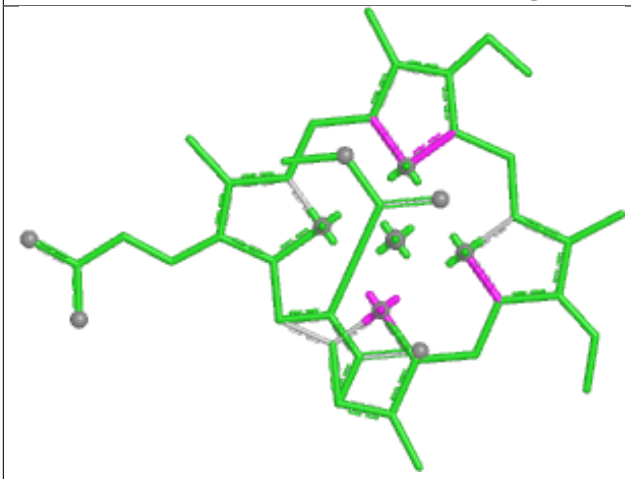


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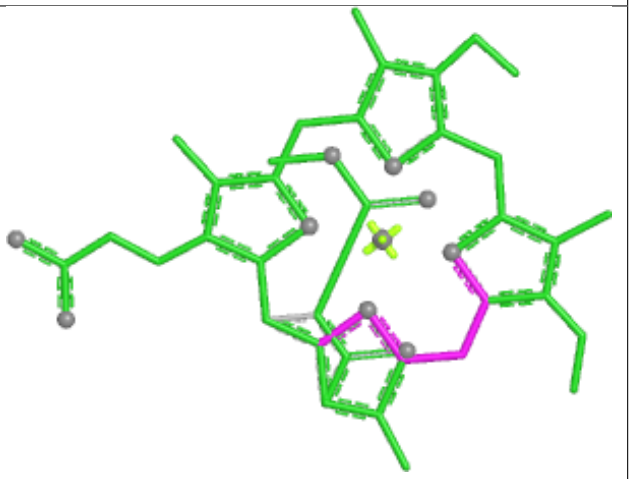


Rings

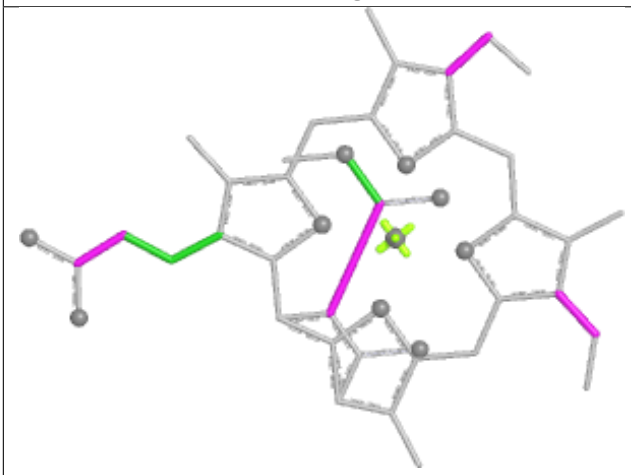
Ligand KC2 Y 309



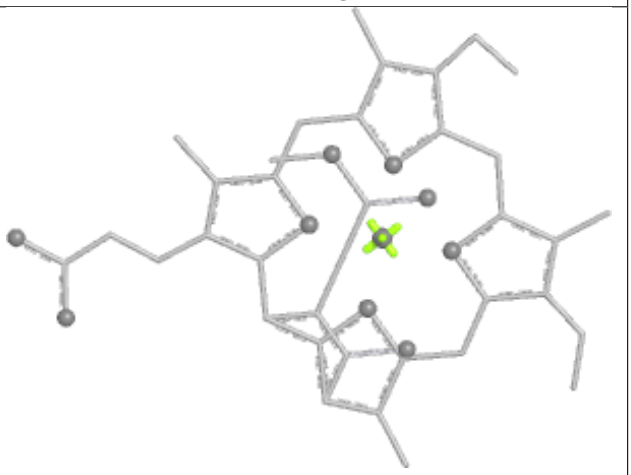
Bond lengths



Bond angles

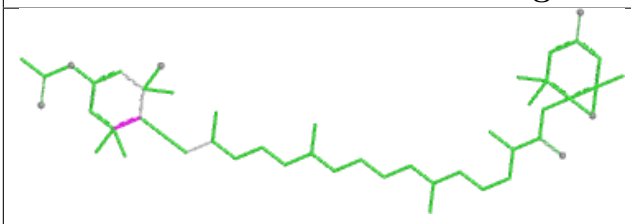


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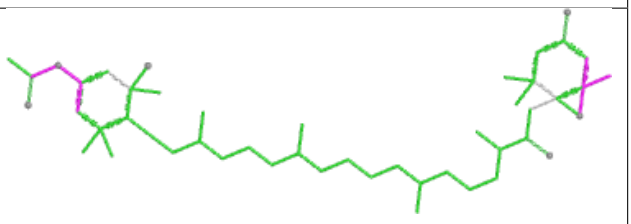


Rings

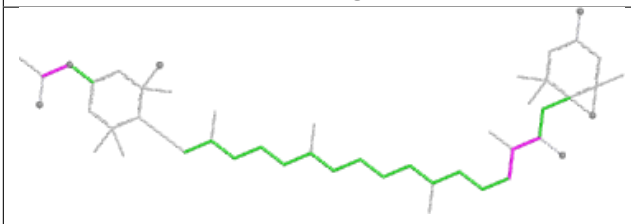
Ligand A86 S 316



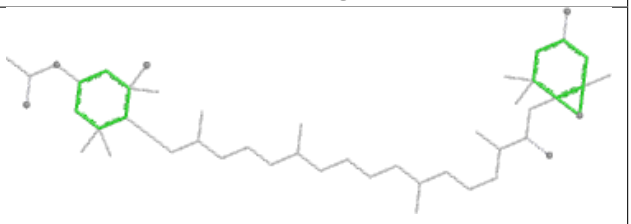
Bond lengths



Bond angles

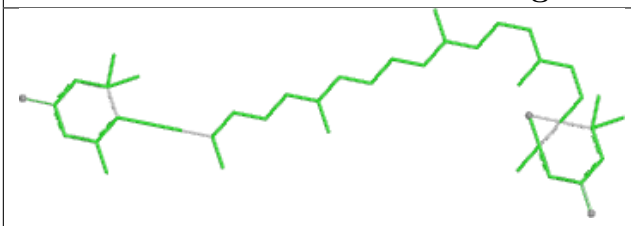


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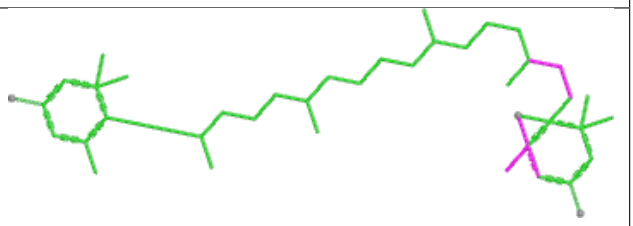


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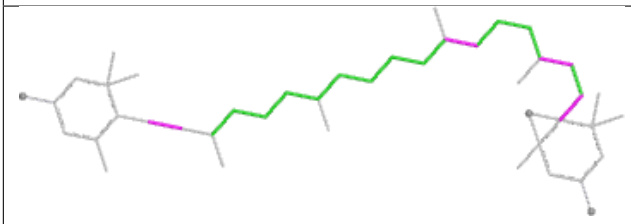
Ligand DD6 I 211



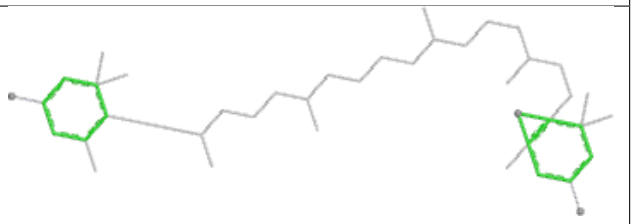
Bond lengths



Bond angles

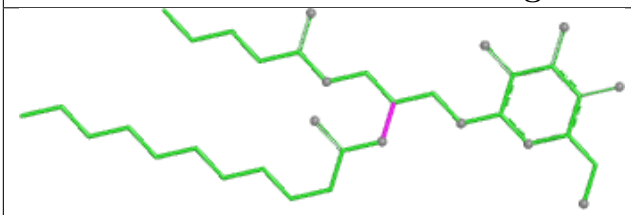


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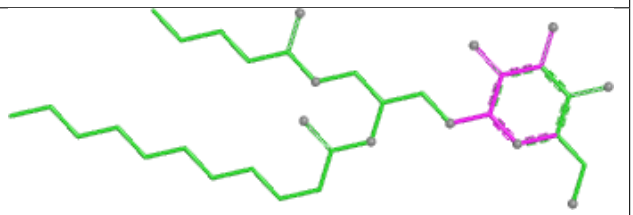


Rings

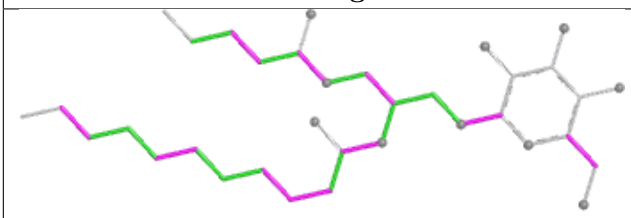
Ligand LMG a 801



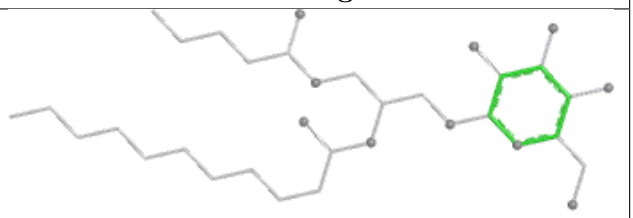
Bond lengths



Bond angles

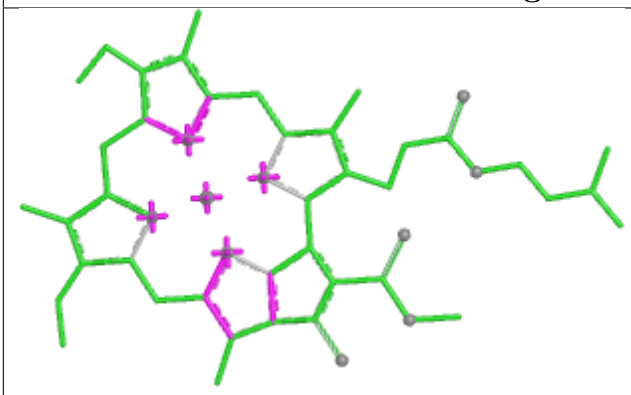


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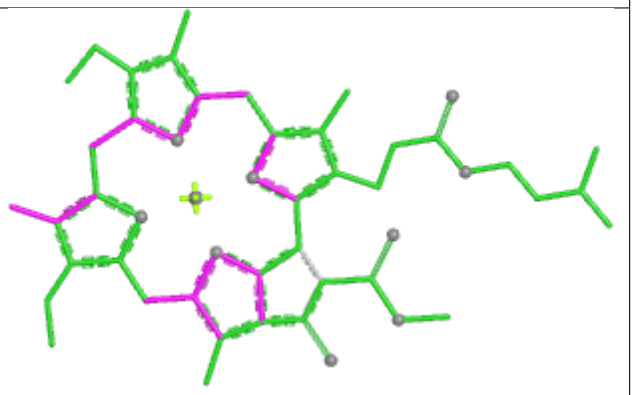


Rings

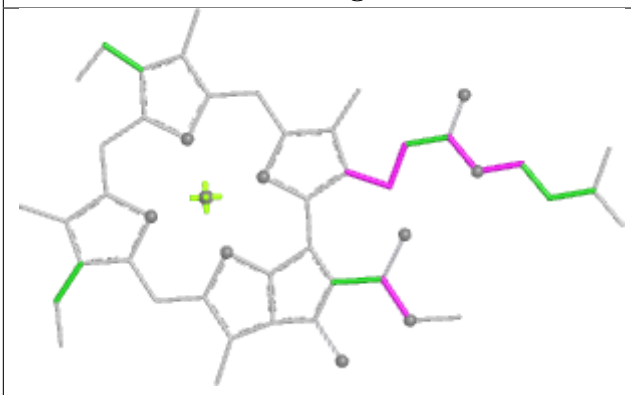
Ligand CLA X 305



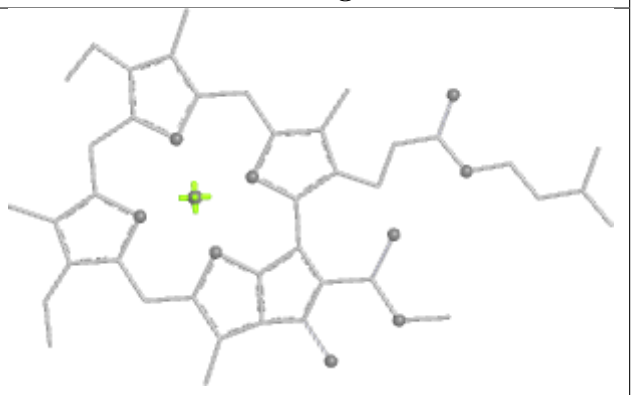
Bond lengths



Bond angles

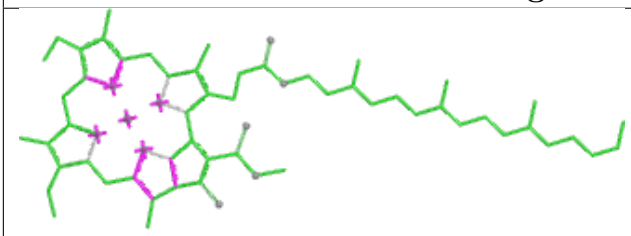


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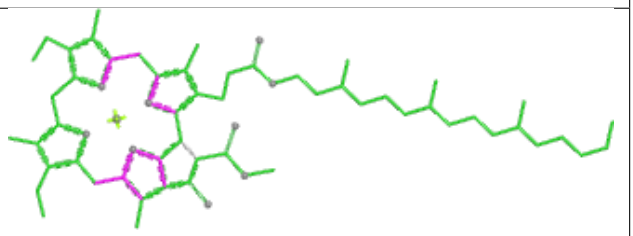


Rings

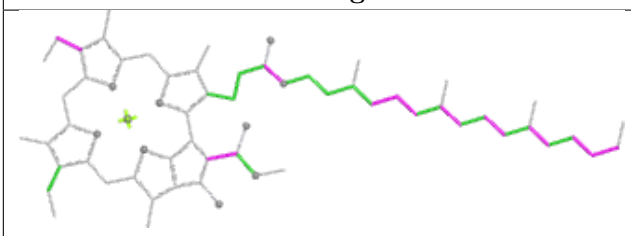
Ligand CLA b 819



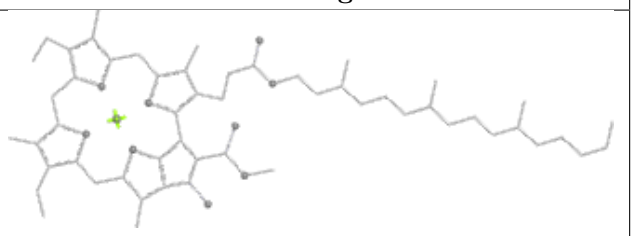
Bond lengths



Bond angles

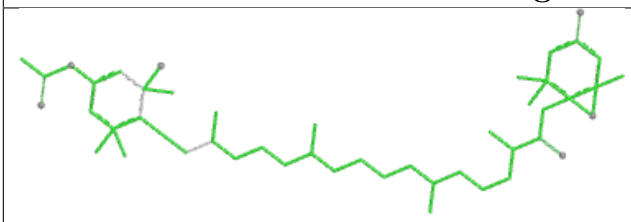


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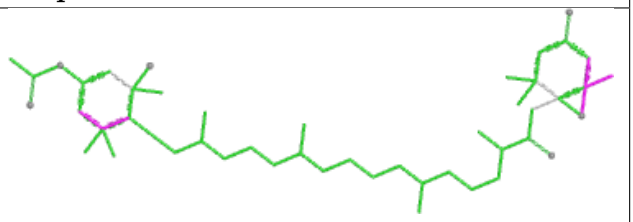


Rings

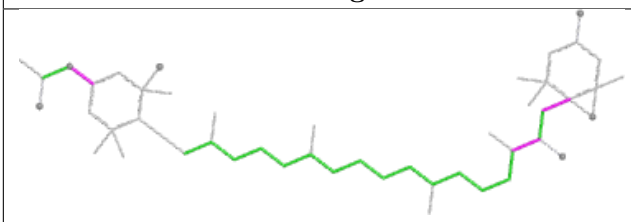
Ligand A86 q 324



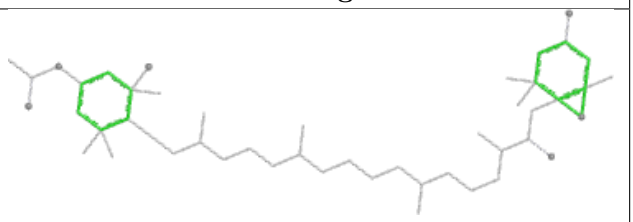
Bond lengths



Bond angles

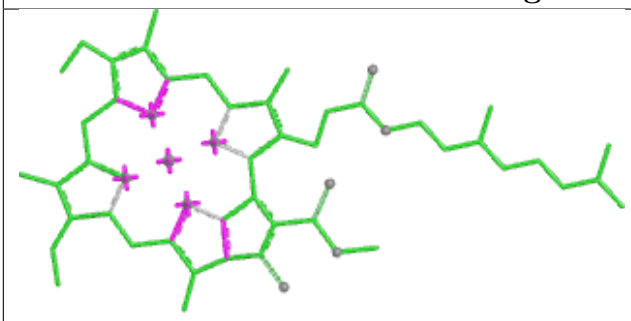


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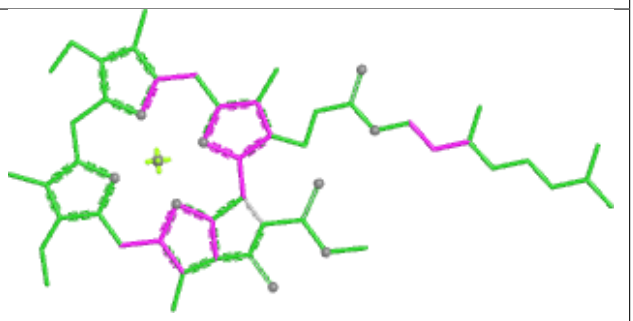


Rings

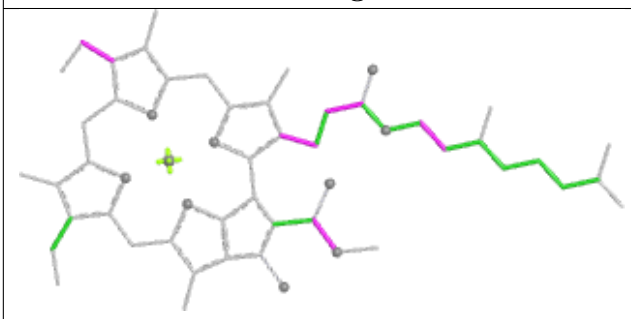
Ligand CLA X 310



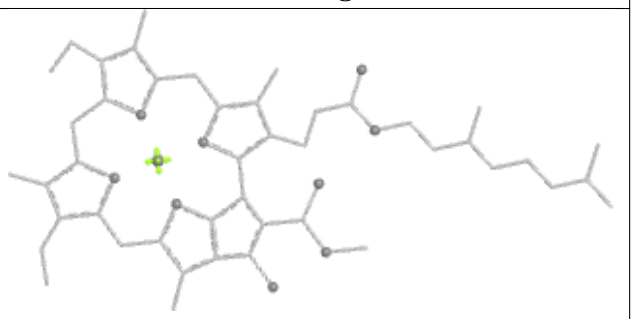
Bond lengths



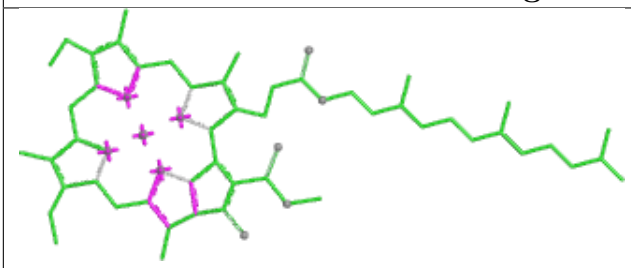
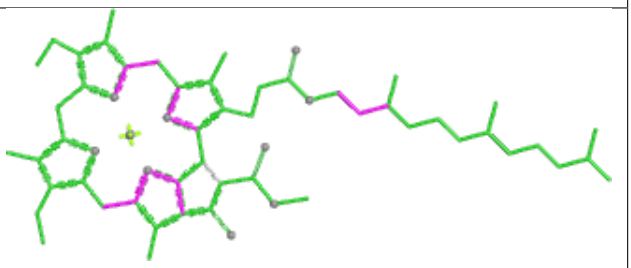
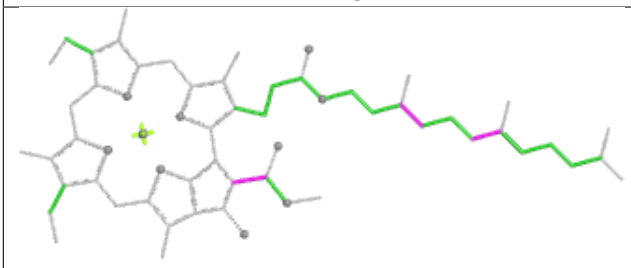
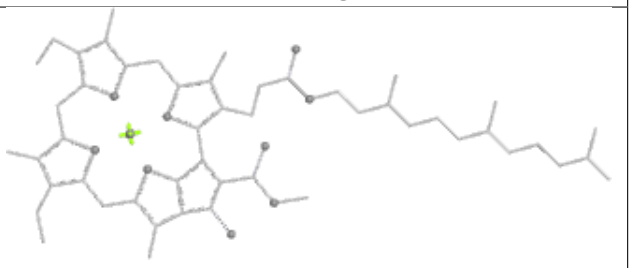
Bond angles

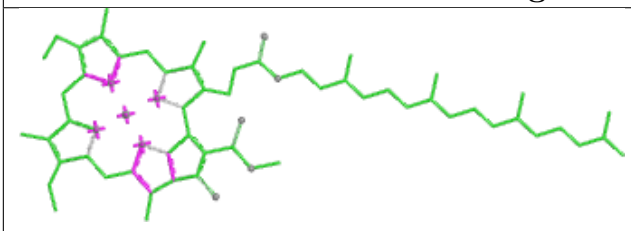
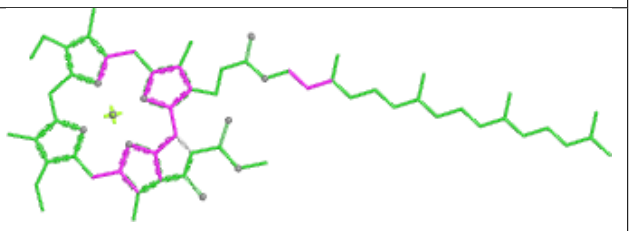
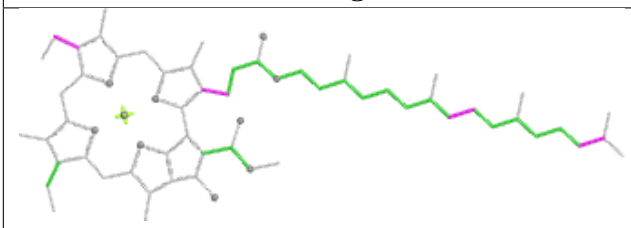
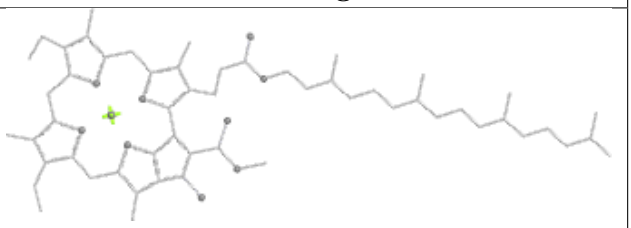


Torsions

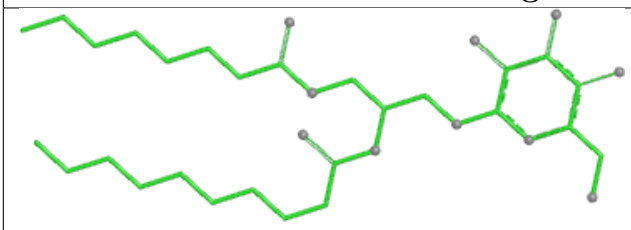


Rings

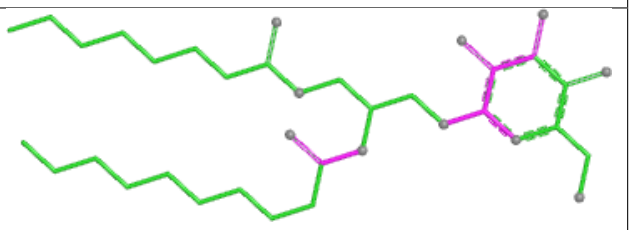
Ligand CLA N 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

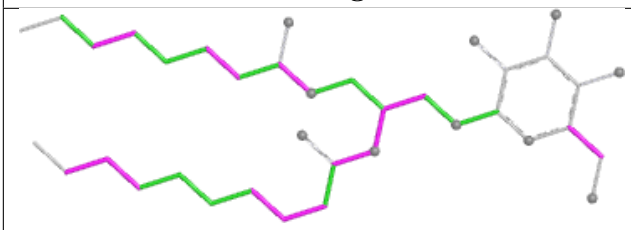
Ligand LMG L 319



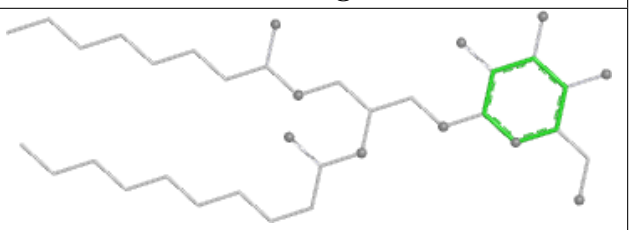
Bond lengths



Bond angles

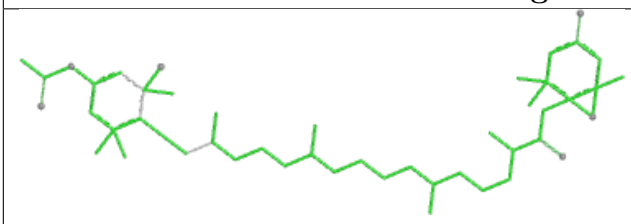


Torsions

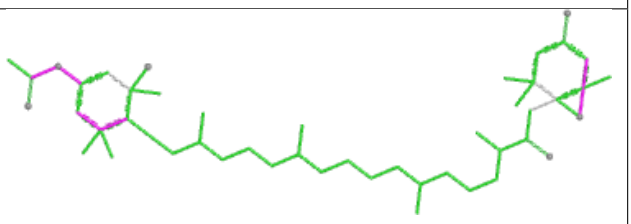


Rings

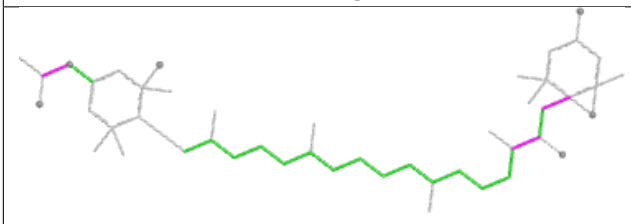
Ligand A86 P 314



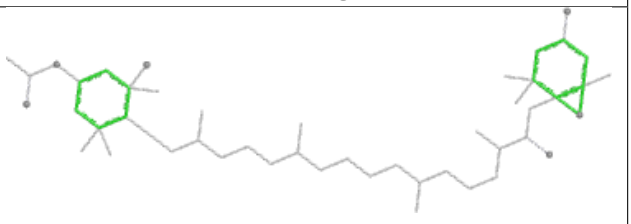
Bond lengths



Bond angles

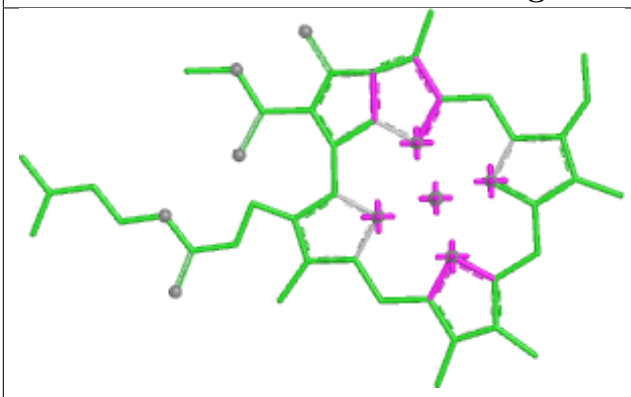


Torsions

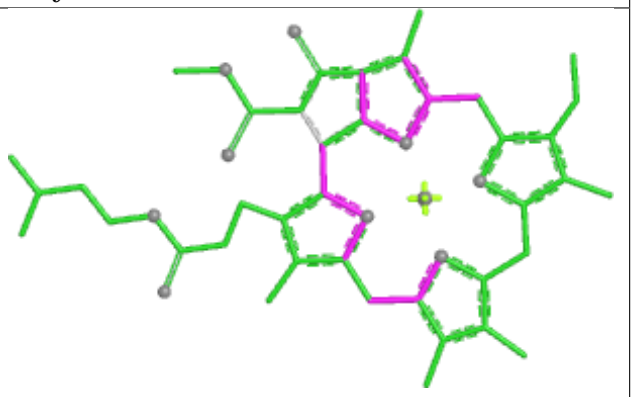


Rings

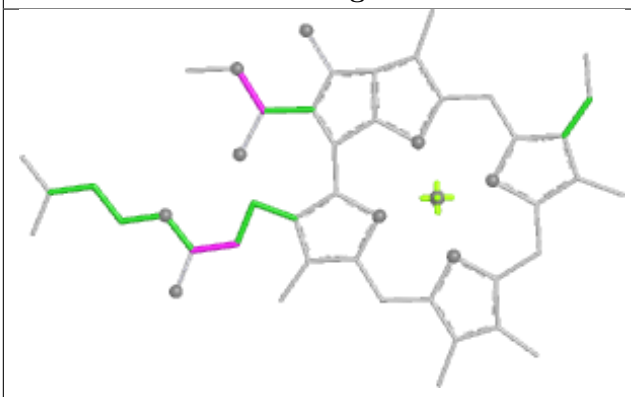
Ligand CLA y 305



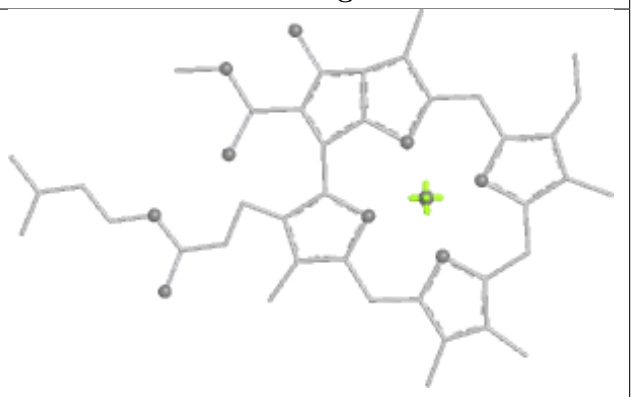
Bond lengths



Bond angles

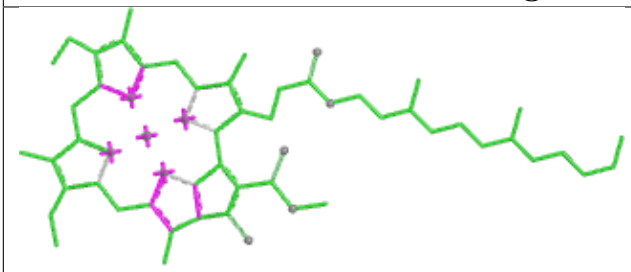


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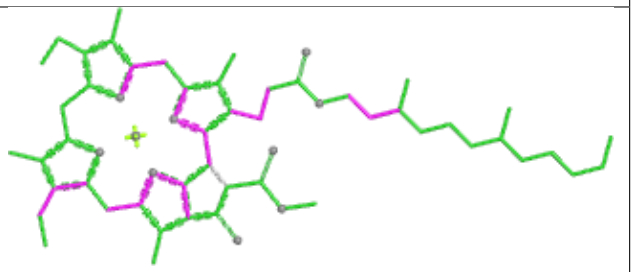


Rings

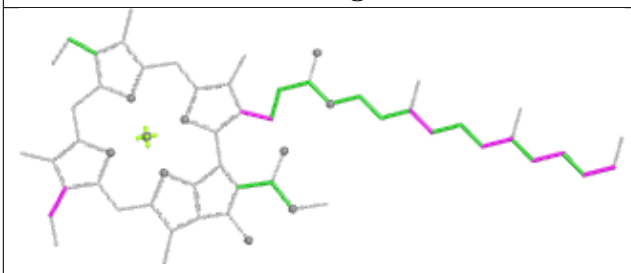
Ligand CLA K 308



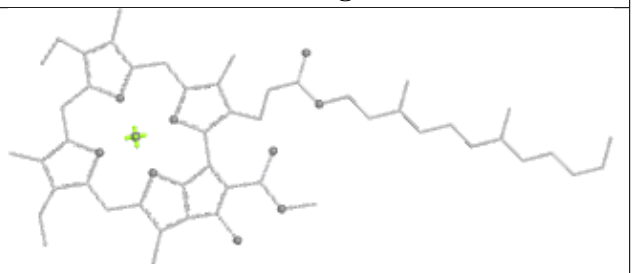
Bond lengths



Bond angles

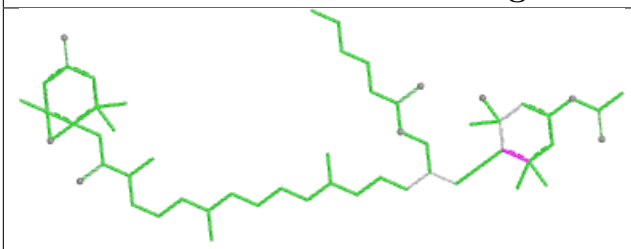


Torsions

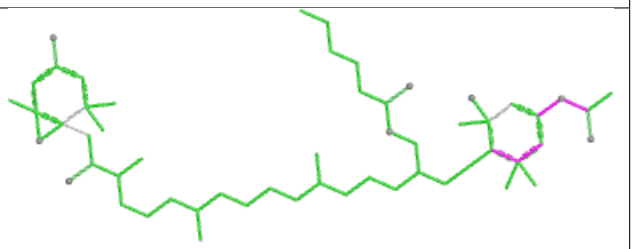


Rings

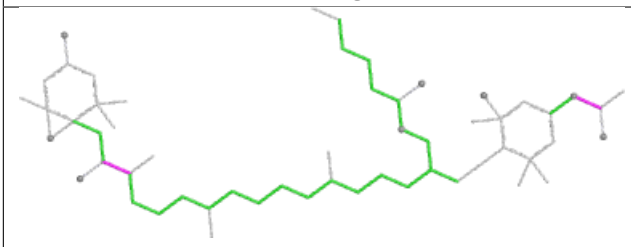
Ligand A1EB1 S 320



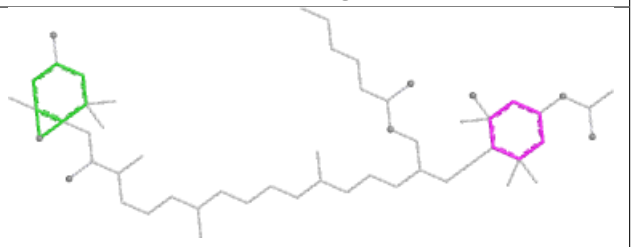
Bond lengths



Bond angles

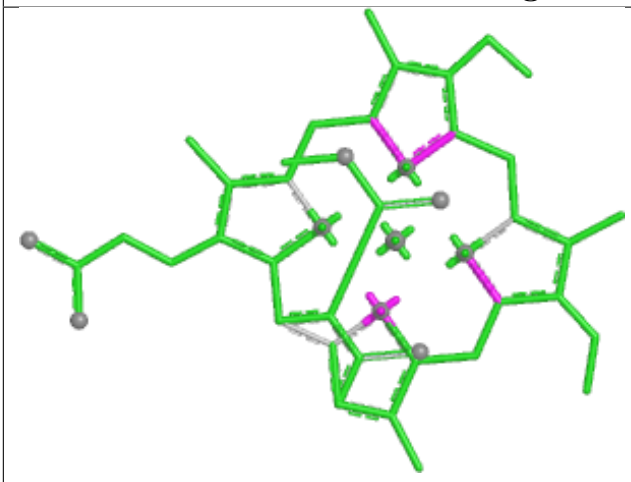


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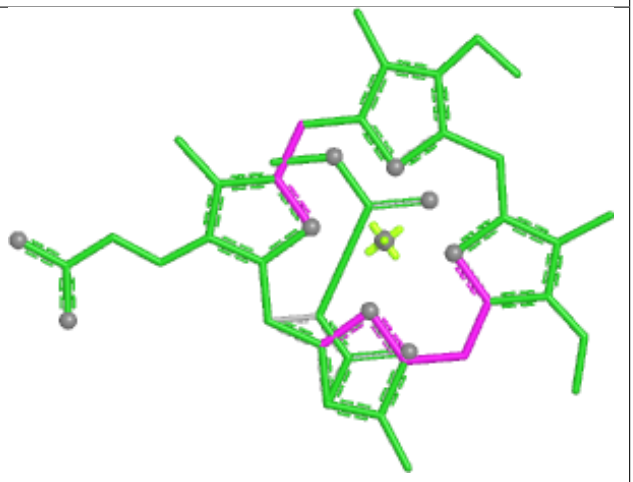


Rings

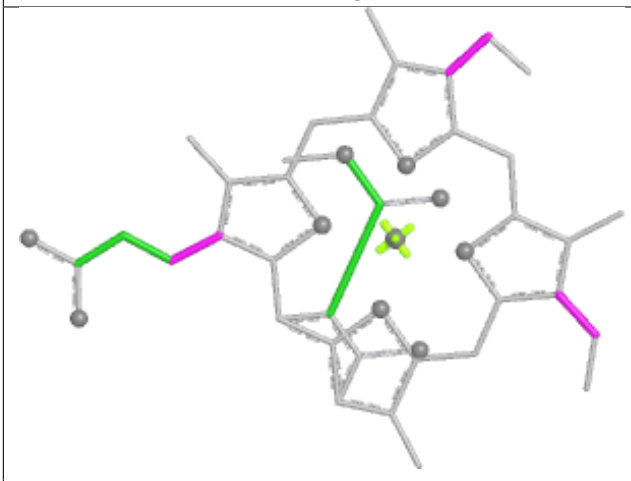
Ligand KC2 M 301



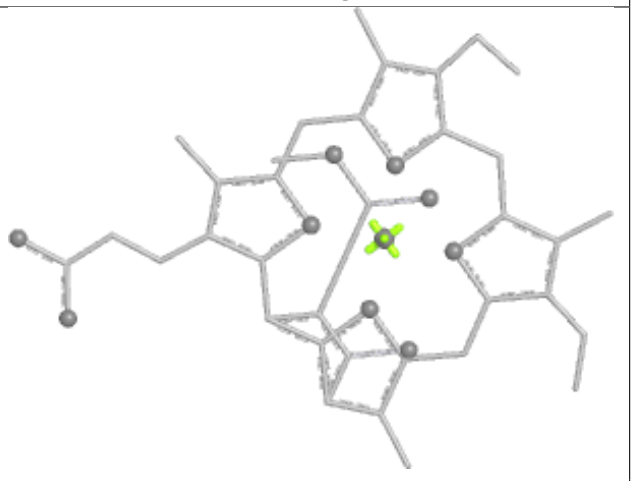
Bond lengths



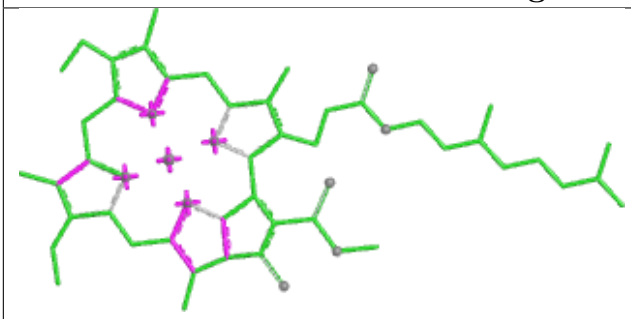
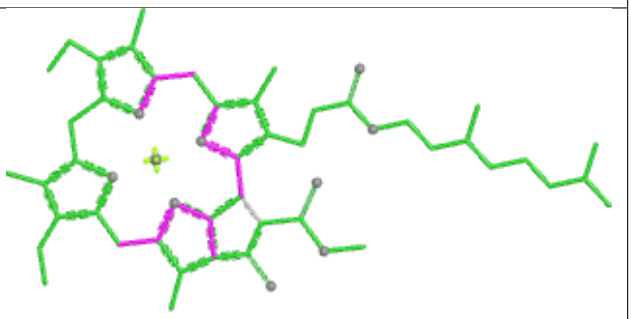
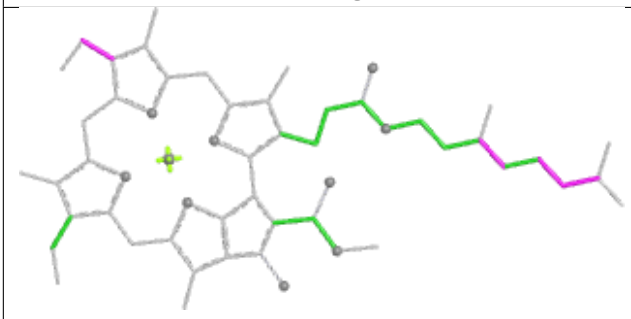
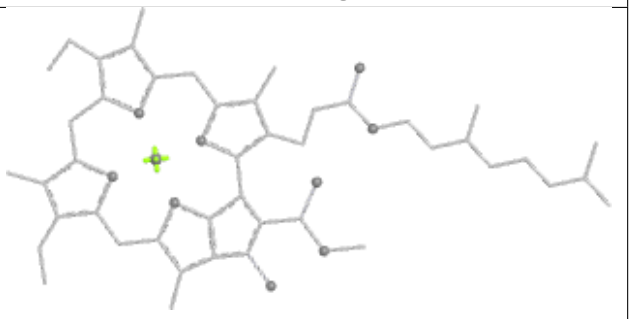
Bond angles

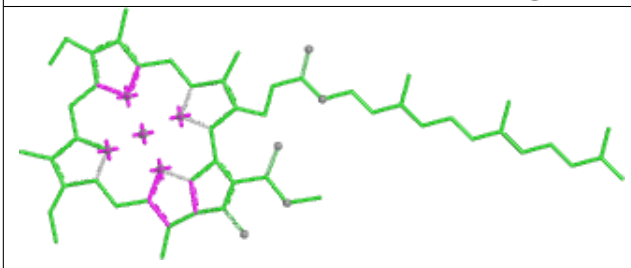
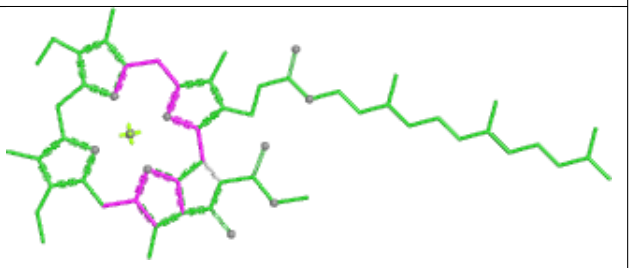
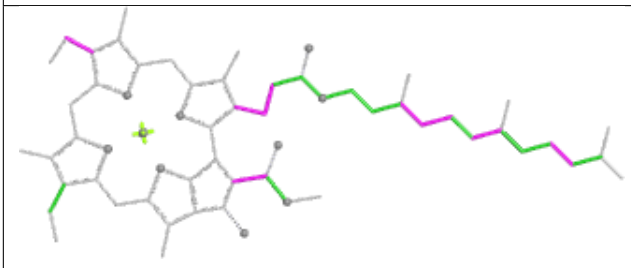
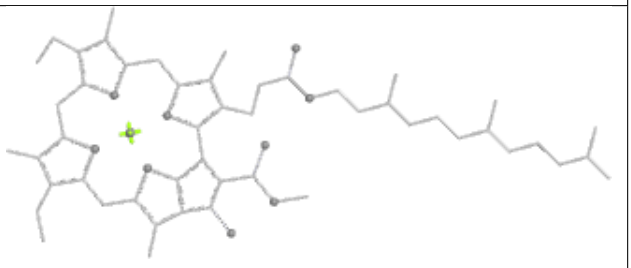


Torsions

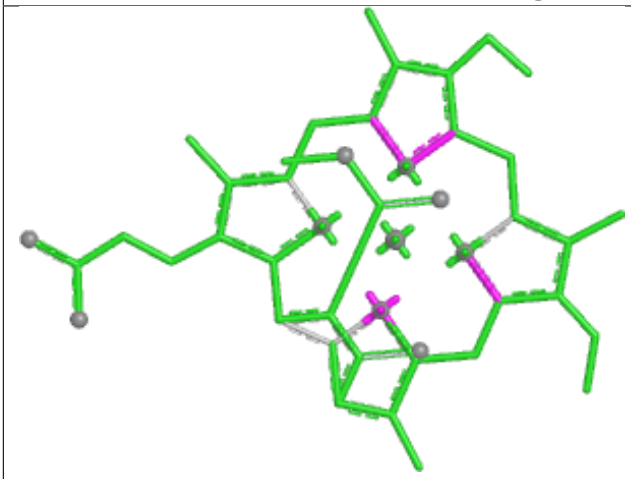


Rings

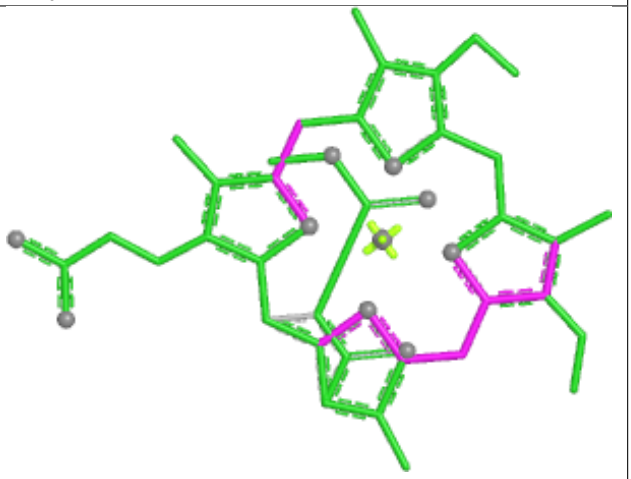
Ligand CLA J 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA F 321	
	
Bond lengths	Bond angles
	
Torsions	Rings

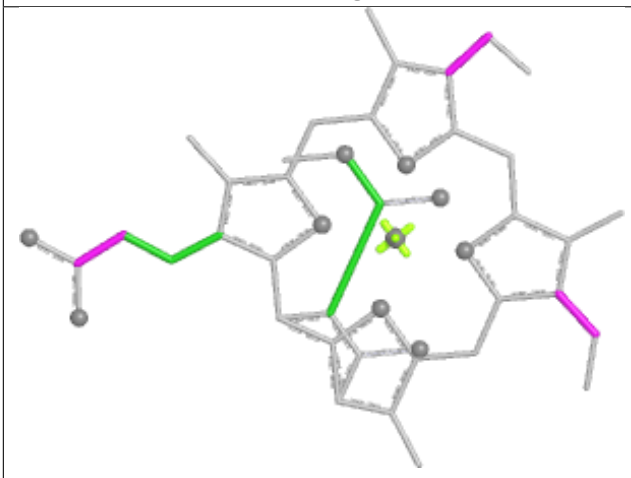
Ligand KC2 y 307



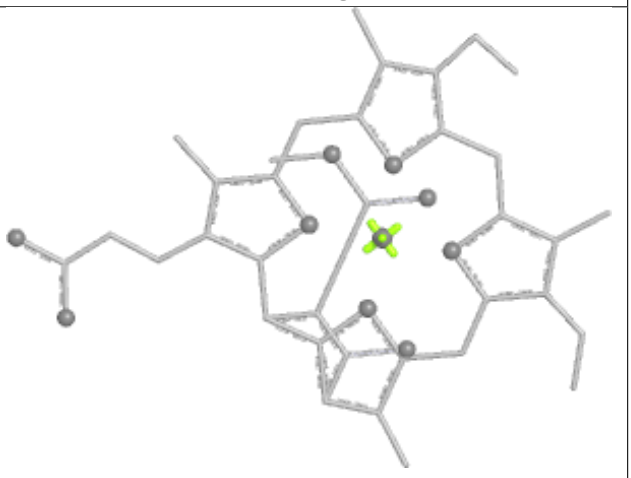
Bond lengths



Bond angles

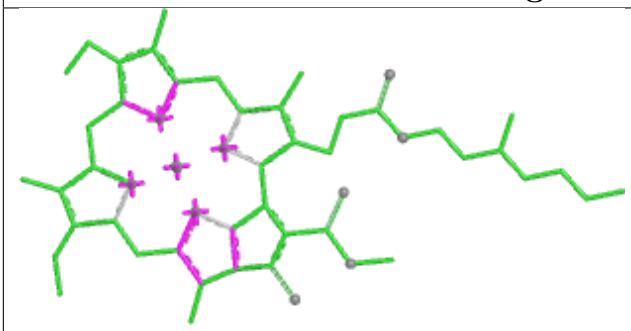


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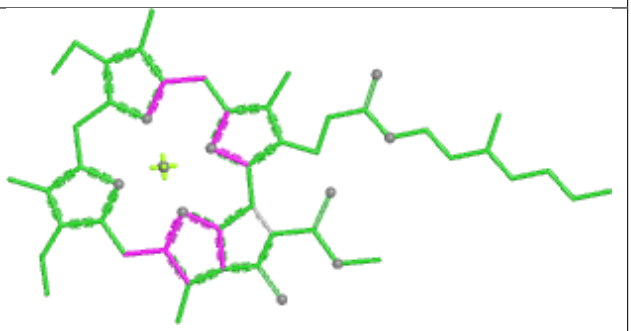


Rings

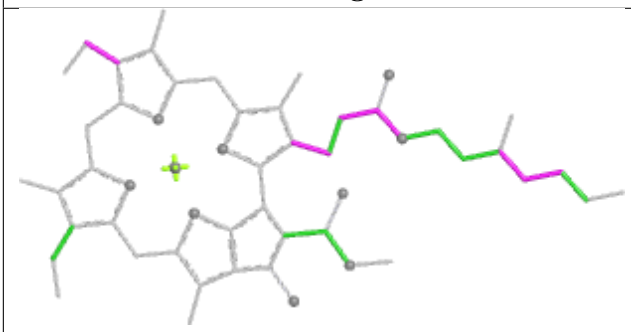
Ligand CLA F 301



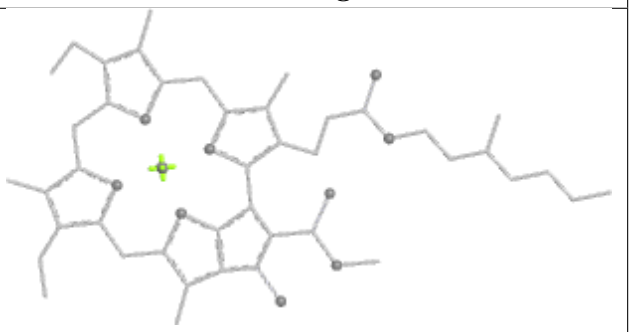
Bond lengths



Bond angles

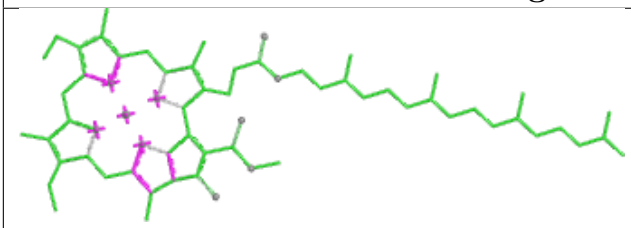


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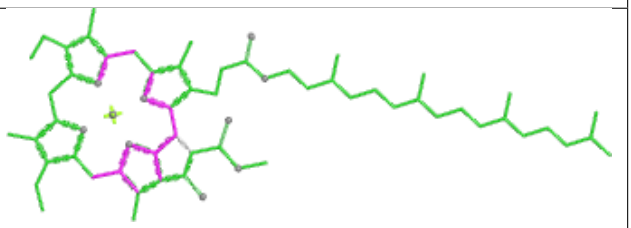


Rings

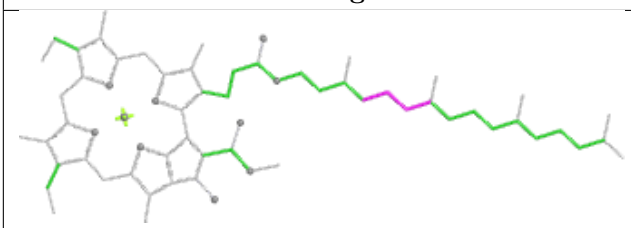
Ligand CLA a 803



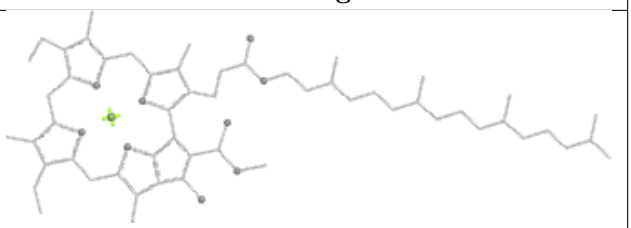
Bond lengths



Bond angles

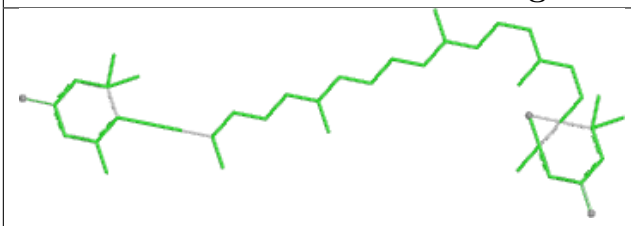


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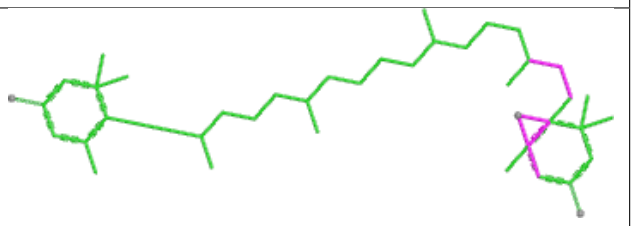


Rings

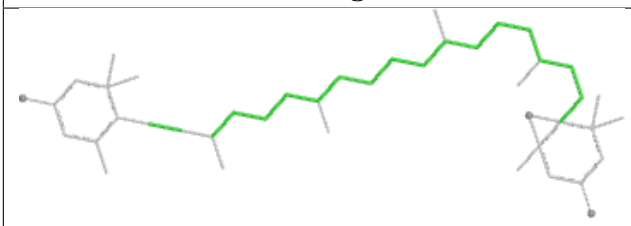
Ligand DD6 J 316



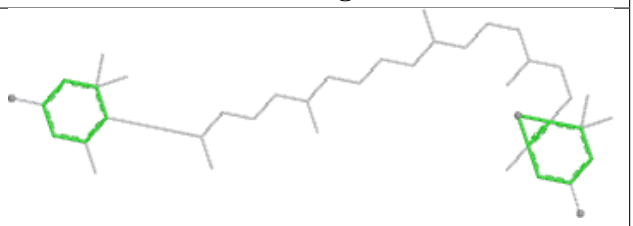
Bond lengths



Bond angles

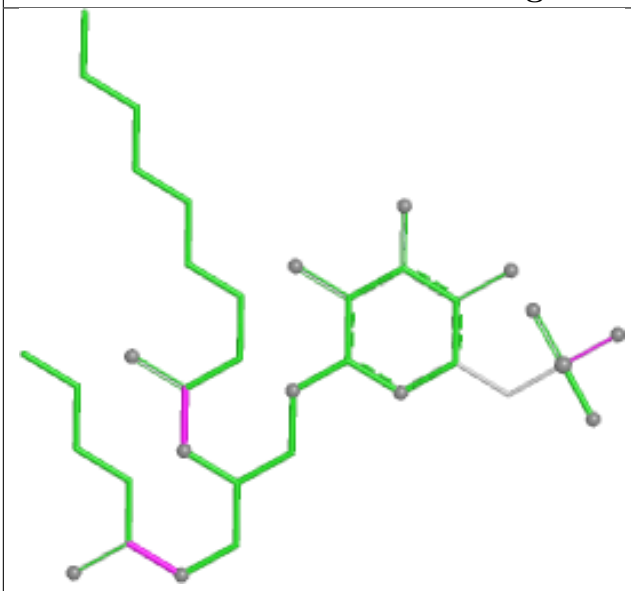


Torsions

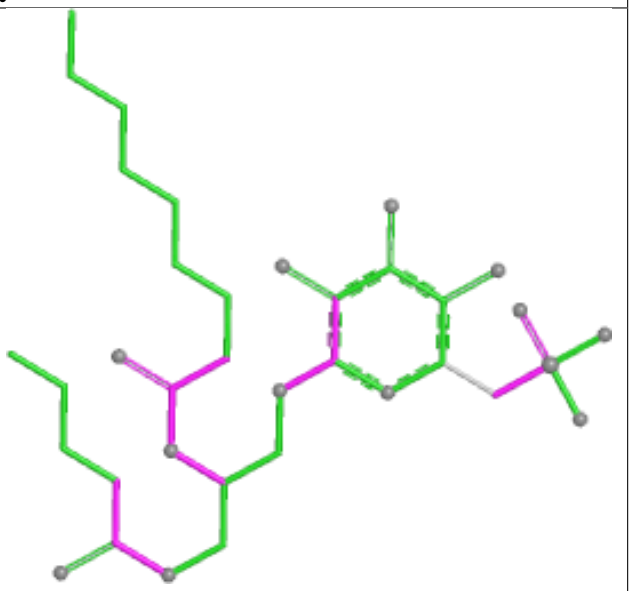


Rings

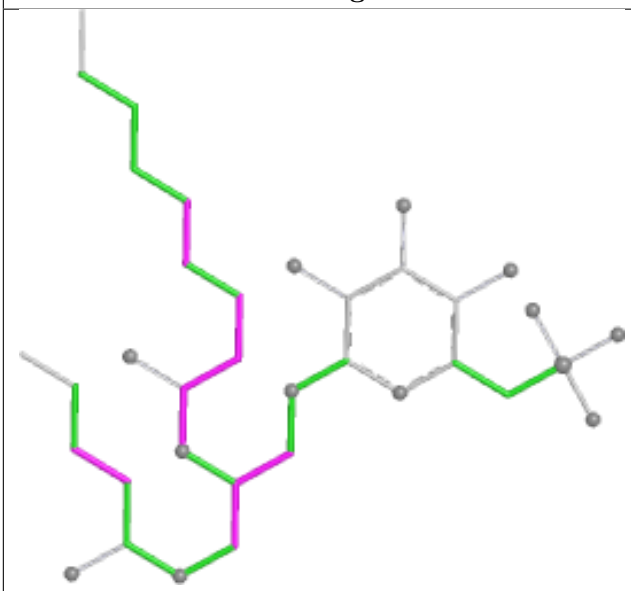
Ligand SQD F 320



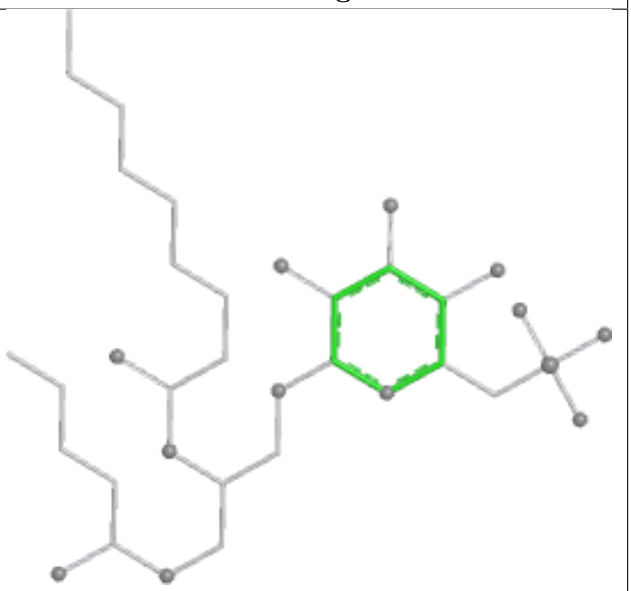
Bond lengths



Bond angles

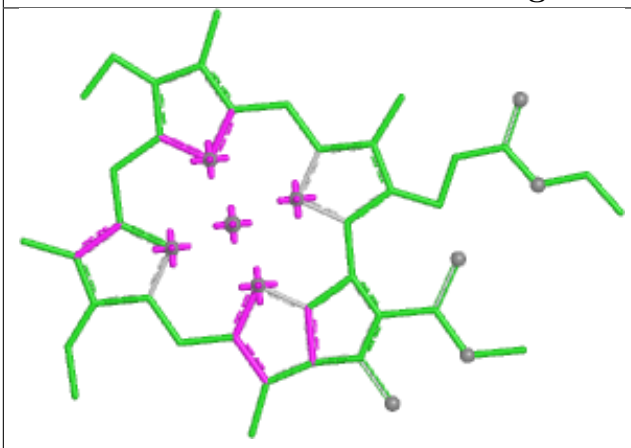


Torsions

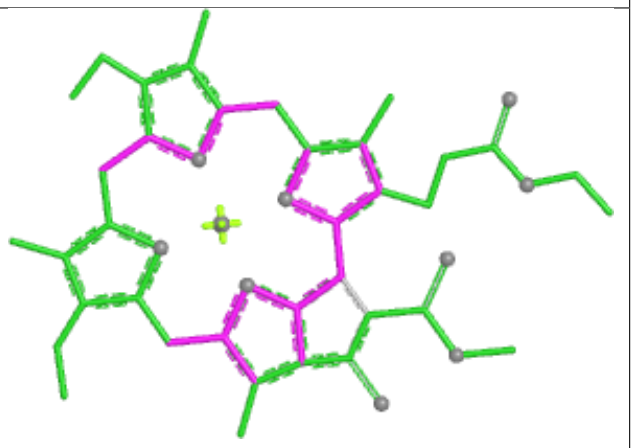


Rings

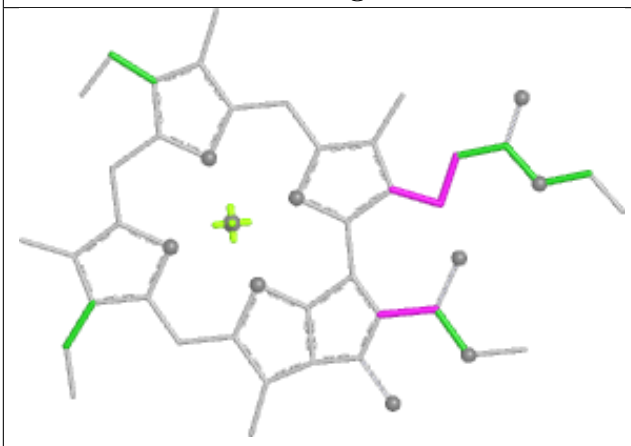
Ligand CLA o 313



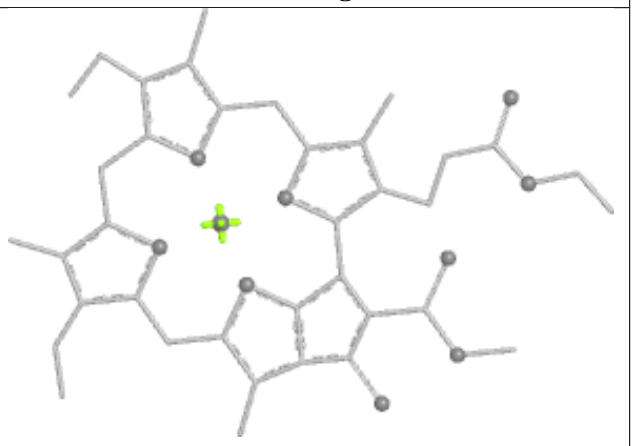
Bond lengths



Bond angles

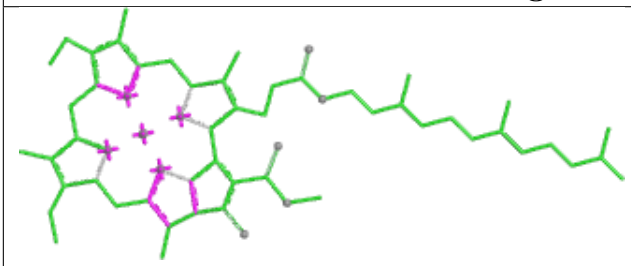


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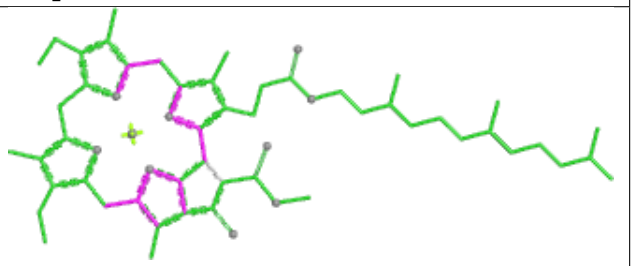


