Full wwPDB EM Validation Report

Mar 5, 2026 – 07:59 AM UTC

PDB ID	:	8WB4 / pdb_00008wb4
EMDB ID	:	EMD-37414
Title	:	Structure of PSII-ACPII supercomplex from cryptophyte algae
Authors	:	Li, X.Y.; Mao, Z.Y.; Shen, J.R.; Han, G.Y.
Deposited on	:	2023-09-08
Resolution	:	2.47 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:

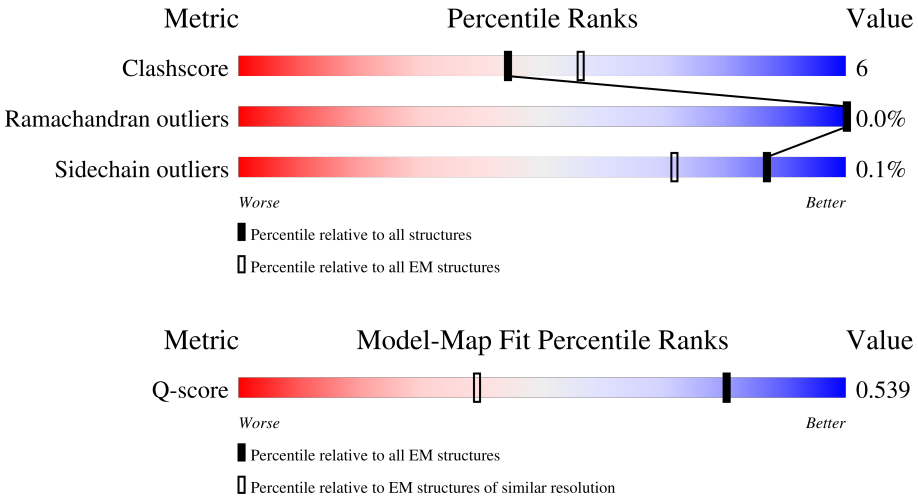
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.47 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	6086 (1.98 - 2.97)

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	M	115	30% · 69%
1	m	115	30% · 69%
2	1	235	30% 69% 14% 17%
2	7	235	29% 71% 12% 17%

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Mol	Chain	Length	Quality of chain
3	2	217	7% 66% 13% 20%
3	8	217	7% 67% 13% 20%
4	3	222	70% 10% 20%
4	9	222	72% 9% 20%
5	0	226	47% 67% 8% 24%
5	4	226	47% 69% 7% 24%
6	5	218	51% 71% 15% 14%
6	p	218	52% 72% 14% 14%
7	6	220	32% 68% 10% 21%
7	P	220	32% 70% 9% 21%
8	A	360	76% 17% 7%
8	a	360	76% 16% 7%
9	D	351	83% 15%
9	d	351	82% 15%
10	E	84	13% 75% 17% 8%
10	e	84	14% 73% 19% 8%
11	F	42	67% 5% 29%
11	f	42	67% 5% 29%
12	H	67	85% 12%
12	h	67	85% 12%
13	I	38	82% 11% 8%
13	i	38	82% 11% 8%
14	J	39	54% 72% 28%
14	j	39	54% 72% 28%
15	K	45	80% 18%

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Mol	Chain	Length	Quality of chain
15	k	45	80% 18%
16	O	330	70% 55% 15% 30%
16	o	330	70% 55% 15% 30%
17	Q	21	100% 100%
17	q	21	100% 100%
18	R	26	42% 100%
18	r	26	50% 100%
19	S	285	17% 60% 11% 29%
19	s	285	17% 61% 10% 29%
20	T	32	91% 9%
20	t	32	91% 9%
21	U	150	61% 51% 11% 38%
21	u	150	61% 47% 15% 38%
22	V	163	80% 69% 11% 20%
22	v	163	80% 68% 12% 20%
23	X	39	97%
23	x	39	97%
24	Y	34	9% 94% 6%
24	y	34	9% 94% 6%
25	Z	62	85% 10%
25	z	62	87% 11%
26	B	509	85% 14%
26	b	509	84% 15%
27	C	461	81% 17%
27	c	461	81% 17%

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Mol	Chain	Length	Quality of chain
28	G	64	58% 98%
28	g	64	59% 97%
29	L	38	87% 13%
29	l	38	87% 13%
30	W	114	33% 6% 61%
30	w	114	33% 6% 61%

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
32	CLA	0	601	X	-	-	-
32	CLA	0	602	X	-	-	-
32	CLA	0	603	X	-	-	-
32	CLA	0	604	X	-	-	-
32	CLA	0	605	X	-	-	-
32	CLA	0	606	X	-	-	-
32	CLA	0	607	X	-	-	-
32	CLA	0	608	X	-	-	-
32	CLA	0	609	X	-	-	-
32	CLA	0	611	X	-	-	-
32	CLA	0	612	X	-	-	-
32	CLA	0	613	X	-	-	-
32	CLA	1	601	X	-	-	-
32	CLA	1	602	X	-	-	-
32	CLA	1	603	X	-	-	-
32	CLA	1	604	X	-	-	-
32	CLA	1	605	X	-	-	-
32	CLA	1	606	X	-	-	-
32	CLA	1	607	X	-	-	-
32	CLA	1	608	X	-	-	-
32	CLA	1	609	X	-	-	-
32	CLA	1	611	X	-	-	-
32	CLA	1	612	X	-	-	-
32	CLA	1	613	X	-	-	-
32	CLA	2	601	X	-	-	-
32	CLA	2	602	X	-	-	-
32	CLA	2	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	2	604	X	-	-	-
32	CLA	2	605	X	-	-	-
32	CLA	2	606	X	-	-	-
32	CLA	2	607	X	-	-	-
32	CLA	2	608	X	-	-	-
32	CLA	2	609	X	-	-	-
32	CLA	2	611	X	-	-	-
32	CLA	2	612	X	-	-	-
32	CLA	3	601	X	-	-	-
32	CLA	3	602	X	-	-	-
32	CLA	3	603	X	-	-	-
32	CLA	3	604	X	-	-	-
32	CLA	3	605	X	-	-	-
32	CLA	3	606	X	-	-	-
32	CLA	3	607	X	-	-	-
32	CLA	3	608	X	-	-	-
32	CLA	3	609	X	-	-	-
32	CLA	3	610	X	-	-	-
32	CLA	3	611	X	-	-	-
32	CLA	4	601	X	-	-	-
32	CLA	4	602	X	-	-	-
32	CLA	4	603	X	-	-	-
32	CLA	4	604	X	-	-	-
32	CLA	4	605	X	-	-	-
32	CLA	4	606	X	-	-	-
32	CLA	4	607	X	-	-	-
32	CLA	4	608	X	-	-	-
32	CLA	4	609	X	-	-	-
32	CLA	4	611	X	-	-	-
32	CLA	4	612	X	-	-	-
32	CLA	4	613	X	-	-	-
32	CLA	5	302	X	-	-	-
32	CLA	5	303	X	-	-	-
32	CLA	5	304	X	-	-	-
32	CLA	5	305	X	-	-	-
32	CLA	5	306	X	-	-	-
32	CLA	5	307	X	-	-	-
32	CLA	5	308	X	-	-	-
32	CLA	5	309	X	-	-	-
32	CLA	5	310	X	-	-	-
32	CLA	5	312	X	-	-	-
32	CLA	5	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	6	601	X	-	-	-
32	CLA	6	602	X	-	-	-
32	CLA	6	603	X	-	-	-
32	CLA	6	604	X	-	-	-
32	CLA	6	606	X	-	-	-
32	CLA	6	607	X	-	-	-
32	CLA	6	608	X	-	-	-
32	CLA	6	610	X	-	-	-
32	CLA	6	611	X	-	-	-
32	CLA	7	601	X	-	-	-
32	CLA	7	602	X	-	-	-
32	CLA	7	603	X	-	-	-
32	CLA	7	604	X	-	-	-
32	CLA	7	605	X	-	-	-
32	CLA	7	606	X	-	-	-
32	CLA	7	607	X	-	-	-
32	CLA	7	608	X	-	-	-
32	CLA	7	609	X	-	-	-
32	CLA	7	611	X	-	-	-
32	CLA	7	612	X	-	-	-
32	CLA	7	613	X	-	-	-
32	CLA	8	601	X	-	-	-
32	CLA	8	602	X	-	-	-
32	CLA	8	603	X	-	-	-
32	CLA	8	604	X	-	-	-
32	CLA	8	605	X	-	-	-
32	CLA	8	606	X	-	-	-
32	CLA	8	607	X	-	-	-
32	CLA	8	608	X	-	-	-
32	CLA	8	609	X	-	-	-
32	CLA	8	611	X	-	-	-
32	CLA	8	612	X	-	-	-
32	CLA	9	601	X	-	-	-
32	CLA	9	602	X	-	-	-
32	CLA	9	603	X	-	-	-
32	CLA	9	604	X	-	-	-
32	CLA	9	605	X	-	-	-
32	CLA	9	606	X	-	-	-
32	CLA	9	607	X	-	-	-
32	CLA	9	608	X	-	-	-
32	CLA	9	609	X	-	-	-
32	CLA	9	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	9	611	X	-	-	-
32	CLA	A	602	X	-	-	-
32	CLA	A	603	X	-	-	-
32	CLA	A	605	X	-	-	-
32	CLA	B	602	X	-	-	-
32	CLA	B	603	X	-	-	-
32	CLA	B	604	X	-	-	-
32	CLA	B	605	X	-	-	-
32	CLA	B	606	X	-	-	-
32	CLA	B	607	X	-	-	-
32	CLA	B	608	X	-	-	-
32	CLA	B	609	X	-	-	-
32	CLA	B	610	X	-	-	-
32	CLA	B	611	X	-	-	-
32	CLA	B	612	X	-	-	-
32	CLA	B	613	X	-	-	-
32	CLA	B	614	X	-	-	-
32	CLA	B	615	X	-	-	-
32	CLA	B	616	X	-	-	-
32	CLA	B	617	X	-	-	-
32	CLA	C	501	X	-	-	-
32	CLA	C	502	X	-	-	-
32	CLA	C	503	X	-	-	-
32	CLA	C	504	X	-	-	-
32	CLA	C	505	X	-	-	-
32	CLA	C	506	X	-	-	-
32	CLA	C	507	X	-	-	-
32	CLA	C	508	X	-	-	-
32	CLA	C	509	X	-	-	-
32	CLA	C	510	X	-	-	-
32	CLA	C	511	X	-	-	-
32	CLA	C	512	X	-	-	-
32	CLA	C	513	X	-	-	-
32	CLA	D	401	X	-	-	-
32	CLA	D	403	X	-	-	-
32	CLA	D	404	X	-	-	-
32	CLA	G	101	X	-	-	-
32	CLA	P	601	X	-	-	-
32	CLA	P	602	X	-	-	-
32	CLA	P	603	X	-	-	-
32	CLA	P	604	X	-	-	-
32	CLA	P	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	P	607	X	-	-	-
32	CLA	P	608	X	-	-	-
32	CLA	P	610	X	-	-	-
32	CLA	P	611	X	-	-	-
32	CLA	S	302	X	-	-	-
32	CLA	S	303	X	-	-	-
32	CLA	a	405	X	-	-	-
32	CLA	a	406	X	-	-	-
32	CLA	a	408	X	-	-	-
32	CLA	b	602	X	-	-	-
32	CLA	b	603	X	-	-	-
32	CLA	b	604	X	-	-	-
32	CLA	b	605	X	-	-	-
32	CLA	b	606	X	-	-	-
32	CLA	b	607	X	-	-	-
32	CLA	b	608	X	-	-	-
32	CLA	b	609	X	-	-	-
32	CLA	b	610	X	-	-	-
32	CLA	b	611	X	-	-	-
32	CLA	b	612	X	-	-	-
32	CLA	b	613	X	-	-	-
32	CLA	b	614	X	-	-	-
32	CLA	b	615	X	-	-	-
32	CLA	b	616	X	-	-	-
32	CLA	b	617	X	-	-	-
32	CLA	c	501	X	-	-	-
32	CLA	c	502	X	-	-	-
32	CLA	c	503	X	-	-	-
32	CLA	c	504	X	-	-	-
32	CLA	c	505	X	-	-	-
32	CLA	c	506	X	-	-	-
32	CLA	c	507	X	-	-	-
32	CLA	c	508	X	-	-	-
32	CLA	c	509	X	-	-	-
32	CLA	c	510	X	-	-	-
32	CLA	c	511	X	-	-	-
32	CLA	c	512	X	-	-	-
32	CLA	c	513	X	-	-	-
32	CLA	d	402	X	-	-	-
32	CLA	d	403	X	-	-	-
32	CLA	d	409	X	-	-	-
32	CLA	g	102	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	p	302	X	-	-	-
32	CLA	p	303	X	-	-	-
32	CLA	p	304	X	-	-	-
32	CLA	p	305	X	-	-	-
32	CLA	p	306	X	-	-	-
32	CLA	p	307	X	-	-	-
32	CLA	p	308	X	-	-	-
32	CLA	p	309	X	-	-	-
32	CLA	p	310	X	-	-	-
32	CLA	p	312	X	-	-	-
32	CLA	p	313	X	-	-	-
32	CLA	s	302	X	-	-	-
32	CLA	s	303	X	-	-	-

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 80246 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II reaction center M.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	m	36	Total 265	C 175	N 42	O 48	0	0
1	M	36	Total 265	C 175	N 42	O 48	0	0

- Molecule 2 is a protein called ACPII-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	194	Total 1472	C 946	N 256	O 262	S 8	0	0
2	7	194	Total 1472	C 946	N 256	O 262	S 8	0	0

- Molecule 3 is a protein called ACPII-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	173	Total 1362	C 899	N 222	O 238	S 3	0	0
3	8	173	Total 1362	C 899	N 222	O 238	S 3	0	0

- Molecule 4 is a protein called ACPII-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	178	Total 1371	C 885	N 230	O 247	S 9	0	0
4	9	178	Total 1371	C 885	N 230	O 247	S 9	0	0

- Molecule 5 is a protein called ACPII-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	172	Total	C	N	O	S	0	0
			1308	845	225	229	9		
5	0	172	Total	C	N	O	S	0	0
			1308	845	225	229	9		

- Molecule 6 is a protein called ACPII-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	187	Total	C	N	O	S	0	0
			1471	956	243	267	5		
6	p	187	Total	C	N	O	S	0	0
			1471	956	243	267	5		

- Molecule 7 is a protein called ACPII-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	173	Total	C	N	O	S	0	0
			1344	878	221	237	8		
7	P	173	Total	C	N	O	S	0	0
			1344	878	221	237	8		

- Molecule 8 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	334	Total	C	N	O	S	0	0
			2618	1712	430	464	12		
8	a	334	Total	C	N	O	S	0	0
			2618	1712	430	464	12		

- Molecule 9 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	342	Total	C	N	O	S	0	0
			2713	1794	444	463	12		
9	d	342	Total	C	N	O	S	0	0
			2713	1794	444	463	12		

- Molecule 10 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	E	77	Total	C	N	O	0	0
			629	409	104	116		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	e	77	Total 629	C 409	N 104	O 116	0	0

- Molecule 11 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	30	Total 247	C 168	N 41	O 37	S 1	0	0
11	f	30	Total 247	C 168	N 41	O 37	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	65	Total 515	C 344	N 81	O 88	S 2	0	0
12	h	65	Total 515	C 344	N 81	O 88	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	35	Total 287	C 191	N 46	O 49	S 1	0	0
13	i	35	Total 287	C 191	N 46	O 49	S 1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	J	28	Total 214	C 147	N 32	O 35	0	0
14	j	28	Total 214	C 147	N 32	O 35	0	0

- Molecule 15 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	K	37	Total 297	C 209	N 44	O 44	0	0
15	k	37	Total 297	C 209	N 44	O 44	0	0

- Molecule 16 is a protein called Photosystem II reaction center protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	231	Total	C	N	O	S	0	0
			1749	1103	282	358	6		
16	o	231	Total	C	N	O	S	0	0
			1749	1103	282	358	6		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	21	Total	C	N	O	0	0
			105	63	21	21		
17	q	21	Total	C	N	O	0	0
			105	63	21	21		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	26	Total	C	N	O	0	0
			130	78	26	26		
18	r	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 19 is a protein called CCPII-S.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	203	Total	C	N	O	S	0	0
			1563	1005	255	299	4		
19	s	203	Total	C	N	O	S	0	0
			1563	1005	255	299	4		

- Molecule 20 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	32	Total	C	N	O	S	0	0
			260	179	40	40	1		
20	t	32	Total	C	N	O	S	0	0
			260	179	40	40	1		

- Molecule 21 is a protein called Photosystem II reaction center protein U.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	93	Total	C	N	O	S	0	0
			742	476	122	142	2		
21	u	93	Total	C	N	O	S	0	0
			742	476	122	142	2		

- Molecule 22 is a protein called Photosystem II cytochrome c550.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	131	Total	C	N	O	S	0	0
			996	626	170	196	4		
22	v	131	Total	C	N	O	S	0	0
			996	626	170	196	4		

- Molecule 23 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	39	Total	C	N	O	S	0	0
			292	192	47	52	1		
23	x	39	Total	C	N	O	S	0	0
			292	192	47	52	1		

- Molecule 24 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	34	Total	C	N	O	S	0	0
			266	180	43	42	1		
24	y	34	Total	C	N	O	S	0	0
			266	180	43	42	1		

- Molecule 25 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	61	Total	C	N	O	S	0	0
			457	315	67	74	1		
25	z	61	Total	C	N	O	S	0	0
			457	315	67	74	1		

- Molecule 26 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	504	Total	C	N	O	S	0	0
			3962	2587	676	688	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	504	Total 3962	C 2587	N 676	O 688	S 11	0	0

- Molecule 27 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	451	Total 3504	C 2290	N 589	O 615	S 10	0	0
27	C	451	Total 3504	C 2290	N 589	O 615	S 10	0	0

- Molecule 28 is a protein called Photosystem II reaction center protein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	g	64	Total 320	C 192	N 64	O 64	0	0
28	G	64	Total 320	C 192	N 64	O 64	0	0

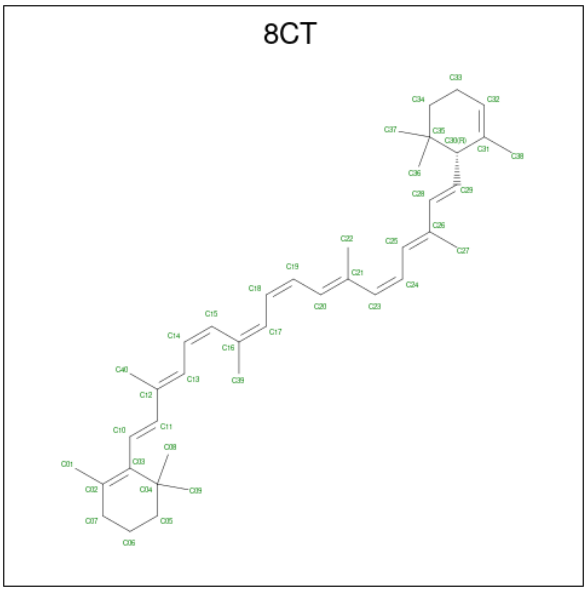
- Molecule 29 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	l	38	Total 310	C 209	N 48	O 52	S 1	0	0
29	L	38	Total 310	C 209	N 48	O 52	S 1	0	0

- Molecule 30 is a protein called Photosystem II reaction center protein W.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	w	45	Total 367	C 238	N 57	O 72	0	0
30	W	45	Total 367	C 238	N 57	O 72	0	0

- Molecule 31 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



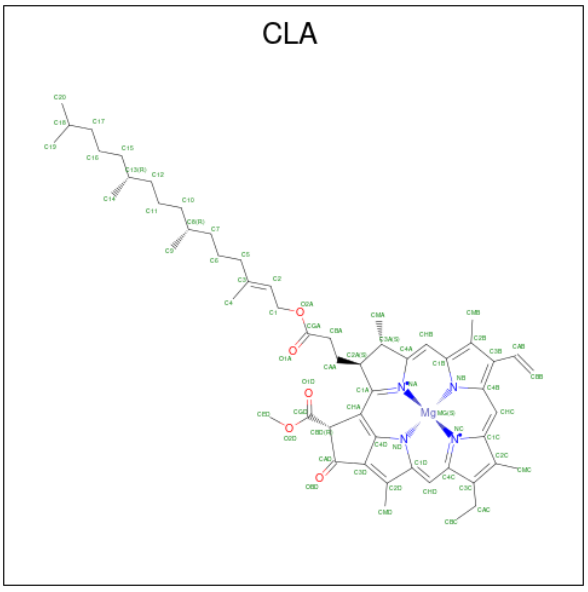
Mol	Chain	Residues	Atoms	AltConf
31	M	1	Total C 40 40	0
31	3	1	Total C 40 40	0
31	6	1	Total C 40 40	0
31	A	1	Total C 40 40	0
31	D	1	Total C 40 40	0
31	H	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	Z	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	d	1	Total C 40 40	0
31	k	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
31	k	1	Total C 40 40	0
31	z	1	Total C 40 40	0
31	9	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	P	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	h	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0

- Molecule 32 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
32	1	1	Total C Mg N O 42 34 1 4 3	0

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Mol	Chain	Residues	Atoms					AltConf
32	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
32	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
32	2	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
32	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
32	3	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
32	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
32	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
32	4	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
32	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
32	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
32	5	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
32	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
32	6	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
32	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
32	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	D	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
32	D	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
32	D	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			61	52	1	4	4	
32	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	c	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
32	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	c	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
32	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	c	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
32	c	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	d	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
32	d	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	d	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	0	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
32	0	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
32	0	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	0	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	0	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	0	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
32	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
32	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
32	8	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
32	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
32	9	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
32	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
32	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	C	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
32	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	C	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
32	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	C	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
32	C	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	P	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
32	P	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

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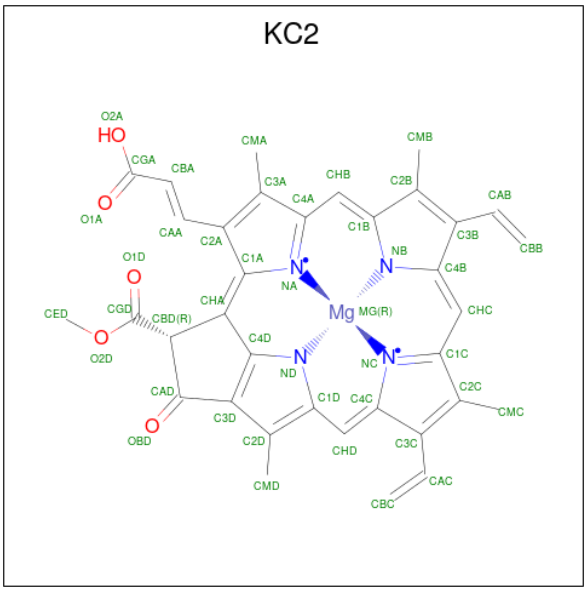
Mol	Chain	Residues	Atoms					AltConf
32	P	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	P	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	p	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
32	p	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
32	p	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	p	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	p	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
32	B	1	Total 61	C 52	Mg 1	N 4	O 4	0
32	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
32	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

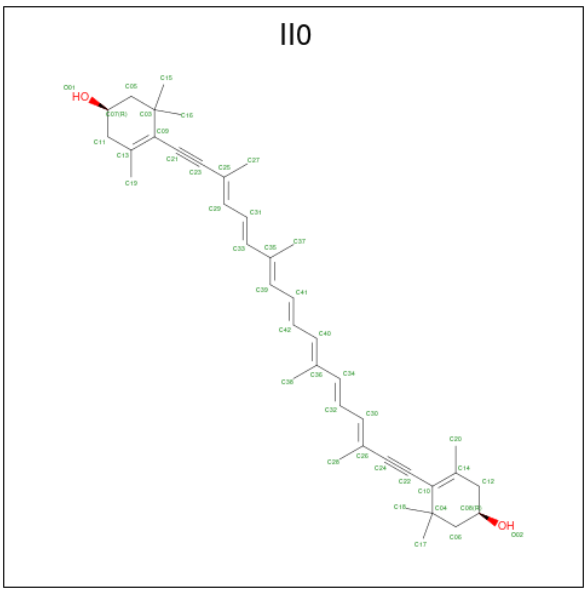
- Molecule 33 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
33	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 34 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: $C_{40}H_{52}O_2$)

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
34	1	1	Total C O 42 40 2	0
34	1	1	Total C O 42 40 2	0
34	1	1	Total C O 42 40 2	0
34	1	1	Total C O 42 40 2	0
34	2	1	Total C O 42 40 2	0
34	2	1	Total C O 42 40 2	0
34	2	1	Total C O 42 40 2	0
34	2	1	Total C O 42 40 2	0
34	3	1	Total C O 42 40 2	0
34	3	1	Total C O 42 40 2	0
34	3	1	Total C O 42 40 2	0
34	4	1	Total C O 42 40 2	0
34	4	1	Total C O 42 40 2	0

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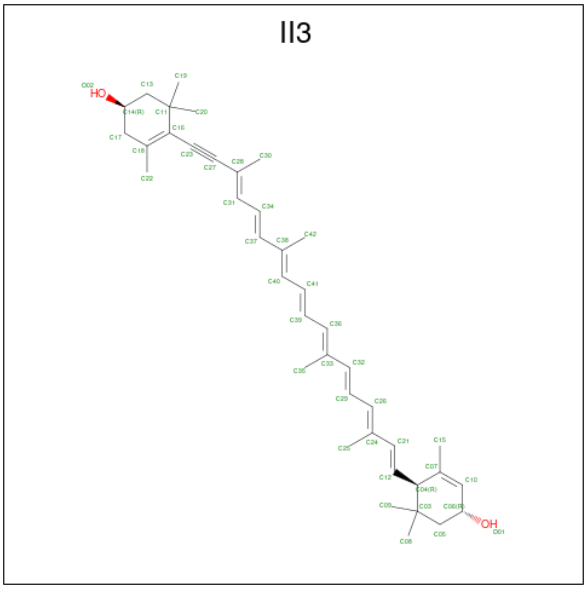
Mol	Chain	Residues	Atoms			AltConf
34	4	1	Total	C	O	0
			42	40	2	
34	5	1	Total	C	O	0
			42	40	2	
34	5	1	Total	C	O	0
			42	40	2	
34	5	1	Total	C	O	0
			42	40	2	
34	5	1	Total	C	O	0
			42	40	2	
34	5	1	Total	C	O	0
			42	40	2	
34	6	1	Total	C	O	0
			42	40	2	
34	6	1	Total	C	O	0
			42	40	2	
34	0	1	Total	C	O	0
			42	40	2	
34	0	1	Total	C	O	0
			42	40	2	
34	0	1	Total	C	O	0
			42	40	2	
34	0	1	Total	C	O	0
			42	40	2	
34	7	1	Total	C	O	0
			42	40	2	
34	7	1	Total	C	O	0
			42	40	2	
34	7	1	Total	C	O	0
			42	40	2	
34	7	1	Total	C	O	0
			42	40	2	
34	8	1	Total	C	O	0
			42	40	2	
34	8	1	Total	C	O	0
			42	40	2	
34	8	1	Total	C	O	0
			42	40	2	
34	8	1	Total	C	O	0
			42	40	2	
34	9	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms	AltConf
34	9	1	Total C O 42 40 2	0
34	9	1	Total C O 42 40 2	0
34	P	1	Total C O 42 40 2	0
34	P	1	Total C O 42 40 2	0
34	p	1	Total C O 42 40 2	0
34	p	1	Total C O 42 40 2	0
34	p	1	Total C O 42 40 2	0
34	p	1	Total C O 42 40 2	0

- Molecule 35 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: II3) (formula: $C_{40}H_{54}O_2$) (labeled as "Ligand of Interest" by depositor).



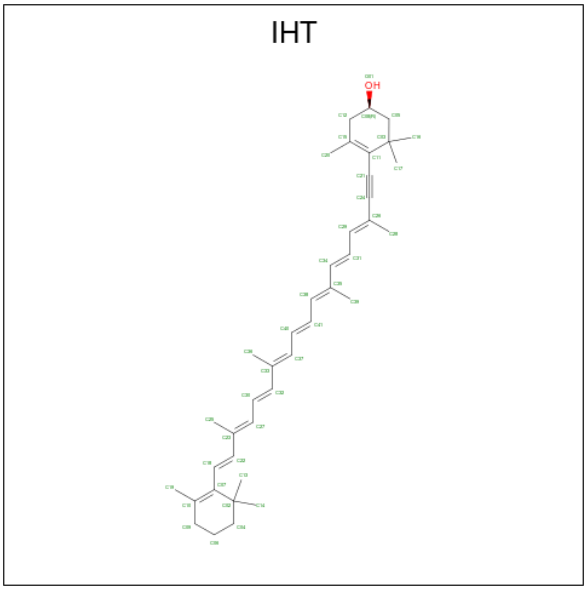
Mol	Chain	Residues	Atoms	AltConf
35	1	1	Total C O 42 40 2	0
35	6	1	Total C O 42 40 2	0

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Mol	Chain	Residues	Atoms	AltConf
35	7	1	Total C O 42 40 2	0
35	P	1	Total C O 42 40 2	0

- Molecule 36 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: $C_{40}H_{54}O$) (labeled as "Ligand of Interest" by depositor).



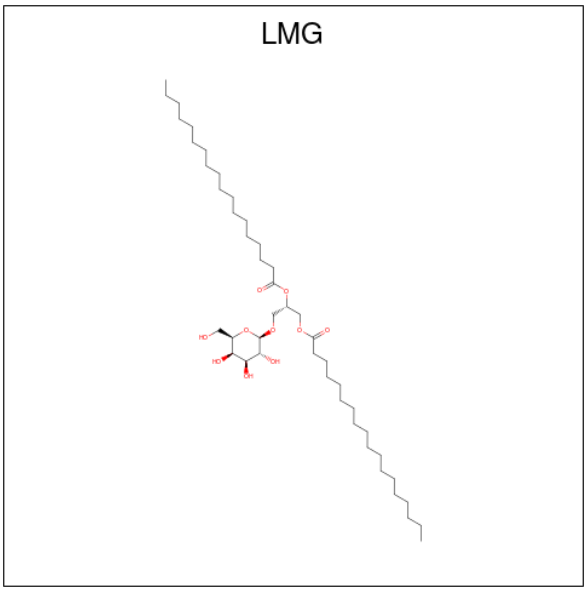
Mol	Chain	Residues	Atoms	AltConf
36	1	1	Total C O 41 40 1	0
36	2	1	Total C O 41 40 1	0
36	4	1	Total C O 41 40 1	0
36	4	1	Total C O 41 40 1	0
36	5	1	Total C O 41 40 1	0
36	0	1	Total C O 41 40 1	0
36	0	1	Total C O 41 40 1	0
36	7	1	Total C O 41 40 1	0

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Mol	Chain	Residues	Atoms	AltConf
36	8	1	Total C O 41 40 1	0
36	p	1	Total C O 41 40 1	0

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



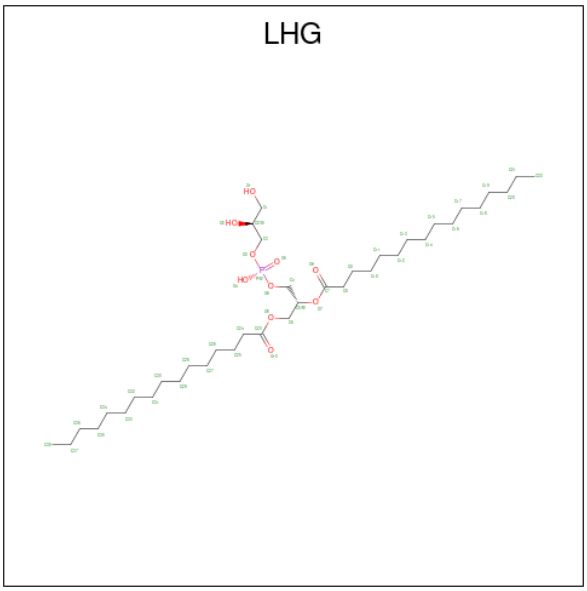
Mol	Chain	Residues	Atoms	AltConf
37	2	1	Total C O 36 26 10	0
37	4	1	Total C O 36 26 10	0
37	6	1	Total C O 28 18 10	0
37	A	1	Total C O 48 38 10	0
37	D	1	Total C O 46 36 10	0
37	D	1	Total C O 40 30 10	0
37	b	1	Total C O 51 41 10	0
37	c	1	Total C O 46 36 10	0
37	d	1	Total C O 40 30 10	0

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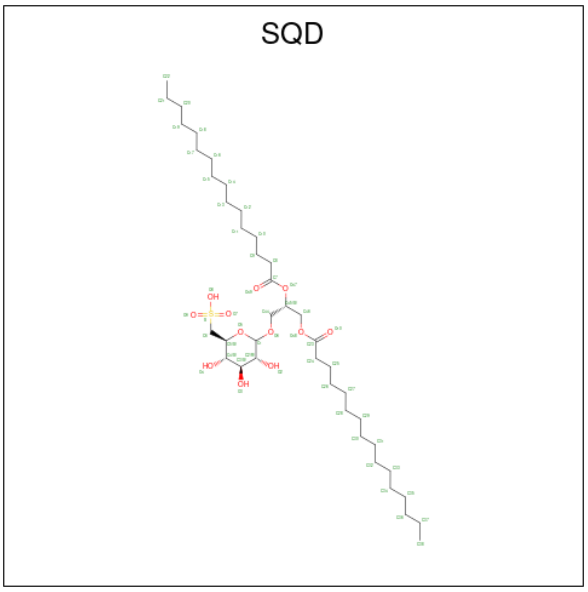
Mol	Chain	Residues	Atoms			AltConf
37	d	1	Total	C	O	0
			46	36	10	
37	g	1	Total	C	O	0
			28	18	10	
37	l	1	Total	C	O	0
			40	30	10	
37	0	1	Total	C	O	0
			36	26	10	
37	8	1	Total	C	O	0
			36	26	10	
37	C	1	Total	C	O	0
			46	36	10	
37	G	1	Total	C	O	0
			28	18	10	
37	L	1	Total	C	O	0
			40	30	10	
37	P	1	Total	C	O	0
			28	18	10	
37	a	1	Total	C	O	0
			48	38	10	
37	B	1	Total	C	O	0
			51	41	10	

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



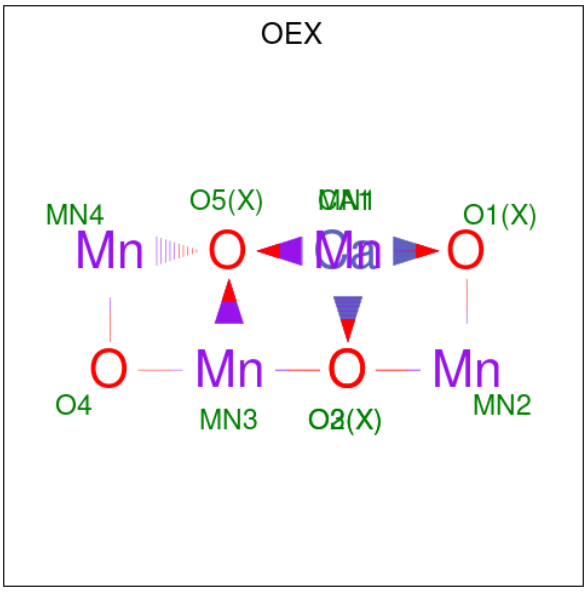
Mol	Chain	Residues	Atoms				AltConf
38	2	1	Total	C	O	P	0
			22	12	9	1	
38	A	1	Total	C	O	P	0
			43	32	10	1	
38	A	1	Total	C	O	P	0
			49	38	10	1	
38	D	1	Total	C	O	P	0
			48	38	9	1	
38	D	1	Total	C	O	P	0
			32	21	10	1	
38	S	1	Total	C	O	P	0
			37	26	10	1	
38	b	1	Total	C	O	P	0
			39	28	10	1	
38	b	1	Total	C	O	P	0
			39	28	10	1	
38	d	1	Total	C	O	P	0
			48	38	9	1	
38	d	1	Total	C	O	P	0
			32	21	10	1	
38	l	1	Total	C	O	P	0
			49	38	10	1	
38	8	1	Total	C	O	P	0
			22	12	9	1	
38	L	1	Total	C	O	P	0
			49	38	10	1	
38	a	1	Total	C	O	P	0
			43	32	10	1	
38	a	1	Total	C	O	P	0
			49	38	10	1	
38	s	1	Total	C	O	P	0
			37	26	10	1	
38	B	1	Total	C	O	P	0
			39	28	10	1	
38	B	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 39 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).



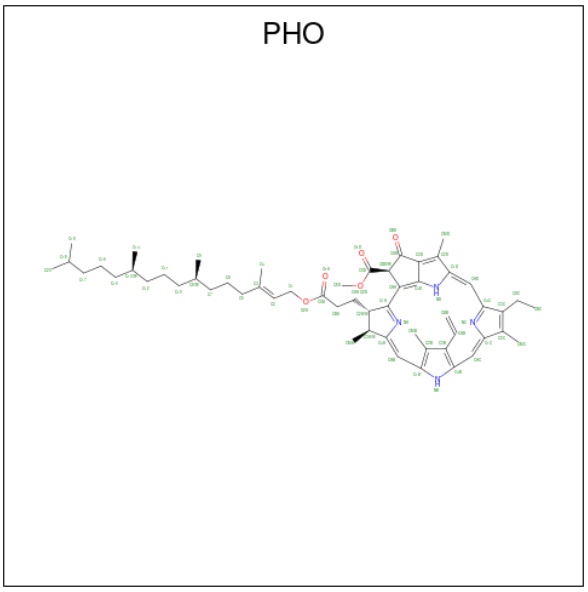
Mol	Chain	Residues	Atoms				AltConf
39	5	1	Total 35	C 22	O 12	S 1	0
39	A	1	Total 54	C 41	O 12	S 1	0
39	b	1	Total 48	C 35	O 12	S 1	0
39	b	1	Total 54	C 41	O 12	S 1	0
39	a	1	Total 54	C 41	O 12	S 1	0
39	p	1	Total 35	C 22	O 12	S 1	0
39	B	1	Total 48	C 35	O 12	S 1	0
39	B	1	Total 54	C 41	O 12	S 1	0

- Molecule 40 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 41 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
41	A	1	Total	C	N	O	0
			64	55	4	5	

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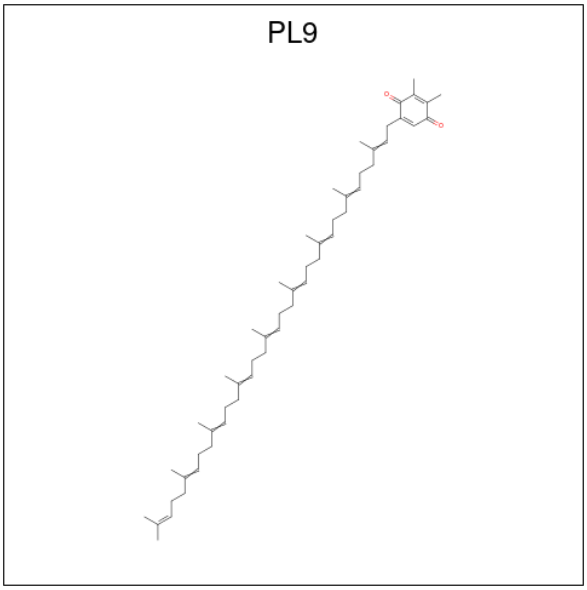
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Mol	Chain	Residues	Atoms				AltConf
41	D	1	Total	C	N	O	0
			64	55	4	5	
41	d	1	Total	C	N	O	0
			64	55	4	5	
41	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 42 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
42	A	1	Total	Cl	0
			1	1	
42	a	1	Total	Cl	0
			1	1	

- Molecule 43 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



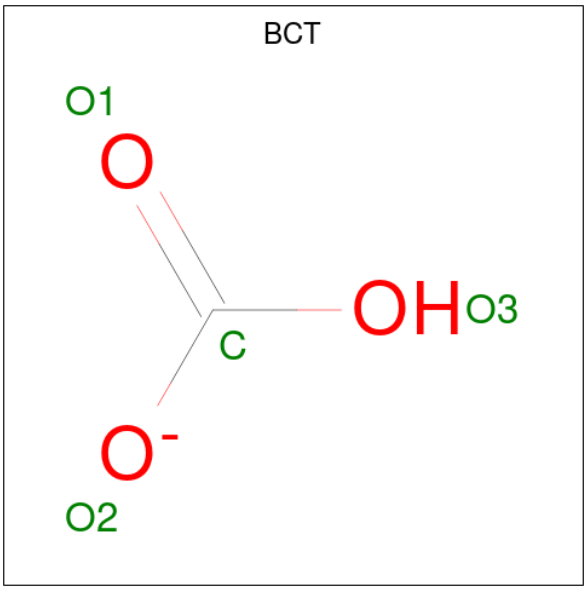
Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total	C	O	0
			13	11	2	
43	D	1	Total	C	O	0
			55	53	2	
43	d	1	Total	C	O	0
			55	53	2	

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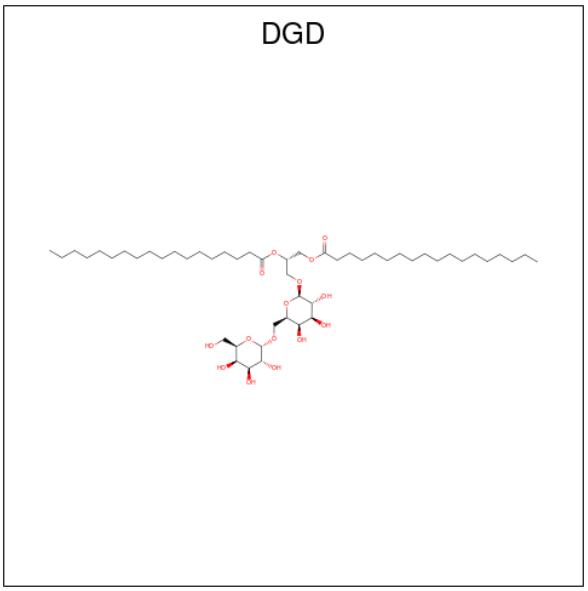
Mol	Chain	Residues	Atoms	AltConf
43	a	1	Total C O 13 11 2	0

- Molecule 44 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 45 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).