Rings

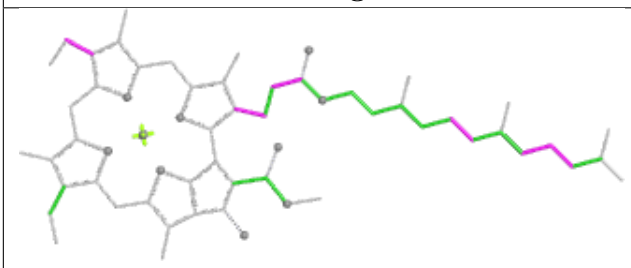
Ligand CLA p 308



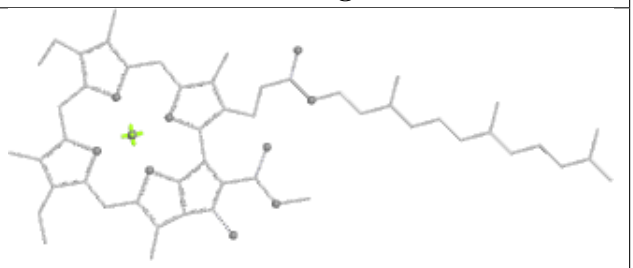
Bond lengths



Bond angles

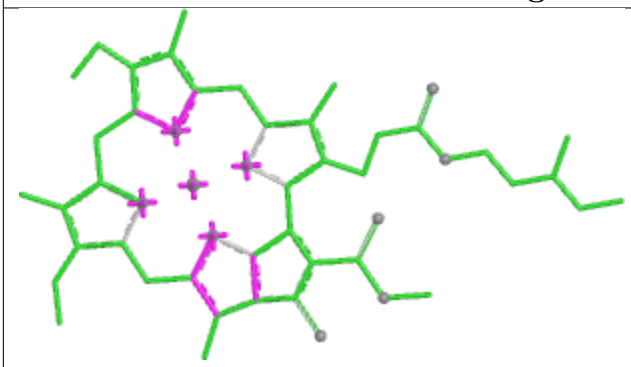


Torsions

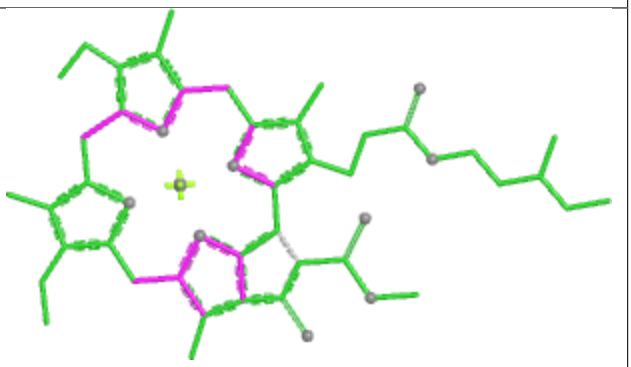


Rings

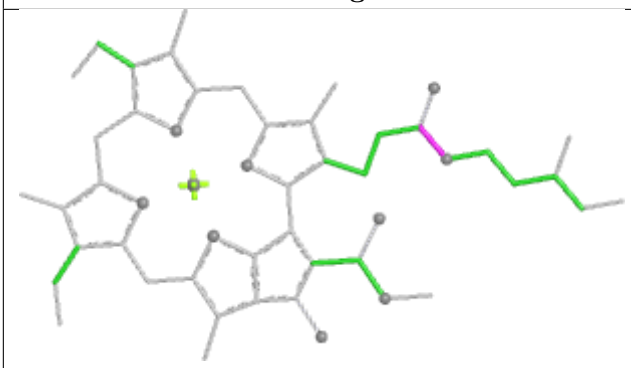
Ligand CLA x 305



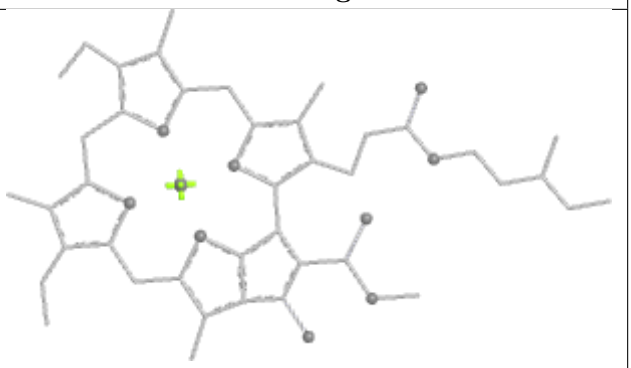
Bond lengths



Bond angles

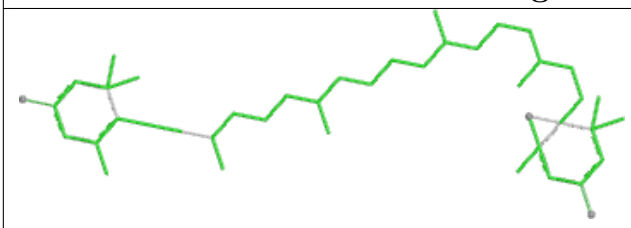


Torsions

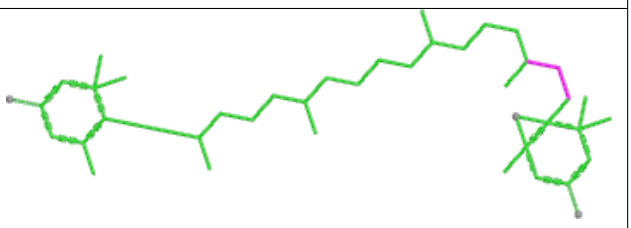


Rings

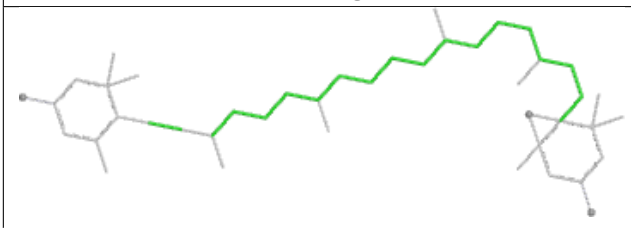
Ligand DD6 I 212



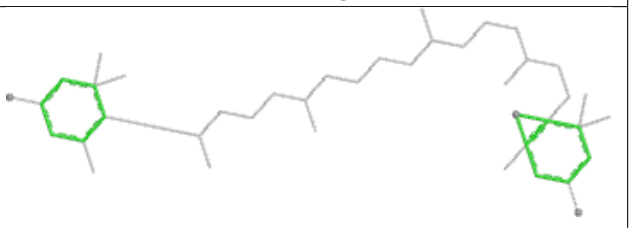
Bond lengths



Bond angles

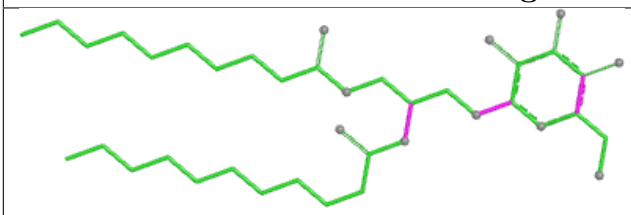


Torsions

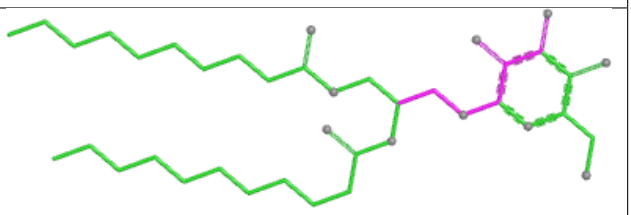


Rings

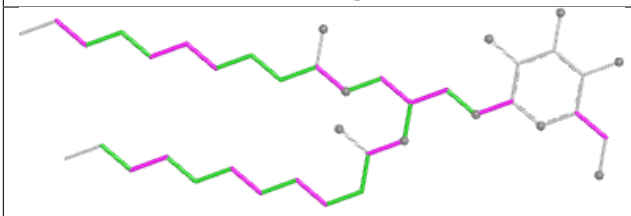
Ligand LMG T 318



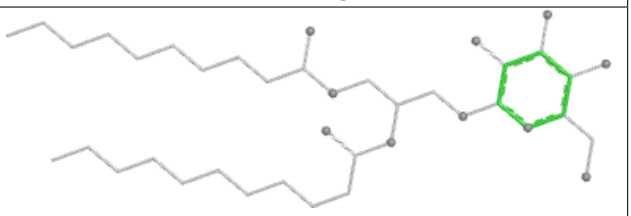
Bond lengths



Bond angles

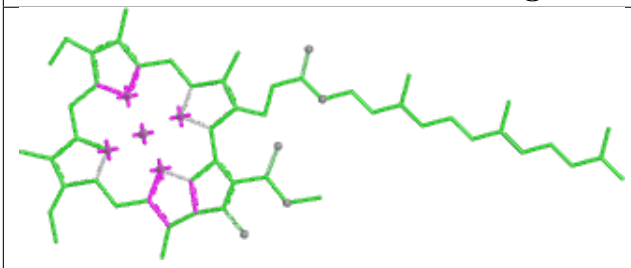


Torsions

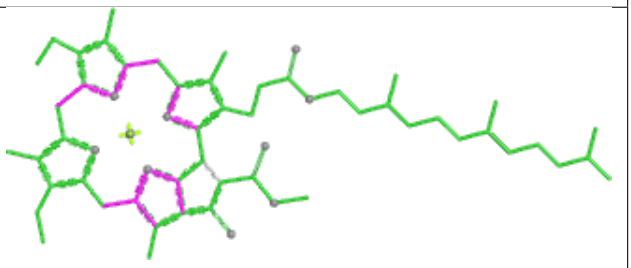


Rings

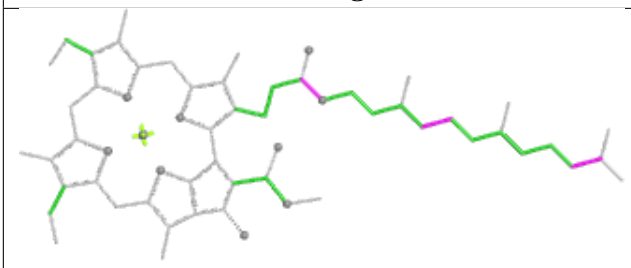
Ligand CLA X 307



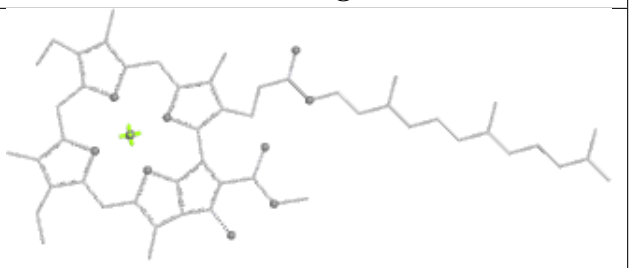
Bond lengths



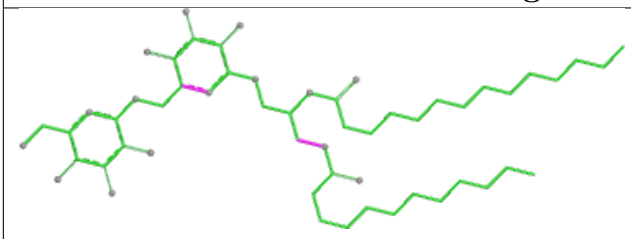
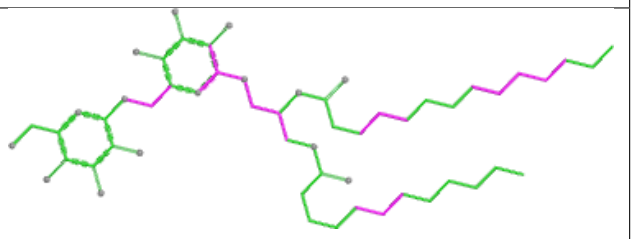
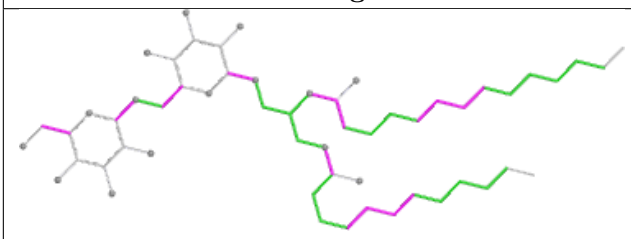
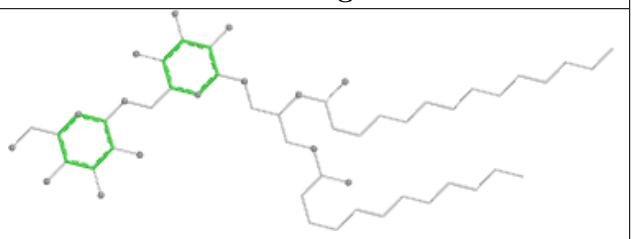
Bond angles

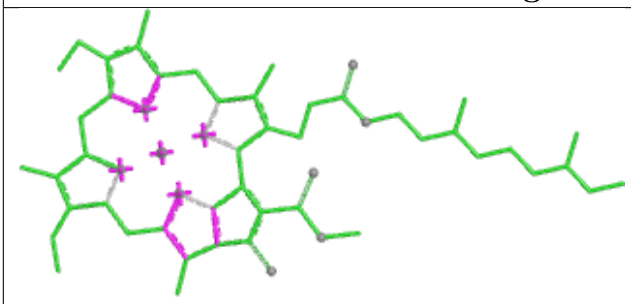
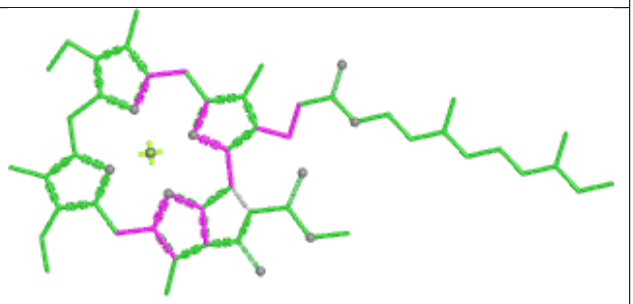
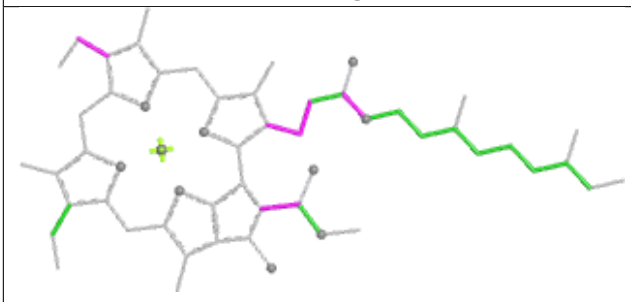
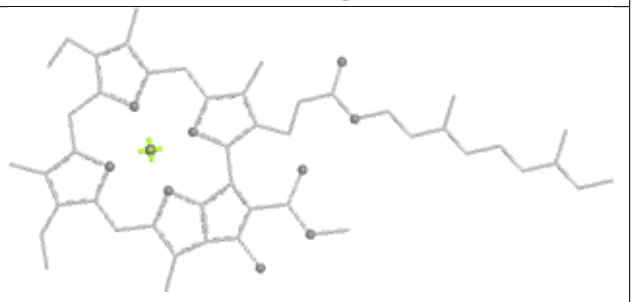


Torsions

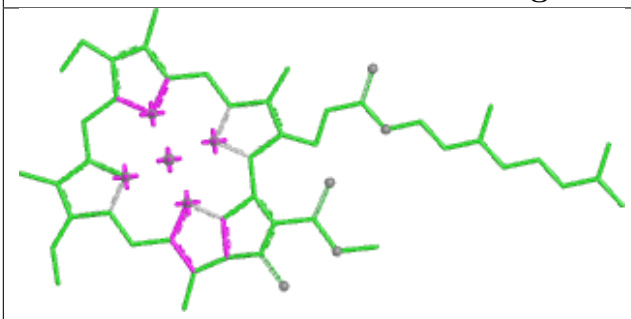


Rings

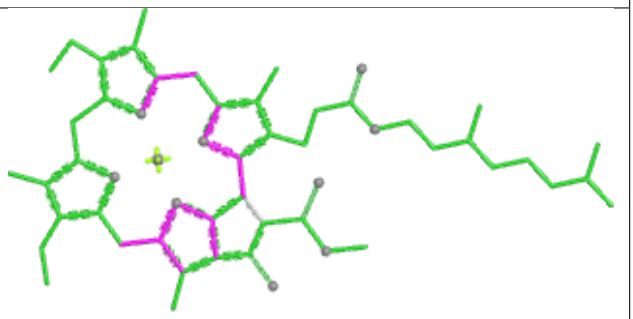
Ligand DGD b 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

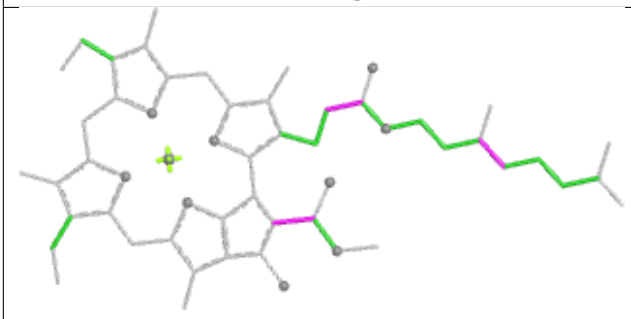
Ligand CLA I 203



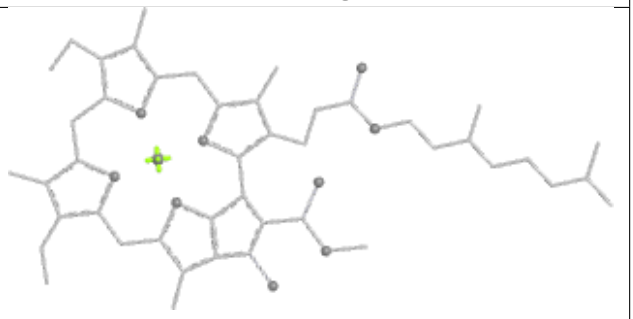
Bond lengths



Bond angles

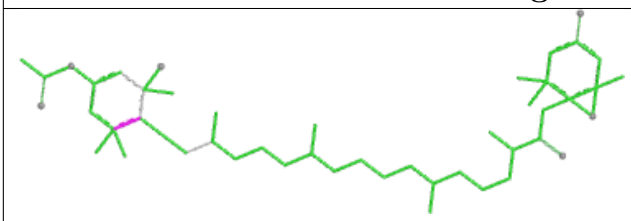


Torsions

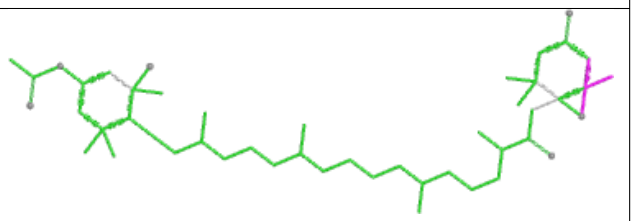


Rings

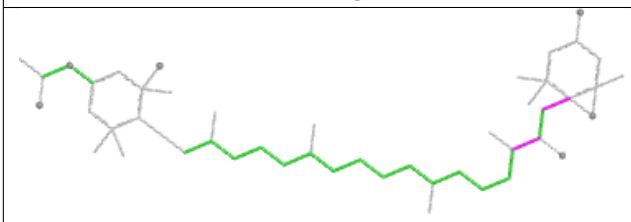
Ligand A86 P 321



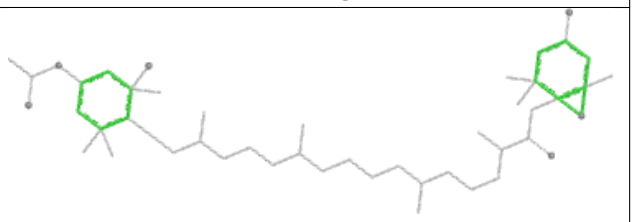
Bond lengths



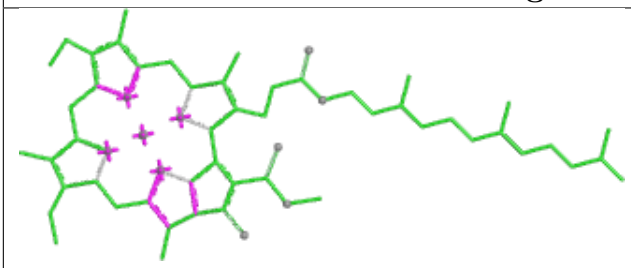
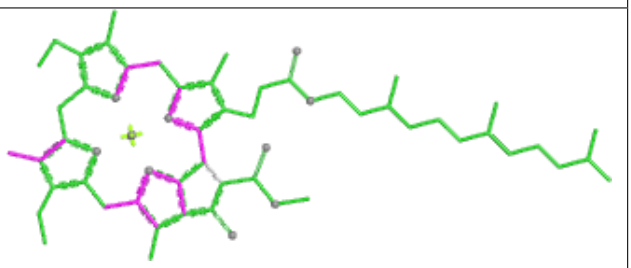
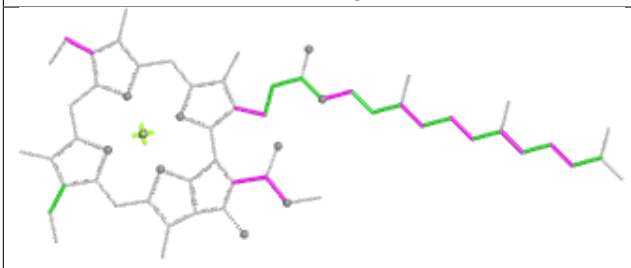
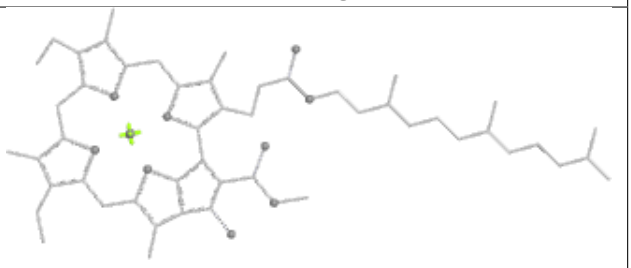
Bond angles

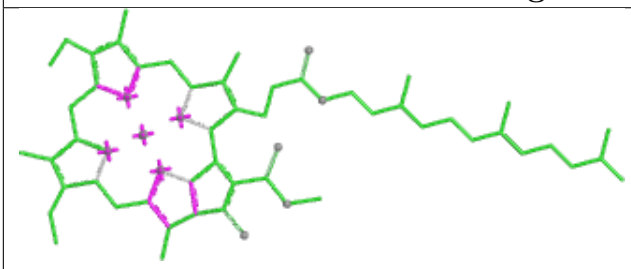
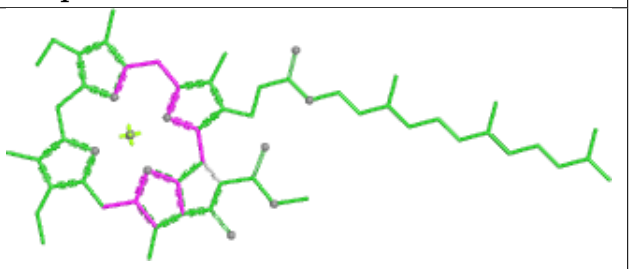
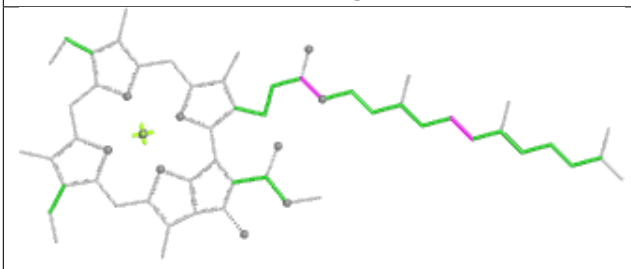
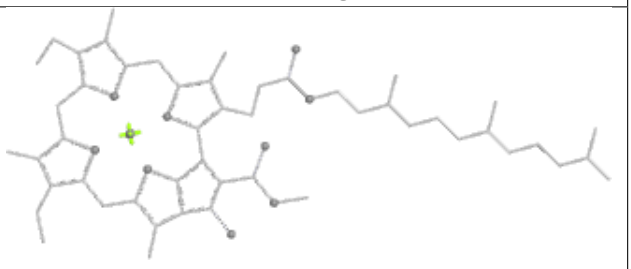


Torsions

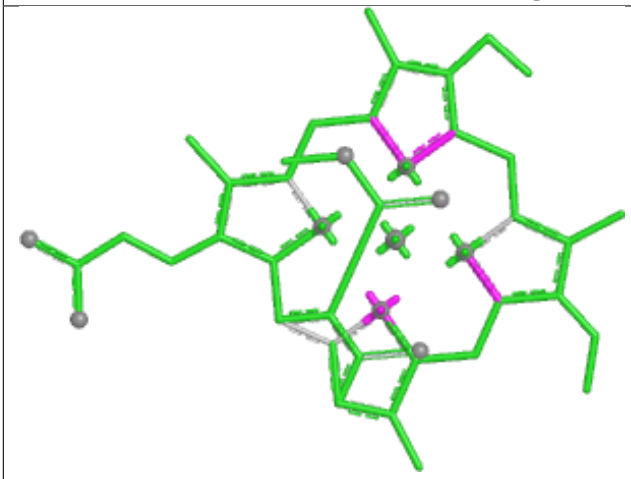


Rings

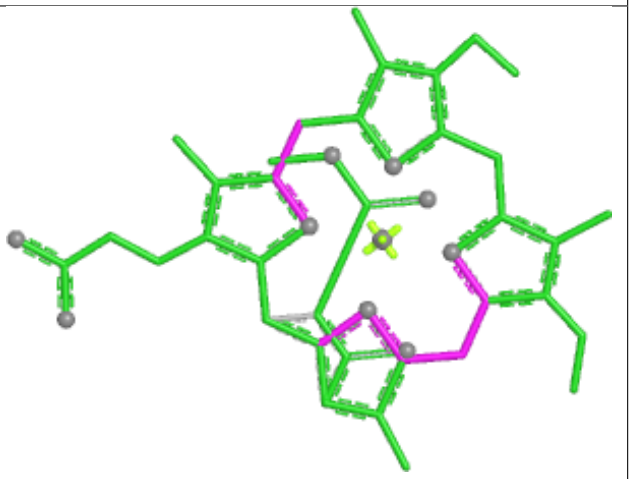
Ligand CLA Z 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA q 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

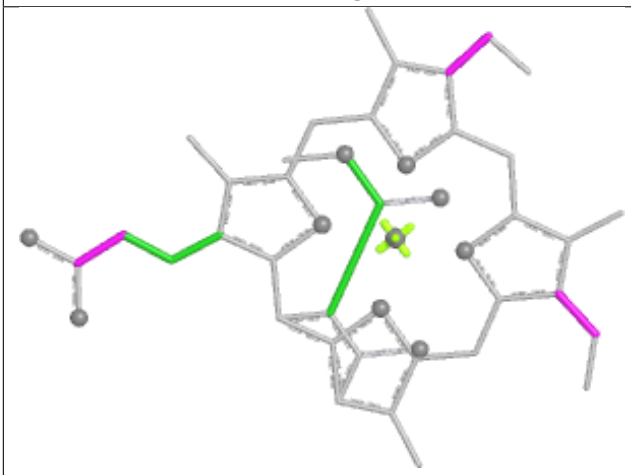
Ligand KC2 Z 308



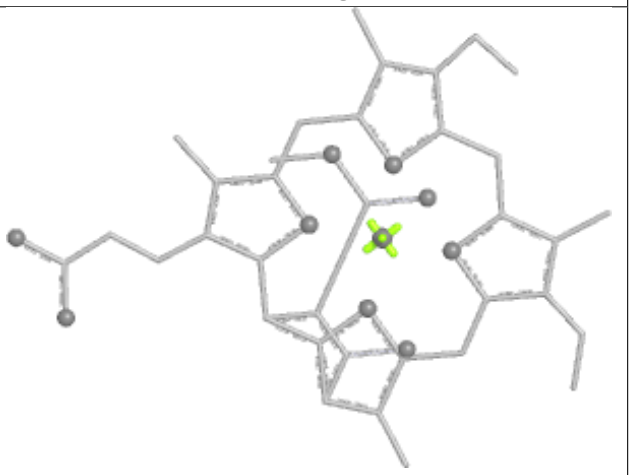
Bond lengths



Bond angles

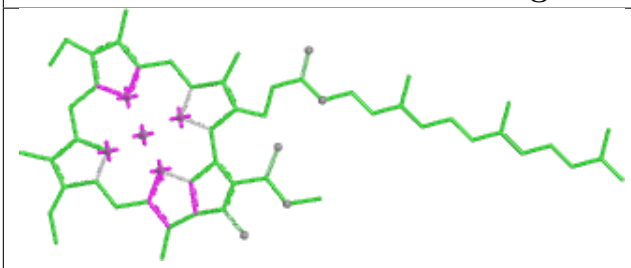


Torsions

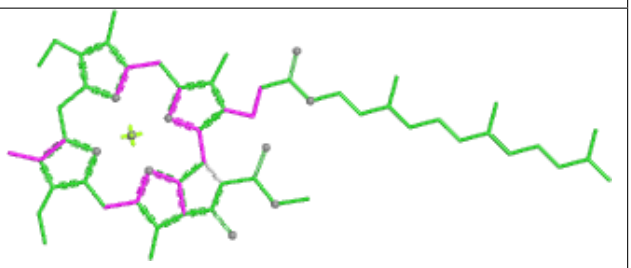


Rings

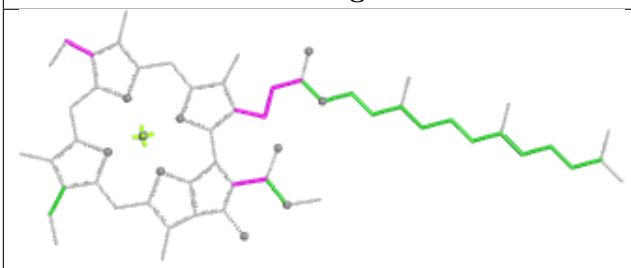
Ligand CLA t 304



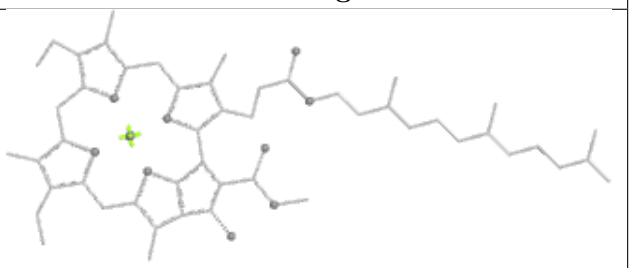
Bond lengths



Bond angles

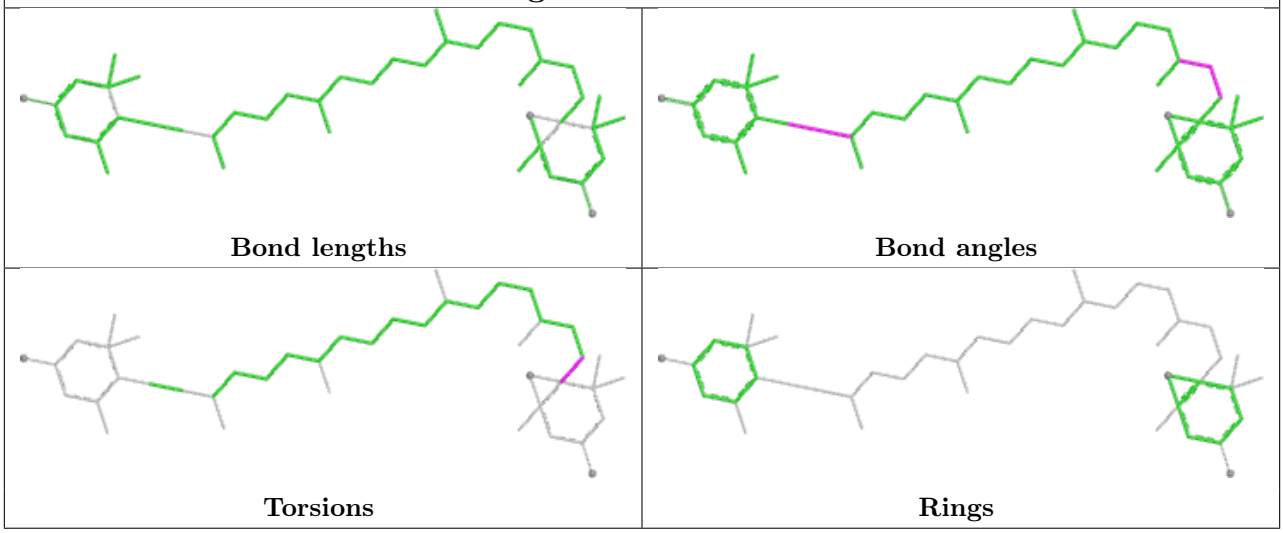


Torsions

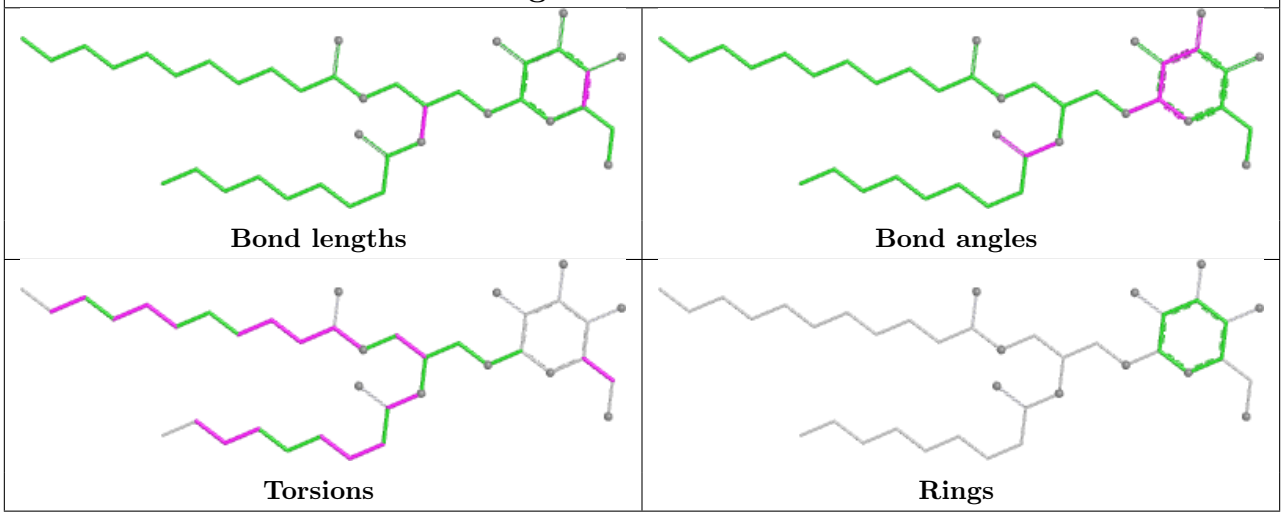


Rings

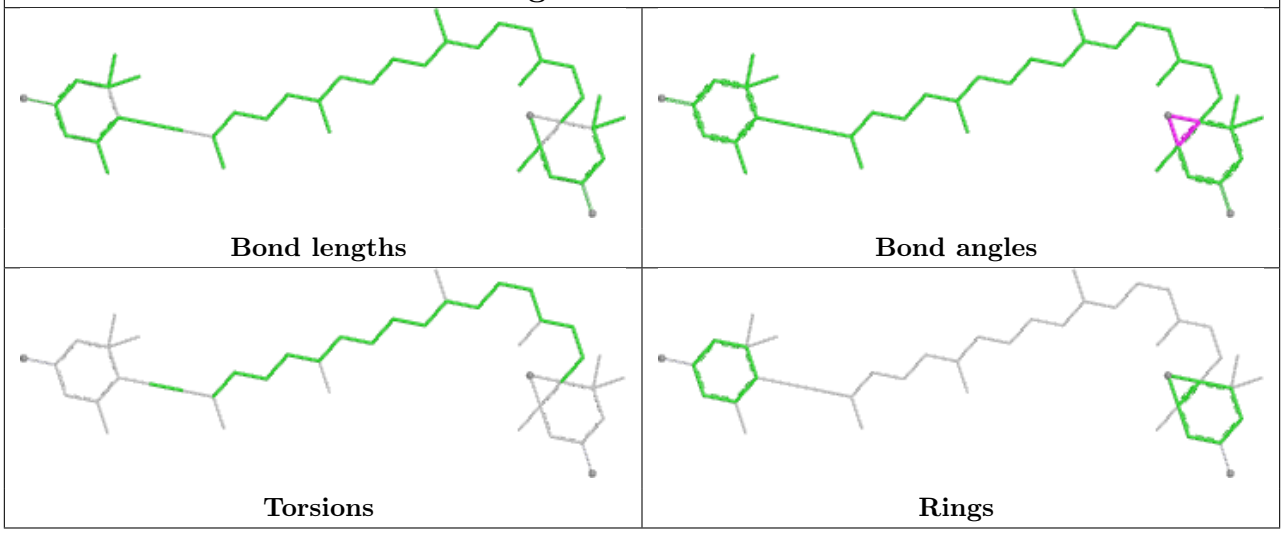
Ligand DD6 F 316



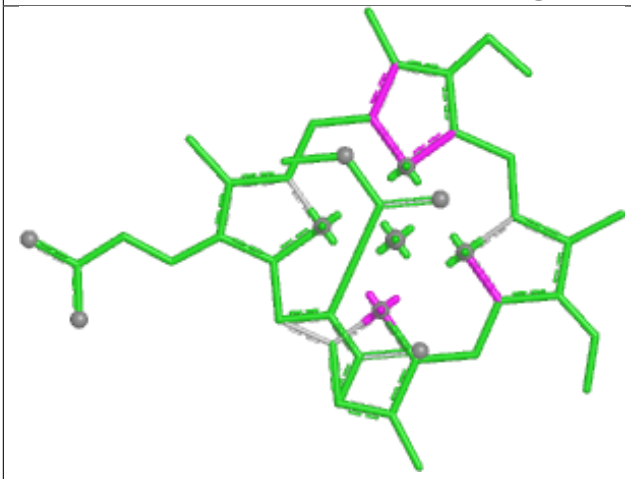
Ligand LMG l 201



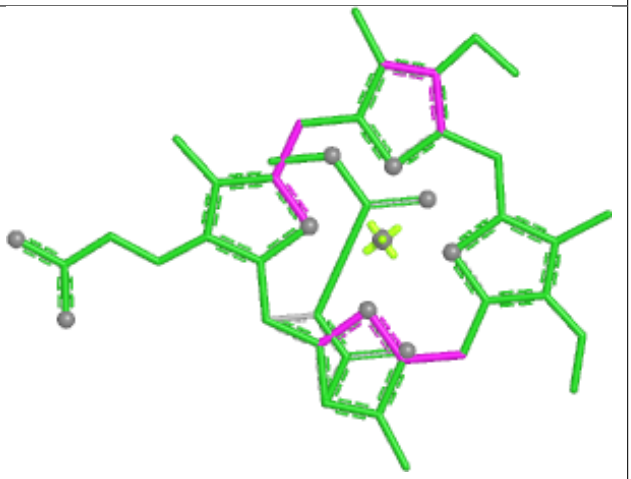
Ligand DD6 L 317



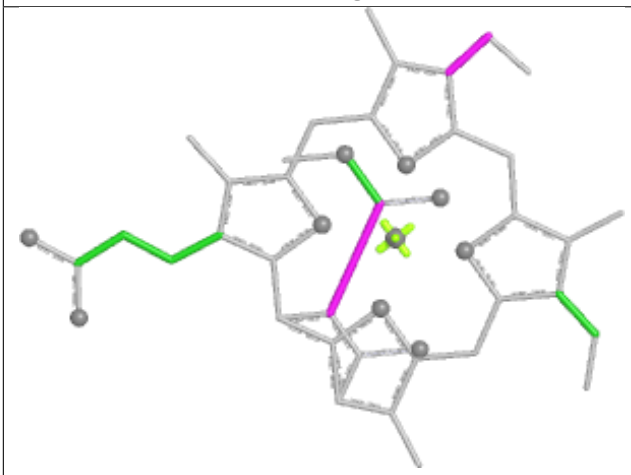
Ligand KC2 o 303



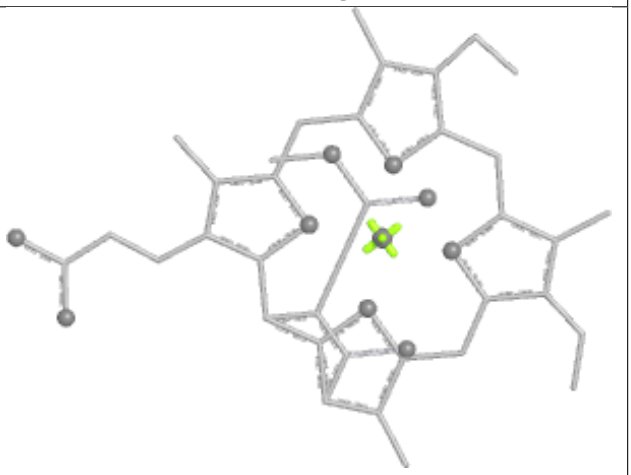
Bond lengths



Bond angles

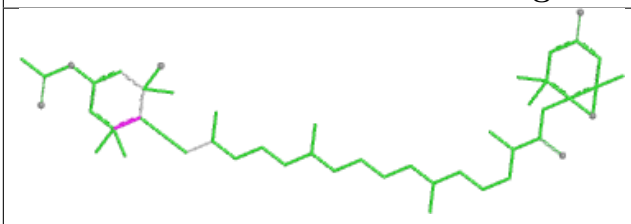


Torsions

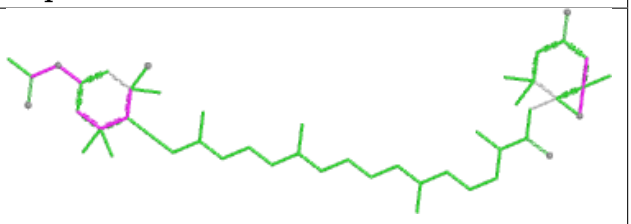


Rings

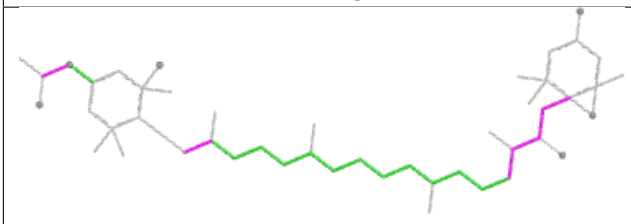
Ligand A86 p 319



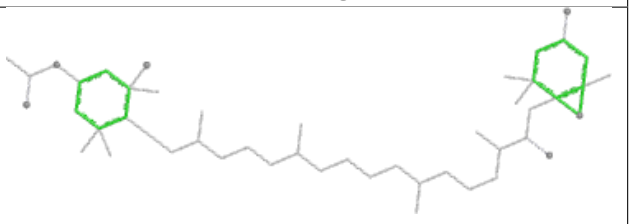
Bond lengths



Bond angles

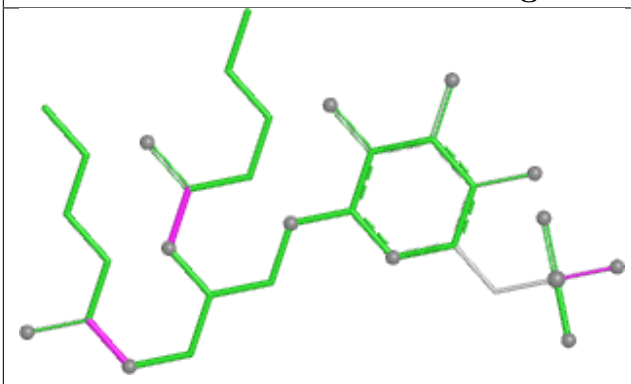


Torsions

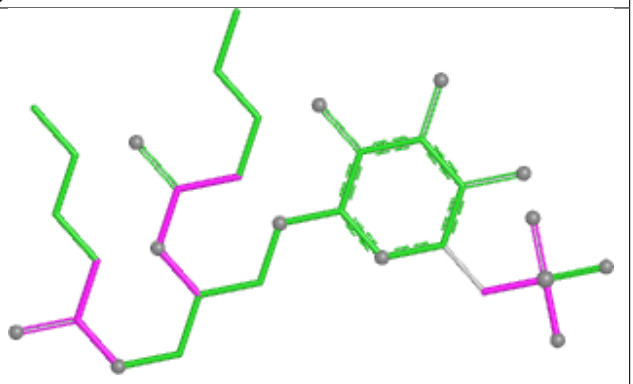


Rings

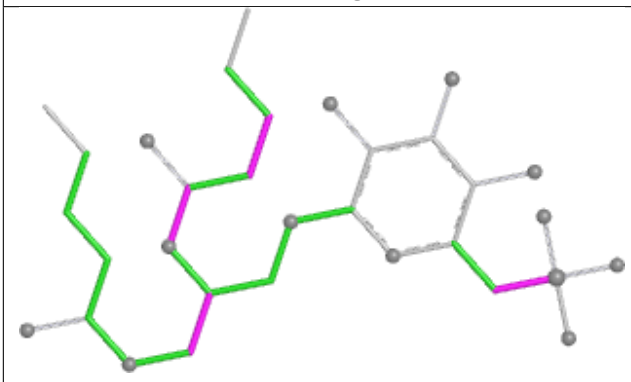
Ligand SQD M 318



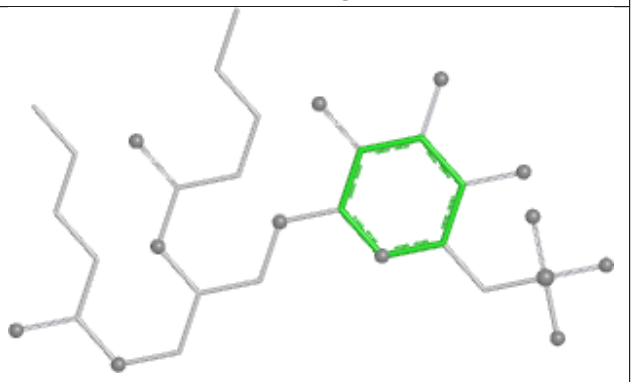
Bond lengths



Bond angles

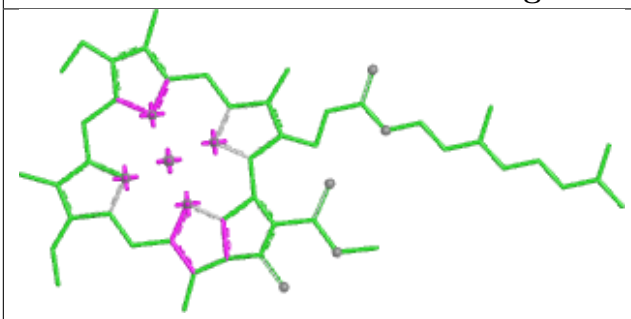


Torsions

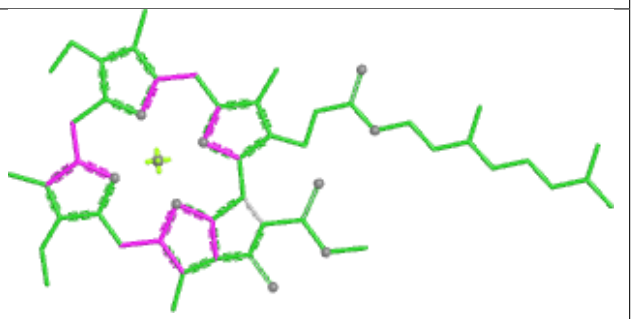


Rings

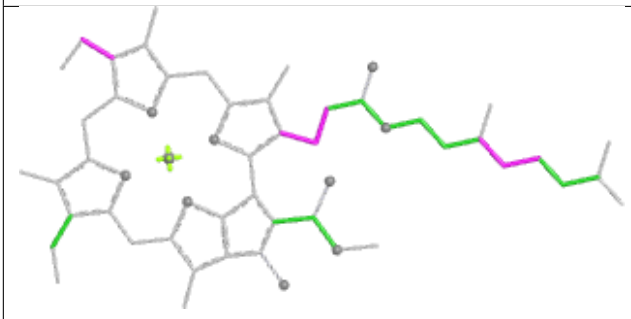
Ligand CLA V 202



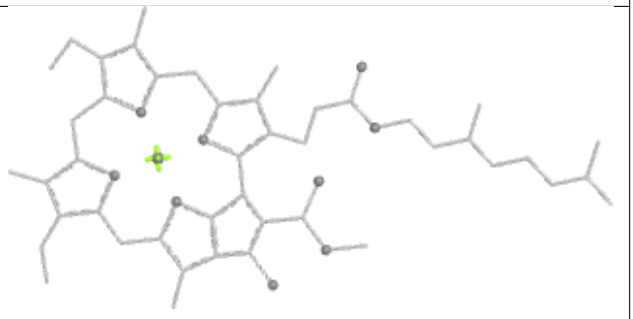
Bond lengths



Bond angles

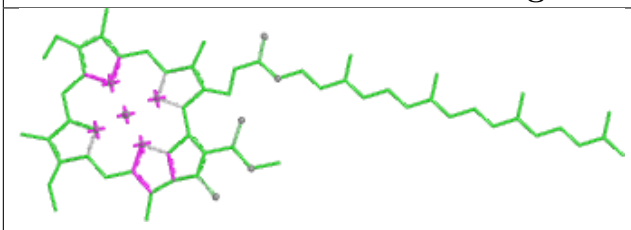


Torsions

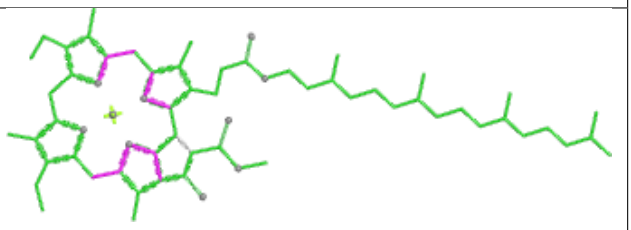


Rings

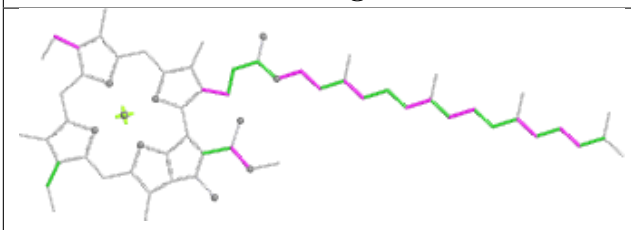
Ligand CLA b 806



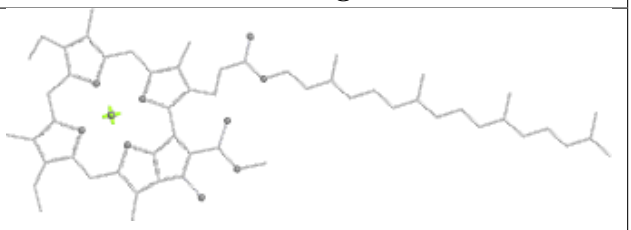
Bond lengths



Bond angles

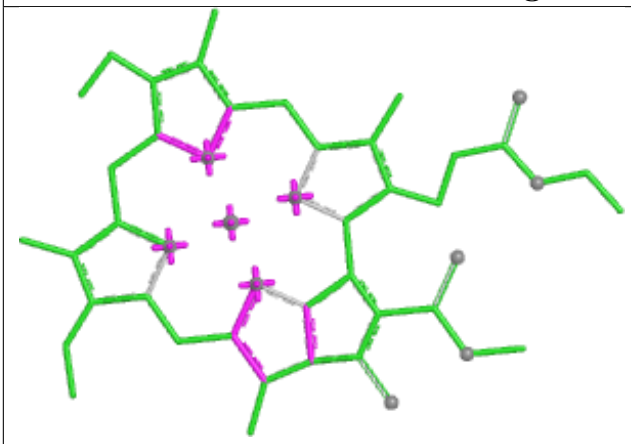


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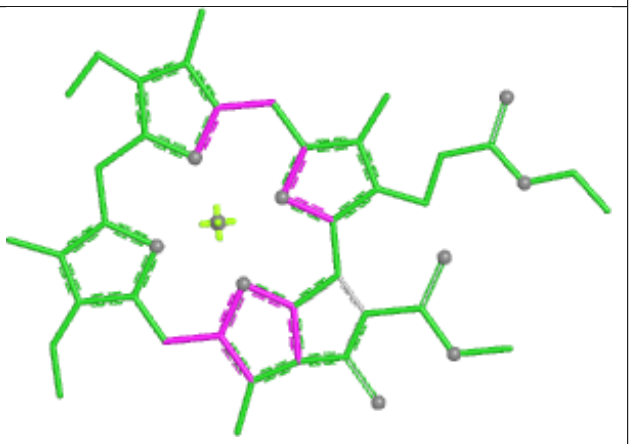


Rings

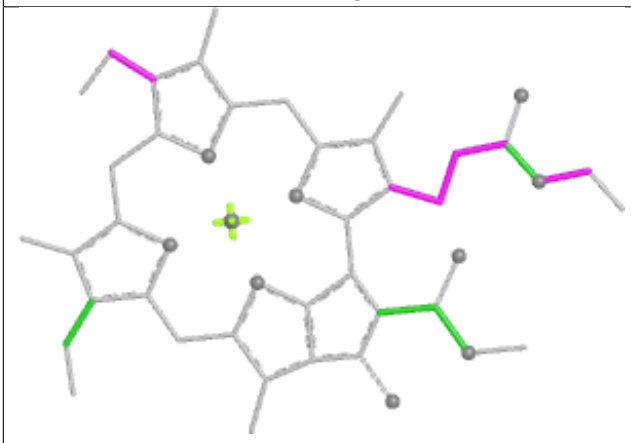
Ligand CLA U 204



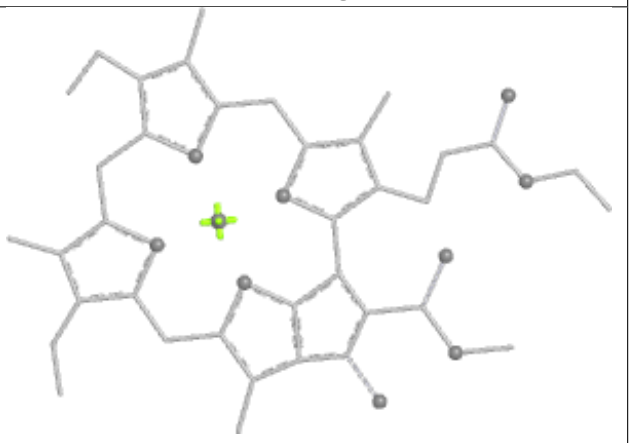
Bond lengths



Bond angles

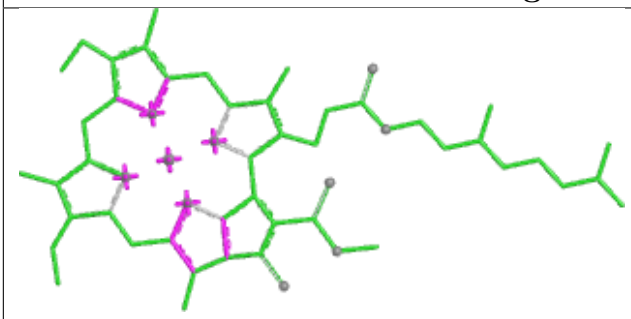


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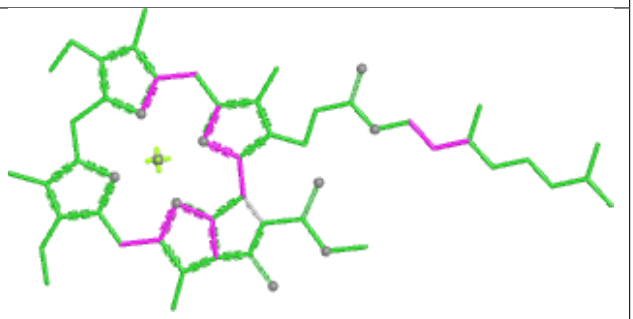


Rings

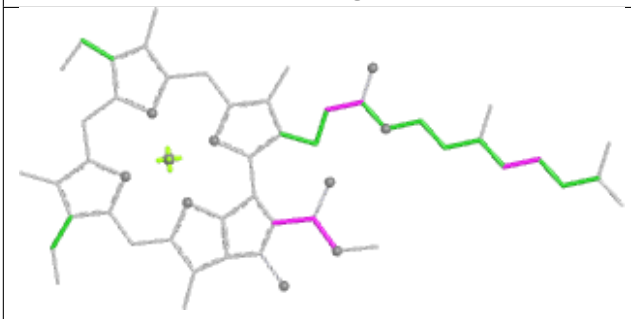
Ligand CLA D 306



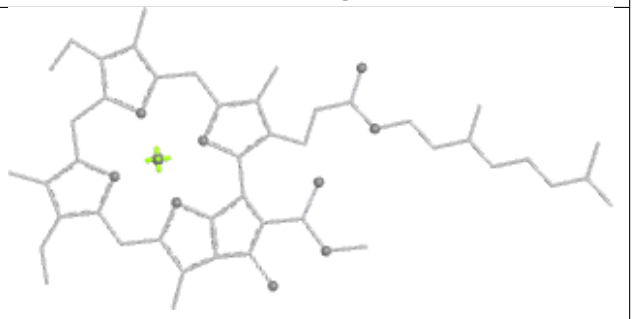
Bond lengths



Bond angles

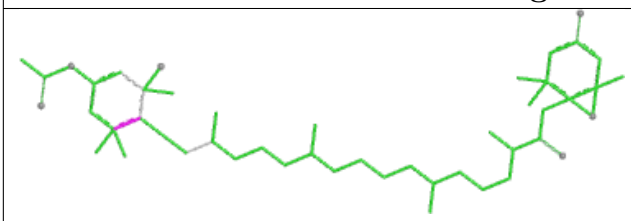


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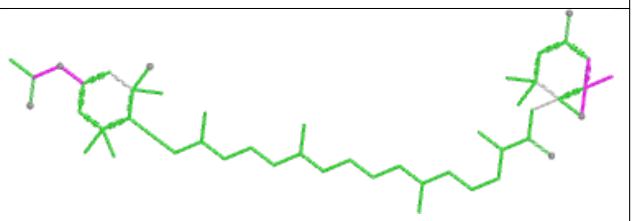


Rings

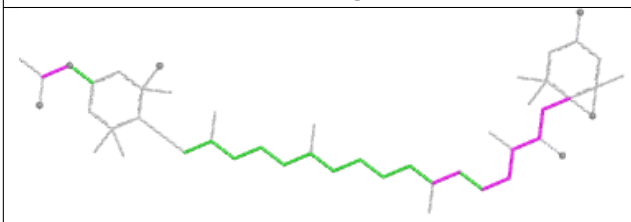
Ligand A86 w 316



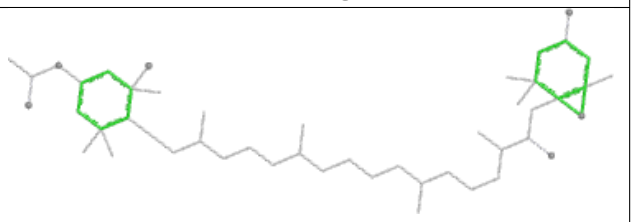
Bond lengths



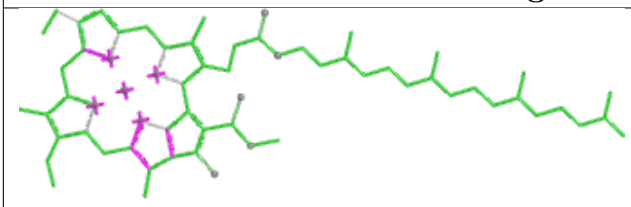
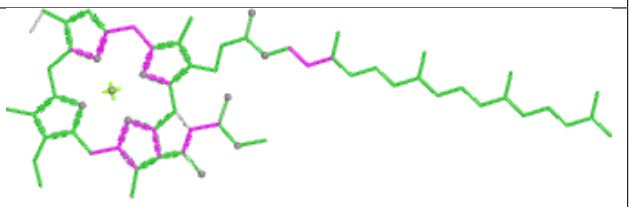
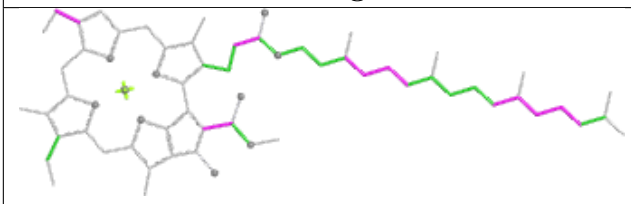
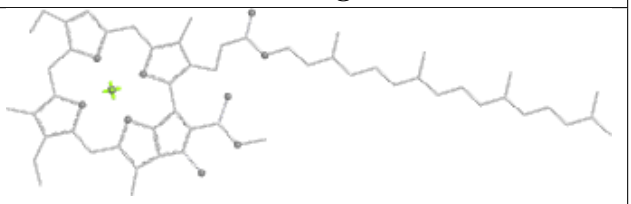
Bond angles

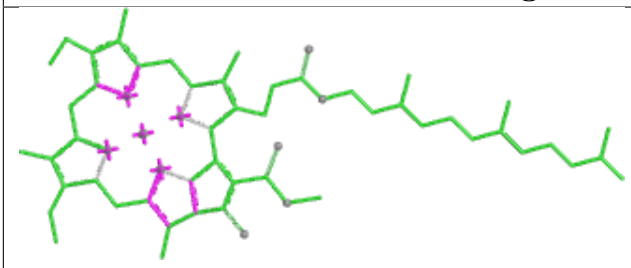
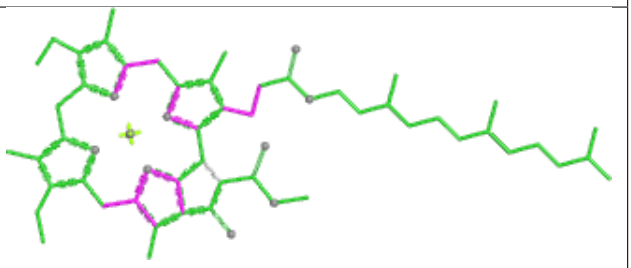
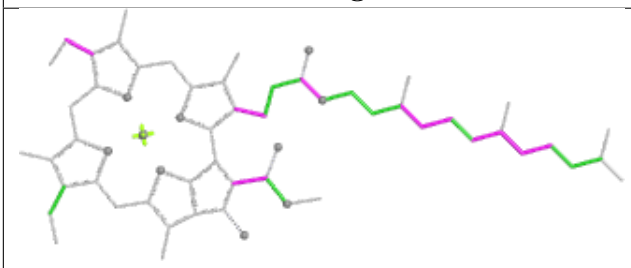
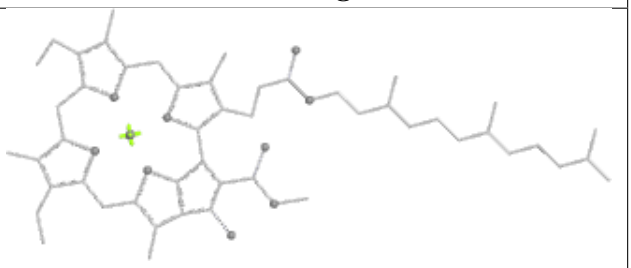


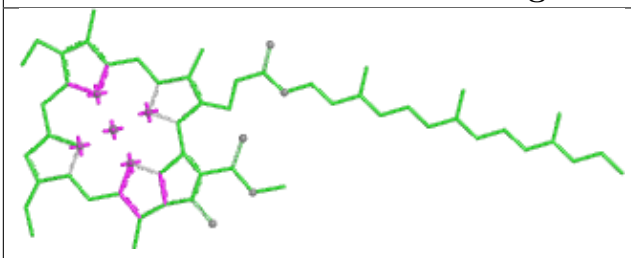
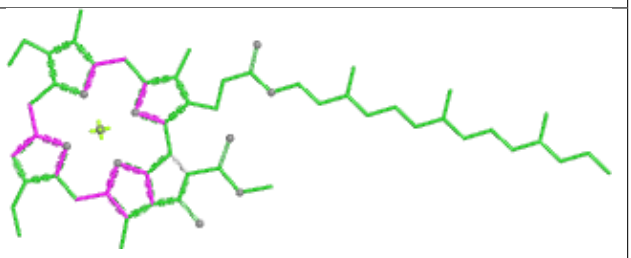
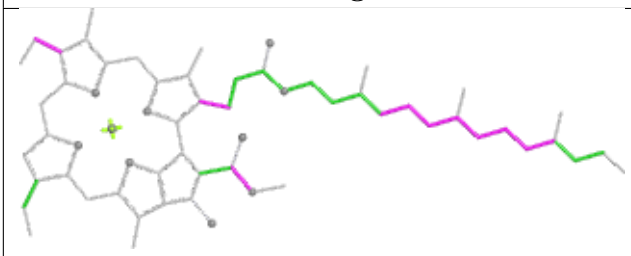
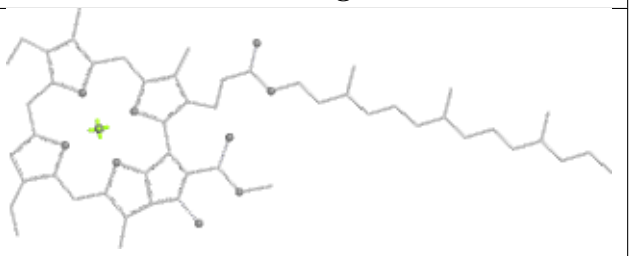
Torsions

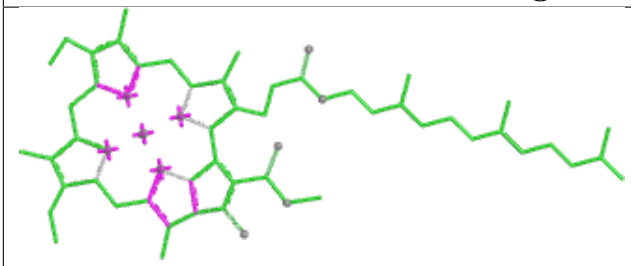
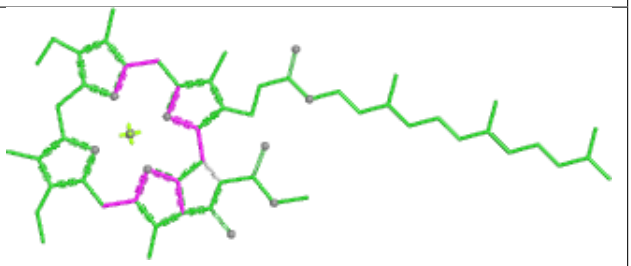
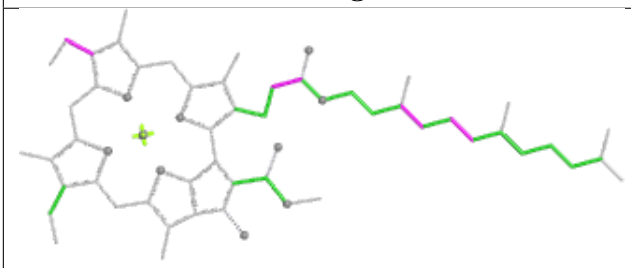
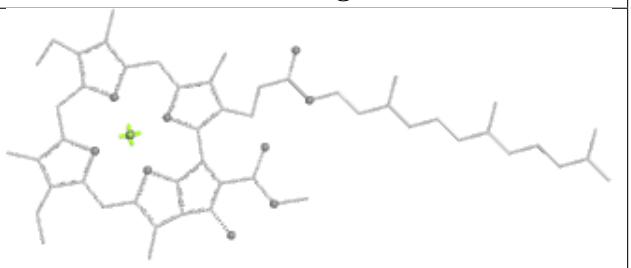


Rings

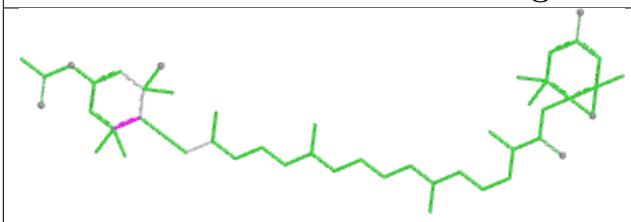
Ligand CLA b 835	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA M 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

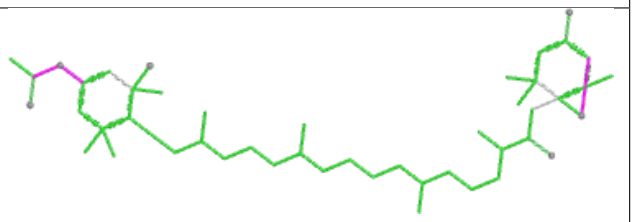
Ligand CLA a 811	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA f 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

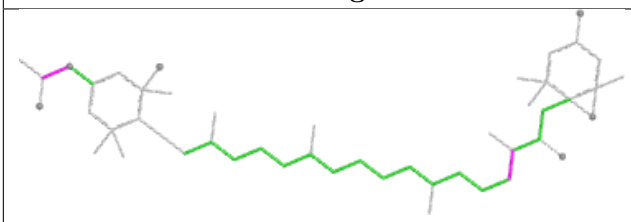
Ligand A86 F 312



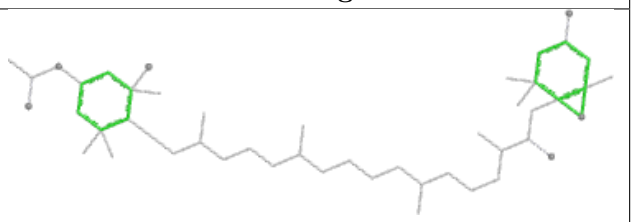
Bond lengths



Bond angles

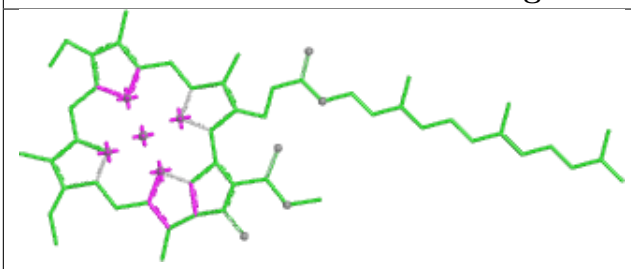


Torsions

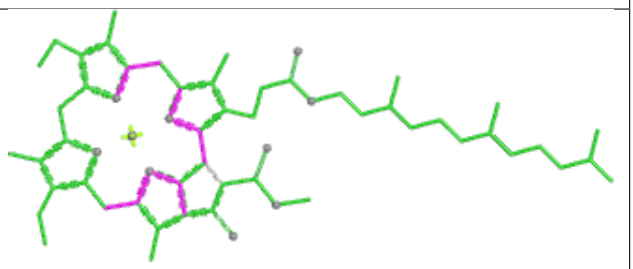


Rings

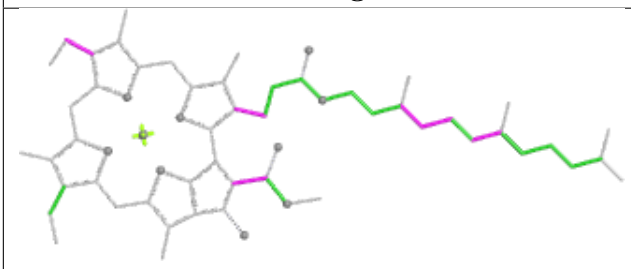
Ligand CLA A 306



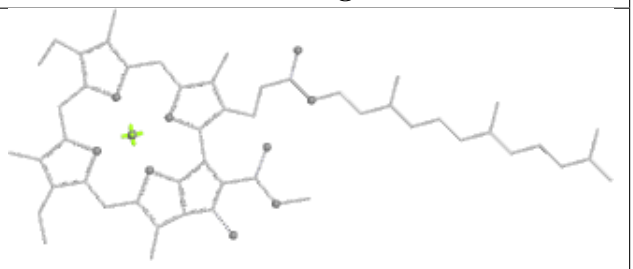
Bond lengths



Bond angles

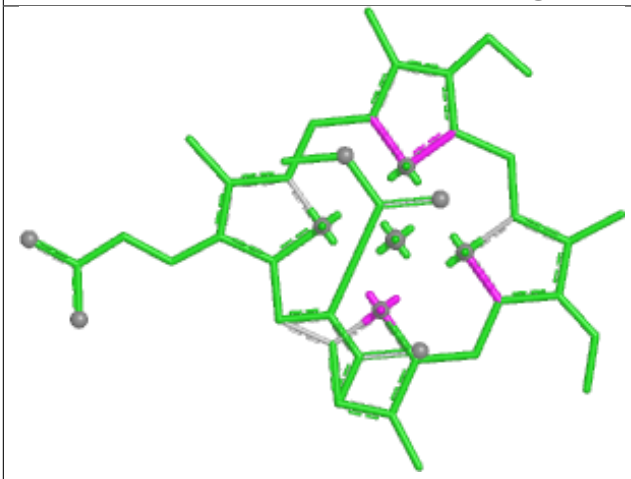


Torsions

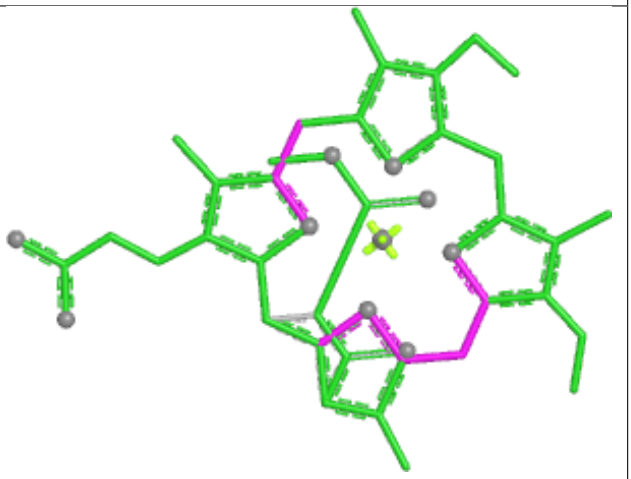


Rings

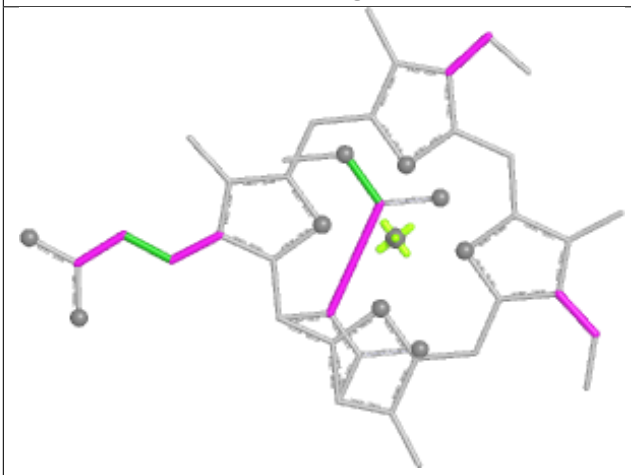
Ligand KC2 v 308



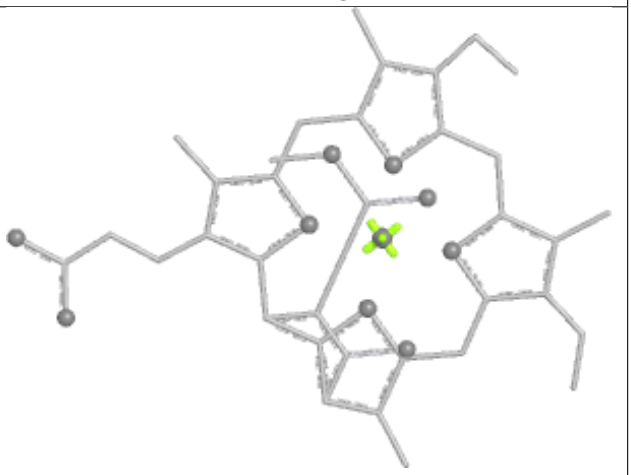
Bond lengths



Bond angles

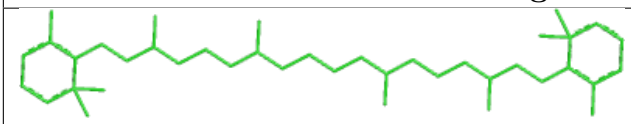


Torsions

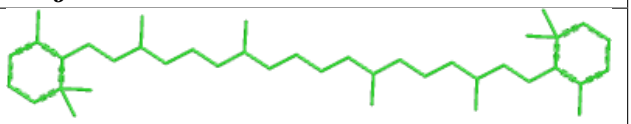


Rings

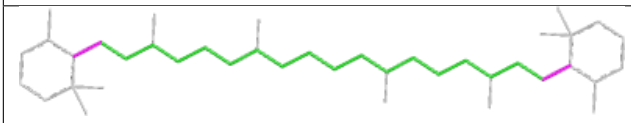
Ligand BCR j 103



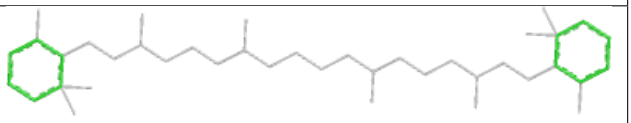
Bond lengths



Bond angles

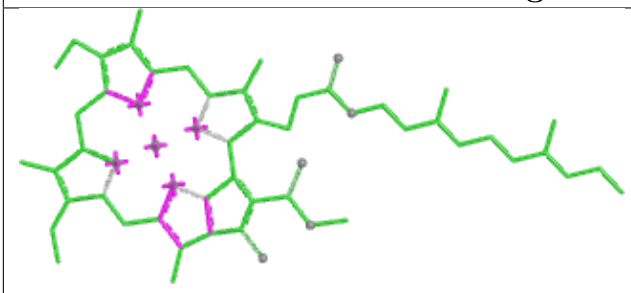


Torsions

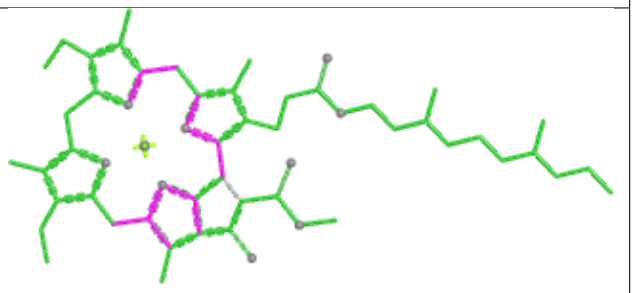


Rings

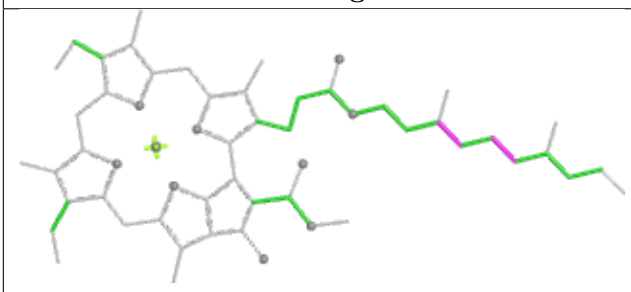
Ligand CLA L 304



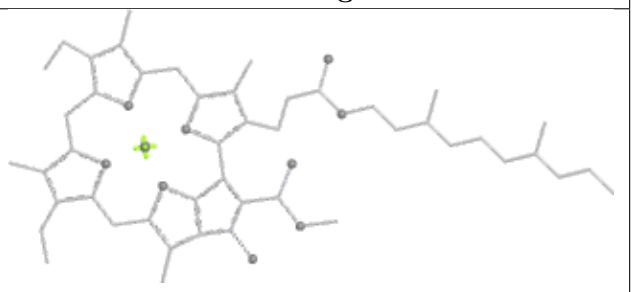
Bond lengths



Bond angles

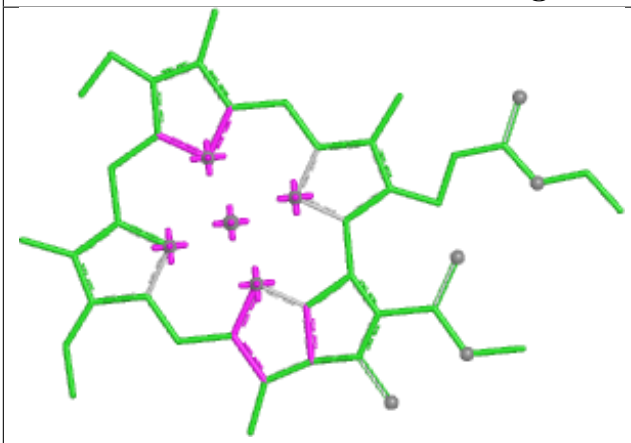


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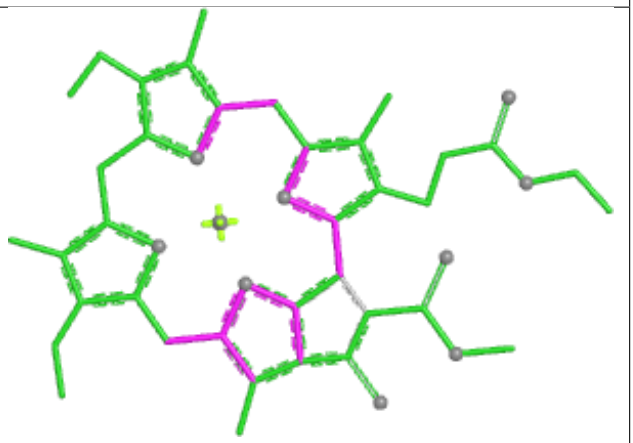


Rings

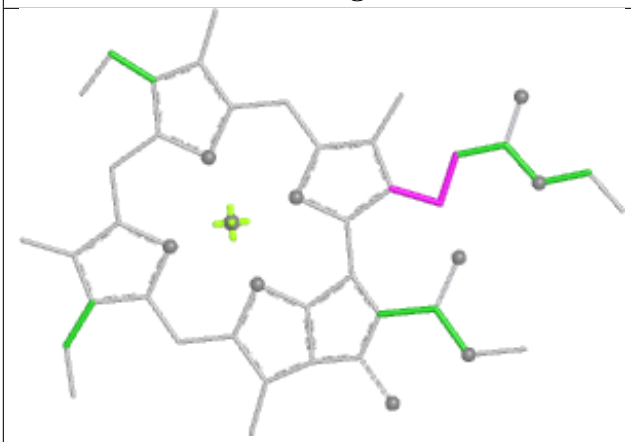
Ligand CLA t 303



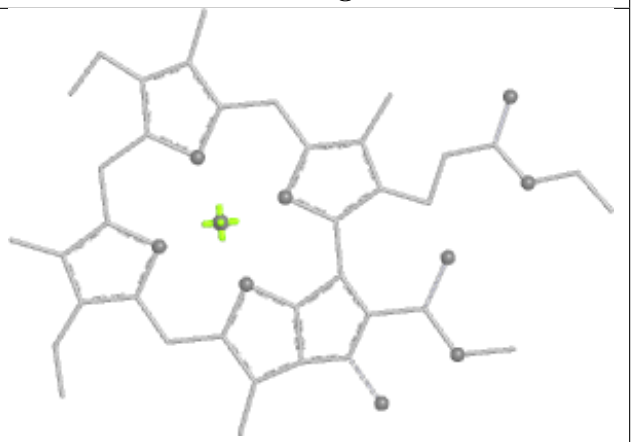
Bond lengths



Bond angles

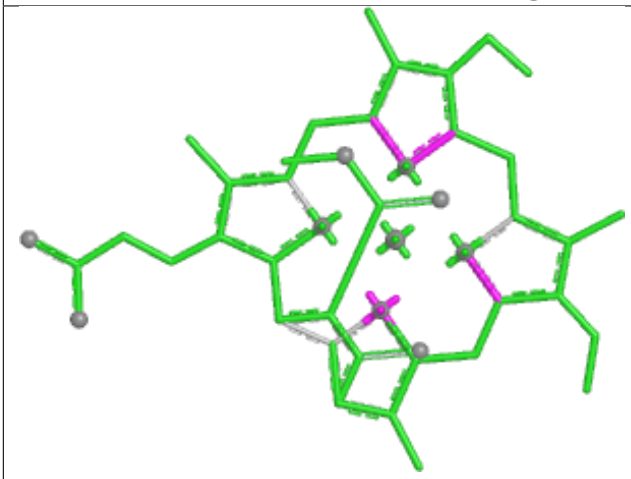


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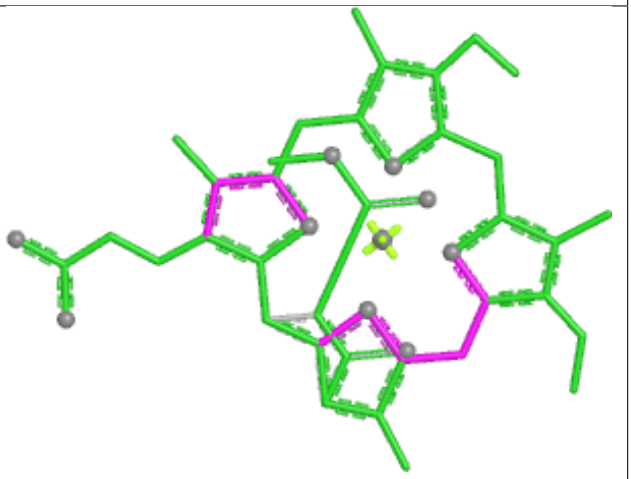


Rings

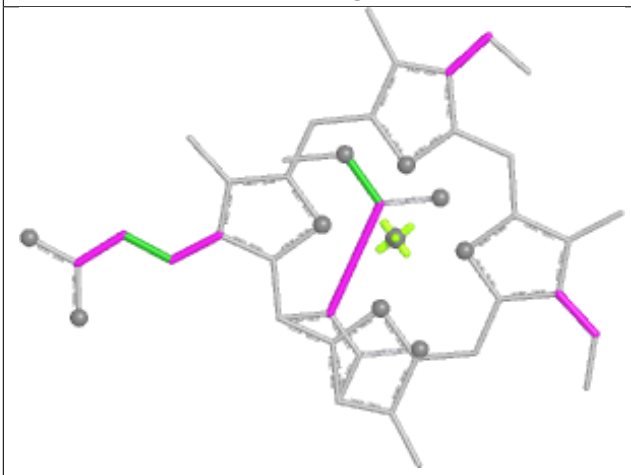
Ligand KC2 G 202



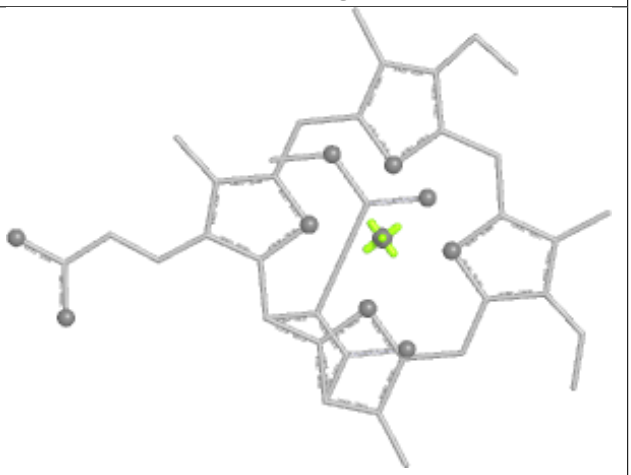
Bond lengths



Bond angles

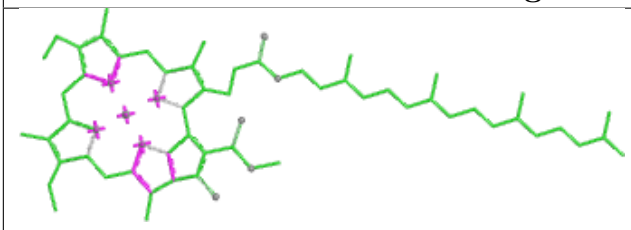


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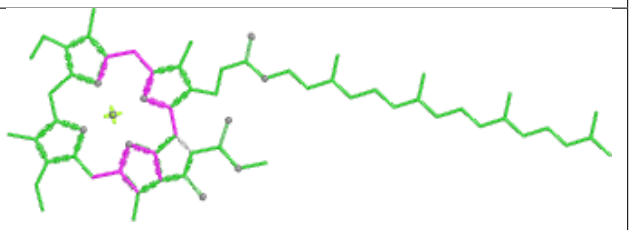


Rings

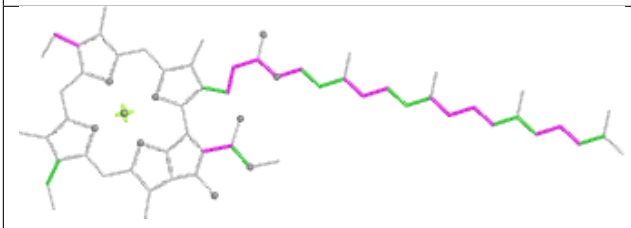
Ligand CLA C 306



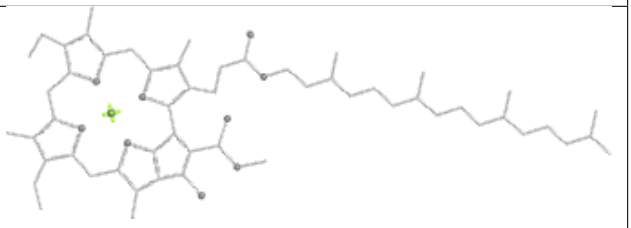
Bond lengths



Bond angles

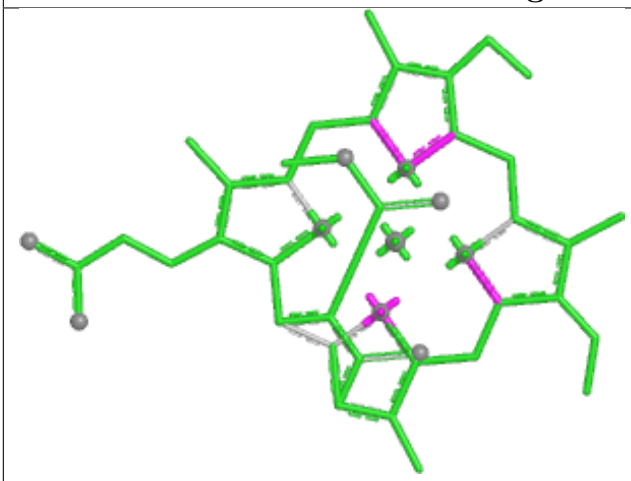


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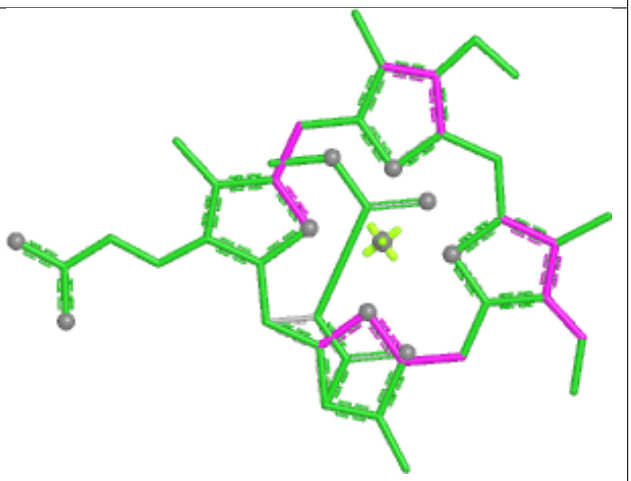


Rings

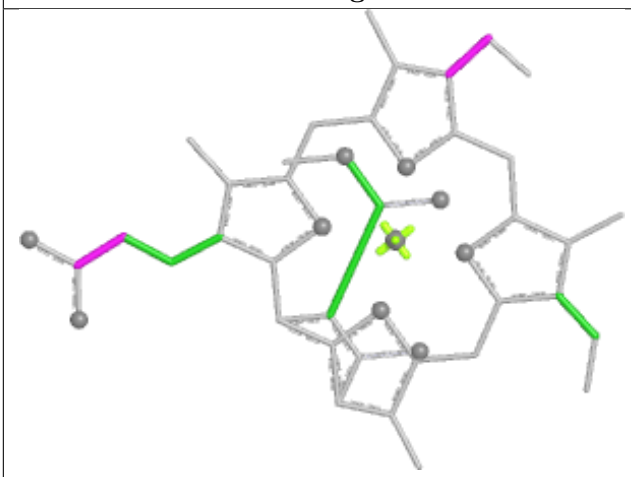
Ligand KC2 T 303



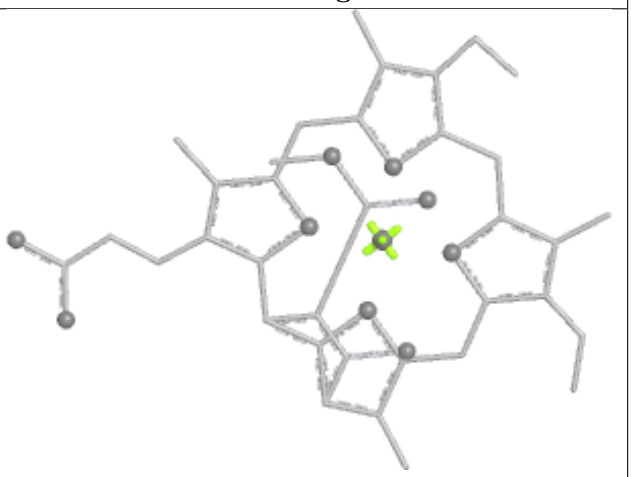
Bond lengths



Bond angles

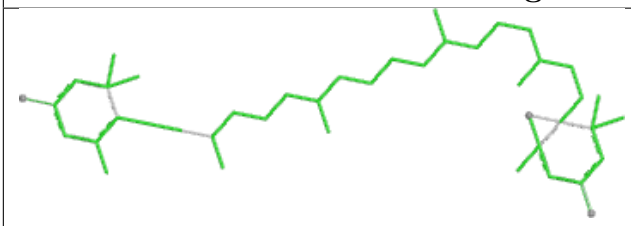


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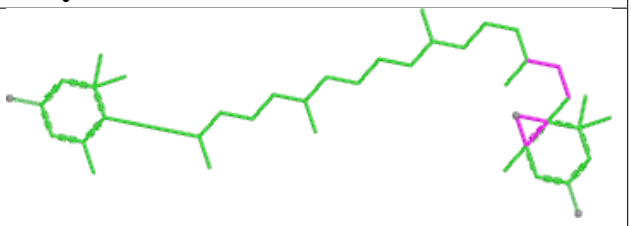


Rings

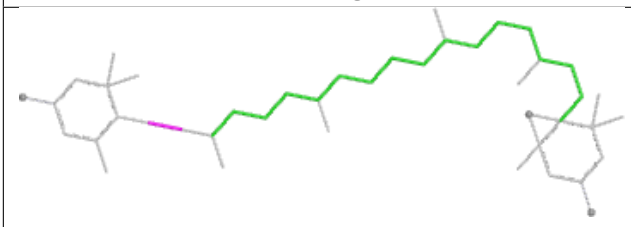
Ligand DD6 Q 212



Bond lengths



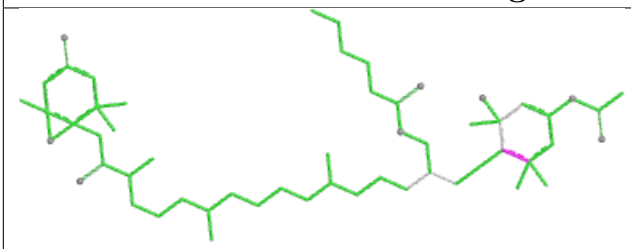
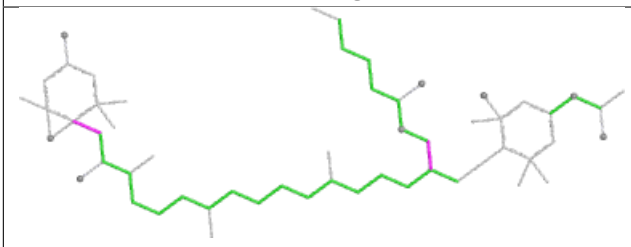
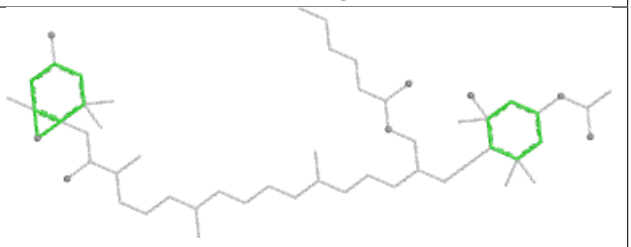
Bond angles

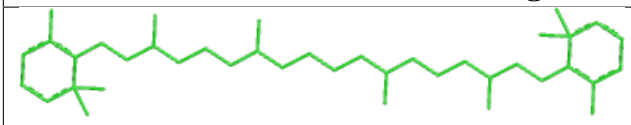
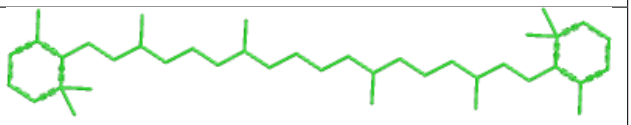
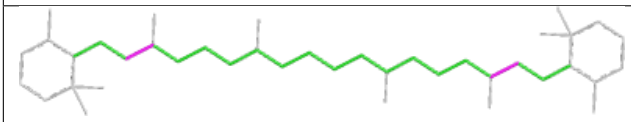
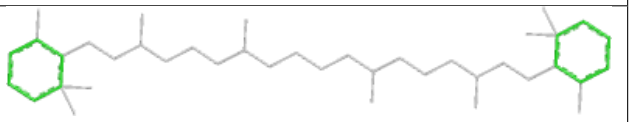


Torsions

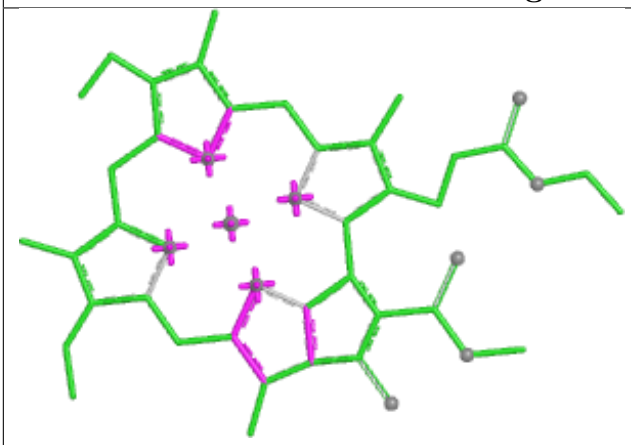


Rings

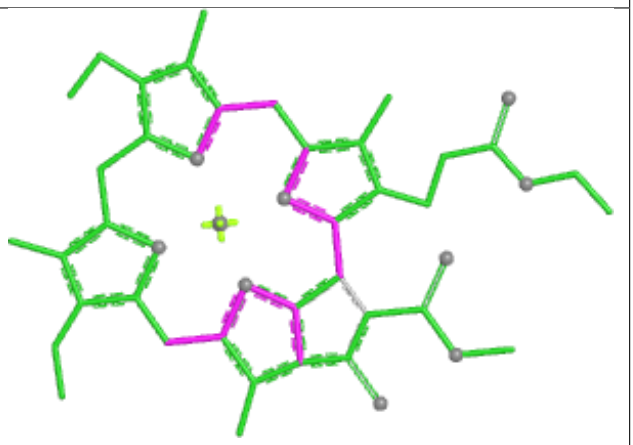
Ligand A1EB1 u 323	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR b 845	
 Bond lengths	 Bond angles
 Torsions	 Rings

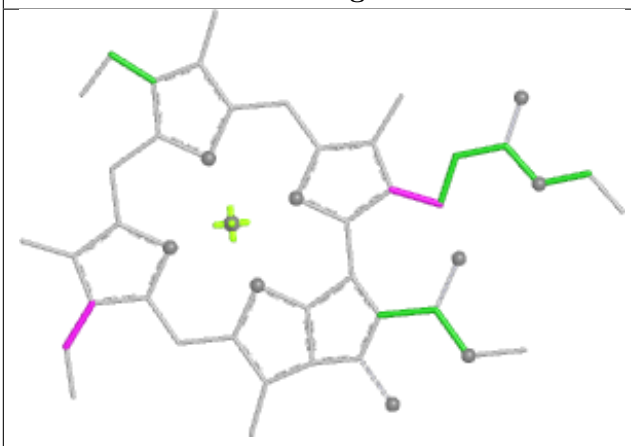
Ligand CLA E 312



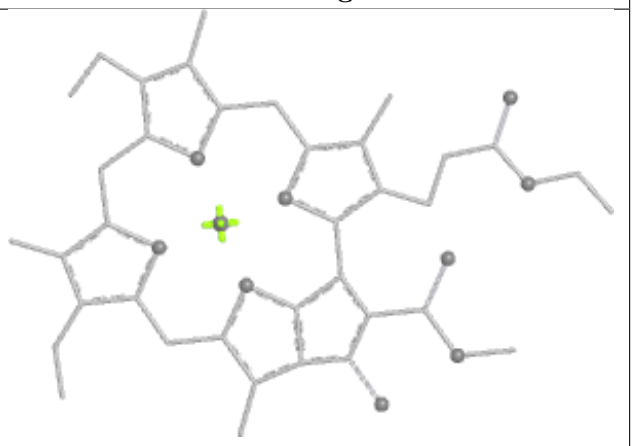
Bond lengths



Bond angles

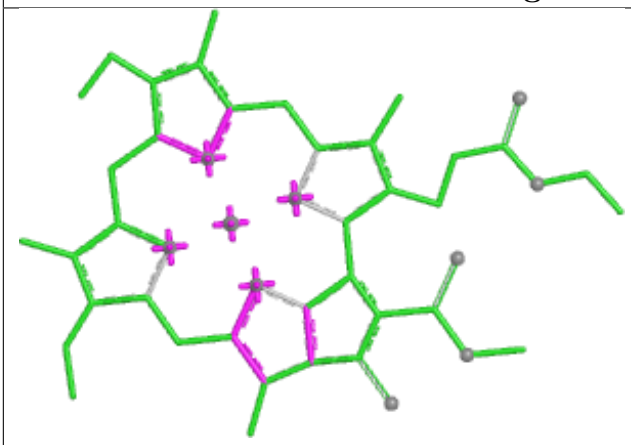


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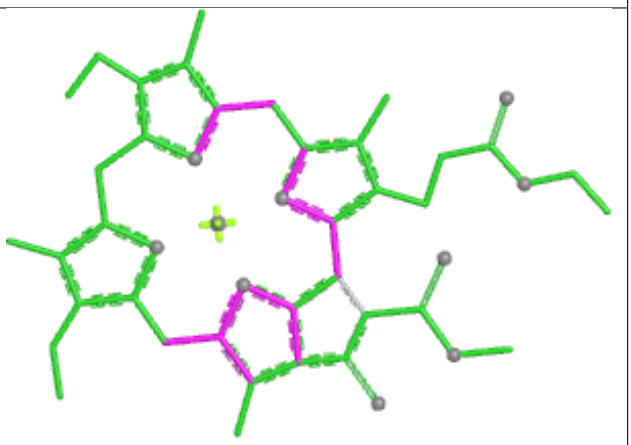


Rings

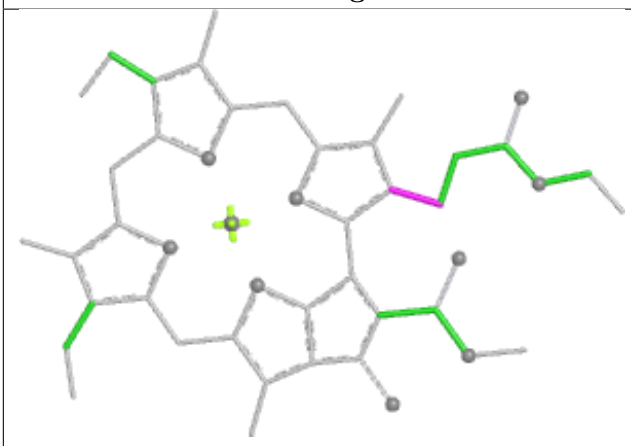
Ligand CLA Y 304



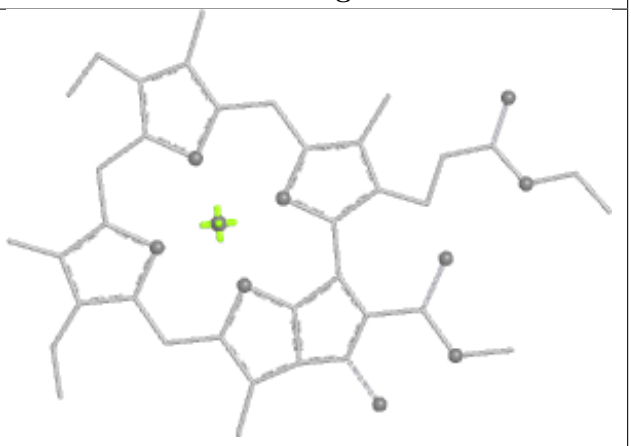
Bond lengths



Bond angles

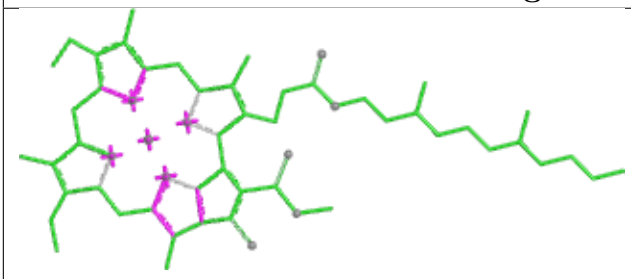


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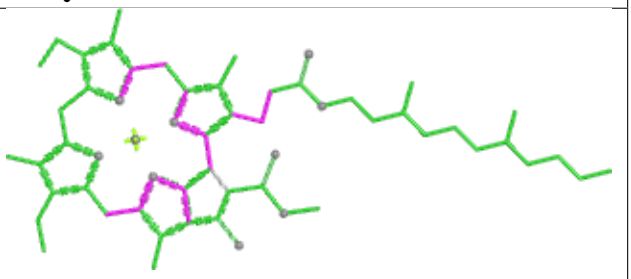


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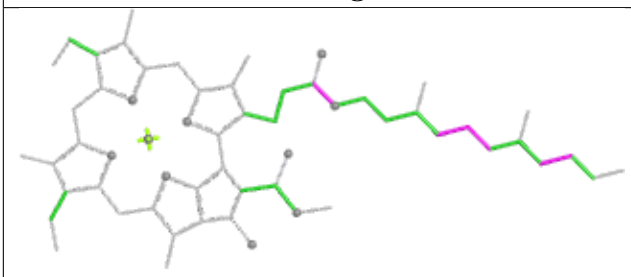
Ligand CLA Q 202



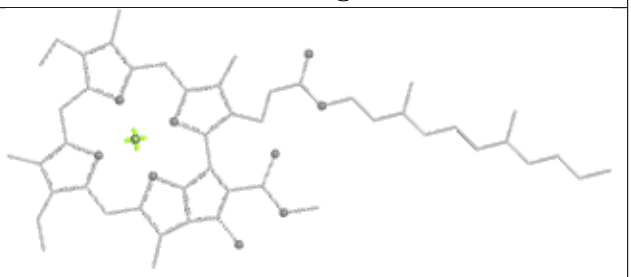
Bond lengths



Bond angles

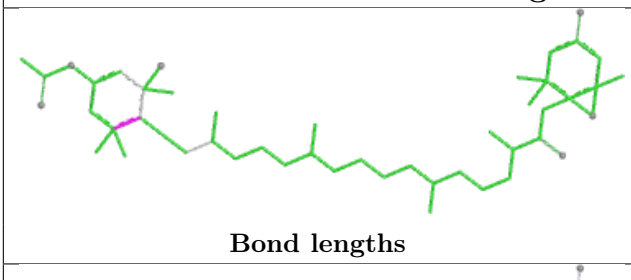


Torsions

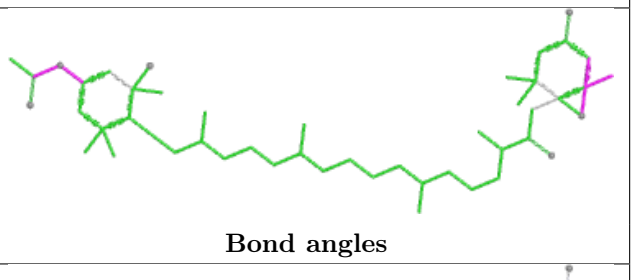


Rings

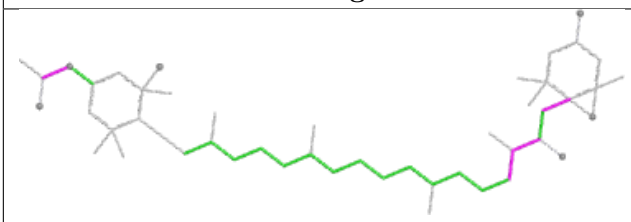
Ligand A86 Y 319



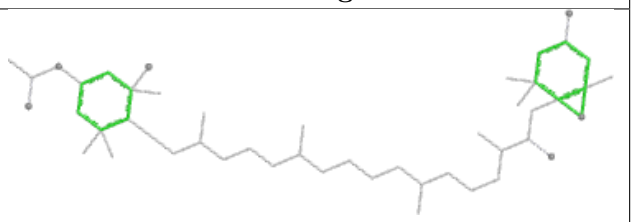
Bond lengths



Bond angles

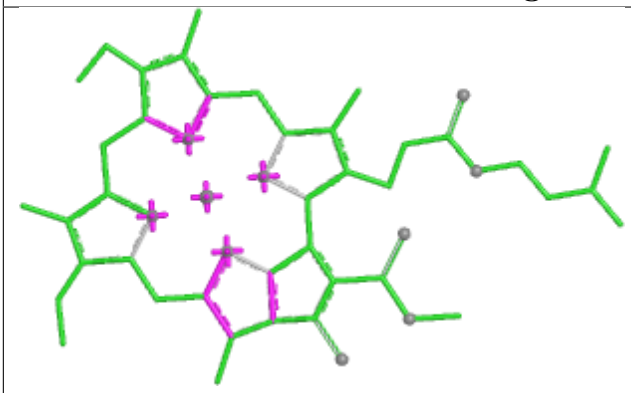


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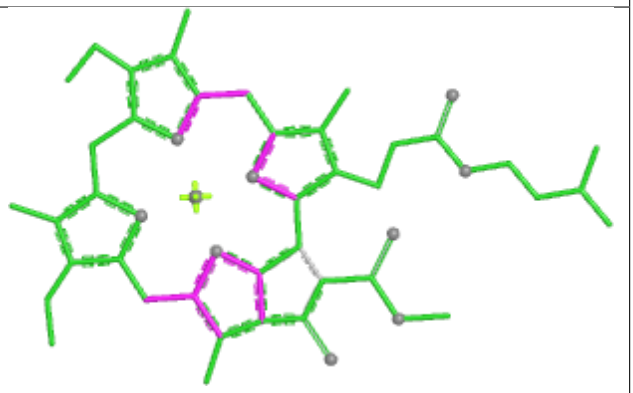


Rings

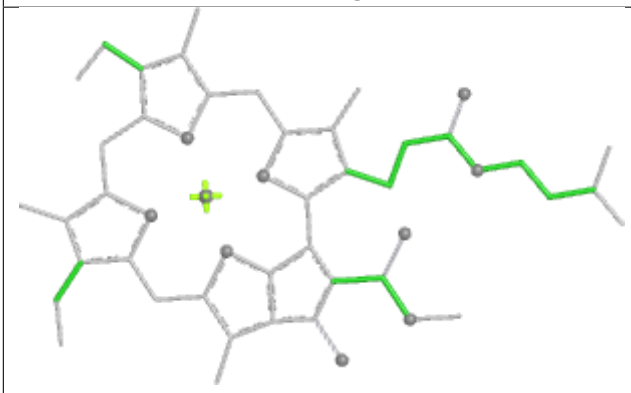
Ligand CLA G 205



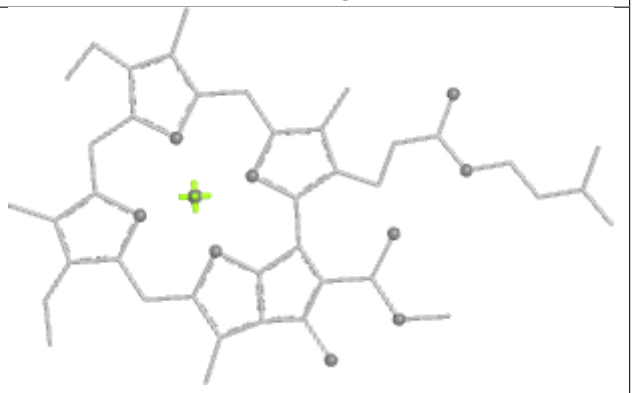
Bond lengths



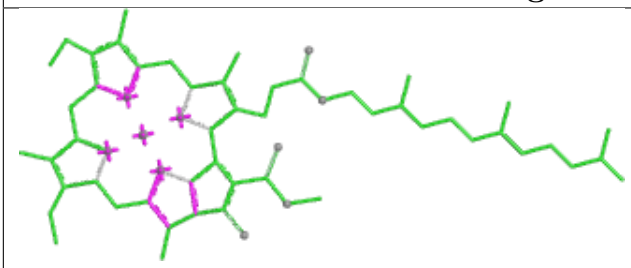
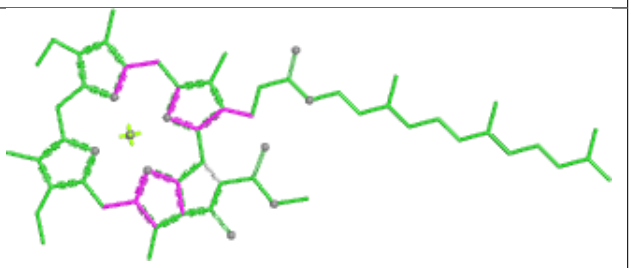
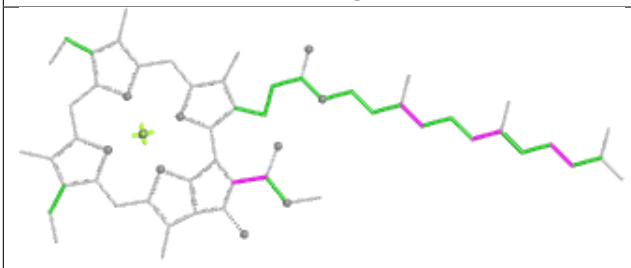
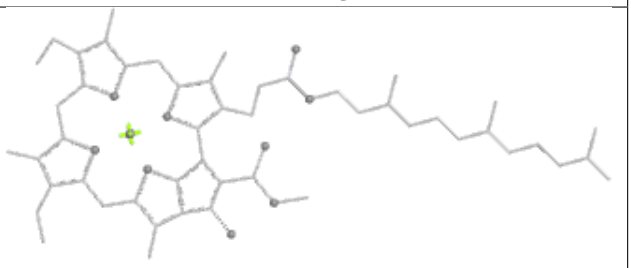
Bond angles

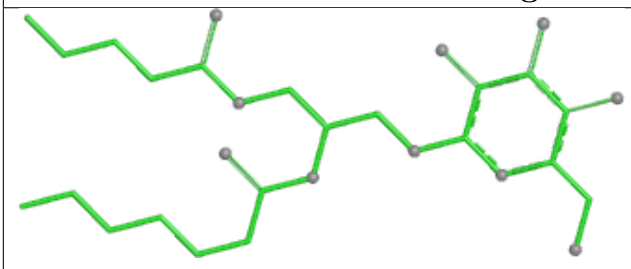
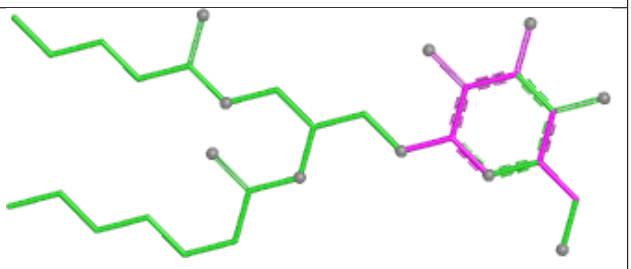
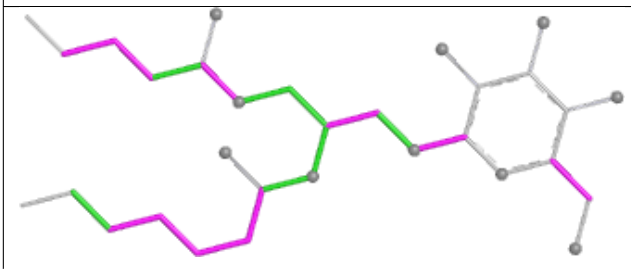
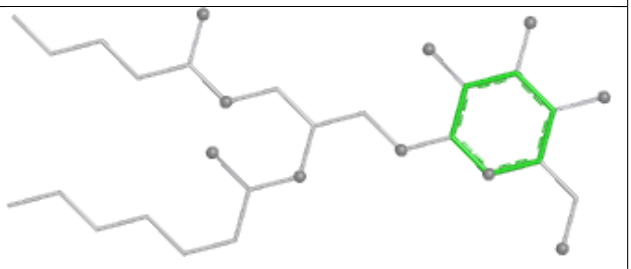


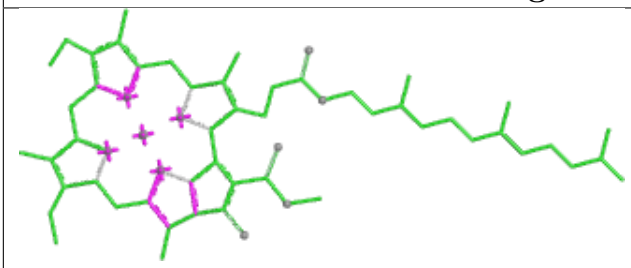
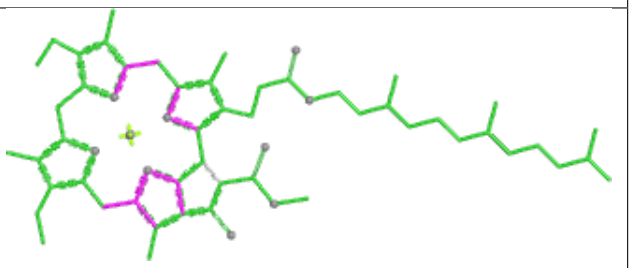
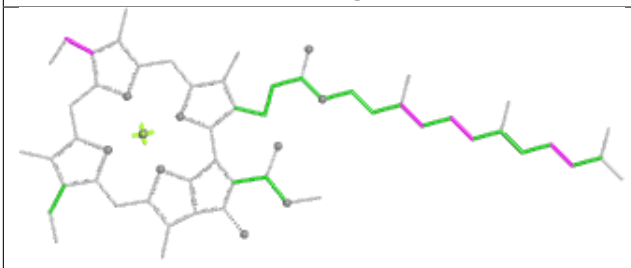
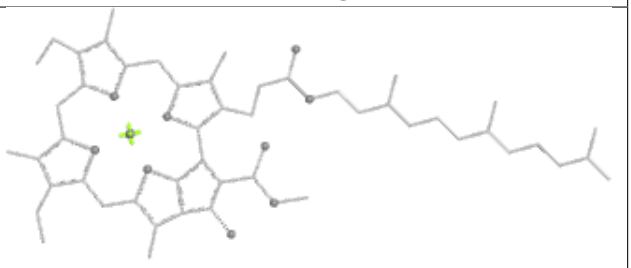
Torsions

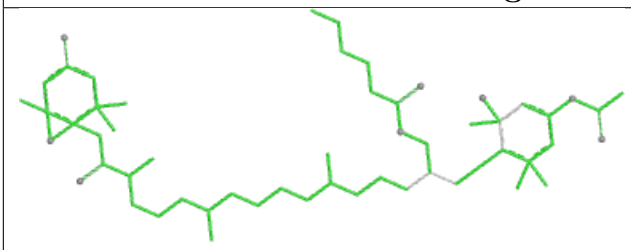
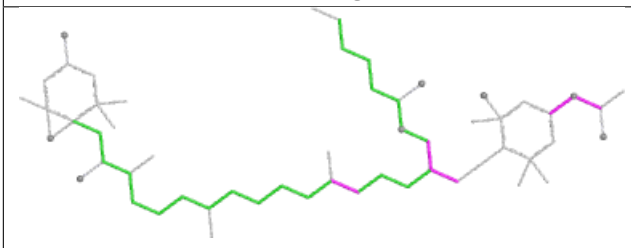
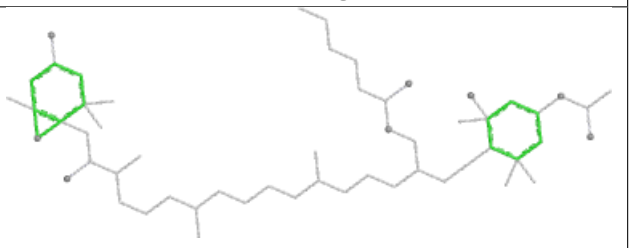