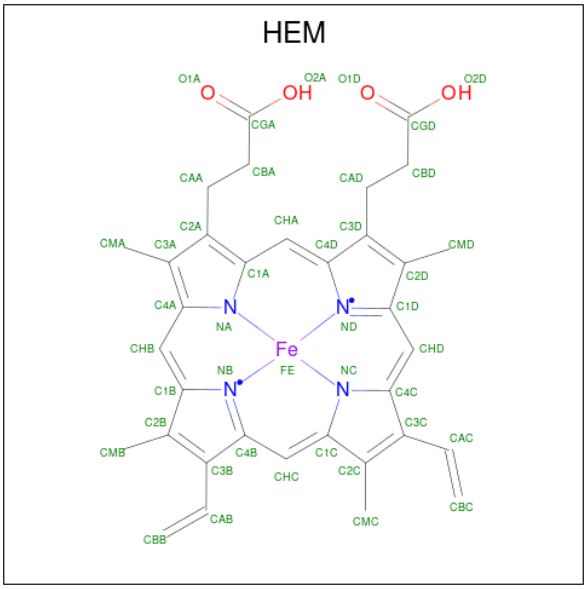


Mol	Chain	Residues	Atoms	AltConf
45	A	1	Total C O 53 39 14	0
45	H	1	Total C O 62 47 15	0
45	c	1	Total C O 55 40 15	0
45	c	1	Total C O 56 41 15	0
45	c	1	Total C O 55 40 15	0
45	C	1	Total C O 55 40 15	0
45	C	1	Total C O 56 41 15	0
45	C	1	Total C O 55 40 15	0
45	a	1	Total C O 53 39 14	0
45	h	1	Total C O 62 47 15	0

- Molecule 46 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	AltConf
46	D	1	Total Fe 1 1	0
46	d	1	Total Fe 1 1	0

- Molecule 47 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



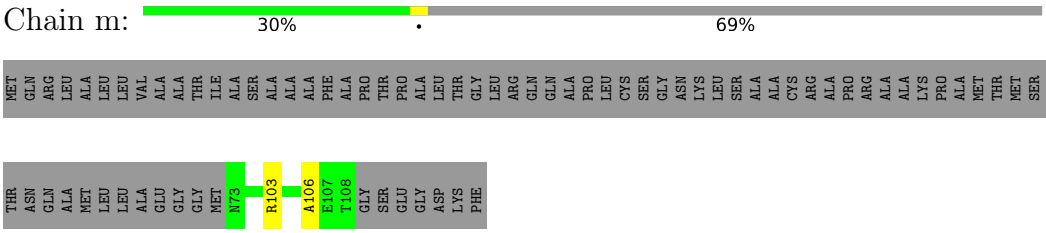
Mol	Chain	Residues	Atoms					AltConf
47	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
47	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
47	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
47	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

3 Residue-property plots (i)

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

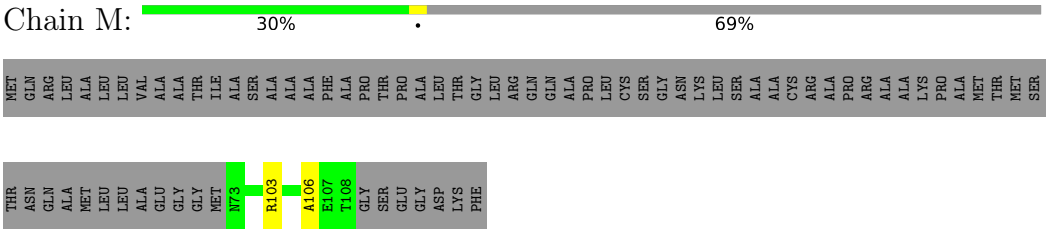
• Molecule 1: Photosystem II reaction center M

Chain m:



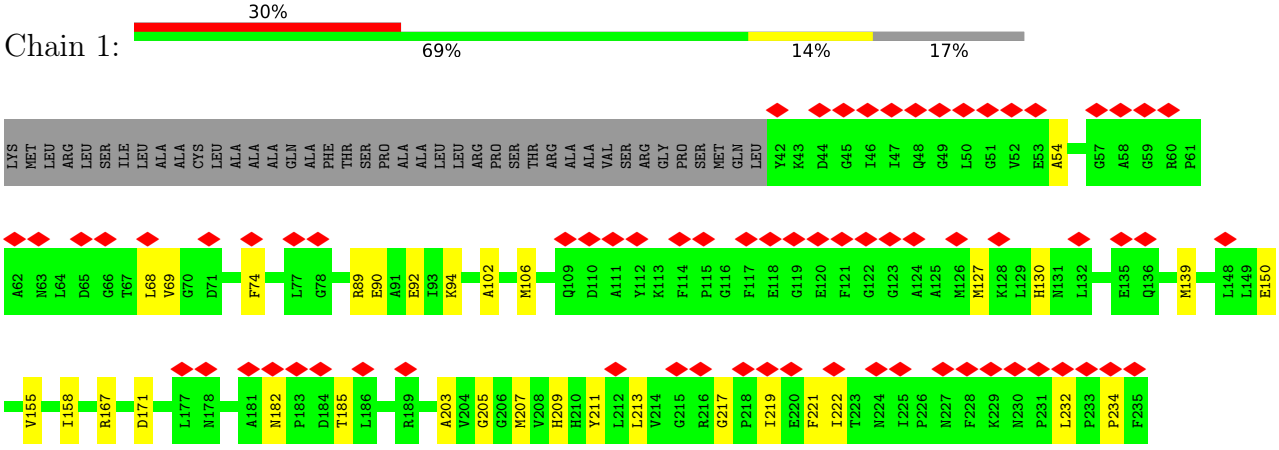
• Molecule 1: Photosystem II reaction center M

Chain M:



• Molecule 2: ACPII-1

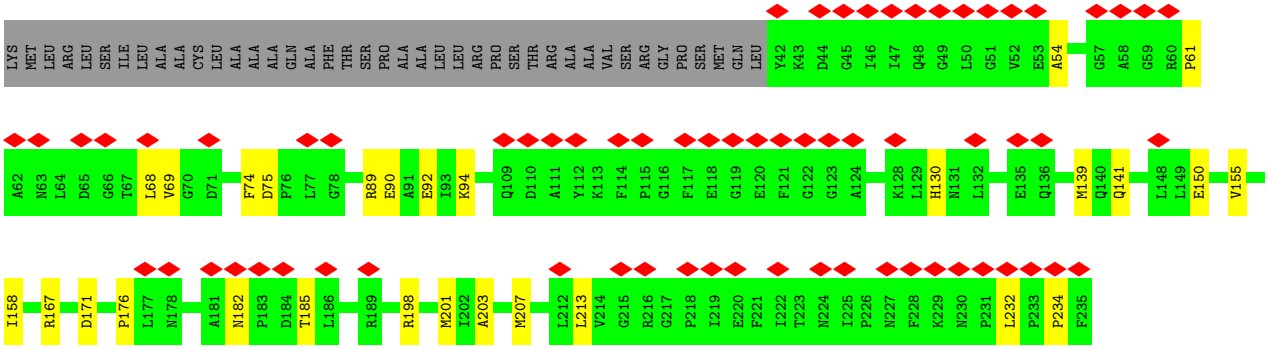
Chain 1:



• Molecule 2: ACPII-1

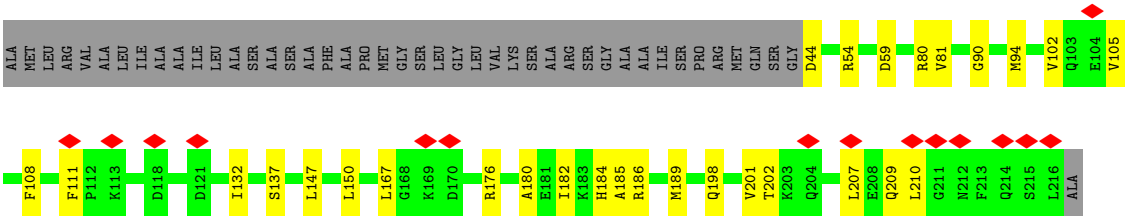
Chain 7:





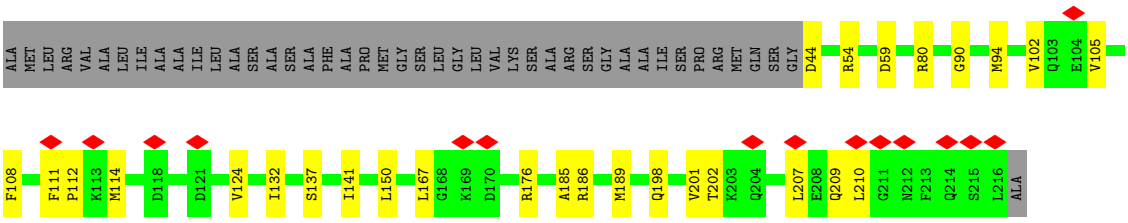
• Molecule 3: ACPII-2





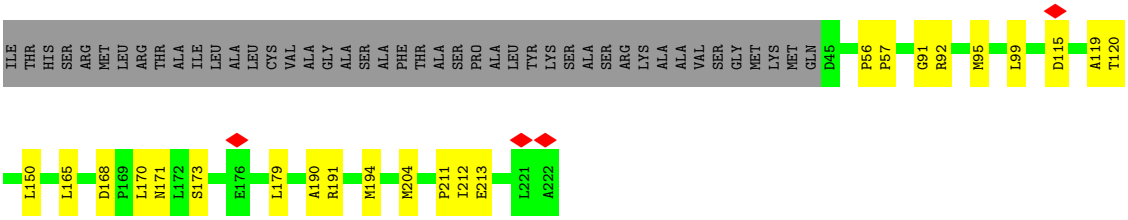
• Molecule 3: ACPII-2





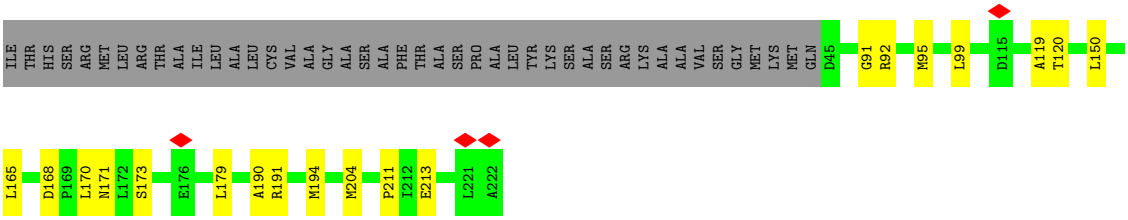
• Molecule 4: ACPII-3





• Molecule 4: ACPII-3

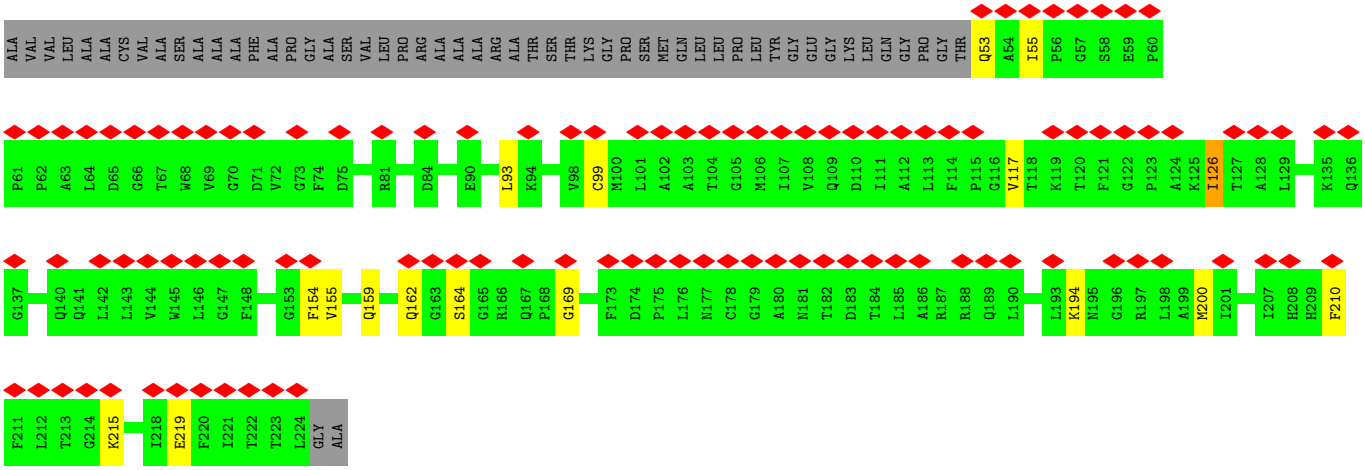




• Molecule 5: ACPII-4

Chain 4:

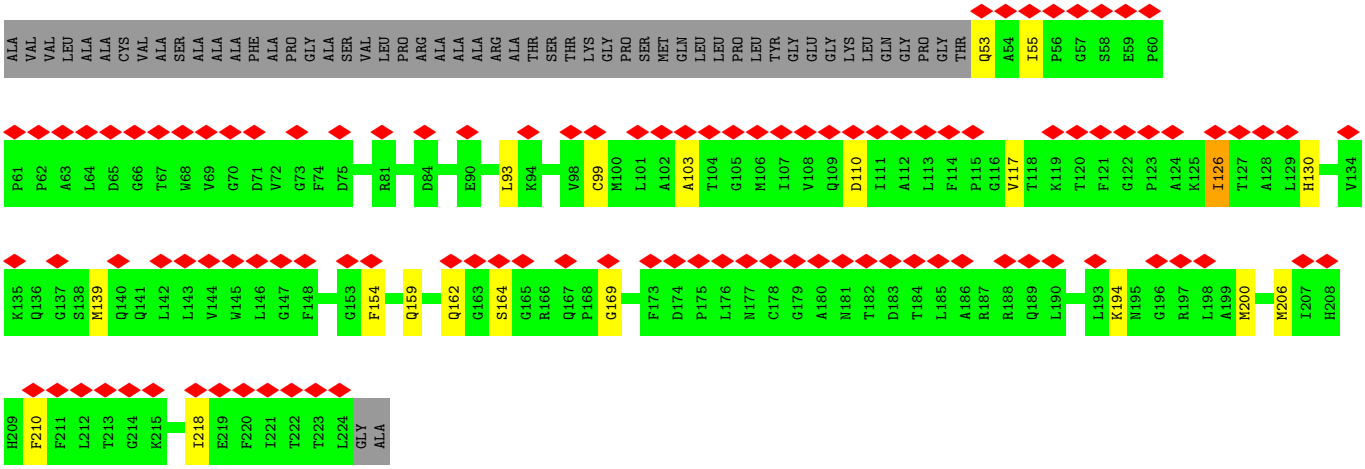




• Molecule 5: ACPII-4

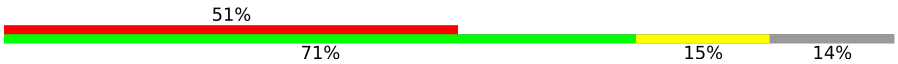
Chain 0:

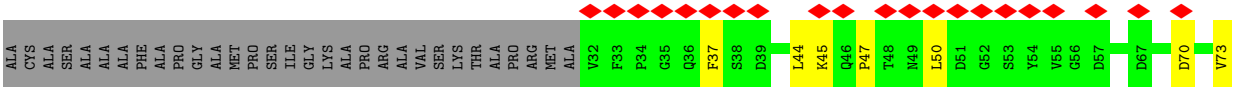


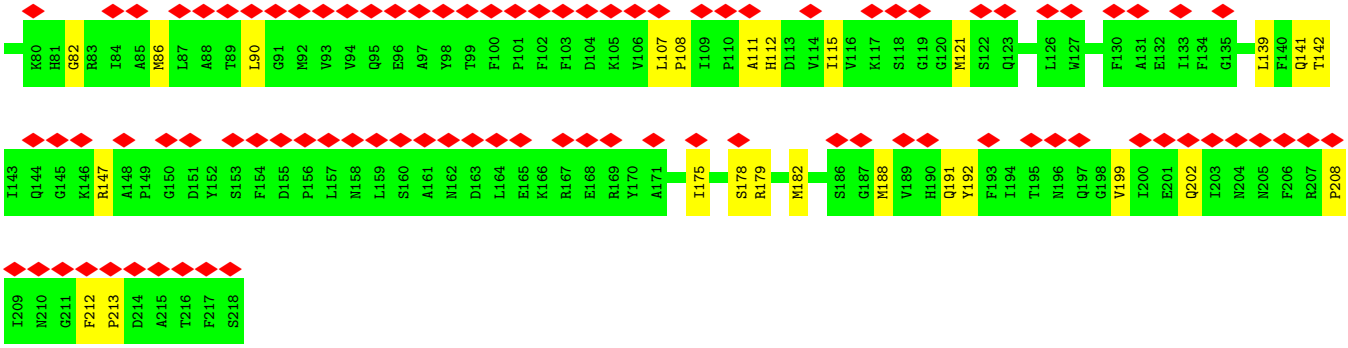


• Molecule 6: ACPII-5

Chain 5:

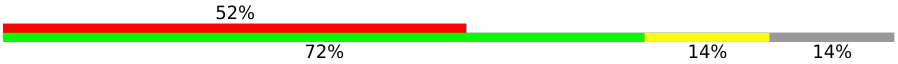


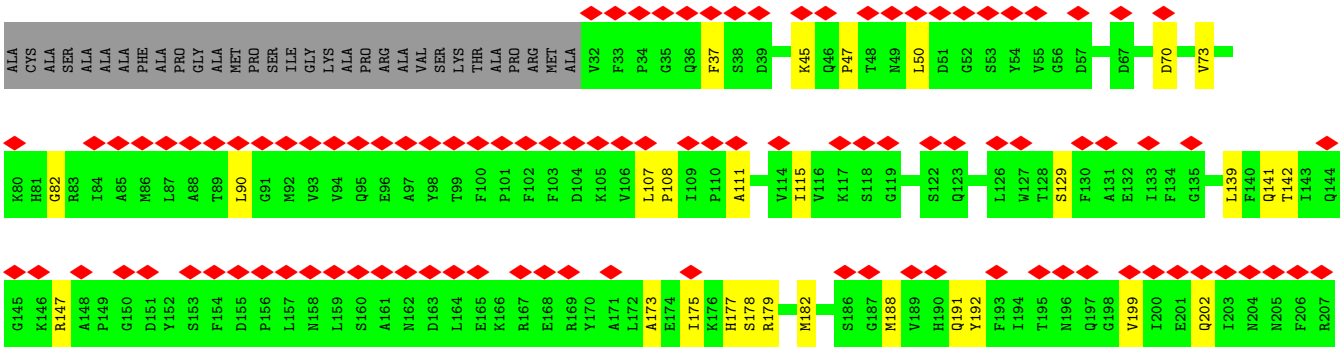




• Molecule 6: ACPII-5

Chain p:

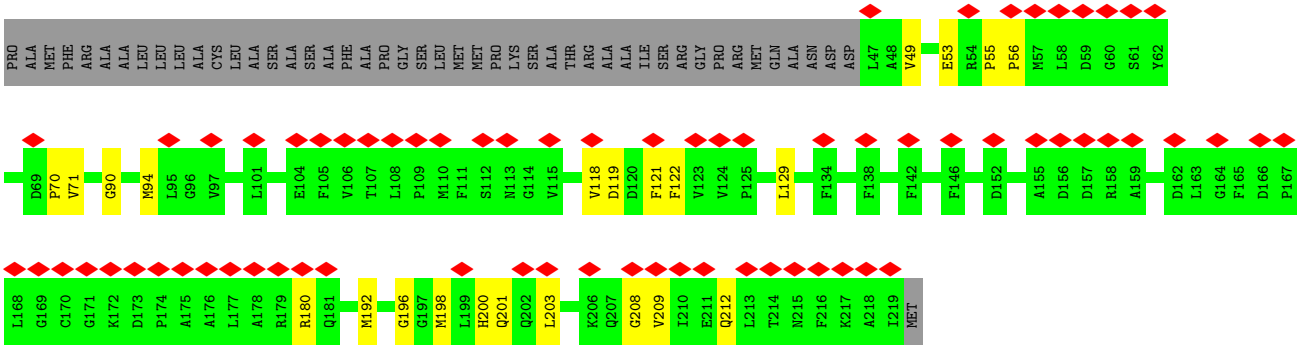




• Molecule 7: ACPII-6

Chain 6:

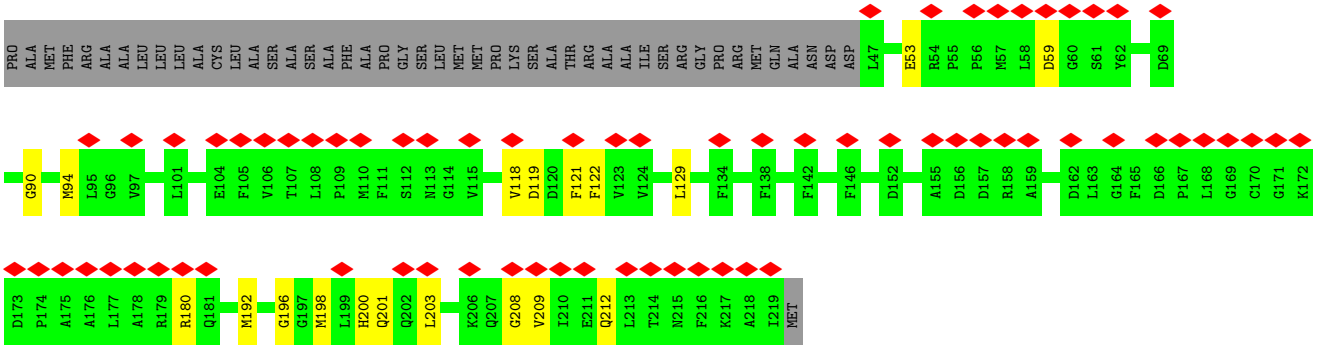




• Molecule 7: ACPII-6

Chain P:





• Molecule 8: Photosystem II protein D1

Chain A:

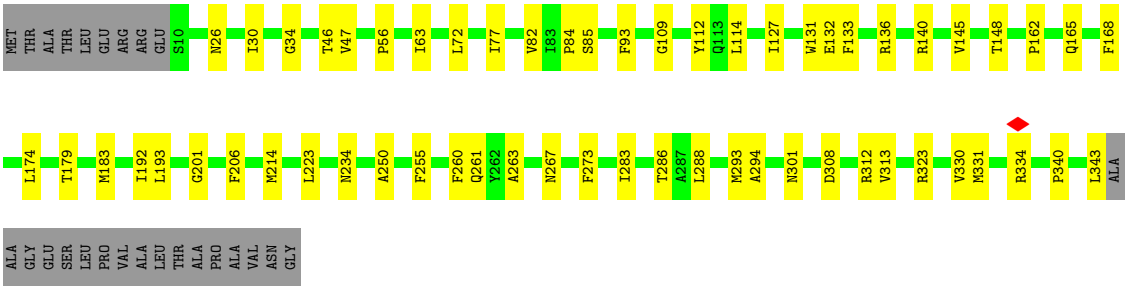




• Molecule 8: Photosystem II protein D1

Chain a:

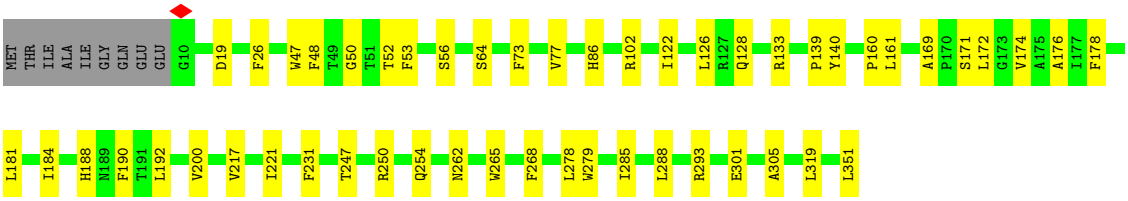




• Molecule 9: Photosystem II D2 protein

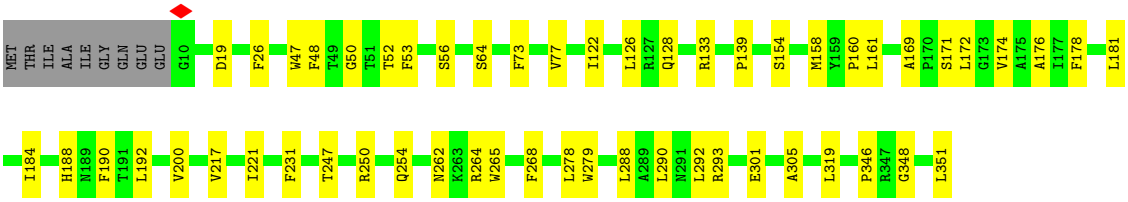
Chain D:





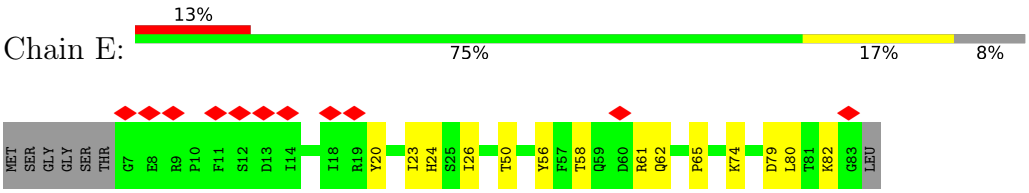
• Molecule 9: Photosystem II D2 protein

Chain d:



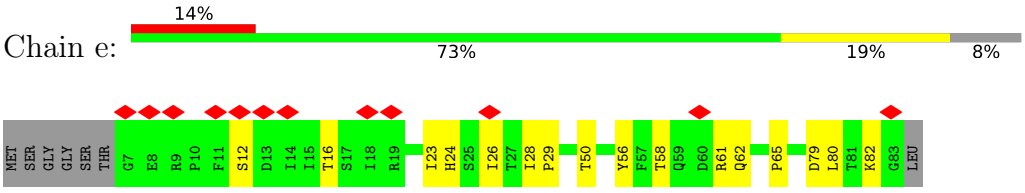
• Molecule 10: Cytochrome b559 subunit alpha

Chain E:



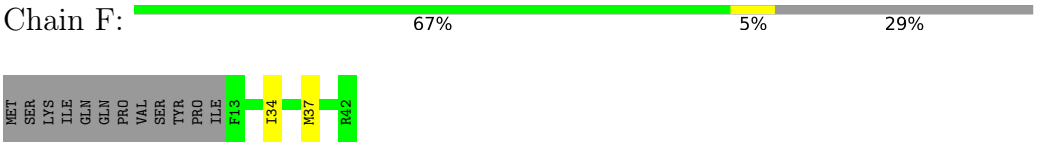
• Molecule 10: Cytochrome b559 subunit alpha

Chain e:



• Molecule 11: Cytochrome b559 subunit beta

Chain F:



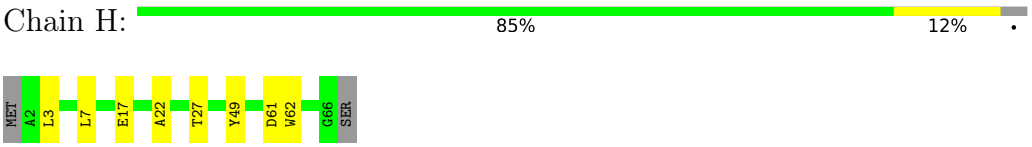
• Molecule 11: Cytochrome b559 subunit beta

Chain f:



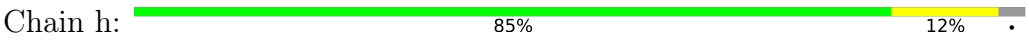
• Molecule 12: Photosystem II reaction center protein H

Chain H:



• Molecule 12: Photosystem II reaction center protein H

Chain h:





• Molecule 13: Photosystem II reaction center protein I

Chain I:

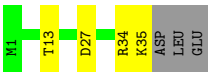




• Molecule 13: Photosystem II reaction center protein I

Chain i:

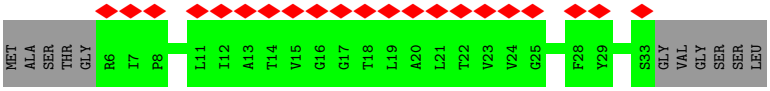




• Molecule 14: Photosystem II reaction center protein J

Chain J:

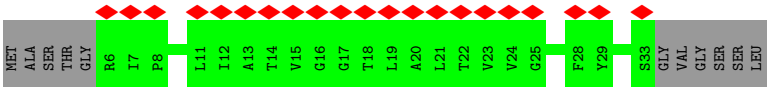




• Molecule 14: Photosystem II reaction center protein J

Chain j:

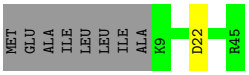




• Molecule 15: Photosystem II reaction center protein K

Chain K:

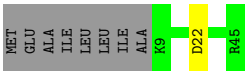




• Molecule 15: Photosystem II reaction center protein K

Chain k:

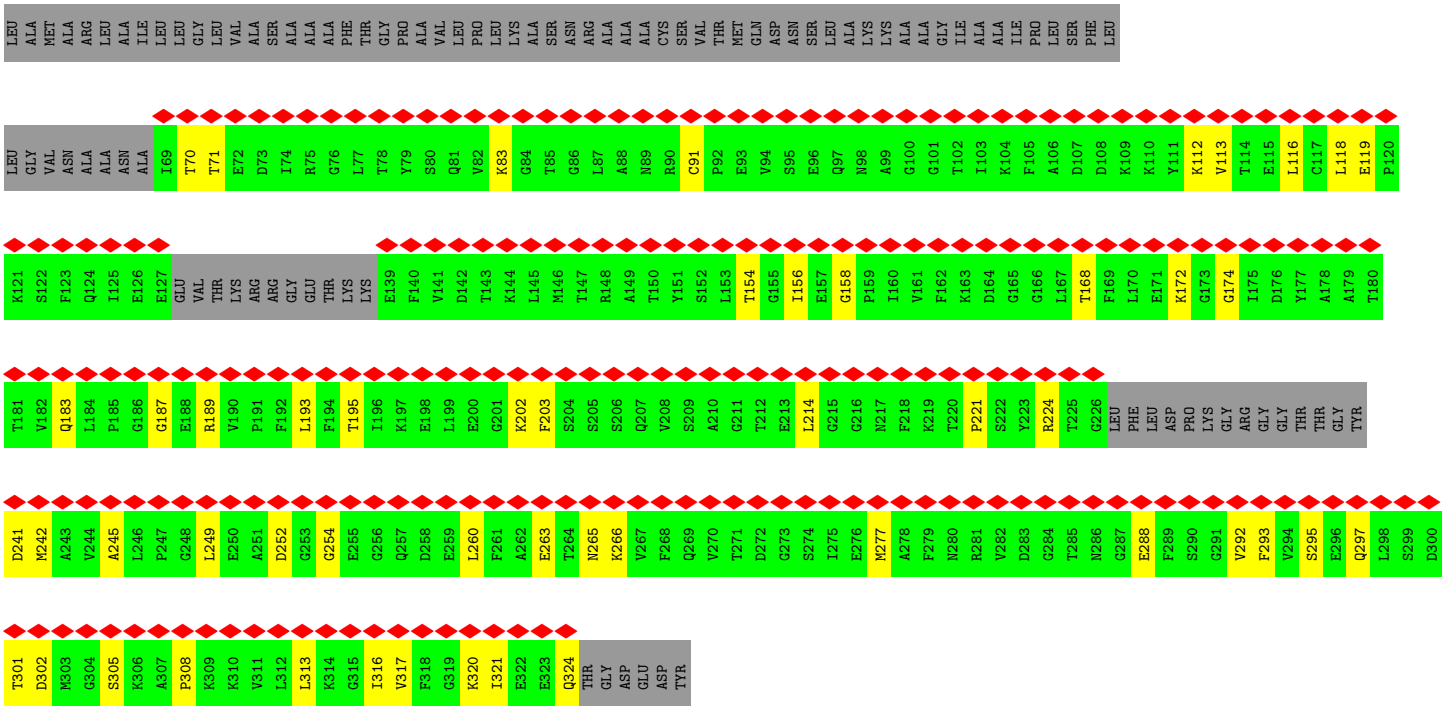




• Molecule 16: Photosystem II reaction center protein O

Chain O:

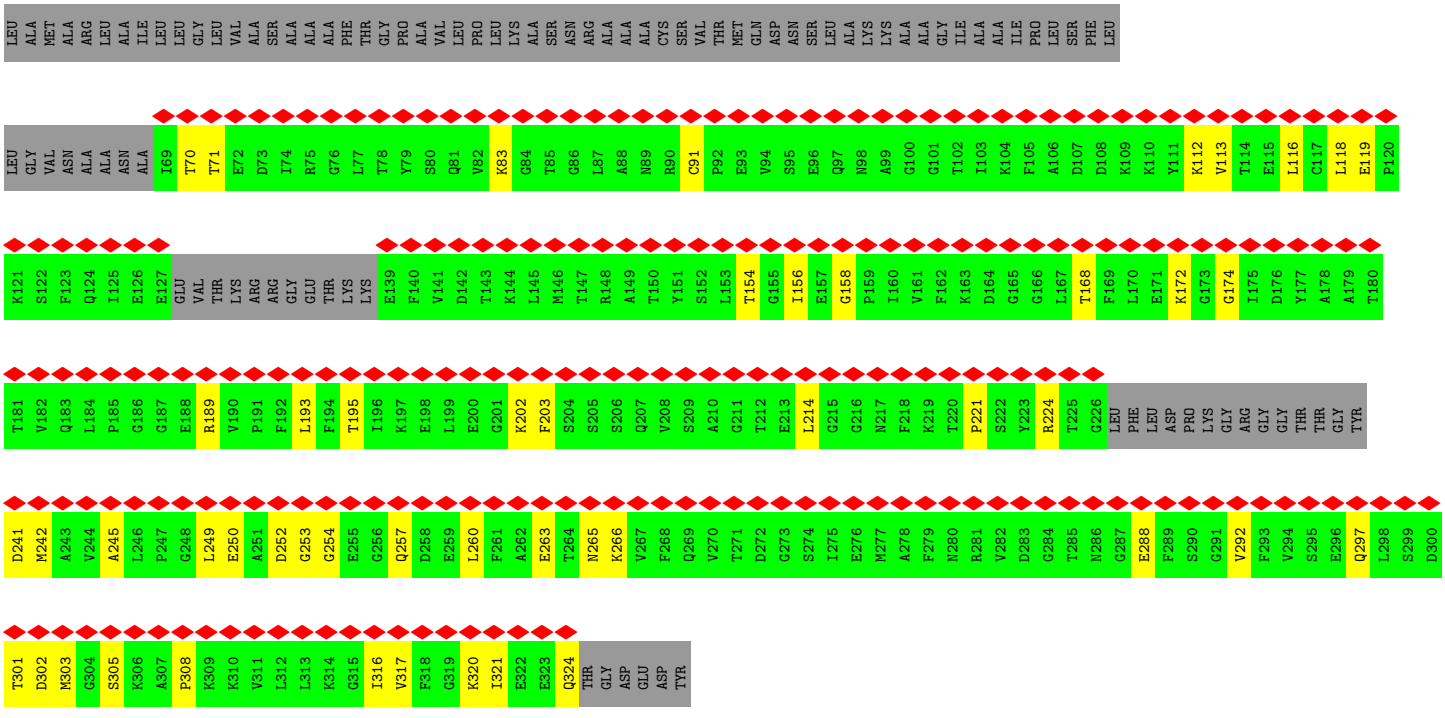




• Molecule 16: Photosystem II reaction center protein O

Chain o:

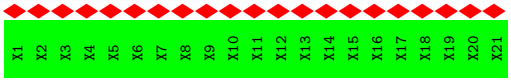




• Molecule 17: Photosystem II reaction center protein Q

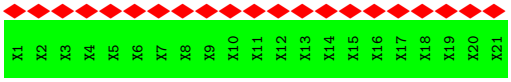
Chain Q:





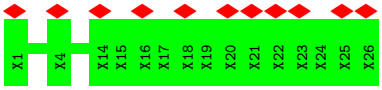
• Molecule 17: Photosystem II reaction center protein Q





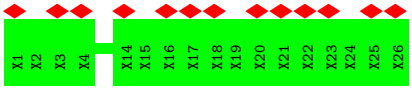
• Molecule 18: Photosystem II reaction center protein R





• Molecule 18: Photosystem II reaction center protein R



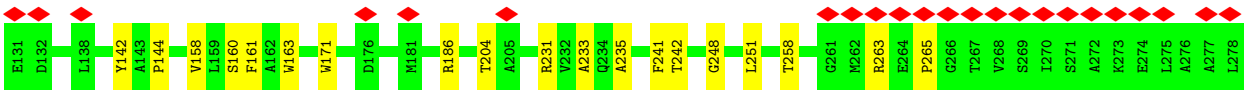


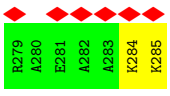
• Molecule 19: CCPII-S







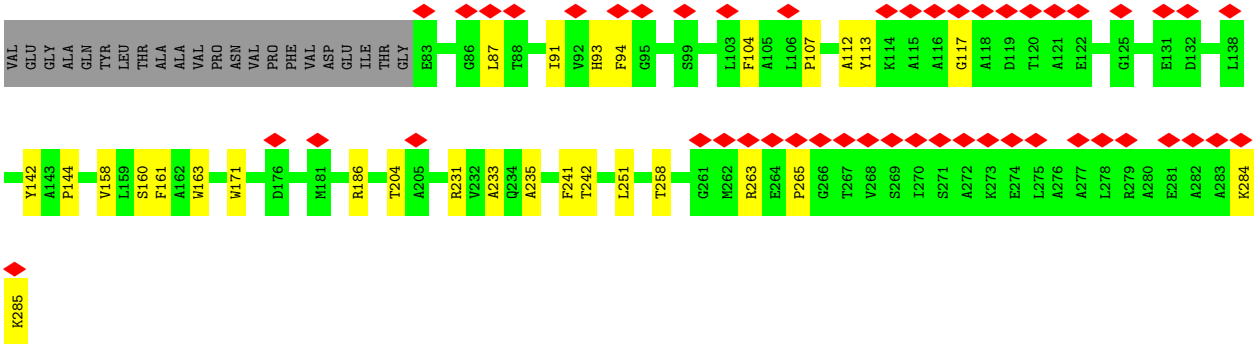




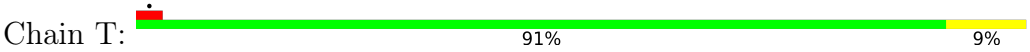
• Molecule 19: CCPII-S

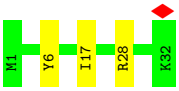




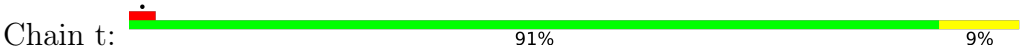


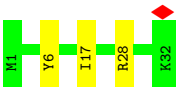
• Molecule 20: Photosystem II reaction center protein T





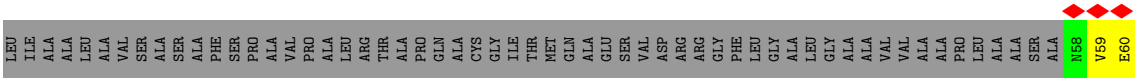
• Molecule 20: Photosystem II reaction center protein T

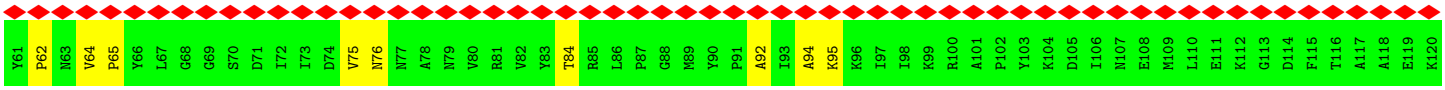


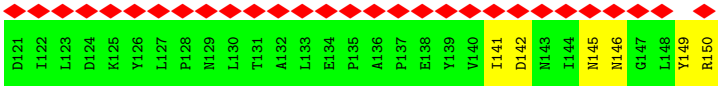


• Molecule 21: Photosystem II reaction center protein U



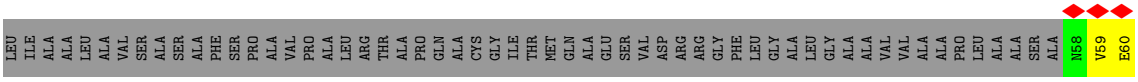


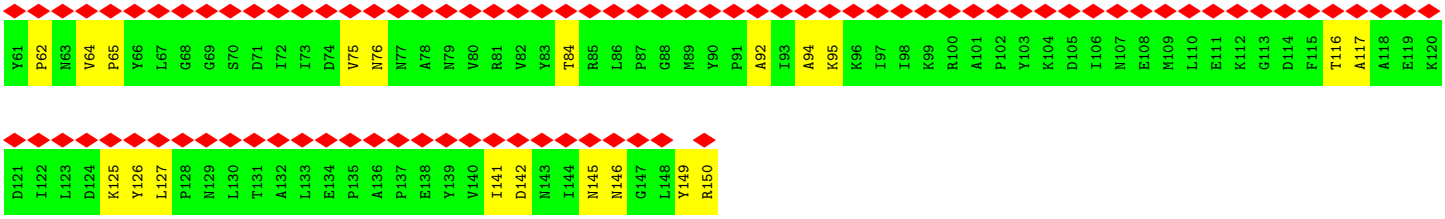




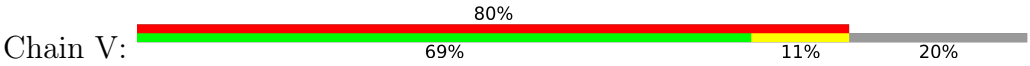
• Molecule 21: Photosystem II reaction center protein U

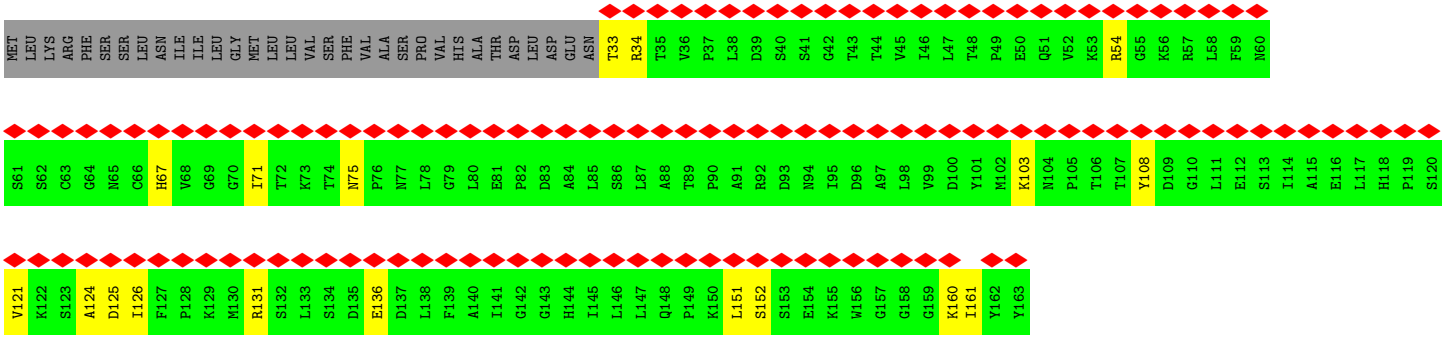




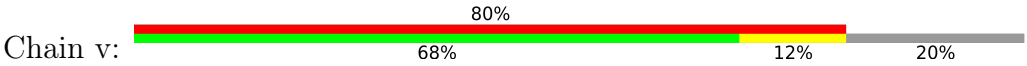


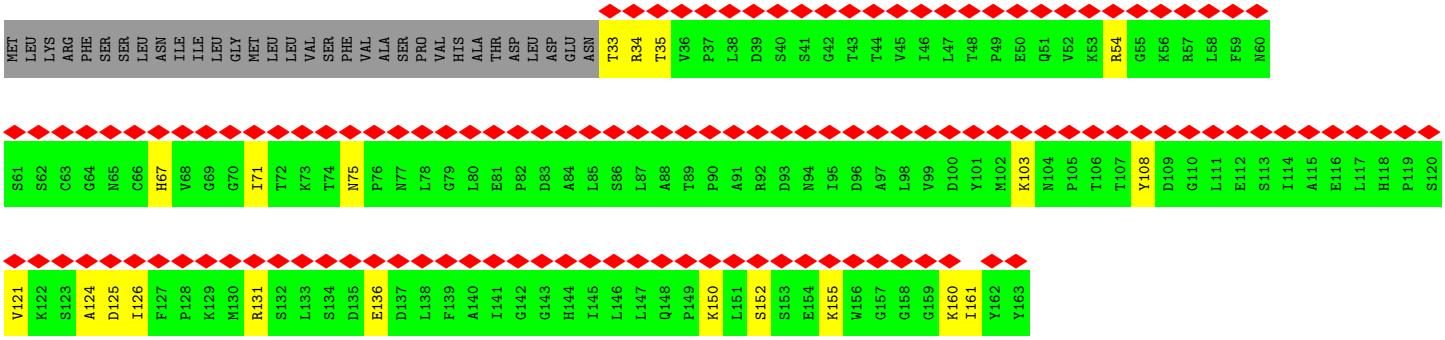
• Molecule 22: Photosystem II cytochrome c550





• Molecule 22: Photosystem II cytochrome c550





• Molecule 23: Photosystem II reaction center X protein





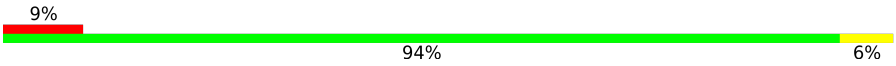
• Molecule 23: Photosystem II reaction center X protein

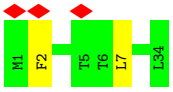




• Molecule 24: Photosystem II reaction center protein Ycf12

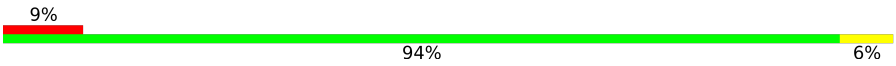
Chain Y:

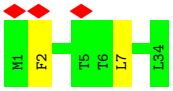




• Molecule 24: Photosystem II reaction center protein Ycf12

Chain y:

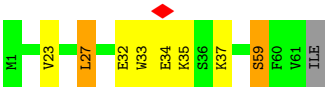




• Molecule 25: Photosystem II reaction center protein Z

Chain Z:

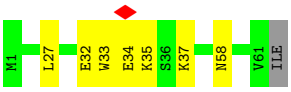




• Molecule 25: Photosystem II reaction center protein Z

Chain z:

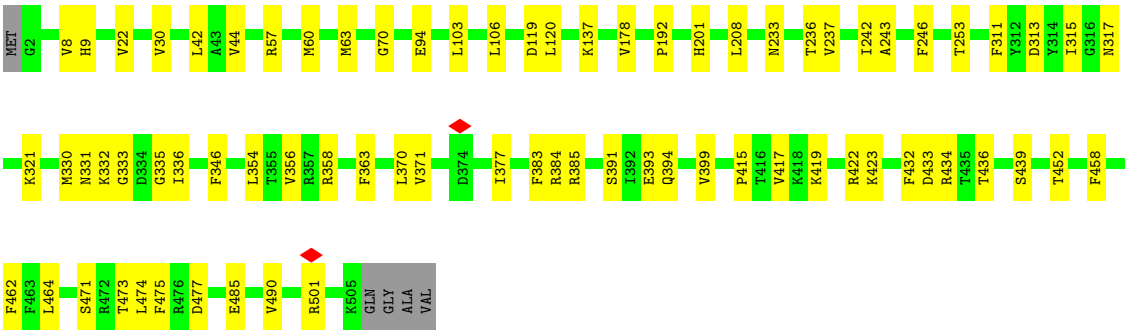




• Molecule 26: Photosystem II CP47 reaction center protein

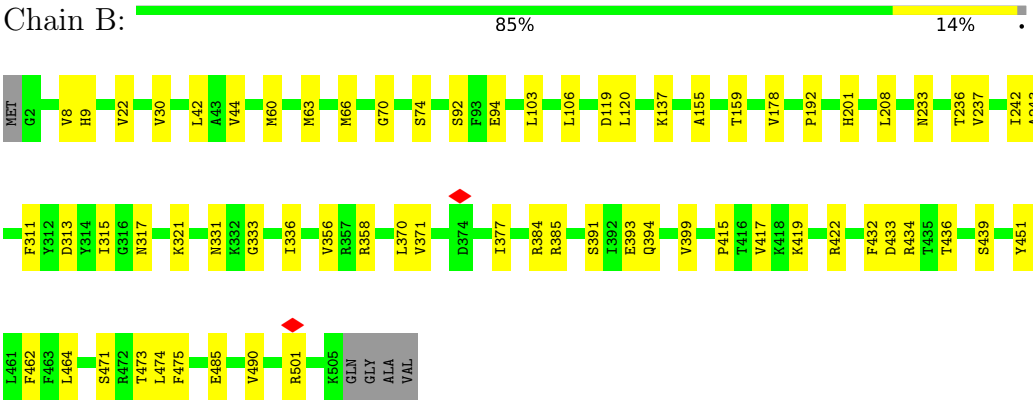
Chain b:





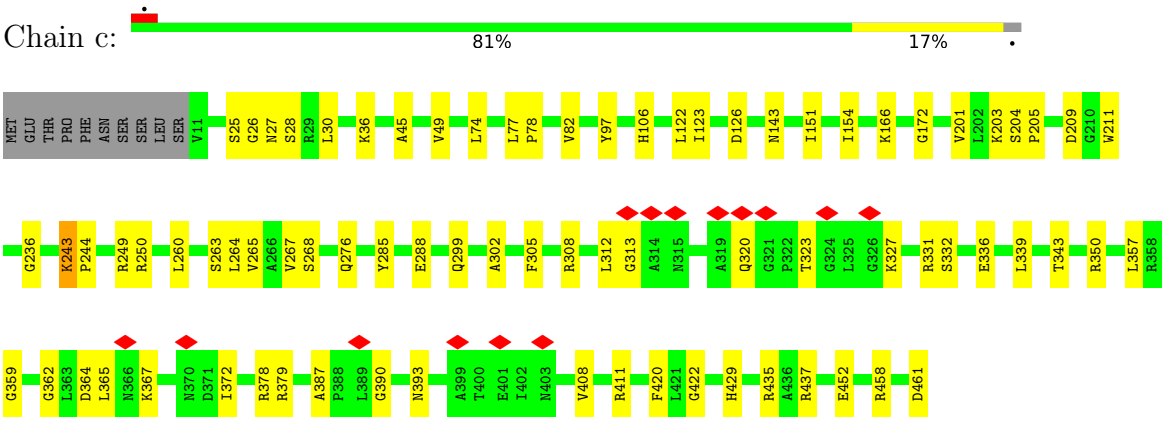
• Molecule 26: Photosystem II CP47 reaction center protein

Chain B:



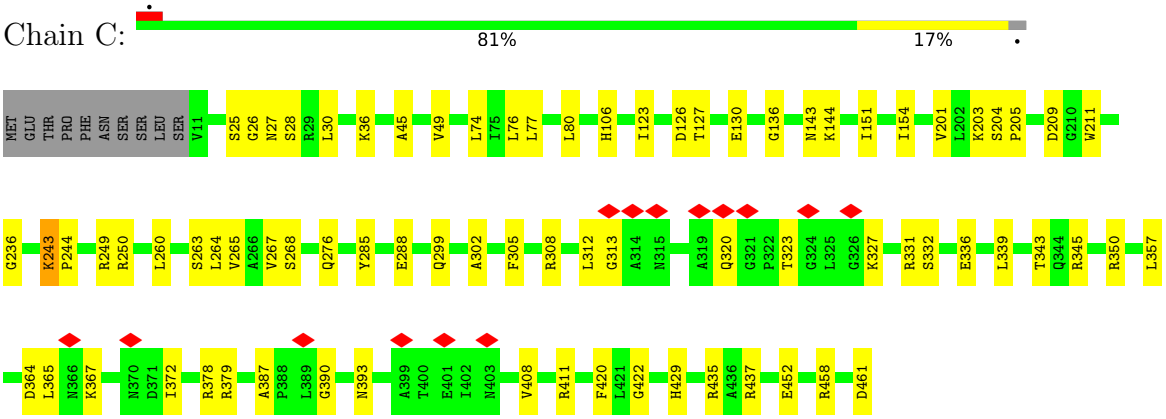
• Molecule 27: Photosystem II CP43 reaction center protein

Chain c:



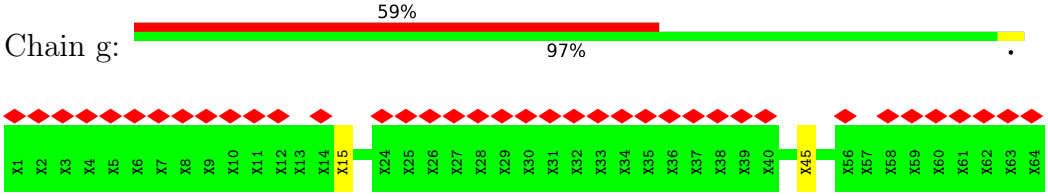
• Molecule 27: Photosystem II CP43 reaction center protein

Chain C:



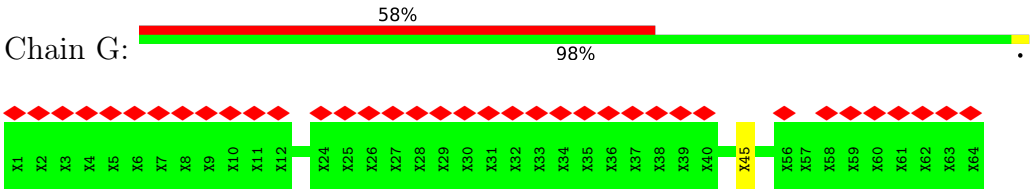
• Molecule 28: Photosystem II reaction center protein G

Chain g:



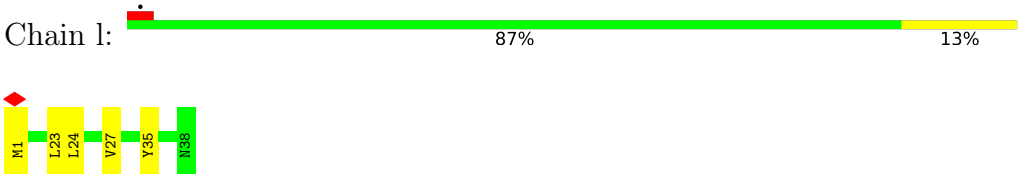
• Molecule 28: Photosystem II reaction center protein G

Chain G:



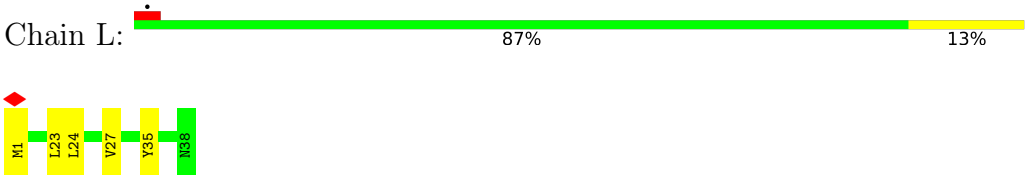
• Molecule 29: Photosystem II reaction center protein L

Chain l:



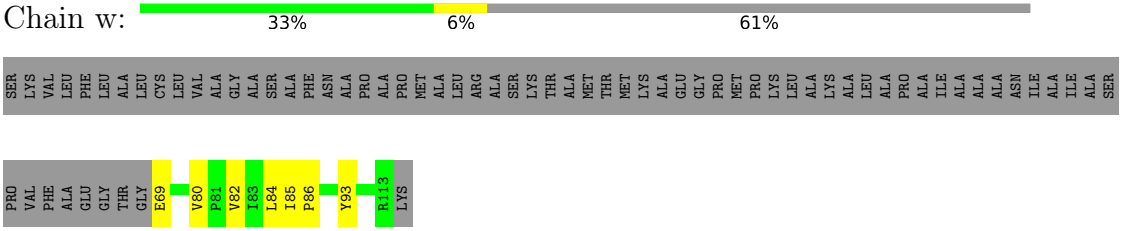
• Molecule 29: Photosystem II reaction center protein L

Chain L:



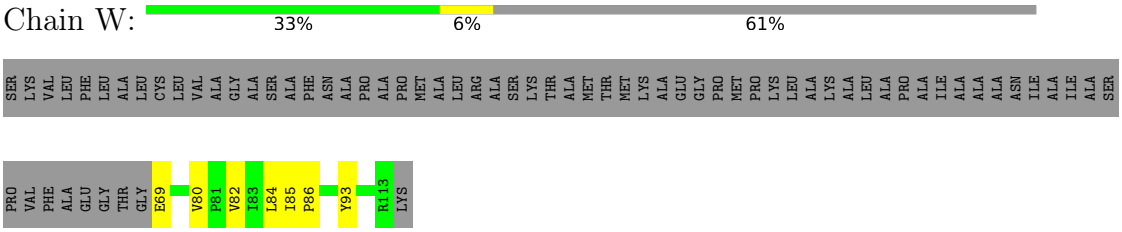
• Molecule 30: Photosystem II reaction center protein W

Chain w:



• Molecule 30: Photosystem II reaction center protein W

Chain W:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	305400	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.307	Depositor
Minimum map value	-0.333	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.253	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SQD, CLA, II3, PL9, FE2, DGD, OEX, CL, IHT, LHG, BCT, 8CT, PHO, HEM, II0, LMG, KC2

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	M	0.19	0/268	0.32	0/367
1	m	0.20	0/268	0.36	0/367
2	1	0.12	0/1507	0.34	0/2043
2	7	0.12	0/1507	0.34	0/2043
3	2	0.12	0/1399	0.28	0/1893
3	8	0.12	0/1399	0.28	0/1893
4	3	0.13	0/1404	0.27	0/1895
4	9	0.13	0/1404	0.25	0/1895
5	0	0.12	0/1339	0.29	0/1814
5	4	0.12	0/1339	0.30	0/1814
6	5	0.11	0/1510	0.30	0/2046
6	p	0.11	0/1510	0.31	0/2046
7	6	0.09	0/1380	0.27	0/1870
7	P	0.10	0/1380	0.27	0/1870
8	A	0.20	0/2702	0.31	0/3688
8	a	0.19	0/2702	0.31	0/3688
9	D	0.19	0/2806	0.29	0/3823
9	d	0.19	0/2806	0.29	0/3823
10	E	0.13	0/647	0.31	0/882
10	e	0.14	0/647	0.36	0/882
11	F	0.15	0/255	0.31	0/344
11	f	0.15	0/255	0.31	0/344
12	H	0.17	0/527	0.29	0/717
12	h	0.17	0/527	0.29	0/717
13	I	0.18	0/294	0.32	0/397
13	i	0.18	0/294	0.31	0/397
14	J	0.11	0/220	0.26	0/301
14	j	0.10	0/220	0.25	0/301
15	K	0.20	0/308	0.34	0/421
15	k	0.20	0/308	0.34	0/421
16	O	0.08	0/1774	0.26	0/2385
16	o	0.08	0/1774	0.26	0/2385

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
19	S	0.13	0/1603	0.31	0/2180
19	s	0.13	0/1603	0.31	0/2180
20	T	0.17	0/267	0.23	0/359
20	t	0.17	0/267	0.22	0/359
21	U	0.11	0/758	0.32	0/1031
21	u	0.12	0/758	0.33	0/1031
22	V	0.08	0/1016	0.25	0/1377
22	v	0.08	0/1016	0.25	0/1377
23	X	0.17	0/296	0.31	0/402
23	x	0.16	0/296	0.26	0/402
24	Y	0.11	0/271	0.26	0/367
24	y	0.11	0/271	0.25	0/367
25	Z	0.21	0/467	0.39	0/638
25	z	0.13	0/467	0.31	0/638
26	B	0.17	0/4093	0.28	0/5569
26	b	0.17	0/4093	0.28	0/5569
27	C	0.19	0/3619	0.32	0/4937
27	c	0.19	0/3619	0.32	0/4937
29	L	0.18	0/320	0.23	0/434
29	l	0.18	0/320	0.23	0/434
30	W	0.19	0/374	0.38	0/509
30	w	0.19	0/374	0.38	0/509
All	All	0.16	0/62848	0.30	0/85378

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	M	265	0	280	5	0
1	m	265	0	280	4	0
2	1	1472	0	1473	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	7	1472	0	1473	20	0
3	2	1362	0	1348	20	0
3	8	1362	0	1348	20	0
4	3	1371	0	1370	16	0
4	9	1371	0	1370	13	0
5	0	1308	0	1323	13	0
5	4	1308	0	1323	12	0
6	5	1471	0	1445	21	0
6	p	1471	0	1445	18	0
7	6	1344	0	1329	17	0
7	P	1344	0	1329	13	0
8	A	2618	0	2514	55	0
8	a	2618	0	2514	54	0
9	D	2713	0	2613	50	0
9	d	2713	0	2613	52	0
10	E	629	0	613	8	0
10	e	629	0	613	10	0
11	F	247	0	250	1	0
11	f	247	0	250	1	0
12	H	515	0	535	7	0
12	h	515	0	535	7	0
13	I	287	0	293	3	0
13	i	287	0	293	3	0
14	J	214	0	222	0	0
14	j	214	0	222	0	0
15	K	297	0	312	1	0
15	k	297	0	312	1	0
16	O	1749	0	1721	36	0
16	o	1749	0	1721	35	0
17	Q	105	0	23	0	0
17	q	105	0	23	0	0
18	R	130	0	29	0	0
18	r	130	0	29	0	0
19	S	1563	0	1540	25	0
19	s	1563	0	1540	23	0
20	T	260	0	278	4	0
20	t	260	0	278	4	0
21	U	742	0	743	15	0
21	u	742	0	743	18	0
22	V	996	0	998	15	0
22	v	996	0	998	16	0
23	X	292	0	318	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	x	292	0	318	1	0
24	Y	266	0	293	1	0
24	y	266	0	293	1	0
25	Z	457	0	501	9	0
25	z	457	0	501	5	0
26	B	3962	0	3858	63	0
26	b	3962	0	3858	63	0
27	C	3504	0	3421	61	0
27	c	3504	0	3421	62	0
28	G	320	0	70	1	0
28	g	320	0	71	2	0
29	L	310	0	313	5	0
29	l	310	0	313	5	0
30	W	367	0	354	5	0
30	w	367	0	354	5	0
31	3	40	0	0	0	0
31	6	40	0	0	0	0
31	9	40	0	0	0	0
31	A	40	0	0	0	0
31	B	120	0	0	0	0
31	C	40	0	0	0	0
31	D	40	0	0	0	0
31	H	40	0	0	0	0
31	K	80	0	0	0	0
31	M	40	0	0	0	0
31	P	40	0	0	0	0
31	Z	40	0	0	1	0
31	a	40	0	0	0	0
31	b	80	0	0	0	0
31	c	40	0	0	0	0
31	d	40	0	0	0	0
31	h	40	0	0	0	0
31	k	80	0	0	0	0
31	z	40	0	0	1	0
32	0	582	0	469	14	0
32	1	582	0	469	15	0
32	2	547	0	456	14	0
32	3	548	0	456	11	0
32	4	582	0	469	15	0
32	5	547	0	456	8	0
32	6	442	0	364	6	0
32	7	582	0	469	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	8	547	0	456	13	0
32	9	548	0	456	12	0
32	A	174	0	170	11	0
32	B	987	0	1039	35	0
32	C	799	0	836	26	0
32	D	176	0	164	5	0
32	G	45	0	33	1	0
32	P	442	0	364	7	0
32	S	110	0	105	5	0
32	a	174	0	170	9	0
32	b	987	0	1039	29	0
32	c	799	0	836	21	0
32	d	176	0	164	2	0
32	g	45	0	33	2	0
32	p	547	0	456	8	0
32	s	110	0	105	4	0
33	0	45	0	0	0	0
33	1	45	0	0	0	0
33	2	45	0	0	0	0
33	4	45	0	0	0	0
33	5	45	0	0	0	0
33	6	90	0	0	0	0
33	7	45	0	0	0	0
33	8	45	0	0	0	0
33	P	90	0	0	3	0
33	p	45	0	0	0	0
34	0	168	0	0	1	0
34	1	168	0	0	1	0
34	2	168	0	0	0	0
34	3	126	0	0	0	0
34	4	126	0	0	1	0
34	5	210	0	0	0	0
34	6	84	0	0	0	0
34	7	168	0	0	1	0
34	8	168	0	0	0	0
34	9	126	0	0	0	0
34	P	84	0	0	0	0
34	p	168	0	0	0	0
35	1	42	0	0	0	0
35	6	42	0	0	0	0
35	7	42	0	0	0	0
35	P	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	0	82	0	0	0	0
36	1	41	0	0	1	0
36	2	41	0	0	0	0
36	4	82	0	0	0	0
36	5	41	0	0	0	0
36	7	41	0	0	0	0
36	8	41	0	0	0	0
36	p	41	0	0	0	0
37	0	36	0	42	0	0
37	2	36	0	42	1	0
37	4	36	0	42	0	0
37	6	28	0	26	0	0
37	8	36	0	42	2	0
37	A	48	0	66	2	0
37	B	51	0	72	0	0
37	C	46	0	62	3	0
37	D	86	0	112	1	0
37	G	28	0	26	0	0
37	L	40	0	50	1	0
37	P	28	0	26	0	0
37	a	48	0	66	3	0
37	b	51	0	72	1	0
37	c	46	0	62	3	0
37	d	86	0	112	1	0
37	g	28	0	26	0	0
37	l	40	0	50	0	0
38	2	22	0	20	0	0
38	8	22	0	20	0	0
38	A	92	0	133	10	0
38	B	78	0	96	3	0
38	D	80	0	108	1	0
38	L	49	0	74	2	0
38	S	37	0	44	1	0
38	a	92	0	133	10	0
38	b	78	0	96	3	0
38	d	80	0	108	1	0
38	l	49	0	74	2	0
38	s	37	0	44	1	0
39	5	35	0	34	4	0
39	A	54	0	78	5	0
39	B	102	0	141	3	0
39	a	54	0	78	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	b	102	0	141	2	0
39	p	35	0	34	3	0
40	A	10	0	0	0	0
40	a	10	0	0	0	0
41	A	64	0	74	1	0
41	D	64	0	74	3	0
41	a	64	0	74	1	0
41	d	64	0	74	3	0
42	A	1	0	0	0	0
42	a	1	0	0	0	0
43	A	13	0	7	0	0
43	D	55	0	80	0	0
43	a	13	0	7	0	0
43	d	55	0	80	0	0
44	A	4	0	1	0	0
44	a	4	0	1	0	0
45	A	53	0	64	1	0
45	C	166	0	206	11	0
45	H	62	0	82	6	0
45	a	53	0	64	1	0
45	c	166	0	206	8	0
45	h	62	0	82	5	0
46	D	1	0	0	0	0
46	d	1	0	0	0	0
47	E	43	0	30	2	0
47	V	43	0	30	3	0
47	f	43	0	30	3	0
47	v	43	0	30	3	0
All	All	80246	0	74543	987	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 6.