Rings

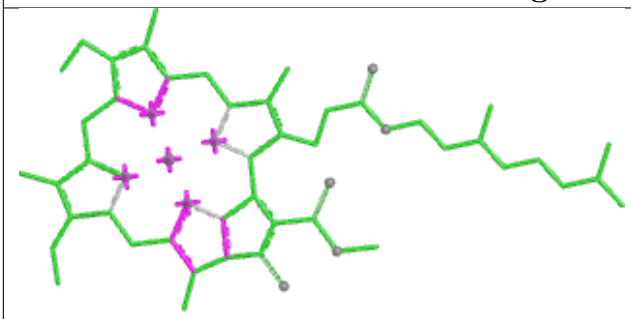
Ligand CLA b 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG E 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

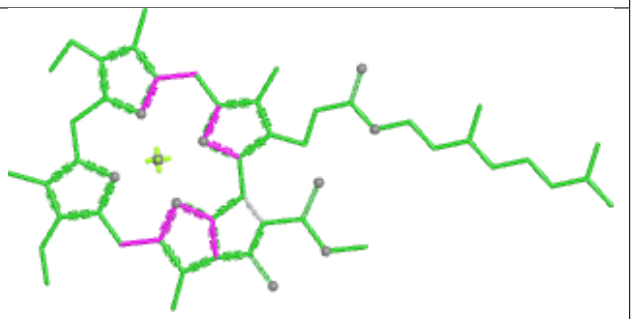
Ligand CLA o 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A1EB1 N 320	
 Bond lengths	 Bond angles
 Torsions	 Rings

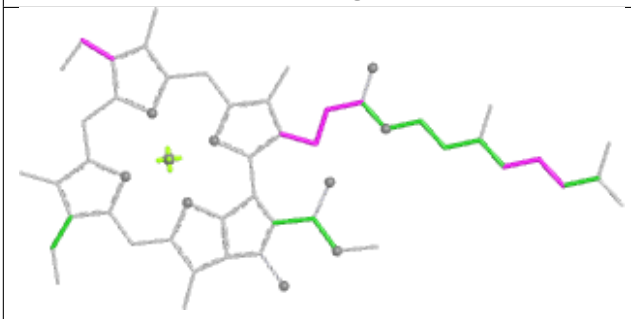
Ligand CLA I 202



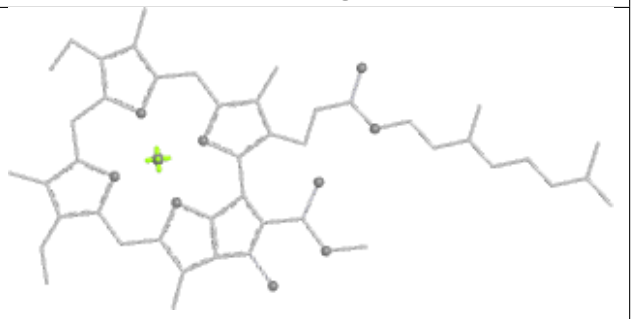
Bond lengths



Bond angles

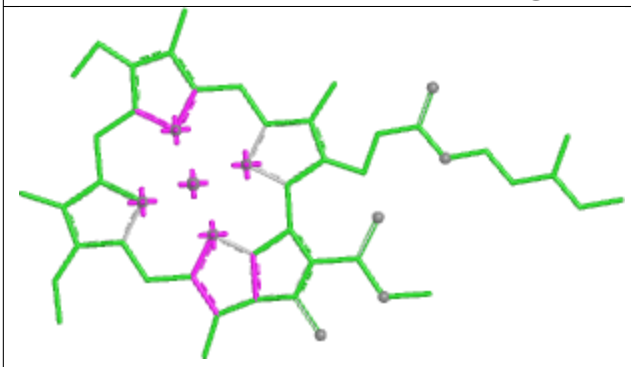


Torsions

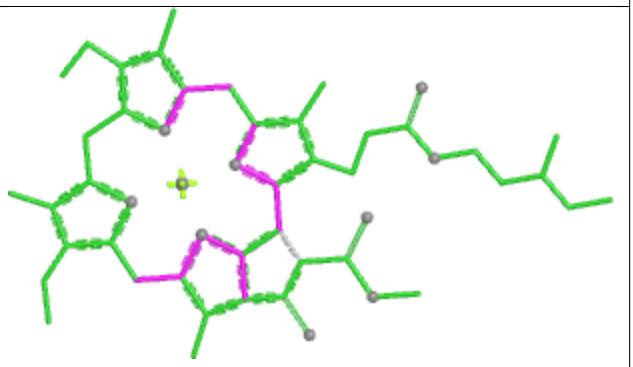


Rings

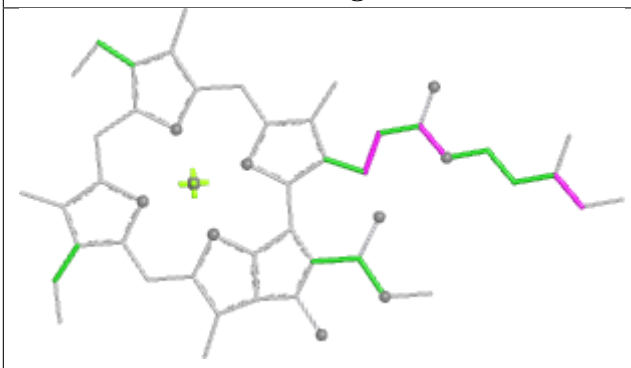
Ligand CLA b 831



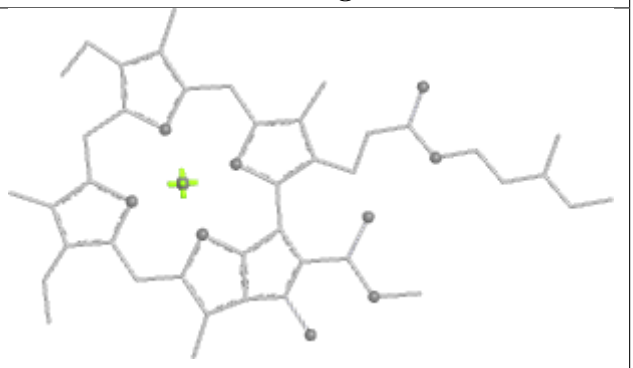
Bond lengths



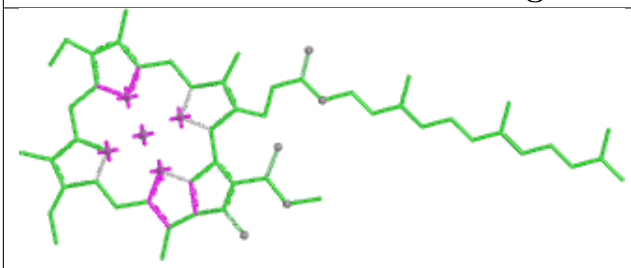
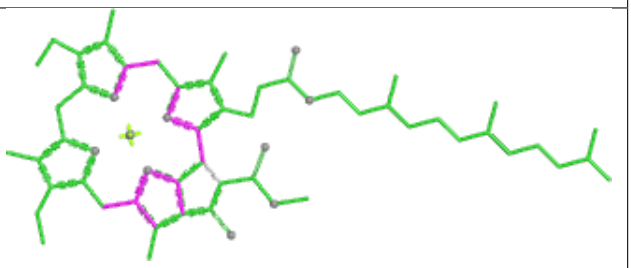
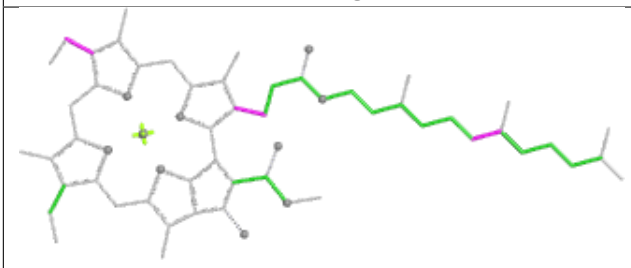
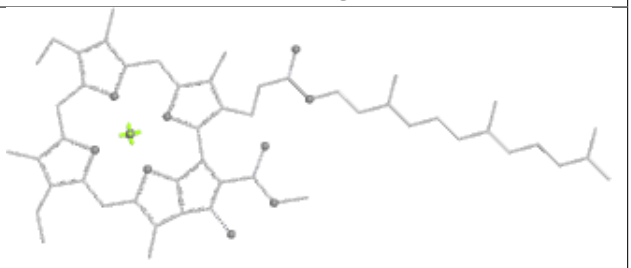
Bond angles

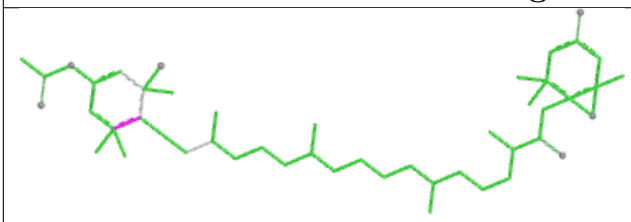
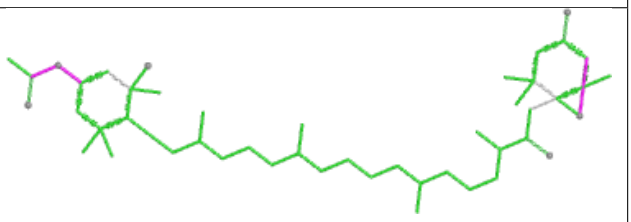
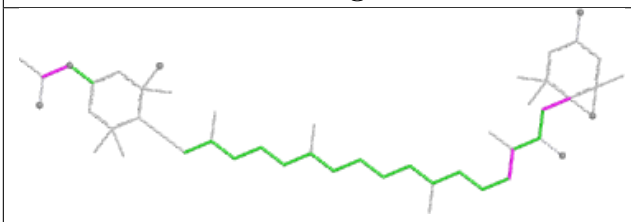
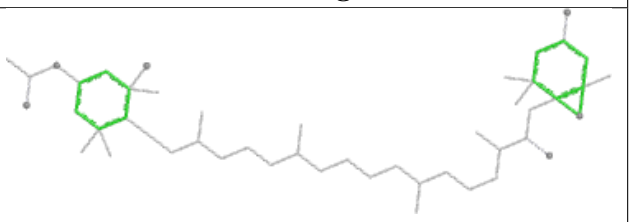


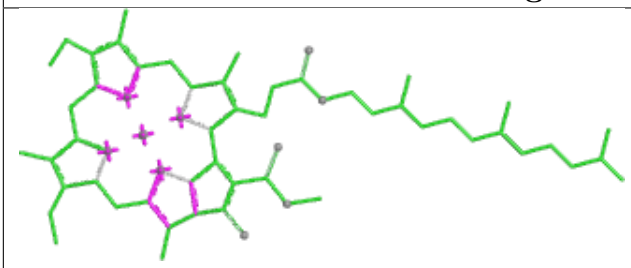
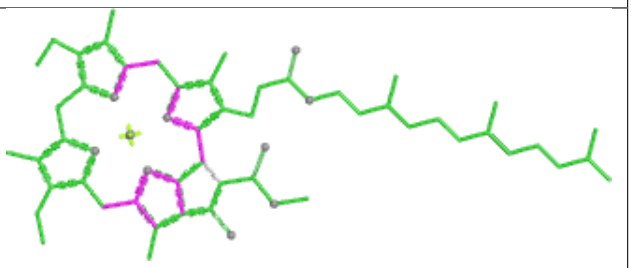
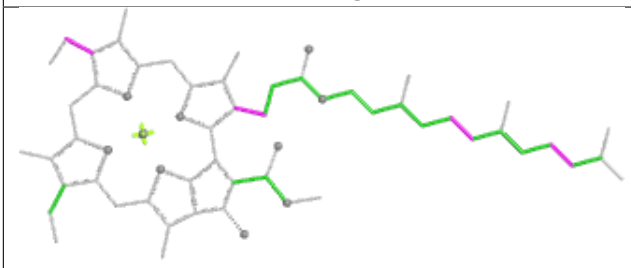
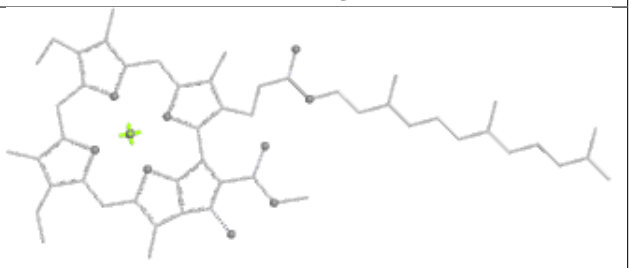
Torsions

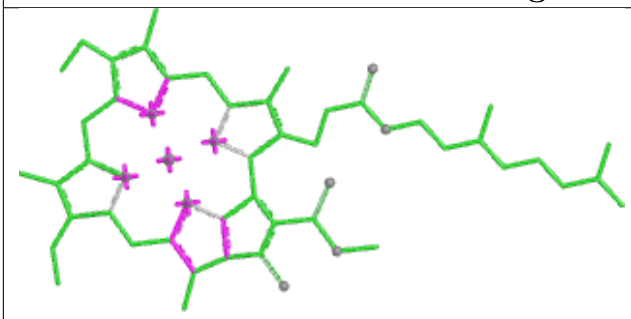
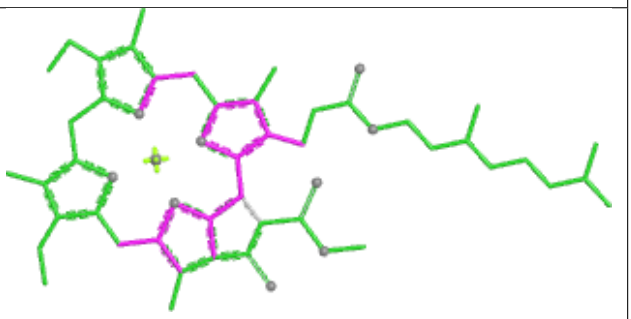
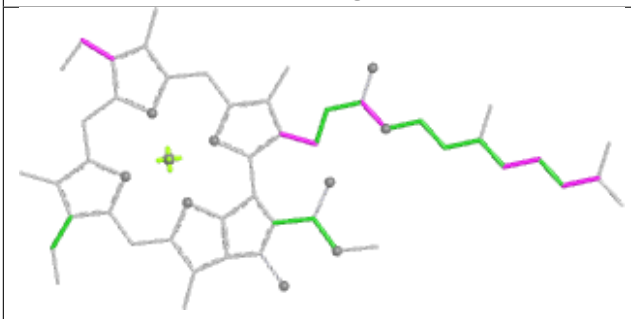
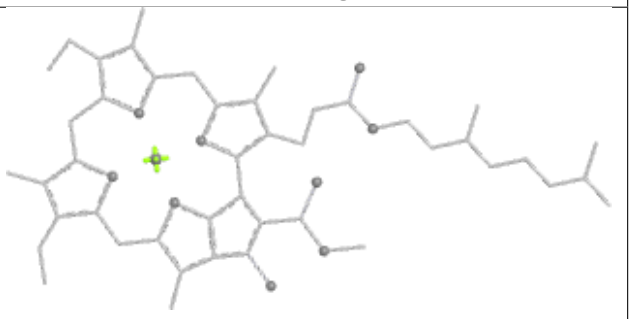


Rings

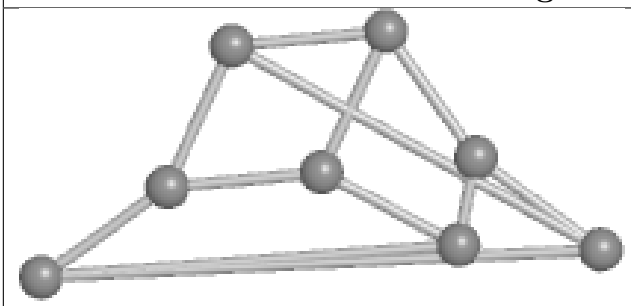
Ligand CLA Z 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A86 D 320	
	
Bond lengths	Bond angles
	
Torsions	Rings

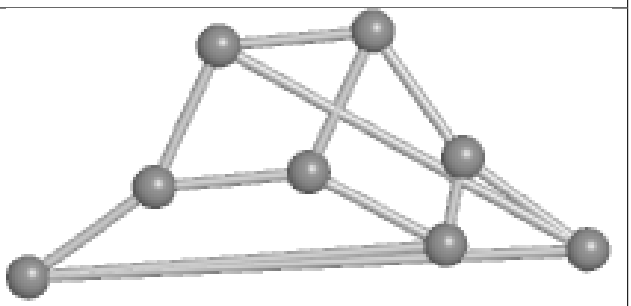
Ligand CLA E 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA o 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

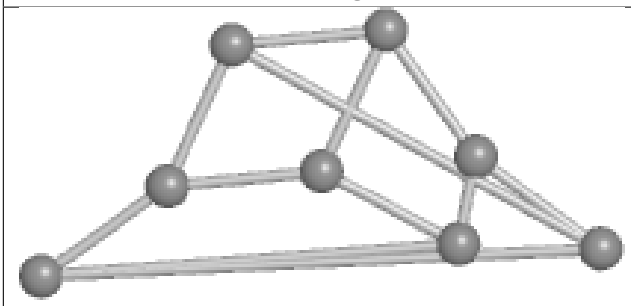
Ligand SF4 c 101



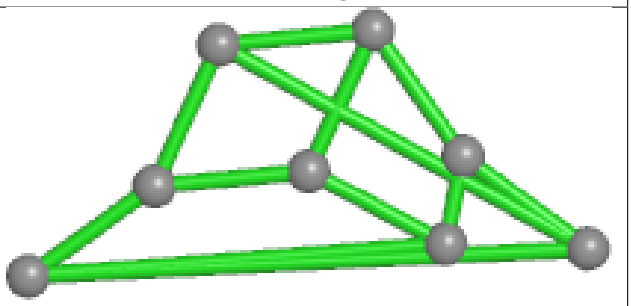
Bond lengths



Bond angles

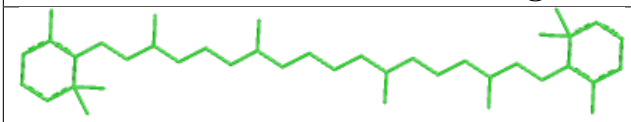


Torsions

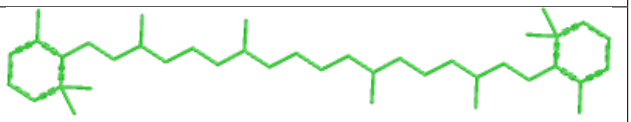


Rings

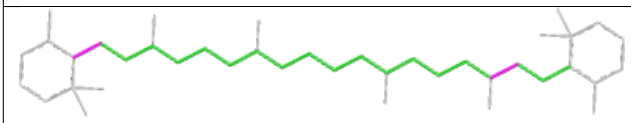
Ligand BCR a 843



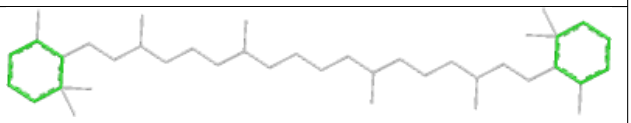
Bond lengths



Bond angles

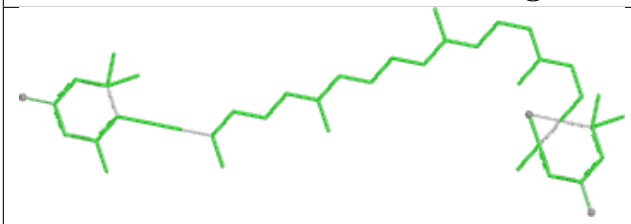


Torsions



Rings

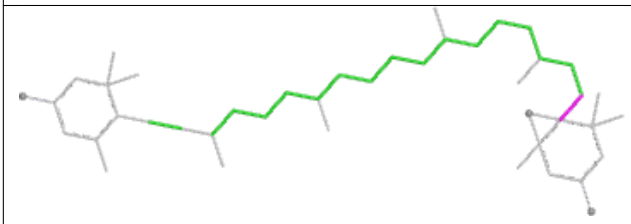
Ligand DD6 A 316



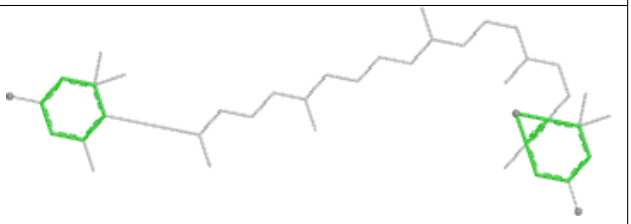
Bond lengths



Bond angles

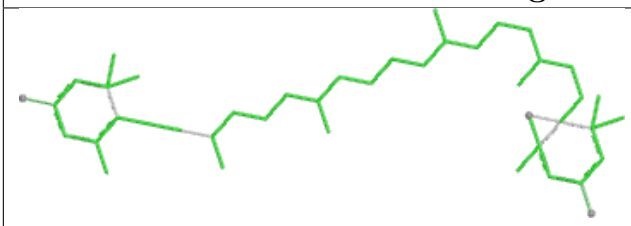


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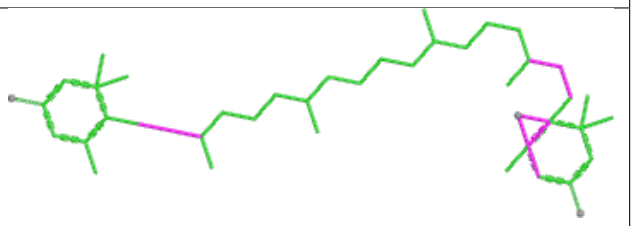


Rings

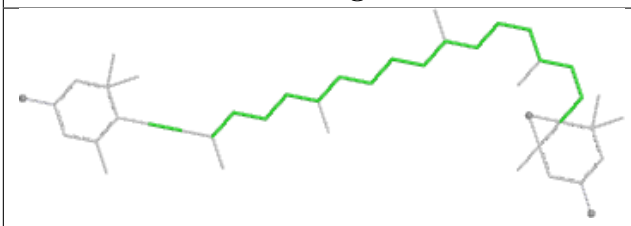
Ligand DD6 v 318



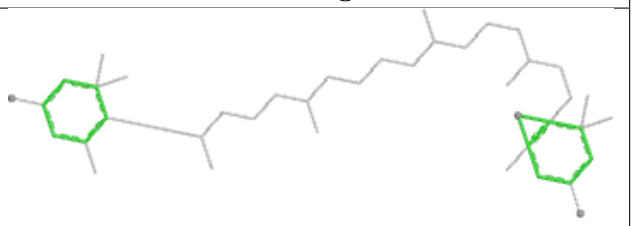
Bond lengths



Bond angles

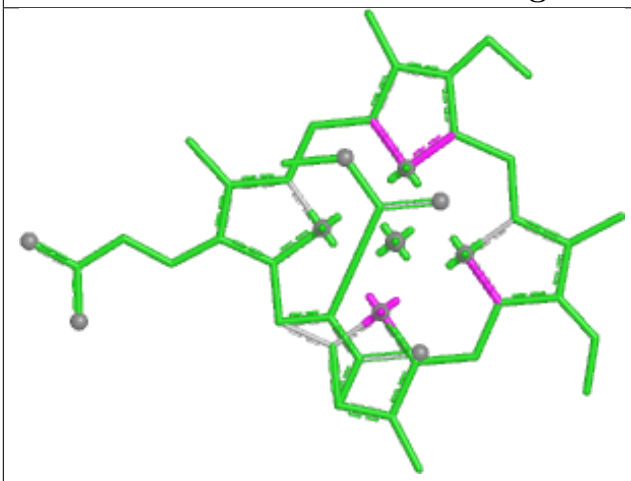


Torsions

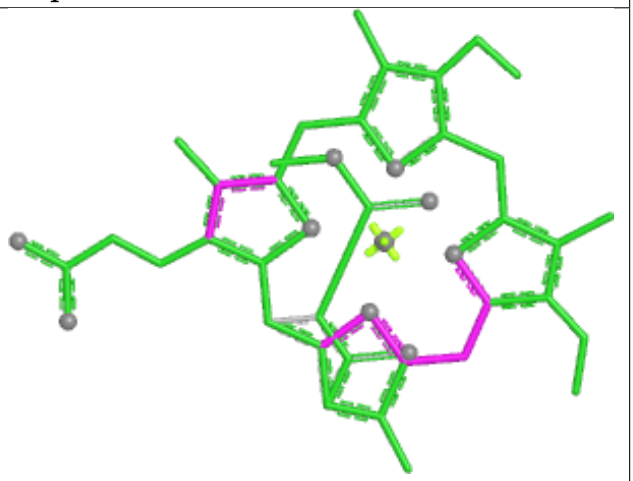


Rings

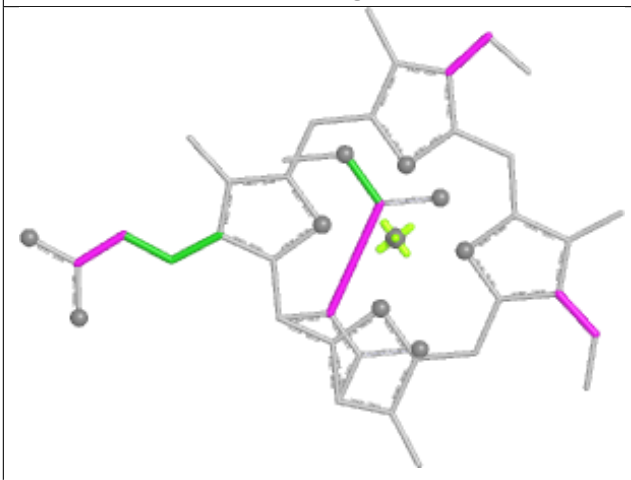
Ligand KC2 p 315



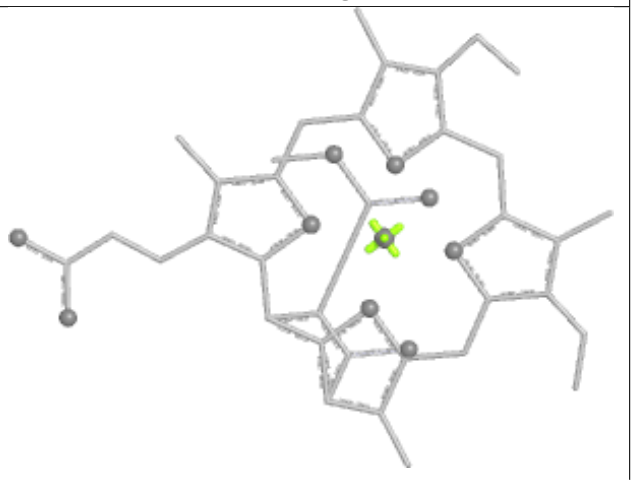
Bond lengths



Bond angles

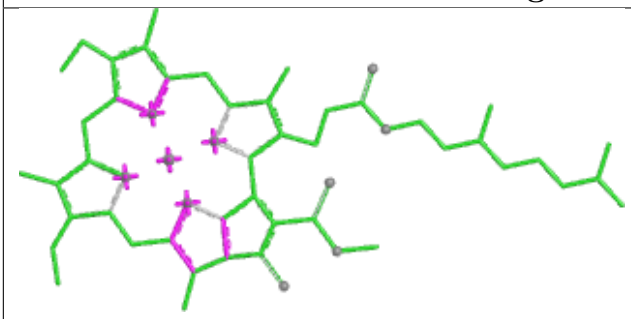


Torsions

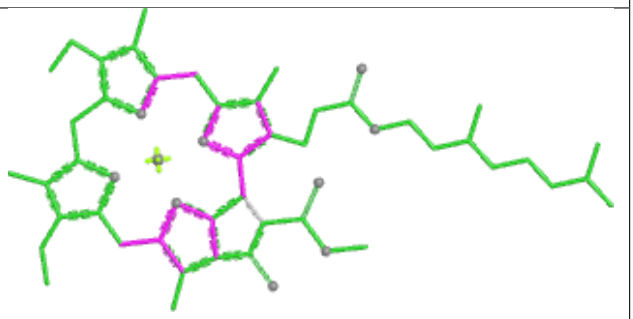


Rings

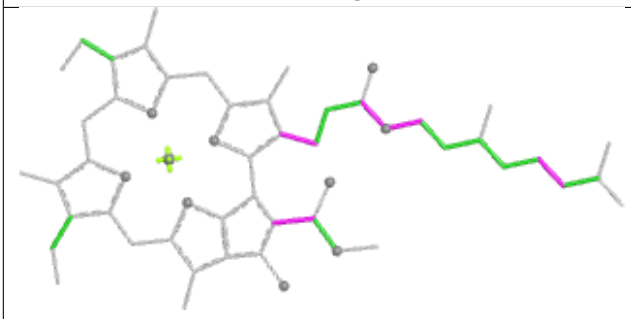
Ligand CLA u 307



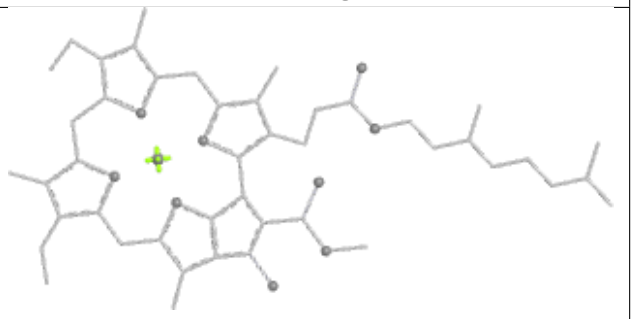
Bond lengths



Bond angles

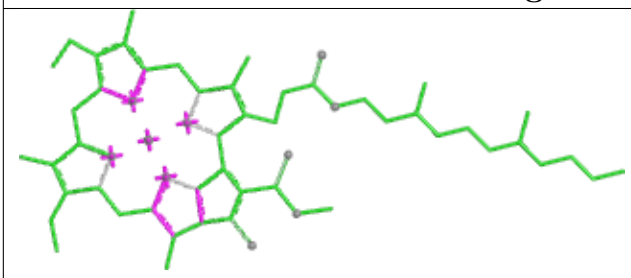


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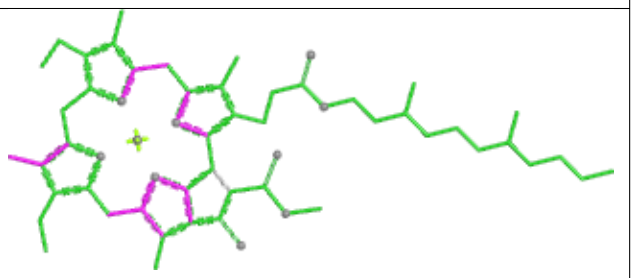


Rings

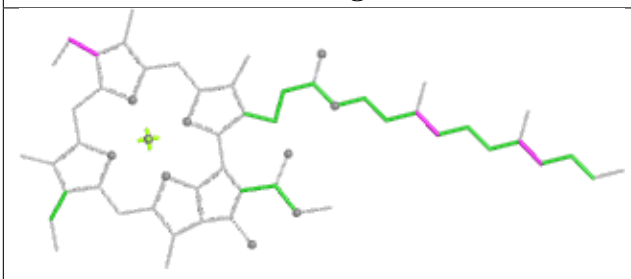
Ligand CLA E 308



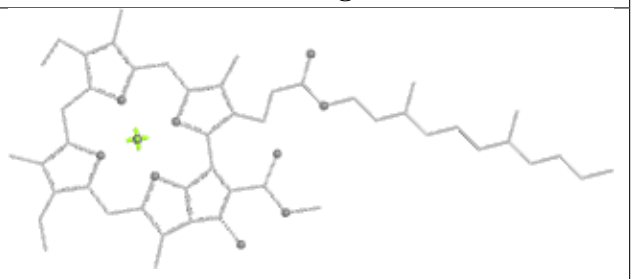
Bond lengths



Bond angles

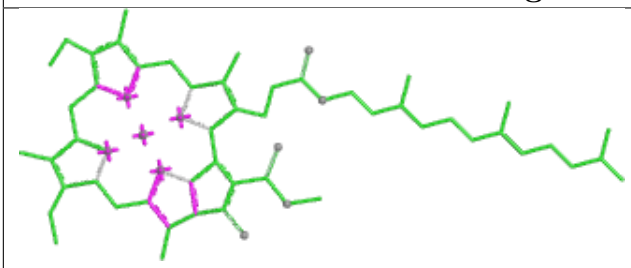


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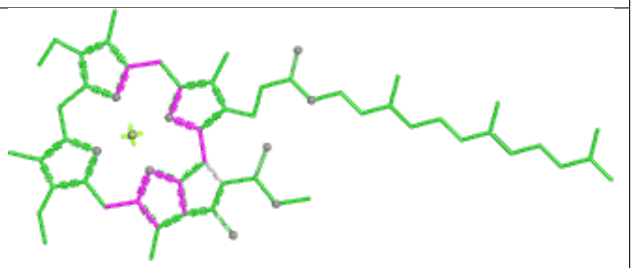


Rings

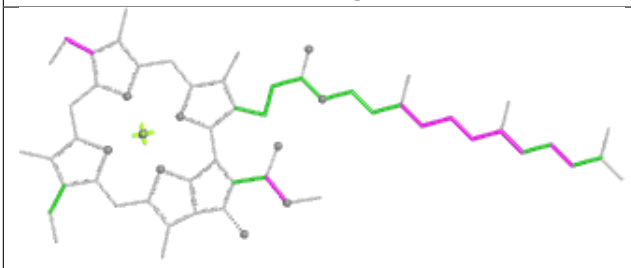
Ligand CLA P 308



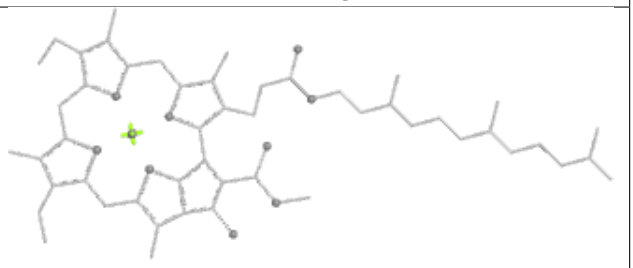
Bond lengths



Bond angles

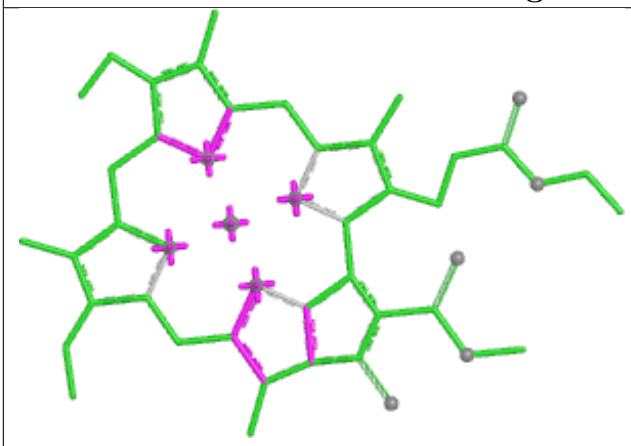


Torsions

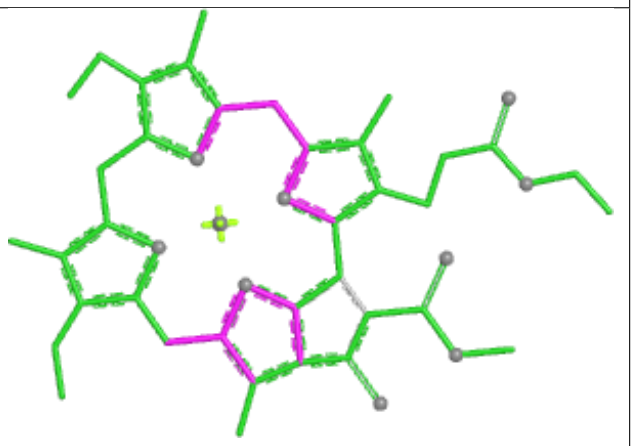


Rings

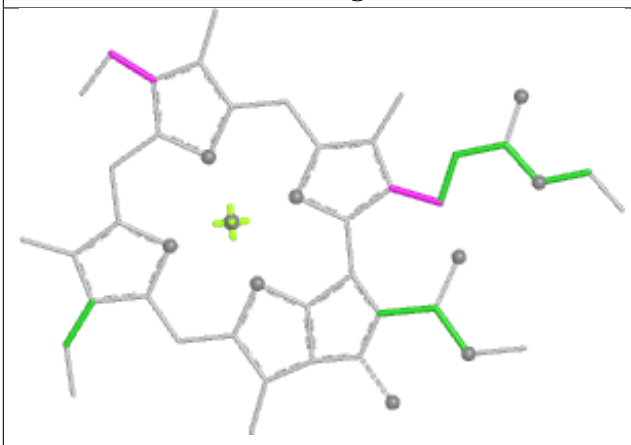
Ligand CLA F 305



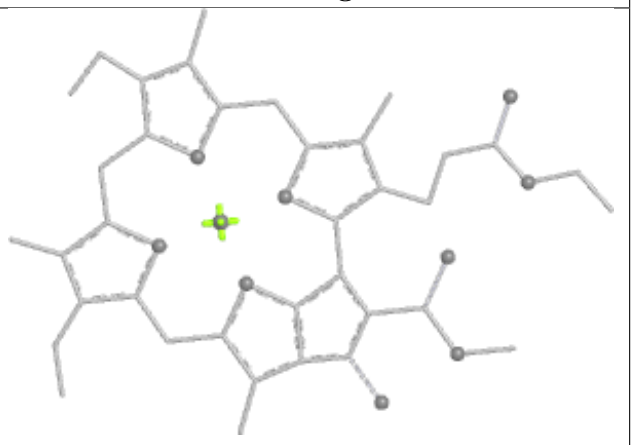
Bond lengths



Bond angles

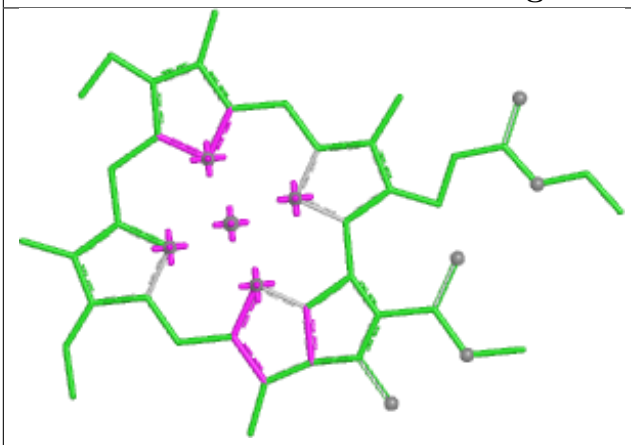


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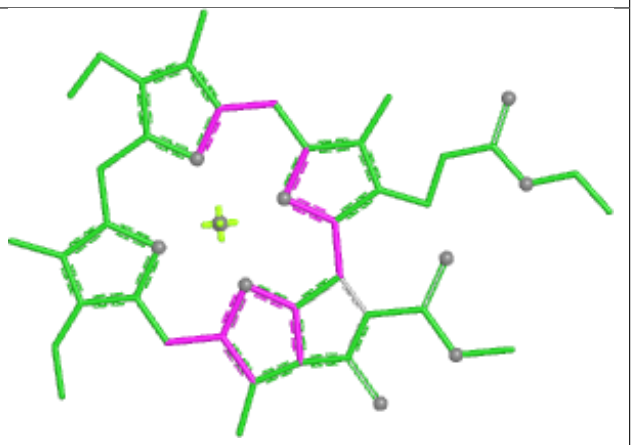


Rings

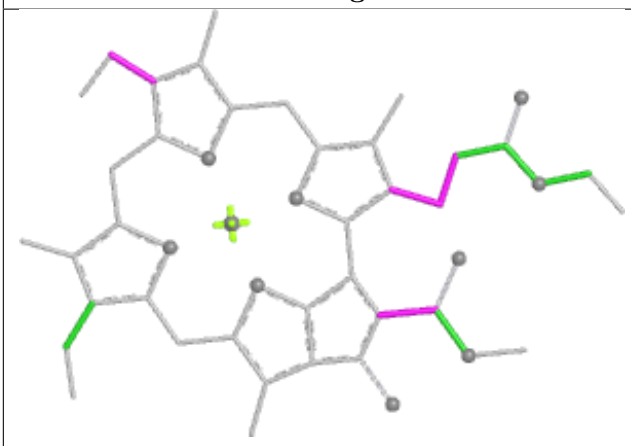
Ligand CLA L 311



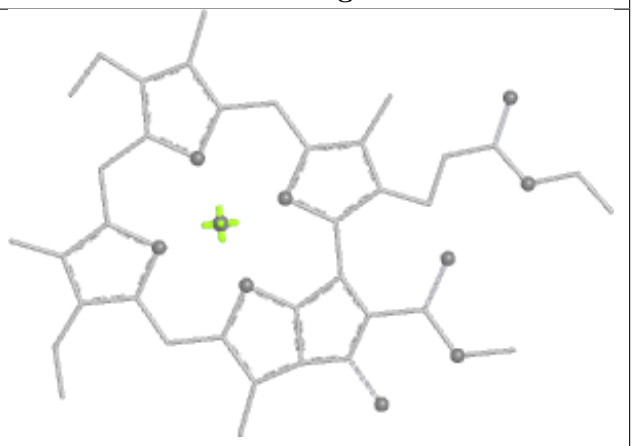
Bond lengths



Bond angles

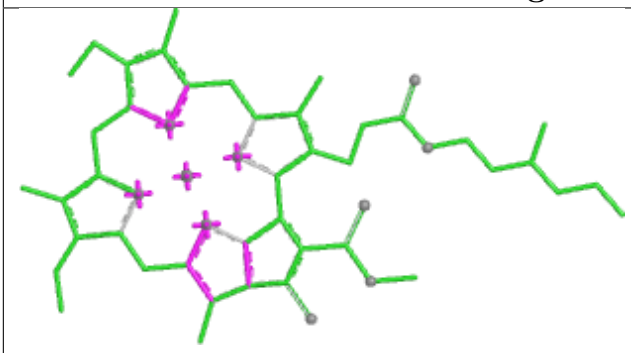


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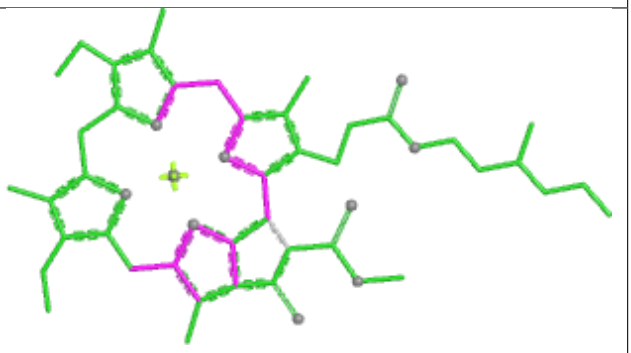


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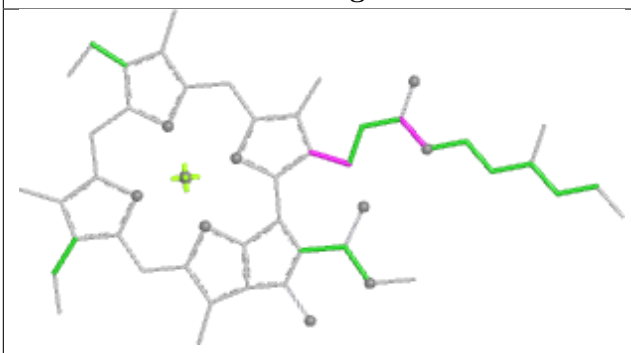
Ligand CLA v 304



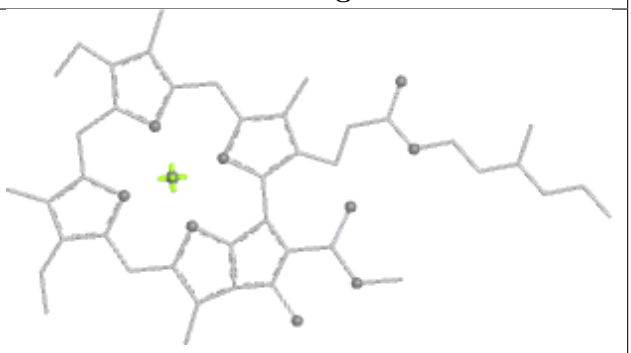
Bond lengths



Bond angles

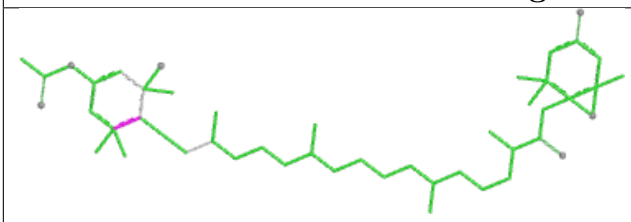


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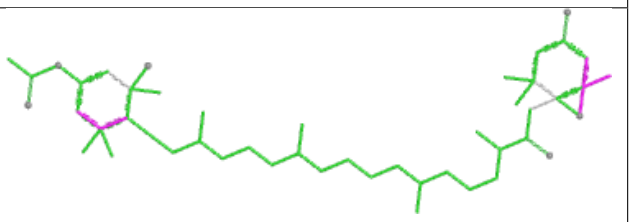


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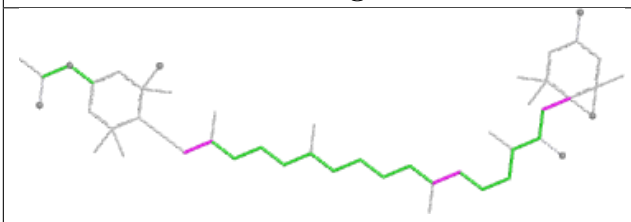
Ligand A86 K 314



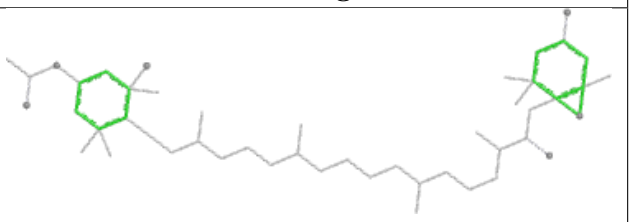
Bond lengths



Bond angles

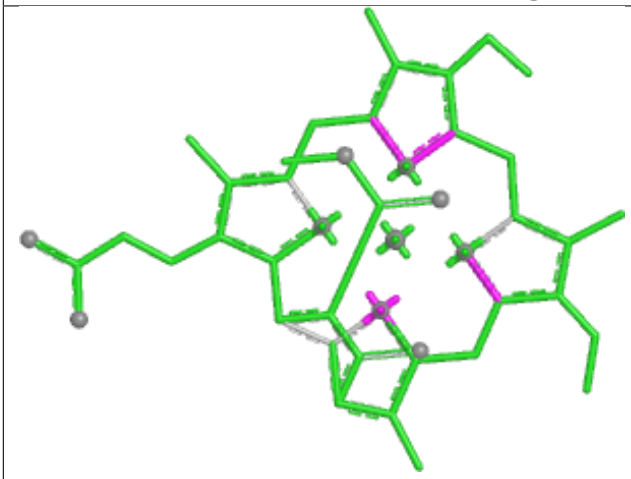


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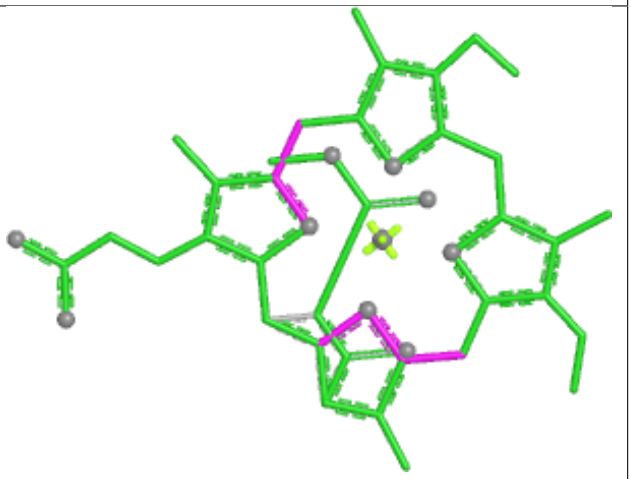


Rings

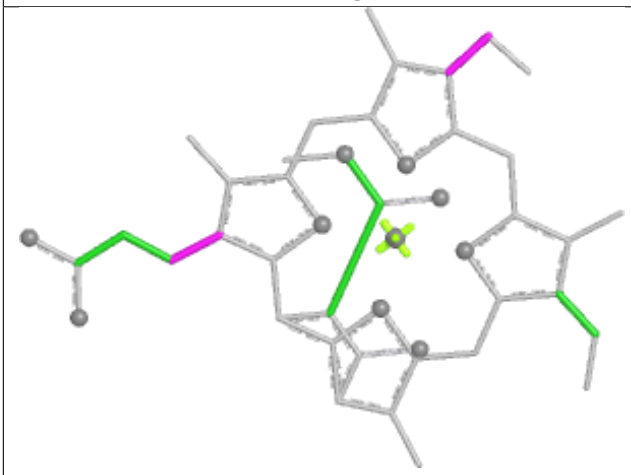
Ligand KC2 G 208



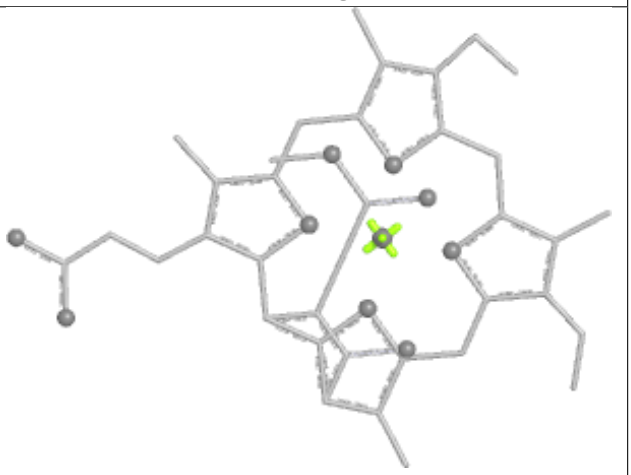
Bond lengths



Bond angles

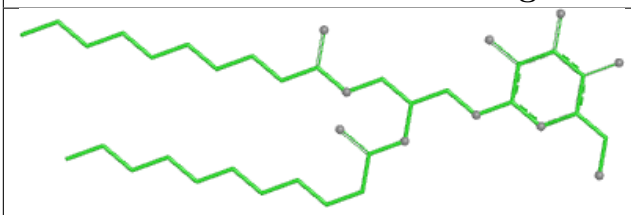


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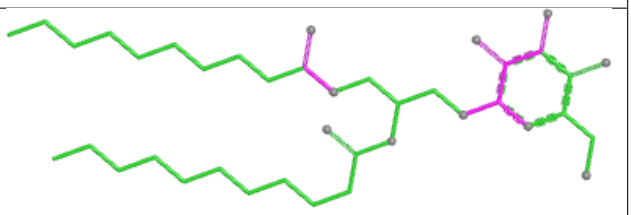


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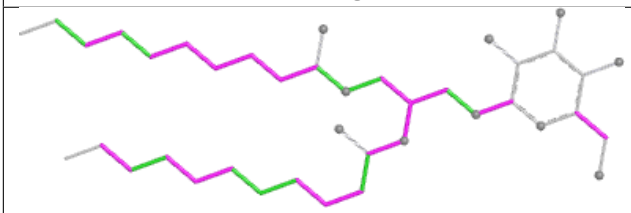
Ligand LMG A 317



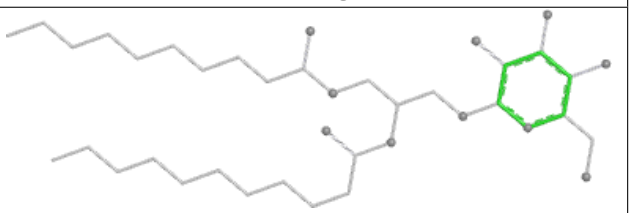
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Bond angles

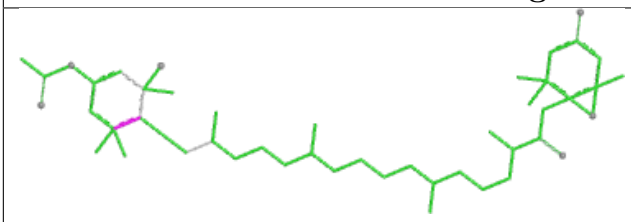


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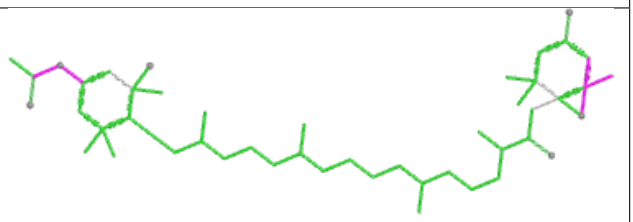


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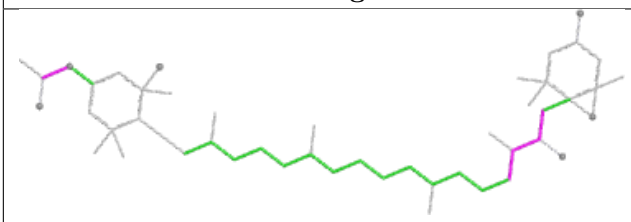
Ligand A86 N 315



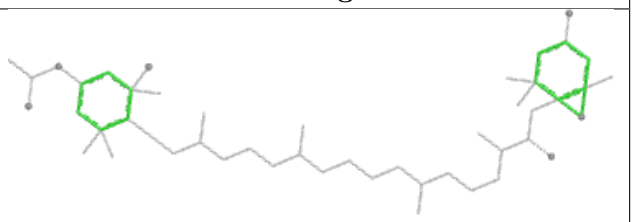
Bond lengths



Bond angles

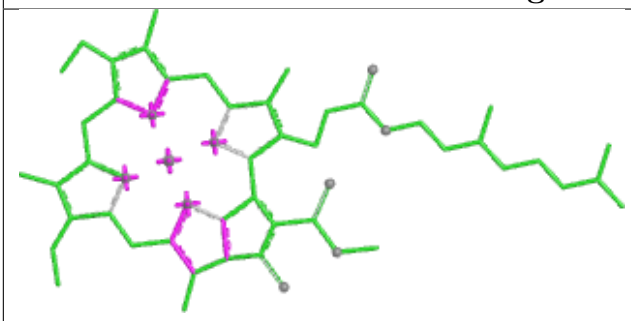


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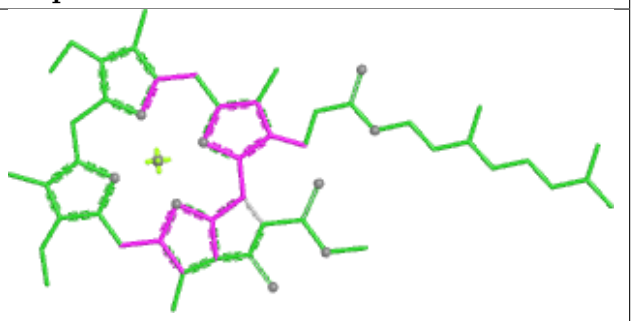


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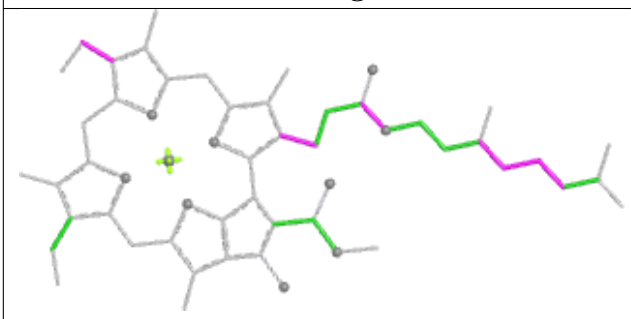
Ligand CLA p 311



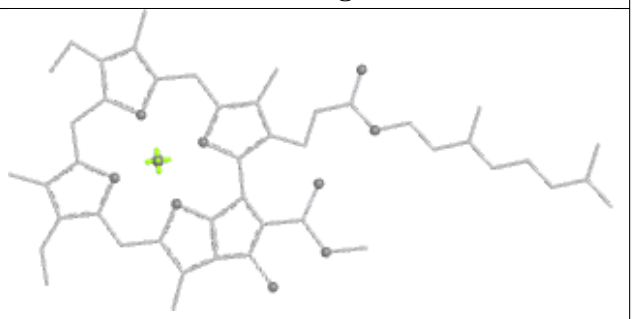
Bond lengths



Bond angles

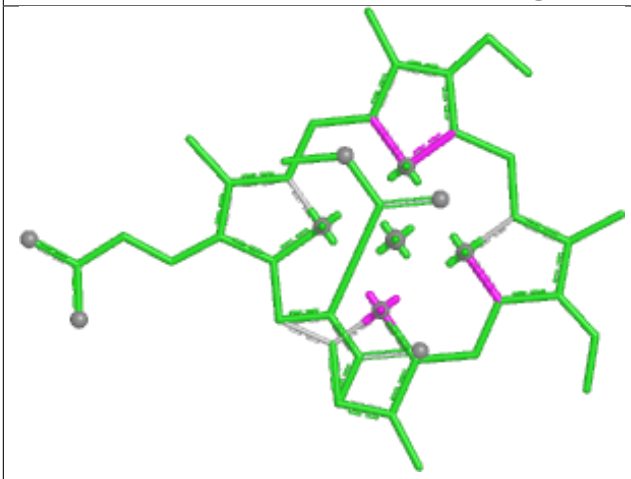


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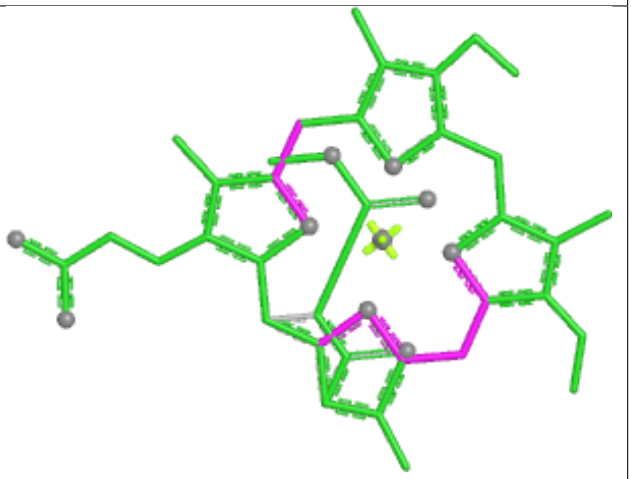


Rings

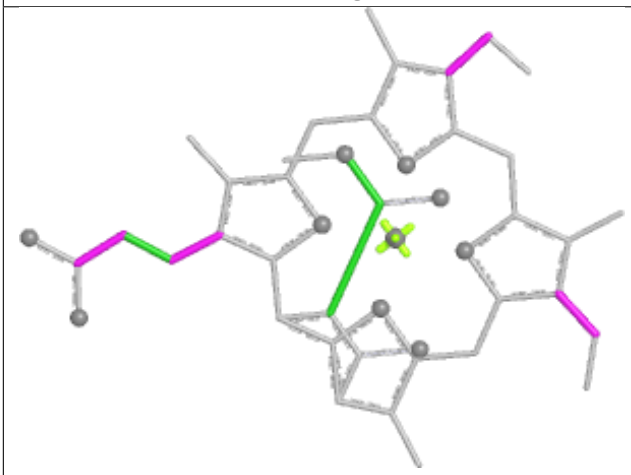
Ligand KC2 o 308



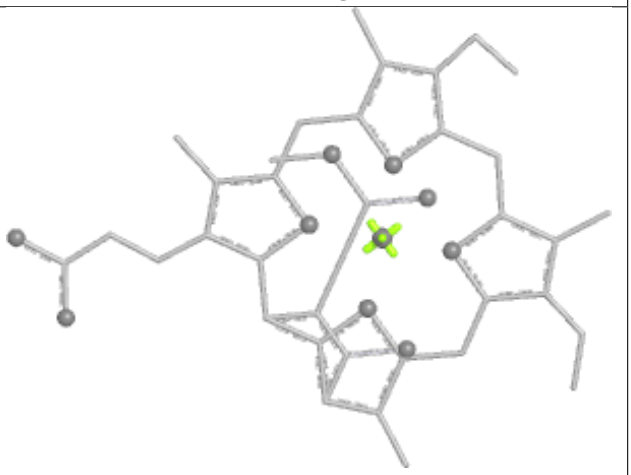
Bond lengths



Bond angles

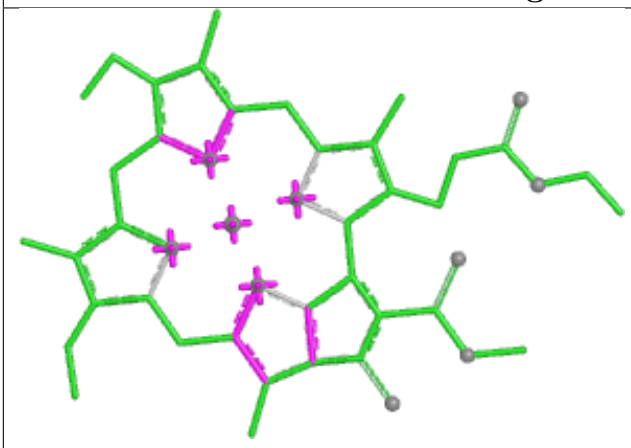


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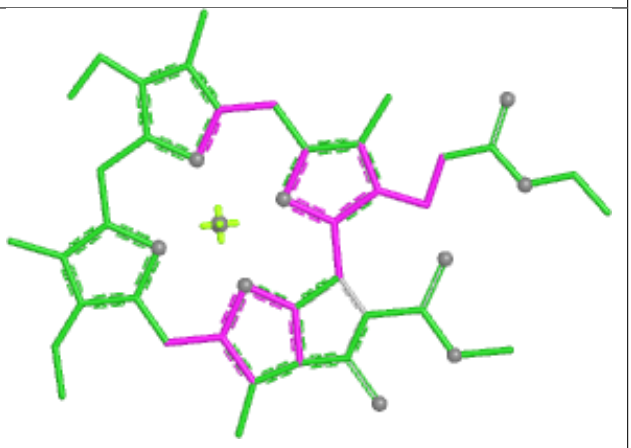


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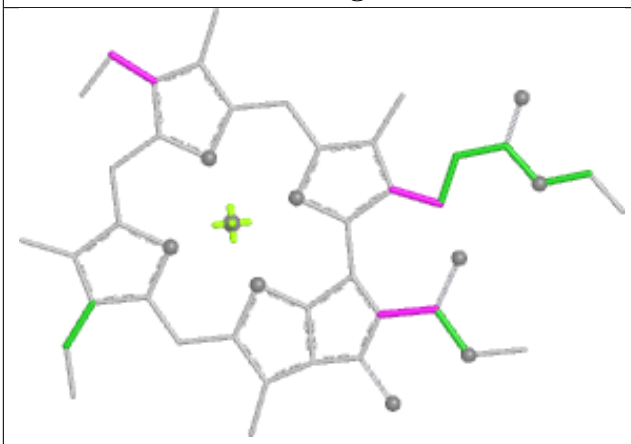
Ligand CLA Z 313



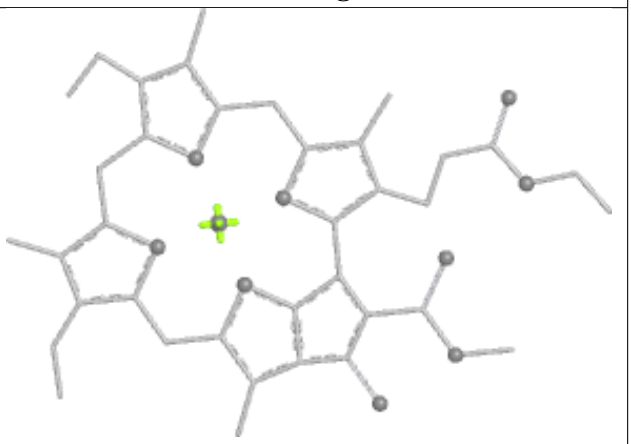
Bond lengths



Bond angles

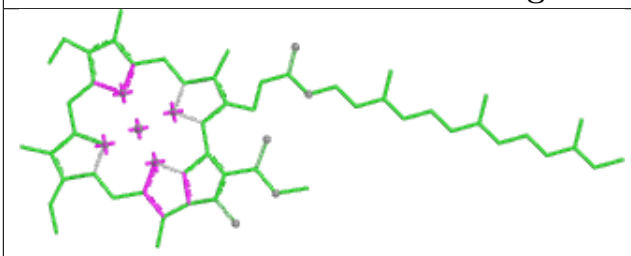


Torsions

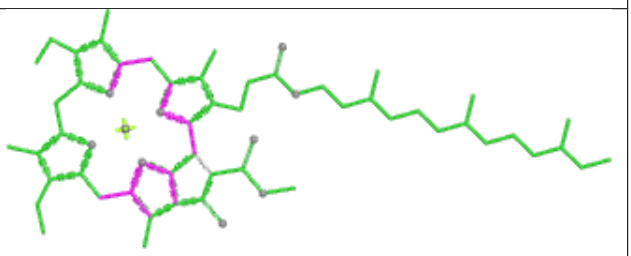


Rings

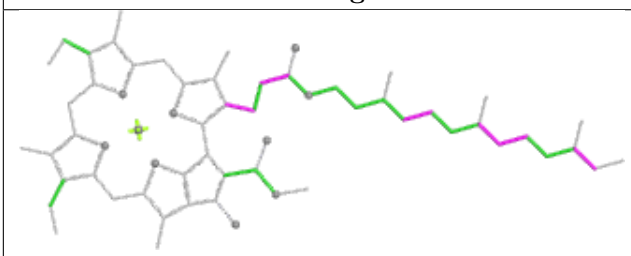
Ligand CLA b 842



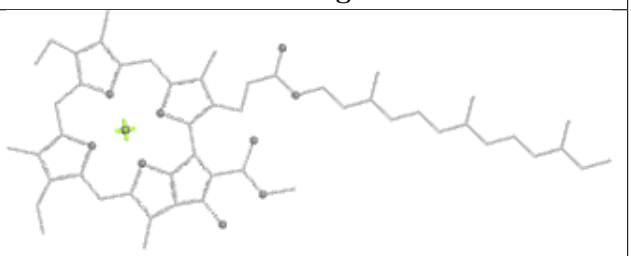
Bond lengths



Bond angles

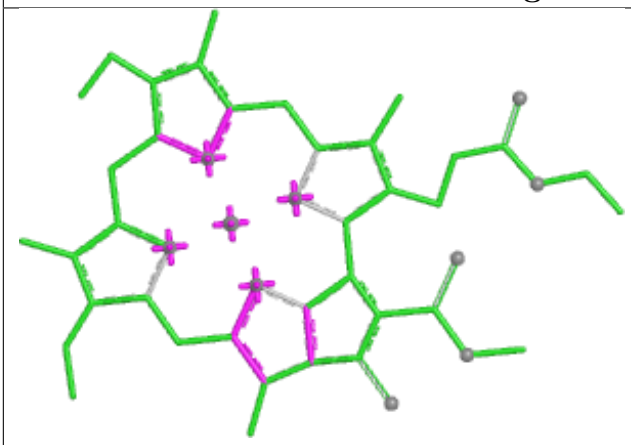


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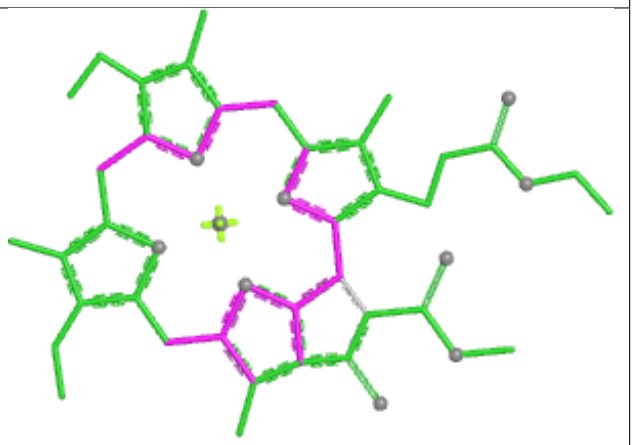


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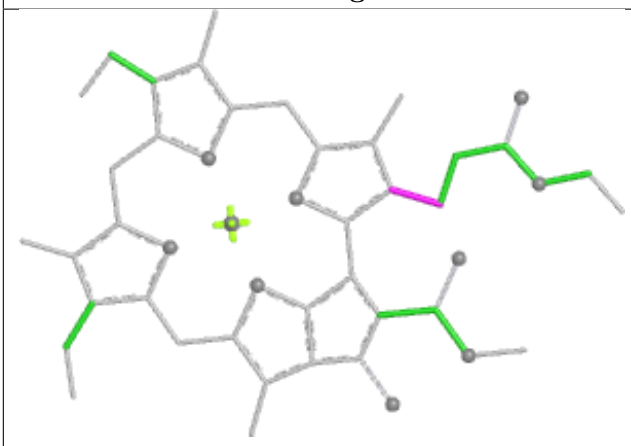
Ligand CLA X 313



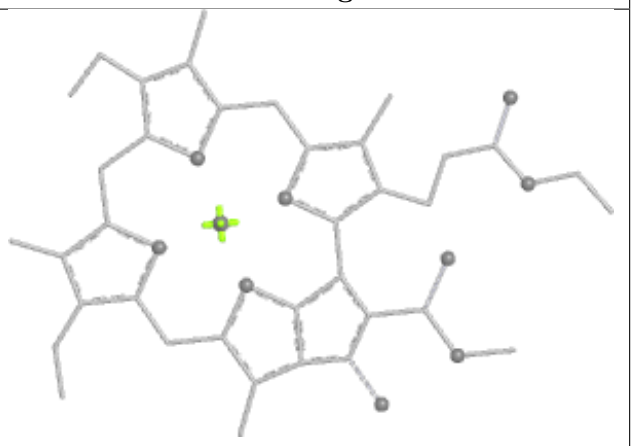
Bond lengths



Bond angles

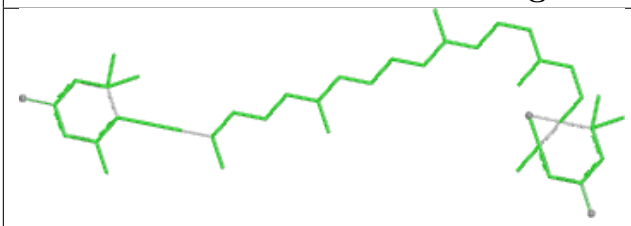


Torsions



Rings

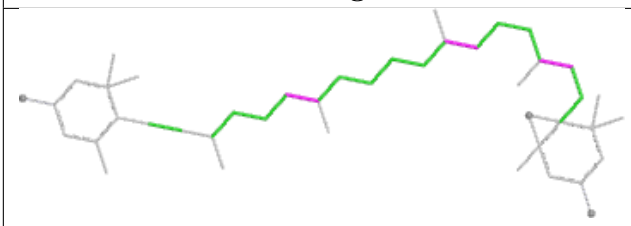
Ligand DD6 q 320



Bond lengths



Bond angles

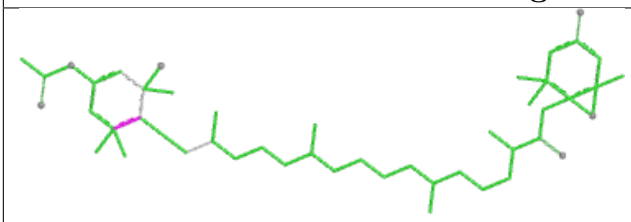


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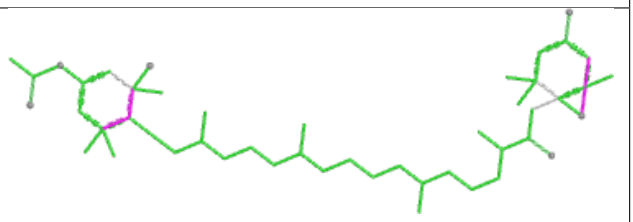


Rings

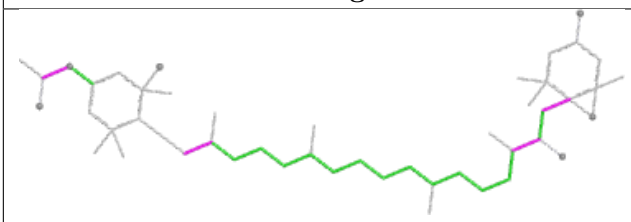
Ligand A86 w 315



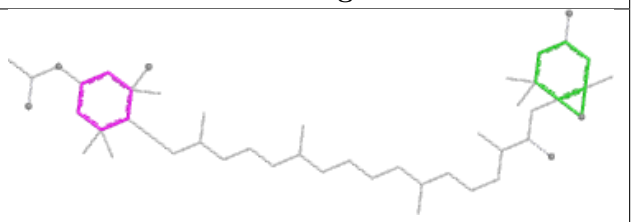
Bond lengths



Bond angles

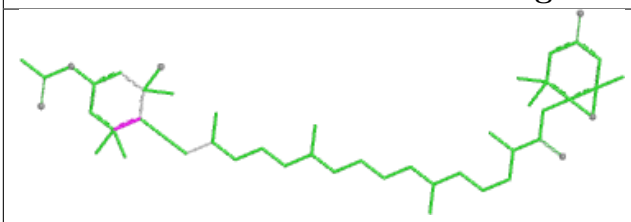


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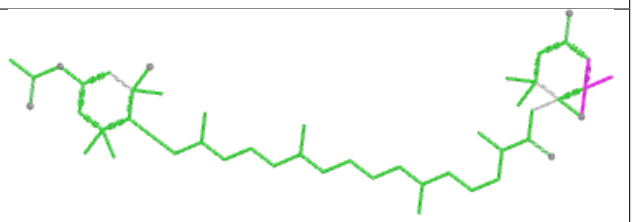


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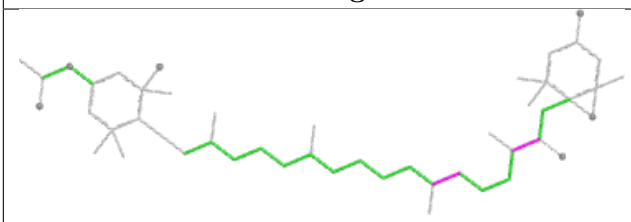
Ligand A86 z 301



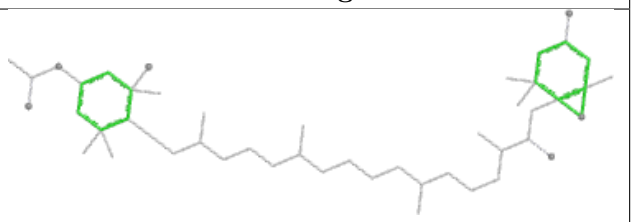
Bond lengths



Bond angles

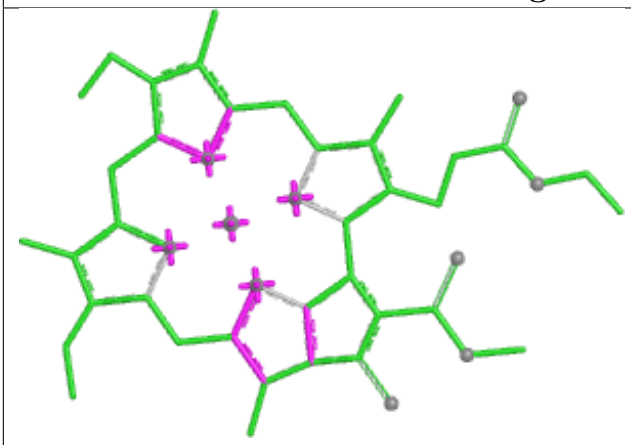


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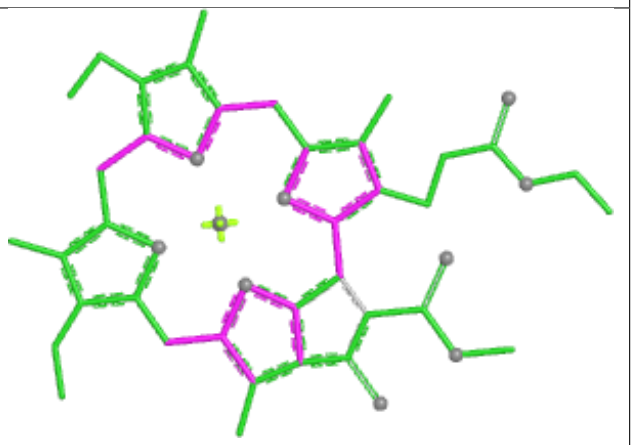


Rings

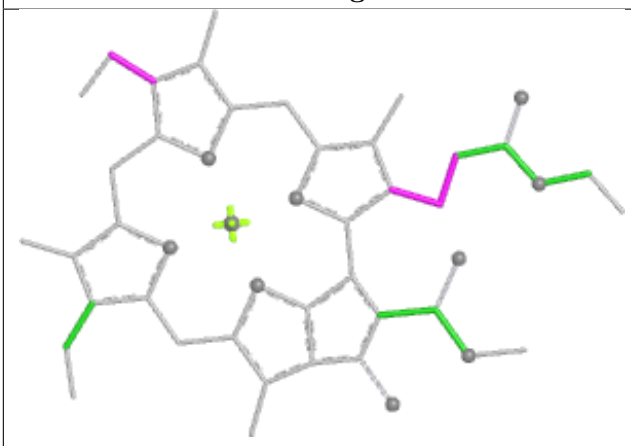
Ligand CLA z 314



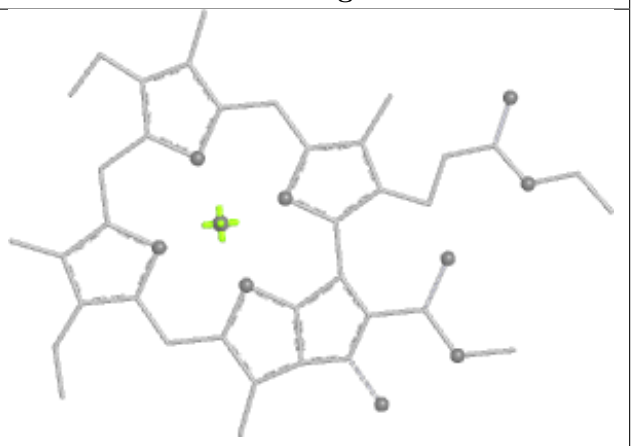
Bond lengths



Bond angles

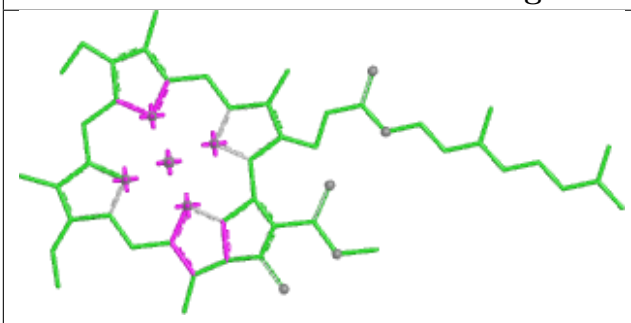


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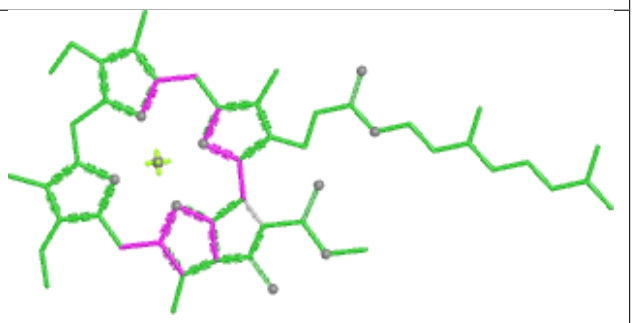


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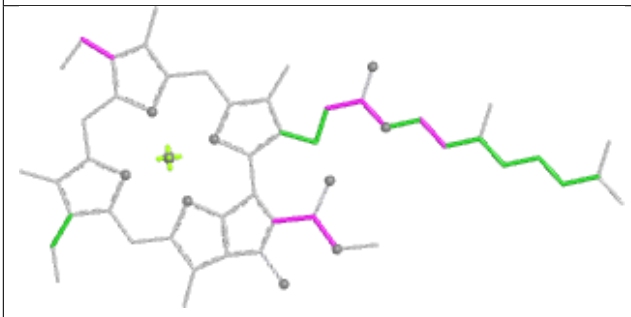
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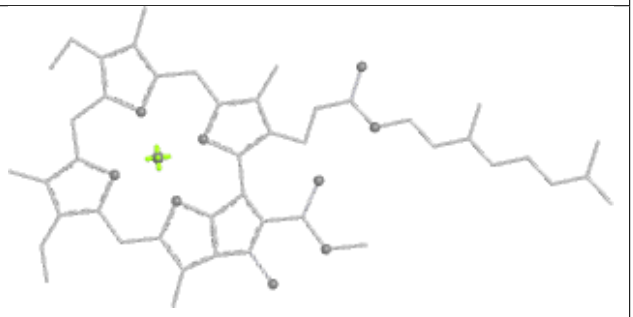
Bond lengths



Bond angles

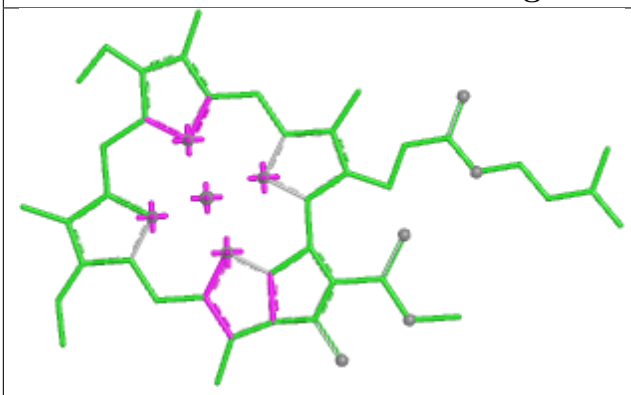


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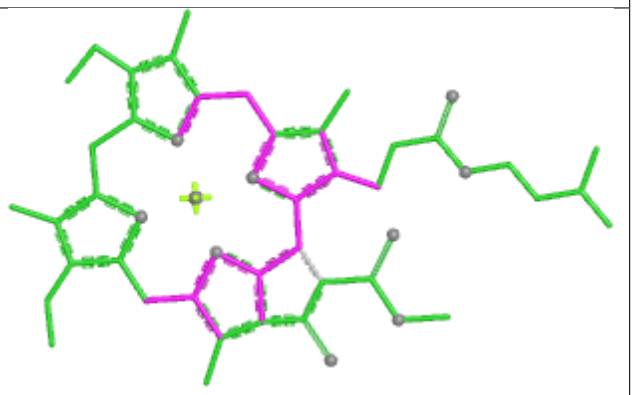


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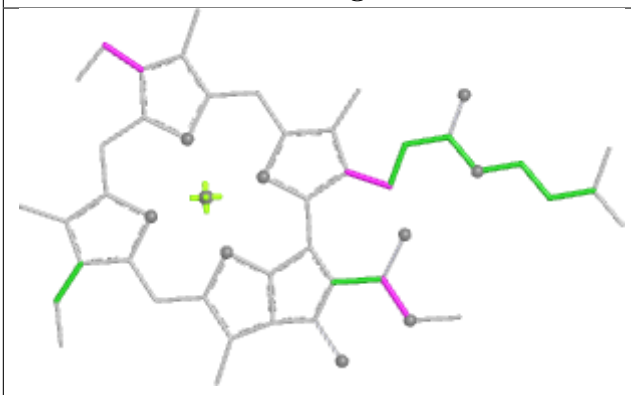
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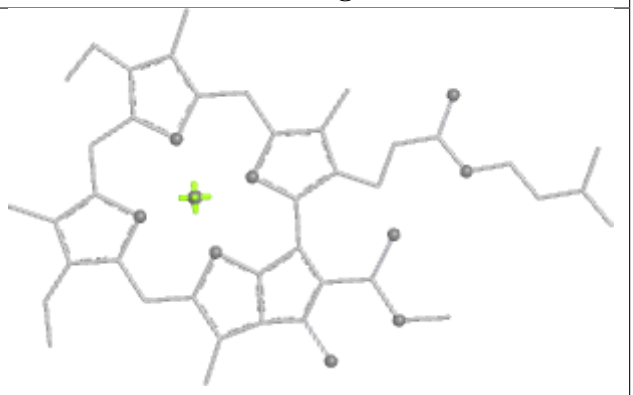
Bond lengths



Bond angles

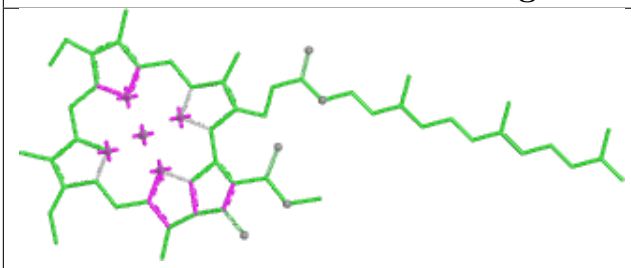


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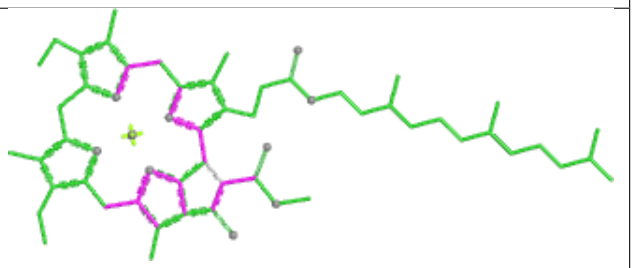


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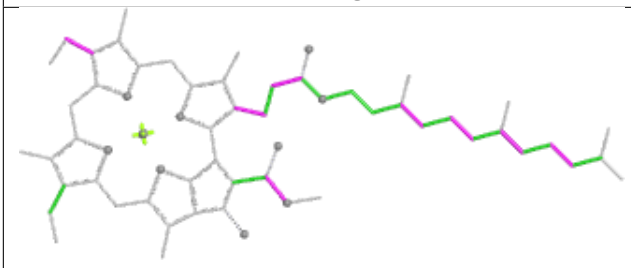
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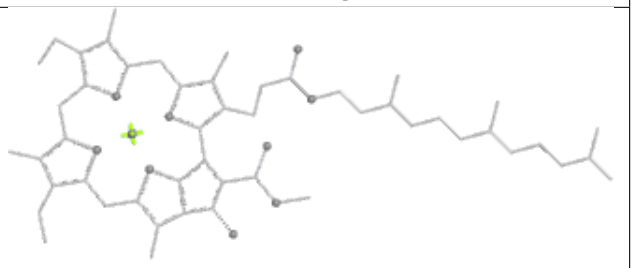
Bond lengths



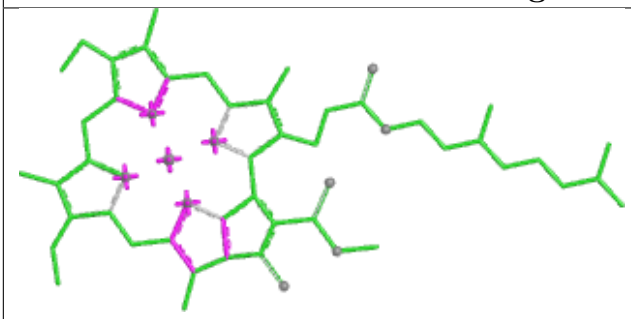
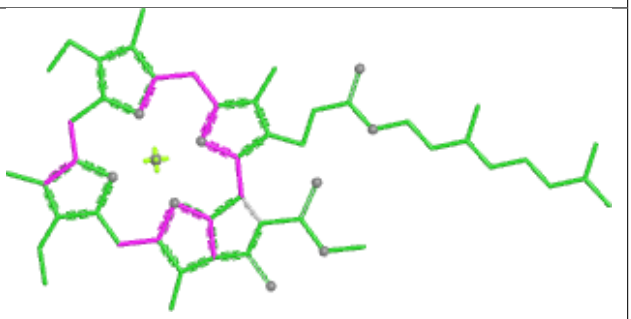
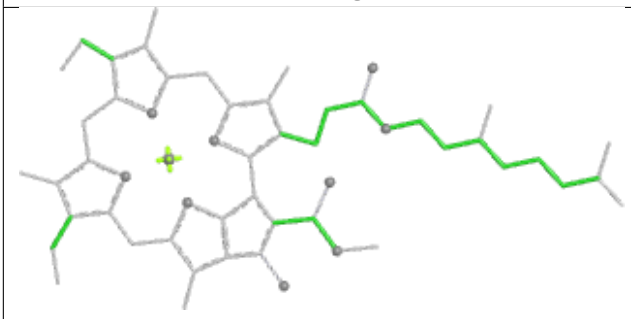
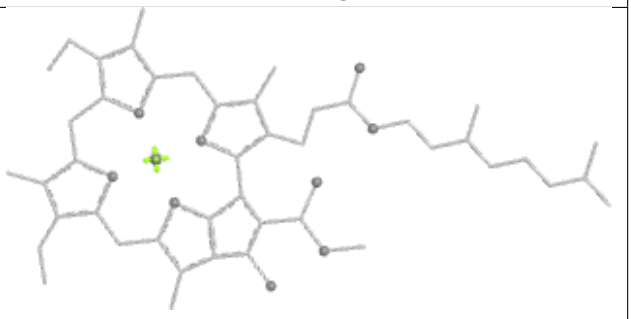
Bond angles

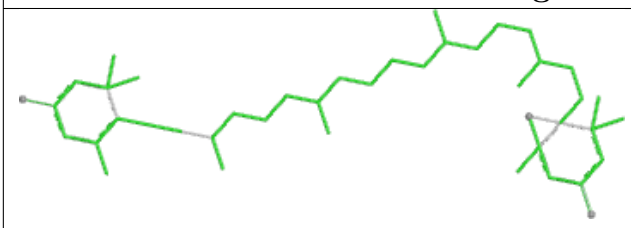
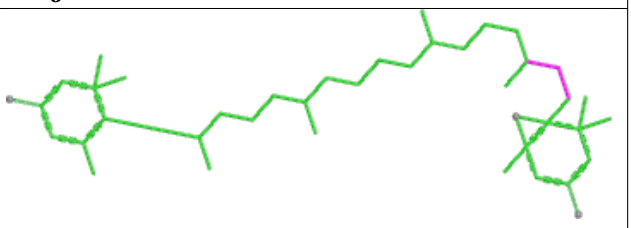
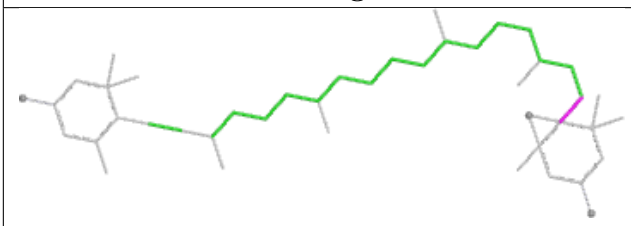
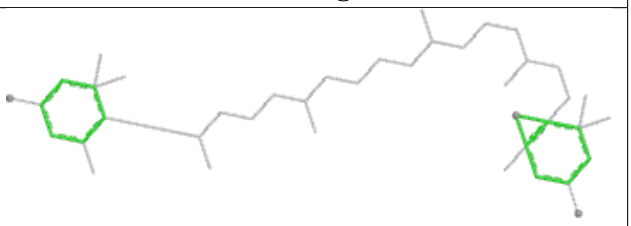


Torsions

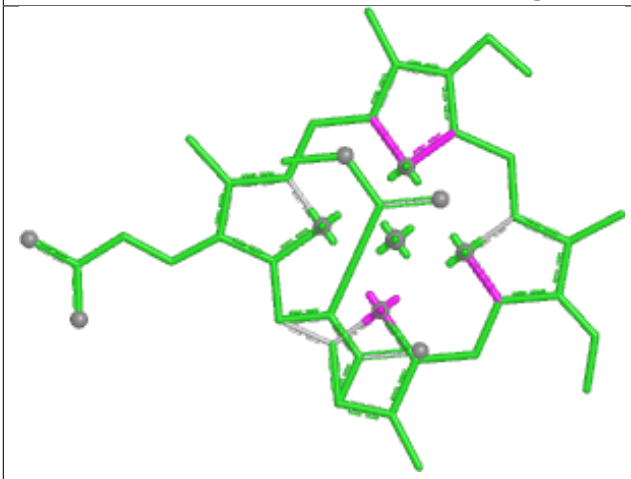


Rings

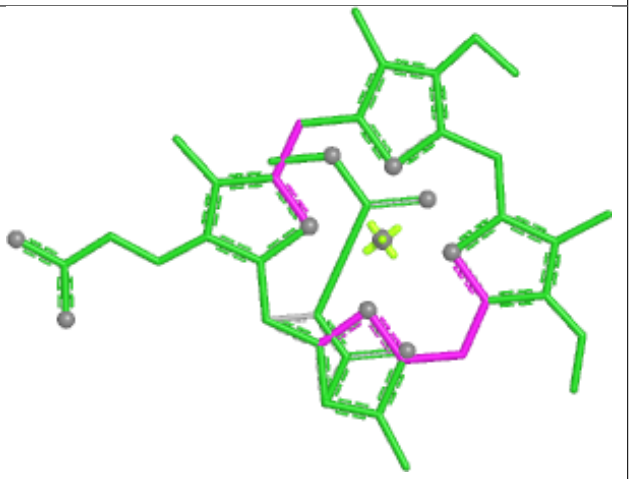
Ligand CLA a 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DD6 j 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

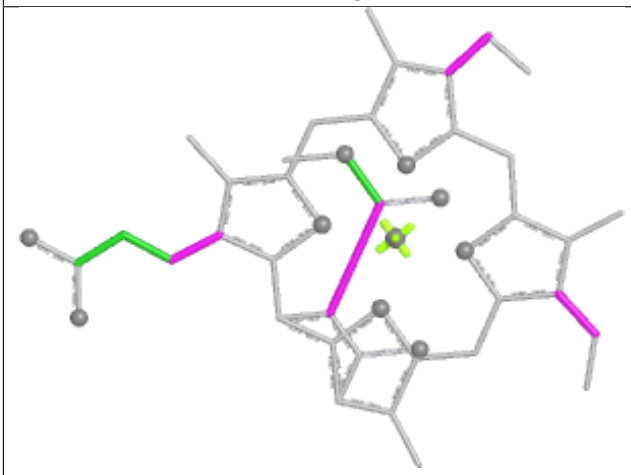
Ligand KC2 L 313



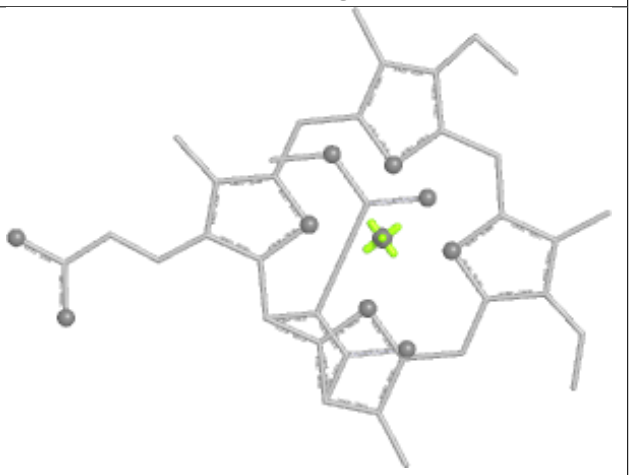
Bond lengths



Bond angles

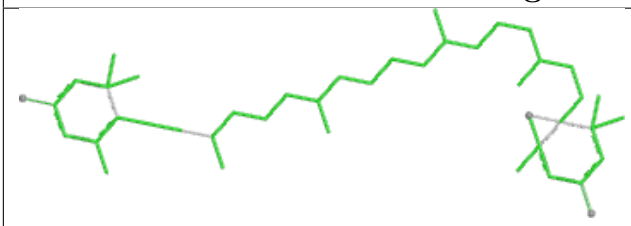


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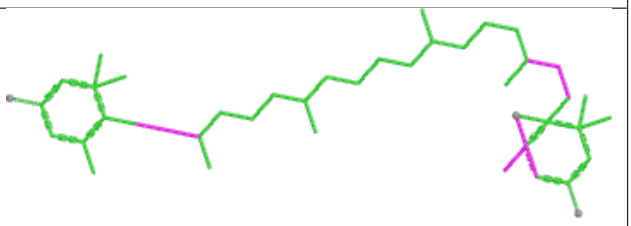


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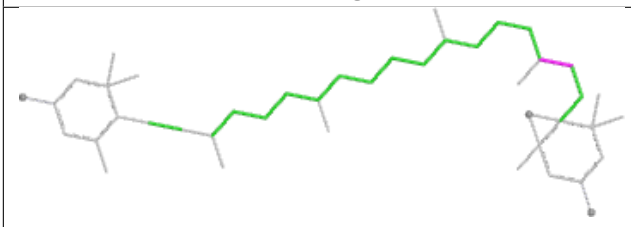
Ligand DD6 H 314



Bond lengths



Bond angles

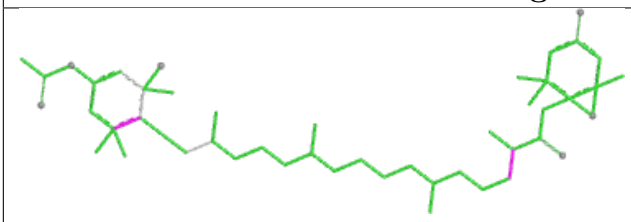


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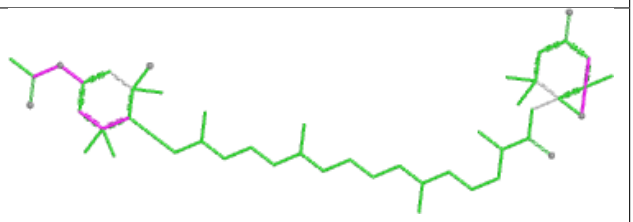


Rings

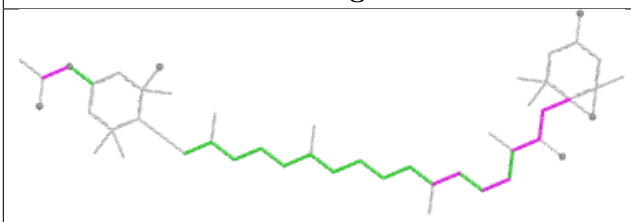
Ligand A86 w 311



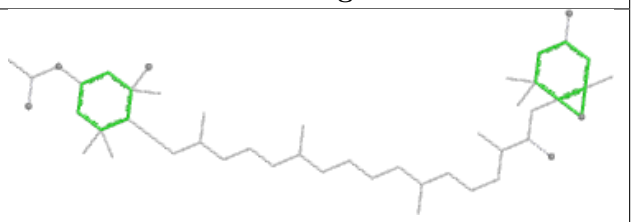
Bond lengths



Bond angles

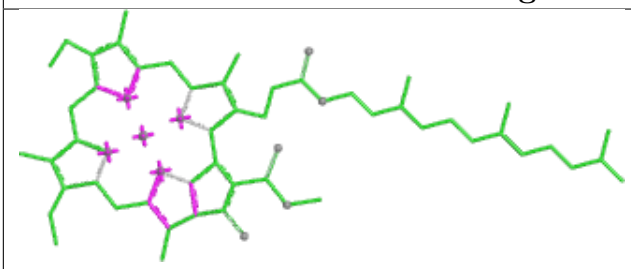


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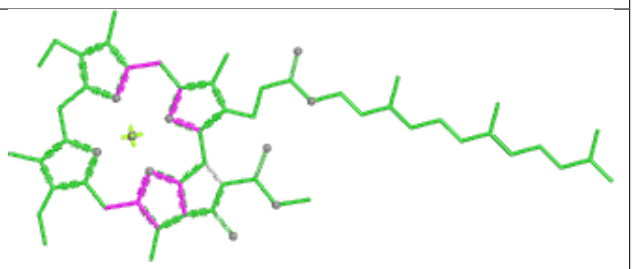


Rings

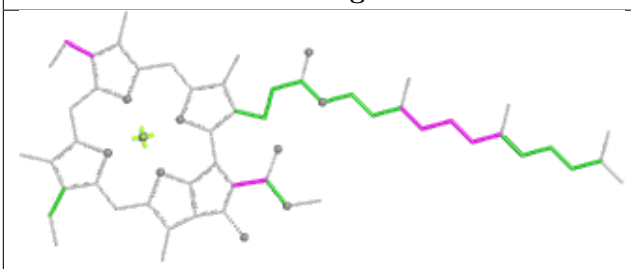
Ligand CLA W 313



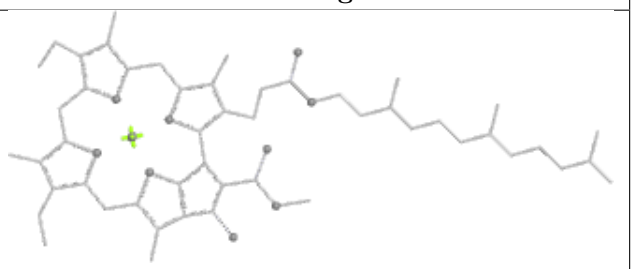
Bond lengths



Bond angles

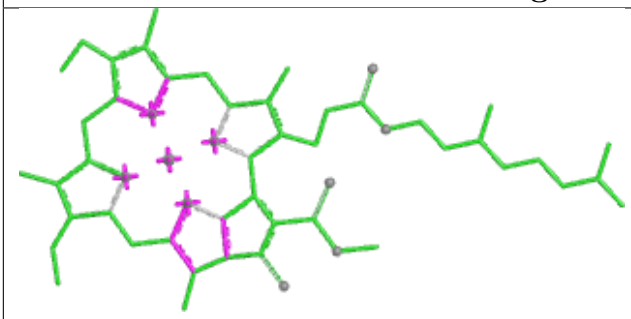


Torsions

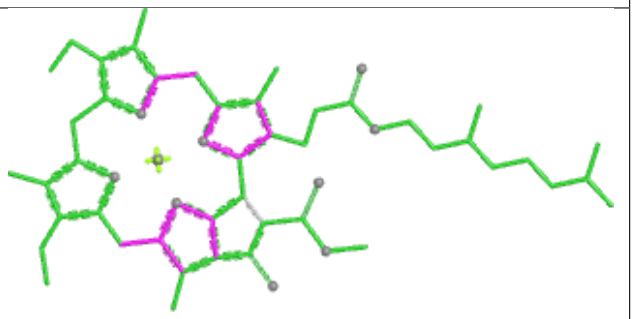


Rings

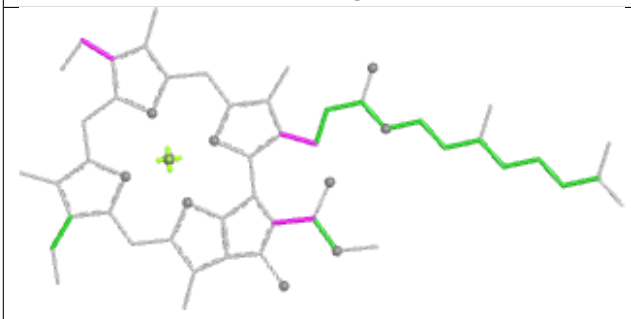
Ligand CLA I 208



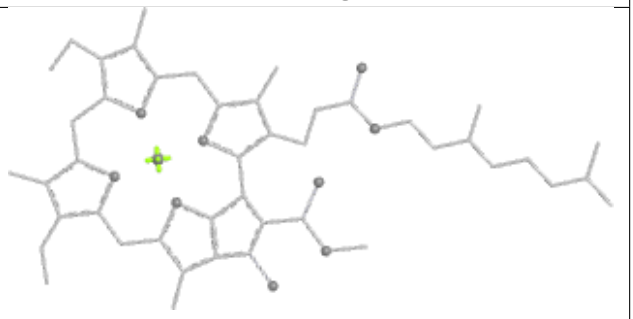
Bond lengths



Bond angles

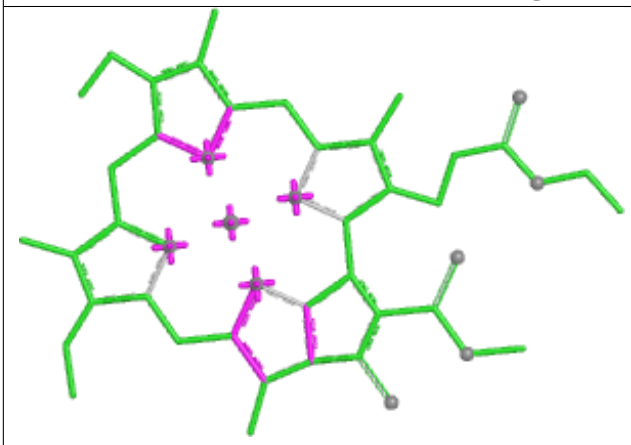


Torsions

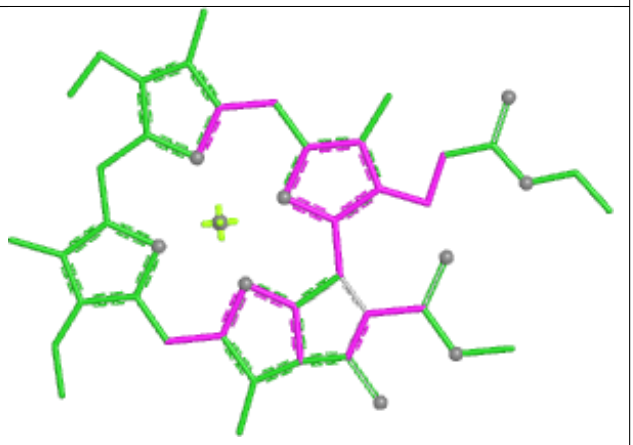


Rings

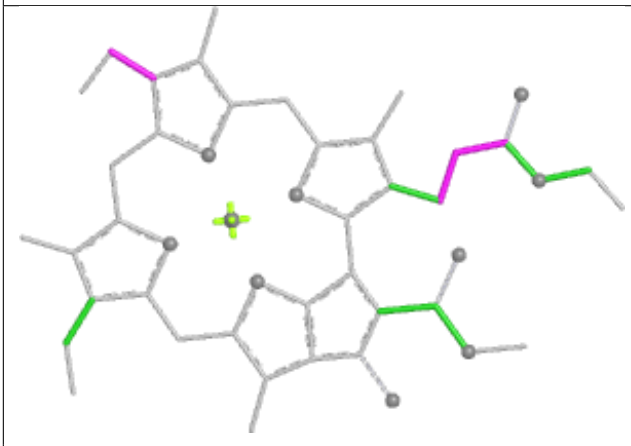
Ligand CLA J 307



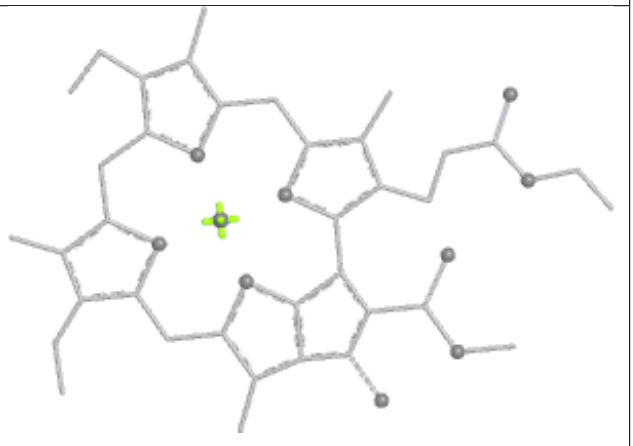
Bond lengths



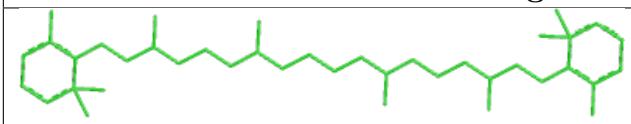
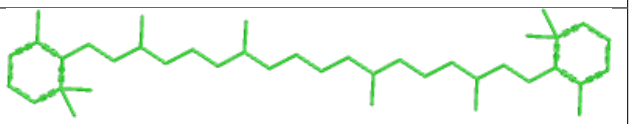
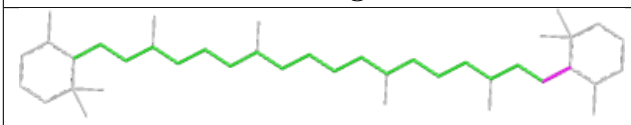
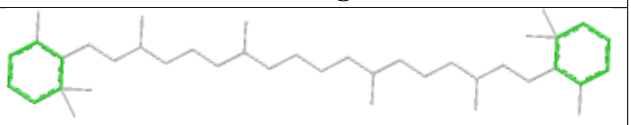
Bond angles

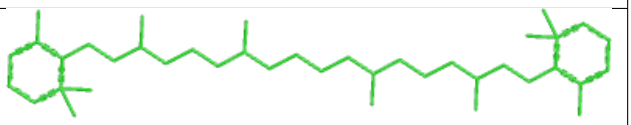
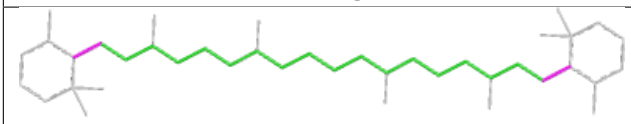
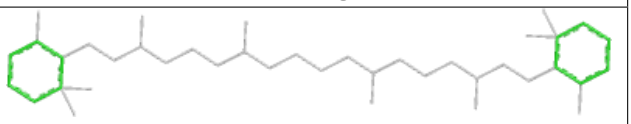


Torsions

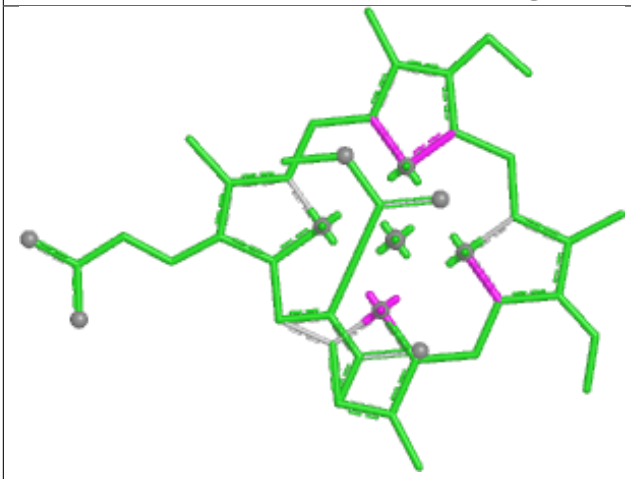


Rings

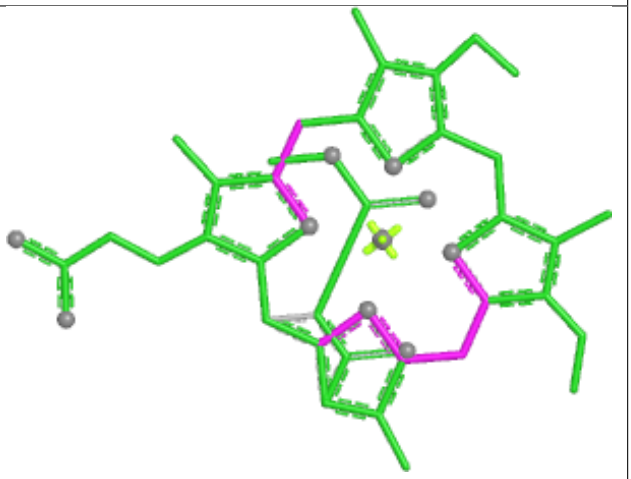
Ligand BCR a 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR i 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

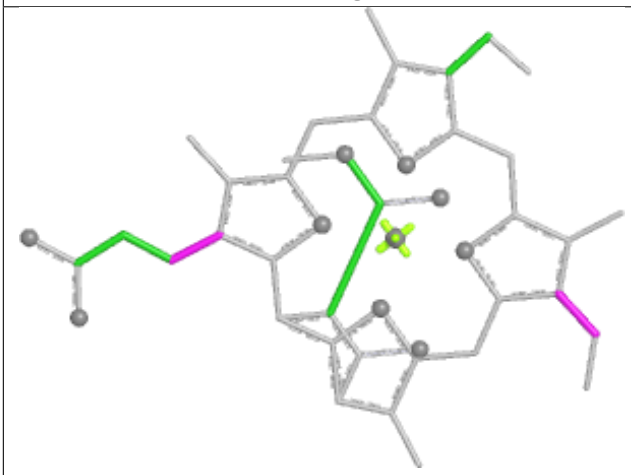
Ligand KC2 X 302



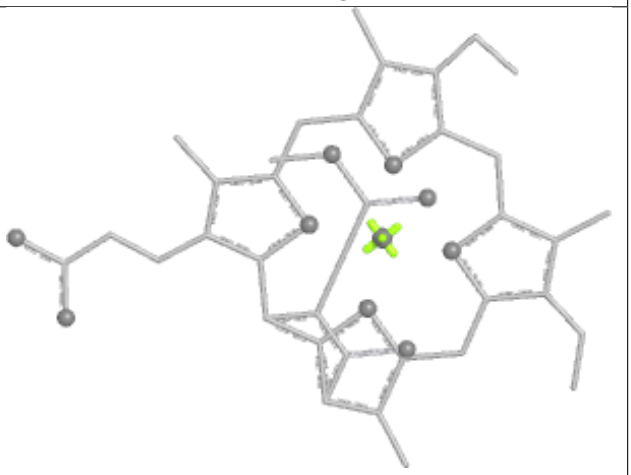
Bond lengths



Bond angles

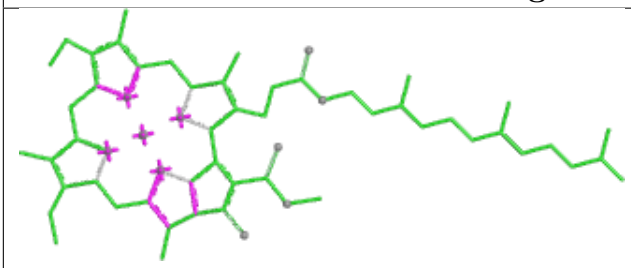


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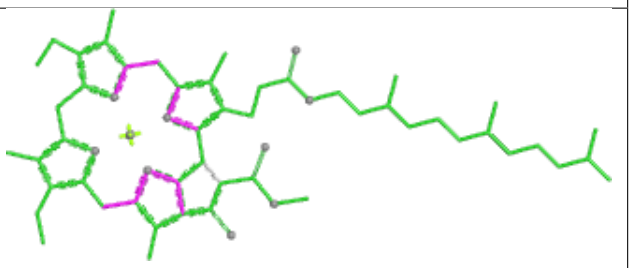


Rings

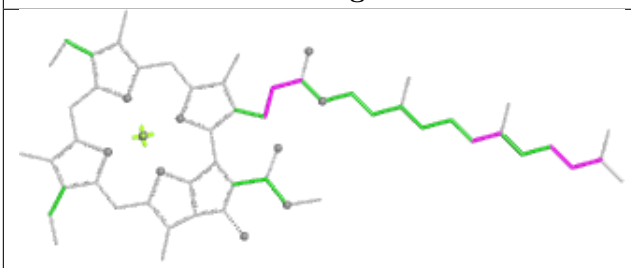
Ligand CLA a 831



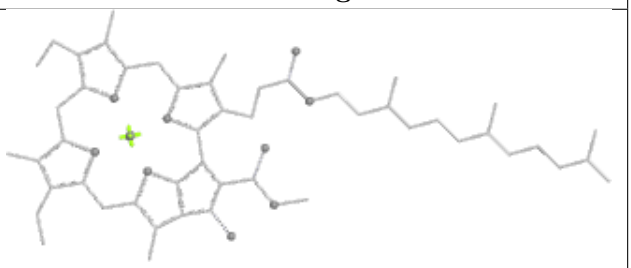
Bond lengths



Bond angles

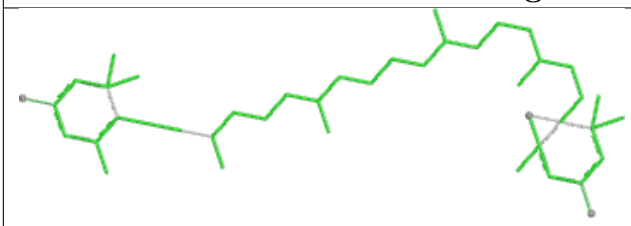


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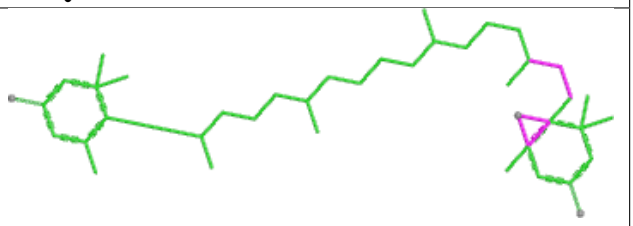


Rings

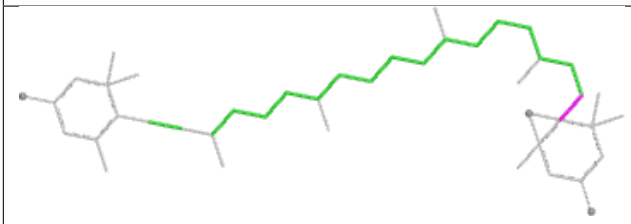
Ligand DD6 Q 211



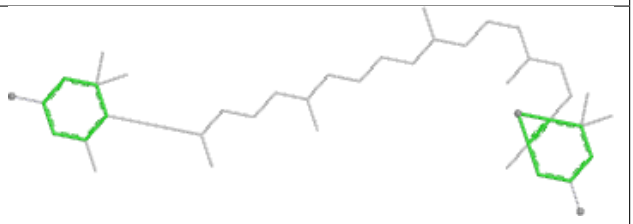
Bond lengths



Bond angles

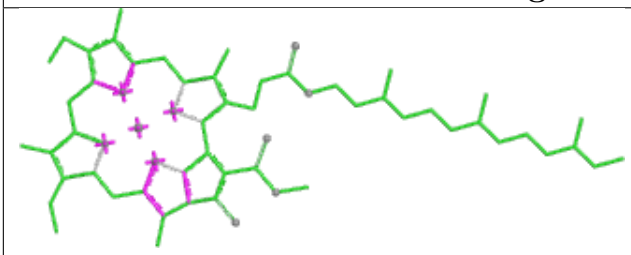


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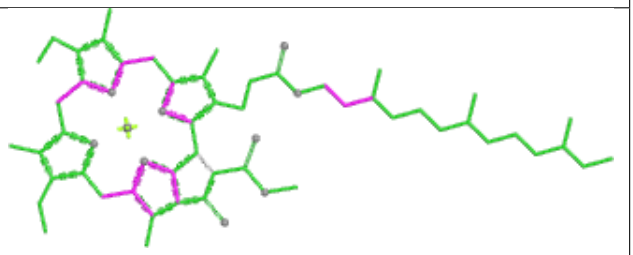


Rings

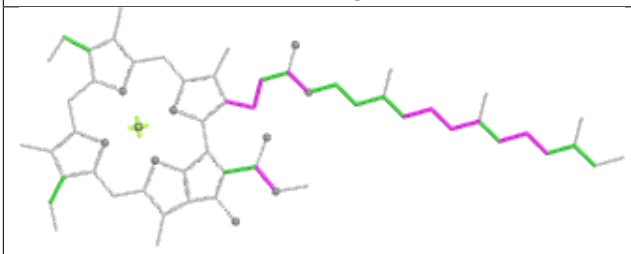
Ligand CLA a 826



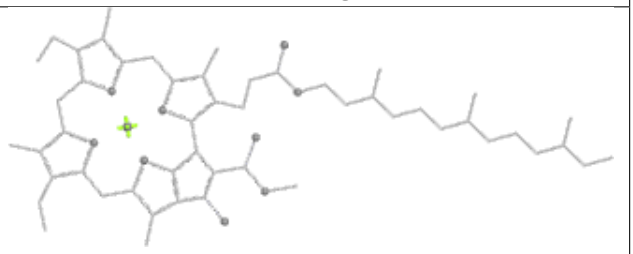
Bond lengths



Bond angles

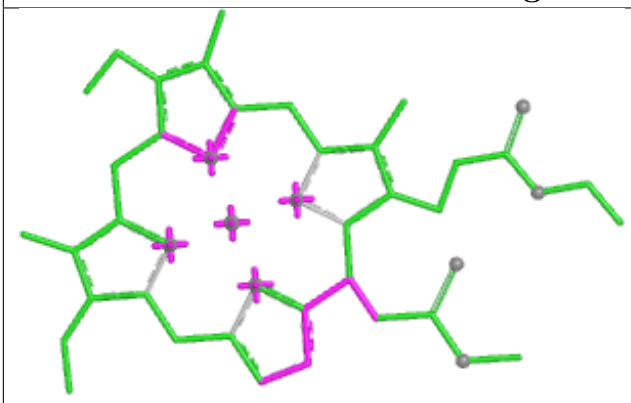


Torsions

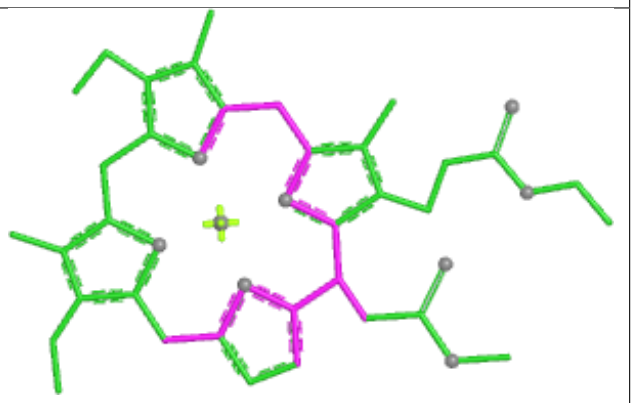


Rings

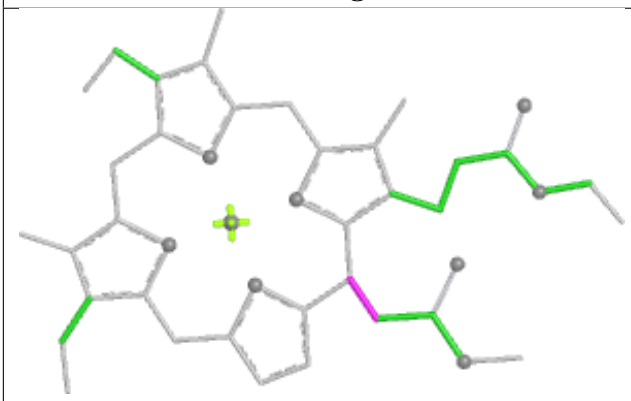
Ligand CLA D 305



Bond lengths



Bond angles

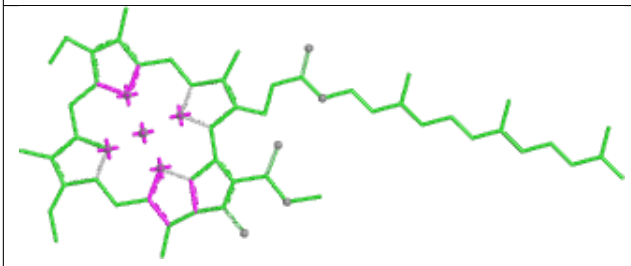


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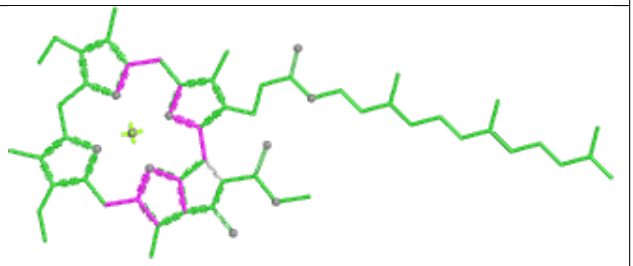