All (987) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:103:ARG:HG3	1:M:106:ALA:HB2	1.64	0.80
26:b:434:ARG:HH12	16:o:249:LEU:HA	1.48	0.79
25:Z:59:SER:HB2	33:P:605:KC2:O1A	1.83	0.77
1:m:106:ALA:HB2	1:M:103:ARG:HG3	1.65	0.76
9:d:351:LEU:HD21	8:a:334:ARG:HE	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:249:LEU:HA	26:B:434:ARG:HH12	1.48	0.76
6:5:82:GLY:HA3	6:5:178:SER:HB3	1.68	0.76
26:B:9:HIS:HB2	32:B:612:CLA:HBA1	1.68	0.75
26:b:9:HIS:HB2	32:b:612:CLA:HBA1	1.68	0.75
6:p:82:GLY:HA3	6:p:178:SER:HB3	1.66	0.75
21:U:64:VAL:HG13	26:B:394:GLN:HE21	1.51	0.74
47:E:101:HEM:HBC2	47:E:101:HEM:HHD	1.68	0.74
2:1:155:VAL:HG22	32:1:607:CLA:HMA1	1.70	0.73
26:b:394:GLN:HE21	21:u:64:VAL:HG13	1.51	0.73
25:Z:59:SER:CB	33:P:605:KC2:O1A	2.35	0.73
4:3:211:PRO:O	4:3:213:GLU:N	2.22	0.73
25:Z:23:VAL:O	25:Z:27:LEU:HB2	1.88	0.73
27:C:357:LEU:HD21	27:C:372:ILE:HG12	1.71	0.73
27:c:357:LEU:HD21	27:c:372:ILE:HG12	1.71	0.73
2:7:155:VAL:HG22	32:7:607:CLA:HMA1	1.69	0.72
8:A:140:ARG:NH2	38:A:613:LHG:O5	2.22	0.72
6:5:208:PRO:HB2	6:5:213:PRO:HD3	1.71	0.72
8:a:140:ARG:NH2	38:a:403:LHG:O5	2.24	0.70
3:2:90:GLY:HA3	3:2:185:ALA:HB1	1.74	0.70
4:9:91:GLY:HA3	4:9:190:ALA:HB1	1.74	0.69
19:S:231:ARG:NH2	27:C:452:GLU:OE1	2.26	0.68
3:8:90:GLY:HA3	3:8:185:ALA:HB1	1.75	0.68
27:c:452:GLU:OE1	19:s:231:ARG:NH2	2.26	0.68
4:3:91:GLY:HA3	4:3:190:ALA:HB1	1.74	0.68
25:Z:33:TRP:O	25:Z:37:LYS:HB3	1.94	0.68
26:b:385:ARG:HD3	9:d:351:LEU:HA	1.75	0.67
1:M:103:ARG:HD3	19:s:251:LEU:HD21	1.77	0.67
22:v:152:SER:H	8:a:312:ARG:HG2	1.59	0.67
25:z:33:TRP:O	25:z:37:LYS:HB3	1.95	0.67
47:f:101:HEM:HHD	47:f:101:HEM:HBC2	1.77	0.66
6:p:182:MET:HE1	32:p:303:CLA:HAB	1.77	0.66
2:7:232:LEU:O	2:7:234:PRO:HD3	1.95	0.66
2:1:232:LEU:O	2:1:234:PRO:HD3	1.95	0.66
4:9:119:ALA:HB3	4:9:204:MET:HE1	1.77	0.66
26:b:394:GLN:NE2	21:u:64:VAL:O	2.29	0.65
32:1:603:CLA:HAC1	32:1:606:CLA:HAB	1.77	0.65
32:B:616:CLA:H2	32:B:617:CLA:HBB2	1.79	0.65
32:A:602:CLA:H122	41:A:604:PHO:H3A	1.78	0.65
1:m:103:ARG:HD3	19:S:251:LEU:HD21	1.79	0.64
21:U:64:VAL:O	26:B:394:GLN:NE2	2.30	0.64
9:d:56:SER:HG	9:d:64:SER:HG	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:616:CLA:H2	32:b:617:CLA:HBB2	1.79	0.64
19:s:284:LYS:HG3	19:s:285:LYS:HG2	1.80	0.64
6:5:182:MET:HE1	32:5:303:CLA:HAB	1.78	0.64
5:0:154:PHE:HB2	32:0:607:CLA:HMA1	1.79	0.64
2:7:130:HIS:HD2	2:7:139:MET:HE2	1.64	0.63
8:a:331:MET:HE3	8:a:334:ARG:HH12	1.62	0.63
32:a:405:CLA:H122	41:a:407:PHO:H3A	1.79	0.63
5:4:154:PHE:HB2	32:4:607:CLA:HMA1	1.80	0.63
9:D:171:SER:HB2	9:D:176:ALA:HB1	1.80	0.63
20:T:28:ARG:NH2	27:C:461:ASP:O	2.32	0.63
21:U:65:PRO:HB3	26:B:394:GLN:HB3	1.81	0.63
9:d:171:SER:HB2	9:d:176:ALA:HB1	1.81	0.62
8:a:93:PHE:HZ	32:a:408:CLA:HAA2	1.64	0.62
4:3:119:ALA:HB3	4:3:204:MET:HE1	1.81	0.62
19:S:284:LYS:HG3	19:S:285:LYS:HG2	1.79	0.62
26:b:394:GLN:HB3	21:u:65:PRO:HB3	1.81	0.62
27:c:267:VAL:HG12	32:c:502:CLA:HAC1	1.80	0.62
27:C:267:VAL:HG12	32:C:502:CLA:HAC1	1.80	0.62
8:A:93:PHE:HZ	32:A:605:CLA:HAA2	1.64	0.62
9:D:19:ASP:OD2	23:X:38:ARG:NH2	2.32	0.62
9:d:19:ASP:OD2	23:x:38:ARG:NH2	2.31	0.62
3:8:201:VAL:HG23	3:8:202:THR:HG23	1.81	0.62
27:c:461:ASP:O	20:t:28:ARG:NH2	2.32	0.62
16:O:116:LEU:HB3	16:O:156:ILE:HB	1.82	0.62
27:c:378:ARG:HE	22:v:126:ILE:HD12	1.65	0.61
32:4:608:CLA:HED3	32:4:608:CLA:H2A	1.81	0.61
27:C:80:LEU:HG	32:C:503:CLA:HED1	1.83	0.61
9:D:301:GLU:HB3	16:O:245:ALA:HB1	1.82	0.61
27:c:97:TYR:OH	25:z:58:ASN:ND2	2.33	0.61
32:0:608:CLA:H2A	32:0:608:CLA:HED3	1.81	0.61
3:2:201:VAL:HG23	3:2:202:THR:HG23	1.81	0.61
32:2:606:CLA:HHC	32:2:606:CLA:HBB1	1.83	0.61
32:9:606:CLA:HHC	32:9:606:CLA:HBB1	1.82	0.61
22:V:75:ASN:HD22	47:V:201:HEM:HAD1	1.66	0.61
22:V:126:ILE:HD12	27:C:378:ARG:HE	1.65	0.61
32:8:606:CLA:HHC	32:8:606:CLA:HBB1	1.83	0.61
6:p:115:ILE:HG13	32:p:305:CLA:HAA2	1.83	0.61
16:o:266:LYS:HD2	16:o:303:MET:HB2	1.83	0.60
47:V:201:HEM:HMB1	47:V:201:HEM:HBB2	1.83	0.60
22:v:75:ASN:HD22	47:v:201:HEM:HAD1	1.65	0.60
26:B:458:PHE:HB3	32:B:605:CLA:HBC2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:v:201:HEM:HMB1	47:v:201:HEM:HBB2	1.82	0.60
8:A:334:ARG:HH12	9:D:351:LEU:HD11	1.65	0.60
22:v:54:ARG:HH12	22:v:136:GLU:HG3	1.67	0.60
9:d:351:LEU:HD12	16:o:224:ARG:HH22	1.65	0.60
5:4:117:VAL:HG23	32:4:613:CLA:HBC3	1.83	0.60
9:d:231:PHE:O	8:a:267:ASN:ND2	2.34	0.60
27:c:143:ASN:HD21	28:g:45:UNK:HA	1.67	0.60
27:C:143:ASN:HD21	28:G:45:UNK:HA	1.67	0.60
8:A:192:ILE:HG13	8:A:293:MET:HE1	1.84	0.59
45:c:515:DGD:HG31	37:c:517:LMG:HC92	1.84	0.59
16:o:116:LEU:HB3	16:o:156:ILE:HB	1.83	0.59
5:0:117:VAL:HG23	32:0:613:CLA:HBC3	1.83	0.59
7:P:201:GLN:HB3	7:P:212:GLN:HE22	1.67	0.59
32:3:606:CLA:HHC	32:3:606:CLA:HBB1	1.82	0.59
7:6:201:GLN:HB3	7:6:212:GLN:HE22	1.68	0.59
8:A:250:ALA:HA	26:B:490:VAL:HG11	1.85	0.59
8:A:323:ARG:NH1	22:V:161:ILE:O	2.36	0.59
8:a:192:ILE:HG13	8:a:293:MET:HE1	1.85	0.59
26:B:311:PHE:O	26:B:317:ASN:ND2	2.35	0.59
26:b:458:PHE:HB3	32:b:605:CLA:HBC2	1.84	0.59
10:E:79:ASP:HA	10:E:82:LYS:HE3	1.85	0.59
26:b:311:PHE:O	26:b:317:ASN:ND2	2.35	0.59
26:b:490:VAL:HG11	8:a:250:ALA:HA	1.84	0.59
11:f:34:ILE:HA	11:f:37:MET:HE3	1.85	0.59
45:C:515:DGD:HG31	37:C:517:LMG:HC92	1.84	0.59
7:6:192:MET:HE1	32:6:602:CLA:HAB	1.83	0.58
11:F:34:ILE:HA	11:F:37:MET:HE3	1.85	0.58
22:V:54:ARG:HH12	22:V:136:GLU:HG3	1.68	0.58
16:o:263:GLU:O	16:o:266:LYS:NZ	2.32	0.58
4:3:120:THR:HG23	4:3:204:MET:HE2	1.86	0.58
26:b:44:VAL:HG23	26:b:60:MET:HE1	1.86	0.58
32:b:605:CLA:HBB1	32:b:614:CLA:HBC2	1.86	0.58
10:e:79:ASP:HA	10:e:82:LYS:HE3	1.85	0.58
26:b:422:ARG:HD2	16:o:250:GLU:HG2	1.85	0.58
26:b:423:LYS:HZ1	16:o:253:GLY:H	1.52	0.58
9:D:73:PHE:HE2	45:C:516:DGD:HA21	1.69	0.57
47:V:201:HEM:HMC1	47:V:201:HEM:HBC2	1.86	0.57
47:v:201:HEM:HMC1	47:v:201:HEM:HBC2	1.86	0.57
4:9:150:LEU:HD22	32:9:606:CLA:HMA1	1.86	0.57
3:8:112:PRO:HG2	3:8:114:MET:HE1	1.86	0.57
26:B:44:VAL:HG23	26:B:60:MET:HE1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:E:101:HEM:HBB2	47:E:101:HEM:HMB2	1.86	0.57
9:d:301:GLU:HB3	16:o:245:ALA:HB1	1.85	0.57
7:P:192:MET:HE1	32:P:602:CLA:HAB	1.87	0.57
4:3:150:LEU:HD22	32:3:606:CLA:HMA1	1.86	0.57
9:D:351:LEU:HB2	26:B:385:ARG:HD3	1.87	0.57
8:a:165:GLN:NE2	8:a:294:ALA:O	2.38	0.57
3:2:108:PHE:HB2	3:2:111:PHE:HD2	1.68	0.57
3:8:108:PHE:HB2	3:8:111:PHE:HD2	1.69	0.57
16:O:288:GLU:HG2	16:O:320:LYS:HG2	1.86	0.57
27:c:285:TYR:O	27:c:411:ARG:NH2	2.37	0.57
32:B:605:CLA:HBB1	32:B:614:CLA:HBC2	1.86	0.57
6:5:70:ASP:H	19:S:112:ALA:HB1	1.70	0.56
27:C:76:LEU:HB3	32:C:503:CLA:HED2	1.87	0.56
27:c:265:VAL:HB	27:c:429:HIS:CG	2.41	0.56
1:m:106:ALA:HB3	1:M:106:ALA:HB3	1.86	0.56
26:b:243:ALA:HA	26:b:246:PHE:CE2	2.41	0.56
47:f:101:HEM:HBB2	47:f:101:HEM:HMB2	1.86	0.56
32:0:603:CLA:HBC1	32:0:607:CLA:HBC2	1.87	0.56
16:o:288:GLU:HG2	16:o:320:LYS:HG2	1.86	0.56
22:v:161:ILE:O	8:a:323:ARG:NH1	2.37	0.56
4:9:120:THR:HG23	4:9:204:MET:HE2	1.87	0.56
32:4:603:CLA:HAC1	32:4:606:CLA:HAB	1.87	0.56
26:b:137:LYS:NZ	12:h:17:GLU:OE1	2.29	0.56
45:c:516:DGD:HA21	9:d:73:PHE:HE2	1.69	0.56
12:H:17:GLU:OE1	26:B:137:LYS:NZ	2.29	0.56
3:2:132:ILE:HD12	32:2:606:CLA:HBC1	1.87	0.56
16:O:168:THR:HG22	16:O:202:LYS:HB3	1.86	0.56
25:Z:23:VAL:O	25:Z:27:LEU:CB	2.53	0.56
3:8:132:ILE:HD12	32:8:606:CLA:HBC1	1.88	0.56
3:8:54:ARG:O	19:s:186:ARG:NH2	2.38	0.55
6:5:115:ILE:HG13	32:5:305:CLA:HAA2	1.87	0.55
21:U:62:PRO:HA	26:B:393:GLU:HB3	1.88	0.55
9:d:184:ILE:O	9:d:188:HIS:HB2	2.05	0.55
26:B:243:ALA:HA	26:B:246:PHE:CE2	2.41	0.55
26:b:432:PHE:HB2	16:o:252:ASP:HA	1.88	0.55
27:C:265:VAL:HB	27:C:429:HIS:CG	2.41	0.55
26:b:393:GLU:HB3	21:u:62:PRO:HA	1.89	0.55
26:b:471:SER:HB2	9:d:139:PRO:HG2	1.89	0.55
27:C:26:GLY:HA3	32:C:511:CLA:HMD2	1.87	0.55
27:c:26:GLY:HA3	32:c:511:CLA:HMD2	1.88	0.55
27:c:435:ARG:HE	38:a:403:LHG:HC2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:145:VAL:O	8:a:148:THR:OG1	2.24	0.55
22:v:124:ALA:HB1	22:v:131:ARG:HG2	1.89	0.55
27:c:25:SER:O	27:c:28:SER:OG	2.24	0.54
8:A:170:ASP:OD2	27:C:345:ARG:NH1	2.40	0.54
12:H:7:LEU:HD21	32:B:616:CLA:H161	1.89	0.54
16:O:263:GLU:O	16:O:266:LYS:NZ	2.40	0.54
27:c:390:GLY:HA3	27:c:408:VAL:HG22	1.89	0.54
8:A:145:VAL:O	8:A:148:THR:OG1	2.24	0.54
8:A:165:GLN:NE2	8:A:294:ALA:O	2.39	0.54
16:o:168:THR:HG22	16:o:202:LYS:HB3	1.88	0.54
2:7:182:ASN:HD22	2:7:185:THR:H	1.55	0.54
9:D:139:PRO:HG2	26:B:471:SER:HB2	1.89	0.54
27:C:285:TYR:O	27:C:411:ARG:NH2	2.37	0.54
32:c:504:CLA:H42	45:c:515:DGD:HB31	1.89	0.54
21:u:142:ASP:HB3	21:u:146:ASN:HA	1.89	0.54
27:C:25:SER:O	27:C:28:SER:OG	2.24	0.54
27:C:390:GLY:HA3	27:C:408:VAL:HG22	1.89	0.54
4:9:211:PRO:O	4:9:213:GLU:N	2.39	0.54
32:C:504:CLA:H42	45:C:515:DGD:HB31	1.88	0.54
26:b:422:ARG:NE	16:o:242:MET:SD	2.80	0.54
8:A:267:ASN:ND2	9:D:231:PHE:O	2.33	0.53
26:b:464:LEU:HD21	38:a:402:LHG:H261	1.91	0.53
9:d:188:HIS:HD1	9:d:293:ARG:HD3	1.73	0.53
8:A:85:SER:HA	8:A:109:GLY:HA3	1.90	0.53
16:O:242:MET:SD	26:B:422:ARG:HD3	2.48	0.53
26:b:485:GLU:O	26:b:501:ARG:NH2	2.41	0.53
8:a:82:VAL:HB	8:a:174:LEU:HB2	1.90	0.53
8:a:84:PRO:HA	8:a:112:TYR:CG	2.44	0.53
2:1:54:ALA:HB3	2:1:74:PHE:HB2	1.89	0.53
2:1:102:ALA:O	2:1:106:MET:HG2	2.08	0.53
8:A:82:VAL:HB	8:A:174:LEU:HB2	1.90	0.53
8:a:283:ILE:HA	8:a:286:THR:HG22	1.90	0.53
8:A:84:PRO:HA	8:A:112:TYR:CG	2.43	0.53
38:A:612:LHG:H261	26:B:464:LEU:HD21	1.90	0.53
21:U:142:ASP:HB3	21:U:146:ASN:HA	1.89	0.53
32:7:608:CLA:H2A	32:7:608:CLA:HED3	1.90	0.53
27:c:74:LEU:HD13	27:c:77:LEU:HD12	1.89	0.53
2:7:89:ARG:NH1	2:7:92:GLU:OE1	2.42	0.53
26:B:485:GLU:O	26:B:501:ARG:NH2	2.42	0.53
27:c:320:GLN:HB3	21:u:141:ILE:HD11	1.91	0.53
2:7:54:ALA:HB3	2:7:74:PHE:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:191:ARG:HA	4:3:194:MET:HE3	1.91	0.53
32:1:608:CLA:H2A	32:1:608:CLA:HED3	1.90	0.53
32:b:604:CLA:HAB	32:b:606:CLA:H152	1.91	0.53
38:A:613:LHG:HC2	27:C:435:ARG:HE	1.73	0.53
32:b:616:CLA:H161	12:h:7:LEU:HD21	1.89	0.53
16:o:241:ASP:HA	21:u:59:VAL:HG22	1.91	0.53
45:C:515:DGD:HB81	37:C:517:LMG:H421	1.91	0.53
32:B:604:CLA:HAB	32:B:606:CLA:H152	1.91	0.52
8:A:312:ARG:HG2	22:V:152:SER:H	1.73	0.52
21:U:141:ILE:HD11	27:C:320:GLN:HB3	1.91	0.52
8:a:162:PRO:HB3	8:a:168:PHE:HA	1.91	0.52
6:p:129:SER:HB3	32:p:308:CLA:HAB	1.91	0.52
2:1:182:ASN:HD22	2:1:185:THR:H	1.55	0.52
22:V:124:ALA:HB1	22:V:131:ARG:HG2	1.89	0.52
8:A:308:ASP:OD1	8:A:312:ARG:N	2.43	0.52
8:A:334:ARG:HD2	9:D:319:LEU:HD13	1.92	0.52
16:O:113:VAL:HG22	16:O:321:ILE:HG12	1.92	0.52
32:b:609:CLA:HBC3	32:b:610:CLA:H122	1.92	0.52
45:c:515:DGD:HB81	37:c:517:LMG:H421	1.91	0.52
4:9:191:ARG:HA	4:9:194:MET:HE3	1.91	0.52
25:z:34:GLU:HA	25:z:37:LYS:HE3	1.91	0.52
2:7:94:LYS:NZ	2:7:150:GLU:OE2	2.40	0.52
38:a:403:LHG:H261	39:a:409:SQD:H241	1.92	0.52
32:0:608:CLA:H51	32:0:608:CLA:HBB1	1.92	0.52
3:8:198:GLN:HB3	3:8:209:GLN:HE22	1.75	0.52
4:9:173:SER:HB2	4:9:179:LEU:HD13	1.92	0.52
4:3:171:ASN:ND2	19:S:117:GLY:O	2.42	0.52
4:3:173:SER:HB2	4:3:179:LEU:HD13	1.92	0.52
32:4:608:CLA:HBB1	32:4:608:CLA:H51	1.91	0.52
6:5:141:GLN:HE22	7:6:53:GLU:HG2	1.75	0.52
32:6:611:CLA:H2A	32:6:611:CLA:HED2	1.92	0.52
21:U:60:GLU:HG3	26:B:415:PRO:HG3	1.91	0.52
32:B:609:CLA:HBC3	32:B:610:CLA:H122	1.92	0.52
21:U:92:ALA:O	21:U:94:ALA:N	2.42	0.52
26:b:415:PRO:HG3	21:u:60:GLU:HG3	1.90	0.52
5:0:103:ALA:HA	5:0:206:MET:HE1	1.92	0.52
3:2:137:SER:HB3	32:2:607:CLA:HAB	1.91	0.51
39:A:606:SQD:H241	38:A:613:LHG:H261	1.92	0.51
9:d:174:VAL:HG11	32:a:406:CLA:HED1	1.92	0.51
38:d:405:LHG:H271	29:l:23:LEU:HD22	1.92	0.51
8:A:283:ILE:HA	8:A:286:THR:HG22	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:d:26:PHE:O	8:a:261:GLN:NE2	2.43	0.51
2:1:89:ARG:NH1	2:1:92:GLU:OE1	2.43	0.51
8:A:286:THR:OG1	32:A:602:CLA:O1D	2.26	0.51
27:C:299:GLN:NE2	27:C:343:THR:OG1	2.43	0.51
26:b:236:THR:HB	26:b:473:THR:HG21	1.93	0.51
9:d:53:PHE:O	10:e:50:THR:OG1	2.26	0.51
3:8:102:VAL:HA	3:8:105:VAL:HG12	1.92	0.51
32:0:607:CLA:HBA1	32:9:609:CLA:H102	1.92	0.51
32:0:607:CLA:HMB2	32:9:609:CLA:H122	1.92	0.51
4:9:171:ASN:ND2	19:s:117:GLY:O	2.41	0.51
38:D:406:LHG:H271	29:L:23:LEU:HD22	1.92	0.51
19:S:113:TYR:O	19:S:117:GLY:N	2.44	0.51
8:a:46:THR:HG21	45:a:414:DGD:HB92	1.93	0.51
8:A:162:PRO:HB3	8:A:168:PHE:HA	1.92	0.51
32:A:603:CLA:HED1	9:D:174:VAL:HG11	1.92	0.51
27:C:244:PRO:HA	32:C:506:CLA:HED3	1.93	0.51
3:2:54:ARG:O	19:S:186:ARG:NH2	2.38	0.51
9:D:53:PHE:O	10:E:50:THR:OG1	2.26	0.51
27:c:244:PRO:HA	32:c:506:CLA:HED3	1.92	0.51
19:s:242:THR:O	20:t:28:ARG:NH1	2.41	0.51
27:c:393:ASN:ND2	8:a:301:ASN:O	2.44	0.51
6:p:107:LEU:HD13	6:p:192:TYR:HE1	1.76	0.51
26:B:236:THR:HB	26:B:473:THR:HG21	1.93	0.51
8:a:85:SER:HA	8:a:109:GLY:HA3	1.91	0.50
3:2:198:GLN:HB3	3:2:209:GLN:HE22	1.75	0.50
9:D:48:PHE:O	9:D:52:THR:OG1	2.28	0.50
16:O:241:ASP:O	26:B:422:ARG:NH1	2.45	0.50
27:c:299:GLN:NE2	27:c:343:THR:OG1	2.44	0.50
32:7:602:CLA:H2A	32:7:602:CLA:HED3	1.93	0.50
19:s:113:TYR:O	19:s:117:GLY:N	2.44	0.50
7:6:198:MET:HE3	7:6:209:VAL:HG11	1.94	0.50
8:a:308:ASP:OD1	8:a:312:ARG:N	2.44	0.50
26:B:22:VAL:HG11	32:B:615:CLA:HMA1	1.93	0.50
6:5:107:LEU:HD13	6:5:192:TYR:HE1	1.75	0.50
15:K:22:ASP:HB3	37:C:517:LMG:H111	1.94	0.50
16:O:252:ASP:HA	26:B:432:PHE:HB2	1.93	0.50
32:b:610:CLA:OBD	12:h:27:THR:OG1	2.30	0.50
3:8:80:ARG:HB3	3:8:150:LEU:HD11	1.94	0.50
4:9:92:ARG:HA	4:9:95:MET:HE3	1.93	0.50
8:a:286:THR:OG1	32:a:405:CLA:O1D	2.26	0.50
9:D:184:ILE:O	9:D:188:HIS:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:193:LEU:O	16:O:297:GLN:NE2	2.43	0.50
27:c:30:LEU:HD21	32:c:511:CLA:H2A	1.92	0.50
16:o:302:ASP:HB3	16:o:305:SER:HB3	1.94	0.50
32:9:609:CLA:H43	39:p:318:SQD:H242	1.92	0.50
37:A:607:LMG:H111	27:C:204:SER:HA	1.93	0.50
9:d:319:LEU:HD13	8:a:334:ARG:CZ	2.42	0.50
16:o:113:VAL:HG22	16:o:321:ILE:HG12	1.93	0.50
6:5:47:PRO:HG2	6:5:50:LEU:HD12	1.93	0.50
19:S:94:PHE:HA	19:S:97:VAL:HG12	1.94	0.50
19:S:258:THR:HA	19:S:263:ARG:HH21	1.76	0.50
6:p:70:ASP:H	19:s:112:ALA:HB1	1.76	0.50
32:1:602:CLA:HED3	32:1:602:CLA:H2A	1.93	0.50
4:3:92:ARG:HA	4:3:95:MET:HE3	1.93	0.50
8:A:261:GLN:NE2	9:D:26:PHE:O	2.44	0.50
32:P:611:CLA:H2A	32:P:611:CLA:HED2	1.93	0.50
21:U:145:ASN:HD22	27:C:327:LYS:HD3	1.77	0.50
27:c:204:SER:HA	37:a:410:LMG:H111	1.94	0.50
21:u:92:ALA:O	21:u:94:ALA:N	2.41	0.49
5:0:159:GLN:HA	5:0:162:GLN:HG2	1.94	0.49
26:B:201:HIS:HB2	32:B:603:CLA:CHB	2.42	0.49
32:3:609:CLA:H122	32:4:607:CLA:HMB2	1.94	0.49
32:0:612:CLA:H2A	32:0:612:CLA:O2D	2.12	0.49
8:a:77:ILE:HD11	20:t:6:TYR:HB3	1.94	0.49
7:6:49:VAL:HG21	7:6:70:PRO:HG3	1.94	0.49
19:s:258:THR:HA	19:s:263:ARG:HH21	1.76	0.49
32:3:609:CLA:H43	39:5:318:SQD:H242	1.93	0.49
27:c:327:LYS:HD3	21:u:145:ASN:HD22	1.77	0.49
7:P:121:PHE:CZ	7:P:129:LEU:HD11	2.47	0.49
5:4:159:GLN:HA	5:4:162:GLN:HG2	1.94	0.49
9:D:77:VAL:HB	9:D:172:LEU:HB2	1.94	0.49
27:c:350:ARG:HH21	16:o:83:LYS:HD2	1.77	0.49
9:d:77:VAL:HB	9:d:172:LEU:HB2	1.94	0.49
3:8:44:ASP:OD1	3:8:44:ASP:N	2.45	0.49
26:B:433:ASP:OD2	26:B:436:THR:OG1	2.27	0.49
9:d:351:LEU:HD23	8:a:334:ARG:HH21	1.78	0.49
5:4:93:LEU:HD22	5:4:169:GLY:HA3	1.94	0.49
16:o:156:ILE:HA	16:o:174:GLY:HA3	1.95	0.49
3:2:44:ASP:N	3:2:44:ASP:OD1	2.45	0.49
26:b:22:VAL:HG11	32:b:615:CLA:HMA1	1.93	0.49
4:3:165:LEU:HB2	32:3:607:CLA:HMD1	1.94	0.49
32:4:612:CLA:O2D	32:4:612:CLA:H2A	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:201:GLY:HA3	8:A:286:THR:HB	1.95	0.49
26:b:201:HIS:HB2	32:b:603:CLA:CHB	2.42	0.49
26:b:233:ASN:O	26:b:236:THR:HG22	2.12	0.49
2:1:94:LYS:NZ	2:1:150:GLU:OE2	2.41	0.48
27:c:123:ILE:HB	25:z:27:LEU:HD21	1.95	0.48
27:c:288:GLU:OE2	27:c:379:ARG:NH1	2.46	0.48
7:P:196:GLY:O	7:P:200:HIS:ND1	2.34	0.48
32:D:404:CLA:H41	32:D:404:CLA:H62	1.58	0.48
16:O:156:ILE:HA	16:O:174:GLY:HA3	1.96	0.48
19:S:87:LEU:HB3	38:S:301:LHG:HC12	1.95	0.48
26:b:391:SER:N	26:b:394:GLN:OE1	2.41	0.48
5:0:93:LEU:HD22	5:0:169:GLY:HA3	1.94	0.48
27:C:74:LEU:HD13	27:C:77:LEU:HD12	1.95	0.48
27:C:332:SER:OG	27:C:336:GLU:OE1	2.25	0.48
6:p:47:PRO:HG2	6:p:50:LEU:HD12	1.94	0.48
27:c:305:PHE:HA	27:c:308:ARG:HG2	1.94	0.48
32:c:505:CLA:HAA2	8:a:131:TRP:CH2	2.49	0.48
37:c:517:LMG:H111	15:k:22:ASP:HB3	1.94	0.48
9:d:50:GLY:HA3	9:d:77:VAL:HG22	1.95	0.48
6:5:212:PHE:N	6:5:213:PRO:HD2	2.28	0.48
32:5:306:CLA:HBA1	32:6:610:CLA:HBD	1.95	0.48
9:D:50:GLY:HA3	9:D:77:VAL:HG22	1.95	0.48
19:S:242:THR:O	20:T:28:ARG:NH1	2.41	0.48
26:B:233:ASN:O	26:B:236:THR:HG22	2.12	0.48
3:2:80:ARG:HB3	3:2:150:LEU:HD11	1.95	0.48
7:6:121:PHE:CZ	7:6:129:LEU:HD11	2.48	0.48
8:A:301:ASN:O	27:C:393:ASN:ND2	2.45	0.48
16:o:193:LEU:O	16:o:297:GLN:NE2	2.43	0.48
25:z:32:GLU:HA	25:z:35:LYS:HB3	1.94	0.48
8:A:46:THR:O	8:A:50:ILE:HG13	2.13	0.48
8:A:311:GLY:HA3	22:V:151:LEU:HD21	1.95	0.48
19:S:100:LEU:HD12	32:S:302:CLA:HBB2	1.96	0.48
10:e:58:THR:O	10:e:62:GLN:NE2	2.47	0.48
27:C:288:GLU:OE2	27:C:379:ARG:NH1	2.46	0.48
32:B:606:CLA:H92	32:B:606:CLA:H61	1.70	0.48
9:D:190:PHE:CD1	9:D:288:LEU:HD11	2.49	0.48
16:O:83:LYS:HD2	27:C:350:ARG:HH21	1.79	0.48
16:O:112:LYS:HE3	16:O:324:GLN:HA	1.95	0.48
16:O:301:THR:HG22	16:O:308:PRO:HG3	1.94	0.48
26:b:384:ARG:HH21	9:d:351:LEU:HD22	1.79	0.48
27:c:276:GLN:HG3	45:c:514:DGD:HB32	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:o:301:THR:HG22	16:o:308:PRO:HG3	1.96	0.48
3:2:102:VAL:HA	3:2:105:VAL:HG12	1.96	0.48
8:A:77:ILE:HD11	20:T:6:TYR:HB3	1.94	0.48
16:o:189:ARG:HH12	8:a:56:PRO:HB2	1.79	0.48
21:u:84:THR:O	22:v:108:TYR:OH	2.31	0.48
21:u:150:ARG:HD3	22:v:160:LYS:H	1.79	0.48
27:C:27:ASN:ND2	32:C:510:CLA:O1A	2.42	0.48
32:2:603:CLA:HAC1	32:2:606:CLA:HAB	1.95	0.48
16:o:189:ARG:HH22	8:a:56:PRO:HB2	1.79	0.48
32:C:513:CLA:H3A	32:C:513:CLA:HBA2	1.45	0.48
7:P:208:GLY:O	7:P:212:GLN:N	2.43	0.48
32:P:610:CLA:HBD	32:p:306:CLA:HBA1	1.96	0.48
32:p:303:CLA:H3A	32:p:303:CLA:HBA2	1.42	0.48
32:3:607:CLA:H142	32:3:607:CLA:H111	1.75	0.48
10:E:58:THR:O	10:E:62:GLN:NE2	2.47	0.48
12:H:27:THR:OG1	32:B:610:CLA:OBD	2.30	0.48
26:b:103:LEU:HB2	32:b:607:CLA:H62	1.96	0.48
27:c:323:THR:HA	16:o:224:ARG:HD2	1.95	0.48
22:v:103:LYS:HA	22:v:121:VAL:HG22	1.96	0.48
26:B:103:LEU:HB2	32:B:607:CLA:H62	1.96	0.48
26:B:237:VAL:HG22	32:B:611:CLA:HBC2	1.95	0.48
32:B:613:CLA:HBB1	32:B:613:CLA:HMB1	1.96	0.48
2:1:213:LEU:HG	32:1:612:CLA:HED3	1.96	0.47
9:D:122:ILE:HD11	45:H:101:DGD:HAE1	1.96	0.47
16:O:224:ARG:HD2	27:C:323:THR:HA	1.96	0.47
22:V:33:THR:OG1	22:V:34:ARG:N	2.46	0.47
22:v:35:THR:O	22:v:150:LYS:NZ	2.46	0.47
3:8:94:MET:HE1	32:8:608:CLA:HAB	1.95	0.47
3:8:137:SER:HB3	32:8:607:CLA:HAB	1.95	0.47
2:1:130:HIS:CD2	2:1:139:MET:HE2	2.49	0.47
32:A:603:CLA:HED1	9:D:174:VAL:CG1	2.44	0.47
10:E:56:TYR:O	10:E:61:ARG:NH2	2.47	0.47
16:O:302:ASP:HB3	16:O:305:SER:HB3	1.95	0.47
19:S:104:PHE:C	19:S:107:PRO:HD2	2.39	0.47
32:c:511:CLA:H202	32:c:511:CLA:H162	1.77	0.47
32:8:603:CLA:HAC1	32:8:606:CLA:HAB	1.96	0.47
37:L:102:LMG:H292	37:L:102:LMG:H111	1.97	0.47
8:A:56:PRO:HB2	16:O:189:ARG:HH12	1.79	0.47
8:A:179:THR:O	8:A:183:MET:HG3	2.15	0.47
26:b:237:VAL:HG22	32:b:611:CLA:HBC2	1.95	0.47
27:C:30:LEU:HD21	32:C:511:CLA:H2A	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:276:GLN:HG3	45:C:514:DGD:HB32	1.95	0.47
19:s:87:LEU:HD21	32:s:302:CLA:C1D	2.44	0.47
16:O:154:THR:OG1	27:C:331:ARG:NH2	2.48	0.47
9:d:190:PHE:CD1	9:d:288:LEU:HD11	2.50	0.47
8:A:131:TRP:CH2	32:C:505:CLA:HAA2	2.49	0.47
9:D:351:LEU:HD13	26:B:384:ARG:HD3	1.96	0.47
32:b:613:CLA:HBB1	32:b:613:CLA:HMB1	1.96	0.47
45:c:515:DGD:HA22	45:c:515:DGD:HA52	1.66	0.47
9:d:122:ILE:HD11	45:h:101:DGD:HAE1	1.96	0.47
13:i:27:ASP:OD1	8:a:136:ARG:NH2	2.44	0.47
2:7:69:VAL:O	2:7:89:ARG:NH2	2.47	0.47
32:8:602:CLA:HBA2	32:8:602:CLA:H3A	1.33	0.47
8:a:201:GLY:HA3	8:a:286:THR:HB	1.95	0.47
4:3:99:LEU:HB3	32:3:604:CLA:HMC2	1.96	0.47
9:d:178:PHE:HA	9:d:181:LEU:HD12	1.95	0.47
32:7:603:CLA:HMA2	32:7:603:CLA:H11	1.96	0.47
32:9:607:CLA:H142	32:9:607:CLA:H111	1.71	0.47
8:a:179:THR:O	8:a:183:MET:HG3	2.14	0.47
32:3:605:CLA:HBA2	32:3:605:CLA:H3A	1.41	0.47
8:A:56:PRO:HB2	16:O:189:ARG:HH22	1.78	0.47
19:S:91:ILE:HA	19:S:94:PHE:CE2	2.50	0.47
32:b:604:CLA:H61	32:b:604:CLA:H41	1.57	0.47
29:l:24:LEU:HD13	38:l:102:LHG:H151	1.97	0.47
16:o:112:LYS:HE3	16:o:324:GLN:HA	1.97	0.47
16:o:195:THR:HG21	16:o:221:PRO:HD2	1.96	0.47
5:0:126:ILE:HD13	5:0:210:PHE:CD1	2.50	0.47
5:0:162:GLN:NE2	39:p:318:SQD:O9	2.47	0.47
19:s:104:PHE:C	19:s:107:PRO:HD2	2.40	0.47
26:B:399:VAL:HG12	26:B:417:VAL:HG22	1.97	0.47
2:1:69:VAL:O	2:1:89:ARG:NH2	2.47	0.47
21:U:150:ARG:HD3	22:V:160:LYS:H	1.79	0.47
26:b:419:LYS:NZ	16:o:254:GLY:O	2.35	0.47
22:v:125:ASP:HA	22:v:131:ARG:HH21	1.79	0.47
19:s:93:HIS:CE1	32:s:302:CLA:HAA1	2.50	0.47
26:B:106:LEU:HD12	32:B:607:CLA:H91	1.96	0.47
3:2:94:MET:HE1	32:2:608:CLA:HAB	1.95	0.47
16:O:158:GLY:HA2	16:O:172:LYS:HG2	1.97	0.47
19:S:158:VAL:O	19:S:161:PHE:HB2	2.15	0.47
26:b:106:LEU:HD12	32:b:607:CLA:H91	1.96	0.47
6:5:142:THR:OG1	6:5:147:ARG:NH1	2.47	0.47
8:A:93:PHE:CZ	32:A:605:CLA:HAA2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:458:ARG:O	9:d:250:ARG:NH1	2.35	0.47
10:e:24:HIS:O	10:e:28:ILE:HG12	2.15	0.47
32:9:605:CLA:H3A	32:9:605:CLA:HBA2	1.41	0.47
2:1:150:GLU:HG2	32:1:607:CLA:NB	2.30	0.46
32:4:603:CLA:HBC1	32:4:607:CLA:HBC2	1.97	0.46
8:A:340:PRO:HB3	21:U:149:TYR:HB3	1.96	0.46
27:c:244:PRO:O	27:c:249:ARG:NH1	2.48	0.46
9:d:48:PHE:O	9:d:52:THR:OG1	2.28	0.46
21:u:149:TYR:HB3	8:a:340:PRO:HB3	1.96	0.46
27:C:201:VAL:O	27:C:211:TRP:NE1	2.42	0.46
9:D:188:HIS:ND1	9:D:293:ARG:HD3	2.30	0.46
22:V:125:ASP:HA	22:V:131:ARG:HH21	1.79	0.46
27:c:27:ASN:ND2	32:c:510:CLA:O1A	2.41	0.46
32:c:504:CLA:H41	32:c:504:CLA:H61	1.47	0.46
9:d:174:VAL:CG1	32:a:406:CLA:HED1	2.45	0.46
39:a:409:SQD:H1	39:a:409:SQD:H45	1.64	0.46
32:1:606:CLA:H3A	32:1:606:CLA:HBA2	1.43	0.46
32:2:602:CLA:HBA2	32:2:602:CLA:H3A	1.33	0.46
32:3:609:CLA:H102	32:4:607:CLA:HBA1	1.98	0.46
9:D:178:PHE:HA	9:D:181:LEU:HD12	1.96	0.46
12:H:49:TYR:CD1	26:B:192:PRO:HG3	2.51	0.46
21:U:84:THR:O	22:V:108:TYR:OH	2.32	0.46
26:b:192:PRO:HG3	12:h:49:TYR:CD1	2.51	0.46
39:a:409:SQD:H371	39:a:409:SQD:H342	1.66	0.46
26:B:103:LEU:HD21	32:B:606:CLA:HMC3	1.97	0.46
32:1:602:CLA:H93	32:1:602:CLA:H61	1.78	0.46
9:D:192:LEU:O	29:L:35:TYR:OH	2.28	0.46
16:O:195:THR:HG21	16:O:221:PRO:HD2	1.97	0.46
22:V:103:LYS:HA	22:V:121:VAL:HG22	1.97	0.46
26:b:433:ASP:OD2	26:b:436:THR:OG1	2.28	0.46
26:b:474:LEU:HD11	32:b:609:CLA:HAA2	1.98	0.46
22:v:152:SER:HB3	8:a:313:VAL:H	1.81	0.46
8:a:206:PHE:HB3	32:a:406:CLA:H11	1.97	0.46
7:6:71:VAL:O	28:g:15:UNK:N	2.48	0.46
38:A:612:LHG:O4	9:D:140:TYR:OH	2.23	0.46
26:b:103:LEU:HD21	32:b:606:CLA:HMC3	1.98	0.46
9:d:348:GLY:N	8:a:330:VAL:O	2.48	0.46
16:o:158:GLY:HA2	16:o:172:LYS:HG2	1.98	0.46
19:s:233:ALA:C	19:s:235:ALA:H	2.24	0.46
32:4:601:CLA:HED3	32:4:601:CLA:H2A	1.97	0.46
32:0:601:CLA:H2A	32:0:601:CLA:HED3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:244:PRO:O	27:C:249:ARG:NH1	2.48	0.46
26:B:451:TYR:OH	32:B:605:CLA:O2D	2.34	0.46
30:W:80:VAL:O	30:W:84:LEU:HB2	2.16	0.46
32:1:612:CLA:H2A	32:1:612:CLA:HED2	1.96	0.46
7:6:180:ARG:HE	32:6:607:CLA:H43	1.81	0.46
2:7:90:GLU:HG2	2:7:158:ILE:HD11	1.97	0.46
45:C:515:DGD:HA22	45:C:515:DGD:HA52	1.67	0.46
26:B:474:LEU:HD11	32:B:609:CLA:HAA2	1.98	0.46
32:B:611:CLA:H202	32:B:611:CLA:H161	1.76	0.46
9:D:250:ARG:NH1	27:C:458:ARG:O	2.35	0.46
10:E:23:ILE:HA	10:E:26:ILE:HG12	1.97	0.46
27:c:420:PHE:CE2	8:a:288:LEU:HD13	2.51	0.46
19:s:241:PHE:HB3	19:s:265:PRO:HG2	1.98	0.46
32:3:602:CLA:H3A	32:3:602:CLA:HBA2	1.36	0.46
7:6:196:GLY:O	7:6:200:HIS:ND1	2.35	0.46
25:Z:32:GLU:HA	25:Z:35:LYS:HB3	1.98	0.46
27:c:387:ALA:HB2	8:a:343:LEU:HD13	1.98	0.46
27:C:250:ARG:NH2	30:W:93:TYR:OH	2.48	0.46
32:s:303:CLA:H122	32:s:303:CLA:H161	1.65	0.46
8:A:136:ARG:NH2	13:I:27:ASP:OD1	2.48	0.46
26:b:242:ILE:HG23	26:b:462:PHE:HD2	1.81	0.46
10:e:56:TYR:O	10:e:61:ARG:NH2	2.48	0.46
38:a:403:LHG:H282	38:a:403:LHG:H311	1.56	0.46
6:p:37:PHE:HA	6:p:45:LYS:HA	1.98	0.46
19:s:142:TYR:CE2	19:s:144:PRO:HB3	2.51	0.46
32:B:617:CLA:H102	32:B:617:CLA:H61	1.54	0.46
32:5:306:CLA:HBA1	32:5:306:CLA:H3A	1.61	0.45
12:H:22:ALA:HA	19:S:204:THR:HG22	1.98	0.45
45:H:101:DGD:HA61	32:B:603:CLA:H202	1.98	0.45
32:b:606:CLA:HBC2	32:b:613:CLA:H111	1.98	0.45
8:A:132:GLU:O	8:A:136:ARG:HG2	2.17	0.45
37:A:607:LMG:H171	27:C:205:PRO:HG3	1.98	0.45
19:S:87:LEU:HD21	32:S:302:CLA:C1D	2.47	0.45
19:S:233:ALA:C	19:S:235:ALA:H	2.24	0.45
19:S:241:PHE:HB3	19:S:265:PRO:HG2	1.98	0.45
9:d:290:LEU:HD21	45:h:101:DGD:HBN2	1.98	0.45
19:s:91:ILE:HA	19:s:94:PHE:CE2	2.52	0.45
19:s:158:VAL:O	19:s:161:PHE:HB2	2.15	0.45
8:A:273:PHE:CE1	38:A:613:LHG:HC61	2.51	0.45
16:O:265:ASN:HA	21:U:59:VAL:HG23	1.97	0.45
25:Z:34:GLU:HA	25:Z:37:LYS:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:L:24:LEU:HD13	38:L:101:LHG:H151	1.97	0.45
8:a:193:LEU:HD11	32:a:405:CLA:HMC2	1.98	0.45
6:p:142:THR:OG1	6:p:147:ARG:NH1	2.49	0.45
26:B:331:ASN:HB3	26:B:336:ILE:HG12	1.97	0.45
5:4:162:GLN:NE2	39:5:318:SQD:O9	2.49	0.45
9:D:133:ARG:NH1	26:B:474:LEU:O	2.46	0.45
27:c:166:LYS:NZ	27:c:172:GLY:O	2.49	0.45
27:c:250:ARG:NH2	30:w:93:TYR:OH	2.48	0.45
19:s:87:LEU:HB3	38:s:301:LHG:HC12	1.97	0.45
19:S:142:TYR:CE2	19:S:144:PRO:HB3	2.51	0.45
9:d:200:VAL:HG22	32:d:402:CLA:C1B	2.47	0.45
16:o:265:ASN:HA	21:u:59:VAL:HG23	1.97	0.45
2:7:150:GLU:HG2	32:7:607:CLA:NB	2.31	0.45
32:C:505:CLA:HBB1	32:C:505:CLA:HMB3	1.98	0.45
7:P:180:ARG:HE	32:P:607:CLA:H43	1.81	0.45
8:a:273:PHE:CE1	38:a:403:LHG:HC61	2.51	0.45
39:a:409:SQD:H272	39:a:409:SQD:H301	1.83	0.45
12:h:22:ALA:HA	19:s:204:THR:HG22	1.98	0.45
13:I:34:ARG:HG2	13:I:35:LYS:HG3	1.99	0.45
21:u:125:LYS:HD2	21:u:126:TYR:CZ	2.52	0.45
5:0:110:ASP:OD2	5:0:218:ILE:HG22	2.16	0.45
32:C:501:CLA:H171	32:C:507:CLA:H101	1.98	0.45
8:a:132:GLU:O	8:a:136:ARG:HG2	2.16	0.45
26:b:399:VAL:HG12	26:b:417:VAL:HG22	1.97	0.45
27:c:205:PRO:HG3	37:a:410:LMG:H171	1.98	0.45
32:1:602:CLA:H3A	32:1:602:CLA:HBA2	1.37	0.45
6:5:191:GLN:HB3	6:5:202:GLN:HE22	1.82	0.45
37:D:411:LMG:HC2	38:B:621:LHG:HC32	1.98	0.45
26:b:331:ASN:HB3	26:b:336:ILE:HG12	1.99	0.45
32:b:609:CLA:H3A	32:b:609:CLA:HBA2	1.81	0.45
32:c:501:CLA:H171	32:c:507:CLA:H101	1.98	0.45
13:i:34:ARG:HG2	13:i:35:LYS:HG3	1.99	0.45
22:v:152:SER:HB2	22:v:155:LYS:HD3	1.99	0.45
3:8:207:LEU:HD23	3:8:210:LEU:HD12	1.99	0.45
4:9:99:LEU:HB3	32:9:604:CLA:HMC2	1.98	0.45
39:B:620:SQD:H342	39:B:620:SQD:H312	1.74	0.45
5:4:53:GLN:HE22	5:4:55:ILE:C	2.25	0.45
8:A:30:ILE:O	8:A:34:GLY:HA3	2.16	0.45
9:D:200:VAL:HG22	32:D:403:CLA:C1B	2.47	0.45
19:S:93:HIS:CE1	32:S:302:CLA:HAA1	2.52	0.45
32:b:603:CLA:H202	45:h:101:DGD:HA61	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:203:LYS:HG2	27:c:209:ASP:HB3	1.99	0.45
5:0:53:GLN:HE22	5:0:55:ILE:C	2.25	0.45
5:0:159:GLN:HB3	5:0:164:SER:HB3	1.98	0.45
5:4:126:ILE:HD13	5:4:210:PHE:CD1	2.51	0.45
6:5:37:PHE:HA	6:5:45:LYS:HA	1.97	0.45
6:5:121:MET:HE2	32:5:307:CLA:C4C	2.47	0.45
9:d:161:LEU:HB3	45:h:101:DGD:HBW2	1.99	0.45
7:P:90:GLY:O	7:P:94:MET:HB2	2.17	0.45
8:a:234:ASN:HD21	38:a:402:LHG:HC12	1.82	0.45
26:B:242:ILE:HG23	26:B:462:PHE:HD2	1.81	0.45
8:A:193:LEU:HD11	32:A:602:CLA:HMC2	1.98	0.44
8:A:288:LEU:HD13	27:C:420:PHE:CE2	2.51	0.44
26:b:477:ASP:OD1	26:b:477:ASP:N	2.50	0.44
27:c:49:VAL:HG13	27:c:106:HIS:HD2	1.82	0.44
32:7:602:CLA:H62	32:7:602:CLA:H41	1.73	0.44
27:C:203:LYS:HG2	27:C:209:ASP:HB3	1.99	0.44
27:C:302:ALA:HB3	27:C:339:LEU:HD13	1.98	0.44
6:p:108:PRO:HA	6:p:111:ALA:HB3	1.99	0.44
4:3:168:ASP:OD1	4:3:168:ASP:N	2.50	0.44
8:A:26:ASN:O	9:D:254:GLN:NE2	2.50	0.44
9:D:161:LEU:HB3	45:H:101:DGD:HBW2	1.99	0.44
26:b:383:PHE:CE2	26:b:384:ARG:HG3	2.52	0.44
22:v:33:THR:OG1	22:v:34:ARG:N	2.48	0.44
27:C:136:GLY:O	27:C:144:LYS:NZ	2.44	0.44
12:h:61:ASP:OD1	12:h:62:TRP:N	2.50	0.44
26:B:30:VAL:HG12	32:B:606:CLA:HHD	1.99	0.44
4:3:115:ASP:OD1	4:3:115:ASP:N	2.48	0.44
9:D:126:LEU:HD13	38:B:621:LHG:H142	1.99	0.44
27:c:437:ARG:HG3	8:a:131:TRP:HZ2	1.82	0.44
8:a:260:PHE:CE1	8:a:263:ALA:HB2	2.52	0.44
26:B:333:GLY:O	26:B:439:SER:HB3	2.17	0.44
2:1:127:MET:HG2	2:1:211:TYR:CD2	2.52	0.44
6:5:188:MET:HE3	6:5:199:VAL:HG11	1.99	0.44
8:A:234:ASN:HD21	38:A:612:LHG:HC12	1.82	0.44
39:A:606:SQD:H45	39:A:606:SQD:H1	1.63	0.44
38:A:612:LHG:H362	38:A:612:LHG:H101	1.99	0.44
32:S:303:CLA:H161	32:S:303:CLA:H122	1.68	0.44
32:d:403:CLA:H62	32:d:403:CLA:H41	1.59	0.44
27:C:49:VAL:HG13	27:C:106:HIS:HD2	1.81	0.44
27:C:243:LYS:HG2	27:C:244:PRO:HD2	2.00	0.44
32:C:503:CLA:H3A	32:C:503:CLA:HBA2	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:p:188:MET:HE3	6:p:199:VAL:HG11	1.99	0.44
26:B:391:SER:N	26:B:394:GLN:OE1	2.41	0.44
30:w:80:VAL:O	30:w:84:LEU:HB2	2.17	0.44
32:5:303:CLA:HBA2	32:5:303:CLA:H3A	1.43	0.44
8:A:131:TRP:HZ2	27:C:437:ARG:HG3	1.83	0.44
38:b:621:LHG:H142	9:d:126:LEU:HD13	1.99	0.44
21:u:75:VAL:HG23	21:u:76:ASN:HD22	1.82	0.44
2:7:213:LEU:HG	32:7:612:CLA:HED3	2.00	0.44
32:1:602:CLA:H62	32:1:602:CLA:H41	1.72	0.44
26:b:356:VAL:HG22	26:b:370:LEU:HG	2.00	0.44
27:c:302:ALA:HB3	27:c:339:LEU:HD13	2.00	0.44
9:d:254:GLN:NE2	8:a:26:ASN:O	2.50	0.44
9:d:292:LEU:HD23	9:d:292:LEU:HA	1.87	0.44
4:9:168:ASP:N	4:9:168:ASP:OD1	2.50	0.44
32:B:606:CLA:HBC2	32:B:613:CLA:H111	1.98	0.44
32:B:616:CLA:H2	32:B:617:CLA:CBB	2.47	0.44
2:1:217:GLY:O	2:1:221:PHE:N	2.44	0.44
32:1:606:CLA:HBB1	36:1:618:IHT:C26	2.47	0.44
3:2:186:ARG:HA	3:2:189:MET:HE3	1.99	0.44
3:2:207:LEU:HD23	3:2:210:LEU:HD12	1.99	0.44
9:D:184:ILE:HG22	9:D:190:PHE:HB2	2.00	0.44
24:Y:2:PHE:HE1	24:Y:7:LEU:HD22	1.83	0.44
26:b:208:LEU:HD23	32:b:603:CLA:HAC2	1.99	0.44
9:d:254:GLN:HB2	8:a:133:PHE:CE2	2.53	0.44
32:7:602:CLA:H3A	32:7:602:CLA:HBA2	1.35	0.44
3:8:167:LEU:HD13	32:8:608:CLA:H42	2.00	0.44
32:9:602:CLA:H3A	32:9:602:CLA:HBA2	1.36	0.44
27:C:263:SER:O	27:C:267:VAL:HG23	2.18	0.44
32:C:507:CLA:H142	32:C:507:CLA:H111	1.80	0.44
8:a:30:ILE:O	8:a:34:GLY:HA3	2.16	0.44
1:M:103:ARG:HG2	19:s:251:LEU:HD11	2.00	0.44
3:2:167:LEU:HD13	32:2:608:CLA:H42	2.00	0.44
5:4:194:LYS:NZ	34:4:616:II0:O02	2.50	0.44
32:4:608:CLA:H91	32:4:608:CLA:H112	1.86	0.44
6:5:90:LEU:HD23	32:5:305:CLA:HMC1	2.00	0.44
7:6:119:ASP:HA	7:6:122:PHE:HD2	1.83	0.44
8:A:343:LEU:HD13	27:C:387:ALA:HB2	1.99	0.44
25:Z:27:LEU:HG	27:C:123:ILE:HD13	1.99	0.44
26:b:42:LEU:HD13	26:b:94:GLU:HG3	2.00	0.44
26:b:201:HIS:HB2	32:b:603:CLA:C1B	2.47	0.44
38:b:621:LHG:HC32	37:d:401:LMG:HC2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:122:LEU:HD11	32:c:511:CLA:H92	1.98	0.44
6:p:175:ILE:HG13	6:p:179:ARG:NE	2.33	0.44
6:p:191:GLN:HB3	6:p:202:GLN:HE22	1.82	0.44
26:B:201:HIS:HB2	32:B:603:CLA:C1B	2.47	0.44
8:A:133:PHE:CE2	9:D:254:GLN:HB2	2.53	0.44
27:c:36:LYS:NZ	27:c:126:ASP:OD1	2.40	0.44
27:c:331:ARG:NH2	16:o:154:THR:OG1	2.51	0.44
27:c:332:SER:OG	27:c:336:GLU:OE1	2.25	0.44
7:P:53:GLU:HG2	6:p:141:GLN:HE22	1.83	0.44
7:P:192:MET:HE1	32:P:602:CLA:HHC	1.99	0.44
26:B:42:LEU:HD13	26:B:94:GLU:HG3	1.99	0.44
2:1:90:GLU:HG2	2:1:158:ILE:HD11	1.99	0.43
27:c:263:SER:O	27:c:267:VAL:HG23	2.18	0.43
16:o:203:PHE:HB3	16:o:214:LEU:HD13	1.99	0.43
5:0:194:LYS:NZ	34:0:616:II0:O02	2.49	0.43
38:a:402:LHG:H362	38:a:402:LHG:H101	2.00	0.43
2:1:207:MET:HE2	34:1:614:II0:C22	2.48	0.43
7:6:90:GLY:O	7:6:94:MET:HB2	2.18	0.43
26:b:30:VAL:HG12	32:b:606:CLA:HHD	1.99	0.43
6:p:90:LEU:HD23	32:p:305:CLA:HMC1	2.00	0.43
32:4:602:CLA:H3A	32:4:602:CLA:HBA2	1.45	0.43
26:b:371:VAL:HG12	26:b:377:ILE:HD13	2.00	0.43
27:c:154:ILE:HG13	27:c:236:GLY:HA3	2.01	0.43
27:c:359:GLY:N	27:c:362:GLY:O	2.50	0.43
9:d:278:LEU:HD12	41:d:410:PHO:HBC3	1.99	0.43
32:g:102:CLA:H3A	32:g:102:CLA:HBA2	1.74	0.43
27:C:308:ARG:O	27:C:312:LEU:HB2	2.19	0.43
26:B:208:LEU:HD23	32:B:603:CLA:HAC2	1.99	0.43
32:B:609:CLA:HBA1	38:B:621:LHG:H101	2.00	0.43
32:2:606:CLA:HBA2	37:2:617:LMG:H291	2.01	0.43
10:e:28:ILE:CG1	10:e:29:PRO:HD3	2.49	0.43
24:y:2:PHE:HE1	24:y:7:LEU:HD22	1.83	0.43
5:0:130:HIS:ND1	5:0:139:MET:SD	2.88	0.43
3:8:186:ARG:HA	3:8:189:MET:HE3	2.00	0.43
32:P:602:CLA:H3A	32:P:602:CLA:HBA2	1.34	0.43
32:1:607:CLA:HBA1	32:1:607:CLA:H3A	1.85	0.43
32:4:604:CLA:HBA2	32:4:604:CLA:H3A	1.65	0.43
32:A:605:CLA:HBA2	32:A:605:CLA:H3A	1.60	0.43
12:H:61:ASP:OD1	12:H:62:TRP:N	2.52	0.43
16:O:254:GLY:O	26:B:419:LYS:NZ	2.35	0.43
26:b:333:GLY:O	26:b:439:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:C:504:CLA:H203	32:C:504:CLA:H162	1.87	0.43
8:a:72:LEU:HD23	8:a:72:LEU:HA	1.85	0.43
4:3:56:PRO:HA	4:3:57:PRO:HD3	1.93	0.43
27:c:243:LYS:HG2	27:c:244:PRO:HD2	2.00	0.43
27:c:260:LEU:O	27:c:264:LEU:HG	2.18	0.43
26:B:356:VAL:HG22	26:B:370:LEU:HG	2.00	0.43
5:4:159:GLN:HB3	5:4:164:SER:HB3	1.99	0.43
32:8:606:CLA:HBA2	37:8:617:LMG:H291	1.99	0.43
27:C:260:LEU:O	27:C:264:LEU:HG	2.18	0.43
32:2:608:CLA:HED3	32:2:608:CLA:H2A	2.01	0.43
8:A:206:PHE:HB3	32:A:603:CLA:H11	2.00	0.43
16:O:203:PHE:HB3	16:O:214:LEU:HD13	2.00	0.43
16:O:292:VAL:HA	16:O:316:ILE:HA	2.01	0.43
26:b:332:LYS:NZ	39:b:620:SQD:O7	2.51	0.43
26:b:474:LEU:O	9:d:133:ARG:NH1	2.46	0.43
37:b:618:LMG:H172	37:b:618:LMG:H141	1.80	0.43
27:c:243:LYS:HE2	27:c:243:LYS:HB3	1.32	0.43
27:c:364:ASP:HB3	27:c:367:LYS:HB2	2.01	0.43
16:o:70:THR:OG1	16:o:71:THR:N	2.52	0.43
3:8:176:ARG:HG2	32:8:609:CLA:HED1	2.01	0.43
8:a:93:PHE:CZ	32:a:408:CLA:HAA2	2.47	0.43
2:1:203:ALA:O	2:1:207:MET:HG3	2.19	0.43
27:C:154:ILE:HG13	27:C:236:GLY:HA3	2.01	0.43
32:C:503:CLA:H62	32:C:503:CLA:H102	1.73	0.43
6:p:212:PHE:N	6:p:213:PRO:HD2	2.34	0.43
41:D:402:PHO:HBB1	41:D:402:PHO:HMB1	2.01	0.43
10:E:65:PRO:HB2	10:E:80:LEU:HD13	2.01	0.43
32:b:612:CLA:H61	32:b:612:CLA:H92	1.69	0.43
32:b:617:CLA:H151	32:b:617:CLA:H18	1.79	0.43
27:c:308:ARG:O	27:c:312:LEU:HB2	2.18	0.43
27:c:365:LEU:HD12	27:c:365:LEU:H	1.83	0.43
27:c:452:GLU:OE2	9:d:247:THR:OG1	2.36	0.43
32:7:602:CLA:H93	32:7:602:CLA:H61	1.73	0.43
32:C:510:CLA:H122	32:C:510:CLA:H8	1.80	0.43
9:D:278:LEU:HD12	41:D:402:PHO:HBC3	2.00	0.42
27:c:313:GLY:HA3	21:u:95:LYS:HE3	2.00	0.42
27:c:323:THR:HG21	8:a:63:ILE:HD12	2.00	0.42
9:d:188:HIS:ND1	9:d:293:ARG:HD3	2.34	0.42
9:d:192:LEU:O	29:l:35:TYR:OH	2.28	0.42
32:7:605:CLA:HBA1	32:7:605:CLA:H3A	1.74	0.42
7:6:192:MET:HE1	32:6:602:CLA:HHC	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:70:THR:OG1	16:O:71:THR:N	2.52	0.42
16:o:292:VAL:HA	16:o:316:ILE:HA	2.01	0.42
32:0:602:CLA:H62	32:0:602:CLA:H41	1.79	0.42
27:C:151:ILE:HD13	32:C:512:CLA:HAB	2.01	0.42
29:L:1:MET:HG2	26:B:119:ASP:HB3	2.02	0.42
6:p:73:VAL:HG13	6:p:139:LEU:HD11	2.00	0.42
19:s:160:SER:HA	19:s:163:TRP:CD1	2.54	0.42
26:B:371:VAL:HG12	26:B:377:ILE:HD13	2.00	0.42
32:B:604:CLA:H41	32:B:604:CLA:H61	1.57	0.42
32:B:609:CLA:H3A	32:B:609:CLA:HBA2	1.81	0.42
3:2:132:ILE:HA	32:2:605:CLA:HBC3	2.01	0.42
8:A:127:ILE:HD13	8:A:148:THR:HG22	2.02	0.42
9:D:47:TRP:HA	9:D:77:VAL:HG21	2.01	0.42
32:b:609:CLA:HBA1	38:b:621:LHG:H101	2.00	0.42
32:c:504:CLA:H203	32:c:504:CLA:H162	1.88	0.42
9:d:128:GLN:NE2	41:d:410:PHO:OBD	2.53	0.42
9:d:217:VAL:O	9:d:221:ILE:HG23	2.18	0.42
3:8:132:ILE:HA	32:8:605:CLA:HBC3	2.01	0.42
27:C:364:ASP:HB3	27:C:367:LYS:HB2	2.00	0.42
32:C:504:CLA:H61	32:C:504:CLA:H41	1.47	0.42
8:a:214:MET:HE2	8:a:255:PHE:CE1	2.54	0.42
32:2:606:CLA:HHC	32:2:606:CLA:CBB	2.49	0.42
6:5:82:GLY:O	6:5:86:MET:HG3	2.20	0.42
26:b:313:ASP:OD1	26:b:358:ARG:NH1	2.44	0.42
32:b:611:CLA:H202	32:b:611:CLA:H161	1.76	0.42
27:c:393:ASN:ND2	45:c:516:DGD:O3D	2.47	0.42
4:9:170:LEU:HD13	39:p:318:SQD:H81	2.02	0.42
32:G:101:CLA:HBA2	32:G:101:CLA:H3A	1.74	0.42
6:5:112:HIS:CD2	6:5:121:MET:HE1	2.55	0.42
9:D:217:VAL:O	9:D:221:ILE:HG23	2.19	0.42
20:T:17:ILE:HG22	39:b:601:SQD:H351	2.01	0.42
9:d:305:ALA:HB1	16:o:260:LEU:HD13	2.02	0.42
41:d:410:PHO:HBB1	41:d:410:PHO:HMB1	2.01	0.42
10:e:28:ILE:HG12	10:e:29:PRO:HD3	2.01	0.42
32:0:604:CLA:H3A	32:0:604:CLA:HBA2	1.67	0.42
32:C:507:CLA:H62	32:C:507:CLA:H41	1.90	0.42
8:a:127:ILE:HD13	8:a:148:THR:HG22	2.02	0.42
32:B:610:CLA:H193	32:B:610:CLA:H162	1.79	0.42
32:B:617:CLA:H141	32:B:617:CLA:H162	1.71	0.42
3:2:176:ARG:HG2	32:2:609:CLA:HED1	2.01	0.42
32:2:605:CLA:HBA2	32:2:605:CLA:H3A	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:63:ILE:HD12	27:C:323:THR:HG21	2.00	0.42
39:A:606:SQD:H342	39:A:606:SQD:H371	1.66	0.42
26:b:60:MET:HB3	26:b:63:MET:HB3	2.02	0.42
26:b:119:ASP:HB3	29:l:1:MET:HG2	2.02	0.42
9:d:160:PRO:HB3	9:d:169:ALA:HB2	2.02	0.42
27:C:393:ASN:ND2	45:C:516:DGD:O3D	2.47	0.42
32:p:304:CLA:HMC3	32:p:307:CLA:HAB	2.01	0.42
26:B:315:ILE:HG12	26:B:321:LYS:HG3	2.00	0.42
4:3:211:PRO:C	4:3:213:GLU:N	2.77	0.42
7:6:118:VAL:HG11	7:6:203:LEU:HG	2.01	0.42
8:A:214:MET:HE2	8:A:255:PHE:CE1	2.55	0.42
31:Z:101:8CT:C07	32:C:513:CLA:H12	2.50	0.42
27:c:308:ARG:NH1	22:v:75:ASN:OD1	2.51	0.42
32:0:602:CLA:H111	32:0:602:CLA:H71	1.83	0.42
27:C:45:ALA:O	27:C:49:VAL:HG23	2.20	0.42
32:C:511:CLA:H202	32:C:511:CLA:H162	1.76	0.42
2:1:167:ARG:NH1	2:1:171:ASP:O	2.52	0.42
4:3:170:LEU:HD13	39:5:318:SQD:H81	2.01	0.42
26:b:317:ASN:HA	26:b:330:MET:HE1	2.01	0.42
27:c:151:ILE:HD13	32:c:512:CLA:HAB	2.01	0.42
32:c:504:CLA:H62	45:c:516:DGD:HB81	2.02	0.42
3:8:59:ASP:OD1	3:8:59:ASP:N	2.53	0.42
7:6:208:GLY:O	7:6:212:GLN:N	2.44	0.42
8:A:46:THR:HG21	45:A:614:DGD:HB92	2.02	0.42
19:S:87:LEU:HD21	32:S:302:CLA:C2D	2.50	0.42
19:S:160:SER:HA	19:S:163:TRP:CD1	2.54	0.42
26:b:70:GLY:HA2	26:b:178:VAL:HG11	2.02	0.42
2:7:141:GLN:HG2	32:7:605:CLA:ND	2.35	0.42
2:7:213:LEU:HD23	2:7:213:LEU:HA	1.89	0.42
38:a:403:LHG:H301	39:a:409:SQD:H122	2.02	0.42
39:B:601:SQD:H241	39:B:601:SQD:H462	1.97	0.42
6:5:108:PRO:HA	6:5:111:ALA:HB3	2.01	0.42
26:b:464:LEU:HB2	9:d:279:TRP:CZ2	2.55	0.42
13:i:13:THR:HG21	30:w:82:VAL:HA	2.02	0.42
29:l:27:VAL:HG11	38:l:102:LHG:H202	2.02	0.42
3:2:182:ILE:HD12	3:2:182:ILE:HA	1.95	0.41
5:4:215:LYS:HB3	5:4:219:GLU:HG3	2.02	0.41
32:D:403:CLA:H93	32:D:403:CLA:H61	1.92	0.41
16:O:91:CYS:HB2	16:O:119:GLU:HB2	2.02	0.41
16:O:252:ASP:OD1	26:B:434:ARG:NH1	2.52	0.41
32:c:505:CLA:H62	32:c:505:CLA:H2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:c:513:CLA:H12	31:z:101:8CT:C07	2.50	0.41
9:d:184:ILE:HG22	9:d:190:PHE:HB2	2.02	0.41
2:7:167:ARG:NH1	2:7:171:ASP:O	2.53	0.41
32:7:612:CLA:HED2	32:7:612:CLA:H2A	2.02	0.41
32:8:608:CLA:H2A	32:8:608:CLA:HED3	2.01	0.41
32:C:509:CLA:HBB1	32:C:509:CLA:HMB1	2.01	0.41
29:L:27:VAL:HG11	38:L:101:LHG:H202	2.02	0.41
32:4:602:CLA:H71	32:4:602:CLA:H111	1.74	0.41
8:A:161:TYR:HB3	8:A:162:PRO:HD3	2.01	0.41
16:O:249:LEU:HA	26:B:434:ARG:NH1	2.27	0.41
21:U:75:VAL:HG23	21:U:76:ASN:HD22	1.85	0.41
32:c:505:CLA:H162	32:c:505:CLA:H202	1.76	0.41
9:d:154:SER:HA	9:d:158:MET:HB2	2.02	0.41
9:d:346:PRO:HB2	8:a:331:MET:SD	2.60	0.41
32:0:602:CLA:H3A	32:0:602:CLA:HBA2	1.44	0.41
2:7:68:LEU:HB3	2:7:89:ARG:HH21	1.85	0.41
2:7:203:ALA:O	2:7:207:MET:HG3	2.20	0.41
32:7:606:CLA:HED2	32:7:606:CLA:H2A	2.02	0.41
27:C:243:LYS:HE2	27:C:243:LYS:HB3	1.34	0.41
26:B:253:THR:HG23	26:B:452:THR:HG23	2.02	0.41
3:2:180:ALA:O	3:2:184:HIS:ND1	2.42	0.41
8:A:183:MET:HA	32:A:602:CLA:HMD1	2.03	0.41
9:D:139:PRO:HG3	26:B:475:PHE:CD1	2.55	0.41
9:D:262:ASN:HB3	9:D:265:TRP:HB3	2.02	0.41
32:c:509:CLA:H141	32:c:509:CLA:H161	1.90	0.41
32:c:510:CLA:H122	32:c:510:CLA:H8	1.81	0.41
32:c:512:CLA:HMB3	32:g:102:CLA:HAB	2.03	0.41
10:e:12:SER:O	10:e:16:THR:OG1	2.34	0.41
16:o:91:CYS:HB2	16:o:119:GLU:HB2	2.02	0.41
27:C:305:PHE:HA	27:C:308:ARG:HG2	2.03	0.41
27:C:365:LEU:HD12	27:C:365:LEU:H	1.85	0.41
32:C:502:CLA:H62	32:C:502:CLA:H41	1.86	0.41
32:1:605:CLA:HBA1	32:1:605:CLA:H3A	1.78	0.41
8:A:105:TRP:NE1	8:A:110:GLY:HA3	2.35	0.41
9:D:102:ARG:HG3	10:E:74:LYS:HG3	2.03	0.41
9:D:247:THR:OG1	27:C:452:GLU:OE2	2.36	0.41
9:D:279:TRP:CZ2	26:B:464:LEU:HB2	2.55	0.41
9:D:305:ALA:HB1	16:O:260:LEU:HD13	2.01	0.41
26:b:57:ARG:NH2	26:b:335:GLY:O	2.53	0.41
32:9:607:CLA:HED3	32:9:607:CLA:HBD	1.87	0.41
45:C:514:DGD:HB71	45:C:514:DGD:HA22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:w:69:GLU:N	30:w:69:GLU:OE1	2.54	0.41
3:2:59:ASP:OD1	3:2:59:ASP:N	2.53	0.41
32:c:513:CLA:H3A	32:c:513:CLA:HBA2	1.47	0.41
10:e:65:PRO:HB2	10:e:80:LEU:HD13	2.01	0.41
5:0:99:CYS:SG	5:0:200:MET:HG3	2.61	0.41
6:5:175:ILE:HG13	6:5:179:ARG:NE	2.35	0.41
7:6:192:MET:HE2	32:6:602:CLA:HMC3	2.02	0.41
8:A:127:ILE:HD11	8:A:151:VAL:HG21	2.03	0.41
9:D:128:GLN:NE2	41:D:402:PHO:OBD	2.53	0.41
16:O:118:LEU:HG	16:O:317:VAL:HG23	2.03	0.41
26:b:346:PHE:O	26:b:354:LEU:N	2.49	0.41
27:c:201:VAL:O	27:c:211:TRP:NE1	2.42	0.41
10:e:23:ILE:HA	10:e:26:ILE:HG12	2.02	0.41
32:7:606:CLA:HMB1	32:7:606:CLA:HBB1	2.03	0.41
26:B:60:MET:HB3	26:B:63:MET:HB3	2.01	0.41
32:B:607:CLA:H143	32:B:607:CLA:H161	1.95	0.41
30:W:69:GLU:OE1	30:W:69:GLU:N	2.54	0.41
8:A:312:ARG:HA	22:V:152:SER:HB3	2.02	0.41
9:D:160:PRO:HB3	9:D:169:ALA:HB2	2.01	0.41
45:H:101:DGD:O5D	45:H:101:DGD:O4D	2.28	0.41
21:u:116:THR:HG22	21:u:117:ALA:H	1.86	0.41
2:7:176:PRO:O	34:7:614:II0:O01	2.38	0.41
7:P:59:ASP:OD1	7:P:59:ASP:N	2.53	0.41
8:a:183:MET:HA	32:a:405:CLA:HMD1	2.02	0.41
37:a:410:LMG:H172	37:a:410:LMG:H201	1.80	0.41
20:t:17:ILE:HG22	39:B:601:SQD:H351	2.02	0.41
26:B:70:GLY:HA2	26:B:178:VAL:HG11	2.03	0.41
32:1:613:CLA:HED2	32:1:613:CLA:HBD	1.92	0.41
32:3:607:CLA:H92	32:3:607:CLA:H62	1.88	0.41
6:5:73:VAL:HG13	6:5:139:LEU:HD11	2.02	0.41
39:5:318:SQD:H121	39:5:318:SQD:H152	1.83	0.41
7:6:198:MET:HB2	7:6:209:VAL:HG11	2.02	0.41
10:E:20:TYR:O	10:E:24:HIS:ND1	2.54	0.41
45:H:101:DGD:HB21	45:H:101:DGD:HB51	1.96	0.41
25:Z:59:SER:HB2	33:P:605:KC2:CGA	2.47	0.41
26:b:120:LEU:HD23	12:h:3:LEU:HD21	2.02	0.41
16:o:118:LEU:HG	16:o:317:VAL:HG23	2.03	0.41
16:o:250:GLU:HB2	16:o:257:GLN:NE2	2.35	0.41
32:C:504:CLA:H62	45:C:516:DGD:HB81	2.03	0.41
32:C:508:CLA:H91	32:C:508:CLA:H111	1.77	0.41
7:P:198:MET:HB2	7:P:209:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:313:ASP:OD1	26:B:358:ARG:NH1	2.44	0.41
2:1:205:GLY:O	2:1:209:HIS:ND1	2.53	0.41
32:2:603:CLA:HBA1	19:S:171:TRP:CH2	2.56	0.41
32:4:602:CLA:H41	32:4:602:CLA:H62	1.70	0.41
8:A:260:PHE:CE1	8:A:263:ALA:HB2	2.56	0.41
38:A:613:LHG:H311	38:A:613:LHG:H282	1.71	0.41
9:D:86:HIS:NE2	9:D:160:PRO:O	2.52	0.41
16:O:242:MET:HE3	16:O:242:MET:HB3	1.94	0.41
27:c:45:ALA:O	27:c:49:VAL:HG23	2.20	0.41
27:c:78:PRO:O	27:c:82:VAL:HG23	2.21	0.41
32:0:608:CLA:H91	32:0:608:CLA:H112	1.87	0.41
3:8:124:VAL:O	37:8:617:LMG:O3	2.34	0.41
27:C:36:LYS:NZ	27:C:126:ASP:OD1	2.37	0.41
39:a:409:SQD:H131	39:a:409:SQD:H102	1.67	0.41
45:h:101:DGD:HB21	45:h:101:DGD:HB51	1.96	0.41
32:p:307:CLA:HBA1	32:p:307:CLA:H3A	1.76	0.41
26:B:74:SER:HA	26:B:92:SER:HB2	2.03	0.41
32:B:612:CLA:H61	32:B:612:CLA:H41	1.64	0.41
39:A:606:SQD:H102	39:A:606:SQD:H131	1.67	0.41
9:D:285:ILE:HG13	32:D:403:CLA:HED2	2.03	0.41
16:O:183:GLN:HE21	16:O:187:GLY:HA2	1.86	0.41
26:b:475:PHE:CD1	9:d:139:PRO:HG3	2.55	0.41
32:b:605:CLA:H93	32:b:605:CLA:H61	1.79	0.41
2:7:198:ARG:HA	2:7:201:MET:HE3	2.03	0.41
27:C:268:SER:OG	27:C:422:GLY:O	2.35	0.41
26:B:8:VAL:HG22	32:B:612:CLA:H12	2.03	0.41
2:1:68:LEU:HB3	2:1:89:ARG:HH21	1.86	0.40
8:A:310:GLN:C	22:V:151:LEU:HD11	2.46	0.40
16:O:295:SER:HB3	16:O:313:LEU:HB2	2.03	0.40
26:b:321:LYS:NZ	26:b:363:PHE:O	2.54	0.40
9:d:268:PHE:CD2	38:a:402:LHG:HC11	2.56	0.40
32:8:603:CLA:HBA1	19:s:171:TRP:CH2	2.56	0.40
7:P:119:ASP:HA	7:P:122:PHE:HD2	1.85	0.40
32:P:604:CLA:H3A	32:P:604:CLA:HBA2	1.77	0.40
26:B:66:MET:HG3	32:B:606:CLA:O1D	2.22	0.40
32:5:304:CLA:HMC3	32:5:307:CLA:HAB	2.02	0.40
9:D:56:SER:OG	9:D:64:SER:OG	2.25	0.40
32:D:404:CLA:HBA1	32:D:404:CLA:H3A	1.87	0.40
45:H:101:DGD:HBH1	26:B:253:THR:HG22	2.04	0.40
13:I:13:THR:HG21	30:W:82:VAL:HA	2.02	0.40
9:d:47:TRP:HA	9:d:77:VAL:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:61:PRO:HG2	2:7:75:ASP:HB3	2.03	0.40
2:7:130:HIS:CD2	2:7:139:MET:HE2	2.51	0.40
8:a:47:VAL:HG21	8:a:114:LEU:HD22	2.03	0.40
6:p:173:ALA:O	6:p:177:HIS:ND1	2.36	0.40
19:s:87:LEU:HD21	32:s:302:CLA:C2D	2.51	0.40
26:B:155:ALA:O	26:B:159:THR:OG1	2.36	0.40
7:6:55:PRO:HA	7:6:56:PRO:HD3	1.90	0.40
9:D:73:PHE:HZ	45:C:516:DGD:HA71	1.87	0.40
9:D:279:TRP:HZ3	26:B:460:LEU:HG	1.86	0.40
21:U:95:LYS:HE3	27:C:313:GLY:HA3	2.04	0.40
26:b:315:ILE:HG12	26:b:321:LYS:HG3	2.02	0.40
9:d:264:ARG:HD3	8:a:223:LEU:HD13	2.03	0.40
45:C:516:DGD:O5D	45:C:516:DGD:O4D	2.39	0.40
3:2:81:VAL:HG13	3:2:147:LEU:HD11	2.03	0.40
32:A:602:CLA:H202	32:A:602:CLA:H161	1.89	0.40
39:A:606:SQD:H301	39:A:606:SQD:H272	1.84	0.40
38:A:612:LHG:HC11	9:D:268:PHE:CD2	2.57	0.40
9:D:250:ARG:NE	9:D:254:GLN:OE1	2.55	0.40
12:H:3:LEU:HD21	26:B:120:LEU:HD23	2.02	0.40
22:V:67:HIS:HA	22:V:71:ILE:O	2.21	0.40
26:b:8:VAL:HG22	32:b:612:CLA:H12	2.04	0.40
9:d:262:ASN:HB3	9:d:265:TRP:HB3	2.02	0.40
3:8:141:ILE:HD13	3:8:141:ILE:HA	1.97	0.40
32:8:606:CLA:HHC	32:8:606:CLA:CBB	2.49	0.40
7:P:118:VAL:HG11	7:P:203:LEU:HG	2.03	0.40
30:w:85:ILE:HB	30:w:86:PRO:HD3	2.03	0.40
30:W:85:ILE:HB	30:W:86:PRO:HD3	2.03	0.40
2:1:219:ILE:HA	2:1:222:ILE:HG22	2.04	0.40
5:4:99:CYS:SG	5:4:200:MET:HG3	2.61	0.40
5:4:155:VAL:HG23	6:5:44:LEU:HD21	2.04	0.40
8:A:238:LYS:NZ	19:S:248:GLY:O	2.46	0.40
16:O:277:MET:HA	16:O:293:PHE:HA	2.04	0.40
26:b:253:THR:HG23	26:b:452:THR:HG23	2.03	0.40
27:c:268:SER:OG	27:c:422:GLY:O	2.36	0.40
47:f:101:HEM:HBC2	47:f:101:HEM:CHD	2.49	0.40
22:v:67:HIS:HA	22:v:71:ILE:O	2.21	0.40
4:9:165:LEU:HD12	32:9:607:CLA:HMD2	2.04	0.40
32:9:607:CLA:H62	32:9:607:CLA:H92	1.88	0.40
27:C:127:THR:OG1	27:C:130:GLU:OE2	2.40	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	M	34/115 (30%)	32 (94%)	2 (6%)	0	100	100
1	m	34/115 (30%)	32 (94%)	2 (6%)	0	100	100
2	1	192/235 (82%)	183 (95%)	9 (5%)	0	100	100
2	7	192/235 (82%)	186 (97%)	6 (3%)	0	100	100
3	2	171/217 (79%)	168 (98%)	3 (2%)	0	100	100
3	8	171/217 (79%)	169 (99%)	2 (1%)	0	100	100
4	3	176/222 (79%)	173 (98%)	2 (1%)	1 (1%)	21	35
4	9	176/222 (79%)	173 (98%)	3 (2%)	0	100	100
5	0	170/226 (75%)	167 (98%)	2 (1%)	1 (1%)	21	35
5	4	170/226 (75%)	167 (98%)	2 (1%)	1 (1%)	21	35
6	5	185/218 (85%)	182 (98%)	3 (2%)	0	100	100
6	p	185/218 (85%)	181 (98%)	4 (2%)	0	100	100
7	6	171/220 (78%)	171 (100%)	0	0	100	100
7	P	171/220 (78%)	171 (100%)	0	0	100	100
8	A	332/360 (92%)	326 (98%)	6 (2%)	0	100	100
8	a	332/360 (92%)	328 (99%)	4 (1%)	0	100	100
9	D	340/351 (97%)	335 (98%)	5 (2%)	0	100	100
9	d	340/351 (97%)	337 (99%)	3 (1%)	0	100	100
10	E	75/84 (89%)	75 (100%)	0	0	100	100
10	e	75/84 (89%)	75 (100%)	0	0	100	100
11	F	28/42 (67%)	28 (100%)	0	0	100	100
11	f	28/42 (67%)	28 (100%)	0	0	100	100
12	H	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
12	h	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
13	I	33/38 (87%)	33 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	i	33/38 (87%)	33 (100%)	0	0	100	100
14	J	26/39 (67%)	26 (100%)	0	0	100	100
14	j	26/39 (67%)	26 (100%)	0	0	100	100
15	K	35/45 (78%)	34 (97%)	1 (3%)	0	100	100
15	k	35/45 (78%)	34 (97%)	1 (3%)	0	100	100
16	O	225/330 (68%)	212 (94%)	13 (6%)	0	100	100
16	o	225/330 (68%)	213 (95%)	12 (5%)	0	100	100
19	S	201/285 (70%)	183 (91%)	18 (9%)	0	100	100
19	s	201/285 (70%)	183 (91%)	18 (9%)	0	100	100
20	T	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
20	t	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
21	U	91/150 (61%)	84 (92%)	7 (8%)	0	100	100
21	u	91/150 (61%)	82 (90%)	9 (10%)	0	100	100
22	V	129/163 (79%)	125 (97%)	4 (3%)	0	100	100
22	v	129/163 (79%)	125 (97%)	4 (3%)	0	100	100
23	X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
23	x	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
24	Y	32/34 (94%)	32 (100%)	0	0	100	100
24	y	32/34 (94%)	32 (100%)	0	0	100	100
25	Z	59/62 (95%)	56 (95%)	3 (5%)	0	100	100
25	z	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
26	B	502/509 (99%)	496 (99%)	6 (1%)	0	100	100
26	b	502/509 (99%)	497 (99%)	5 (1%)	0	100	100
27	C	449/461 (97%)	443 (99%)	6 (1%)	0	100	100
27	c	449/461 (97%)	442 (98%)	7 (2%)	0	100	100
29	L	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
29	l	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
30	W	43/114 (38%)	43 (100%)	0	0	100	100
30	w	43/114 (38%)	43 (100%)	0	0	100	100
All	All	7730/9392 (82%)	7539 (98%)	188 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	3	212	ILE
5	4	126	ILE
5	0	126	ILE