Rings

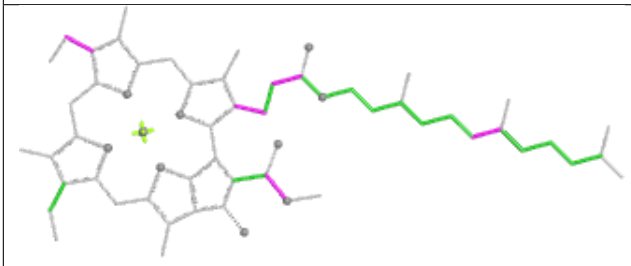
Ligand CLA a 813



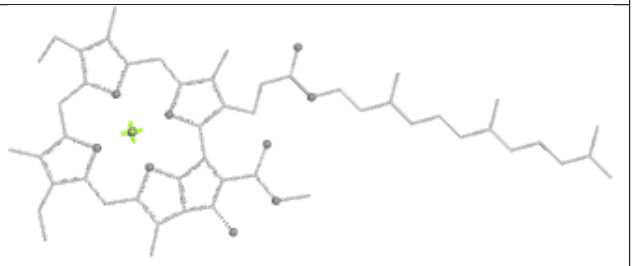
Bond lengths



Bond angles

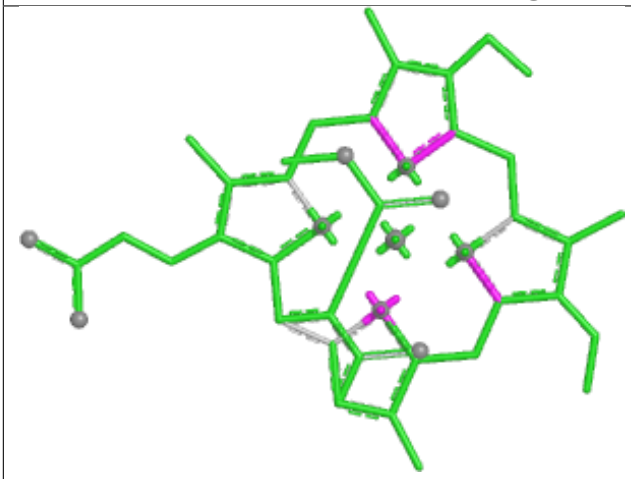


Torsions

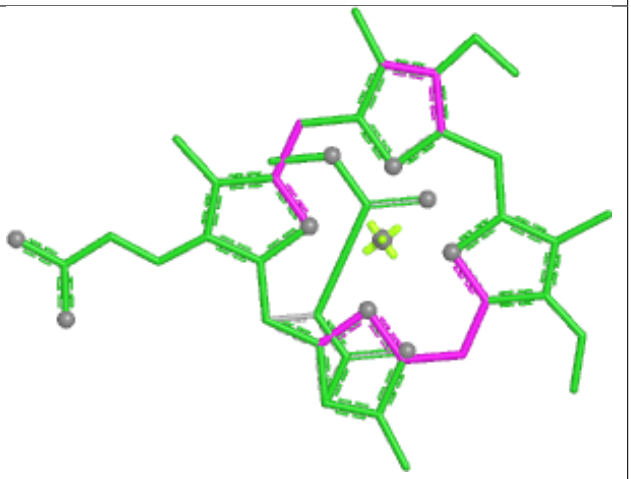


Rings

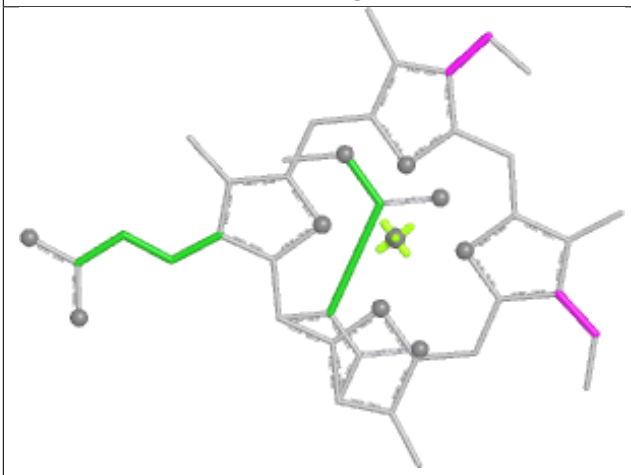
Ligand KC2 N 309



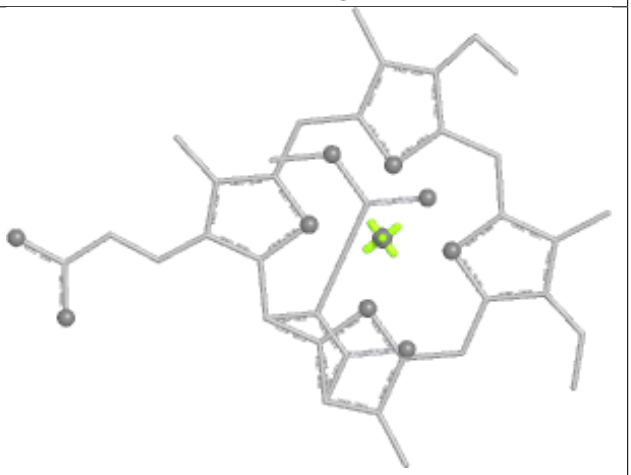
Bond lengths



Bond angles

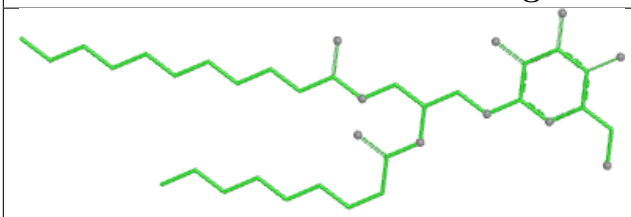


Torsions

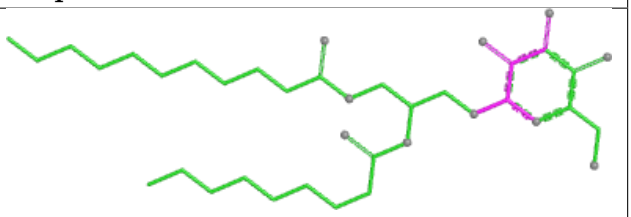


Rings

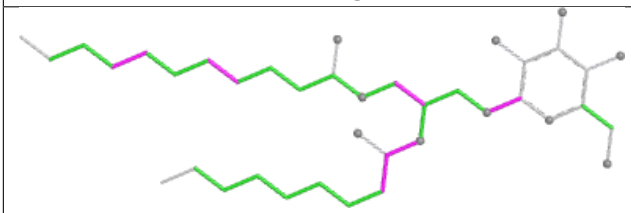
Ligand LMG p 301



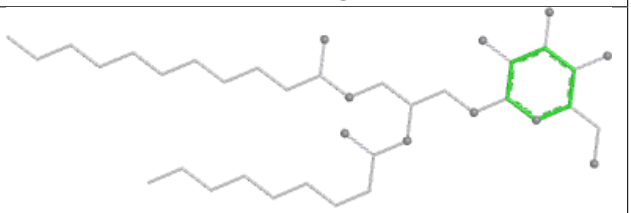
Bond lengths



Bond angles

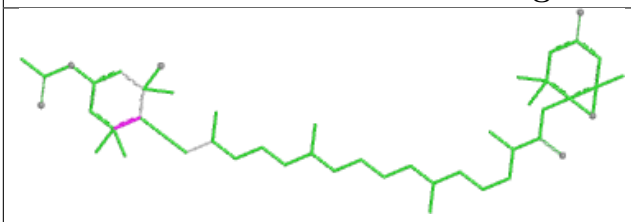


Torsions

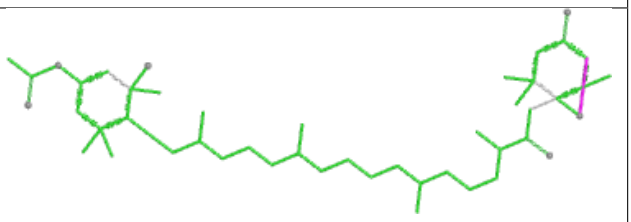


Rings

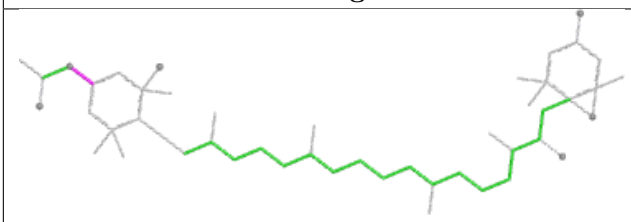
Ligand A86 S 318



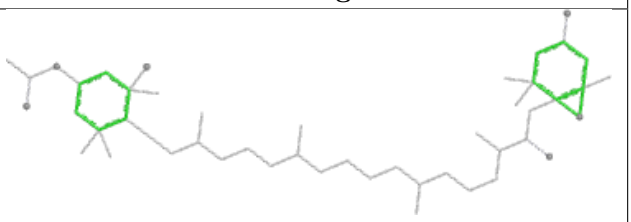
Bond lengths



Bond angles

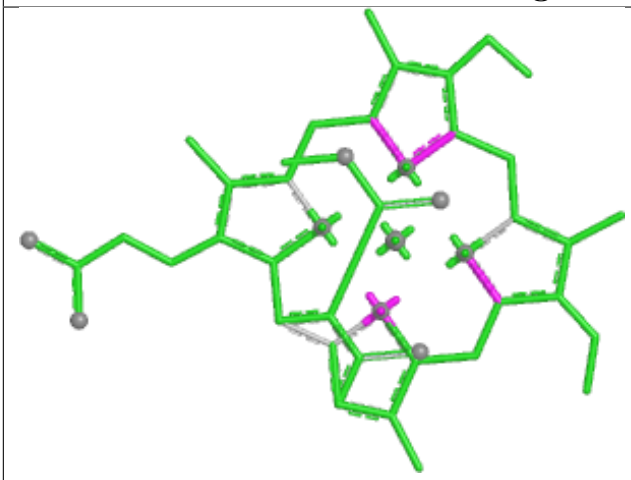


Torsions

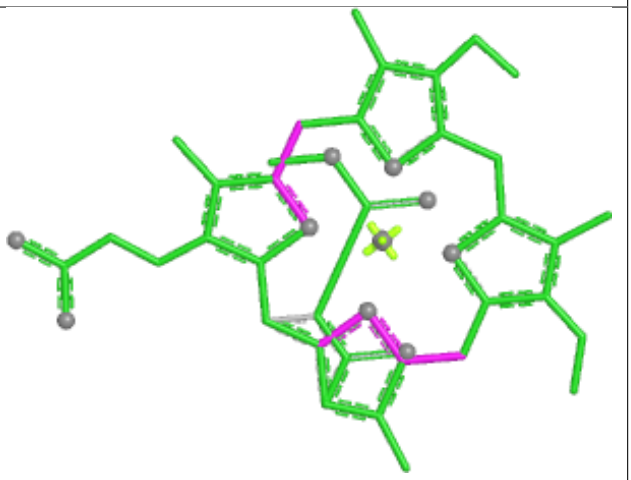


Rings

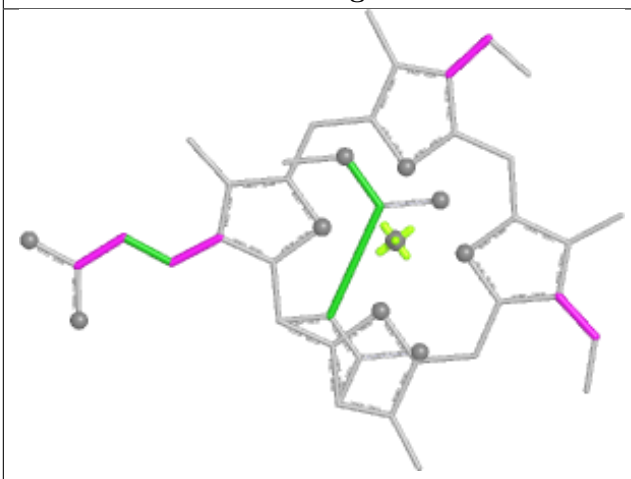
Ligand KC2 I 214



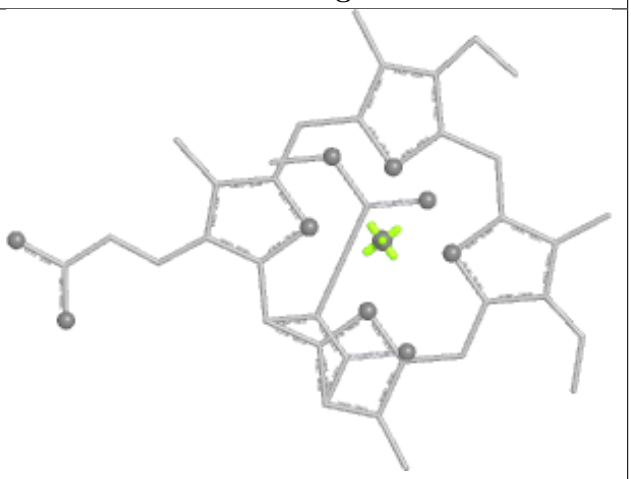
Bond lengths



Bond angles

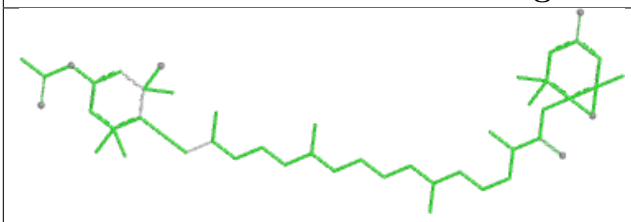


Torsions

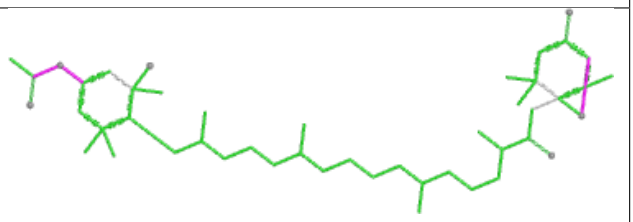


Rings

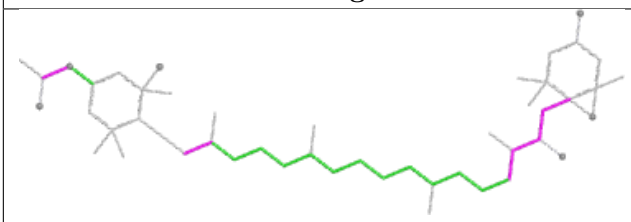
Ligand A86 x 319



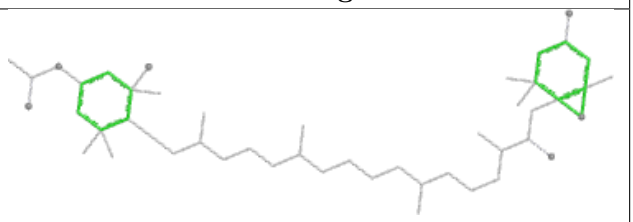
Bond lengths



Bond angles

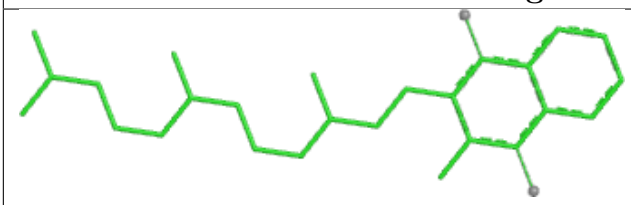


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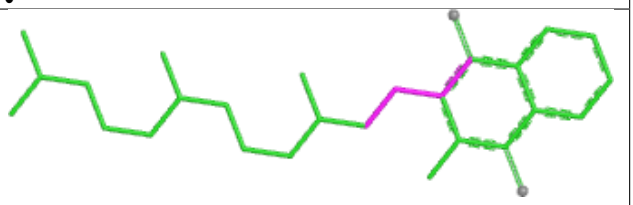


Rings

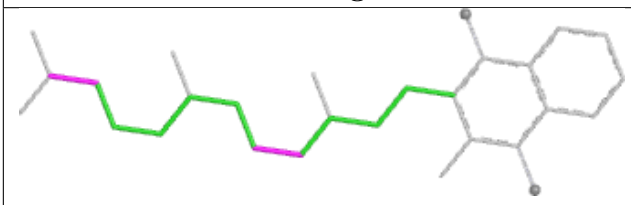
Ligand PQN a 847



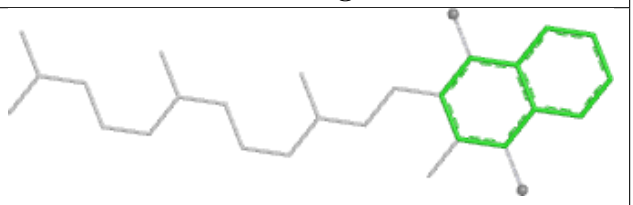
Bond lengths



Bond angles

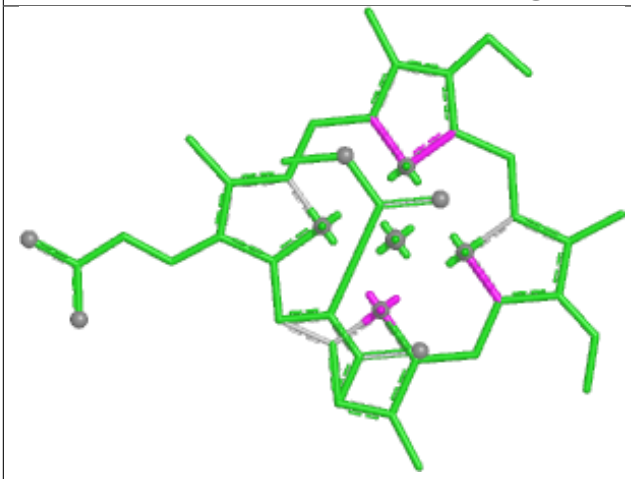


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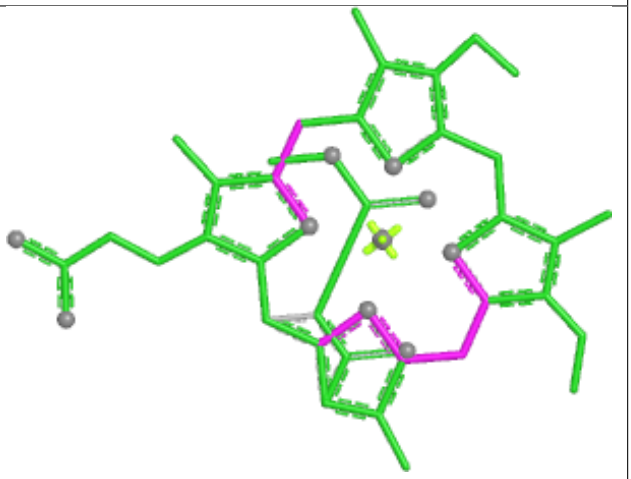


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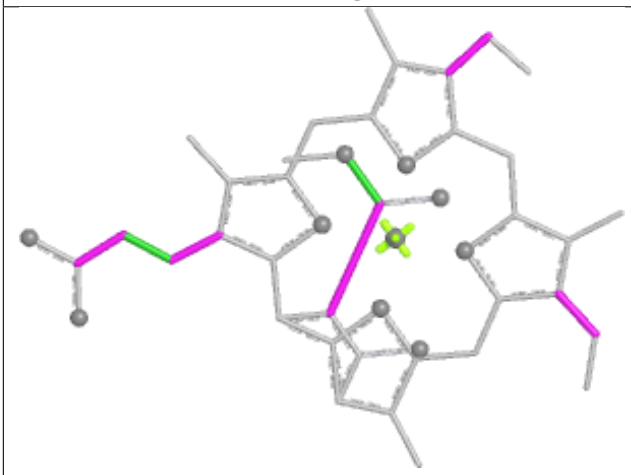
Ligand KC2 E 319



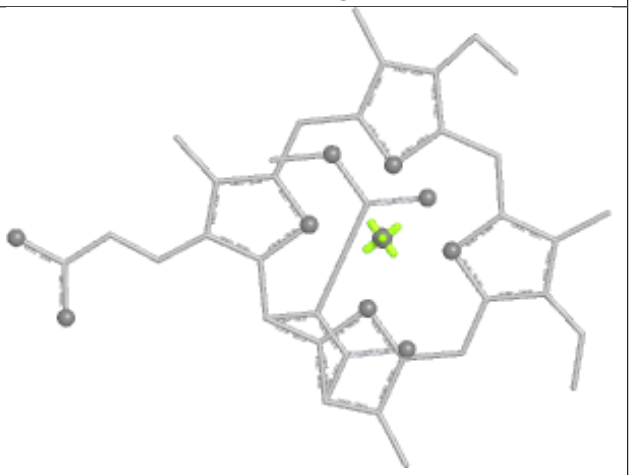
Bond lengths



Bond angles

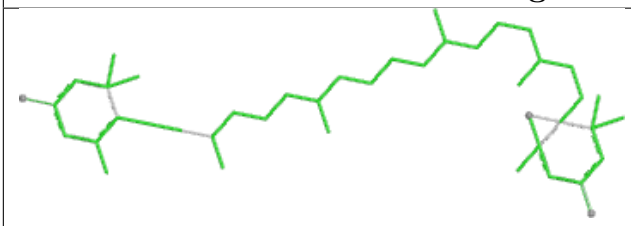


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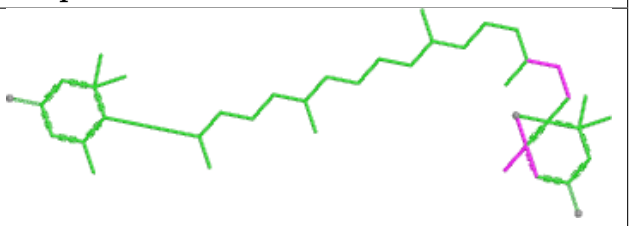


Rings

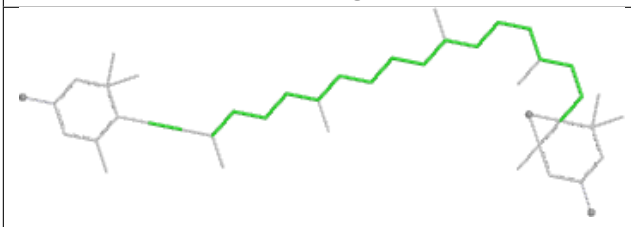
Ligand DD6 q 318



Bond lengths



Bond angles

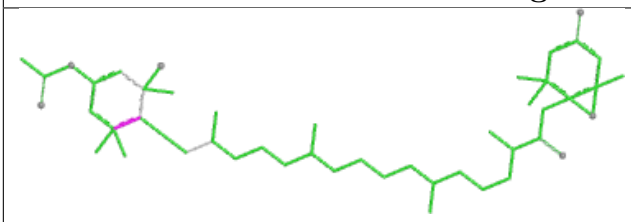


Torsions

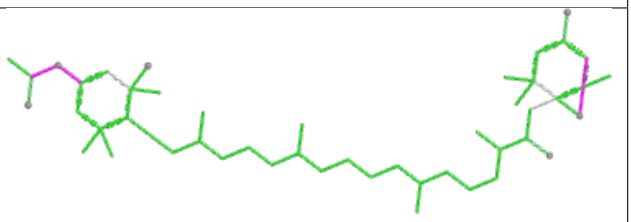


Rings

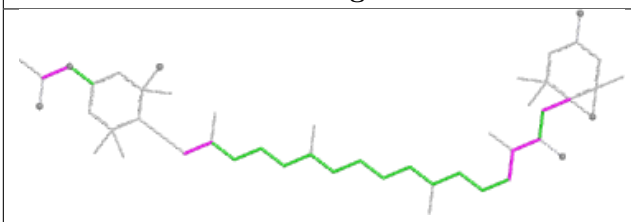
Ligand A86 w 310



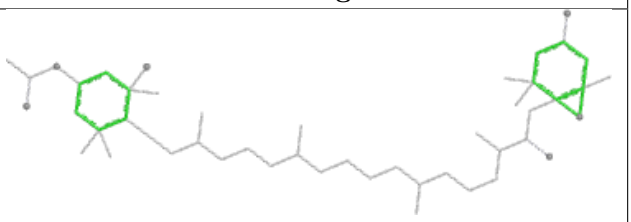
Bond lengths



Bond angles

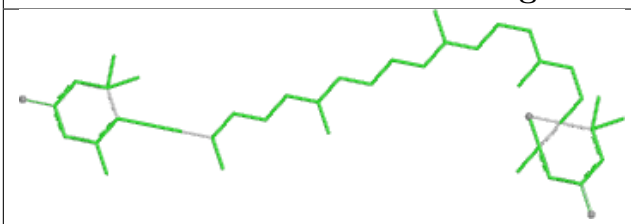


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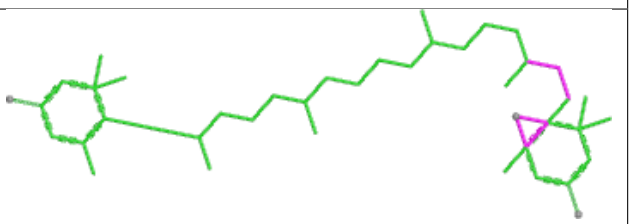


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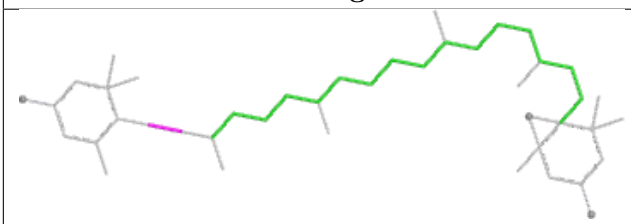
Ligand DD6 W 315



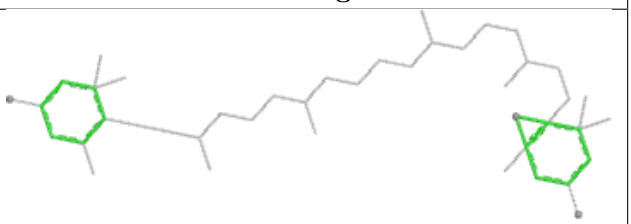
Bond lengths



Bond angles

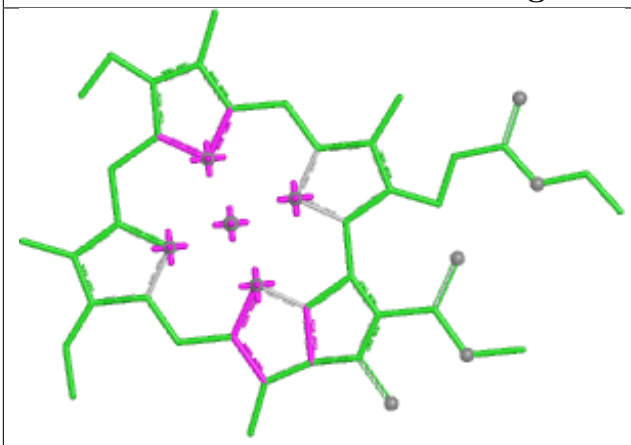


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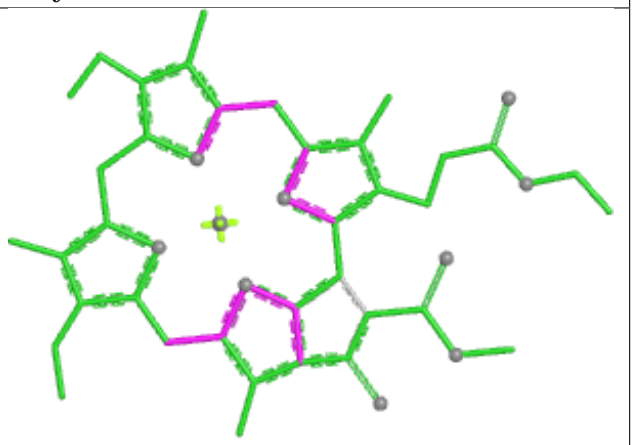


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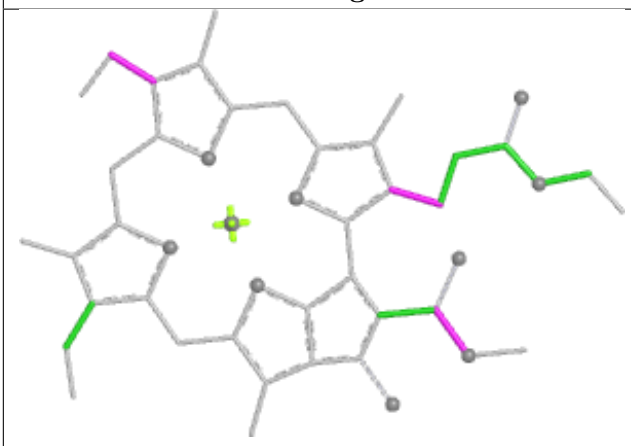
Ligand CLA y 308



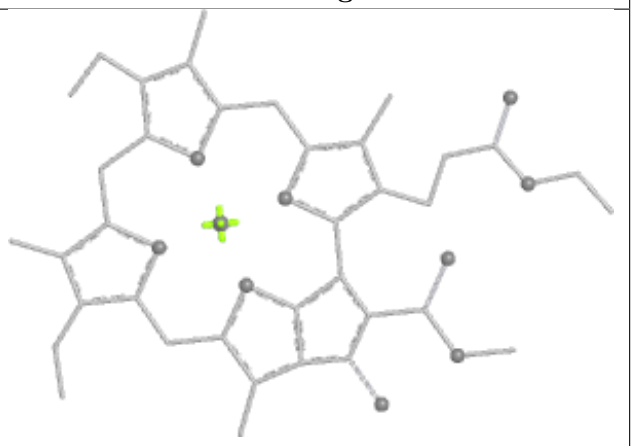
Bond lengths



Bond angles

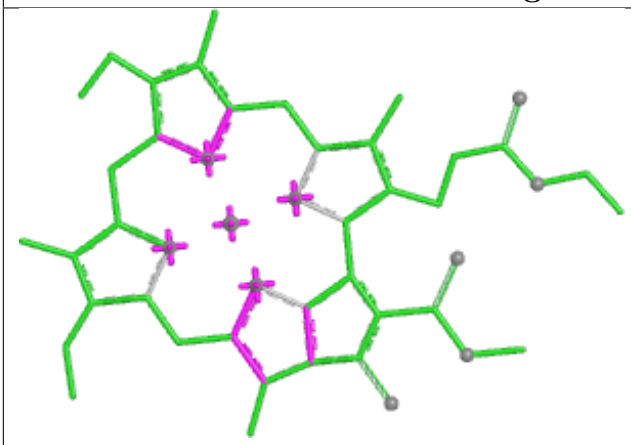


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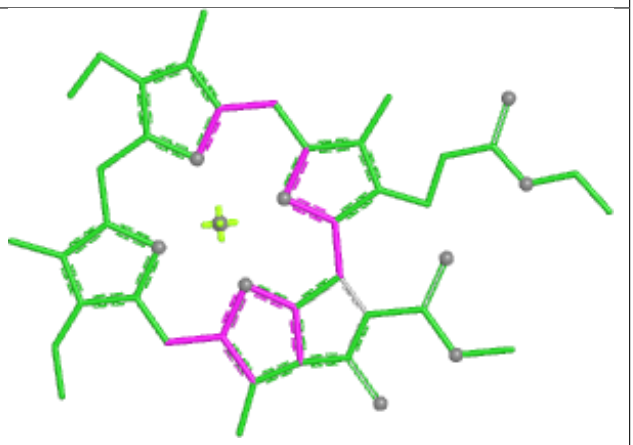


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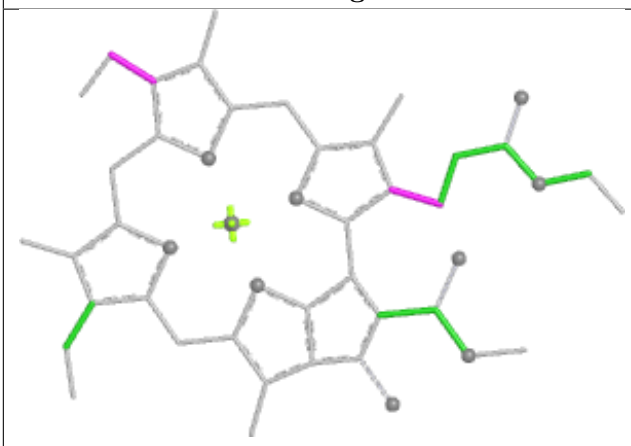
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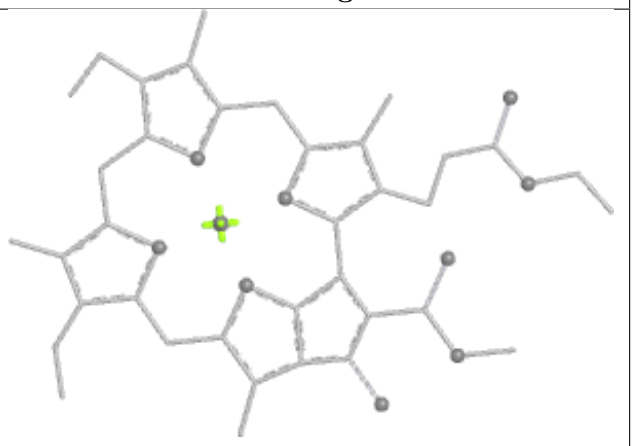
Bond lengths



Bond angles

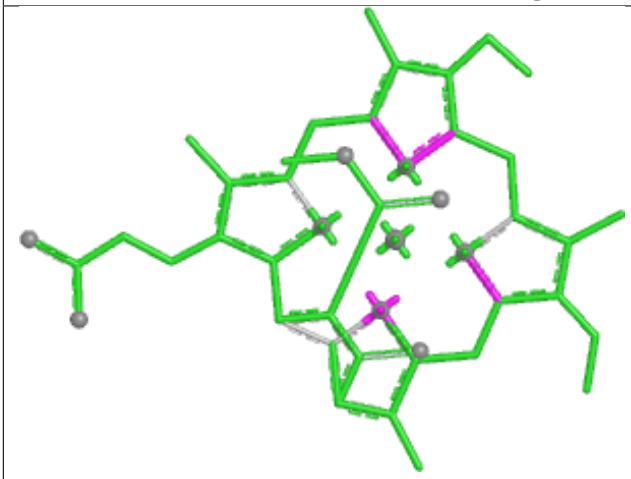


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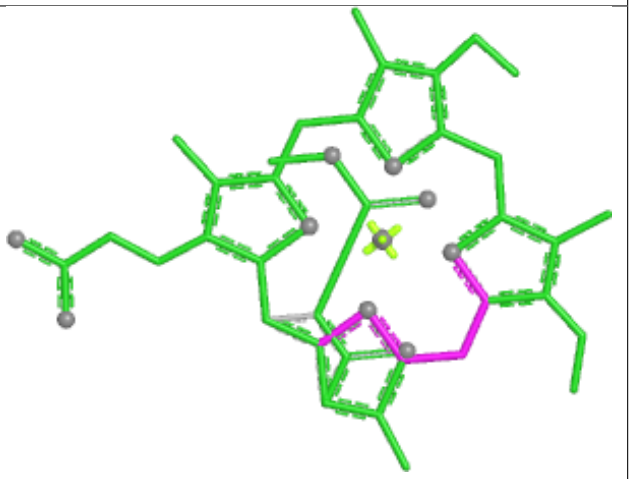


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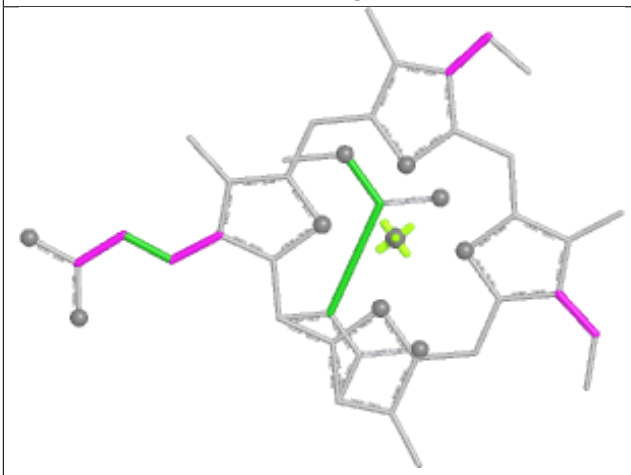
Ligand KC2 L 309



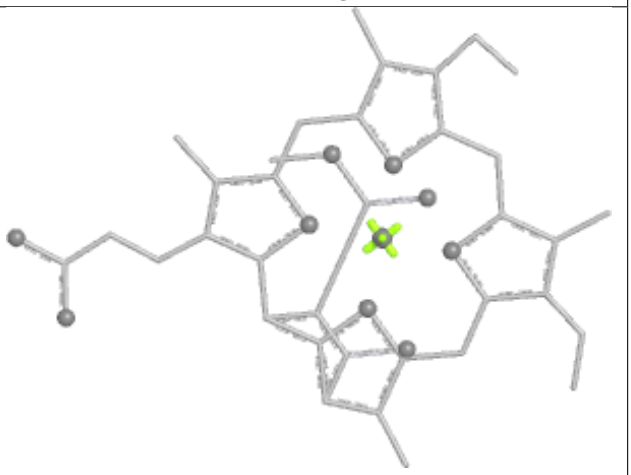
Bond lengths



Bond angles

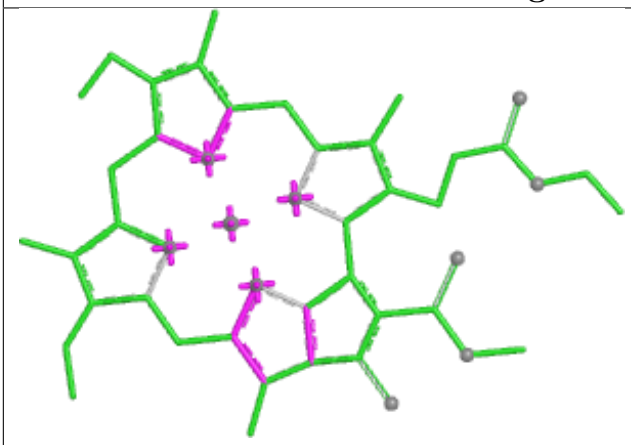


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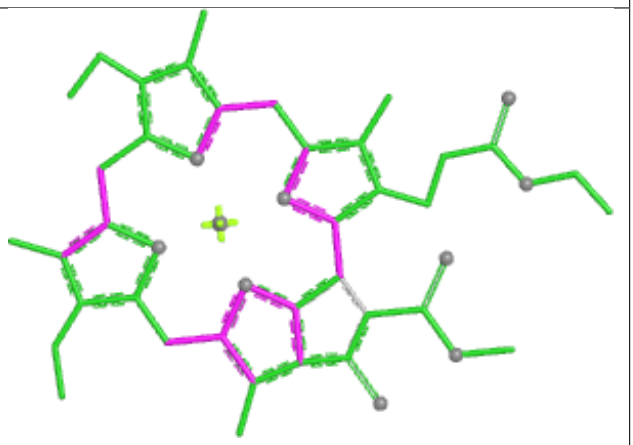


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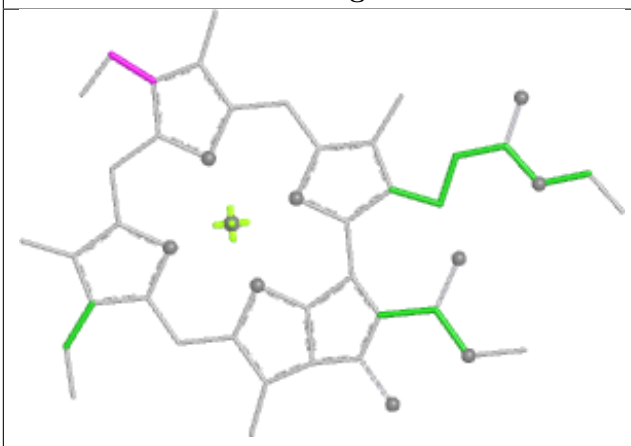
Ligand CLA a 818



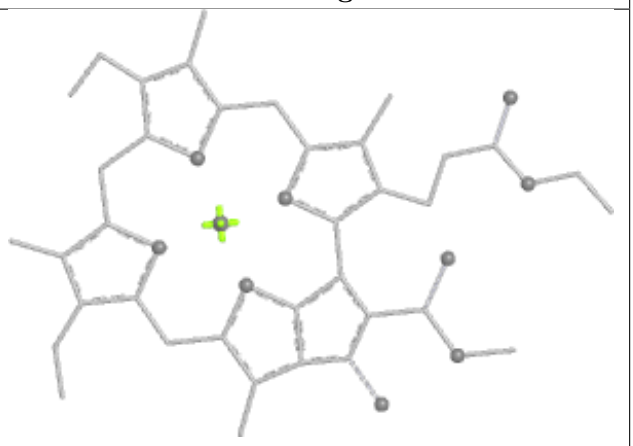
Bond lengths



Bond angles

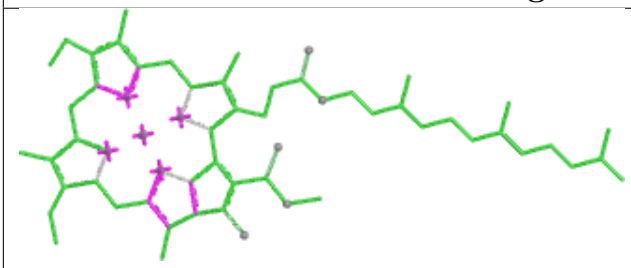


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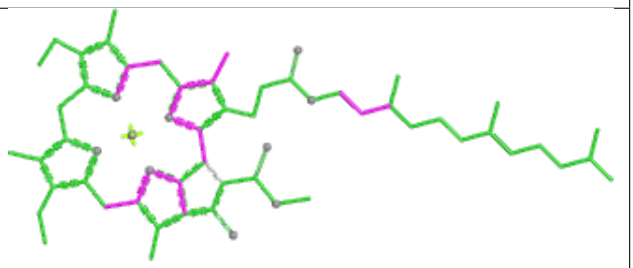


Rings

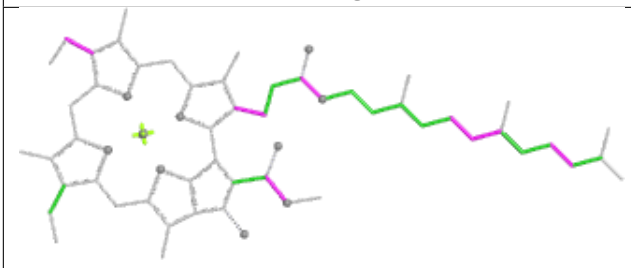
Ligand CLA x 312



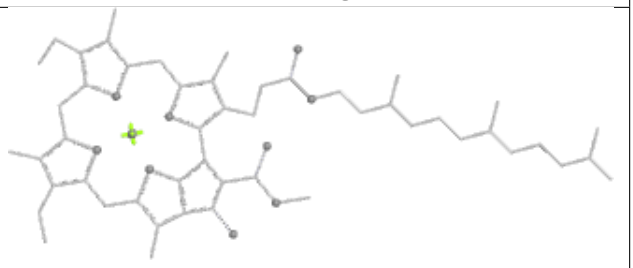
Bond lengths



Bond angles

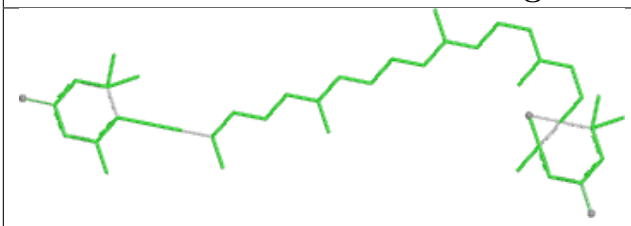


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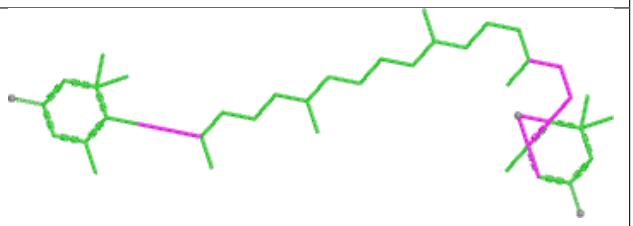


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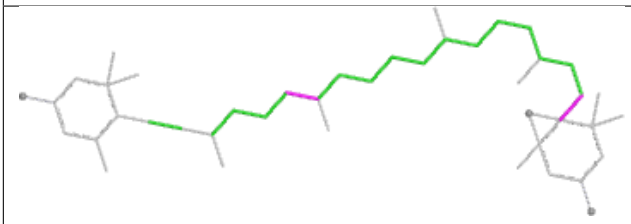
Ligand DD6 N 317



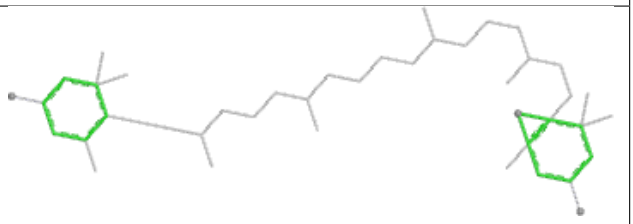
Bond lengths



Bond angles

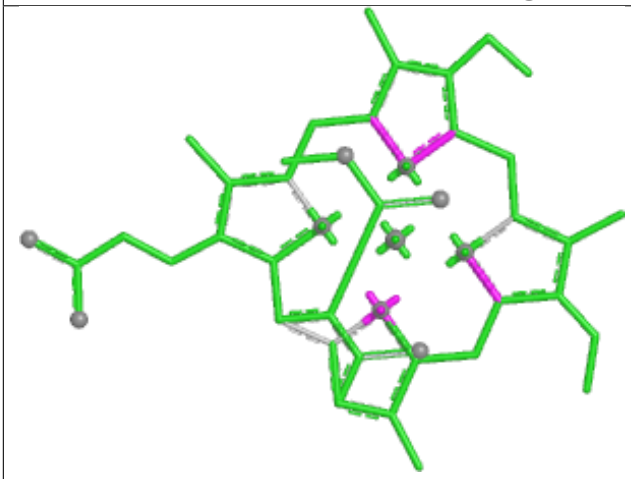


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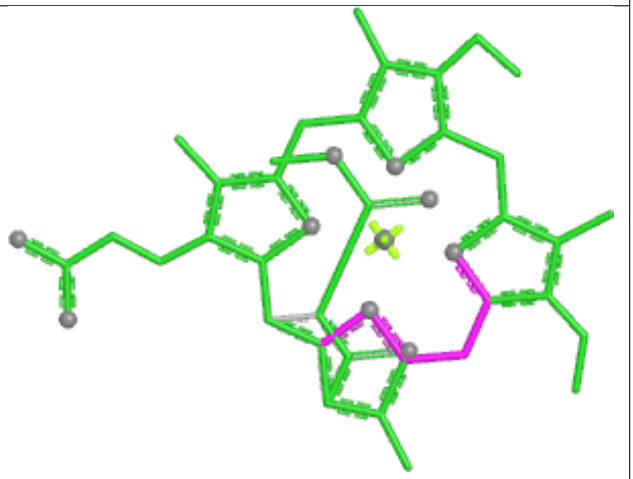


Rings

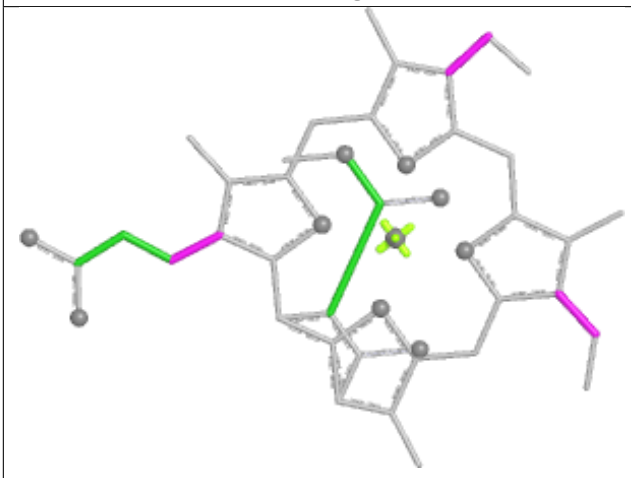
Ligand KC2 W 302



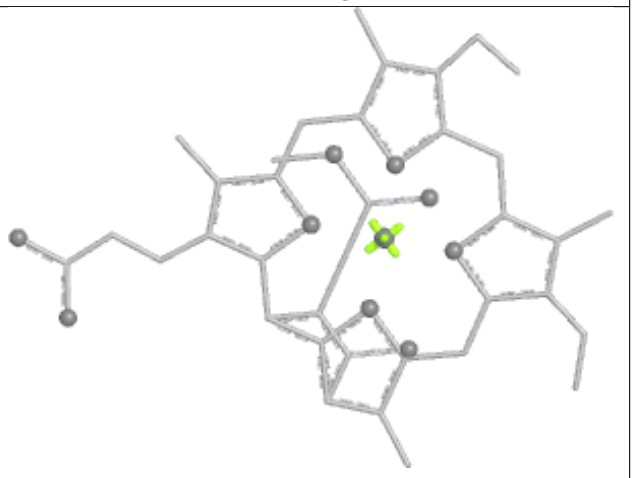
Bond lengths



Bond angles

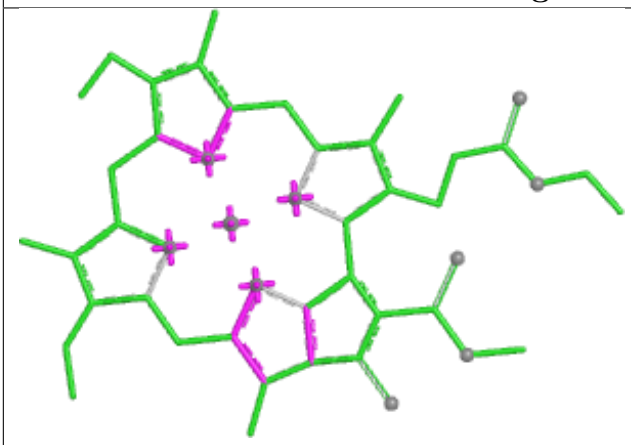


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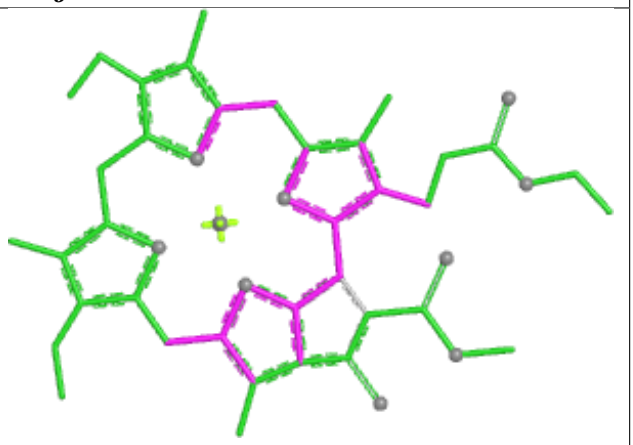


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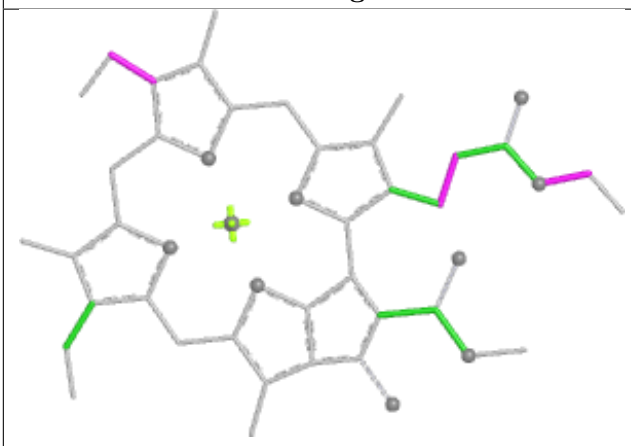
Ligand CLA j 102



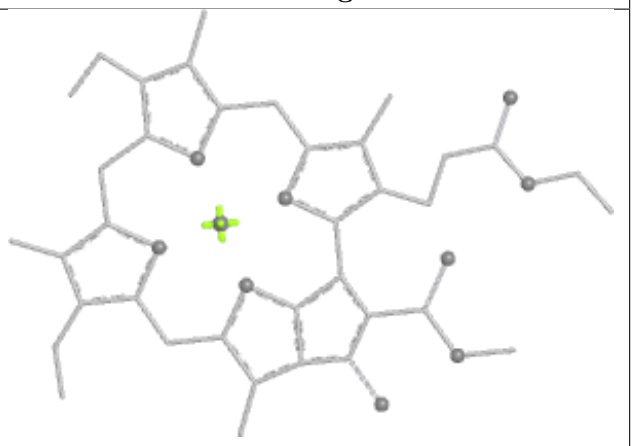
Bond lengths



Bond angles



Torsions



Rings

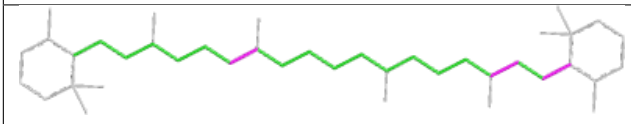
Ligand BCR l 206



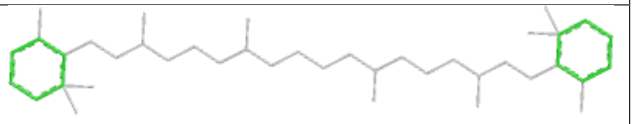
Bond lengths



Bond angles

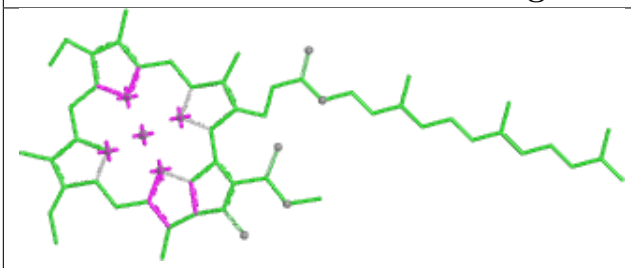


Torsions

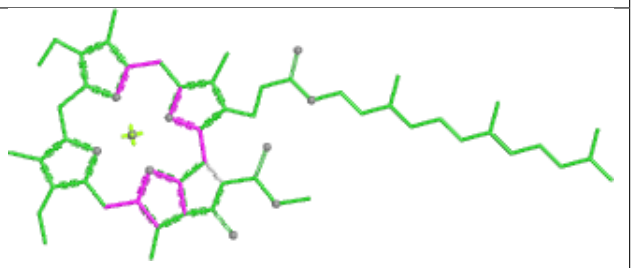


Rings

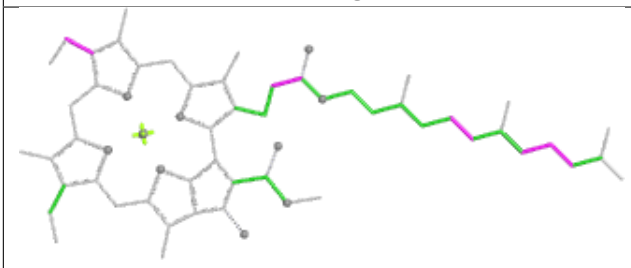
Ligand CLA x 308



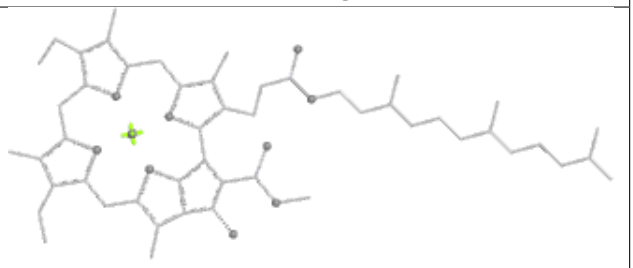
Bond lengths



Bond angles

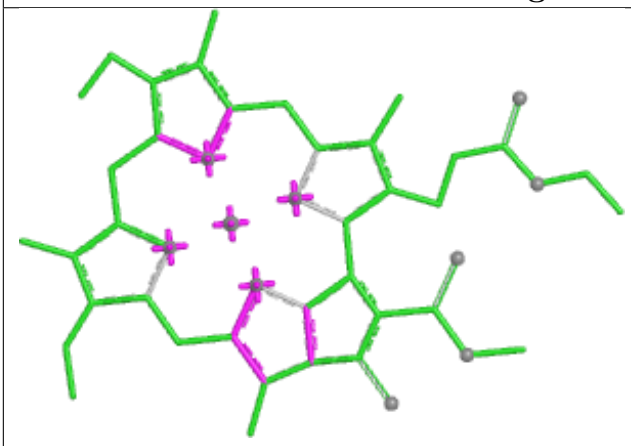


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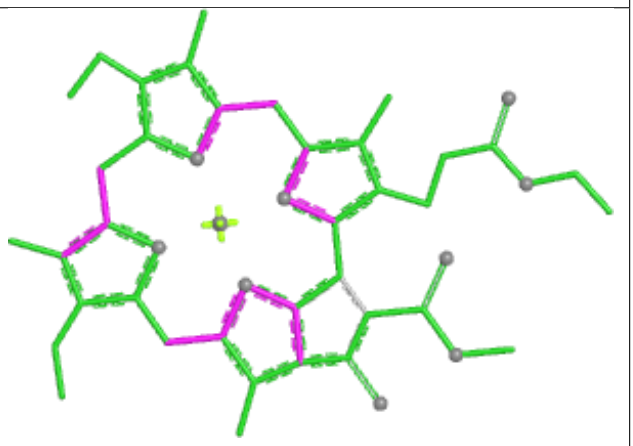


Rings

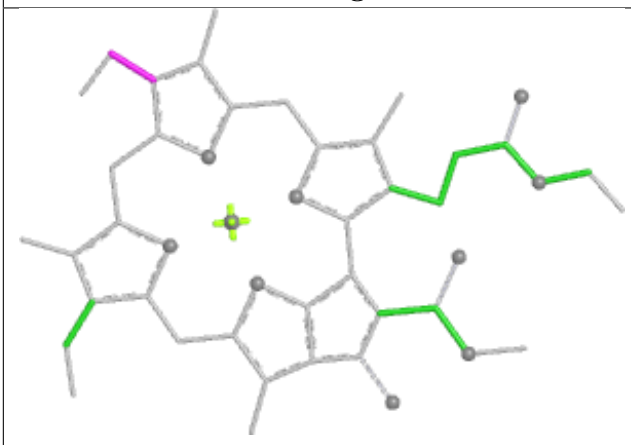
Ligand CLA J 309



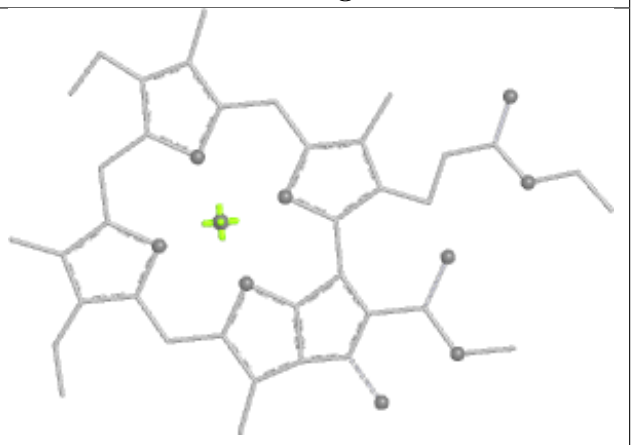
Bond lengths



Bond angles

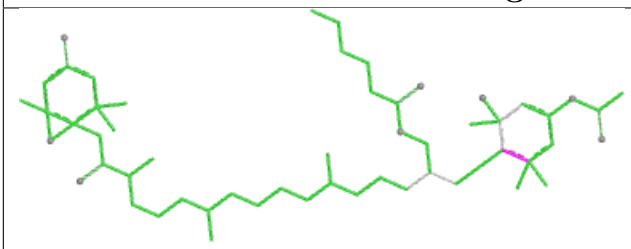


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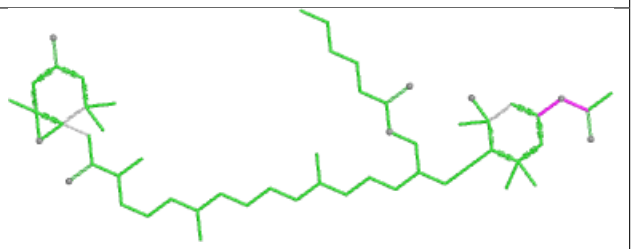


Rings

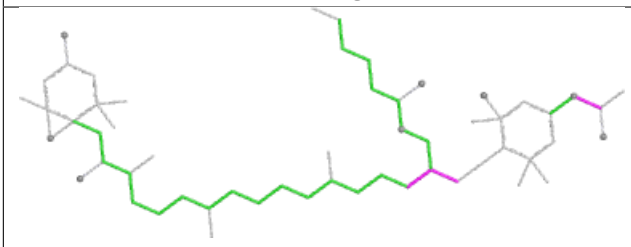
Ligand A1EB1 T 316



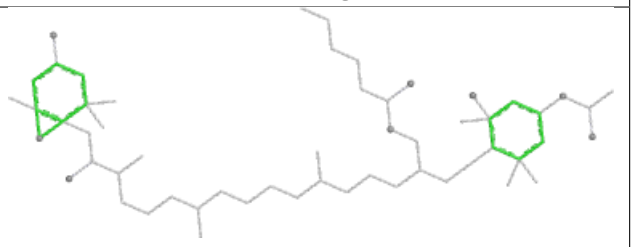
Bond lengths



Bond angles

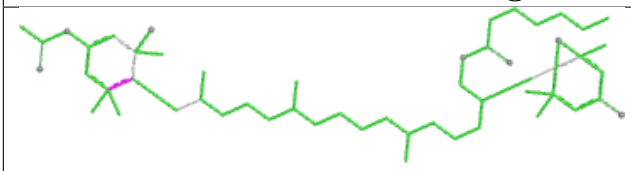


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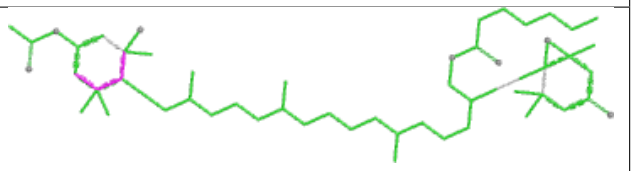


Rings

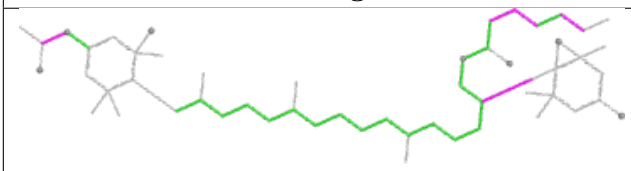
Ligand A1EB4 P 320



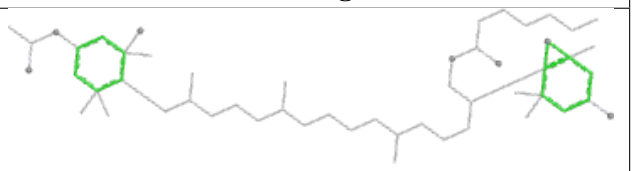
Bond lengths



Bond angles

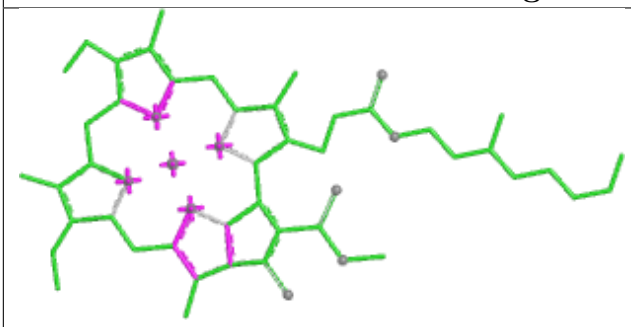


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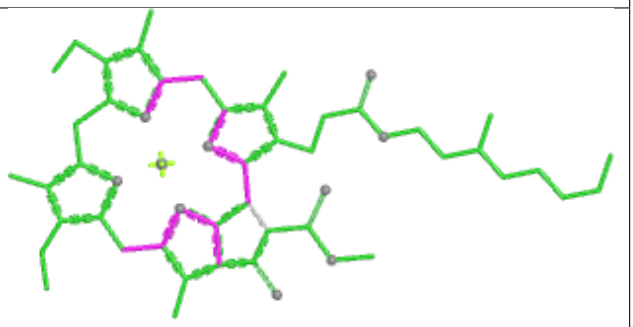