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	M	28/84 (33%)	28 (100%)	0	100	100
1	m	28/84 (33%)	28 (100%)	0	100	100
2	1	149/179 (83%)	149 (100%)	0	100	100
2	7	149/179 (83%)	149 (100%)	0	100	100
3	2	139/167 (83%)	139 (100%)	0	100	100
3	8	139/167 (83%)	139 (100%)	0	100	100
4	3	143/175 (82%)	143 (100%)	0	100	100
4	9	143/175 (82%)	143 (100%)	0	100	100
5	0	136/169 (80%)	136 (100%)	0	100	100
5	4	136/169 (80%)	136 (100%)	0	100	100
6	5	157/175 (90%)	157 (100%)	0	100	100
6	p	157/175 (90%)	157 (100%)	0	100	100
7	6	141/174 (81%)	141 (100%)	0	100	100
7	P	141/174 (81%)	141 (100%)	0	100	100
8	A	271/289 (94%)	271 (100%)	0	100	100
8	a	271/289 (94%)	271 (100%)	0	100	100
9	D	274/281 (98%)	274 (100%)	0	100	100
9	d	274/281 (98%)	274 (100%)	0	100	100
10	E	68/73 (93%)	68 (100%)	0	100	100
10	e	68/73 (93%)	68 (100%)	0	100	100
11	F	25/37 (68%)	25 (100%)	0	100	100
11	f	25/37 (68%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	H	56/58 (97%)	56 (100%)	0	100	100
12	h	56/58 (97%)	56 (100%)	0	100	100
13	I	33/36 (92%)	33 (100%)	0	100	100
13	i	33/36 (92%)	33 (100%)	0	100	100
14	J	22/29 (76%)	22 (100%)	0	100	100
14	j	22/29 (76%)	22 (100%)	0	100	100
15	K	30/36 (83%)	30 (100%)	0	100	100
15	k	30/36 (83%)	30 (100%)	0	100	100
16	O	189/258 (73%)	189 (100%)	0	100	100
16	o	189/258 (73%)	189 (100%)	0	100	100
19	S	159/219 (73%)	159 (100%)	0	100	100
19	s	159/219 (73%)	159 (100%)	0	100	100
20	T	27/27 (100%)	27 (100%)	0	100	100
20	t	27/27 (100%)	27 (100%)	0	100	100
21	U	80/115 (70%)	80 (100%)	0	100	100
21	u	80/115 (70%)	79 (99%)	1 (1%)	61	80
22	V	112/141 (79%)	112 (100%)	0	100	100
22	v	112/141 (79%)	112 (100%)	0	100	100
23	X	34/34 (100%)	34 (100%)	0	100	100
23	x	34/34 (100%)	34 (100%)	0	100	100
24	Y	29/29 (100%)	29 (100%)	0	100	100
24	y	29/29 (100%)	29 (100%)	0	100	100
25	Z	50/51 (98%)	48 (96%)	2 (4%)	28	51
25	z	50/51 (98%)	50 (100%)	0	100	100
26	B	401/404 (99%)	401 (100%)	0	100	100
26	b	401/404 (99%)	401 (100%)	0	100	100
27	C	356/366 (97%)	355 (100%)	1 (0%)	86	93
27	c	356/366 (97%)	355 (100%)	1 (0%)	86	93
29	L	35/35 (100%)	35 (100%)	0	100	100
29	l	35/35 (100%)	35 (100%)	0	100	100
30	W	40/85 (47%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	w	40/85 (47%)	40 (100%)	0	100 100
All	All	6368/7452 (86%)	6363 (100%)	5 (0%)	87 95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	Z	27	LEU
25	Z	59	SER
27	c	243	LYS
21	u	127	LEU
27	C	243	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	109	GLN
2	1	168	GLN
2	1	182	ASN
3	2	120	HIS
3	2	198	GLN
3	2	209	GLN
4	3	104	GLN
4	3	209	GLN
5	4	53	GLN
5	4	109	GLN
5	4	208	HIS
6	5	49	ASN
6	5	190	HIS
6	5	202	GLN
6	5	205	ASN
7	6	103	GLN
7	6	212	GLN
7	6	215	ASN
8	A	215	HIS
8	A	234	ASN
8	A	261	GLN
8	A	335	ASN
8	A	338	ASN
9	D	185	GLN
9	D	196	HIS
10	E	62	GLN

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Mol	Chain	Res	Type
11	F	21	HIS
11	F	41	GLN
16	O	183	GLN
16	O	257	GLN
16	O	324	GLN
21	U	76	ASN
21	U	145	ASN
22	V	65	ASN
22	V	104	ASN
26	b	26	HIS
26	b	114	HIS
26	b	216	HIS
26	b	274	GLN
26	b	425	GLN
27	c	62	HIS
27	c	106	HIS
27	c	143	ASN
27	c	276	GLN
27	c	299	GLN
27	c	310	GLN
27	c	320	GLN
27	c	406	ASN
9	d	185	GLN
10	e	62	GLN
16	o	183	GLN
16	o	257	GLN
21	u	63	ASN
21	u	76	ASN
21	u	145	ASN
22	v	65	ASN
5	0	53	GLN
5	0	208	HIS
2	7	81	ASN
2	7	182	ASN
3	8	120	HIS
3	8	198	GLN
3	8	209	GLN
4	9	104	GLN
4	9	209	GLN
27	C	41	HIS
27	C	44	HIS
27	C	62	HIS

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Mol	Chain	Res	Type
27	C	106	HIS
27	C	143	ASN
27	C	276	GLN
27	C	299	GLN
27	C	320	GLN
27	C	361	ASN
27	C	406	ASN
7	P	103	GLN
7	P	131	GLN
7	P	212	GLN
7	P	215	ASN
8	a	215	HIS
8	a	234	ASN
8	a	338	ASN
6	p	49	ASN
6	p	190	HIS
6	p	202	GLN
6	p	205	ASN
6	p	210	ASN
26	B	26	HIS
26	B	216	HIS
26	B	274	GLN
26	B	425	GLN
30	w	102	ASN
30	w	111	GLN
30	W	102	ASN
30	W	111	GLN

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 (i)

Of 376 ligands modelled in this entry, 4 are monoatomic - leaving 372 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
38	LHG	L	101	-	48,48,48	0.65	1 (2%)	51,54,54	1.30	7 (13%)
32	CLA	5	312	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	4 (6%)
43	PL9	d	404	-	55,55,55	1.27	5 (9%)	68,69,69	1.51	13 (19%)
37	LMG	c	517	-	46,46,55	0.77	1 (2%)	54,54,63	1.32	6 (11%)
32	CLA	p	313	-	49,53,73	1.39	8 (16%)	58,89,113	1.37	4 (6%)
33	KC2	P	609	-	49,53,53	1.74	8 (16%)	60,89,89	1.87	15 (25%)
32	CLA	3	610	4	49,53,73	1.39	9 (18%)	58,89,113	1.43	4 (6%)
32	CLA	1	609	-	45,49,73	1.42	8 (17%)	54,84,113	1.47	5 (9%)
32	CLA	c	502	-	68,72,73	1.17	8 (11%)	80,111,113	1.29	5 (6%)
33	KC2	6	605	7	49,53,53	1.78	8 (16%)	60,89,89	1.83	14 (23%)
32	CLA	B	610	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
34	II0	5	314	-	39,43,43	2.02	2 (5%)	48,60,60	1.71	13 (27%)
32	CLA	1	601	-	46,50,73	1.41	8 (17%)	53,85,113	1.40	4 (7%)
33	KC2	8	610	-	49,53,53	1.76	9 (18%)	60,89,89	1.87	14 (23%)
32	CLA	7	607	-	49,53,73	1.39	8 (16%)	58,89,113	1.35	4 (6%)
32	CLA	d	403	-	64,68,73	1.19	9 (14%)	76,107,113	1.35	9 (11%)
32	CLA	1	612	-	49,53,73	1.39	7 (14%)	58,89,113	1.36	4 (6%)
32	CLA	P	611	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	4 (6%)
31	8CT	k	101	-	40,41,41	4.79	23 (57%)	51,56,56	2.72	20 (39%)
32	CLA	c	505	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	7 (8%)
38	LHG	d	405	-	44,47,48	0.56	1 (2%)	44,51,54	1.20	6 (13%)
34	II0	7	619	-	39,43,43	2.00	2 (5%)	48,60,60	1.57	9 (18%)
34	II0	p	315	-	39,43,43	2.05	2 (5%)	48,60,60	1.62	10 (20%)
31	8CT	B	624	-	40,41,41	4.81	23 (57%)	51,56,56	2.84	17 (33%)
32	CLA	4	613	5	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
47	HEM	v	201	-	50,50,50	1.45	9 (18%)	67,82,82	1.05	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	8CT	M	201	-	40,41,41	4.78	23 (57%)	51,56,56	3.01	19 (37%)
45	DGD	H	101	-	63,63,67	0.88	2 (3%)	77,77,81	1.37	8 (10%)
32	CLA	5	310	-	45,49,73	1.42	8 (17%)	54,84,113	1.46	5 (9%)
33	KC2	0	610	5	49,53,53	1.74	8 (16%)	60,89,89	1.89	15 (25%)
37	LMG	B	618	-	51,51,55	0.74	1 (1%)	59,59,63	1.35	6 (10%)
32	CLA	9	610	4	49,53,73	1.39	8 (16%)	58,89,113	1.44	4 (6%)
32	CLA	0	608	5	64,68,73	1.21	8 (12%)	76,107,113	1.28	5 (6%)
34	II0	2	613	-	39,43,43	2.02	2 (5%)	48,60,60	1.62	9 (18%)
38	LHG	a	402	-	42,42,48	0.68	1 (2%)	45,48,54	1.25	4 (8%)
32	CLA	p	304	-	54,58,73	1.32	8 (14%)	64,95,113	1.38	6 (9%)
32	CLA	B	603	-	64,69,73	1.17	9 (14%)	73,106,113	1.21	4 (5%)
32	CLA	c	501	-	69,73,73	1.14	9 (13%)	82,113,113	1.30	6 (7%)
32	CLA	g	102	-	49,53,73	1.40	8 (16%)	58,89,113	1.37	4 (6%)
32	CLA	4	607	5	49,53,73	1.39	8 (16%)	58,89,113	1.34	4 (6%)
32	CLA	5	304	-	54,58,73	1.33	8 (14%)	64,95,113	1.39	6 (9%)
32	CLA	c	506	-	49,53,73	1.37	9 (18%)	58,89,113	1.44	5 (8%)
32	CLA	7	601	-	46,50,73	1.41	8 (17%)	53,85,113	1.40	4 (7%)
32	CLA	0	603	-	54,58,73	1.32	8 (14%)	64,95,113	1.38	6 (9%)
32	CLA	1	603	-	54,58,73	1.32	8 (14%)	64,95,113	1.38	6 (9%)
34	II0	1	616	-	39,43,43	2.05	2 (5%)	48,60,60	1.63	11 (22%)
34	II0	7	617	-	39,43,43	2.05	2 (5%)	48,60,60	1.63	9 (18%)
33	KC2	7	610	-	49,53,53	1.74	8 (16%)	60,89,89	1.88	15 (25%)
32	CLA	0	609	-	45,49,73	1.43	8 (17%)	54,84,113	1.46	5 (9%)
45	DGD	c	514	-	56,56,67	0.98	2 (3%)	70,70,81	1.47	10 (14%)
32	CLA	2	605	3	64,68,73	1.23	8 (12%)	76,107,113	1.29	5 (6%)
32	CLA	c	507	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	5 (6%)
32	CLA	B	609	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	6 (7%)
38	LHG	l	102	-	48,48,48	0.65	1 (2%)	51,54,54	1.30	6 (11%)
31	8CT	B	623	-	40,41,41	4.81	23 (57%)	51,56,56	2.52	17 (33%)
34	II0	2	615	-	39,43,43	2.04	3 (7%)	48,60,60	1.67	11 (22%)
32	CLA	4	604	-	59,63,73	1.27	8 (13%)	70,101,113	1.35	8 (11%)
32	CLA	8	603	-	54,58,73	1.31	8 (14%)	64,95,113	1.40	6 (9%)
31	8CT	k	102	-	40,41,41	4.81	23 (57%)	51,56,56	2.81	18 (35%)
32	CLA	7	603	-	54,58,73	1.32	7 (12%)	64,95,113	1.40	8 (12%)
32	CLA	8	607	3	49,53,73	1.37	8 (16%)	58,89,113	1.40	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	SQD	A	606	-	52,54,54	1.54	7 (13%)	62,65,65	1.35	8 (12%)
32	CLA	b	611	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)
32	CLA	3	601	4	46,50,73	1.40	8 (17%)	53,85,113	1.44	4 (7%)
32	CLA	8	608	3	64,68,73	1.21	9 (14%)	76,107,113	1.29	5 (6%)
34	II0	9	612	-	39,43,43	2.02	2 (5%)	48,60,60	1.57	11 (22%)
32	CLA	p	312	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	4 (6%)
32	CLA	p	302	6	46,50,73	1.41	8 (17%)	53,85,113	1.42	4 (7%)
32	CLA	b	614	-	69,73,73	1.15	9 (13%)	82,113,113	1.25	6 (7%)
32	CLA	b	608	-	45,49,73	1.38	9 (20%)	54,84,113	1.48	5 (9%)
32	CLA	9	601	4	46,50,73	1.40	8 (17%)	53,85,113	1.46	5 (9%)
32	CLA	s	303	19	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
38	LHG	D	406	-	44,47,48	0.56	1 (2%)	44,51,54	1.21	6 (13%)
32	CLA	5	302	6	46,50,73	1.41	8 (17%)	53,85,113	1.42	4 (7%)
32	CLA	P	608	-	45,49,73	1.41	8 (17%)	54,84,113	1.44	5 (9%)
32	CLA	0	601	5	46,50,73	1.41	8 (17%)	53,85,113	1.42	4 (7%)
47	HEM	E	101	-	50,50,50	1.44	7 (14%)	67,82,82	1.13	4 (5%)
32	CLA	B	613	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	8 (9%)
32	CLA	4	606	-	49,53,73	1.40	8 (16%)	58,89,113	1.33	4 (6%)
32	CLA	8	609	38	45,49,73	1.41	8 (17%)	54,84,113	1.46	5 (9%)
32	CLA	C	501	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	6 (7%)
38	LHG	a	403	-	48,48,48	0.66	1 (2%)	51,54,54	1.28	6 (11%)
32	CLA	C	502	-	68,72,73	1.17	9 (13%)	80,111,113	1.29	5 (6%)
34	II0	P	614	-	39,43,43	2.02	2 (5%)	48,60,60	1.60	10 (20%)
32	CLA	C	504	-	68,72,73	1.15	9 (13%)	80,111,113	1.30	6 (7%)
33	KC2	6	609	-	49,53,53	1.74	8 (16%)	60,89,89	1.86	15 (25%)
36	IHT	2	616	-	40,42,42	1.53	2 (5%)	52,58,58	1.93	13 (25%)
32	CLA	8	601	3	46,50,73	1.40	8 (17%)	53,85,113	1.41	4 (7%)
32	CLA	P	607	7	64,68,73	1.22	9 (14%)	76,107,113	1.29	5 (6%)
32	CLA	5	308	6	49,53,73	1.39	9 (18%)	58,89,113	1.40	4 (6%)
32	CLA	7	612	-	49,53,73	1.39	8 (16%)	58,89,113	1.37	4 (6%)
32	CLA	p	305	-	59,63,73	1.27	8 (13%)	70,101,113	1.35	6 (8%)
32	CLA	p	308	6	49,53,73	1.40	9 (18%)	58,89,113	1.41	4 (6%)
34	II0	0	616	-	39,43,43	2.04	2 (5%)	48,60,60	1.63	11 (22%)
34	II0	9	613	-	39,43,43	2.03	2 (5%)	48,60,60	1.58	9 (18%)
32	CLA	6	601	7	46,50,73	1.41	8 (17%)	53,85,113	1.40	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	3	611	-	49,53,73	1.37	9 (18%)	58,89,113	1.39	4 (6%)
32	CLA	b	615	-	68,72,73	1.15	9 (13%)	80,111,113	1.27	5 (6%)
39	SQD	p	318	-	33,35,54	1.77	7 (21%)	43,46,65	1.50	6 (13%)
34	II0	0	615	-	39,43,43	2.01	2 (5%)	48,60,60	1.62	12 (25%)
32	CLA	D	404	-	64,68,73	1.19	9 (14%)	76,107,113	1.35	9 (11%)
31	8CT	d	408	-	40,41,41	4.84	23 (57%)	51,56,56	2.49	16 (31%)
32	CLA	1	607	-	49,53,73	1.38	8 (16%)	58,89,113	1.36	4 (6%)
32	CLA	3	607	4	64,68,73	1.21	9 (14%)	76,107,113	1.31	4 (5%)
41	PHO	a	407	-	58,69,69	2.10	11 (18%)	55,99,99	1.44	7 (12%)
34	II0	p	314	-	39,43,43	2.02	2 (5%)	48,60,60	1.71	13 (27%)
32	CLA	b	602	-	51,55,73	1.33	9 (17%)	60,91,113	1.38	5 (8%)
32	CLA	S	303	19	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
32	CLA	C	505	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	7 (8%)
45	DGD	c	515	-	57,57,67	0.95	2 (3%)	71,71,81	1.41	9 (12%)
34	II0	5	319	-	39,43,43	2.04	2 (5%)	48,60,60	1.71	12 (25%)
36	IHT	1	618	-	40,42,42	1.52	1 (2%)	52,58,58	1.90	12 (23%)
32	CLA	a	406	-	53,57,73	1.30	9 (16%)	61,93,113	1.46	5 (8%)
32	CLA	3	606	-	49,53,73	1.38	9 (18%)	58,89,113	1.33	4 (6%)
32	CLA	B	612	-	68,72,73	1.16	9 (13%)	80,111,113	1.29	6 (7%)
34	II0	6	614	-	39,43,43	2.04	3 (7%)	48,60,60	1.59	8 (16%)
34	II0	7	614	-	39,43,43	2.03	2 (5%)	48,60,60	1.61	6 (12%)
36	IHT	4	614	-	40,42,42	1.51	1 (2%)	52,58,58	1.79	10 (19%)
32	CLA	c	503	-	69,73,73	1.16	9 (13%)	82,113,113	1.35	7 (8%)
43	PL9	A	609	-	13,13,55	1.58	2 (15%)	17,17,69	1.79	4 (23%)
34	II0	6	612	-	39,43,43	2.01	2 (5%)	48,60,60	1.67	11 (22%)
44	BCT	a	401	46	3,3,3	1.10	0	2,3,3	4.56	2 (100%)
32	CLA	0	602	5	63,67,73	1.22	8 (12%)	74,105,113	1.31	6 (8%)
31	8CT	h	102	-	40,41,41	4.84	23 (57%)	51,56,56	2.79	13 (25%)
32	CLA	p	310	-	45,49,73	1.42	8 (17%)	54,84,113	1.46	5 (9%)
32	CLA	2	603	-	54,58,73	1.32	8 (14%)	64,95,113	1.40	6 (9%)
32	CLA	9	608	-	45,49,73	1.40	8 (17%)	54,84,113	1.47	6 (11%)
35	II3	6	613	-	40,43,43	1.50	1 (2%)	47,60,60	1.68	11 (23%)
31	8CT	c	518	-	40,41,41	4.86	22 (55%)	51,56,56	2.89	17 (33%)
37	LMG	d	406	-	46,46,55	0.78	1 (2%)	54,54,63	1.34	5 (9%)
31	8CT	B	622	-	40,41,41	4.78	23 (57%)	51,56,56	3.00	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	II0	8	615	-	39,43,43	2.04	2 (5%)	48,60,60	1.69	10 (20%)
37	LMG	A	607	-	48,48,55	0.78	1 (2%)	56,56,63	1.34	5 (8%)
32	CLA	2	609	38	45,49,73	1.41	8 (17%)	54,84,113	1.45	5 (9%)
32	CLA	C	506	-	49,53,73	1.36	9 (18%)	58,89,113	1.44	5 (8%)
32	CLA	P	603	-	54,58,73	1.31	8 (14%)	64,95,113	1.41	5 (7%)
31	8CT	D	409	-	40,41,41	4.84	23 (57%)	51,56,56	2.48	16 (31%)
32	CLA	5	307	-	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
32	CLA	6	604	-	59,63,73	1.27	7 (11%)	70,101,113	1.33	6 (8%)
32	CLA	P	610	-	49,53,73	1.40	9 (18%)	58,89,113	1.44	4 (6%)
32	CLA	4	612	-	49,53,73	1.40	7 (14%)	58,89,113	1.46	5 (8%)
32	CLA	4	602	5	63,67,73	1.22	8 (12%)	74,105,113	1.31	6 (8%)
32	CLA	3	609	-	64,68,73	1.21	8 (12%)	76,107,113	1.29	5 (6%)
32	CLA	D	401	-	63,67,73	1.19	9 (14%)	74,105,113	1.37	8 (10%)
31	8CT	P	615	-	40,41,41	4.87	23 (57%)	51,56,56	2.60	17 (33%)
34	II0	9	614	-	39,43,43	2.01	2 (5%)	48,60,60	1.57	12 (25%)
34	II0	8	619	-	39,43,43	2.07	2 (5%)	48,60,60	1.61	10 (20%)
34	II0	p	316	-	39,43,43	2.03	2 (5%)	48,60,60	1.58	9 (18%)
32	CLA	B	616	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	5 (6%)
37	LMG	2	617	-	36,36,55	0.86	1 (2%)	44,44,63	1.25	5 (11%)
34	II0	2	614	-	39,43,43	2.02	2 (5%)	48,60,60	1.61	11 (22%)
32	CLA	8	612	-	49,53,73	1.38	8 (16%)	58,89,113	1.38	4 (6%)
32	CLA	8	605	3	64,68,73	1.22	9 (14%)	76,107,113	1.27	5 (6%)
32	CLA	B	617	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	5 (6%)
32	CLA	B	602	-	51,55,73	1.33	9 (17%)	60,91,113	1.39	5 (8%)
32	CLA	P	604	-	59,63,73	1.27	7 (11%)	70,101,113	1.32	6 (8%)
47	HEM	f	101	11	50,50,50	1.47	7 (14%)	67,82,82	1.12	1 (1%)
32	CLA	p	303	6	63,67,73	1.23	8 (12%)	74,105,113	1.31	6 (8%)
32	CLA	C	503	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	7 (8%)
34	II0	5	316	-	39,43,43	2.04	2 (5%)	48,60,60	1.60	9 (18%)
38	LHG	8	618	32	21,21,48	0.77	0	23,26,54	1.31	2 (8%)
37	LMG	l	101	-	40,40,55	0.88	2 (5%)	48,48,63	1.29	6 (12%)
34	II0	5	315	-	39,43,43	2.03	2 (5%)	48,60,60	1.61	10 (20%)
37	LMG	D	411	-	40,40,55	0.81	0	48,48,63	1.25	6 (12%)
32	CLA	7	609	-	45,49,73	1.42	8 (17%)	54,84,113	1.48	5 (9%)
37	LMG	0	619	-	36,36,55	0.87	1 (2%)	44,44,63	1.26	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	II0	0	620	-	39,43,43	2.04	2 (5%)	48,60,60	1.65	13 (27%)
34	II0	3	613	-	39,43,43	2.04	2 (5%)	48,60,60	1.60	9 (18%)
32	CLA	9	602	4	63,67,73	1.21	9 (14%)	74,105,113	1.32	6 (8%)
32	CLA	2	612	-	49,53,73	1.38	8 (16%)	58,89,113	1.38	4 (6%)
32	CLA	4	611	-	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
32	CLA	b	616	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	5 (6%)
34	II0	3	612	-	39,43,43	2.02	2 (5%)	48,60,60	1.59	11 (22%)
32	CLA	c	508	-	69,73,73	1.14	9 (13%)	82,113,113	1.30	6 (7%)
32	CLA	7	604	2	59,63,73	1.27	8 (13%)	70,101,113	1.35	6 (8%)
37	LMG	6	616	-	28,28,55	0.98	1 (3%)	36,36,63	1.27	6 (16%)
31	8CT	Z	101	-	40,41,41	4.77	23 (57%)	51,56,56	2.63	21 (41%)
32	CLA	S	302	-	49,53,73	1.39	7 (14%)	58,89,113	1.40	4 (6%)
31	8CT	b	623	-	40,41,41	4.80	23 (57%)	51,56,56	2.85	16 (31%)
32	CLA	4	608	5	64,68,73	1.21	8 (12%)	76,107,113	1.28	5 (6%)
36	IHT	0	614	-	40,42,42	1.49	1 (2%)	52,58,58	1.77	10 (19%)
32	CLA	7	605	-	54,58,73	1.32	8 (14%)	64,95,113	1.35	6 (9%)
45	DGD	C	514	-	56,56,67	0.98	2 (3%)	70,70,81	1.47	10 (14%)
32	CLA	P	602	7	63,67,73	1.22	8 (12%)	74,105,113	1.32	6 (8%)
31	8CT	K	101	-	40,41,41	4.81	23 (57%)	51,56,56	2.81	18 (35%)
32	CLA	b	604	-	68,72,73	1.16	9 (13%)	80,111,113	1.27	6 (7%)
33	KC2	5	311	-	49,53,53	1.75	9 (18%)	60,89,89	1.91	15 (25%)
38	LHG	2	618	32	21,21,48	0.77	0	23,26,54	1.31	2 (8%)
32	CLA	6	606	7	49,53,73	1.38	6 (12%)	58,89,113	1.32	4 (6%)
32	CLA	9	606	-	49,53,73	1.39	9 (18%)	58,89,113	1.34	4 (6%)
41	PHO	d	410	-	58,69,69	2.10	9 (15%)	55,99,99	1.49	7 (12%)
32	CLA	4	605	-	54,58,73	1.32	8 (14%)	64,95,113	1.38	6 (9%)
32	CLA	C	507	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	5 (6%)
31	8CT	A	610	-	40,41,41	4.77	23 (57%)	51,56,56	2.77	21 (41%)
45	DGD	C	516	-	56,56,67	0.93	2 (3%)	70,70,81	1.41	8 (11%)
32	CLA	1	604	2	59,63,73	1.27	8 (13%)	70,101,113	1.36	6 (8%)
34	II0	4	615	-	39,43,43	2.01	2 (5%)	48,60,60	1.63	10 (20%)
32	CLA	b	607	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	8 (9%)
45	DGD	C	515	-	57,57,67	0.95	2 (3%)	71,71,81	1.41	9 (12%)
32	CLA	b	605	-	65,69,73	1.20	8 (12%)	77,108,113	1.36	7 (9%)
32	CLA	4	609	-	45,49,73	1.42	8 (17%)	54,84,113	1.47	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	IHT	8	616	-	40,42,42	1.53	2 (5%)	52,58,58	1.92	13 (25%)
36	IHT	4	617	-	40,42,42	1.56	2 (5%)	52,58,58	1.93	13 (25%)
32	CLA	b	606	-	69,73,73	1.15	9 (13%)	82,113,113	1.26	4 (4%)
32	CLA	C	512	-	61,65,73	1.22	9 (14%)	71,102,113	1.36	5 (7%)
32	CLA	G	101	-	49,53,73	1.40	8 (16%)	58,89,113	1.38	4 (6%)
32	CLA	6	610	-	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
34	II0	8	613	-	39,43,43	2.04	2 (5%)	48,60,60	1.60	9 (18%)
32	CLA	p	306	-	64,68,73	1.22	8 (12%)	76,107,113	1.27	4 (5%)
34	II0	1	617	-	39,43,43	2.06	2 (5%)	48,60,60	1.65	9 (18%)
39	SQD	B	620	-	52,54,54	1.55	7 (13%)	62,65,65	1.35	6 (9%)
38	LHG	D	410	-	31,31,48	0.77	1 (3%)	34,37,54	1.30	3 (8%)
32	CLA	P	601	7	46,50,73	1.40	8 (17%)	53,85,113	1.40	4 (7%)
32	CLA	0	605	-	54,58,73	1.32	8 (14%)	64,95,113	1.37	6 (9%)
32	CLA	c	510	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	5 (6%)
32	CLA	C	509	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	8 (9%)
34	II0	1	614	-	39,43,43	2.02	2 (5%)	48,60,60	1.57	8 (16%)
32	CLA	5	306	-	64,68,73	1.22	8 (12%)	76,107,113	1.29	4 (5%)
38	LHG	b	621	-	38,38,48	0.70	2 (5%)	41,44,54	1.29	4 (9%)
32	CLA	C	508	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	6 (7%)
45	DGD	A	614	-	54,54,67	1.04	4 (7%)	67,67,81	1.47	10 (14%)
32	CLA	a	408	-	64,68,73	1.18	9 (14%)	76,107,113	1.31	6 (7%)
34	II0	7	616	-	39,43,43	2.05	2 (5%)	48,60,60	1.65	10 (20%)
32	CLA	9	609	-	64,68,73	1.21	9 (14%)	76,107,113	1.29	6 (7%)
32	CLA	b	610	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
37	LMG	D	407	-	46,46,55	0.78	1 (2%)	54,54,63	1.34	5 (9%)
38	LHG	d	411	-	31,31,48	0.77	1 (3%)	34,37,54	1.30	3 (8%)
34	II0	0	617	-	39,43,43	2.01	2 (5%)	48,60,60	1.67	10 (20%)
32	CLA	9	611	-	49,53,73	1.38	9 (18%)	58,89,113	1.40	4 (6%)
34	II0	4	616	-	39,43,43	2.04	2 (5%)	48,60,60	1.62	11 (22%)
31	8CT	K	102	-	40,41,41	4.78	23 (57%)	51,56,56	2.73	20 (39%)
33	KC2	p	311	-	49,53,53	1.75	9 (18%)	60,89,89	1.92	15 (25%)
37	LMG	a	410	-	48,48,55	0.77	1 (2%)	56,56,63	1.34	5 (8%)
32	CLA	1	602	2	63,67,73	1.22	8 (12%)	74,105,113	1.31	6 (8%)
32	CLA	2	601	3	46,50,73	1.40	8 (17%)	53,85,113	1.40	4 (7%)
32	CLA	B	615	-	68,72,73	1.15	9 (13%)	80,111,113	1.27	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	PL9	a	412	-	13,13,55	1.58	2 (15%)	17,17,69	1.78	4 (23%)
32	CLA	9	607	4	64,68,73	1.20	9 (14%)	76,107,113	1.32	4 (5%)
33	KC2	2	610	-	49,53,53	1.76	9 (18%)	60,89,89	1.88	14 (23%)
32	CLA	c	512	-	61,65,73	1.21	9 (14%)	71,102,113	1.36	5 (7%)
32	CLA	8	604	-	59,63,73	1.26	8 (13%)	70,101,113	1.36	6 (8%)
39	SQD	b	601	-	46,48,54	1.60	7 (15%)	56,59,65	1.44	5 (8%)
33	KC2	1	610	-	49,53,53	1.75	9 (18%)	60,89,89	1.88	14 (23%)
32	CLA	b	603	-	64,69,73	1.16	9 (14%)	73,106,113	1.21	4 (5%)
32	CLA	4	603	-	54,58,73	1.33	8 (14%)	64,95,113	1.38	6 (9%)
32	CLA	0	607	5	49,53,73	1.39	8 (16%)	58,89,113	1.33	4 (6%)
34	II0	8	614	-	39,43,43	2.03	2 (5%)	48,60,60	1.59	11 (22%)
32	CLA	D	403	-	61,65,73	1.33	10 (16%)	74,103,113	1.35	7 (9%)
37	LMG	G	102	-	28,28,55	0.98	1 (3%)	36,36,63	1.29	5 (13%)
32	CLA	3	604	4	59,63,73	1.26	9 (15%)	70,101,113	1.34	6 (8%)
32	CLA	c	509	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	8 (9%)
32	CLA	3	608	-	45,49,73	1.39	8 (17%)	54,84,113	1.48	6 (11%)
32	CLA	0	613	5	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
32	CLA	7	611	-	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
32	CLA	9	604	4	59,63,73	1.26	9 (15%)	70,101,113	1.34	6 (8%)
32	CLA	6	602	7	63,67,73	1.22	9 (14%)	74,105,113	1.31	7 (9%)
31	8CT	H	102	-	40,41,41	4.84	23 (57%)	51,56,56	2.78	13 (25%)
38	LHG	A	612	-	42,42,48	0.68	1 (2%)	45,48,54	1.25	4 (8%)
40	OEX	A	601	8	0,15,15	-	-	-		
32	CLA	1	606	-	49,53,73	1.38	8 (16%)	58,89,113	1.41	4 (6%)
32	CLA	0	604	-	59,63,73	1.27	7 (11%)	70,101,113	1.34	8 (11%)
32	CLA	a	405	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	5 (6%)
32	CLA	A	602	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	5 (6%)
41	PHO	D	402	-	58,69,69	2.10	9 (15%)	55,99,99	1.49	7 (12%)
32	CLA	B	604	-	68,72,73	1.16	9 (13%)	80,111,113	1.26	6 (7%)
43	PL9	D	405	-	55,55,55	1.27	5 (9%)	68,69,69	1.51	13 (19%)
31	8CT	a	413	-	40,41,41	4.77	23 (57%)	51,56,56	3.10	18 (35%)
38	LHG	B	619	-	38,38,48	0.70	1 (2%)	41,44,54	1.31	4 (9%)
32	CLA	c	504	-	68,72,73	1.16	9 (13%)	80,111,113	1.30	6 (7%)
31	8CT	z	101	-	40,41,41	4.76	23 (57%)	51,56,56	2.67	22 (43%)
35	II3	7	615	-	40,43,43	1.50	1 (2%)	47,60,60	1.60	10 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	0	606	-	49,53,73	1.40	8 (16%)	58,89,113	1.35	4 (6%)
36	IHT	7	618	-	40,42,42	1.53	1 (2%)	52,58,58	1.89	10 (19%)
45	DGD	a	414	-	54,54,67	1.04	5 (9%)	67,67,81	1.46	10 (14%)
32	CLA	B	607	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	8 (9%)
32	CLA	5	305	-	59,63,73	1.28	8 (13%)	70,101,113	1.35	6 (8%)
32	CLA	c	513	-	53,57,73	1.30	9 (16%)	61,93,113	1.42	6 (9%)
32	CLA	7	606	-	49,53,73	1.38	7 (14%)	58,89,113	1.44	6 (10%)
32	CLA	b	612	-	68,72,73	1.16	9 (13%)	80,111,113	1.29	6 (7%)
44	BCT	A	611	46	3,3,3	1.11	0	2,3,3	4.58	2 (100%)
32	CLA	5	303	6	63,67,73	1.23	9 (14%)	74,105,113	1.32	6 (8%)
38	LHG	b	619	-	38,38,48	0.69	1 (2%)	41,44,54	1.30	4 (9%)
32	CLA	C	511	27	69,73,73	1.16	9 (13%)	82,113,113	1.29	4 (4%)
32	CLA	4	601	5	46,50,73	1.41	8 (17%)	53,85,113	1.41	4 (7%)
36	IHT	0	618	-	40,42,42	1.51	2 (5%)	52,58,58	1.92	13 (25%)
33	KC2	P	605	-	49,53,53	1.77	8 (16%)	60,89,89	1.80	15 (25%)
32	CLA	7	608	2	64,68,73	1.21	8 (12%)	76,107,113	1.27	4 (5%)
32	CLA	C	510	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
32	CLA	c	511	27	69,73,73	1.16	9 (13%)	82,113,113	1.28	4 (4%)
32	CLA	p	309	6	64,68,73	1.21	8 (12%)	76,107,113	1.28	5 (6%)
31	8CT	9	615	-	40,41,41	4.83	23 (57%)	51,56,56	2.79	18 (35%)
32	CLA	b	613	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	8 (9%)
38	LHG	A	613	-	48,48,48	0.66	1 (2%)	51,54,54	1.28	6 (11%)
39	SQD	a	409	-	52,54,54	1.54	7 (13%)	62,65,65	1.34	8 (12%)
32	CLA	2	604	-	59,63,73	1.26	8 (13%)	70,101,113	1.36	6 (8%)
32	CLA	0	612	-	49,53,73	1.40	8 (16%)	58,89,113	1.46	5 (8%)
32	CLA	2	602	3	63,67,73	1.22	9 (14%)	74,105,113	1.31	6 (8%)
34	II0	5	301	-	39,43,43	2.00	2 (5%)	48,60,60	1.66	9 (18%)
32	CLA	1	611	-	49,53,73	1.40	7 (14%)	58,89,113	1.43	4 (6%)
32	CLA	8	611	-	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
47	HEM	V	201	-	50,50,50	1.46	8 (16%)	67,82,82	1.04	4 (5%)
36	IHT	5	317	-	40,42,42	1.50	1 (2%)	52,58,58	1.77	13 (25%)
32	CLA	7	613	-	49,53,73	1.39	7 (14%)	58,89,113	1.42	4 (6%)
32	CLA	B	608	-	45,49,73	1.38	9 (20%)	54,84,113	1.48	5 (9%)
32	CLA	9	603	-	54,58,73	1.30	8 (14%)	64,95,113	1.41	6 (9%)
32	CLA	8	606	-	49,53,73	1.39	8 (16%)	58,89,113	1.36	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	B	606	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	4 (4%)
32	CLA	1	605	-	54,58,73	1.32	8 (14%)	64,95,113	1.35	6 (9%)
31	8CT	b	622	-	40,41,41	4.80	23 (57%)	51,56,56	2.52	17 (33%)
37	LMG	d	401	-	40,40,55	0.80	0	48,48,63	1.24	6 (12%)
32	CLA	3	603	-	54,58,73	1.30	9 (16%)	64,95,113	1.42	6 (9%)
34	II0	4	619	-	39,43,43	2.03	2 (5%)	48,60,60	1.64	13 (27%)
41	PHO	A	604	-	58,69,69	2.10	11 (18%)	55,99,99	1.46	7 (12%)
36	IHT	p	317	-	40,42,42	1.50	1 (2%)	52,58,58	1.81	13 (25%)
35	II3	P	613	-	40,43,43	1.49	1 (2%)	47,60,60	1.67	10 (21%)
32	CLA	2	611	-	49,53,73	1.39	7 (14%)	58,89,113	1.43	4 (6%)
37	LMG	4	618	-	36,36,55	0.87	1 (2%)	44,44,63	1.26	5 (11%)
32	CLA	1	613	-	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
32	CLA	b	617	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	5 (6%)
32	CLA	B	614	-	69,73,73	1.15	9 (13%)	82,113,113	1.24	6 (7%)
32	CLA	6	611	-	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
38	LHG	B	621	-	38,38,48	0.70	2 (5%)	41,44,54	1.29	4 (9%)
40	OEX	a	404	8	0,15,15	-	-	-		
32	CLA	d	409	-	63,67,73	1.18	9 (14%)	74,105,113	1.36	8 (10%)
37	LMG	P	616	-	28,28,55	0.98	1 (3%)	36,36,63	1.27	6 (16%)
32	CLA	6	603	-	54,58,73	1.31	8 (14%)	64,95,113	1.40	5 (7%)
37	LMG	b	618	-	51,51,55	0.73	1 (1%)	59,59,63	1.36	6 (10%)
32	CLA	6	607	7	64,68,73	1.21	8 (12%)	76,107,113	1.29	5 (6%)
37	LMG	8	617	-	36,36,55	0.85	1 (2%)	44,44,63	1.25	5 (11%)
32	CLA	7	602	2	63,67,73	1.22	8 (12%)	74,105,113	1.32	6 (8%)
32	CLA	6	608	-	45,49,73	1.42	8 (17%)	54,84,113	1.45	5 (9%)
32	CLA	C	513	-	53,57,73	1.30	9 (16%)	61,93,113	1.41	5 (8%)
32	CLA	d	402	-	61,65,73	1.32	10 (16%)	74,103,113	1.35	7 (9%)
32	CLA	2	607	3	49,53,73	1.38	8 (16%)	58,89,113	1.37	4 (6%)
32	CLA	9	605	-	50,54,73	1.35	9 (18%)	59,90,113	1.36	4 (6%)
32	CLA	0	611	-	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
39	SQD	5	318	-	33,35,54	1.77	8 (24%)	43,46,65	1.49	6 (13%)
37	LMG	g	101	-	28,28,55	0.98	1 (3%)	36,36,63	1.28	5 (13%)
32	CLA	2	608	3	64,68,73	1.20	9 (14%)	76,107,113	1.30	5 (6%)
39	SQD	B	601	-	46,48,54	1.60	7 (15%)	56,59,65	1.44	5 (8%)
32	CLA	B	611	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	P	606	7	49,53,73	1.39	6 (12%)	58,89,113	1.31	4 (6%)
32	CLA	5	309	-	64,68,73	1.21	8 (12%)	76,107,113	1.29	5 (6%)
34	II0	2	619	-	39,43,43	2.05	2 (5%)	48,60,60	1.63	10 (20%)
31	8CT	C	518	-	40,41,41	4.85	22 (55%)	51,56,56	2.89	17 (33%)
32	CLA	A	605	-	64,68,73	1.18	9 (14%)	76,107,113	1.30	6 (7%)
37	LMG	L	102	-	40,40,55	0.88	2 (5%)	48,48,63	1.29	6 (12%)
39	SQD	b	620	-	52,54,54	1.55	7 (13%)	62,65,65	1.34	6 (9%)
32	CLA	p	307	-	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
32	CLA	2	606	-	49,53,73	1.39	8 (16%)	58,89,113	1.37	4 (6%)
37	LMG	C	517	-	46,46,55	0.77	1 (2%)	54,54,63	1.32	6 (11%)
34	II0	3	614	-	39,43,43	2.01	2 (5%)	48,60,60	1.57	10 (20%)
38	LHG	s	301	-	36,36,48	0.72	1 (2%)	39,42,54	1.27	4 (10%)
32	CLA	s	302	-	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
31	8CT	3	615	-	40,41,41	4.83	23 (57%)	51,56,56	2.79	17 (33%)
38	LHG	S	301	-	36,36,48	0.72	1 (2%)	39,42,54	1.27	4 (10%)
35	II3	1	615	-	40,43,43	1.50	1 (2%)	47,60,60	1.56	6 (12%)
45	DGD	c	516	-	56,56,67	0.93	2 (3%)	70,70,81	1.41	7 (10%)
32	CLA	3	605	-	50,54,73	1.35	8 (16%)	59,90,113	1.35	4 (6%)
32	CLA	b	609	-	69,73,73	1.14	9 (13%)	82,113,113	1.29	7 (8%)
34	II0	p	301	-	39,43,43	2.03	2 (5%)	48,60,60	1.67	12 (25%)
34	II0	P	612	-	39,43,43	1.99	2 (5%)	48,60,60	1.66	12 (25%)
32	CLA	B	605	-	65,69,73	1.20	8 (12%)	77,108,113	1.36	7 (9%)
32	CLA	8	602	3	63,67,73	1.22	9 (14%)	74,105,113	1.31	6 (8%)
32	CLA	A	603	-	53,57,73	1.28	8 (15%)	61,93,113	1.43	5 (8%)
32	CLA	3	602	4	63,67,73	1.21	9 (14%)	74,105,113	1.33	6 (8%)
32	CLA	1	608	2	64,68,73	1.21	9 (14%)	76,107,113	1.28	4 (5%)
32	CLA	5	313	-	49,53,73	1.39	7 (14%)	58,89,113	1.37	4 (6%)
31	8CT	6	615	-	40,41,41	4.87	23 (57%)	51,56,56	2.59	18 (35%)
33	KC2	4	610	5	49,53,53	1.74	8 (16%)	60,89,89	1.88	15 (25%)
45	DGD	h	101	-	63,63,67	0.88	2 (3%)	77,77,81	1.37	8 (10%)
34	II0	1	619	-	39,43,43	1.99	2 (5%)	48,60,60	1.59	9 (18%)

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
38	LHG	L	101	-	-	19/53/53/53	-
32	CLA	5	312	-	1/1/11/20	7/15/91/115	-
43	PL9	d	404	-	-	3/53/73/73	0/1/1/1
37	LMG	c	517	-	-	25/41/61/70	0/1/1/1
32	CLA	p	313	-	1/1/11/20	10/15/91/115	-
33	KC2	P	609	-	-	12/15/71/71	-
32	CLA	3	610	4	1/1/11/20	7/15/91/115	-
32	CLA	1	609	-	1/1/10/20	4/10/86/115	-
32	CLA	c	502	-	1/1/14/20	17/37/113/115	-
33	KC2	6	605	7	-	9/15/71/71	-
32	CLA	B	610	-	1/1/15/20	9/39/115/115	-
34	II0	5	314	-	-	2/21/67/67	0/2/2/2
32	CLA	1	601	-	1/1/10/20	4/12/88/115	-
33	KC2	8	610	-	-	11/15/71/71	-
32	CLA	7	607	-	1/1/11/20	8/15/91/115	-
32	CLA	d	403	-	1/1/14/20	10/33/109/115	-
32	CLA	1	612	-	1/1/11/20	7/15/91/115	-
32	CLA	P	611	-	1/1/11/20	9/15/91/115	-
31	8CT	k	101	-	-	6/29/63/63	0/2/2/2
32	CLA	c	505	-	1/1/15/20	13/39/115/115	-
38	LHG	d	405	-	-	17/47/51/53	-
34	II0	7	619	-	-	1/21/67/67	0/2/2/2
34	II0	p	315	-	-	4/21/67/67	0/2/2/2
31	8CT	B	624	-	-	7/29/63/63	0/2/2/2
32	CLA	4	613	5	1/1/11/20	8/15/91/115	-
47	HEM	v	201	-	-	1/14/54/54	-
31	8CT	M	201	-	-	16/29/63/63	0/2/2/2
45	DGD	H	101	-	-	19/51/91/95	0/2/2/2
32	CLA	5	310	-	1/1/10/20	4/10/86/115	-
33	KC2	0	610	5	-	12/15/71/71	-
37	LMG	B	618	-	-	19/46/66/70	0/1/1/1
32	CLA	9	610	4	1/1/11/20	7/15/91/115	-
32	CLA	0	608	5	1/1/14/20	9/33/109/115	-
34	II0	2	613	-	-	1/21/67/67	0/2/2/2
38	LHG	a	402	-	-	10/47/47/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	p	304	-	1/1/12/20	11/21/97/115	-
32	CLA	B	603	-	1/1/12/20	13/29/107/115	-
32	CLA	c	501	-	1/1/15/20	17/39/115/115	-
32	CLA	g	102	-	1/1/11/20	5/15/91/115	-
32	CLA	5	304	-	1/1/12/20	11/21/97/115	-
32	CLA	4	607	5	1/1/11/20	4/15/91/115	-
32	CLA	c	506	-	1/1/11/20	4/15/91/115	-
32	CLA	7	601	-	1/1/10/20	5/12/88/115	-
32	CLA	0	603	-	1/1/12/20	4/21/97/115	-
32	CLA	1	603	-	1/1/12/20	7/21/97/115	-
34	II0	1	616	-	-	4/21/67/67	0/2/2/2
34	II0	7	617	-	-	4/21/67/67	0/2/2/2
33	KC2	7	610	-	-	12/15/71/71	-
32	CLA	0	609	-	1/1/10/20	2/10/86/115	-
45	DGD	c	514	-	-	19/44/84/95	0/2/2/2
32	CLA	2	605	3	1/1/14/20	11/33/109/115	-
32	CLA	c	507	-	1/1/15/20	15/39/115/115	-
32	CLA	B	609	-	1/1/15/20	8/39/115/115	-
38	LHG	l	102	-	-	19/53/53/53	-
31	8CT	B	623	-	-	8/29/63/63	0/2/2/2
34	II0	2	615	-	-	2/21/67/67	0/2/2/2
32	CLA	4	604	-	1/1/13/20	11/27/103/115	-
32	CLA	8	603	-	1/1/12/20	6/21/97/115	-
31	8CT	k	102	-	-	13/29/63/63	0/2/2/2
32	CLA	7	603	-	1/1/12/20	7/21/97/115	-
32	CLA	8	607	3	1/1/11/20	4/15/91/115	-
39	SQD	A	606	-	-	27/49/69/69	0/1/1/1
32	CLA	b	611	-	1/1/15/20	7/39/115/115	-
32	CLA	3	601	4	1/1/10/20	5/12/88/115	-
32	CLA	8	608	3	1/1/14/20	10/33/109/115	-
34	II0	9	612	-	-	3/21/67/67	0/2/2/2
32	CLA	p	312	-	1/1/11/20	7/15/91/115	-
32	CLA	p	302	6	1/1/10/20	4/12/88/115	-
32	CLA	b	614	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	b	608	-	1/1/10/20	3/10/86/115	-
32	CLA	9	601	4	1/1/10/20	5/12/88/115	-
32	CLA	s	303	19	1/1/15/20	17/39/115/115	-
38	LHG	D	406	-	-	17/47/51/53	-
32	CLA	5	302	6	1/1/10/20	4/12/88/115	-
32	CLA	P	608	-	1/1/10/20	2/10/86/115	-
32	CLA	0	601	5	1/1/10/20	4/12/88/115	-
47	HEM	E	101	-	-	4/14/54/54	-
32	CLA	B	613	-	1/1/15/20	15/39/115/115	-
32	CLA	4	606	-	1/1/11/20	6/15/91/115	-
32	CLA	8	609	38	1/1/10/20	4/10/86/115	-
32	CLA	C	501	-	1/1/15/20	17/39/115/115	-
38	LHG	a	403	-	-	24/53/53/53	-
32	CLA	C	502	-	1/1/14/20	17/37/113/115	-
34	II0	P	614	-	-	2/21/67/67	0/2/2/2
32	CLA	C	504	-	1/1/14/20	12/37/113/115	-
33	KC2	6	609	-	-	12/15/71/71	-
36	IHT	2	616	-	-	1/25/65/65	0/2/2/2
32	CLA	8	601	3	1/1/10/20	4/12/88/115	-
32	CLA	P	607	7	1/1/14/20	7/33/109/115	-
32	CLA	5	308	6	1/1/11/20	5/15/91/115	-
32	CLA	7	612	-	1/1/11/20	7/15/91/115	-
32	CLA	p	305	-	1/1/13/20	8/27/103/115	-
32	CLA	p	308	6	1/1/11/20	5/15/91/115	-
34	II0	0	616	-	-	4/21/67/67	0/2/2/2
34	II0	9	613	-	-	1/21/67/67	0/2/2/2
32	CLA	6	601	7	1/1/10/20	2/12/88/115	-
32	CLA	3	611	-	1/1/11/20	7/15/91/115	-
32	CLA	b	615	-	1/1/14/20	13/37/113/115	-
39	SQD	p	318	-	-	19/30/50/69	0/1/1/1
34	II0	0	615	-	-	1/21/67/67	0/2/2/2
32	CLA	D	404	-	1/1/14/20	11/33/109/115	-
31	8CT	d	408	-	-	13/29/63/63	0/2/2/2
32	CLA	1	607	-	1/1/11/20	8/15/91/115	-
32	CLA	3	607	4	1/1/14/20	8/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	PHO	a	407	-	-	8/37/103/103	0/5/6/6
34	II0	p	314	-	-	0/21/67/67	0/2/2/2
32	CLA	b	602	-	1/1/11/20	6/18/94/115	-
32	CLA	S	303	19	1/1/15/20	17/39/115/115	-
32	CLA	C	505	-	1/1/15/20	13/39/115/115	-
45	DGD	c	515	-	-	18/45/85/95	0/2/2/2
34	II0	5	319	-	-	2/21/67/67	0/2/2/2
36	IHT	1	618	-	-	4/25/65/65	0/2/2/2
32	CLA	a	406	-	1/1/11/20	4/20/96/115	-
32	CLA	3	606	-	1/1/11/20	0/15/91/115	-
32	CLA	B	612	-	1/1/14/20	15/37/113/115	-
34	II0	6	614	-	-	3/21/67/67	0/2/2/2
34	II0	7	614	-	-	1/21/67/67	0/2/2/2
36	IHT	4	614	-	-	5/25/65/65	0/2/2/2
32	CLA	c	503	-	1/1/15/20	16/39/115/115	-
43	PL9	A	609	-	-	1/5/18/73	0/1/1/1
34	II0	6	612	-	-	1/21/67/67	0/2/2/2
32	CLA	0	602	5	1/1/13/20	11/32/108/115	-
31	8CT	h	102	-	-	9/29/63/63	0/2/2/2
32	CLA	p	310	-	1/1/10/20	4/10/86/115	-
32	CLA	2	603	-	1/1/12/20	6/21/97/115	-
32	CLA	9	608	-	1/1/10/20	2/10/86/115	-
35	II3	6	613	-	-	1/25/67/67	0/2/2/2
31	8CT	c	518	-	-	10/29/63/63	0/2/2/2
37	LMG	d	406	-	-	18/41/61/70	0/1/1/1
31	8CT	B	622	-	-	16/29/63/63	0/2/2/2
34	II0	8	615	-	-	2/21/67/67	0/2/2/2
37	LMG	A	607	-	-	16/43/63/70	0/1/1/1
32	CLA	2	609	38	1/1/10/20	4/10/86/115	-
32	CLA	C	506	-	1/1/11/20	4/15/91/115	-
32	CLA	P	603	-	1/1/12/20	2/21/97/115	-
31	8CT	D	409	-	-	13/29/63/63	0/2/2/2
32	CLA	5	307	-	1/1/11/20	5/15/91/115	-
32	CLA	6	604	-	1/1/13/20	6/27/103/115	-
32	CLA	P	610	-	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	4	612	-	1/1/11/20	9/15/91/115	-
32	CLA	4	602	5	1/1/13/20	11/32/108/115	-
32	CLA	3	609	-	1/1/14/20	7/33/109/115	-
32	CLA	D	401	-	1/1/13/20	3/32/108/115	-
31	8CT	P	615	-	-	4/29/63/63	0/2/2/2
34	II0	9	614	-	-	3/21/67/67	0/2/2/2
34	II0	8	619	-	-	1/21/67/67	0/2/2/2
34	II0	p	316	-	-	3/21/67/67	0/2/2/2
32	CLA	B	616	-	1/1/15/20	7/39/115/115	-
37	LMG	2	617	-	-	10/31/51/70	0/1/1/1
34	II0	2	614	-	-	0/21/67/67	0/2/2/2
32	CLA	8	612	-	1/1/11/20	7/15/91/115	-
32	CLA	8	605	3	1/1/14/20	11/33/109/115	-
32	CLA	B	617	-	1/1/15/20	13/39/115/115	-
32	CLA	B	602	-	1/1/11/20	6/18/94/115	-
32	CLA	P	604	-	1/1/13/20	6/27/103/115	-
47	HEM	f	101	11	-	4/14/54/54	-
32	CLA	p	303	6	1/1/13/20	12/32/108/115	-
32	CLA	C	503	-	1/1/15/20	14/39/115/115	-
34	II0	5	316	-	-	2/21/67/67	0/2/2/2
38	LHG	8	618	32	-	10/24/24/53	-
37	LMG	l	101	-	-	17/35/55/70	0/1/1/1
34	II0	5	315	-	-	3/21/67/67	0/2/2/2
37	LMG	D	411	-	-	26/35/55/70	0/1/1/1
32	CLA	7	609	-	1/1/10/20	4/10/86/115	-
37	LMG	0	619	-	-	10/31/51/70	0/1/1/1
34	II0	0	620	-	-	1/21/67/67	0/2/2/2
34	II0	3	613	-	-	0/21/67/67	0/2/2/2
32	CLA	9	602	4	1/1/13/20	9/32/108/115	-
32	CLA	2	612	-	1/1/11/20	7/15/91/115	-
32	CLA	4	611	-	1/1/11/20	7/15/91/115	-
32	CLA	b	616	-	1/1/15/20	7/39/115/115	-
34	II0	3	612	-	-	2/21/67/67	0/2/2/2
32	CLA	c	508	-	1/1/15/20	9/39/115/115	-
32	CLA	7	604	2	1/1/13/20	6/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LMG	6	616	-	-	10/23/43/70	0/1/1/1
31	8CT	Z	101	-	-	12/29/63/63	0/2/2/2
32	CLA	S	302	-	1/1/11/20	7/15/91/115	-
31	8CT	b	623	-	-	7/29/63/63	0/2/2/2
32	CLA	4	608	5	1/1/14/20	9/33/109/115	-
36	IHT	0	614	-	-	5/25/65/65	0/2/2/2
32	CLA	7	605	-	1/1/12/20	8/21/97/115	-
45	DGD	C	514	-	-	19/44/84/95	0/2/2/2
32	CLA	P	602	7	1/1/13/20	14/32/108/115	-
31	8CT	K	101	-	-	12/29/63/63	0/2/2/2
32	CLA	b	604	-	1/1/14/20	8/37/113/115	-
33	KC2	5	311	-	-	10/15/71/71	-
38	LHG	2	618	32	-	11/24/24/53	-
32	CLA	6	606	7	1/1/11/20	4/15/91/115	-
32	CLA	9	606	-	1/1/11/20	0/15/91/115	-
41	PHO	d	410	-	-	8/37/103/103	0/5/6/6
32	CLA	4	605	-	1/1/12/20	7/21/97/115	-
32	CLA	C	507	-	1/1/15/20	15/39/115/115	-
31	8CT	A	610	-	-	5/29/63/63	0/2/2/2
45	DGD	C	516	-	-	18/44/84/95	0/2/2/2
32	CLA	1	604	2	1/1/13/20	6/27/103/115	-
34	II0	4	615	-	-	0/21/67/67	0/2/2/2
32	CLA	b	607	-	1/1/15/20	7/39/115/115	-
45	DGD	C	515	-	-	18/45/85/95	0/2/2/2
32	CLA	b	605	-	1/1/14/20	8/35/111/115	-
32	CLA	4	609	-	1/1/10/20	2/10/86/115	-
36	IHT	8	616	-	-	0/25/65/65	0/2/2/2
36	IHT	4	617	-	-	6/25/65/65	0/2/2/2
32	CLA	b	606	-	1/1/15/20	12/39/115/115	-
32	CLA	C	512	-	1/1/12/20	10/29/105/115	-
32	CLA	G	101	-	1/1/11/20	5/15/91/115	-
32	CLA	6	610	-	1/1/11/20	6/15/91/115	-
34	II0	8	613	-	-	0/21/67/67	0/2/2/2
32	CLA	p	306	-	1/1/14/20	14/33/109/115	-
34	II0	1	617	-	-	3/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	SQD	B	620	-	-	23/49/69/69	0/1/1/1
38	LHG	D	410	-	-	18/36/36/53	-
32	CLA	P	601	7	1/1/10/20	2/12/88/115	-
32	CLA	0	605	-	1/1/12/20	7/21/97/115	-
32	CLA	c	510	-	1/1/15/20	8/39/115/115	-
32	CLA	C	509	-	1/1/15/20	6/39/115/115	-
34	II0	1	614	-	-	0/21/67/67	0/2/2/2
32	CLA	5	306	-	1/1/14/20	15/33/109/115	-
38	LHG	b	621	-	-	14/43/43/53	-
32	CLA	C	508	-	1/1/15/20	9/39/115/115	-
45	DGD	A	614	-	-	15/43/79/95	0/2/2/2
32	CLA	a	408	-	1/1/14/20	3/33/109/115	-
34	II0	7	616	-	-	3/21/67/67	0/2/2/2
32	CLA	9	609	-	1/1/14/20	7/33/109/115	-
32	CLA	b	610	-	1/1/15/20	9/39/115/115	-
37	LMG	D	407	-	-	18/41/61/70	0/1/1/1
38	LHG	d	411	-	-	18/36/36/53	-
34	II0	0	617	-	-	2/21/67/67	0/2/2/2
32	CLA	9	611	-	1/1/11/20	7/15/91/115	-
34	II0	4	616	-	-	4/21/67/67	0/2/2/2
31	8CT	K	102	-	-	6/29/63/63	0/2/2/2
33	KC2	p	311	-	-	10/15/71/71	-
37	LMG	a	410	-	-	16/43/63/70	0/1/1/1
32	CLA	1	602	2	1/1/13/20	12/32/108/115	-
32	CLA	2	601	3	1/1/10/20	4/12/88/115	-
32	CLA	B	615	-	1/1/14/20	13/37/113/115	-
43	PL9	a	412	-	-	1/5/18/73	0/1/1/1
32	CLA	9	607	4	1/1/14/20	8/33/109/115	-
33	KC2	2	610	-	-	11/15/71/71	-
32	CLA	c	512	-	1/1/12/20	10/29/105/115	-
32	CLA	8	604	-	1/1/13/20	2/27/103/115	-
39	SQD	b	601	-	-	23/43/63/69	0/1/1/1
33	KC2	1	610	-	-	12/15/71/71	-
32	CLA	b	603	-	1/1/12/20	13/29/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	4	603	-	1/1/12/20	4/21/97/115	-
32	CLA	0	607	5	1/1/11/20	2/15/91/115	-
34	II0	8	614	-	-	0/21/67/67	0/2/2/2
32	CLA	D	403	-	1/1/13/20	8/28/104/115	-
37	LMG	G	102	-	-	9/23/43/70	0/1/1/1
32	CLA	3	604	4	1/1/13/20	5/27/103/115	-
32	CLA	c	509	-	1/1/15/20	6/39/115/115	-
32	CLA	3	608	-	1/1/10/20	2/10/86/115	-
32	CLA	0	613	5	1/1/11/20	8/15/91/115	-
32	CLA	7	611	-	1/1/11/20	6/15/91/115	-
32	CLA	9	604	4	1/1/13/20	5/27/103/115	-
32	CLA	6	602	7	1/1/13/20	14/32/108/115	-
31	8CT	H	102	-	-	9/29/63/63	0/2/2/2
38	LHG	A	612	-	-	10/47/47/53	-
32	CLA	1	606	-	1/1/11/20	12/15/91/115	-
32	CLA	0	604	-	1/1/13/20	11/27/103/115	-
32	CLA	a	405	-	1/1/15/20	7/39/115/115	-
32	CLA	A	602	-	1/1/15/20	7/39/115/115	-
41	PHO	D	402	-	-	8/37/103/103	0/5/6/6
32	CLA	B	604	-	1/1/14/20	8/37/113/115	-
43	PL9	D	405	-	-	3/53/73/73	0/1/1/1
31	8CT	a	413	-	-	6/29/63/63	0/2/2/2
38	LHG	B	619	-	-	19/43/43/53	-
32	CLA	c	504	-	1/1/14/20	12/37/113/115	-
31	8CT	z	101	-	-	12/29/63/63	0/2/2/2
35	II3	7	615	-	-	2/25/67/67	0/2/2/2
32	CLA	0	606	-	1/1/11/20	6/15/91/115	-
36	IHT	7	618	-	-	2/25/65/65	0/2/2/2
45	DGD	a	414	-	-	13/43/79/95	0/2/2/2
32	CLA	B	607	-	1/1/15/20	7/39/115/115	-
32	CLA	5	305	-	1/1/13/20	8/27/103/115	-
32	CLA	c	513	-	1/1/11/20	10/20/96/115	-
32	CLA	7	606	-	1/1/11/20	11/15/91/115	-
32	CLA	b	612	-	1/1/14/20	15/37/113/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	5	303	6	1/1/13/20	11/32/108/115	-
38	LHG	b	619	-	-	19/43/43/53	-
32	CLA	C	511	27	1/1/15/20	8/39/115/115	-
32	CLA	4	601	5	1/1/10/20	4/12/88/115	-
36	IHT	0	618	-	-	5/25/65/65	0/2/2/2
33	KC2	P	605	-	-	10/15/71/71	-
32	CLA	7	608	2	1/1/14/20	10/33/109/115	-
32	CLA	C	510	-	1/1/15/20	8/39/115/115	-
32	CLA	c	511	27	1/1/15/20	8/39/115/115	-
32	CLA	p	309	6	1/1/14/20	10/33/109/115	-
32	CLA	b	613	-	1/1/15/20	15/39/115/115	-
31	8CT	9	615	-	-	10/29/63/63	0/2/2/2
38	LHG	A	613	-	-	23/53/53/53	-
39	SQD	a	409	-	-	27/49/69/69	0/1/1/1
32	CLA	2	604	-	1/1/13/20	2/27/103/115	-
32	CLA	0	612	-	1/1/11/20	9/15/91/115	-
32	CLA	2	602	3	1/1/13/20	9/32/108/115	-
34	II0	5	301	-	-	3/21/67/67	0/2/2/2
32	CLA	1	611	-	1/1/11/20	6/15/91/115	-
32	CLA	8	611	-	1/1/11/20	5/15/91/115	-
47	HEM	V	201	-	-	1/14/54/54	-
36	IHT	5	317	-	-	1/25/65/65	0/2/2/2
32	CLA	7	613	-	1/1/11/20	6/15/91/115	-
32	CLA	B	608	-	1/1/10/20	2/10/86/115	-
32	CLA	9	603	-	1/1/12/20	8/21/97/115	-
32	CLA	8	606	-	1/1/11/20	4/15/91/115	-
32	CLA	B	606	-	1/1/15/20	12/39/115/115	-
32	CLA	1	605	-	1/1/12/20	9/21/97/115	-
31	8CT	b	622	-	-	8/29/63/63	0/2/2/2
37	LMG	d	401	-	-	26/35/55/70	0/1/1/1
32	CLA	3	603	-	1/1/12/20	8/21/97/115	-
34	II0	4	619	-	-	2/21/67/67	0/2/2/2
41	PHO	A	604	-	-	8/37/103/103	0/5/6/6
36	IHT	p	317	-	-	0/25/65/65	0/2/2/2
35	II3	P	613	-	-	3/25/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	2	611	-	1/1/11/20	5/15/91/115	-
37	LMG	4	618	-	-	11/31/51/70	0/1/1/1
32	CLA	1	613	-	1/1/11/20	6/15/91/115	-
32	CLA	b	617	-	1/1/15/20	13/39/115/115	-
32	CLA	B	614	-	1/1/15/20	13/39/115/115	-
32	CLA	6	611	-	1/1/11/20	9/15/91/115	-
38	LHG	B	621	-	-	14/43/43/53	-
32	CLA	d	409	-	1/1/13/20	3/32/108/115	-
37	LMG	P	616	-	-	10/23/43/70	0/1/1/1
32	CLA	6	603	-	1/1/12/20	2/21/97/115	-
37	LMG	b	618	-	-	17/46/66/70	0/1/1/1
32	CLA	6	607	7	1/1/14/20	7/33/109/115	-
37	LMG	8	617	-	-	10/31/51/70	0/1/1/1
32	CLA	7	602	2	1/1/13/20	12/32/108/115	-
32	CLA	6	608	-	1/1/10/20	2/10/86/115	-
32	CLA	C	513	-	1/1/11/20	10/20/96/115	-
32	CLA	d	402	-	1/1/13/20	8/28/104/115	-
32	CLA	2	607	3	1/1/11/20	4/15/91/115	-
32	CLA	9	605	-	1/1/11/20	8/17/93/115	-
32	CLA	0	611	-	1/1/11/20	7/15/91/115	-
39	SQD	5	318	-	-	19/30/50/69	0/1/1/1
37	LMG	g	101	-	-	10/23/43/70	0/1/1/1
32	CLA	2	608	3	1/1/14/20	10/33/109/115	-
39	SQD	B	601	-	-	23/43/63/69	0/1/1/1
32	CLA	B	611	-	1/1/15/20	7/39/115/115	-
32	CLA	P	606	7	1/1/11/20	4/15/91/115	-
32	CLA	5	309	-	1/1/14/20	10/33/109/115	-
34	II0	2	619	-	-	2/21/67/67	0/2/2/2
32	CLA	A	605	-	1/1/14/20	3/33/109/115	-
31	8CT	C	518	-	-	10/29/63/63	0/2/2/2
37	LMG	L	102	-	-	19/35/55/70	0/1/1/1
39	SQD	b	620	-	-	24/49/69/69	0/1/1/1
32	CLA	p	307	-	1/1/11/20	5/15/91/115	-
32	CLA	2	606	-	1/1/11/20	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LMG	C	517	-	-	25/41/61/70	0/1/1/1
34	II0	3	614	-	-	4/21/67/67	0/2/2/2
38	LHG	s	301	-	-	19/41/41/53	-
32	CLA	s	302	-	1/1/11/20	6/15/91/115	-
31	8CT	3	615	-	-	10/29/63/63	0/2/2/2
38	LHG	S	301	-	-	20/41/41/53	-
35	II3	1	615	-	-	2/25/67/67	0/2/2/2
45	DGD	c	516	-	-	19/44/84/95	0/2/2/2
32	CLA	3	605	-	1/1/11/20	8/17/93/115	-
32	CLA	b	609	-	1/1/15/20	8/39/115/115	-
34	II0	p	301	-	-	2/21/67/67	0/2/2/2
34	II0	P	612	-	-	0/21/67/67	0/2/2/2
32	CLA	B	605	-	1/1/14/20	8/35/111/115	-
32	CLA	8	602	3	1/1/13/20	10/32/108/115	-
32	CLA	A	603	-	1/1/11/20	4/20/96/115	-
32	CLA	3	602	4	1/1/13/20	9/32/108/115	-
32	CLA	1	608	2	1/1/14/20	10/33/109/115	-
32	CLA	5	313	-	1/1/11/20	10/15/91/115	-
31	8CT	6	615	-	-	4/29/63/63	0/2/2/2
33	KC2	4	610	5	-	12/15/71/71	-
45	DGD	h	101	-	-	19/51/91/95	0/2/2/2
34	II0	1	619	-	-	2/21/67/67	0/2/2/2