Rings

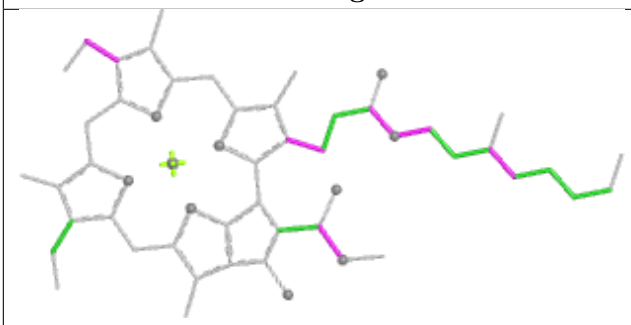
Ligand CLA K 307



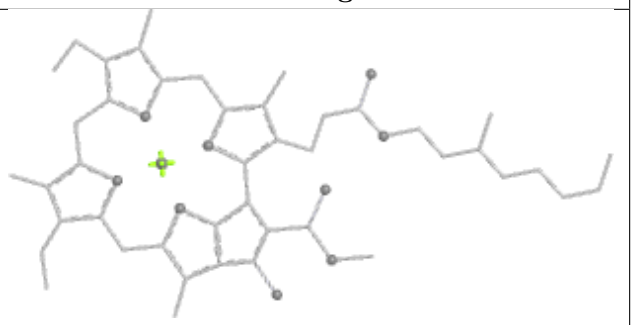
Bond lengths



Bond angles

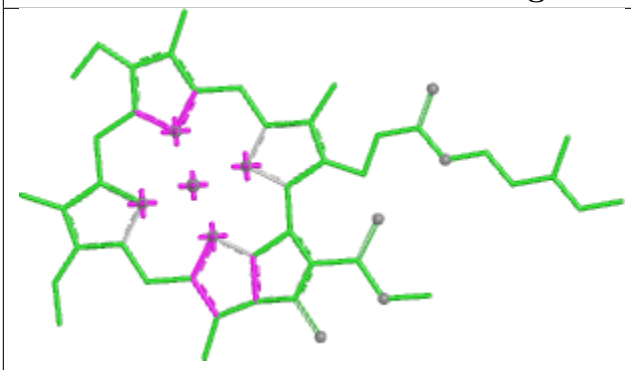


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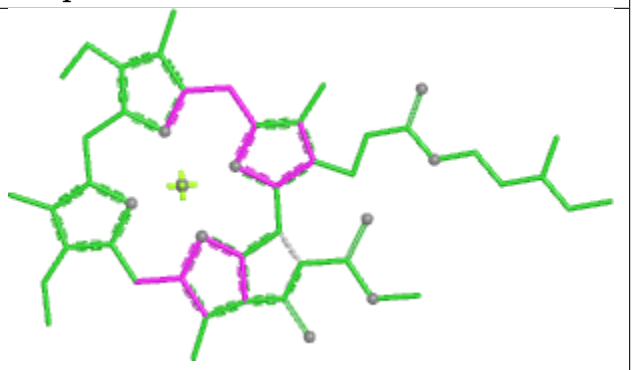


Rings

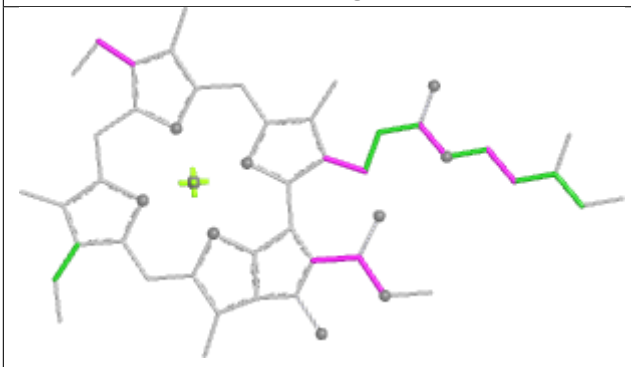
Ligand CLA q 310



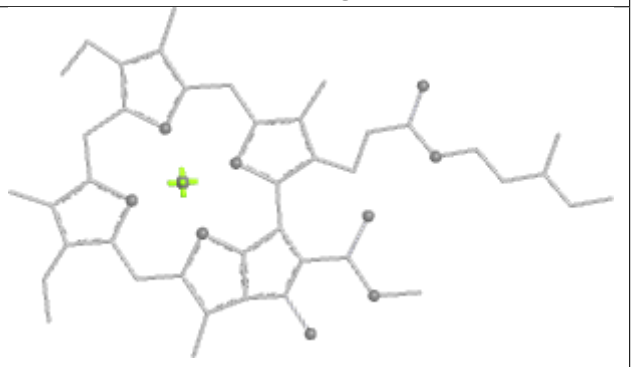
Bond lengths



Bond angles

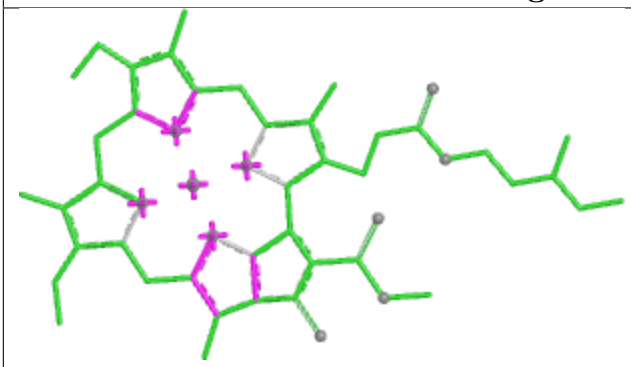


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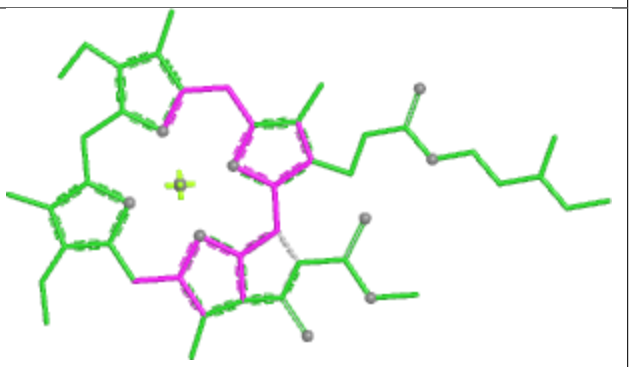


Rings

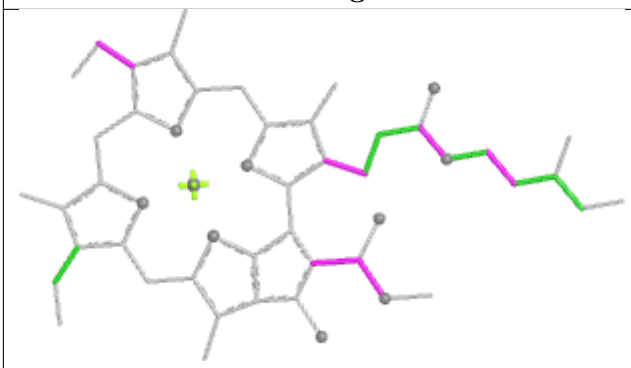
Ligand CLA v 310



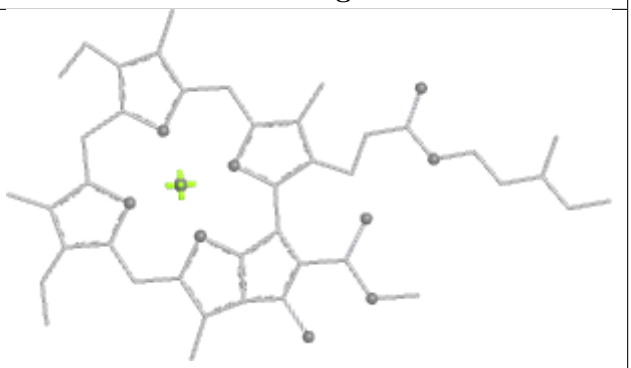
Bond lengths



Bond angles

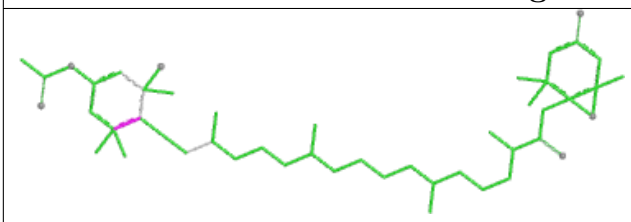


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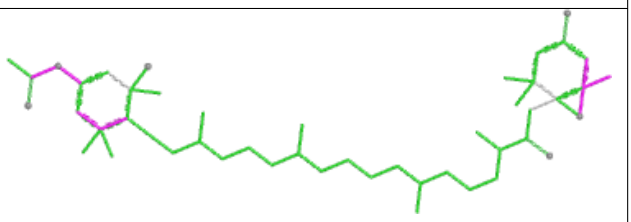


Rings

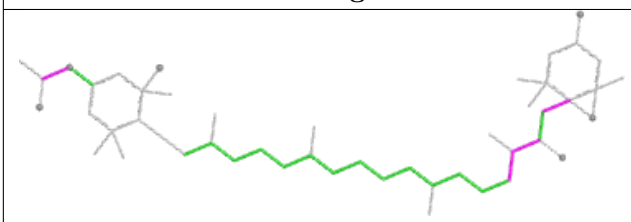
Ligand A86 X 319



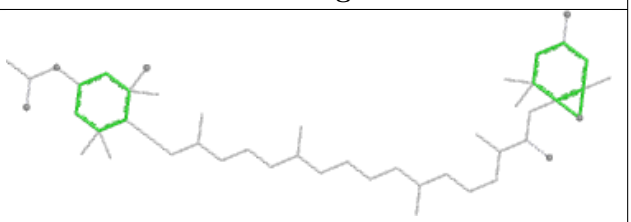
Bond lengths



Bond angles

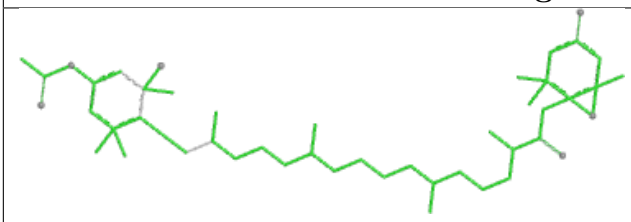


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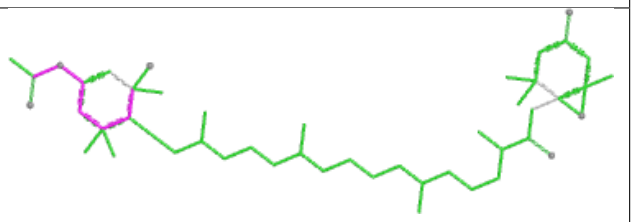


Rings

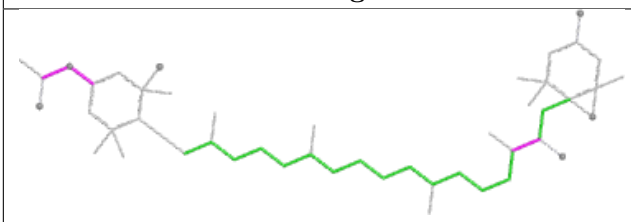
Ligand A86 z 315



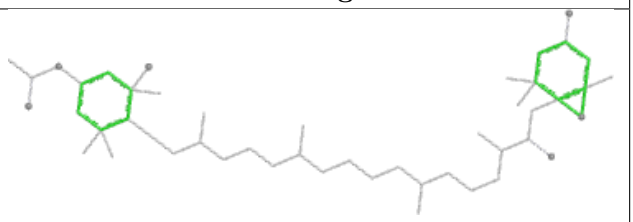
Bond lengths



Bond angles

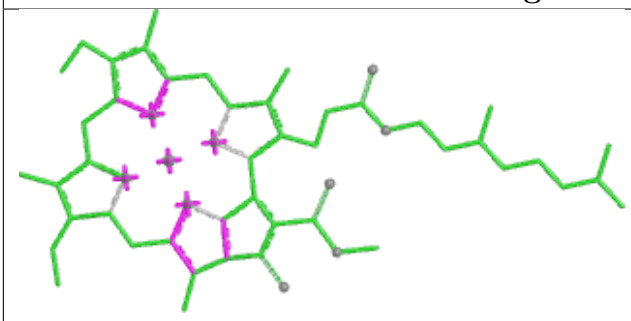


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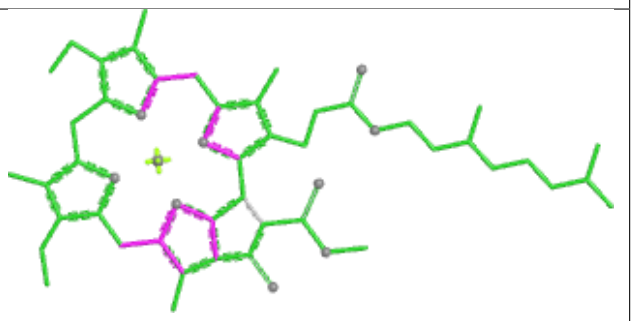


Rings

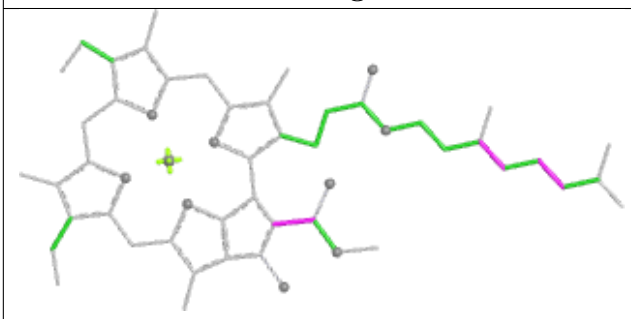
Ligand CLA R 307



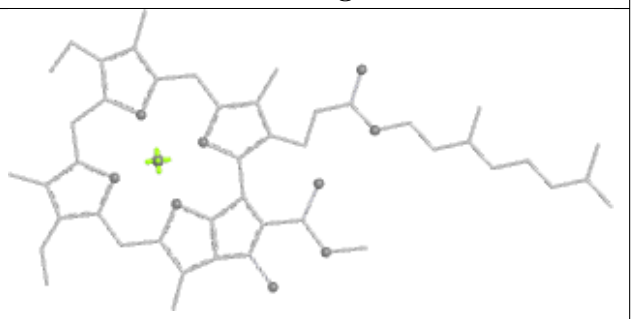
Bond lengths



Bond angles

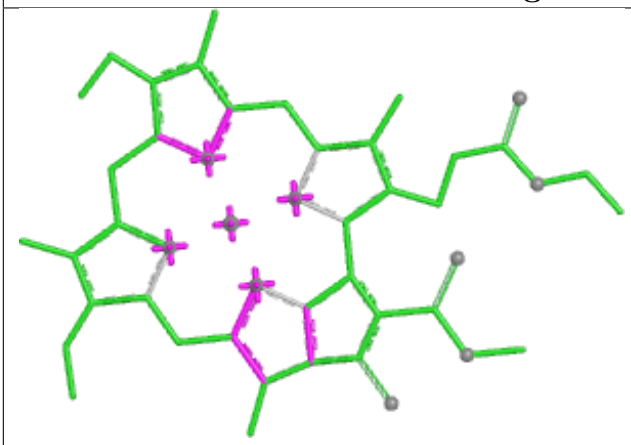


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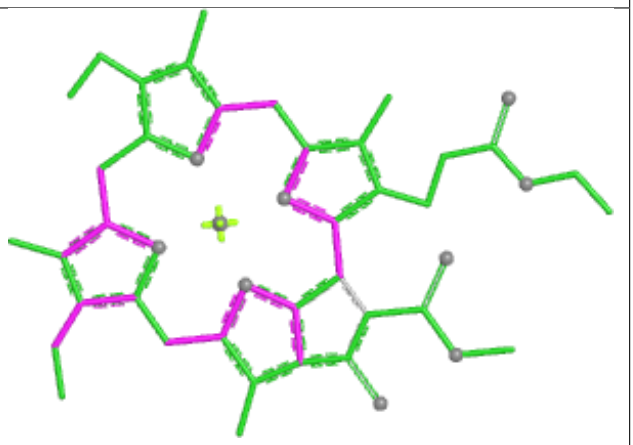


Rings

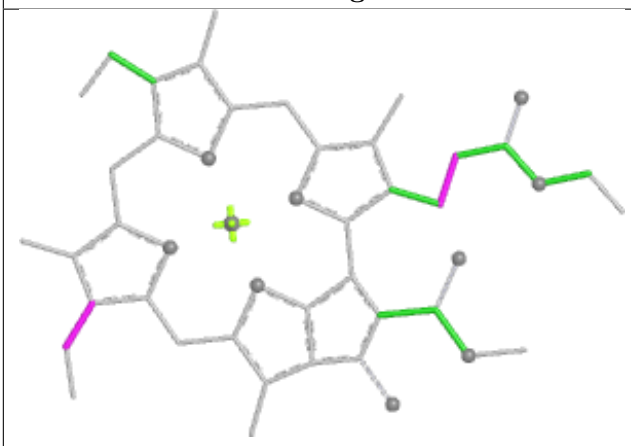
Ligand CLA A 301



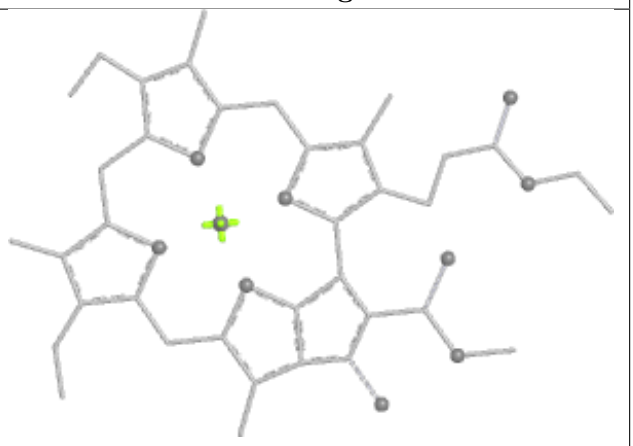
Bond lengths



Bond angles

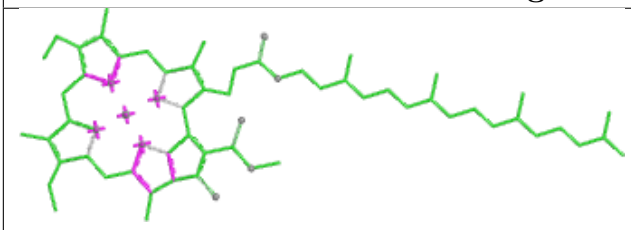


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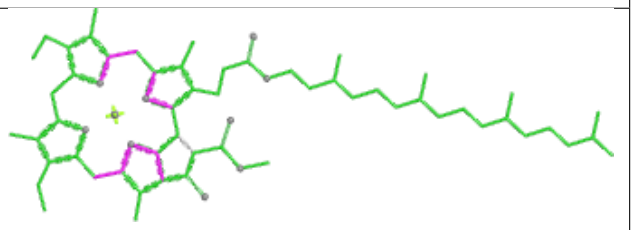


Rings

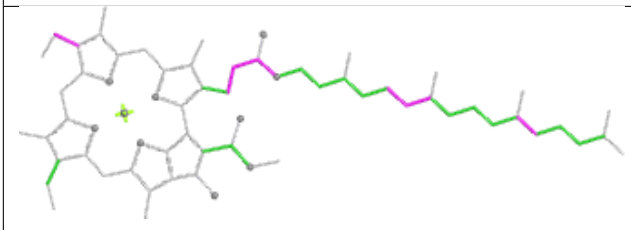
Ligand CLA b 814



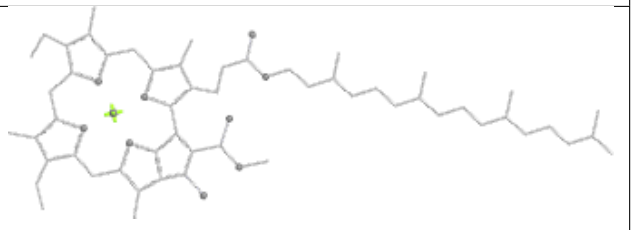
Bond lengths



Bond angles

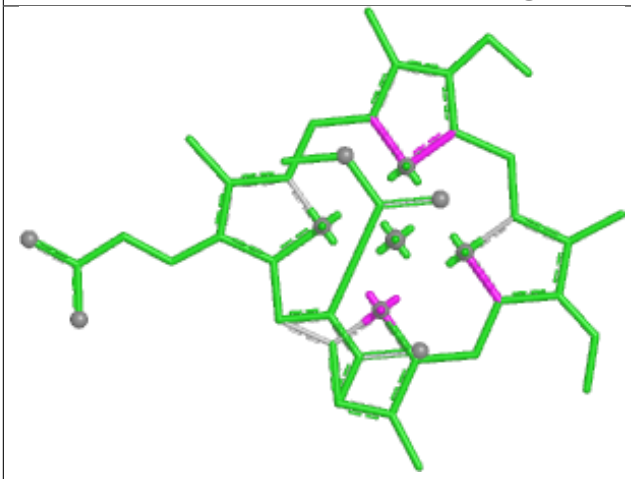


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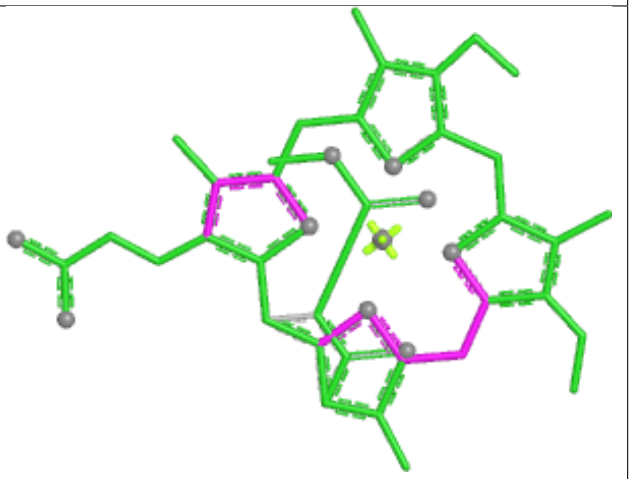


Rings

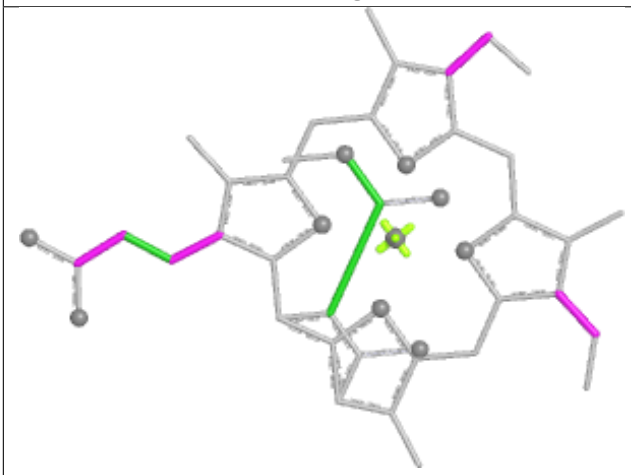
Ligand KC2 W 309



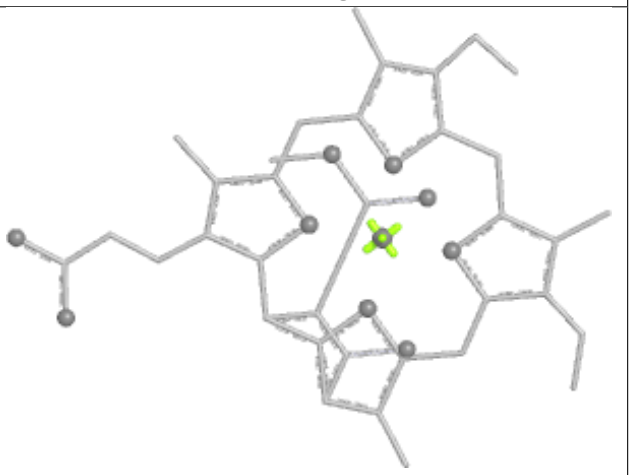
Bond lengths



Bond angles

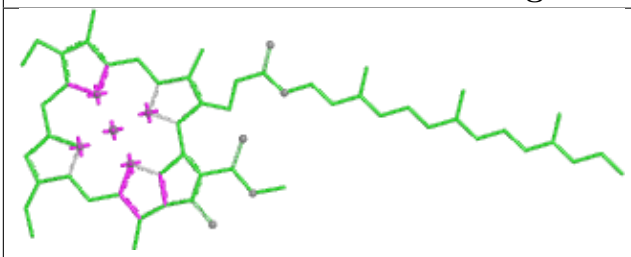


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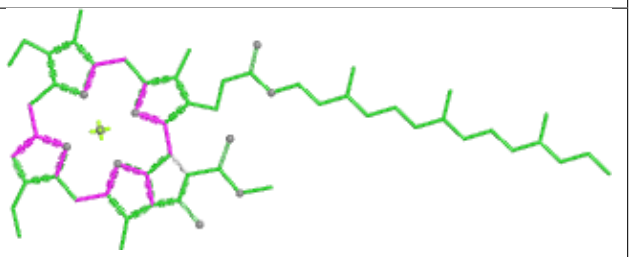


Rings

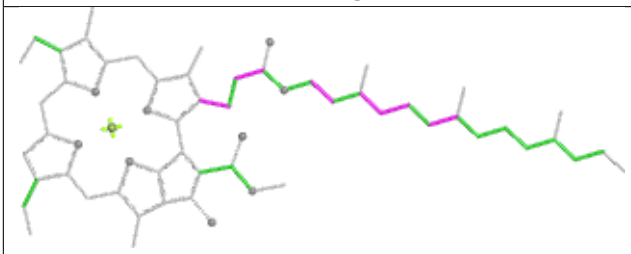
Ligand CLA F 303



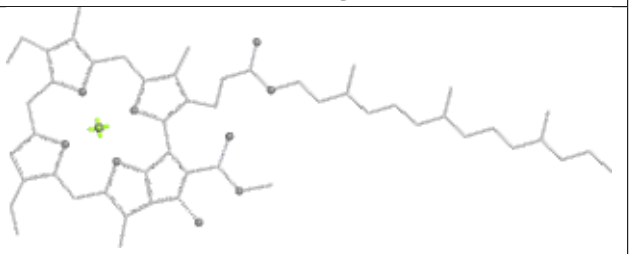
Bond lengths



Bond angles

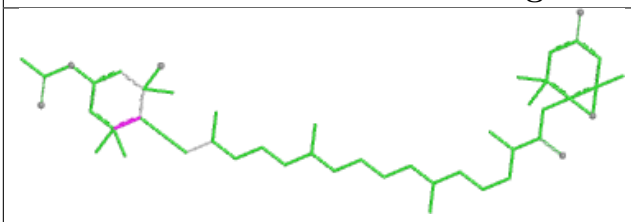


Torsions

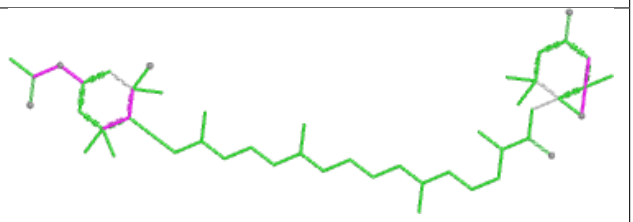


Rings

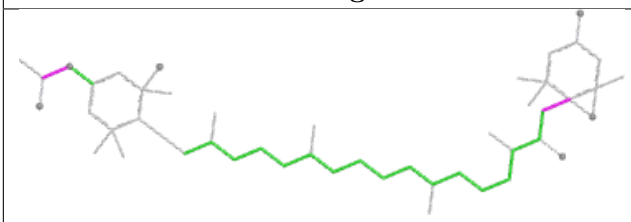
Ligand A86 M 313



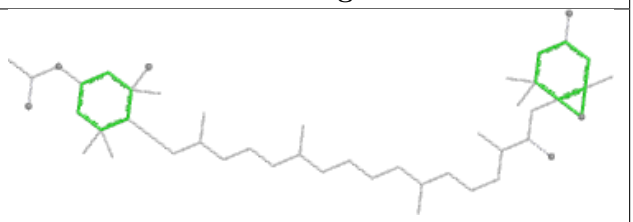
Bond lengths



Bond angles

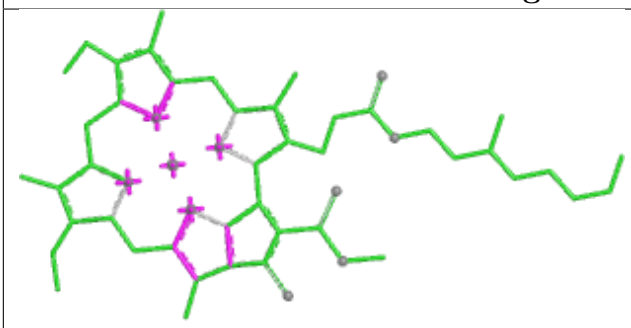


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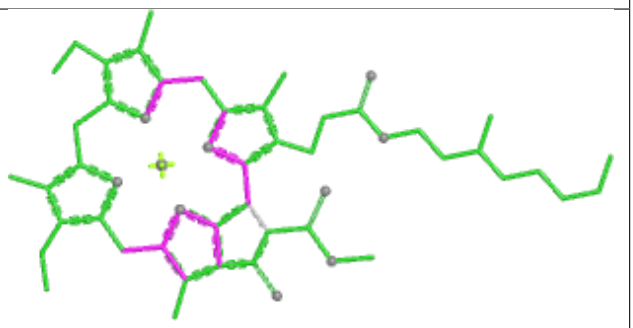


Rings

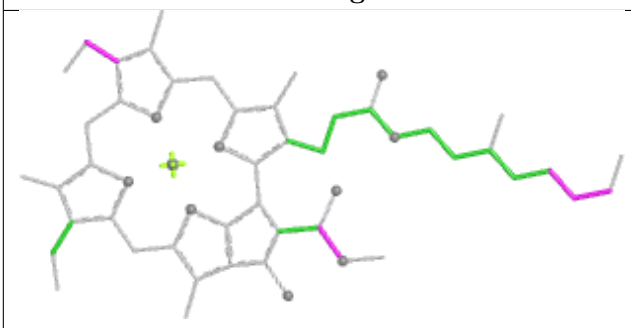
Ligand CLA G 207



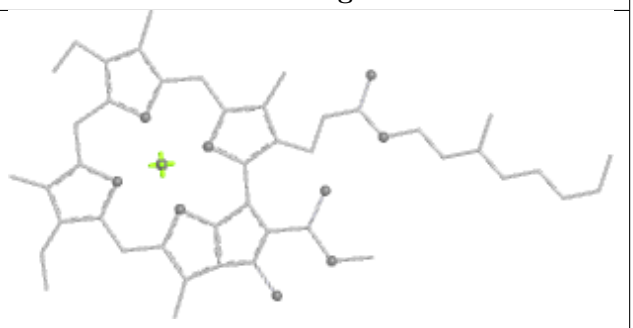
Bond lengths



Bond angles

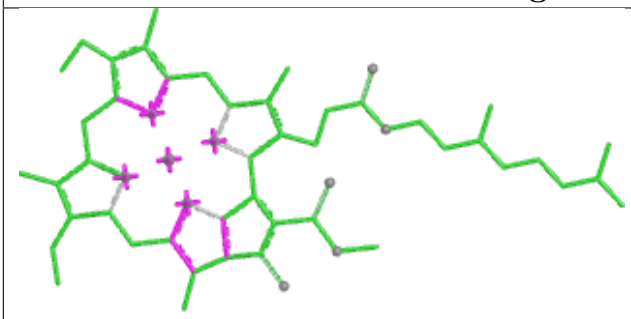


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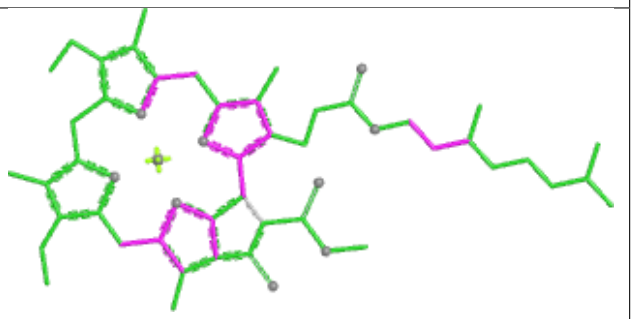


Rings

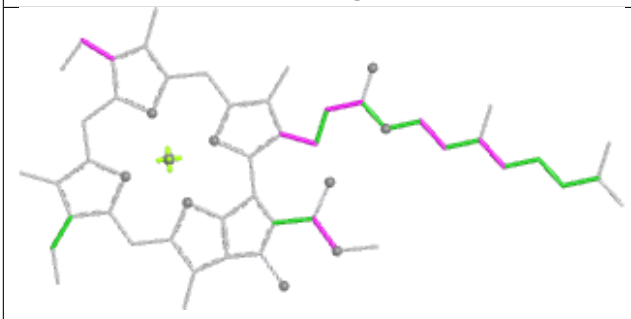
Ligand CLA z 311



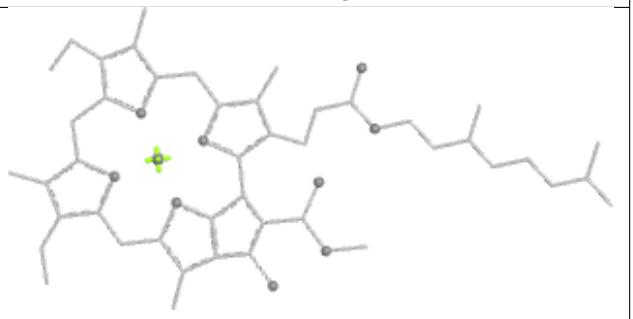
Bond lengths



Bond angles

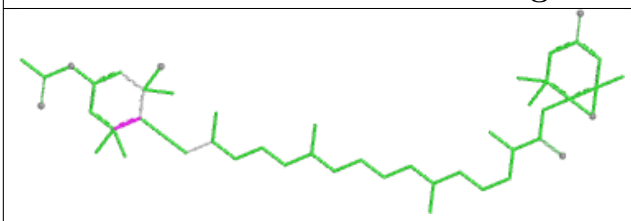


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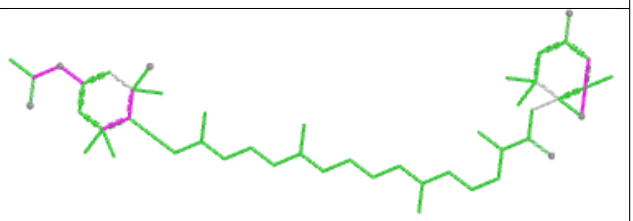


Rings

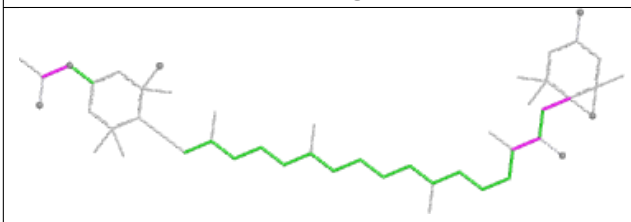
Ligand A86 P 316



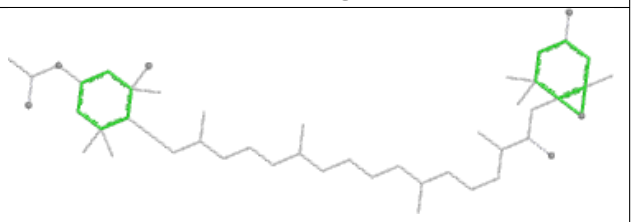
Bond lengths



Bond angles

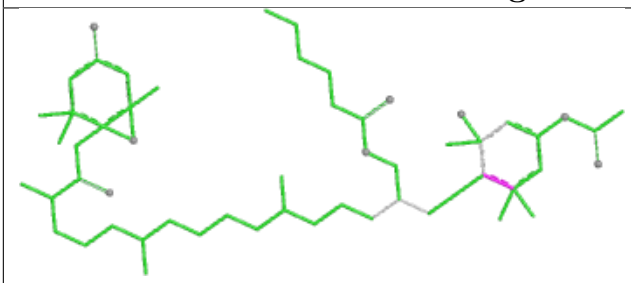


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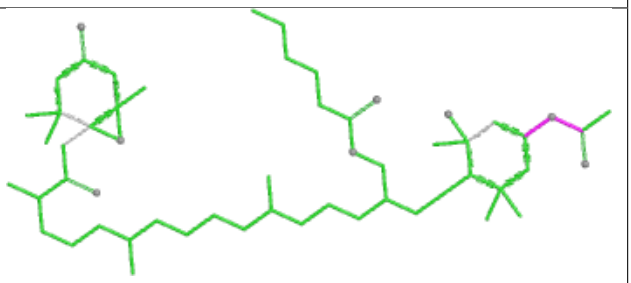


Rings

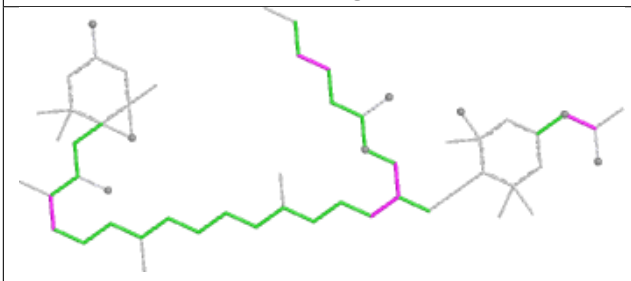
Ligand A1EB1 S 321



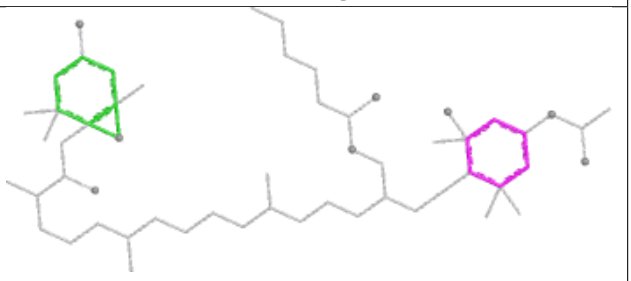
Bond lengths



Bond angles

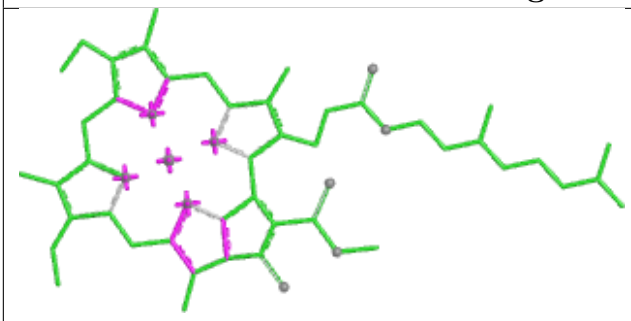


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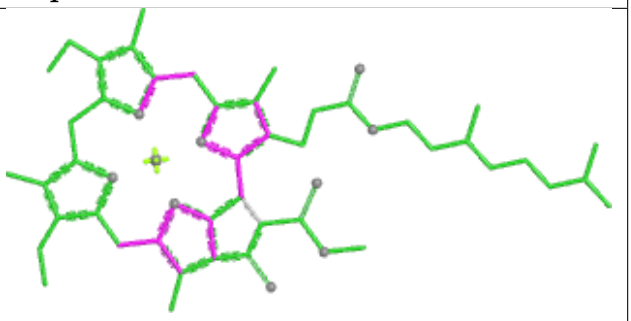


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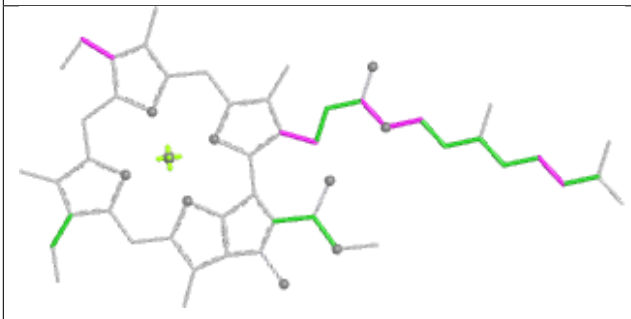
Ligand CLA p 307



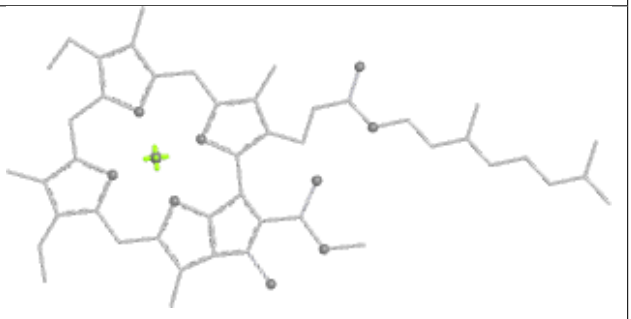
Bond lengths



Bond angles

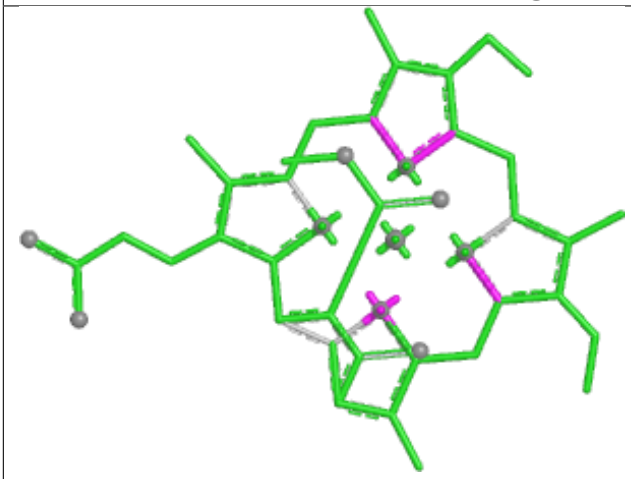


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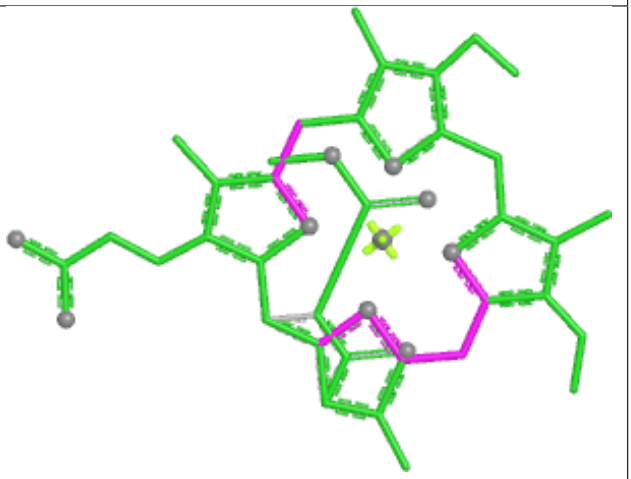


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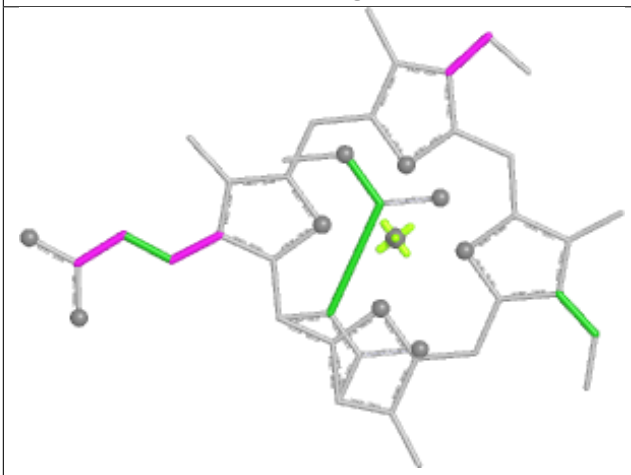
Ligand KC2 F 309



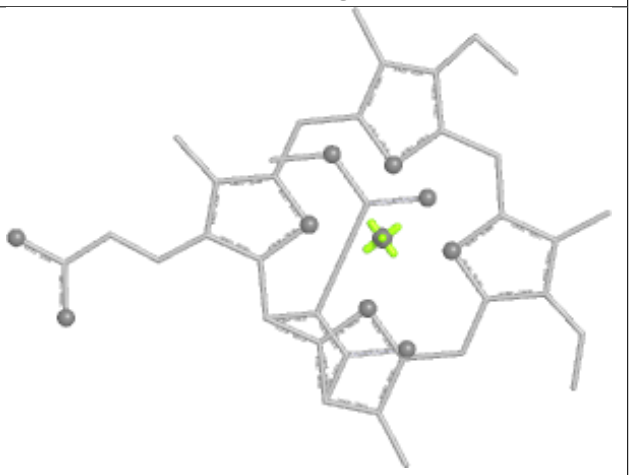
Bond lengths



Bond angles

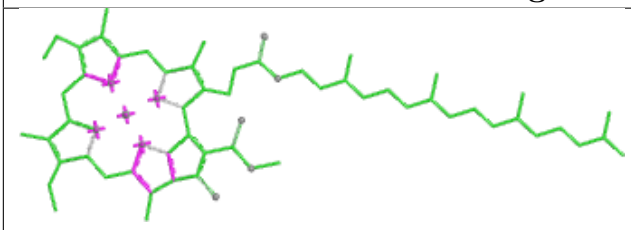


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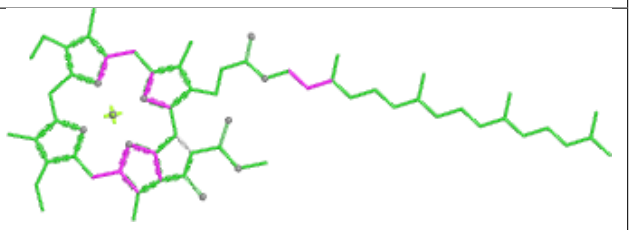


Rings

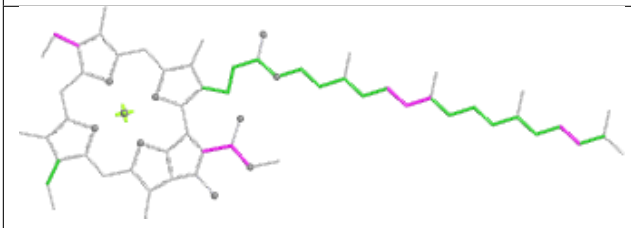
Ligand CLA a 841



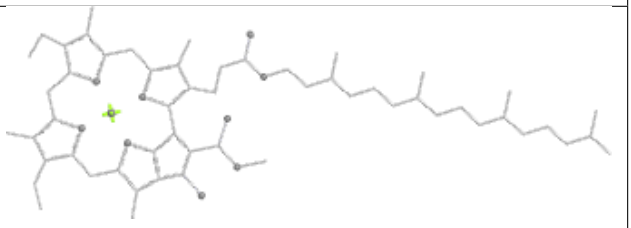
Bond lengths



Bond angles

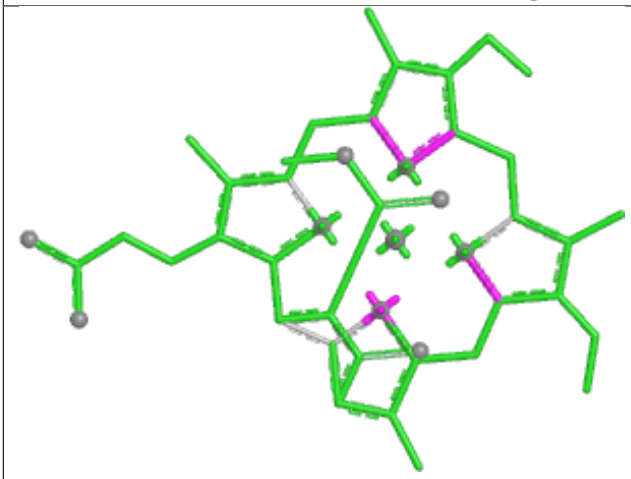


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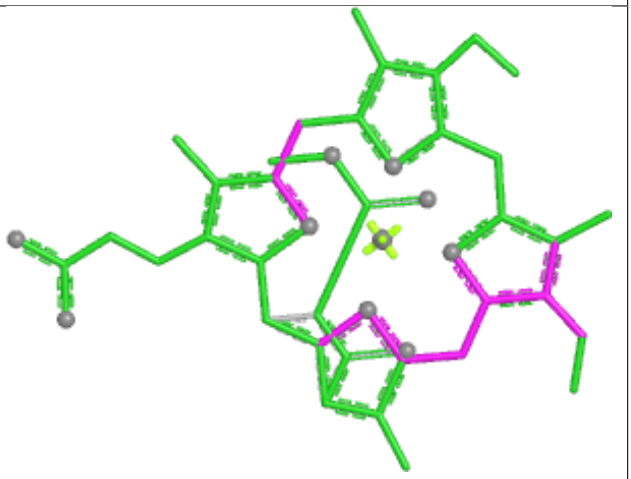


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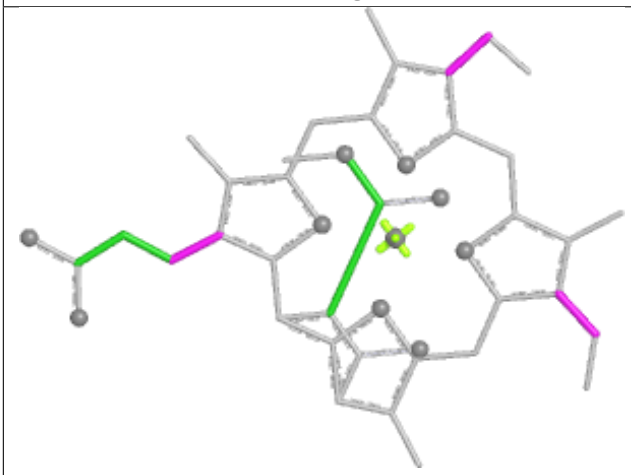
Ligand KC2 N 303



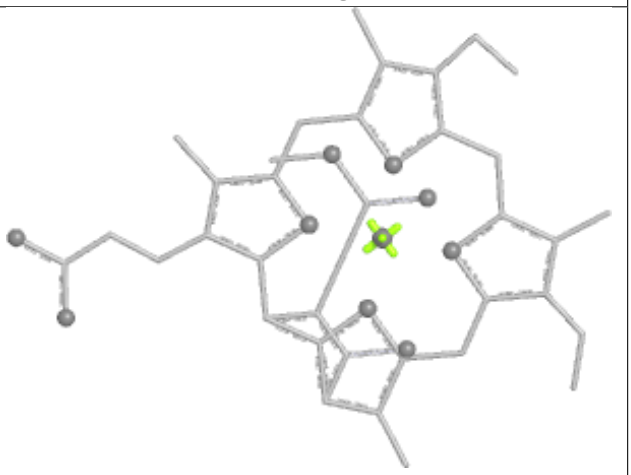
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Bond angles

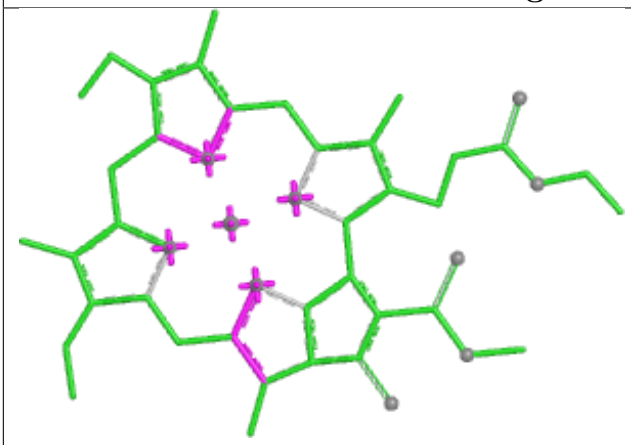


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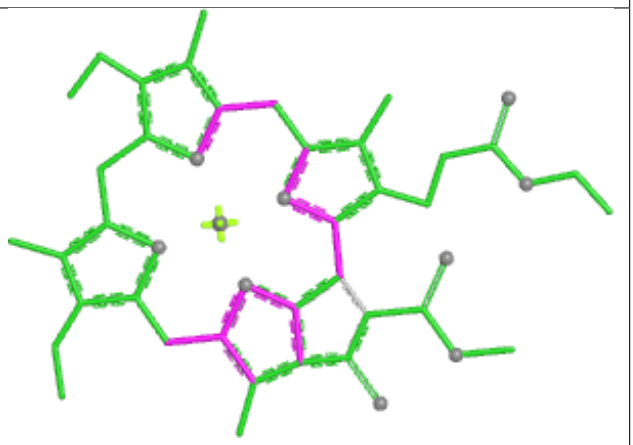


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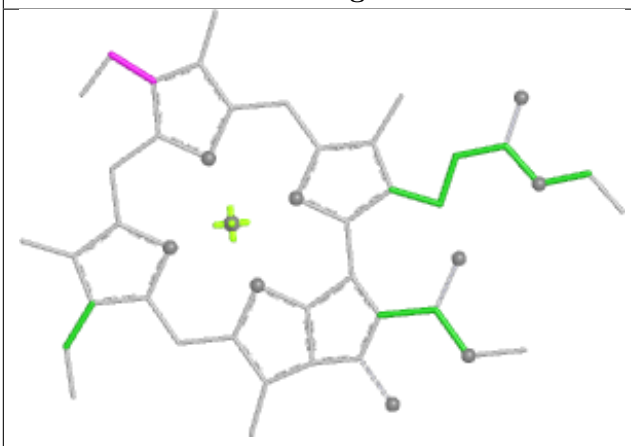
Ligand CLA L 301



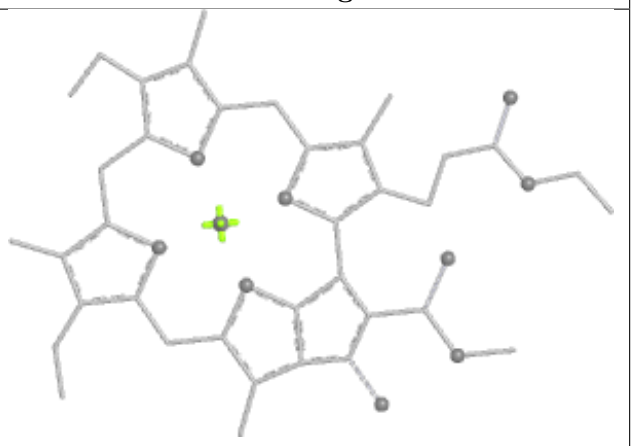
Bond lengths



Bond angles

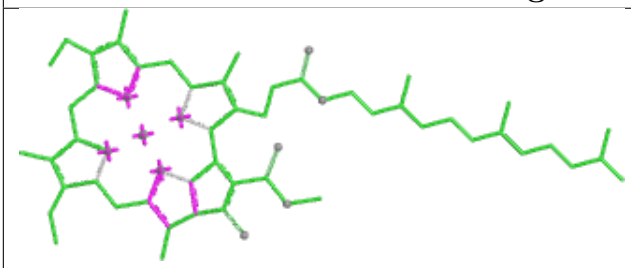


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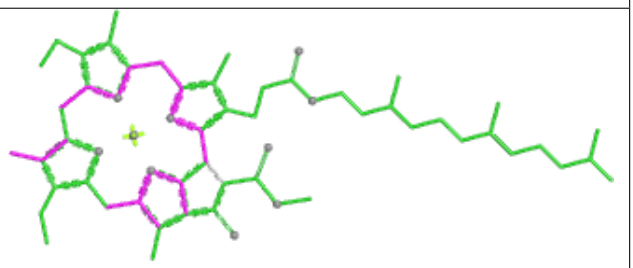


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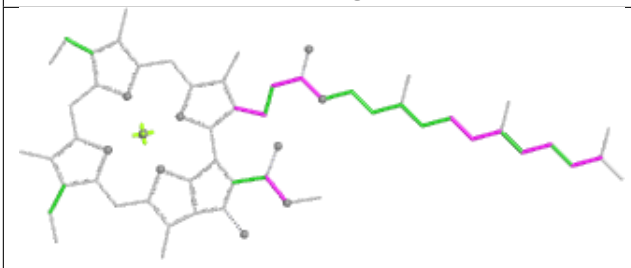
Ligand CLA v 307



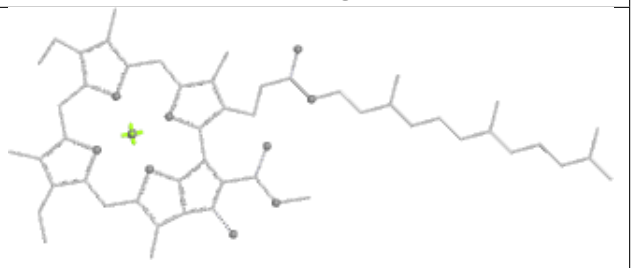
Bond lengths



Bond angles

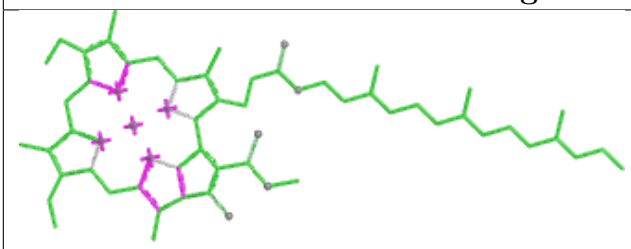


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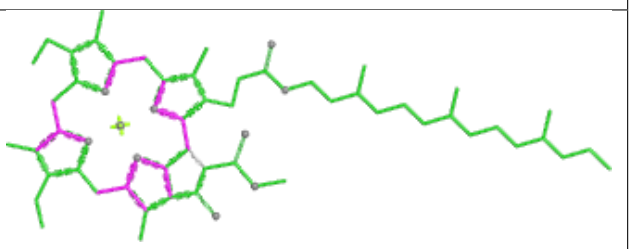


Rings

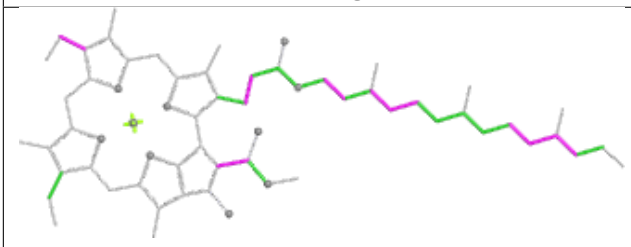
Ligand CLA M 311



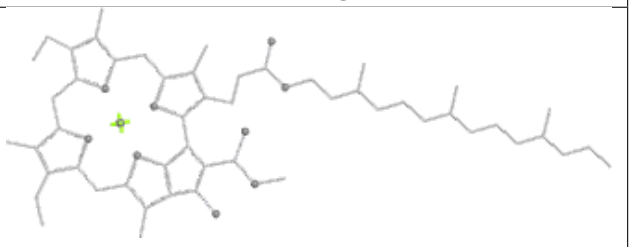
Bond lengths



Bond angles

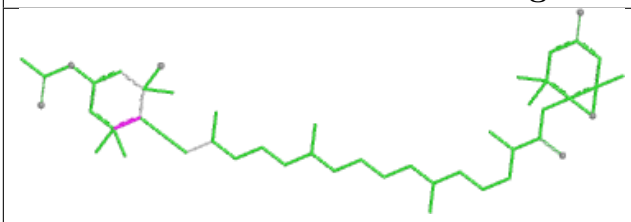


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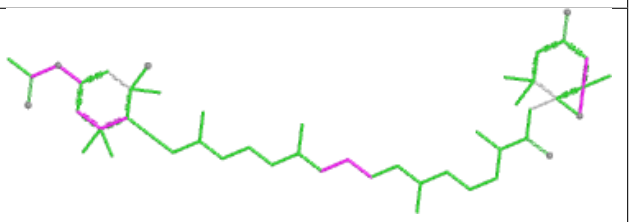