All (2699) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	408	8CT	C02-C03	14.93	1.59	1.34
31	D	409	8CT	C02-C03	14.90	1.59	1.34
31	b	622	8CT	C02-C03	14.84	1.59	1.34
31	h	102	8CT	C02-C03	14.83	1.59	1.34
31	H	102	8CT	C02-C03	14.83	1.59	1.34
31	K	102	8CT	C02-C03	14.78	1.59	1.34
31	B	623	8CT	C02-C03	14.78	1.59	1.34
31	k	101	8CT	C02-C03	14.77	1.59	1.34
31	a	413	8CT	C02-C03	14.76	1.59	1.34
31	B	624	8CT	C02-C03	14.70	1.59	1.34
31	b	623	8CT	C02-C03	14.69	1.59	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Z	101	8CT	C02-C03	14.68	1.59	1.34
31	A	610	8CT	C02-C03	14.67	1.59	1.34
31	z	101	8CT	C02-C03	14.64	1.59	1.34
31	P	615	8CT	C02-C03	14.63	1.59	1.34
31	6	615	8CT	C02-C03	14.63	1.59	1.34
31	K	101	8CT	C02-C03	14.62	1.59	1.34
31	k	102	8CT	C02-C03	14.60	1.59	1.34
31	B	622	8CT	C02-C03	14.53	1.58	1.34
31	c	518	8CT	C02-C03	14.53	1.58	1.34
31	C	518	8CT	C02-C03	14.53	1.58	1.34
31	3	615	8CT	C02-C03	14.52	1.58	1.34
31	M	201	8CT	C02-C03	14.49	1.58	1.34
31	9	615	8CT	C02-C03	14.49	1.58	1.34
31	6	615	8CT	C32-C31	14.41	1.60	1.32
31	P	615	8CT	C32-C31	14.38	1.60	1.32
31	3	615	8CT	C32-C31	14.31	1.59	1.32
31	9	615	8CT	C32-C31	14.29	1.59	1.32
31	B	623	8CT	C32-C31	14.28	1.59	1.32
31	b	622	8CT	C32-C31	14.25	1.59	1.32
31	d	408	8CT	C32-C31	14.25	1.59	1.32
31	D	409	8CT	C32-C31	14.25	1.59	1.32
31	k	101	8CT	C32-C31	14.25	1.59	1.32
31	c	518	8CT	C32-C31	14.24	1.59	1.32
31	K	102	8CT	C32-C31	14.22	1.59	1.32
31	A	610	8CT	C32-C31	14.20	1.59	1.32
31	C	518	8CT	C32-C31	14.19	1.59	1.32
31	h	102	8CT	C32-C31	14.16	1.59	1.32
31	H	102	8CT	C32-C31	14.13	1.59	1.32
31	Z	101	8CT	C32-C31	14.12	1.59	1.32
31	k	102	8CT	C32-C31	14.10	1.59	1.32
31	M	201	8CT	C32-C31	14.08	1.59	1.32
31	B	624	8CT	C32-C31	14.08	1.59	1.32
31	K	101	8CT	C32-C31	14.08	1.59	1.32
31	b	623	8CT	C32-C31	14.07	1.59	1.32
31	a	413	8CT	C32-C31	14.07	1.59	1.32
31	B	622	8CT	C32-C31	14.06	1.59	1.32
31	z	101	8CT	C32-C31	14.03	1.59	1.32
41	A	604	PHO	C1B-C2B	9.45	1.49	1.39
41	a	407	PHO	C1B-C2B	9.38	1.49	1.39
41	d	410	PHO	C1B-C2B	9.38	1.49	1.39
41	D	402	PHO	C1B-C2B	9.34	1.49	1.39
31	9	615	8CT	C34-C35	-8.82	1.37	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	k	101	8CT	C34-C35	-8.81	1.37	1.54
31	d	408	8CT	C34-C35	-8.81	1.37	1.54
31	a	413	8CT	C34-C35	-8.79	1.37	1.54
31	D	409	8CT	C34-C35	-8.79	1.37	1.54
31	K	102	8CT	C34-C35	-8.79	1.37	1.54
31	3	615	8CT	C34-C35	-8.77	1.37	1.54
31	P	615	8CT	C34-C35	-8.77	1.37	1.54
31	6	615	8CT	C34-C35	-8.74	1.37	1.54
31	A	610	8CT	C34-C35	-8.70	1.37	1.54
31	B	623	8CT	C34-C35	-8.70	1.37	1.54
31	C	518	8CT	C34-C35	-8.66	1.37	1.54
31	b	622	8CT	C34-C35	-8.64	1.37	1.54
31	c	518	8CT	C34-C35	-8.63	1.37	1.54
34	7	616	II0	C22-C10	-8.63	1.25	1.42
31	Z	101	8CT	C34-C35	-8.62	1.37	1.54
34	8	619	II0	C22-C10	-8.58	1.25	1.42
34	1	617	II0	C21-C09	-8.55	1.25	1.42
31	H	102	8CT	C34-C35	-8.55	1.38	1.54
34	p	315	II0	C22-C10	-8.55	1.25	1.42
31	z	101	8CT	C34-C35	-8.54	1.38	1.54
36	2	616	IHT	C21-C11	-8.53	1.25	1.42
31	h	102	8CT	C34-C35	-8.53	1.38	1.54
36	7	618	IHT	C21-C11	-8.53	1.25	1.42
34	2	619	II0	C22-C10	-8.53	1.25	1.42
34	1	616	II0	C21-C09	-8.52	1.25	1.42
34	5	319	II0	C22-C10	-8.51	1.25	1.42
34	1	617	II0	C22-C10	-8.51	1.26	1.42
34	7	617	II0	C21-C09	-8.51	1.26	1.42
34	7	617	II0	C22-C10	-8.50	1.26	1.42
34	p	301	II0	C22-C10	-8.50	1.26	1.42
36	1	618	IHT	C21-C11	-8.49	1.26	1.42
34	1	616	II0	C22-C10	-8.49	1.26	1.42
34	5	301	II0	C22-C10	-8.49	1.26	1.42
34	3	613	II0	C22-C10	-8.49	1.26	1.42
34	4	619	II0	C22-C10	-8.49	1.26	1.42
34	9	614	II0	C22-C10	-8.48	1.26	1.42
34	8	619	II0	C21-C09	-8.48	1.26	1.42
34	4	616	II0	C22-C10	-8.48	1.26	1.42
34	5	316	II0	C22-C10	-8.48	1.26	1.42
31	B	624	8CT	C34-C35	-8.47	1.38	1.54
36	8	616	IHT	C21-C11	-8.47	1.26	1.42
34	8	614	II0	C22-C10	-8.47	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	7	616	II0	C21-C09	-8.47	1.26	1.42
34	2	614	II0	C22-C10	-8.46	1.26	1.42
31	K	101	8CT	C34-C35	-8.46	1.38	1.54
34	5	314	II0	C21-C09	-8.46	1.26	1.42
34	7	614	II0	C22-C10	-8.46	1.26	1.42
34	5	316	II0	C21-C09	-8.46	1.26	1.42
34	0	617	II0	C22-C10	-8.46	1.26	1.42
34	0	620	II0	C22-C10	-8.46	1.26	1.42
34	p	316	II0	C22-C10	-8.45	1.26	1.42
34	3	614	II0	C22-C10	-8.45	1.26	1.42
36	p	317	IHT	C21-C11	-8.45	1.26	1.42
31	k	102	8CT	C34-C35	-8.45	1.38	1.54
34	0	616	II0	C22-C10	-8.44	1.26	1.42
36	4	617	IHT	C21-C11	-8.44	1.26	1.42
34	9	613	II0	C22-C10	-8.43	1.26	1.42
34	8	613	II0	C21-C09	-8.42	1.26	1.42
34	5	315	II0	C22-C10	-8.42	1.26	1.42
34	0	620	II0	C21-C09	-8.42	1.26	1.42
31	b	623	8CT	C34-C35	-8.42	1.38	1.54
34	5	314	II0	C22-C10	-8.41	1.26	1.42
34	1	614	II0	C22-C10	-8.41	1.26	1.42
34	3	612	II0	C21-C09	-8.41	1.26	1.42
34	8	615	II0	C21-C09	-8.41	1.26	1.42
34	p	314	II0	C21-C09	-8.41	1.26	1.42
34	7	614	II0	C21-C09	-8.41	1.26	1.42
31	B	622	8CT	C34-C35	-8.41	1.38	1.54
36	5	317	IHT	C21-C11	-8.40	1.26	1.42
34	p	315	II0	C21-C09	-8.40	1.26	1.42
34	9	613	II0	C21-C09	-8.40	1.26	1.42
35	6	613	II3	C23-C16	-8.40	1.26	1.42
34	P	614	II0	C22-C10	-8.40	1.26	1.42
34	2	619	II0	C21-C09	-8.40	1.26	1.42
34	3	613	II0	C21-C09	-8.39	1.26	1.42
34	2	615	II0	C22-C10	-8.39	1.26	1.42
34	1	614	II0	C21-C09	-8.39	1.26	1.42
34	6	614	II0	C21-C09	-8.39	1.26	1.42
34	2	613	II0	C22-C10	-8.39	1.26	1.42
34	4	616	II0	C21-C09	-8.38	1.26	1.42
34	0	616	II0	C21-C09	-8.38	1.26	1.42
34	6	614	II0	C22-C10	-8.38	1.26	1.42
34	4	615	II0	C21-C09	-8.38	1.26	1.42
34	5	319	II0	C21-C09	-8.38	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	4	615	II0	C22-C10	-8.38	1.26	1.42
34	p	316	II0	C21-C09	-8.38	1.26	1.42
34	5	315	II0	C21-C09	-8.38	1.26	1.42
34	2	613	II0	C21-C09	-8.38	1.26	1.42
34	8	614	II0	C21-C09	-8.38	1.26	1.42
34	3	612	II0	C22-C10	-8.37	1.26	1.42
34	8	613	II0	C22-C10	-8.37	1.26	1.42
31	M	201	8CT	C34-C35	-8.37	1.38	1.54
34	P	614	II0	C21-C09	-8.37	1.26	1.42
34	p	301	II0	C21-C09	-8.37	1.26	1.42
34	9	612	II0	C22-C10	-8.37	1.26	1.42
34	9	612	II0	C21-C09	-8.36	1.26	1.42
35	P	613	II3	C23-C16	-8.36	1.26	1.42
34	8	615	II0	C22-C10	-8.36	1.26	1.42
34	6	612	II0	C21-C09	-8.35	1.26	1.42
36	0	618	IHT	C21-C11	-8.35	1.26	1.42
35	1	615	II3	C23-C16	-8.35	1.26	1.42
35	7	615	II3	C23-C16	-8.35	1.26	1.42
34	3	614	II0	C21-C09	-8.35	1.26	1.42
34	2	615	II0	C21-C09	-8.34	1.26	1.42
34	0	617	II0	C21-C09	-8.34	1.26	1.42
34	p	314	II0	C22-C10	-8.34	1.26	1.42
34	0	615	II0	C22-C10	-8.34	1.26	1.42
34	P	612	II0	C21-C09	-8.34	1.26	1.42
36	4	614	IHT	C21-C11	-8.34	1.26	1.42
34	4	619	II0	C21-C09	-8.33	1.26	1.42
34	6	612	II0	C22-C10	-8.32	1.26	1.42
34	2	614	II0	C21-C09	-8.31	1.26	1.42
34	7	619	II0	C22-C10	-8.31	1.26	1.42
34	9	614	II0	C21-C09	-8.31	1.26	1.42
36	0	614	IHT	C21-C11	-8.30	1.26	1.42
34	0	615	II0	C21-C09	-8.29	1.26	1.42
41	d	410	PHO	C3B-C4B	8.28	1.49	1.41
34	1	619	II0	C22-C10	-8.28	1.26	1.42
41	D	402	PHO	C3B-C4B	8.27	1.49	1.41
34	P	612	II0	C22-C10	-8.27	1.26	1.42
34	5	301	II0	C21-C09	-8.27	1.26	1.42
34	7	619	II0	C21-C09	-8.24	1.26	1.42
34	1	619	II0	C21-C09	-8.22	1.26	1.42
41	A	604	PHO	C3B-C4B	8.11	1.49	1.41
41	a	407	PHO	C3B-C4B	8.06	1.49	1.41
31	H	102	8CT	C05-C06	-6.99	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	h	102	8CT	C05-C06	-6.96	1.36	1.52
31	z	101	8CT	C05-C06	-6.87	1.36	1.52
31	Z	101	8CT	C05-C06	-6.85	1.36	1.52
31	k	101	8CT	C05-C06	-6.84	1.36	1.52
31	a	413	8CT	C05-C06	-6.82	1.36	1.52
31	d	408	8CT	C05-C06	-6.82	1.36	1.52
31	K	102	8CT	C05-C06	-6.81	1.36	1.52
31	D	409	8CT	C05-C06	-6.81	1.36	1.52
31	b	622	8CT	C05-C06	-6.81	1.36	1.52
31	b	623	8CT	C05-C06	-6.81	1.36	1.52
31	B	624	8CT	C05-C06	-6.81	1.36	1.52
31	B	623	8CT	C05-C06	-6.79	1.36	1.52
31	M	201	8CT	C05-C06	-6.77	1.36	1.52
31	B	622	8CT	C05-C06	-6.76	1.36	1.52
31	K	101	8CT	C05-C06	-6.75	1.36	1.52
31	c	518	8CT	C05-C06	-6.75	1.36	1.52
31	C	518	8CT	C05-C06	-6.73	1.36	1.52
31	k	102	8CT	C05-C06	-6.73	1.36	1.52
31	P	615	8CT	C05-C06	-6.68	1.36	1.52
31	A	610	8CT	C05-C06	-6.65	1.36	1.52
31	6	615	8CT	C05-C06	-6.63	1.36	1.52
31	3	615	8CT	C05-C06	-6.61	1.36	1.52
31	9	615	8CT	C05-C06	-6.61	1.36	1.52
31	P	615	8CT	C15-C16	6.48	1.59	1.46
31	c	518	8CT	C15-C16	6.48	1.59	1.46
31	6	615	8CT	C15-C16	6.48	1.59	1.46
31	C	518	8CT	C15-C16	6.46	1.59	1.46
31	P	615	8CT	C28-C26	6.40	1.59	1.46
31	B	624	8CT	C15-C16	6.39	1.59	1.46
31	6	615	8CT	C28-C26	6.39	1.59	1.46
31	b	623	8CT	C15-C16	6.39	1.59	1.46
31	9	615	8CT	C15-C16	6.38	1.59	1.46
31	3	615	8CT	C15-C16	6.37	1.59	1.46
31	c	518	8CT	C28-C26	6.36	1.59	1.46
31	H	102	8CT	C15-C16	6.36	1.59	1.46
31	a	413	8CT	C15-C16	6.35	1.59	1.46
31	9	615	8CT	C28-C26	6.35	1.59	1.46
31	D	409	8CT	C15-C16	6.33	1.59	1.46
31	d	408	8CT	C15-C16	6.33	1.59	1.46
31	C	518	8CT	C28-C26	6.31	1.59	1.46
31	K	101	8CT	C28-C26	6.30	1.59	1.46
31	h	102	8CT	C15-C16	6.30	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	k	102	8CT	C28-C26	6.29	1.59	1.46
31	d	408	8CT	C28-C26	6.28	1.59	1.46
31	D	409	8CT	C28-C26	6.28	1.59	1.46
31	3	615	8CT	C28-C26	6.28	1.59	1.46
31	B	623	8CT	C15-C16	6.28	1.59	1.46
31	M	201	8CT	C15-C16	6.28	1.59	1.46
31	B	622	8CT	C15-C16	6.26	1.59	1.46
31	k	102	8CT	C15-C16	6.26	1.59	1.46
31	K	101	8CT	C15-C16	6.25	1.59	1.46
31	h	102	8CT	C28-C26	6.24	1.59	1.46
31	b	622	8CT	C15-C16	6.24	1.59	1.46
31	H	102	8CT	C28-C26	6.24	1.59	1.46
31	B	624	8CT	C28-C26	6.23	1.59	1.46
31	b	623	8CT	C28-C26	6.21	1.59	1.46
31	b	622	8CT	C28-C26	6.19	1.59	1.46
31	K	102	8CT	C15-C16	6.18	1.59	1.46
31	B	623	8CT	C28-C26	6.17	1.59	1.46
31	k	101	8CT	C15-C16	6.16	1.59	1.46
31	B	622	8CT	C28-C26	6.14	1.59	1.46
31	z	101	8CT	C28-C26	6.12	1.59	1.46
31	A	610	8CT	C04-C03	-6.11	1.46	1.53
31	b	623	8CT	C04-C03	-6.10	1.46	1.53
31	B	624	8CT	C04-C03	-6.10	1.46	1.53
31	A	610	8CT	C15-C16	6.09	1.59	1.46
31	Z	101	8CT	C28-C26	6.09	1.59	1.46
31	M	201	8CT	C28-C26	6.07	1.58	1.46
31	z	101	8CT	C15-C16	6.07	1.58	1.46
31	c	518	8CT	C34-C33	6.06	1.66	1.52
31	C	518	8CT	C34-C33	6.06	1.66	1.52
31	k	101	8CT	C04-C03	-6.05	1.46	1.53
31	K	102	8CT	C04-C03	-6.03	1.46	1.53
31	Z	101	8CT	C15-C16	6.02	1.58	1.46
31	K	102	8CT	C28-C26	6.01	1.58	1.46
31	k	101	8CT	C28-C26	6.01	1.58	1.46
31	A	610	8CT	C28-C26	6.00	1.58	1.46
31	C	518	8CT	C04-C03	-6.00	1.46	1.53
31	a	413	8CT	C34-C33	5.98	1.66	1.52
31	B	622	8CT	C04-C03	-5.97	1.46	1.53
31	c	518	8CT	C04-C03	-5.96	1.46	1.53
31	c	518	8CT	C23-C21	5.96	1.58	1.46
31	M	201	8CT	C34-C33	5.95	1.66	1.52
31	3	615	8CT	C04-C03	-5.94	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	622	8CT	C34-C33	5.94	1.66	1.52
31	9	615	8CT	C04-C03	-5.94	1.46	1.53
31	P	615	8CT	C23-C21	5.94	1.58	1.46
31	K	101	8CT	C23-C21	5.93	1.58	1.46
31	C	518	8CT	C23-C21	5.93	1.58	1.46
31	M	201	8CT	C04-C03	-5.92	1.46	1.53
31	k	102	8CT	C23-C21	5.91	1.58	1.46
31	6	615	8CT	C23-C21	5.90	1.58	1.46
31	9	615	8CT	C23-C21	5.88	1.58	1.46
31	3	615	8CT	C23-C21	5.87	1.58	1.46
31	H	102	8CT	C04-C03	-5.86	1.46	1.53
31	h	102	8CT	C04-C03	-5.86	1.46	1.53
31	a	413	8CT	C28-C26	5.86	1.58	1.46
31	h	102	8CT	C23-C21	5.84	1.58	1.46
31	b	623	8CT	C23-C21	5.83	1.58	1.46
31	B	624	8CT	C23-C21	5.83	1.58	1.46
31	H	102	8CT	C23-C21	5.83	1.58	1.46
31	D	409	8CT	C23-C21	5.81	1.58	1.46
31	d	408	8CT	C23-C21	5.79	1.58	1.46
31	b	622	8CT	C04-C03	-5.77	1.46	1.53
31	B	623	8CT	C04-C03	-5.76	1.46	1.53
31	k	102	8CT	C04-C03	-5.73	1.46	1.53
31	B	622	8CT	C23-C21	5.73	1.58	1.46
31	K	101	8CT	C34-C33	5.73	1.65	1.52
31	B	623	8CT	C34-C33	5.71	1.65	1.52
31	k	102	8CT	C34-C33	5.71	1.65	1.52
31	M	201	8CT	C23-C21	5.71	1.58	1.46
31	B	623	8CT	C23-C21	5.70	1.58	1.46
31	b	622	8CT	C34-C33	5.69	1.65	1.52
31	a	413	8CT	C04-C03	-5.69	1.46	1.53
31	b	622	8CT	C23-C21	5.68	1.58	1.46
31	B	624	8CT	C34-C33	5.66	1.65	1.52
31	P	615	8CT	C04-C03	-5.65	1.46	1.53
31	b	623	8CT	C34-C33	5.65	1.65	1.52
31	K	101	8CT	C04-C03	-5.65	1.46	1.53
31	A	610	8CT	C34-C33	5.63	1.65	1.52
31	6	615	8CT	C04-C03	-5.62	1.46	1.53
31	Z	101	8CT	C04-C03	-5.59	1.46	1.53
31	Z	101	8CT	C23-C21	5.58	1.57	1.46
31	z	101	8CT	C23-C21	5.58	1.57	1.46
31	d	408	8CT	C34-C33	5.55	1.65	1.52
31	A	610	8CT	C23-C21	5.55	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	409	8CT	C34-C33	5.55	1.65	1.52
31	k	101	8CT	C23-C21	5.54	1.57	1.46
31	a	413	8CT	C23-C21	5.54	1.57	1.46
31	K	102	8CT	C34-C33	5.53	1.65	1.52
31	K	102	8CT	C23-C21	5.52	1.57	1.46
31	z	101	8CT	C04-C03	-5.50	1.46	1.53
31	k	101	8CT	C34-C33	5.50	1.65	1.52
31	6	615	8CT	C34-C33	5.47	1.64	1.52
31	h	102	8CT	C34-C33	5.46	1.64	1.52
31	z	101	8CT	C34-C33	5.46	1.64	1.52
31	P	615	8CT	C34-C33	5.45	1.64	1.52
31	H	102	8CT	C34-C33	5.44	1.64	1.52
31	3	615	8CT	C34-C33	5.42	1.64	1.52
31	D	409	8CT	C04-C03	-5.42	1.46	1.53
31	d	408	8CT	C04-C03	-5.41	1.46	1.53
31	Z	101	8CT	C34-C33	5.41	1.64	1.52
31	9	615	8CT	C34-C33	5.40	1.64	1.52
33	6	605	KC2	CHD-C4C	5.34	1.49	1.38
33	P	605	KC2	CHD-C4C	5.33	1.49	1.38
33	0	610	KC2	CHD-C4C	5.28	1.49	1.38
33	2	610	KC2	CHD-C4C	5.27	1.49	1.38
33	1	610	KC2	CHD-C4C	5.27	1.49	1.38
33	4	610	KC2	CHD-C4C	5.26	1.49	1.38
33	p	311	KC2	CHD-C4C	5.25	1.49	1.38
33	8	610	KC2	CHD-C4C	5.24	1.49	1.38
33	6	609	KC2	CHD-C4C	5.24	1.49	1.38
31	K	101	8CT	C05-C04	5.24	1.66	1.54
31	P	615	8CT	C05-C04	5.22	1.66	1.54
33	P	609	KC2	CHD-C4C	5.21	1.48	1.38
33	7	610	KC2	CHD-C4C	5.21	1.48	1.38
33	5	311	KC2	CHD-C4C	5.20	1.48	1.38
31	k	102	8CT	C05-C04	5.20	1.66	1.54
31	D	409	8CT	C05-C04	5.18	1.66	1.54
31	6	615	8CT	C05-C04	5.18	1.66	1.54
31	d	408	8CT	C05-C04	5.17	1.65	1.54
31	z	101	8CT	C05-C04	5.14	1.65	1.54
31	Z	101	8CT	C05-C04	5.12	1.65	1.54
31	3	615	8CT	C05-C04	5.11	1.65	1.54
31	a	413	8CT	C05-C04	5.11	1.65	1.54
31	9	615	8CT	C05-C04	5.11	1.65	1.54
31	c	518	8CT	C05-C04	5.10	1.65	1.54
31	C	518	8CT	C05-C04	5.08	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	H	102	8CT	C05-C04	5.08	1.65	1.54
31	h	102	8CT	C05-C04	5.05	1.65	1.54
31	B	622	8CT	C05-C04	5.01	1.65	1.54
31	B	623	8CT	C05-C04	5.01	1.65	1.54
31	B	624	8CT	C05-C04	5.00	1.65	1.54
31	M	201	8CT	C05-C04	5.00	1.65	1.54
31	b	622	8CT	C05-C04	4.99	1.65	1.54
31	b	623	8CT	C05-C04	4.99	1.65	1.54
31	A	610	8CT	C05-C04	4.95	1.65	1.54
31	K	102	8CT	C05-C04	4.92	1.65	1.54
31	k	101	8CT	C05-C04	4.91	1.65	1.54
31	3	615	8CT	C06-C07	4.70	1.67	1.52
31	9	615	8CT	C06-C07	4.70	1.67	1.52
39	B	620	SQD	O48-C23	4.69	1.47	1.33
31	A	610	8CT	C06-C07	4.69	1.67	1.52
39	b	620	SQD	O48-C23	4.68	1.47	1.33
31	c	518	8CT	C06-C07	4.67	1.67	1.52
31	C	518	8CT	C06-C07	4.67	1.67	1.52
31	P	615	8CT	C06-C07	4.66	1.67	1.52
39	B	601	SQD	O48-C23	4.65	1.46	1.33
39	p	318	SQD	O48-C23	4.65	1.46	1.33
31	6	615	8CT	C19-C20	4.65	1.57	1.43
31	6	615	8CT	C06-C07	4.64	1.67	1.52
31	P	615	8CT	C19-C20	4.64	1.57	1.43
39	5	318	SQD	O48-C23	4.64	1.46	1.33
39	b	601	SQD	O48-C23	4.63	1.46	1.33
31	c	518	8CT	C19-C20	4.62	1.57	1.43
31	C	518	8CT	C19-C20	4.62	1.57	1.43
31	K	101	8CT	C06-C07	4.61	1.66	1.52
31	B	624	8CT	C06-C07	4.60	1.66	1.52
31	b	623	8CT	C06-C07	4.60	1.66	1.52
31	B	622	8CT	C06-C07	4.60	1.66	1.52
31	k	102	8CT	C06-C07	4.59	1.66	1.52
39	a	409	SQD	O48-C23	4.58	1.46	1.33
31	B	623	8CT	C06-C07	4.58	1.66	1.52
31	M	201	8CT	C06-C07	4.57	1.66	1.52
31	K	102	8CT	C06-C07	4.56	1.66	1.52
31	b	623	8CT	C19-C20	4.56	1.57	1.43
31	b	622	8CT	C06-C07	4.56	1.66	1.52
39	A	606	SQD	O48-C23	4.56	1.46	1.33
31	k	102	8CT	C19-C20	4.55	1.57	1.43
31	k	101	8CT	C06-C07	4.55	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	9	615	8CT	C19-C20	4.54	1.57	1.43
31	B	624	8CT	C19-C20	4.54	1.57	1.43
31	H	102	8CT	C19-C20	4.54	1.57	1.43
31	K	101	8CT	C19-C20	4.53	1.57	1.43
31	3	615	8CT	C19-C20	4.53	1.57	1.43
31	h	102	8CT	C19-C20	4.52	1.57	1.43
31	d	408	8CT	C06-C07	4.51	1.66	1.52
31	D	409	8CT	C19-C20	4.50	1.57	1.43
33	2	610	KC2	MG-ND	-4.49	1.96	2.05
31	D	409	8CT	C06-C07	4.49	1.66	1.52
31	H	102	8CT	C06-C07	4.49	1.66	1.52
31	Z	101	8CT	C06-C07	4.49	1.66	1.52
31	d	408	8CT	C19-C20	4.49	1.57	1.43
31	z	101	8CT	C06-C07	4.49	1.66	1.52
33	6	605	KC2	MG-ND	-4.48	1.96	2.05
33	8	610	KC2	MG-ND	-4.47	1.96	2.05
31	h	102	8CT	C06-C07	4.46	1.66	1.52
31	a	413	8CT	C06-C07	4.46	1.66	1.52
33	P	605	KC2	MG-ND	-4.46	1.97	2.05
31	b	622	8CT	C19-C20	4.44	1.56	1.43
31	B	623	8CT	C19-C20	4.44	1.56	1.43
31	M	201	8CT	C19-C20	4.43	1.56	1.43
31	B	622	8CT	C19-C20	4.43	1.56	1.43
33	1	610	KC2	MG-ND	-4.41	1.97	2.05
31	a	413	8CT	C19-C20	4.40	1.56	1.43
33	6	609	KC2	MG-ND	-4.39	1.97	2.05
33	5	311	KC2	MG-ND	-4.38	1.97	2.05
33	7	610	KC2	MG-ND	-4.38	1.97	2.05
33	4	610	KC2	MG-ND	-4.38	1.97	2.05
33	0	610	KC2	MG-ND	-4.37	1.97	2.05
31	k	101	8CT	C19-C20	4.35	1.56	1.43
33	P	609	KC2	MG-ND	-4.35	1.97	2.05
33	p	311	KC2	MG-ND	-4.35	1.97	2.05
31	A	610	8CT	C19-C20	4.35	1.56	1.43
31	K	102	8CT	C19-C20	4.34	1.56	1.43
31	z	101	8CT	C19-C20	4.34	1.56	1.43
31	Z	101	8CT	C19-C20	4.31	1.56	1.43
31	C	518	8CT	C24-C25	4.31	1.56	1.43
33	6	605	KC2	MG-NB	-4.30	1.97	2.05
31	P	615	8CT	C24-C25	4.29	1.56	1.43
31	c	518	8CT	C24-C25	4.29	1.56	1.43
31	6	615	8CT	C24-C25	4.28	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	P	605	KC2	CHC-C1C	4.26	1.48	1.39
31	9	615	8CT	C24-C25	4.25	1.56	1.43
33	6	605	KC2	CHC-C1C	4.25	1.48	1.39
31	3	615	8CT	C24-C25	4.24	1.56	1.43
31	k	102	8CT	C24-C25	4.24	1.56	1.43
33	p	311	KC2	CHC-C1C	4.23	1.48	1.39
31	K	101	8CT	C24-C25	4.23	1.56	1.43
33	P	605	KC2	MG-NB	-4.22	1.97	2.05
31	h	102	8CT	C24-C25	4.21	1.56	1.43
31	H	102	8CT	C24-C25	4.20	1.56	1.43
33	0	610	KC2	CHC-C1C	4.20	1.48	1.39
33	P	609	KC2	CHC-C1C	4.19	1.48	1.39
31	D	409	8CT	C24-C25	4.19	1.56	1.43
33	6	609	KC2	CHC-C1C	4.19	1.48	1.39
33	5	311	KC2	CHC-C1C	4.19	1.48	1.39
31	b	623	8CT	C24-C25	4.18	1.56	1.43
31	B	624	8CT	C24-C25	4.18	1.56	1.43
33	2	610	KC2	MG-NB	-4.18	1.97	2.05
33	6	605	KC2	CHC-C4B	4.18	1.46	1.38
31	d	408	8CT	C24-C25	4.17	1.56	1.43
33	1	610	KC2	CHC-C1C	4.17	1.48	1.39
33	7	610	KC2	CHC-C1C	4.16	1.48	1.39
33	4	610	KC2	CHC-C1C	4.16	1.48	1.39
33	8	610	KC2	MG-NB	-4.15	1.97	2.05
33	2	610	KC2	CHC-C1C	4.15	1.48	1.39
31	B	622	8CT	C24-C25	4.15	1.56	1.43
33	P	605	KC2	CHC-C4B	4.14	1.46	1.38
31	B	623	8CT	C24-C25	4.12	1.56	1.43
31	b	622	8CT	C24-C25	4.12	1.56	1.43
31	M	201	8CT	C24-C25	4.12	1.56	1.43
43	A	609	PL9	C3-C4	-4.11	1.43	1.49
43	a	412	PL9	C3-C4	-4.11	1.43	1.49
33	8	610	KC2	CHC-C1C	4.10	1.48	1.39
31	Z	101	8CT	C24-C25	4.08	1.55	1.43
33	4	610	KC2	MG-NB	-4.08	1.97	2.05
31	z	101	8CT	C24-C25	4.08	1.55	1.43
33	0	610	KC2	MG-NB	-4.07	1.97	2.05
33	P	609	KC2	CHC-C4B	4.06	1.46	1.38
33	7	610	KC2	MG-NB	-4.06	1.97	2.05
33	1	610	KC2	MG-NB	-4.06	1.97	2.05
33	5	311	KC2	CHC-C4B	4.05	1.46	1.38
33	6	609	KC2	MG-NB	-4.05	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	P	609	KC2	MG-NB	-4.05	1.97	2.05
33	p	311	KC2	MG-NB	-4.05	1.97	2.05
33	p	311	KC2	CHC-C4B	4.04	1.46	1.38
33	5	311	KC2	MG-NB	-4.04	1.97	2.05
33	6	609	KC2	CHC-C4B	4.03	1.46	1.38
33	1	610	KC2	CHC-C4B	4.03	1.46	1.38
33	0	610	KC2	CHC-C4B	4.02	1.46	1.38
31	K	102	8CT	C24-C25	4.01	1.55	1.43
33	4	610	KC2	CHC-C4B	4.01	1.46	1.38
31	k	101	8CT	C24-C25	3.99	1.55	1.43
33	8	610	KC2	CHC-C4B	3.99	1.46	1.38
33	7	610	KC2	CHC-C4B	3.99	1.46	1.38
31	A	610	8CT	C24-C25	3.97	1.55	1.43
33	2	610	KC2	CHC-C4B	3.97	1.46	1.38
31	P	615	8CT	C14-C13	3.95	1.55	1.43
31	c	518	8CT	C14-C13	3.94	1.55	1.43
31	C	518	8CT	C14-C13	3.94	1.55	1.43
31	a	413	8CT	C24-C25	3.94	1.55	1.43
31	6	615	8CT	C14-C13	3.92	1.55	1.43
31	b	623	8CT	C14-C13	3.89	1.55	1.43
31	3	615	8CT	C14-C13	3.88	1.55	1.43
31	B	624	8CT	C14-C13	3.87	1.55	1.43
31	6	615	8CT	C11-C12	3.87	1.54	1.46
31	D	409	8CT	C14-C13	3.84	1.55	1.43
31	d	408	8CT	C14-C13	3.84	1.55	1.43
31	H	102	8CT	C14-C13	3.84	1.55	1.43
31	K	101	8CT	C14-C13	3.84	1.55	1.43
31	H	102	8CT	C28-C29	3.84	1.41	1.32
31	9	615	8CT	C14-C13	3.83	1.55	1.43
31	k	102	8CT	C14-C13	3.83	1.55	1.43
31	P	615	8CT	C11-C12	3.82	1.54	1.46
31	h	102	8CT	C14-C13	3.82	1.55	1.43
31	a	413	8CT	C14-C13	3.82	1.55	1.43
31	6	615	8CT	C28-C29	3.81	1.40	1.32
31	b	622	8CT	C14-C13	3.80	1.55	1.43
31	B	623	8CT	C14-C13	3.80	1.55	1.43
31	h	102	8CT	C28-C29	3.80	1.40	1.32
41	d	410	PHO	C4D-CHA	3.79	1.45	1.39
31	d	408	8CT	C28-C29	3.79	1.40	1.32
39	B	601	SQD	O47-C45	-3.77	1.37	1.46
31	c	518	8CT	C30-C29	3.77	1.55	1.50
31	C	518	8CT	C30-C29	3.77	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	P	615	8CT	C28-C29	3.77	1.40	1.32
31	K	102	8CT	C14-C13	3.76	1.54	1.43
31	M	201	8CT	C14-C13	3.76	1.54	1.43
31	k	101	8CT	C14-C13	3.75	1.54	1.43
41	a	407	PHO	C1D-C2D	3.75	1.43	1.39
31	B	622	8CT	C14-C13	3.75	1.54	1.43
31	D	409	8CT	C28-C29	3.75	1.40	1.32
31	K	101	8CT	C28-C29	3.74	1.40	1.32
39	b	601	SQD	O47-C45	-3.74	1.37	1.46
31	b	623	8CT	C11-C12	3.74	1.54	1.46
41	D	402	PHO	C4D-CHA	3.74	1.45	1.39
47	f	101	HEM	FE-ND	3.74	2.06	1.94
31	c	518	8CT	C28-C29	3.73	1.40	1.32
31	C	518	8CT	C28-C29	3.73	1.40	1.32
31	9	615	8CT	C11-C12	3.72	1.53	1.46
31	D	409	8CT	C11-C12	3.72	1.53	1.46
43	d	404	PL9	C3-C4	-3.72	1.43	1.49
31	d	408	8CT	C11-C12	3.72	1.53	1.46
31	B	624	8CT	C11-C12	3.72	1.53	1.46
31	A	610	8CT	C14-C13	3.71	1.54	1.43
41	A	604	PHO	C1D-C2D	3.71	1.43	1.39
43	D	405	PL9	C3-C4	-3.70	1.43	1.49
31	k	102	8CT	C28-C29	3.69	1.40	1.32
31	3	615	8CT	C28-C29	3.69	1.40	1.32
31	M	201	8CT	C28-C29	3.68	1.40	1.32
39	b	620	SQD	O47-C45	-3.68	1.37	1.46
39	B	620	SQD	O47-C45	-3.68	1.37	1.46
41	d	410	PHO	C1D-C2D	3.68	1.43	1.39
31	k	102	8CT	C11-C12	3.68	1.53	1.46
31	3	615	8CT	C11-C12	3.67	1.53	1.46
31	9	615	8CT	C28-C29	3.67	1.40	1.32
47	f	101	HEM	FE-NB	3.67	2.06	1.94
31	Z	101	8CT	C28-C29	3.67	1.40	1.32
31	z	101	8CT	C28-C29	3.67	1.40	1.32
31	H	102	8CT	C11-C12	3.67	1.53	1.46
31	K	101	8CT	C11-C12	3.66	1.53	1.46
32	0	612	CLA	C1D-ND	3.66	1.42	1.37
32	4	612	CLA	C1D-ND	3.66	1.42	1.37
47	V	201	HEM	FE-NB	3.66	2.06	1.94
39	a	409	SQD	O47-C45	-3.65	1.38	1.46
31	B	622	8CT	C28-C29	3.65	1.40	1.32
41	D	402	PHO	C1D-C2D	3.65	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	E	101	HEM	FE-ND	3.64	2.06	1.94
39	A	606	SQD	O47-C45	-3.64	1.38	1.46
31	H	102	8CT	C30-C29	3.64	1.55	1.50
31	h	102	8CT	C30-C29	3.64	1.55	1.50
31	b	623	8CT	C28-C29	3.63	1.40	1.32
31	B	624	8CT	C28-C29	3.63	1.40	1.32
31	z	101	8CT	C14-C13	3.63	1.54	1.43
31	c	518	8CT	C11-C12	3.63	1.53	1.46
31	C	518	8CT	C11-C12	3.63	1.53	1.46
31	b	622	8CT	C11-C12	3.63	1.53	1.46
31	h	102	8CT	C11-C12	3.63	1.53	1.46
32	1	613	CLA	C1D-ND	3.62	1.42	1.37
31	Z	101	8CT	C14-C13	3.62	1.54	1.43
32	p	313	CLA	C1D-ND	3.61	1.42	1.37
31	B	623	8CT	C28-C29	3.61	1.40	1.32
32	7	613	CLA	C1D-ND	3.61	1.42	1.37
31	B	623	8CT	C11-C12	3.61	1.53	1.46
41	A	604	PHO	C4D-CHA	3.60	1.44	1.39
32	0	609	CLA	C1D-ND	3.60	1.42	1.37
31	b	622	8CT	C28-C29	3.60	1.40	1.32
32	5	313	CLA	C1D-ND	3.60	1.42	1.37
41	a	407	PHO	C4D-CHA	3.60	1.44	1.39
32	7	604	CLA	C1D-ND	3.60	1.42	1.37
32	4	613	CLA	C1D-ND	3.60	1.42	1.37
32	0	611	CLA	C1D-ND	3.59	1.42	1.37
32	4	609	CLA	C1D-ND	3.59	1.42	1.37
32	4	604	CLA	C1D-ND	3.59	1.42	1.37
32	4	611	CLA	C1D-ND	3.58	1.42	1.37
32	0	606	CLA	C1D-ND	3.58	1.42	1.37
32	7	603	CLA	C1D-ND	3.58	1.42	1.37
32	6	611	CLA	C1D-ND	3.58	1.42	1.37
32	1	604	CLA	C1D-ND	3.58	1.42	1.37
47	v	201	HEM	FE-NB	3.58	2.05	1.94
32	p	302	CLA	C1D-ND	3.57	1.42	1.37
32	5	305	CLA	C1D-ND	3.57	1.42	1.37
31	k	101	8CT	C11-C12	3.57	1.53	1.46
32	6	608	CLA	C1D-ND	3.56	1.42	1.37
31	P	615	8CT	C35-C30	3.56	1.66	1.56
32	0	613	CLA	C1D-ND	3.56	1.42	1.37
32	0	601	CLA	C1D-ND	3.55	1.42	1.37
32	6	604	CLA	C1D-ND	3.55	1.42	1.37
32	p	307	CLA	C1D-ND	3.55	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	413	8CT	C11-C12	3.55	1.53	1.46
32	7	611	CLA	C1D-ND	3.55	1.42	1.37
32	4	603	CLA	C1D-ND	3.55	1.42	1.37
32	7	601	CLA	C1D-ND	3.55	1.42	1.37
32	2	611	CLA	C1D-ND	3.55	1.42	1.37
32	1	611	CLA	C1D-ND	3.54	1.42	1.37
32	4	606	CLA	C1D-ND	3.54	1.42	1.37
32	5	304	CLA	C1D-ND	3.54	1.42	1.37
31	B	622	8CT	C30-C29	3.54	1.55	1.50
32	P	610	CLA	C1D-ND	3.54	1.42	1.37
32	5	302	CLA	C1D-ND	3.54	1.42	1.37
32	1	612	CLA	C1D-ND	3.54	1.42	1.37
32	1	601	CLA	C1D-ND	3.53	1.42	1.37
32	6	606	CLA	C1D-ND	3.53	1.42	1.37
32	5	306	CLA	C1D-ND	3.53	1.42	1.37
32	P	611	CLA	C1D-ND	3.53	1.42	1.37
31	K	102	8CT	C11-C12	3.53	1.53	1.46
32	S	302	CLA	C1D-ND	3.53	1.42	1.37
32	1	609	CLA	C1D-ND	3.53	1.42	1.37
32	P	606	CLA	C1D-ND	3.52	1.42	1.37
31	Z	101	8CT	C35-C30	3.52	1.66	1.56
32	1	603	CLA	C1D-ND	3.52	1.42	1.37
32	P	604	CLA	C1D-ND	3.52	1.42	1.37
32	p	310	CLA	C1D-ND	3.52	1.42	1.37
47	E	101	HEM	FE-NB	3.52	2.05	1.94
32	5	310	CLA	C1D-ND	3.52	1.42	1.37
32	0	604	CLA	C1D-ND	3.52	1.42	1.37
32	0	605	CLA	C1D-ND	3.52	1.42	1.37
32	P	601	CLA	C1D-ND	3.52	1.42	1.37
32	P	602	CLA	C1D-ND	3.52	1.42	1.37
32	2	601	CLA	C1D-ND	3.52	1.42	1.37
32	p	305	CLA	C1D-ND	3.52	1.42	1.37
32	5	307	CLA	C1D-ND	3.51	1.42	1.37
32	7	609	CLA	C1D-ND	3.51	1.42	1.37
32	s	302	CLA	C1D-ND	3.51	1.42	1.37
32	4	601	CLA	C1D-ND	3.51	1.42	1.37
32	4	605	CLA	C1D-ND	3.51	1.42	1.37
32	1	607	CLA	C1D-ND	3.51	1.42	1.37
32	8	606	CLA	C1D-ND	3.51	1.42	1.37
31	H	102	8CT	C35-C30	3.51	1.66	1.56
32	P	608	CLA	C1D-ND	3.51	1.42	1.37
31	A	610	8CT	C11-C12	3.51	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	M	201	8CT	C11-C12	3.51	1.53	1.46
32	g	102	CLA	C1D-ND	3.50	1.42	1.37
31	z	101	8CT	C35-C30	3.50	1.66	1.56
32	p	304	CLA	C1D-ND	3.50	1.42	1.37
32	p	306	CLA	C1D-ND	3.50	1.42	1.37
47	v	201	HEM	FE-ND	3.50	2.05	1.94
31	6	615	8CT	C35-C30	3.50	1.66	1.56
32	6	610	CLA	C1D-ND	3.50	1.42	1.37
32	6	601	CLA	C1D-ND	3.49	1.42	1.37
32	G	101	CLA	C1D-ND	3.49	1.42	1.37
31	M	201	8CT	C30-C29	3.49	1.55	1.50
31	B	622	8CT	C11-C12	3.49	1.53	1.46
32	P	607	CLA	C1D-ND	3.49	1.42	1.37
47	V	201	HEM	FE-ND	3.49	2.05	1.94
32	8	601	CLA	C1D-ND	3.48	1.42	1.37
31	h	102	8CT	C35-C30	3.48	1.66	1.56
32	8	611	CLA	C1D-ND	3.48	1.42	1.37
32	2	605	CLA	C1D-ND	3.48	1.42	1.37
32	0	603	CLA	C1D-ND	3.48	1.42	1.37
32	7	605	CLA	C1D-ND	3.48	1.42	1.37
31	9	615	8CT	C35-C30	3.48	1.66	1.56
32	2	604	CLA	C1D-ND	3.48	1.42	1.37
32	p	308	CLA	C1D-ND	3.48	1.42	1.37
32	2	607	CLA	C1D-ND	3.48	1.42	1.37
32	6	603	CLA	C1D-ND	3.47	1.42	1.37
32	2	606	CLA	C1D-ND	3.47	1.42	1.37
32	3	605	CLA	C1D-ND	3.47	1.42	1.37
32	7	612	CLA	C1D-ND	3.47	1.42	1.37
32	7	607	CLA	C1D-ND	3.47	1.42	1.37
32	P	603	CLA	C1D-ND	3.47	1.42	1.37
31	d	408	8CT	C01-C02	3.47	1.56	1.50
32	9	604	CLA	C1D-ND	3.47	1.42	1.37
31	z	101	8CT	C11-C12	3.47	1.53	1.46
31	k	102	8CT	C30-C29	3.47	1.55	1.50
32	8	609	CLA	C1D-ND	3.47	1.42	1.37
32	S	303	CLA	C1D-ND	3.46	1.42	1.37
32	s	303	CLA	C1D-ND	3.46	1.42	1.37
32	4	602	CLA	C1D-ND	3.46	1.42	1.37
32	8	612	CLA	C1D-ND	3.46	1.42	1.37
31	D	409	8CT	C01-C02	3.46	1.56	1.50
31	Z	101	8CT	C11-C12	3.46	1.53	1.46
32	2	609	CLA	C1D-ND	3.46	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	603	CLA	C1D-ND	3.46	1.42	1.37
32	b	605	CLA	C1D-ND	3.46	1.42	1.37
32	6	602	CLA	C1D-ND	3.46	1.42	1.37
32	0	608	CLA	C1D-ND	3.45	1.42	1.37
32	8	604	CLA	C1D-ND	3.45	1.42	1.37
32	2	612	CLA	C1D-ND	3.45	1.42	1.37
32	9	601	CLA	C1D-ND	3.45	1.42	1.37
32	b	616	CLA	C1D-ND	3.45	1.42	1.37
32	5	303	CLA	C1D-ND	3.45	1.42	1.37
32	4	607	CLA	C1D-ND	3.44	1.42	1.37
32	2	602	CLA	C1D-ND	3.44	1.42	1.37
32	1	605	CLA	C1D-ND	3.44	1.42	1.37
32	0	602	CLA	C1D-ND	3.44	1.42	1.37
32	6	607	CLA	C1D-ND	3.44	1.42	1.37
32	0	607	CLA	C1D-ND	3.44	1.42	1.37
32	8	603	CLA	C1D-ND	3.44	1.42	1.37
32	9	606	CLA	C1D-ND	3.44	1.42	1.37
31	3	615	8CT	C35-C30	3.44	1.65	1.56
31	B	622	8CT	C35-C30	3.44	1.65	1.56
32	8	605	CLA	C1D-ND	3.43	1.42	1.37
32	9	608	CLA	C1D-ND	3.43	1.42	1.37
32	p	312	CLA	C1D-ND	3.43	1.42	1.37
33	6	605	KC2	CHD-C1D	3.43	1.47	1.39
32	p	303	CLA	C1D-ND	3.43	1.42	1.37
32	5	308	CLA	C1D-ND	3.43	1.42	1.37
32	9	605	CLA	C1D-ND	3.43	1.42	1.37
31	k	101	8CT	C28-C29	3.43	1.40	1.32
31	a	413	8CT	C28-C29	3.43	1.40	1.32
32	1	606	CLA	C1D-ND	3.43	1.42	1.37
31	K	101	8CT	C30-C29	3.43	1.55	1.50
32	4	608	CLA	C1D-ND	3.43	1.42	1.37
31	A	610	8CT	C28-C29	3.43	1.40	1.32
31	K	102	8CT	C28-C29	3.42	1.40	1.32
32	7	606	CLA	C1D-ND	3.42	1.42	1.37
32	p	309	CLA	C1D-ND	3.42	1.42	1.37
33	0	610	KC2	CHD-C1D	3.42	1.47	1.39
32	8	607	CLA	C1D-ND	3.42	1.42	1.37
31	6	615	8CT	C01-C02	3.42	1.56	1.50
32	5	309	CLA	C1D-ND	3.42	1.42	1.37
32	3	611	CLA	C1D-ND	3.41	1.42	1.37
33	P	605	KC2	CHD-C1D	3.41	1.47	1.39
39	p	318	SQD	O47-C45	-3.41	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	622	8CT	C01-C02	3.41	1.56	1.50
32	3	606	CLA	C1D-ND	3.41	1.42	1.37
32	3	610	CLA	C1D-ND	3.41	1.42	1.37
31	B	623	8CT	C01-C02	3.41	1.56	1.50
32	B	605	CLA	C1D-ND	3.41	1.42	1.37
32	9	611	CLA	C1D-ND	3.40	1.42	1.37
39	p	318	SQD	O5-C1	3.40	1.50	1.41
31	c	518	8CT	C35-C30	3.40	1.65	1.56
32	B	616	CLA	C1D-ND	3.40	1.42	1.37
31	C	518	8CT	C35-C30	3.40	1.65	1.56