Rings

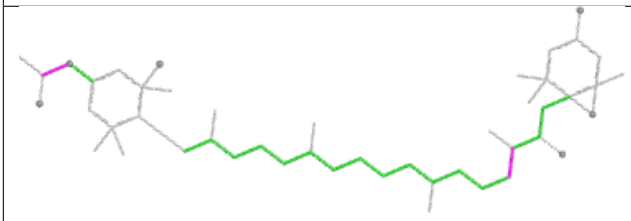
Ligand A86 X 314



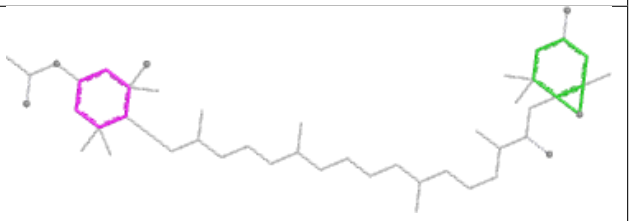
Bond lengths



Bond angles

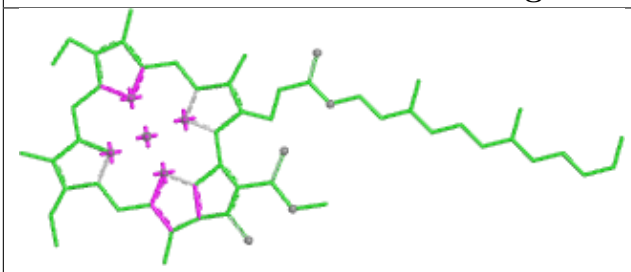


Torsions

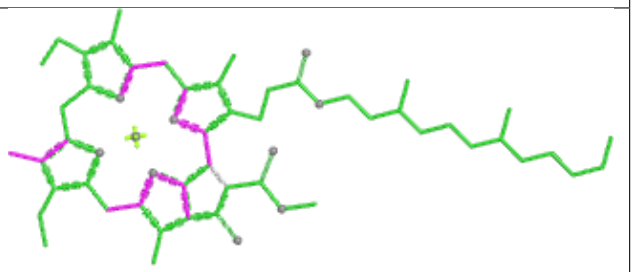


Rings

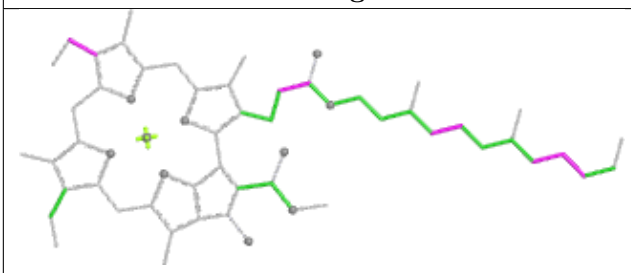
Ligand CLA P 307



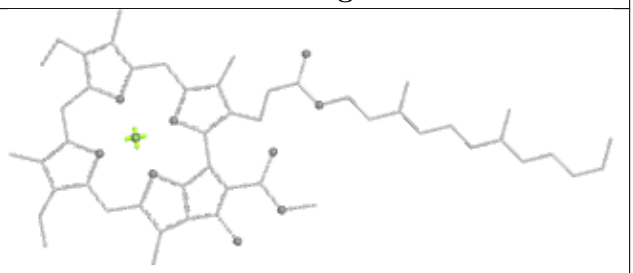
Bond lengths



Bond angles

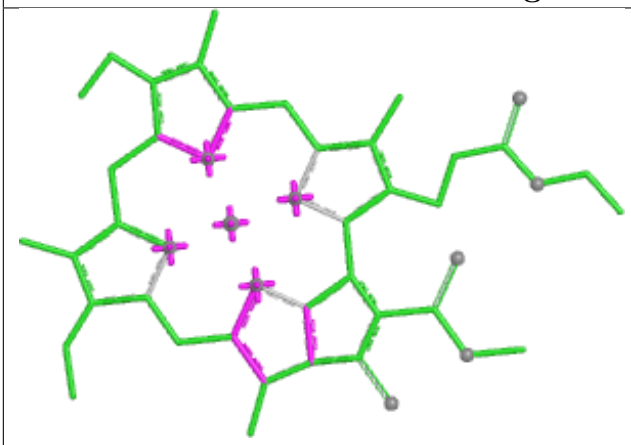


Torsions

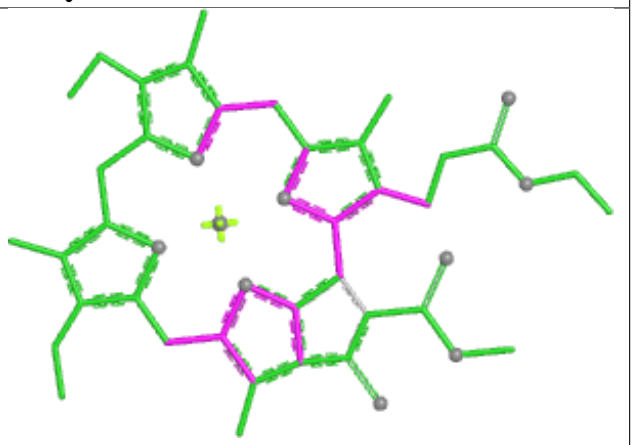


Rings

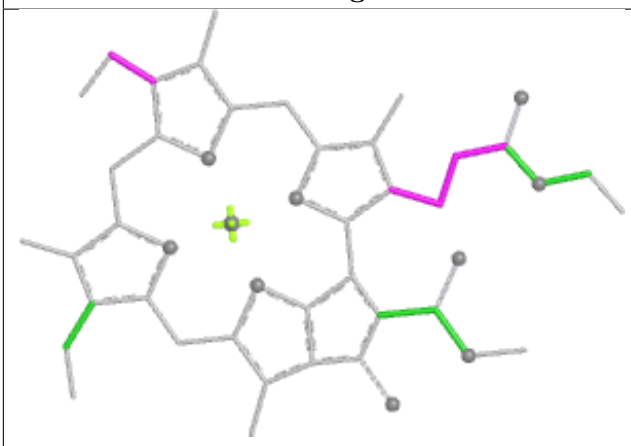
Ligand CLA Q 209



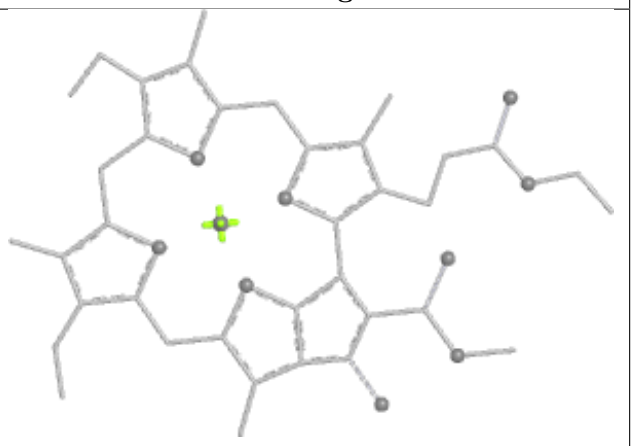
Bond lengths



Bond angles

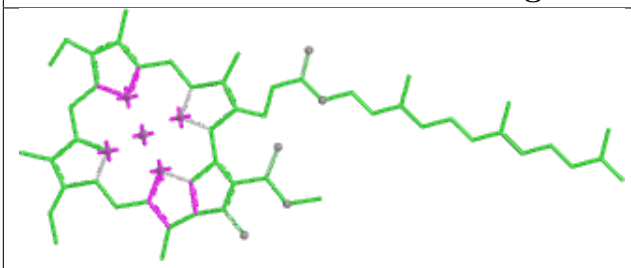


Torsions

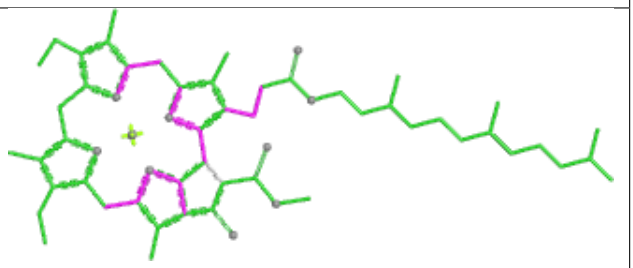


Rings

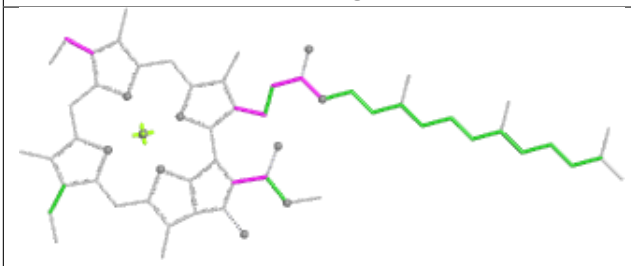
Ligand CLA w 304



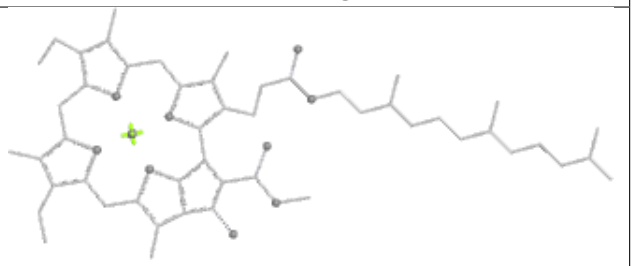
Bond lengths



Bond angles

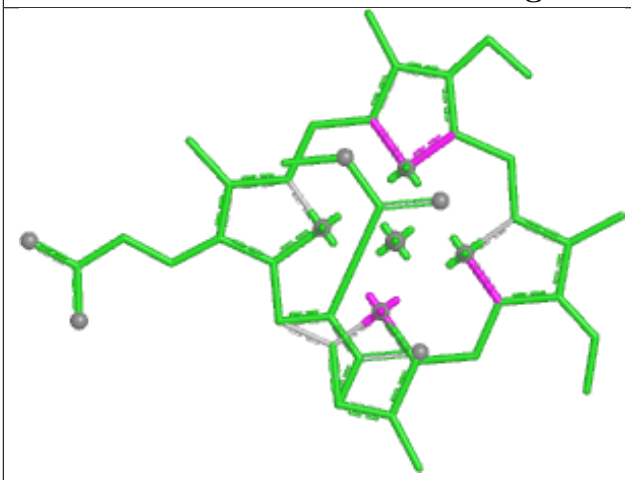


Torsions

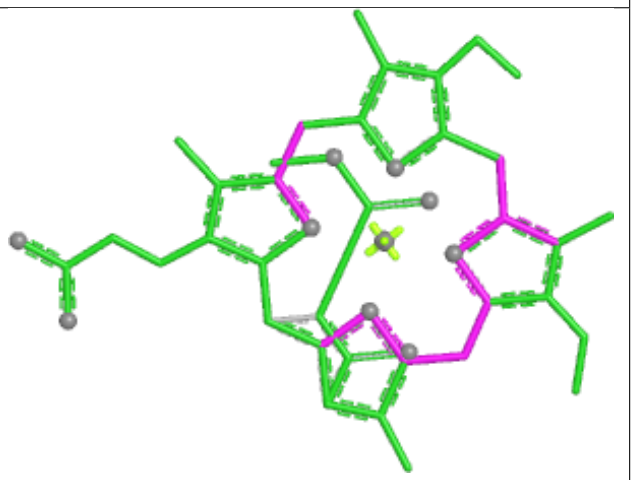


Rings

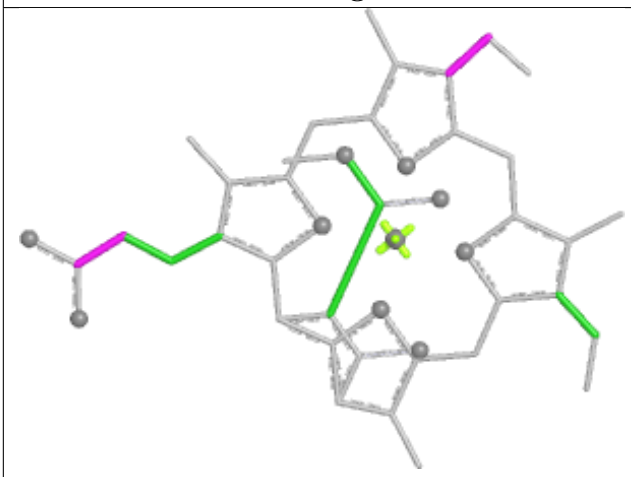
Ligand KC2 H 316



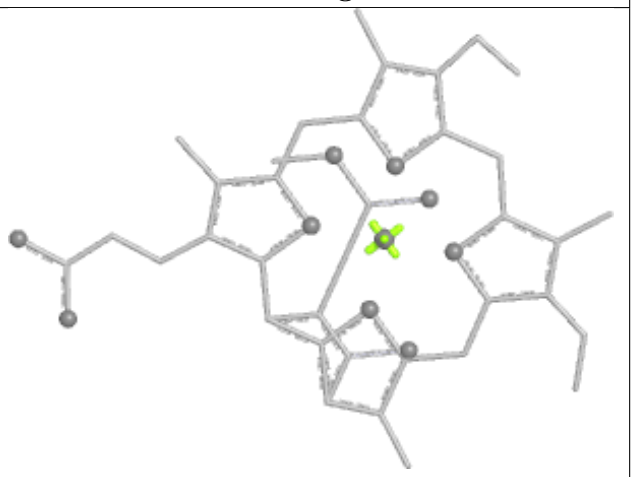
Bond lengths



Bond angles

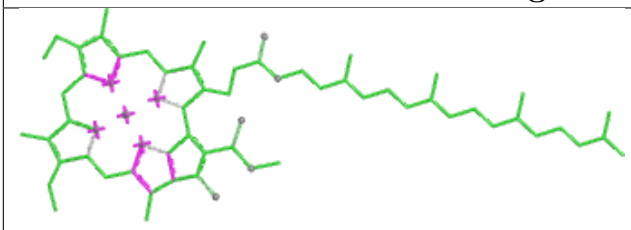


Torsions

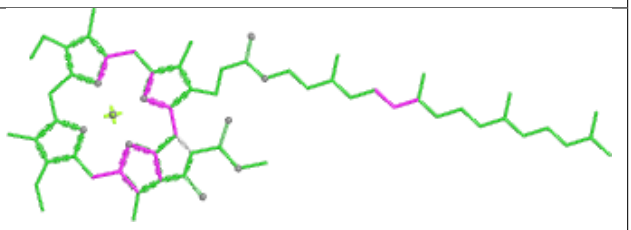


Rings

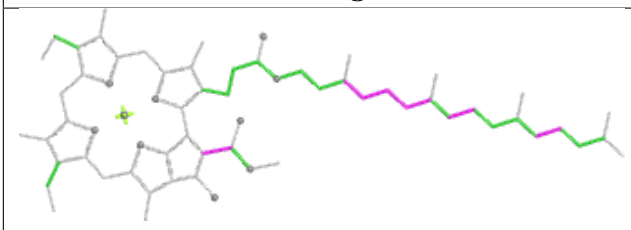
Ligand CLA a 836



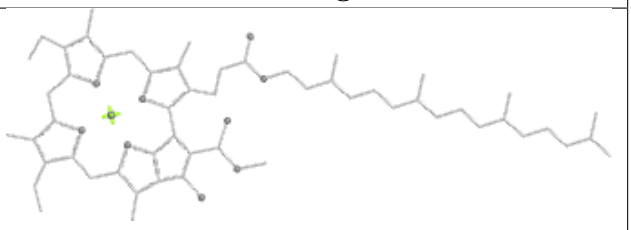
Bond lengths



Bond angles

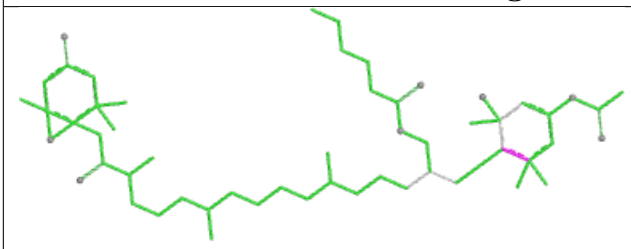


Torsions

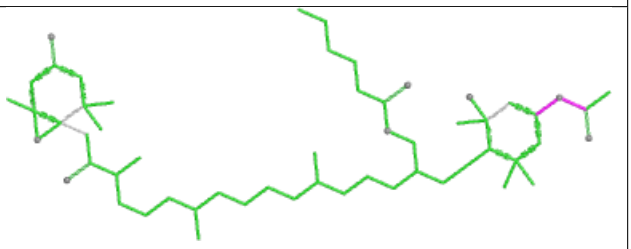


Rings

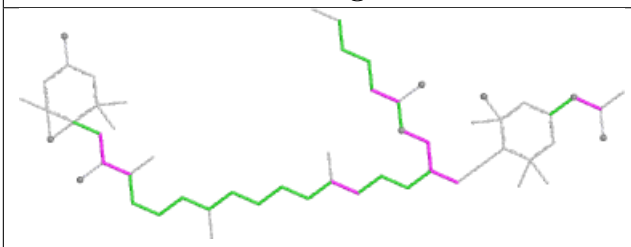
Ligand A1EB1 T 320



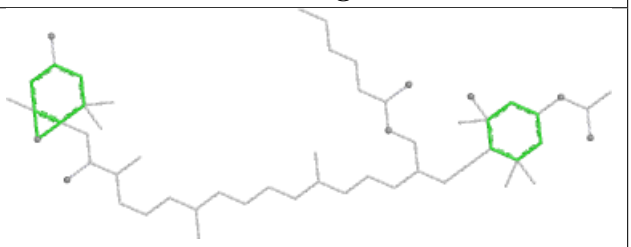
Bond lengths



Bond angles

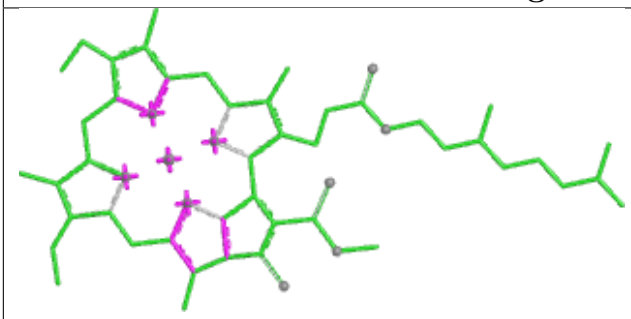


Torsions

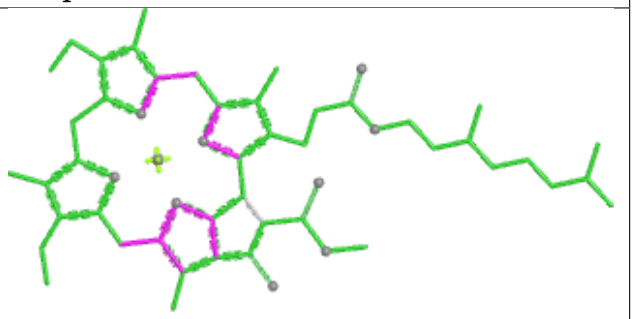


Rings

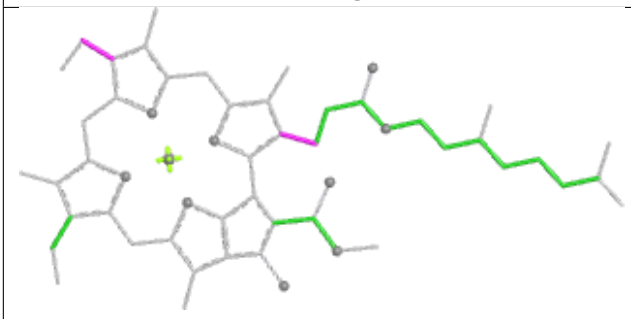
Ligand CLA q 301



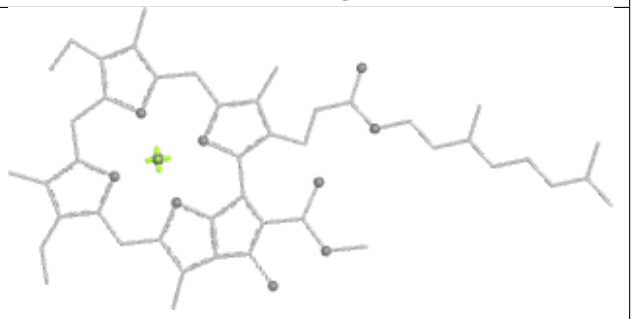
Bond lengths



Bond angles

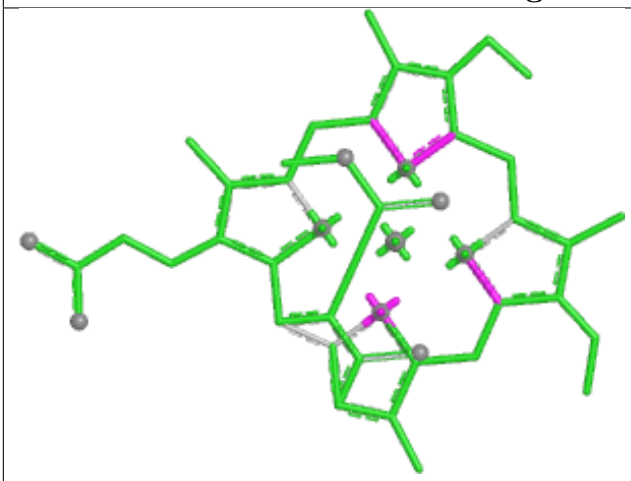


Torsions

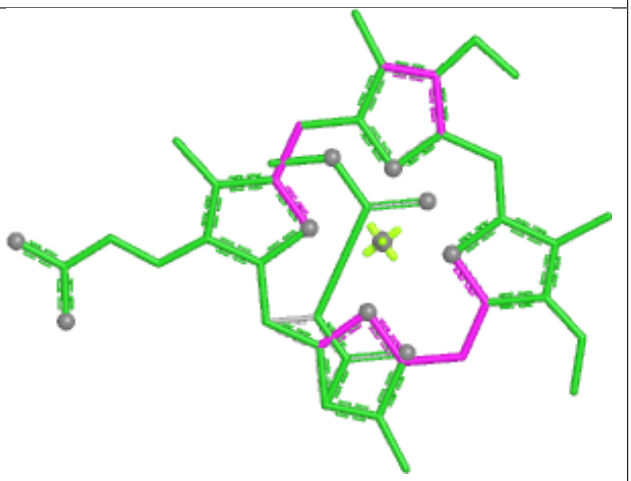


Rings

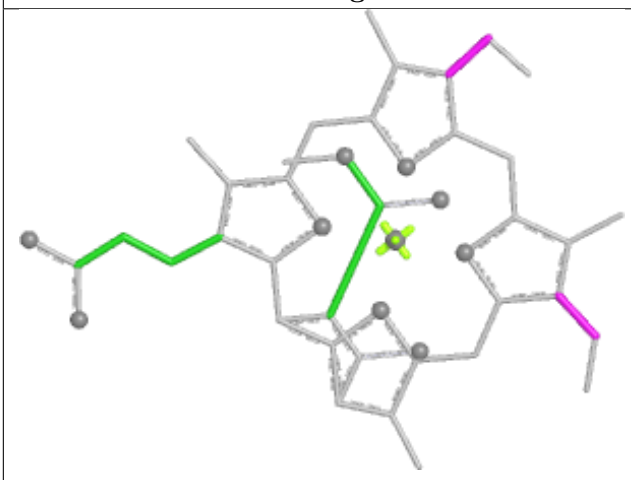
Ligand KC2 R 301



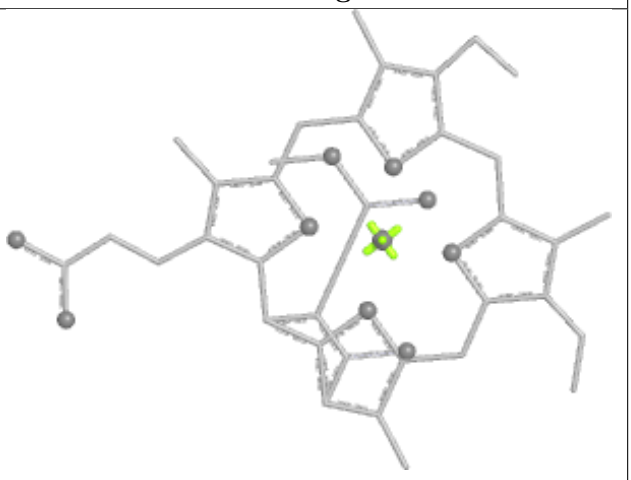
Bond lengths



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.

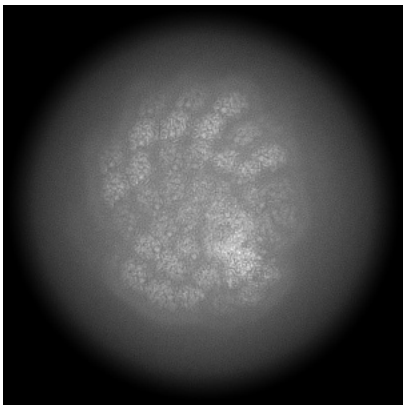
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-64087. These allow visual inspection of the internal detail of the map and identification of artifacts.

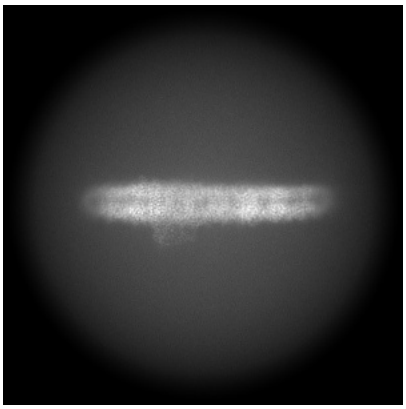
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

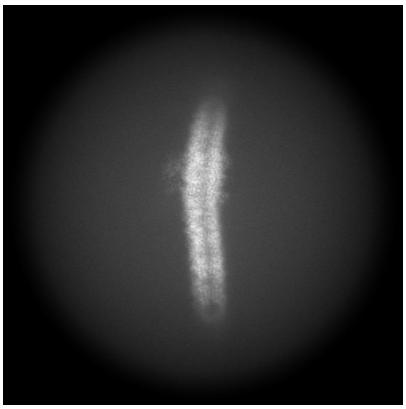
6.1.1 Primary map



X

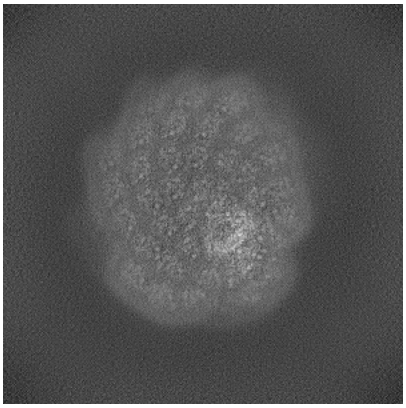


Y

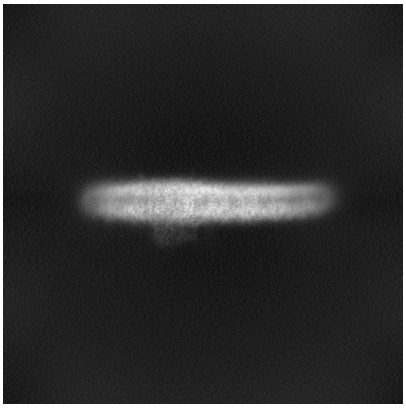


Z

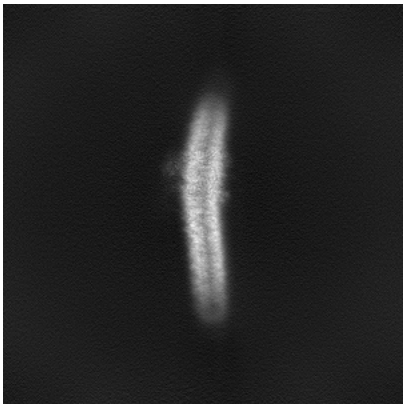
6.1.2 Raw map



X



Y

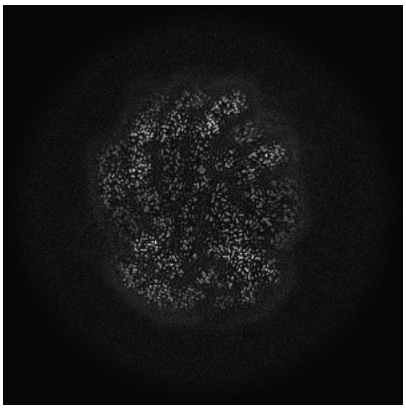


Z

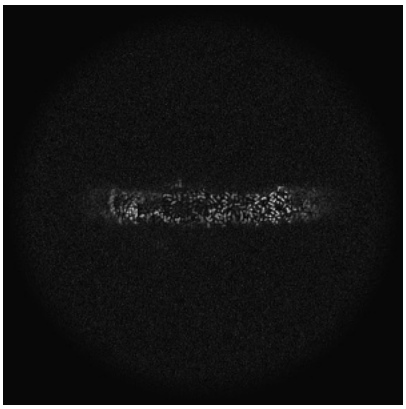
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

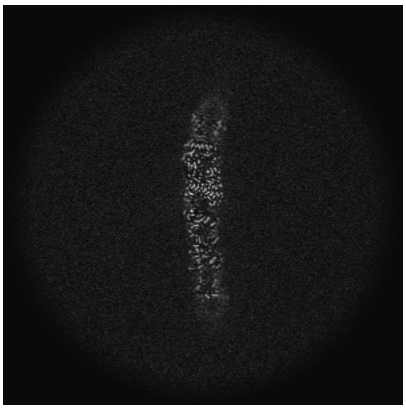
6.2.1 Primary map



X Index: 250

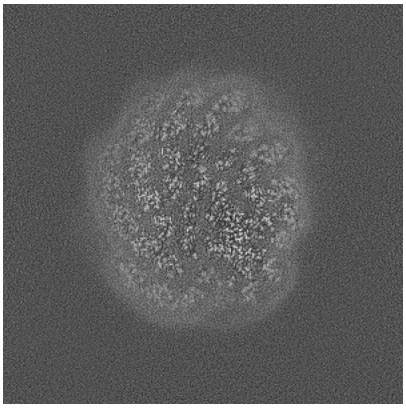


Y Index: 250

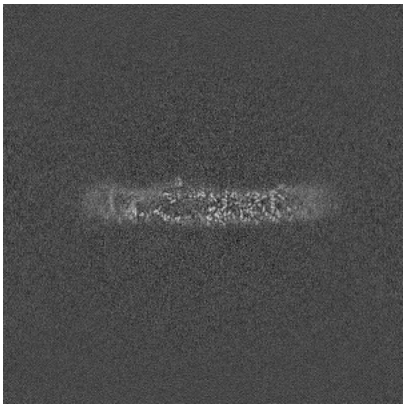


Z Index: 250

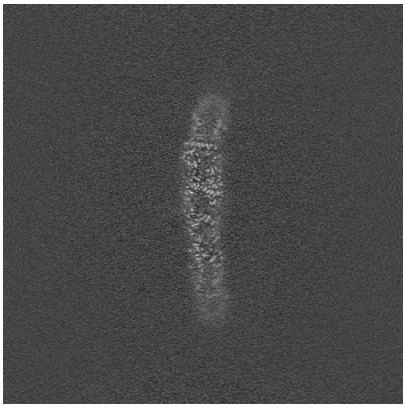
6.2.2 Raw map



X Index: 250



Y Index: 250

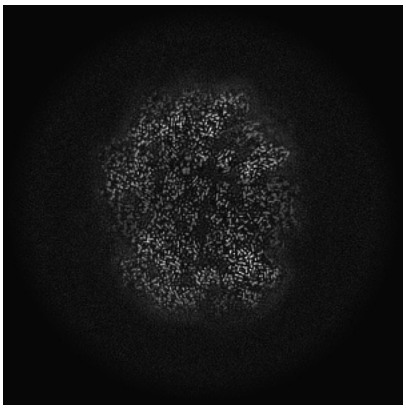


Z Index: 250

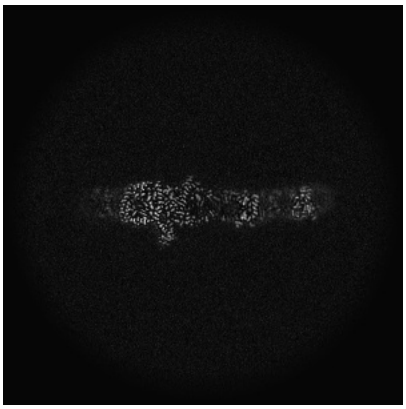
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

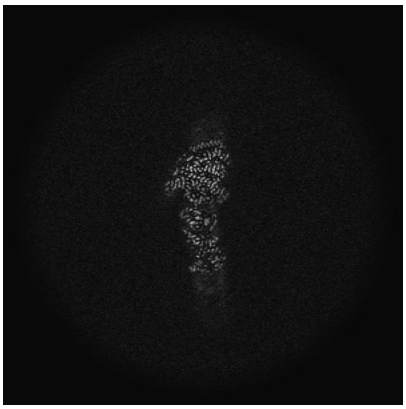
6.3.1 Primary map



X Index: 244

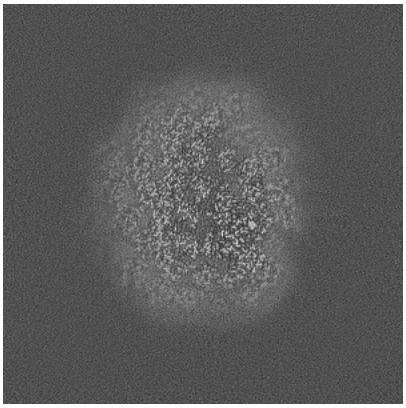


Y Index: 285

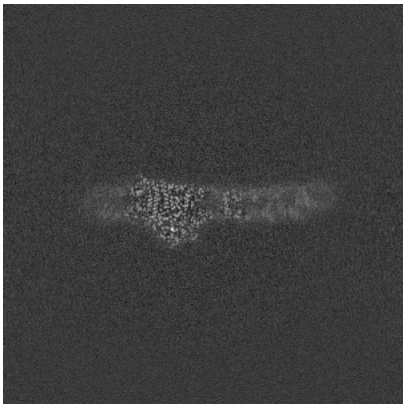


Z Index: 191

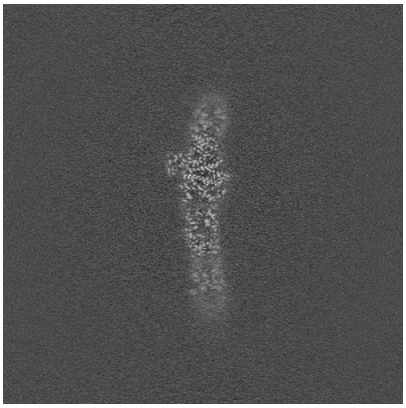
6.3.2 Raw map



X Index: 242



Y Index: 295

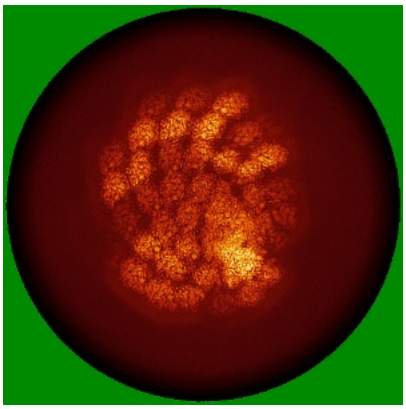


Z Index: 230

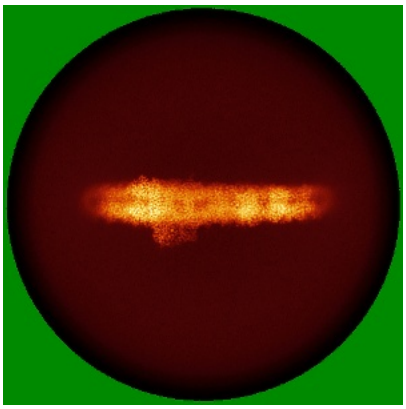
The images above show the largest variance slices of the map in three orthogonal directions.

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

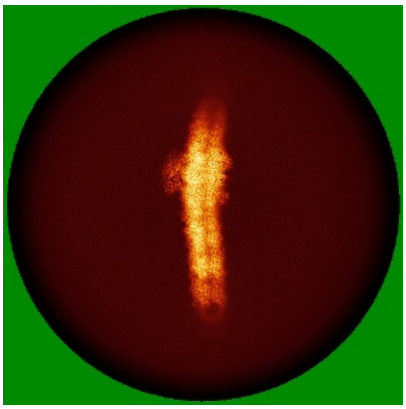
6.4.1 Primary map



X

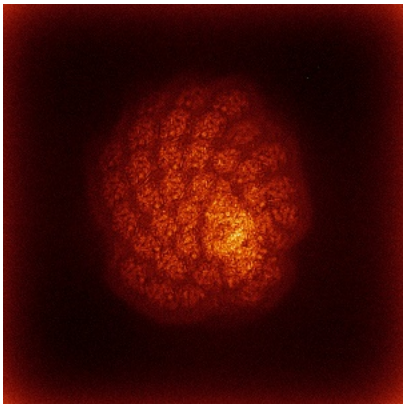


Y

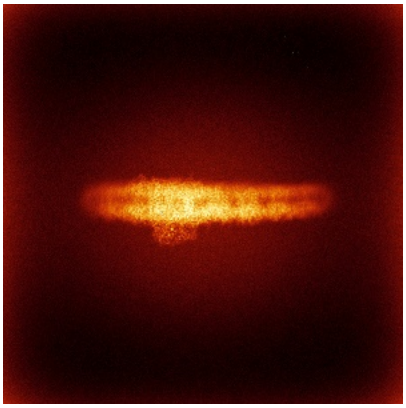


Z

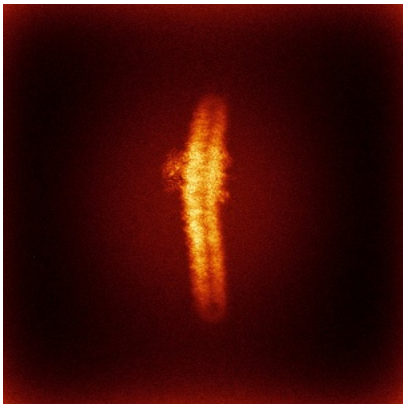
6.4.2 Raw map



X



Y

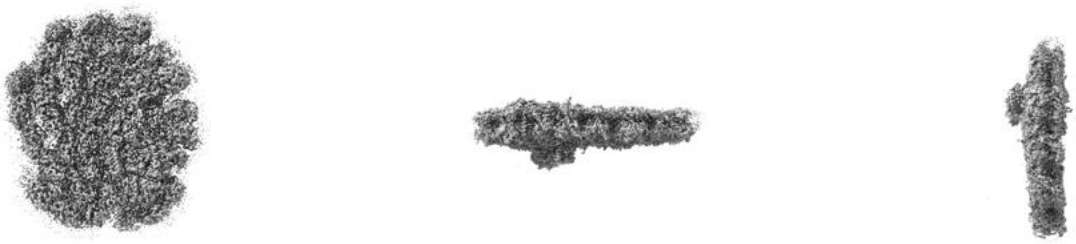


Z

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 0.19. 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.

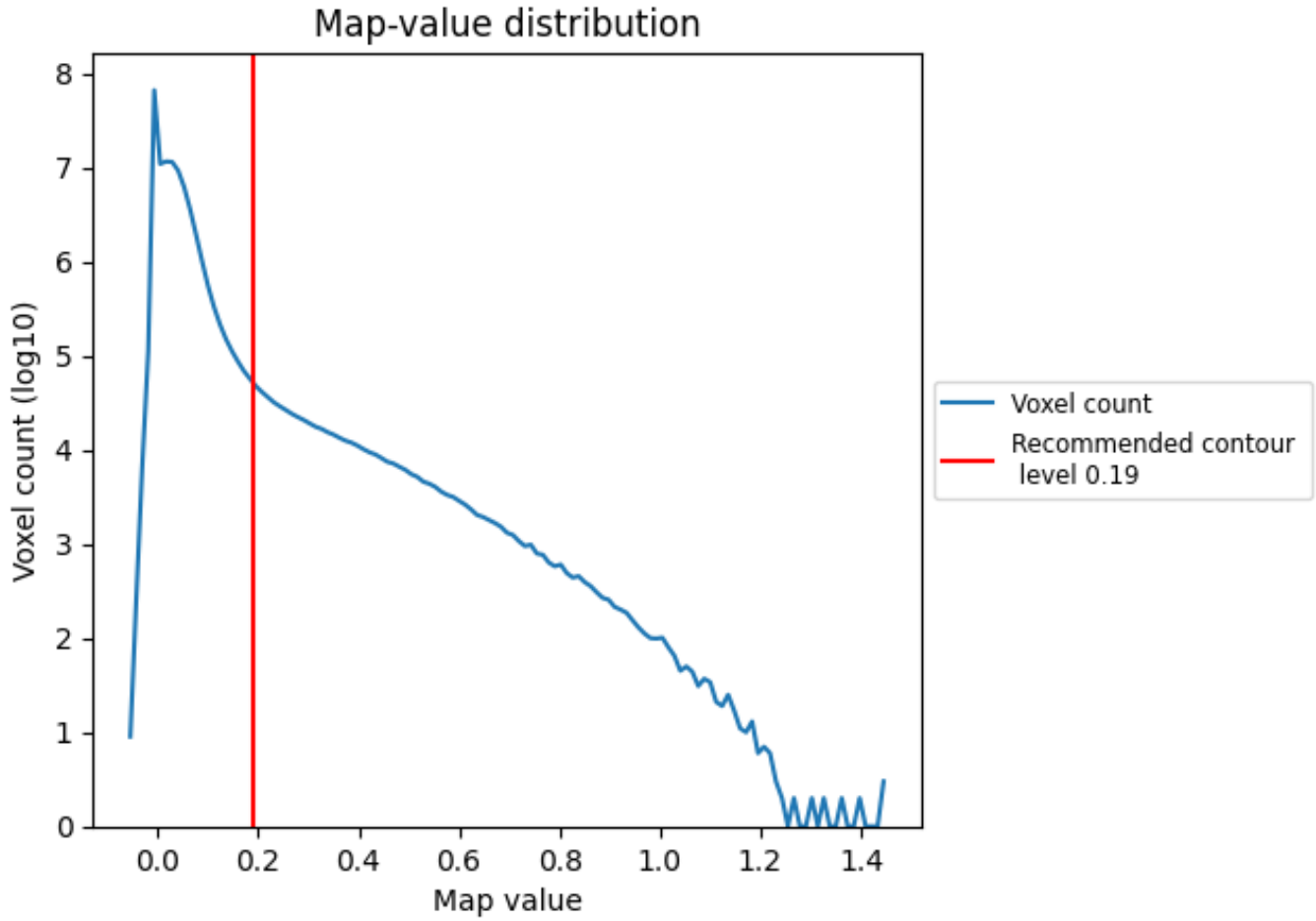
6.6 Mask visualisation (i)

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

7 Map analysis

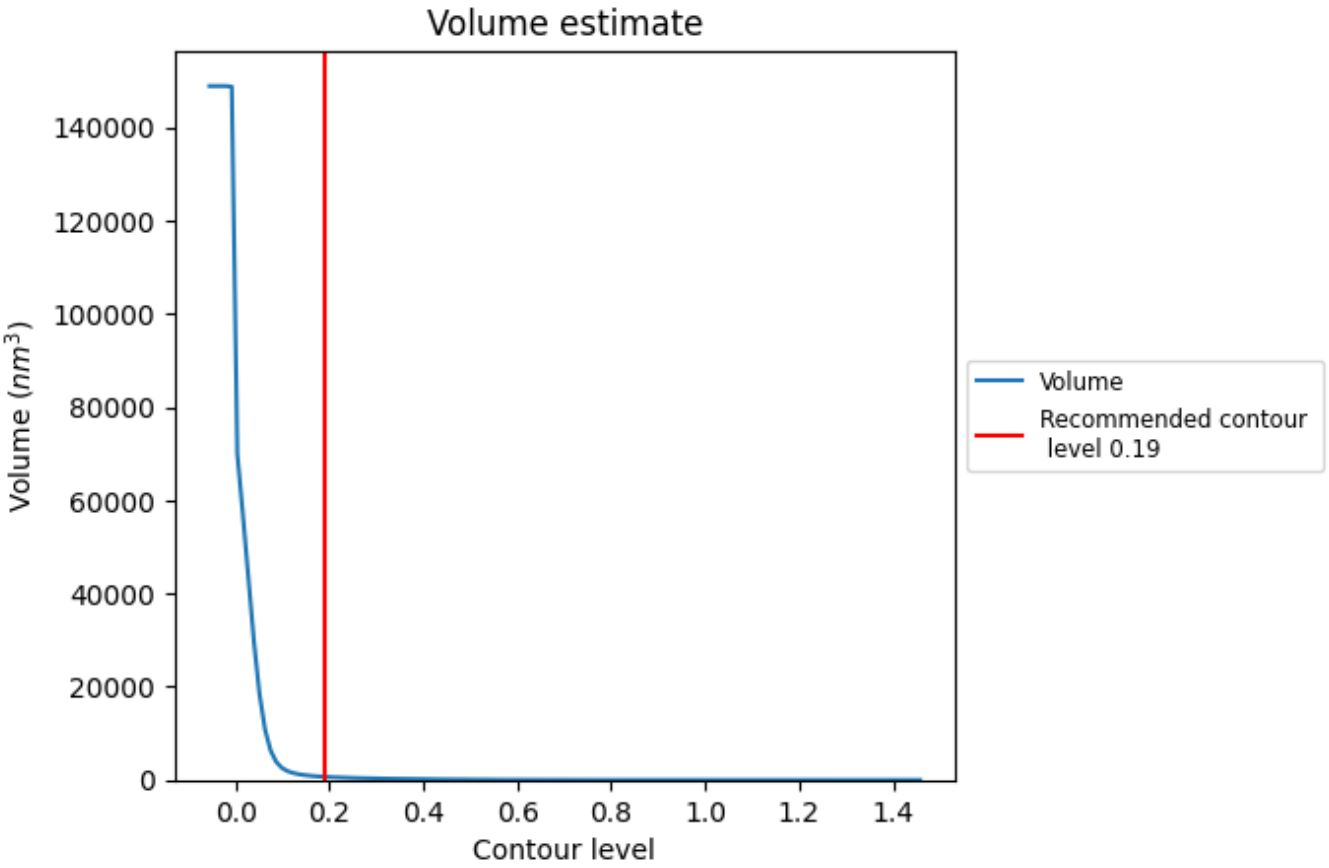
This section contains the results of statistical analysis of the map.

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.

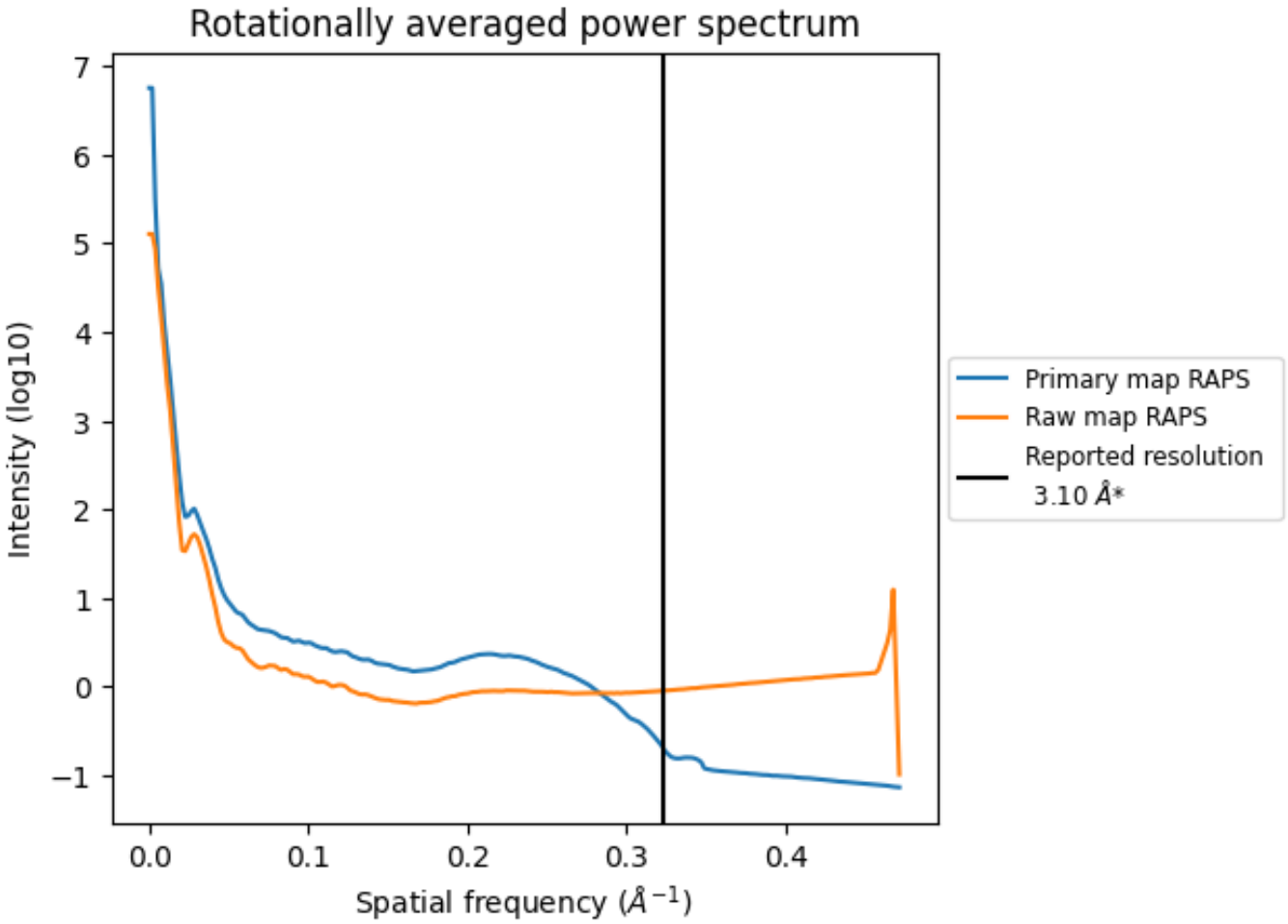
7.2 Volume estimate



The volume at the recommended contour level is 675 nm^3; this corresponds to an approximate mass of 610 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)

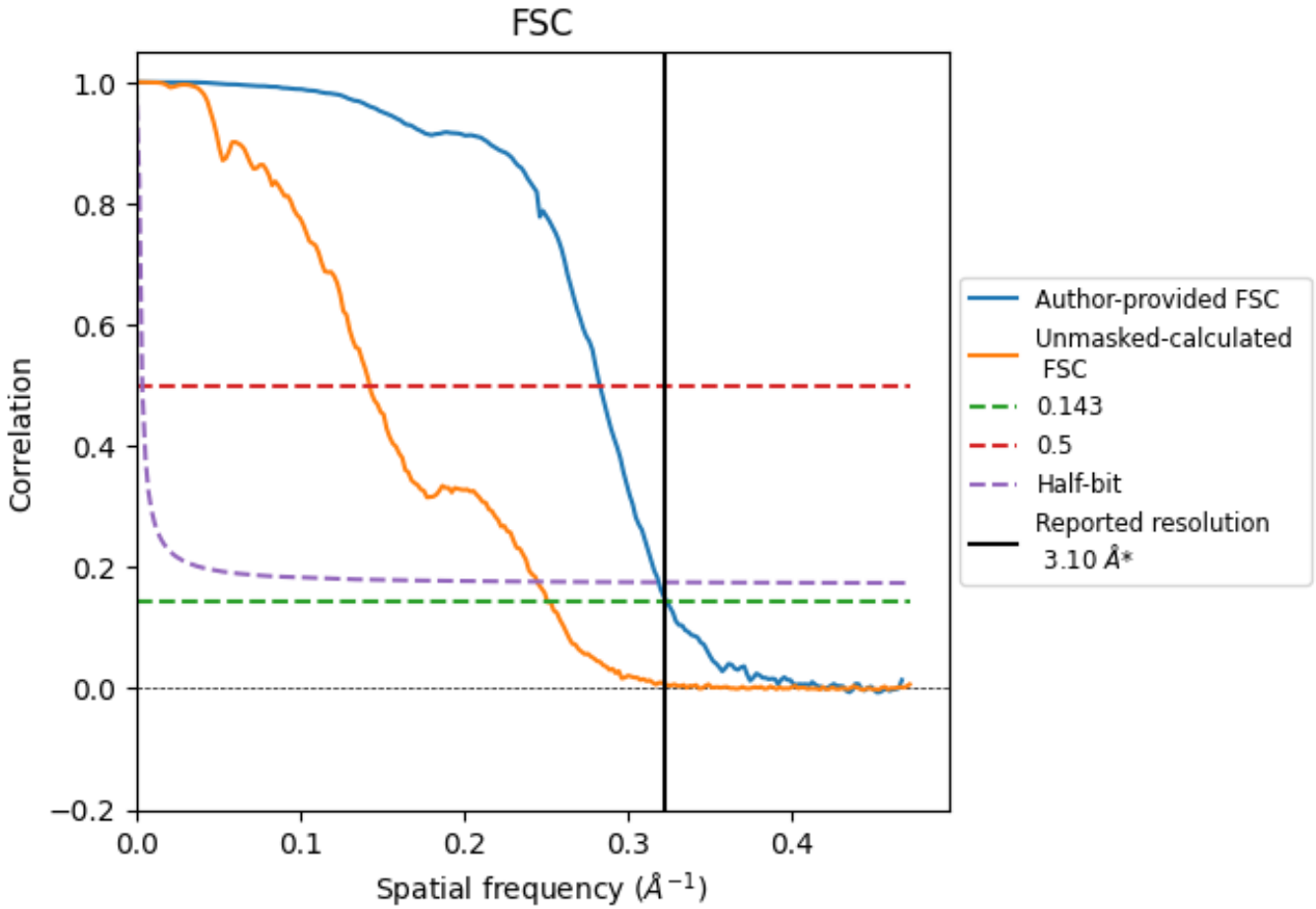


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

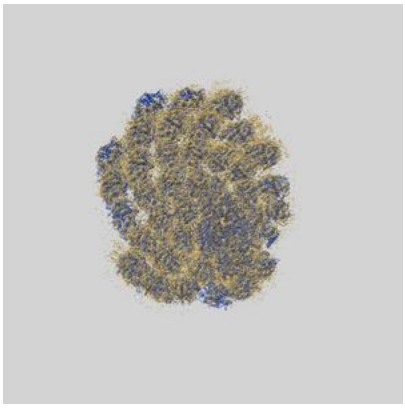
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.09	3.54	3.14
Unmasked-calculated*	3.99	7.02	4.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.99 differs from the reported value 3.1 by more than 10 %

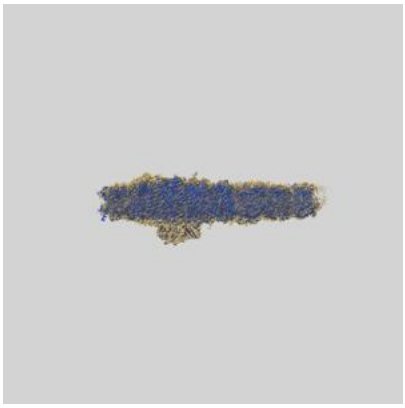
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-64087 and PDB model 9UEN. Per-residue inclusion information can be found in section 3 on page 66.

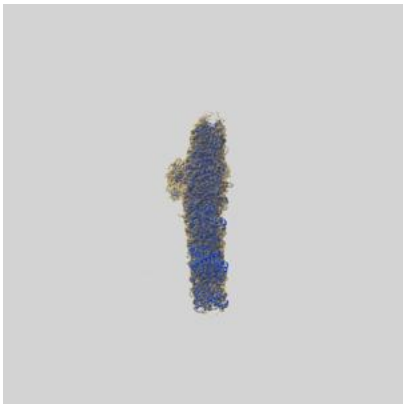
9.1 Map-model overlay



X



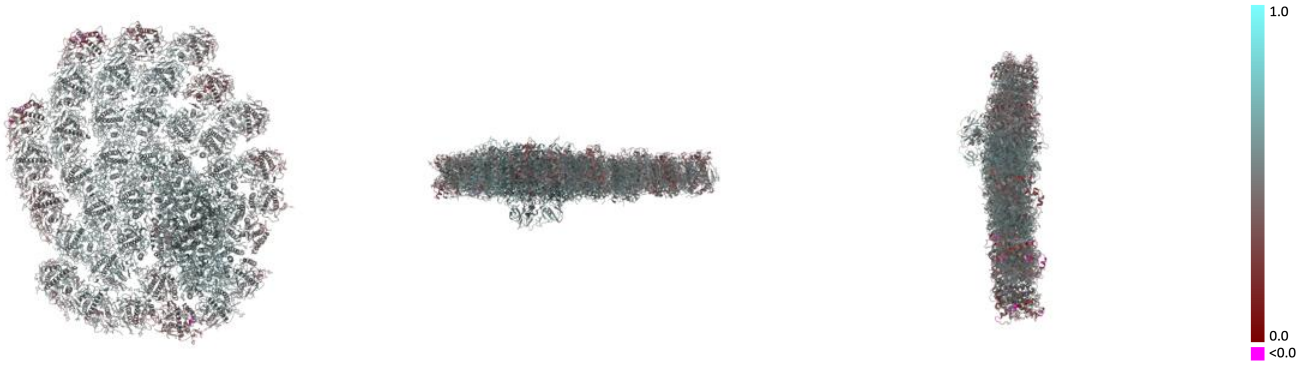
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

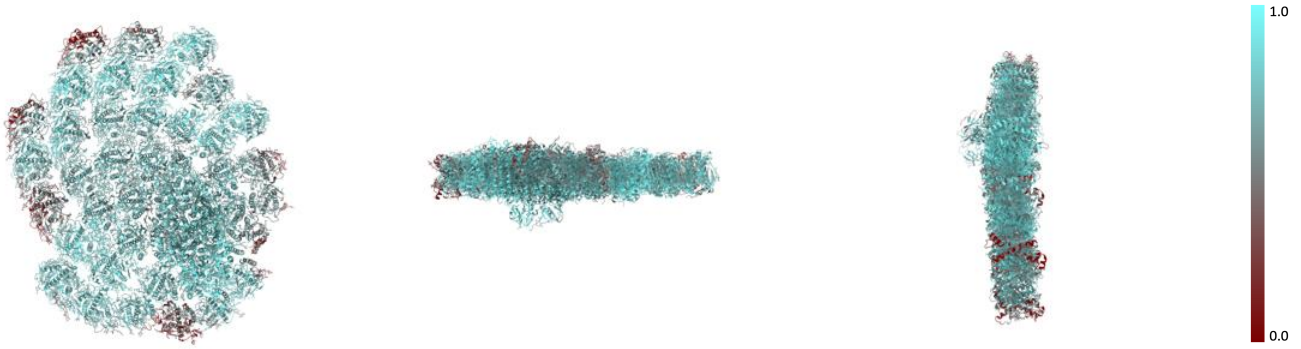
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

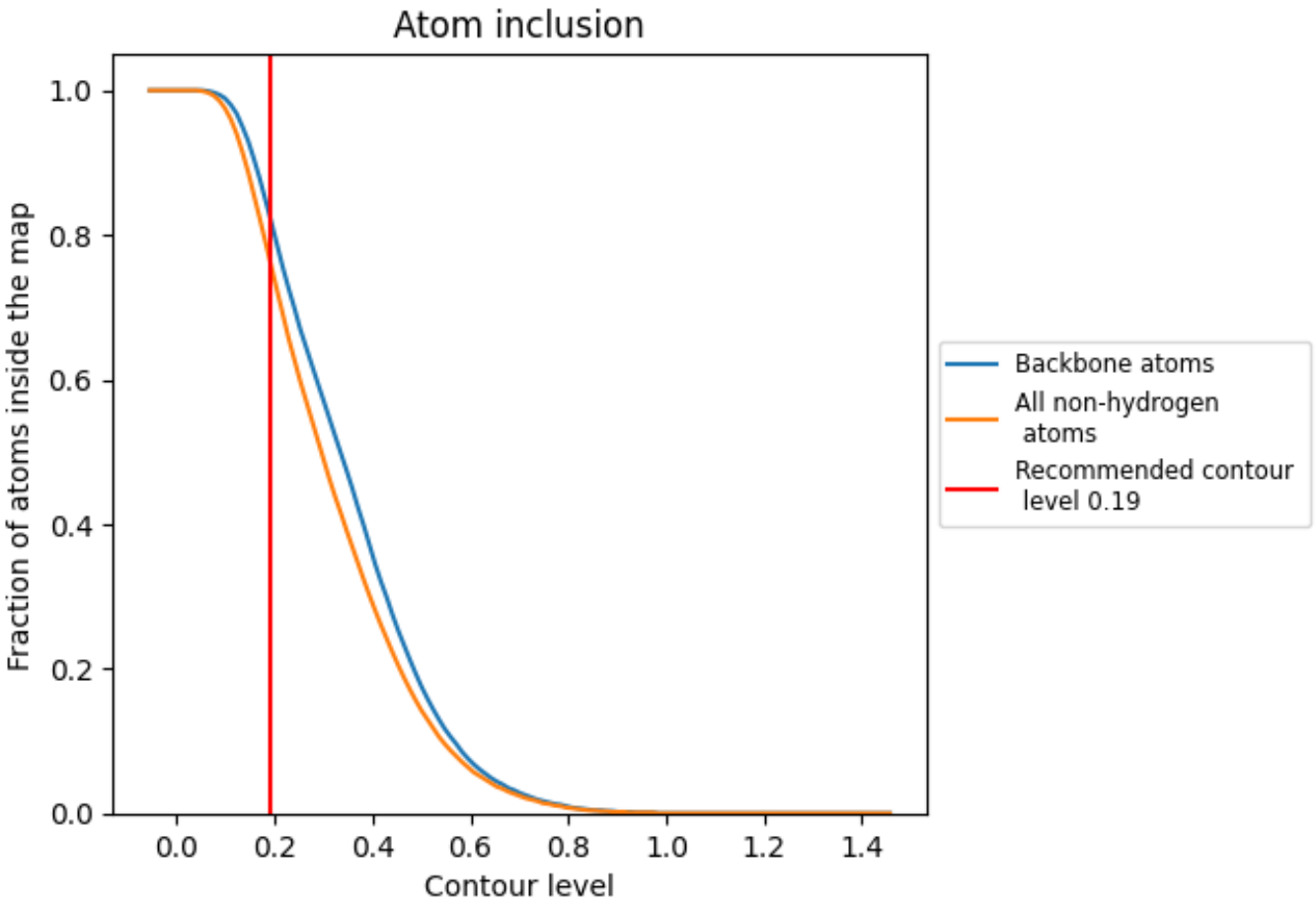
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.19).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 77% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7660	0.5070
A	0.8540	0.5430
B	0.5090	0.4400
C	0.7470	0.4950
D	0.8110	0.5570
E	0.8030	0.5560
F	0.8020	0.4930
G	0.8550	0.5160
H	0.7410	0.4910
I	0.7790	0.5340
J	0.3120	0.3700
K	0.8660	0.5290
L	0.5510	0.4440
M	0.7940	0.5510
N	0.8930	0.5440
O	0.7300	0.5150
P	0.8450	0.5380
Q	0.7710	0.4710
R	0.7610	0.5210
S	0.7700	0.4820
T	0.8420	0.5370
U	0.5700	0.4500
V	0.6860	0.5350
W	0.8160	0.5330
X	0.8200	0.4800
Y	0.6790	0.3930
Z	0.8280	0.4820
a	0.8520	0.5670
b	0.9260	0.5770
c	0.8680	0.5250
d	0.7420	0.5330
e	0.8640	0.5520
f	0.8090	0.5240
i	0.8080	0.5410
j	0.7870	0.5320



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Chain	Atom inclusion	Q-score
k	0.7620	0.5340
l	0.7870	0.5340
m	0.7740	0.5160
o	0.7600	0.4860
p	0.4340	0.4220
q	0.7230	0.4690
r	0.8990	0.5550
t	0.4880	0.3920
u	0.8180	0.5080
v	0.8360	0.5130
w	0.3790	0.3720
x	0.8920	0.5460
y	0.5790	0.4230
z	0.9090	0.5450