32	9	603	CLA	C1D-ND	3.40	1.42	1.37
31	M	201	8CT	C35-C30	3.40	1.65	1.56
33	P	609	KC2	CHD-C1D	3.40	1.47	1.39
31	P	615	8CT	C01-C02	3.40	1.56	1.50
31	a	413	8CT	C01-C02	3.40	1.56	1.50
39	5	318	SQD	O47-C45	-3.40	1.38	1.46
32	3	601	CLA	C1D-ND	3.40	1.42	1.37
32	8	608	CLA	C1D-ND	3.40	1.42	1.37
32	8	602	CLA	C1D-ND	3.39	1.42	1.37
39	p	318	SQD	O47-C7	3.39	1.43	1.34
32	1	608	CLA	C1D-ND	3.39	1.42	1.37
32	1	602	CLA	C1D-ND	3.39	1.42	1.37
31	3	615	8CT	C01-C02	3.39	1.56	1.50
32	7	608	CLA	C1D-ND	3.38	1.42	1.37
32	9	607	CLA	C1D-ND	3.38	1.42	1.37
39	5	318	SQD	O5-C1	3.38	1.50	1.41
31	9	615	8CT	C01-C02	3.38	1.56	1.50
33	4	610	KC2	CHD-C1D	3.38	1.47	1.39
31	P	615	8CT	C30-C29	3.38	1.55	1.50
32	3	604	CLA	C1D-ND	3.38	1.42	1.37
32	7	602	CLA	C1D-ND	3.38	1.42	1.37
31	Z	101	8CT	C30-C29	3.38	1.55	1.50
32	5	312	CLA	C1D-ND	3.38	1.42	1.37
32	c	503	CLA	C1D-ND	3.38	1.42	1.37
31	k	102	8CT	C01-C02	3.37	1.56	1.50
39	5	318	SQD	O47-C7	3.37	1.43	1.34
32	3	609	CLA	C1D-ND	3.37	1.42	1.37
32	3	603	CLA	C1D-ND	3.37	1.42	1.37
33	6	609	KC2	CHD-C1D	3.37	1.47	1.39
31	z	101	8CT	C01-C02	3.37	1.56	1.50
33	p	311	KC2	CHD-C1D	3.37	1.47	1.39
32	3	608	CLA	C1D-ND	3.37	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	5	311	KC2	CHD-C1D	3.36	1.47	1.39
31	Z	101	8CT	C01-C02	3.36	1.56	1.50
32	b	602	CLA	C1D-ND	3.36	1.42	1.37
31	k	101	8CT	C01-C02	3.36	1.56	1.50
32	2	608	CLA	C1D-ND	3.36	1.42	1.37
31	K	101	8CT	C01-C02	3.36	1.56	1.50
31	C	518	8CT	C01-C02	3.36	1.56	1.50
31	k	102	8CT	C35-C30	3.36	1.65	1.56
32	9	609	CLA	C1D-ND	3.36	1.42	1.37
31	3	615	8CT	C30-C29	3.35	1.55	1.50
31	A	610	8CT	C01-C02	3.35	1.56	1.50
31	K	102	8CT	C01-C02	3.35	1.56	1.50
32	9	610	CLA	C1D-ND	3.35	1.42	1.37
31	c	518	8CT	C01-C02	3.34	1.56	1.50
32	3	607	CLA	C1D-ND	3.34	1.42	1.37
32	C	504	CLA	C1D-ND	3.34	1.42	1.37
32	B	602	CLA	C1D-ND	3.34	1.42	1.37
32	9	602	CLA	C1D-ND	3.34	1.42	1.37
31	6	615	8CT	C30-C29	3.34	1.55	1.50
32	C	502	CLA	C1D-ND	3.34	1.42	1.37
31	9	615	8CT	C30-C29	3.34	1.55	1.50
31	z	101	8CT	C30-C29	3.33	1.55	1.50
33	7	610	KC2	CHD-C1D	3.33	1.46	1.39
39	A	606	SQD	O47-C7	3.33	1.43	1.34
32	c	504	CLA	C1D-ND	3.33	1.42	1.37
33	1	610	KC2	CHD-C1D	3.33	1.46	1.39
32	B	610	CLA	C1D-ND	3.33	1.42	1.37
31	D	409	8CT	C35-C30	3.32	1.65	1.56
31	M	201	8CT	C01-C02	3.32	1.56	1.50
32	C	501	CLA	C1D-ND	3.32	1.42	1.37
31	K	101	8CT	C35-C30	3.32	1.65	1.56
32	3	602	CLA	C1D-ND	3.32	1.42	1.37
31	k	101	8CT	C35-C30	3.31	1.65	1.56
32	C	503	CLA	C1D-ND	3.31	1.42	1.37
32	b	607	CLA	C1D-ND	3.31	1.42	1.37
32	c	502	CLA	C1D-ND	3.31	1.42	1.37
33	8	610	KC2	CHD-C1D	3.31	1.46	1.39
31	d	408	8CT	C35-C30	3.30	1.65	1.56
31	K	102	8CT	C35-C30	3.30	1.65	1.56
32	b	611	CLA	C1D-ND	3.30	1.42	1.37
32	b	610	CLA	C1D-ND	3.30	1.42	1.37
32	c	501	CLA	C1D-ND	3.30	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	622	8CT	C01-C02	3.29	1.56	1.50
31	b	623	8CT	C01-C02	3.29	1.56	1.50
31	B	624	8CT	C01-C02	3.29	1.56	1.50
32	c	513	CLA	C1D-ND	3.28	1.42	1.37
33	2	610	KC2	CHD-C1D	3.28	1.46	1.39
32	B	603	CLA	C1D-ND	3.28	1.42	1.37
32	B	607	CLA	C1D-ND	3.28	1.42	1.37
39	b	601	SQD	O47-C7	3.28	1.43	1.34
32	B	606	CLA	C1D-ND	3.28	1.42	1.37
39	b	620	SQD	O5-C1	3.28	1.50	1.41
39	B	601	SQD	O5-C1	3.28	1.50	1.41
39	b	601	SQD	O5-C1	3.28	1.50	1.41
39	a	409	SQD	O47-C7	3.28	1.43	1.34
32	C	509	CLA	C1D-ND	3.28	1.42	1.37
31	d	408	8CT	C30-C29	3.28	1.55	1.50
32	b	617	CLA	C1D-ND	3.27	1.42	1.37
32	B	617	CLA	C1D-ND	3.27	1.42	1.37
32	C	507	CLA	C1D-ND	3.27	1.42	1.37
39	B	601	SQD	O47-C7	3.27	1.43	1.34
32	b	603	CLA	C1D-ND	3.27	1.42	1.37
32	c	506	CLA	C1D-ND	3.26	1.42	1.37
31	H	102	8CT	C01-C02	3.26	1.56	1.50
31	6	615	8CT	C18-C17	3.26	1.53	1.43
32	C	510	CLA	C1D-ND	3.26	1.42	1.37
32	d	403	CLA	C1D-ND	3.26	1.42	1.37
31	P	615	8CT	C18-C17	3.26	1.53	1.43
32	D	401	CLA	C1D-ND	3.26	1.42	1.37
32	C	513	CLA	C1D-ND	3.26	1.42	1.37
32	b	604	CLA	C1D-ND	3.26	1.42	1.37
32	D	404	CLA	C1D-ND	3.26	1.42	1.37
32	c	511	CLA	C1D-ND	3.25	1.42	1.37
32	b	614	CLA	C1D-ND	3.25	1.42	1.37
31	C	518	8CT	C18-C17	3.25	1.53	1.43
32	C	512	CLA	C1D-ND	3.24	1.42	1.37
31	D	409	8CT	C30-C29	3.24	1.55	1.50
32	d	409	CLA	C1D-ND	3.24	1.42	1.37
31	c	518	8CT	C18-C17	3.24	1.53	1.43
39	B	620	SQD	O5-C1	3.23	1.50	1.41
32	c	509	CLA	C1D-ND	3.23	1.42	1.37
32	B	604	CLA	C1D-ND	3.23	1.42	1.37
39	B	620	SQD	O47-C7	3.23	1.43	1.34
32	D	403	CLA	C1D-ND	3.23	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	610	8CT	C35-C30	3.22	1.65	1.56
32	C	511	CLA	C1D-ND	3.22	1.42	1.37
32	a	406	CLA	C1D-ND	3.22	1.42	1.37
32	C	506	CLA	C1D-ND	3.22	1.42	1.37
39	b	620	SQD	O47-C7	3.22	1.43	1.34
32	c	510	CLA	C1D-ND	3.22	1.42	1.37
32	d	402	CLA	CAB-C3B	-3.22	1.44	1.50
32	b	608	CLA	C1D-ND	3.22	1.42	1.37
32	B	611	CLA	C1D-ND	3.22	1.42	1.37
32	D	403	CLA	CAB-C3B	-3.21	1.44	1.50
32	A	605	CLA	C1D-ND	3.21	1.42	1.37
32	c	507	CLA	C1D-ND	3.21	1.42	1.37
32	B	614	CLA	C1D-ND	3.21	1.42	1.37
32	B	612	CLA	C1D-ND	3.21	1.42	1.37
32	a	408	CLA	C1D-ND	3.21	1.42	1.37
32	a	405	CLA	C1D-ND	3.21	1.42	1.37
39	A	606	SQD	O5-C1	3.21	1.50	1.41
31	h	102	8CT	C01-C02	3.21	1.56	1.50
32	b	609	CLA	C1D-ND	3.21	1.42	1.37
32	b	606	CLA	C1D-ND	3.20	1.42	1.37
32	b	615	CLA	C1D-ND	3.20	1.42	1.37
31	b	623	8CT	C18-C17	3.20	1.53	1.43
32	C	508	CLA	C1D-ND	3.20	1.42	1.37
39	a	409	SQD	O5-C1	3.20	1.50	1.41
31	K	101	8CT	C18-C17	3.20	1.53	1.43
32	A	602	CLA	C1D-ND	3.20	1.42	1.37
32	d	402	CLA	C1D-ND	3.20	1.42	1.37
32	B	608	CLA	C1D-ND	3.20	1.42	1.37
32	c	512	CLA	C1D-ND	3.20	1.42	1.37
32	8	606	CLA	C4B-NB	3.19	1.42	1.37
31	3	615	8CT	C18-C17	3.19	1.53	1.43
31	B	624	8CT	C18-C17	3.18	1.53	1.43
32	4	606	CLA	C4B-NB	3.18	1.42	1.37
32	0	612	CLA	C4B-NB	3.18	1.42	1.37
32	c	508	CLA	C1D-ND	3.17	1.42	1.37
32	0	606	CLA	C4B-NB	3.17	1.42	1.37
47	f	101	HEM	FE-NA	3.17	2.05	1.95
32	2	606	CLA	C4B-NB	3.17	1.42	1.37
31	h	102	8CT	C18-C17	3.17	1.53	1.43
31	k	102	8CT	C18-C17	3.17	1.53	1.43
32	1	613	CLA	C4B-NB	3.17	1.42	1.37
31	P	615	8CT	C10-C03	3.16	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	9	615	8CT	C18-C17	3.16	1.53	1.43
31	b	623	8CT	C35-C30	3.16	1.65	1.56
31	H	102	8CT	C18-C17	3.16	1.53	1.43
32	b	612	CLA	C1D-ND	3.15	1.42	1.37
31	B	624	8CT	C35-C30	3.15	1.65	1.56
32	C	505	CLA	C1D-ND	3.15	1.42	1.37
31	6	615	8CT	C10-C03	3.15	1.55	1.45
32	A	603	CLA	C1D-ND	3.15	1.42	1.37
32	B	609	CLA	C1D-ND	3.14	1.42	1.37
47	V	201	HEM	CAB-C3B	3.14	1.55	1.47
32	c	505	CLA	C1D-ND	3.14	1.42	1.37
47	V	201	HEM	FE-NA	3.14	2.05	1.95
47	v	201	HEM	CAB-C3B	3.14	1.55	1.47
32	6	601	CLA	C4B-NB	3.13	1.42	1.37
32	7	601	CLA	C4B-NB	3.13	1.42	1.37
32	0	604	CLA	C4B-NB	3.13	1.42	1.37
47	V	201	HEM	CAC-C3C	3.13	1.55	1.47
31	D	409	8CT	C18-C17	3.12	1.52	1.43
31	d	408	8CT	C18-C17	3.12	1.52	1.43
31	a	413	8CT	C18-C17	3.12	1.52	1.43
47	V	201	HEM	FE-NC	3.12	2.05	1.95
32	B	615	CLA	C1D-ND	3.12	1.42	1.37
47	v	201	HEM	FE-NA	3.12	2.05	1.95
32	0	609	CLA	C4B-NB	3.11	1.42	1.37
47	v	201	HEM	CAC-C3C	3.11	1.55	1.47
31	b	622	8CT	C18-C17	3.11	1.52	1.43
32	1	601	CLA	C4B-NB	3.11	1.41	1.37
32	4	601	CLA	C4B-NB	3.11	1.41	1.37
32	P	610	CLA	C4B-NB	3.11	1.41	1.37
32	0	611	CLA	C4B-NB	3.11	1.41	1.37
32	4	604	CLA	C4B-NB	3.10	1.41	1.37
32	4	612	CLA	C4B-NB	3.10	1.41	1.37
32	7	613	CLA	C4B-NB	3.10	1.41	1.37
31	B	623	8CT	C18-C17	3.10	1.52	1.43
31	M	201	8CT	C18-C17	3.10	1.52	1.43
32	5	313	CLA	C4B-NB	3.10	1.41	1.37
31	B	624	8CT	C10-C03	3.10	1.55	1.45
39	B	601	SQD	C24-C23	3.10	1.59	1.50
32	7	612	CLA	C4B-NB	3.10	1.41	1.37
32	2	601	CLA	C4B-NB	3.09	1.41	1.37
31	Z	101	8CT	C07-C02	-3.09	1.45	1.51
32	5	310	CLA	C4B-NB	3.09	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	f	101	HEM	FE-NC	3.09	2.05	1.95
31	D	409	8CT	C10-C03	3.09	1.55	1.45
31	z	101	8CT	C07-C02	-3.08	1.45	1.51
31	k	102	8CT	C10-C03	3.08	1.55	1.45
32	P	606	CLA	C4B-NB	3.08	1.41	1.37
32	0	613	CLA	C4B-NB	3.08	1.41	1.37
32	7	605	CLA	C4B-NB	3.08	1.41	1.37
32	p	313	CLA	C4B-NB	3.08	1.41	1.37
32	g	102	CLA	C4B-NB	3.08	1.41	1.37
31	b	623	8CT	C10-C03	3.08	1.55	1.45
32	4	611	CLA	C4B-NB	3.08	1.41	1.37
32	p	312	CLA	C4B-NB	3.08	1.41	1.37
47	v	201	HEM	FE-NC	3.07	2.05	1.95
32	6	604	CLA	C4B-NB	3.07	1.41	1.37
39	b	601	SQD	C24-C23	3.07	1.59	1.50
32	3	606	CLA	C4B-NB	3.07	1.41	1.37
31	B	622	8CT	C18-C17	3.07	1.52	1.43
32	4	609	CLA	C4B-NB	3.07	1.41	1.37
31	3	615	8CT	C10-C03	3.07	1.55	1.45
31	d	408	8CT	C10-C03	3.07	1.55	1.45
32	5	312	CLA	C4B-NB	3.07	1.41	1.37
32	1	612	CLA	C4B-NB	3.07	1.41	1.37
32	0	607	CLA	C4B-NB	3.07	1.41	1.37
32	P	604	CLA	C4B-NB	3.07	1.41	1.37
47	f	101	HEM	CAB-C3B	3.06	1.55	1.47
31	9	615	8CT	C10-C03	3.06	1.55	1.45
32	7	611	CLA	C4B-NB	3.06	1.41	1.37
31	B	623	8CT	C10-C03	3.06	1.55	1.45
32	0	601	CLA	C4B-NB	3.06	1.41	1.37
31	b	622	8CT	C10-C03	3.06	1.55	1.45
32	5	302	CLA	C4B-NB	3.06	1.41	1.37
32	6	610	CLA	C4B-NB	3.06	1.41	1.37
32	p	310	CLA	C4B-NB	3.06	1.41	1.37
32	G	101	CLA	C4B-NB	3.06	1.41	1.37
32	6	606	CLA	C4B-NB	3.06	1.41	1.37
43	a	412	PL9	C7-C3	-3.05	1.47	1.51
32	5	306	CLA	C4B-NB	3.05	1.41	1.37
32	1	605	CLA	C4B-NB	3.05	1.41	1.37
32	2	605	CLA	C4B-NB	3.05	1.41	1.37
32	7	609	CLA	C4B-NB	3.05	1.41	1.37
31	c	518	8CT	C10-C03	3.05	1.55	1.45
31	C	518	8CT	C10-C03	3.05	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	5	304	CLA	C4B-NB	3.05	1.41	1.37
31	B	623	8CT	C35-C30	3.05	1.64	1.56
32	4	613	CLA	C4B-NB	3.05	1.41	1.37
31	K	101	8CT	C10-C03	3.05	1.55	1.45
32	4	605	CLA	C4B-NB	3.04	1.41	1.37
32	9	606	CLA	C4B-NB	3.04	1.41	1.37
31	a	413	8CT	C35-C30	3.04	1.64	1.56
32	0	605	CLA	C4B-NB	3.04	1.41	1.37
32	1	611	CLA	C4B-NB	3.04	1.41	1.37
32	6	608	CLA	C4B-NB	3.04	1.41	1.37
32	7	603	CLA	C4B-NB	3.04	1.41	1.37
43	A	609	PL9	C7-C3	-3.04	1.47	1.51
47	E	101	HEM	CAB-C3B	3.04	1.55	1.47
31	H	102	8CT	C10-C03	3.03	1.55	1.45
31	h	102	8CT	C10-C03	3.03	1.55	1.45
32	5	305	CLA	C4B-NB	3.03	1.41	1.37
32	b	613	CLA	C1D-ND	3.03	1.41	1.37
31	b	622	8CT	C35-C30	3.03	1.64	1.56
32	p	305	CLA	C4B-NB	3.03	1.41	1.37
31	K	102	8CT	C18-C17	3.02	1.52	1.43
31	k	101	8CT	C10-C03	3.02	1.55	1.45
32	p	307	CLA	C4B-NB	3.02	1.41	1.37
32	B	613	CLA	C1D-ND	3.02	1.41	1.37
31	k	101	8CT	C18-C17	3.02	1.52	1.43
32	p	302	CLA	C4B-NB	3.01	1.41	1.37
32	4	607	CLA	C4B-NB	3.01	1.41	1.37
43	d	404	PL9	C6-C1	-3.01	1.43	1.48
32	1	609	CLA	C4B-NB	3.01	1.41	1.37
32	p	306	CLA	C4B-NB	3.01	1.41	1.37
32	p	303	CLA	C4B-NB	3.01	1.41	1.37
32	8	611	CLA	C4B-NB	3.01	1.41	1.37
31	M	201	8CT	C07-C02	-3.01	1.45	1.51
31	B	622	8CT	C07-C02	-3.01	1.45	1.51
31	a	413	8CT	C10-C03	3.00	1.55	1.45
32	3	601	CLA	C4B-NB	3.00	1.41	1.37
32	s	303	CLA	C4B-NB	3.00	1.41	1.37
32	S	303	CLA	C4B-NB	3.00	1.41	1.37
32	8	605	CLA	C4B-NB	3.00	1.41	1.37
32	p	308	CLA	C4B-NB	3.00	1.41	1.37
31	K	102	8CT	C10-C03	3.00	1.55	1.45
32	P	601	CLA	C4B-NB	3.00	1.41	1.37
31	A	610	8CT	C18-C17	3.00	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	z	101	8CT	C10-C03	3.00	1.55	1.45
31	Z	101	8CT	C10-C03	2.99	1.55	1.45
31	A	610	8CT	C10-C03	2.99	1.55	1.45
32	1	608	CLA	C4B-NB	2.99	1.41	1.37
32	6	607	CLA	C4B-NB	2.99	1.41	1.37
32	P	607	CLA	C4B-NB	2.99	1.41	1.37
32	7	604	CLA	C4B-NB	2.99	1.41	1.37
32	2	612	CLA	C4B-NB	2.99	1.41	1.37
32	0	603	CLA	C4B-NB	2.99	1.41	1.37
32	8	612	CLA	C4B-NB	2.99	1.41	1.37
32	1	603	CLA	C4B-NB	2.99	1.41	1.37
32	7	607	CLA	C4B-NB	2.99	1.41	1.37
39	B	620	SQD	C24-C23	2.99	1.59	1.50
39	a	409	SQD	C24-C23	2.99	1.59	1.50
32	7	608	CLA	C4B-NB	2.99	1.41	1.37
32	s	302	CLA	C4B-NB	2.99	1.41	1.37
43	D	405	PL9	C6-C1	-2.98	1.43	1.48
32	5	309	CLA	C4B-NB	2.98	1.41	1.37
32	8	601	CLA	C4B-NB	2.98	1.41	1.37
32	8	609	CLA	C4B-NB	2.98	1.41	1.37
32	6	611	CLA	C4B-NB	2.98	1.41	1.37
32	5	303	CLA	C4B-NB	2.98	1.41	1.37
31	z	101	8CT	C18-C17	2.98	1.52	1.43
31	Z	101	8CT	C18-C17	2.98	1.52	1.43
32	9	601	CLA	C4B-NB	2.98	1.41	1.37
32	4	603	CLA	C4B-NB	2.98	1.41	1.37
31	M	201	8CT	C10-C03	2.97	1.55	1.45
32	6	603	CLA	C4B-NB	2.97	1.41	1.37
39	A	606	SQD	C24-C23	2.97	1.59	1.50
39	b	620	SQD	C24-C23	2.97	1.59	1.50
32	P	603	CLA	C4B-NB	2.97	1.41	1.37
32	4	608	CLA	C4B-NB	2.97	1.41	1.37
32	S	302	CLA	C4B-NB	2.97	1.41	1.37
32	2	607	CLA	C4B-NB	2.96	1.41	1.37
32	2	611	CLA	C4B-NB	2.96	1.41	1.37
32	2	609	CLA	C4B-NB	2.96	1.41	1.37
32	9	611	CLA	C4B-NB	2.96	1.41	1.37
32	9	605	CLA	C4B-NB	2.96	1.41	1.37
32	5	308	CLA	C4B-NB	2.95	1.41	1.37
32	0	608	CLA	C4B-NB	2.95	1.41	1.37
32	p	309	CLA	C4B-NB	2.95	1.41	1.37
31	B	622	8CT	C10-C03	2.95	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1	607	CLA	C4B-NB	2.95	1.41	1.37
31	a	413	8CT	C07-C02	-2.95	1.45	1.51
32	P	608	CLA	C4B-NB	2.95	1.41	1.37
32	0	602	CLA	C4B-NB	2.94	1.41	1.37
32	9	608	CLA	C4B-NB	2.94	1.41	1.37
47	E	101	HEM	FE-NC	2.94	2.04	1.95
32	3	609	CLA	C4B-NB	2.94	1.41	1.37
47	E	101	HEM	CAC-C3C	2.94	1.55	1.47
32	1	602	CLA	C4B-NB	2.93	1.41	1.37
32	3	603	CLA	C4B-NB	2.93	1.41	1.37
32	3	610	CLA	C4B-NB	2.93	1.41	1.37
32	9	610	CLA	C4B-NB	2.93	1.41	1.37
47	f	101	HEM	CAC-C3C	2.93	1.55	1.47
32	1	604	CLA	C4B-NB	2.93	1.41	1.37
32	9	609	CLA	C4B-NB	2.93	1.41	1.37
32	5	307	CLA	C4B-NB	2.92	1.41	1.37
31	c	518	8CT	C07-C02	-2.92	1.45	1.51
32	3	605	CLA	C4B-NB	2.92	1.41	1.37
31	H	102	8CT	C07-C02	-2.92	1.45	1.51
32	3	604	CLA	C4B-NB	2.92	1.41	1.37
32	2	603	CLA	C4B-NB	2.92	1.41	1.37
32	p	304	CLA	C4B-NB	2.92	1.41	1.37
32	P	611	CLA	C4B-NB	2.92	1.41	1.37
31	K	101	8CT	C07-C02	-2.92	1.45	1.51
31	d	408	8CT	C07-C02	-2.91	1.45	1.51
32	2	604	CLA	C4B-NB	2.91	1.41	1.37
32	4	602	CLA	C4B-NB	2.91	1.41	1.37
32	7	602	CLA	C4B-NB	2.91	1.41	1.37
32	3	611	CLA	C4B-NB	2.91	1.41	1.37
31	k	102	8CT	C07-C02	-2.91	1.45	1.51
32	c	511	CLA	C4B-NB	2.91	1.41	1.37
32	9	604	CLA	C4B-NB	2.90	1.41	1.37
31	C	518	8CT	C07-C02	-2.90	1.45	1.51
32	3	607	CLA	C4B-NB	2.90	1.41	1.37
32	8	608	CLA	C4B-NB	2.90	1.41	1.37
31	P	615	8CT	C07-C02	-2.89	1.45	1.51
31	h	102	8CT	C07-C02	-2.89	1.45	1.51
32	C	511	CLA	C4B-NB	2.89	1.41	1.37
47	E	101	HEM	FE-NA	2.89	2.04	1.95
32	D	403	CLA	C4B-NB	2.89	1.41	1.37
31	A	610	8CT	C07-C02	-2.89	1.45	1.51
32	3	608	CLA	C4B-NB	2.88	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	409	8CT	C07-C02	-2.88	1.45	1.51
32	8	602	CLA	C4B-NB	2.88	1.41	1.37
32	d	402	CLA	C4B-NB	2.88	1.41	1.37
32	8	604	CLA	C4B-NB	2.87	1.41	1.37
32	2	602	CLA	C4B-NB	2.87	1.41	1.37
32	b	611	CLA	C4B-NB	2.87	1.41	1.37
32	B	611	CLA	C4B-NB	2.87	1.41	1.37
31	6	615	8CT	C07-C02	-2.87	1.45	1.51
32	b	606	CLA	C4B-NB	2.86	1.41	1.37
32	7	606	CLA	C4B-NB	2.85	1.41	1.37
32	b	602	CLA	C4B-NB	2.85	1.41	1.37
32	P	602	CLA	C4B-NB	2.85	1.41	1.37
32	1	606	CLA	C4B-NB	2.84	1.41	1.37
32	C	512	CLA	C4B-NB	2.84	1.41	1.37
32	c	506	CLA	C4B-NB	2.84	1.41	1.37
32	9	603	CLA	C4B-NB	2.84	1.41	1.37
32	8	603	CLA	C4B-NB	2.83	1.41	1.37
32	c	513	CLA	C4B-NB	2.83	1.41	1.37
32	8	607	CLA	C4B-NB	2.83	1.41	1.37
32	2	608	CLA	C4B-NB	2.83	1.41	1.37
32	9	607	CLA	C4B-NB	2.83	1.41	1.37
31	K	102	8CT	C07-C02	-2.82	1.45	1.51
31	B	623	8CT	C07-C02	-2.82	1.45	1.51
32	C	513	CLA	C4B-NB	2.82	1.41	1.37
32	B	602	CLA	C4B-NB	2.82	1.41	1.37
32	B	603	CLA	C4B-NB	2.82	1.41	1.37
32	C	508	CLA	C4B-NB	2.82	1.41	1.37
31	b	622	8CT	C07-C02	-2.81	1.45	1.51
32	c	512	CLA	C4B-NB	2.81	1.41	1.37
32	6	602	CLA	C4B-NB	2.81	1.41	1.37
32	b	610	CLA	C4B-NB	2.81	1.41	1.37
32	B	612	CLA	C4B-NB	2.81	1.41	1.37
43	d	404	PL9	C7-C3	-2.81	1.47	1.51
32	C	510	CLA	C4B-NB	2.81	1.41	1.37
43	D	405	PL9	C7-C3	-2.80	1.47	1.51
32	6	608	CLA	C1B-C2B	2.80	1.49	1.43
32	c	504	CLA	C4B-NB	2.80	1.41	1.37
31	k	101	8CT	C07-C02	-2.80	1.45	1.51
31	B	624	8CT	C07-C02	-2.80	1.45	1.51
32	3	602	CLA	C4B-NB	2.80	1.41	1.37
32	B	607	CLA	C4B-NB	2.80	1.41	1.37
32	7	611	CLA	C1B-C2B	2.80	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	P	608	CLA	C1B-C2B	2.80	1.49	1.43
32	B	610	CLA	C4B-NB	2.79	1.41	1.37
32	C	504	CLA	C4B-NB	2.79	1.41	1.37
32	B	606	CLA	C4B-NB	2.79	1.41	1.37
31	3	615	8CT	C07-C02	-2.79	1.45	1.51
32	c	508	CLA	C4B-NB	2.79	1.41	1.37
32	9	602	CLA	C4B-NB	2.78	1.41	1.37
32	B	605	CLA	C4B-NB	2.78	1.41	1.37
32	5	312	CLA	C1B-C2B	2.78	1.49	1.43
32	c	503	CLA	C4B-NB	2.78	1.41	1.37
32	b	612	CLA	C4B-NB	2.78	1.41	1.37
32	b	603	CLA	C4B-NB	2.78	1.41	1.37
32	B	609	CLA	C4B-NB	2.78	1.41	1.37
32	p	313	CLA	C1B-C2B	2.77	1.49	1.43
32	1	611	CLA	C1B-C2B	2.77	1.49	1.43
32	c	505	CLA	C4B-NB	2.77	1.41	1.37
31	b	623	8CT	C30-C29	2.77	1.54	1.50
32	4	611	CLA	C1B-C2B	2.77	1.49	1.43
32	1	601	CLA	C1B-C2B	2.77	1.49	1.43
32	7	613	CLA	C1B-C2B	2.77	1.49	1.43
32	C	503	CLA	C4B-NB	2.76	1.41	1.37
31	b	623	8CT	C07-C02	-2.76	1.45	1.51
31	B	624	8CT	C30-C29	2.76	1.54	1.50
32	C	501	CLA	C4B-NB	2.76	1.41	1.37
32	0	611	CLA	C1B-C2B	2.76	1.49	1.43
32	p	310	CLA	C1B-C2B	2.76	1.49	1.43
32	b	608	CLA	C4B-NB	2.76	1.41	1.37
32	B	608	CLA	C4B-NB	2.76	1.41	1.37
32	P	606	CLA	C1B-C2B	2.76	1.49	1.43
41	a	407	PHO	CMC-C2C	-2.76	1.46	1.50
31	K	102	8CT	C30-C29	2.76	1.54	1.50
32	0	613	CLA	C1B-C2B	2.76	1.49	1.43
32	5	305	CLA	C1B-C2B	2.76	1.49	1.43
32	5	313	CLA	C1B-C2B	2.75	1.49	1.43
32	C	506	CLA	C4B-NB	2.75	1.41	1.37
32	D	404	CLA	C4B-NB	2.75	1.41	1.37
32	p	304	CLA	C1B-C2B	2.75	1.49	1.43
32	7	605	CLA	C1B-C2B	2.75	1.49	1.43
32	8	611	CLA	C1B-C2B	2.75	1.49	1.43
32	7	602	CLA	C1B-C2B	2.75	1.49	1.43
32	b	607	CLA	C4B-NB	2.75	1.41	1.37
32	p	306	CLA	C1B-C2B	2.75	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	p	302	CLA	C1B-C2B	2.75	1.49	1.43
32	0	601	CLA	C1B-C2B	2.75	1.49	1.43
32	5	306	CLA	C1B-C2B	2.75	1.49	1.43
31	b	622	8CT	C30-C29	2.74	1.54	1.50
32	p	305	CLA	C1B-C2B	2.74	1.49	1.43
32	b	605	CLA	C4B-NB	2.74	1.41	1.37
32	1	613	CLA	C1B-C2B	2.74	1.49	1.43
32	4	605	CLA	C1B-C2B	2.74	1.49	1.43
32	c	501	CLA	C4B-NB	2.74	1.41	1.37
32	1	604	CLA	C1B-C2B	2.74	1.49	1.43
32	5	310	CLA	C1B-C2B	2.74	1.49	1.43
32	b	609	CLA	C4B-NB	2.73	1.41	1.37
31	9	615	8CT	C07-C02	-2.73	1.45	1.51
32	4	612	CLA	C1B-C2B	2.73	1.49	1.43
32	0	608	CLA	C1B-C2B	2.73	1.49	1.43
32	6	610	CLA	C1B-C2B	2.73	1.49	1.43
32	P	610	CLA	C1B-C2B	2.73	1.49	1.43
32	0	603	CLA	C1B-C2B	2.73	1.49	1.43
32	0	612	CLA	C1B-C2B	2.73	1.49	1.43
32	0	605	CLA	C1B-C2B	2.73	1.49	1.43
32	4	608	CLA	C1B-C2B	2.73	1.49	1.43
41	d	410	PHO	CMC-C2C	-2.73	1.46	1.50
32	4	601	CLA	C1B-C2B	2.73	1.49	1.43
32	1	606	CLA	C1B-C2B	2.72	1.49	1.43
32	5	304	CLA	C1B-C2B	2.72	1.49	1.43
32	p	312	CLA	C1B-C2B	2.72	1.49	1.43
32	2	603	CLA	C1B-C2B	2.72	1.49	1.43
32	0	606	CLA	C1B-C2B	2.72	1.49	1.43
31	B	623	8CT	C30-C29	2.72	1.54	1.50
32	1	602	CLA	C1B-C2B	2.72	1.49	1.43
32	4	609	CLA	C1B-C2B	2.72	1.49	1.43
32	6	611	CLA	C1B-C2B	2.72	1.49	1.43
32	b	616	CLA	C4B-NB	2.72	1.41	1.37
32	B	616	CLA	C4B-NB	2.72	1.41	1.37
32	2	611	CLA	C1B-C2B	2.72	1.49	1.43
32	6	606	CLA	C1B-C2B	2.72	1.49	1.43
32	7	609	CLA	C1B-C2B	2.72	1.49	1.43
32	c	502	CLA	C4B-NB	2.72	1.41	1.37
32	1	603	CLA	C1B-C2B	2.72	1.49	1.43
32	8	603	CLA	C1B-C2B	2.72	1.49	1.43
32	5	308	CLA	C1B-C2B	2.72	1.49	1.43
32	7	601	CLA	C1B-C2B	2.72	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C	514	DGD	O1G-C1G	-2.72	1.39	1.45
32	2	609	CLA	C1B-C2B	2.72	1.49	1.43
32	P	607	CLA	C1B-C2B	2.72	1.49	1.43
32	0	602	CLA	C1B-C2B	2.72	1.49	1.43
32	5	302	CLA	C1B-C2B	2.72	1.49	1.43
32	p	309	CLA	C1B-C2B	2.72	1.49	1.43
45	A	614	DGD	O2G-C2G	-2.72	1.40	1.46
41	A	604	PHO	CMC-C2C	-2.72	1.46	1.50
32	A	605	CLA	C4B-NB	2.71	1.41	1.37
32	c	507	CLA	C4B-NB	2.71	1.41	1.37
32	C	507	CLA	C4B-NB	2.71	1.41	1.37
32	4	603	CLA	C1B-C2B	2.71	1.49	1.43
32	7	603	CLA	C1B-C2B	2.71	1.49	1.43
32	0	609	CLA	C1B-C2B	2.71	1.49	1.43
32	P	611	CLA	C1B-C2B	2.71	1.49	1.43
32	C	502	CLA	C4B-NB	2.71	1.41	1.37
32	6	601	CLA	C1B-C2B	2.71	1.49	1.43
32	b	614	CLA	C4B-NB	2.71	1.41	1.37
32	B	614	CLA	C4B-NB	2.71	1.41	1.37
32	1	612	CLA	C1B-C2B	2.71	1.49	1.43
32	7	604	CLA	C1B-C2B	2.71	1.49	1.43
32	s	303	CLA	C1B-C2B	2.71	1.49	1.43
45	c	514	DGD	O1G-C1G	-2.71	1.39	1.45
32	6	607	CLA	C1B-C2B	2.71	1.49	1.43
32	C	505	CLA	C4B-NB	2.71	1.41	1.37
32	4	606	CLA	C1B-C2B	2.71	1.49	1.43
32	B	617	CLA	C4B-NB	2.70	1.41	1.37
32	3	607	CLA	C1B-C2B	2.70	1.49	1.43
32	4	607	CLA	C1B-C2B	2.70	1.49	1.43
32	4	613	CLA	C1B-C2B	2.70	1.49	1.43
32	8	609	CLA	C1B-C2B	2.70	1.49	1.43
32	b	617	CLA	C4B-NB	2.70	1.41	1.37
32	3	608	CLA	C1B-C2B	2.70	1.49	1.43
32	6	603	CLA	C1B-C2B	2.70	1.49	1.43
32	2	612	CLA	C1B-C2B	2.70	1.49	1.43
32	3	610	CLA	C1B-C2B	2.70	1.49	1.43
32	9	610	CLA	C1B-C2B	2.70	1.49	1.43
32	c	510	CLA	C4B-NB	2.70	1.41	1.37
32	7	607	CLA	C1B-C2B	2.70	1.49	1.43
32	p	308	CLA	C1B-C2B	2.70	1.49	1.43
32	2	601	CLA	C1B-C2B	2.70	1.49	1.43
32	P	604	CLA	C1B-C2B	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	s	302	CLA	C1B-C2B	2.70	1.49	1.43
32	1	605	CLA	C1B-C2B	2.70	1.49	1.43
32	4	602	CLA	C1B-C2B	2.70	1.49	1.43
32	3	601	CLA	C1B-C2B	2.70	1.49	1.43
32	5	309	CLA	C1B-C2B	2.70	1.49	1.43
32	9	607	CLA	C1B-C2B	2.70	1.49	1.43
45	a	414	DGD	O2G-C2G	-2.69	1.40	1.46
32	a	408	CLA	C4B-NB	2.69	1.41	1.37
32	2	607	CLA	C1B-C2B	2.69	1.49	1.43
32	2	608	CLA	C1B-C2B	2.69	1.49	1.43
32	b	604	CLA	C4B-NB	2.69	1.41	1.37
32	c	509	CLA	C4B-NB	2.69	1.41	1.37
32	8	607	CLA	C1B-C2B	2.69	1.49	1.43
32	2	602	CLA	C1B-C2B	2.69	1.49	1.43
32	S	302	CLA	C1B-C2B	2.69	1.49	1.43
32	S	303	CLA	C1B-C2B	2.69	1.49	1.43
32	1	609	CLA	C1B-C2B	2.69	1.49	1.43
45	c	514	DGD	O2G-C2G	-2.69	1.40	1.46
41	D	402	PHO	CMC-C2C	-2.69	1.46	1.50
32	6	604	CLA	C1B-C2B	2.69	1.49	1.43
32	9	611	CLA	C1B-C2B	2.69	1.49	1.43
32	b	613	CLA	C4B-NB	2.69	1.41	1.37
32	B	615	CLA	C4B-NB	2.69	1.41	1.37
32	3	611	CLA	C1B-C2B	2.69	1.49	1.43
32	8	612	CLA	C1B-C2B	2.69	1.49	1.43
32	P	601	CLA	C1B-C2B	2.69	1.49	1.43
32	b	605	CLA	C1B-C2B	2.68	1.49	1.43
32	B	604	CLA	C4B-NB	2.68	1.41	1.37
32	2	604	CLA	C1B-C2B	2.68	1.49	1.43
32	8	604	CLA	C1B-C2B	2.68	1.49	1.43
32	9	608	CLA	C1B-C2B	2.68	1.49	1.43
32	7	606	CLA	C1B-C2B	2.68	1.49	1.43
32	8	602	CLA	C1B-C2B	2.68	1.49	1.43
32	7	608	CLA	C1B-C2B	2.68	1.49	1.43
32	B	605	CLA	C1B-C2B	2.68	1.49	1.43
32	c	511	CLA	C1B-C2B	2.68	1.49	1.43
32	b	616	CLA	C1B-C2B	2.68	1.49	1.43
32	c	503	CLA	C1B-C2B	2.68	1.49	1.43
32	B	616	CLA	C1B-C2B	2.68	1.49	1.43
32	0	607	CLA	C1B-C2B	2.68	1.49	1.43
32	8	601	CLA	C1B-C2B	2.68	1.49	1.43
31	k	101	8CT	C30-C29	2.68	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	7	612	CLA	C1B-C2B	2.68	1.49	1.43
32	b	615	CLA	C4B-NB	2.68	1.41	1.37
32	D	403	CLA	C4B-C3B	2.67	1.49	1.43
32	9	605	CLA	C1B-C2B	2.67	1.49	1.43
32	c	502	CLA	C1B-C2B	2.67	1.49	1.43
32	C	503	CLA	C1B-C2B	2.67	1.49	1.43
32	B	613	CLA	C4B-NB	2.67	1.41	1.37
32	C	511	CLA	C1B-C2B	2.67	1.49	1.43
32	1	608	CLA	C1B-C2B	2.66	1.49	1.43
32	p	307	CLA	C1B-C2B	2.66	1.49	1.43
32	d	403	CLA	C4B-NB	2.66	1.41	1.37
32	a	405	CLA	C4B-NB	2.66	1.41	1.37
32	3	605	CLA	C1B-C2B	2.66	1.49	1.43
32	9	601	CLA	C1B-C2B	2.66	1.49	1.43
32	1	607	CLA	C1B-C2B	2.66	1.49	1.43
32	8	608	CLA	C1B-C2B	2.65	1.49	1.43
45	C	514	DGD	O2G-C2G	-2.65	1.40	1.46
32	C	501	CLA	C1B-C2B	2.65	1.49	1.43
32	a	405	CLA	C1B-C2B	2.65	1.49	1.43
32	c	501	CLA	C1B-C2B	2.65	1.49	1.43
32	9	603	CLA	C1B-C2B	2.65	1.49	1.43
32	9	609	CLA	C1B-C2B	2.65	1.49	1.43
32	C	502	CLA	C1B-C2B	2.65	1.49	1.43
32	p	303	CLA	C1B-C2B	2.64	1.49	1.43
32	2	605	CLA	C1B-C2B	2.64	1.49	1.43
32	5	307	CLA	C1B-C2B	2.64	1.49	1.43
32	b	608	CLA	C1B-C2B	2.64	1.49	1.43
32	6	602	CLA	C1B-C2B	2.64	1.49	1.43
32	b	617	CLA	C1B-C2B	2.64	1.49	1.43
32	B	617	CLA	C1B-C2B	2.64	1.49	1.43
32	P	602	CLA	C1B-C2B	2.64	1.49	1.43
31	A	610	8CT	C30-C29	2.64	1.54	1.50
32	4	604	CLA	C1B-C2B	2.64	1.49	1.43
32	5	303	CLA	C1B-C2B	2.64	1.49	1.43
32	B	608	CLA	C1B-C2B	2.64	1.49	1.43
32	D	401	CLA	C4B-NB	2.64	1.41	1.37
32	P	603	CLA	C1B-C2B	2.63	1.49	1.43
32	d	402	CLA	C4B-C3B	2.63	1.49	1.43
32	C	513	CLA	C1B-C2B	2.63	1.49	1.43
32	2	606	CLA	C1B-C2B	2.63	1.49	1.43
32	3	602	CLA	C1B-C2B	2.63	1.49	1.43
32	b	606	CLA	C1B-C2B	2.63	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	513	CLA	C1B-C2B	2.63	1.49	1.43
32	A	602	CLA	C1B-C2B	2.63	1.49	1.43
32	8	605	CLA	C1B-C2B	2.63	1.49	1.43
32	d	403	CLA	C1B-C2B	2.62	1.49	1.43
32	8	606	CLA	C1B-C2B	2.62	1.49	1.43
38	D	406	LHG	O7-C5	-2.62	1.40	1.46
32	A	602	CLA	C4B-NB	2.62	1.41	1.37
32	C	510	CLA	C1B-C2B	2.62	1.49	1.43
38	d	405	LHG	O7-C5	-2.62	1.40	1.46
32	0	604	CLA	C1B-C2B	2.62	1.49	1.43
32	g	102	CLA	C1B-C2B	2.62	1.49	1.43
32	c	510	CLA	C1B-C2B	2.62	1.49	1.43
32	3	609	CLA	C1B-C2B	2.62	1.49	1.43
41	a	407	PHO	CAC-C3C	-2.62	1.47	1.51
32	3	603	CLA	C1B-C2B	2.61	1.49	1.43
32	G	101	CLA	C1B-C2B	2.61	1.49	1.43
32	B	614	CLA	C1B-C2B	2.61	1.49	1.43
32	C	509	CLA	C4B-NB	2.61	1.41	1.37
41	A	604	PHO	CMD-C2D	-2.61	1.46	1.51
32	B	606	CLA	C1B-C2B	2.61	1.49	1.43
32	9	602	CLA	C1B-C2B	2.60	1.49	1.43
32	b	614	CLA	C1B-C2B	2.60	1.49	1.43
38	l	102	LHG	O7-C5	-2.60	1.40	1.46
32	c	509	CLA	C1B-C2B	2.59	1.49	1.43
32	3	604	CLA	C1B-C2B	2.59	1.49	1.43
41	A	604	PHO	CAC-C3C	-2.59	1.47	1.51
32	c	507	CLA	C1B-C2B	2.59	1.49	1.43
41	D	402	PHO	CMD-C2D	-2.59	1.46	1.51
32	C	505	CLA	C1B-C2B	2.59	1.49	1.43
32	B	610	CLA	C1B-C2B	2.59	1.49	1.43
32	b	612	CLA	C1B-C2B	2.58	1.49	1.43
32	D	404	CLA	C1B-C2B	2.58	1.49	1.43
32	B	615	CLA	C1B-C2B	2.58	1.49	1.43
41	a	407	PHO	CMD-C2D	-2.58	1.46	1.51
32	D	401	CLA	C1B-C2B	2.58	1.49	1.43
32	B	604	CLA	C1B-C2B	2.58	1.49	1.43
32	c	512	CLA	C1B-C2B	2.58	1.49	1.43
38	L	101	LHG	O7-C5	-2.58	1.40	1.46
32	9	604	CLA	C1B-C2B	2.58	1.49	1.43
32	C	507	CLA	C1B-C2B	2.58	1.49	1.43
32	C	509	CLA	C1B-C2B	2.58	1.49	1.43
32	B	612	CLA	C1B-C2B	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	607	CLA	C1B-C2B	2.57	1.49	1.43
32	C	504	CLA	C1B-C2B	2.57	1.49	1.43
32	b	610	CLA	C1B-C2B	2.57	1.49	1.43
32	C	512	CLA	C1B-C2B	2.57	1.49	1.43
41	d	410	PHO	CMD-C2D	-2.57	1.46	1.51
32	c	504	CLA	C1B-C2B	2.57	1.49	1.43
31	a	413	8CT	C30-C29	2.57	1.54	1.50
33	7	610	KC2	CBA-CGA	-2.56	1.42	1.48
41	A	604	PHO	CMB-C2B	-2.56	1.46	1.51
32	9	606	CLA	C3B-C4B	2.56	1.50	1.42
32	b	607	CLA	C1B-C2B	2.56	1.49	1.43
32	b	613	CLA	C1B-C2B	2.56	1.49	1.43
32	B	613	CLA	C1B-C2B	2.56	1.49	1.43
32	d	409	CLA	C4B-NB	2.56	1.41	1.37
32	c	505	CLA	C1B-C2B	2.56	1.49	1.43
32	b	615	CLA	C1B-C2B	2.56	1.49	1.43
32	b	604	CLA	C1B-C2B	2.55	1.49	1.43
33	P	605	KC2	CBA-CGA	-2.55	1.42	1.48
32	3	606	CLA	C3B-C4B	2.55	1.50	1.42
32	C	508	CLA	C1B-C2B	2.54	1.49	1.43
41	a	407	PHO	CMB-C2B	-2.54	1.46	1.51
32	A	605	CLA	C1B-C2B	2.54	1.49	1.43
33	5	311	KC2	CBA-CGA	-2.54	1.42	1.48
32	c	508	CLA	C1B-C2B	2.53	1.49	1.43
33	1	610	KC2	CBA-CGA	-2.53	1.42	1.48
33	6	605	KC2	CBA-CGA	-2.53	1.42	1.48
33	6	605	KC2	C4B-NB	-2.53	1.34	1.37
32	d	409	CLA	C1B-C2B	2.52	1.49	1.43
32	D	403	CLA	C1B-C2B	2.52	1.49	1.43
32	8	606	CLA	C3B-C4B	2.52	1.50	1.42
32	b	602	CLA	C1B-C2B	2.52	1.49	1.43
45	c	515	DGD	O2G-C2G	-2.52	1.40	1.46
32	A	603	CLA	C4B-NB	2.52	1.41	1.37
32	B	603	CLA	C1B-C2B	2.52	1.49	1.43
32	9	606	CLA	C1B-C2B	2.52	1.49	1.43
33	4	610	KC2	CBA-CGA	-2.51	1.42	1.48
32	a	408	CLA	C1B-C2B	2.51	1.49	1.43
32	d	402	CLA	C1B-C2B	2.51	1.49	1.43
33	0	610	KC2	CBA-CGA	-2.50	1.42	1.48
33	8	610	KC2	CBA-CGA	-2.50	1.42	1.48
33	p	311	KC2	CBA-CGA	-2.50	1.42	1.48
32	2	606	CLA	C3B-C4B	2.50	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	602	CLA	C1B-C2B	2.50	1.49	1.43
32	b	603	CLA	C1B-C2B	2.50	1.49	1.43
32	b	611	CLA	C1B-C2B	2.50	1.49	1.43
45	C	515	DGD	O2G-C2G	-2.49	1.40	1.46
33	2	610	KC2	CBA-CGA	-2.49	1.42	1.48
37	L	102	LMG	O7-C8	-2.49	1.40	1.46
43	D	405	PL9	C53-C6	-2.49	1.45	1.50
41	D	402	PHO	CMB-C2B	-2.48	1.46	1.51
32	3	606	CLA	C1B-C2B	2.48	1.48	1.43
38	A	612	LHG	O7-C5	-2.48	1.40	1.46
32	B	611	CLA	C1B-C2B	2.47	1.48	1.43
33	8	610	KC2	C4B-NB	-2.47	1.34	1.37
33	6	609	KC2	CBA-CGA	-2.47	1.42	1.48
43	d	404	PL9	C53-C6	-2.47	1.45	1.50
37	l	101	LMG	O7-C8	-2.46	1.40	1.46
33	P	605	KC2	C4B-NB	-2.45	1.34	1.37
32	C	506	CLA	C1B-C2B	2.45	1.48	1.43
38	a	402	LHG	O7-C5	-2.45	1.40	1.46
41	d	410	PHO	CMB-C2B	-2.45	1.46	1.51
33	P	609	KC2	CBA-CGA	-2.44	1.42	1.48
32	a	406	CLA	MG-NB	-2.43	2.01	2.05
38	A	613	LHG	O7-C5	-2.43	1.40	1.46
32	c	506	CLA	C1B-C2B	2.43	1.48	1.43
32	b	613	CLA	CMD-C2D	-2.43	1.45	1.50
32	G	101	CLA	CMB-C2B	-2.43	1.45	1.50
32	A	603	CLA	C1B-C2B	2.42	1.48	1.43
37	A	607	LMG	O7-C8	-2.42	1.40	1.46
45	c	516	DGD	O2G-C2G	-2.41	1.40	1.46
33	0	610	KC2	C4B-NB	-2.41	1.34	1.37
32	D	403	CLA	CMD-C2D	-2.41	1.45	1.50
32	d	402	CLA	CMD-C2D	-2.41	1.45	1.50
33	1	610	KC2	C4B-NB	-2.41	1.34	1.37
38	a	403	LHG	O7-C5	-2.41	1.40	1.46
33	2	610	KC2	C4B-NB	-2.40	1.34	1.37
32	b	609	CLA	C1B-C2B	2.40	1.48	1.43
32	0	604	CLA	C3B-C4B	2.40	1.49	1.42
32	g	102	CLA	CMB-C2B	-2.40	1.45	1.50
45	C	516	DGD	O2G-C2G	-2.39	1.41	1.46
32	a	406	CLA	C4B-NB	2.39	1.41	1.37
32	B	613	CLA	CMD-C2D	-2.39	1.45	1.50
37	a	410	LMG	O7-C8	-2.39	1.41	1.46
32	a	406	CLA	C1B-C2B	2.39	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	7	610	KC2	C4B-NB	-2.39	1.34	1.37
45	a	414	DGD	O1G-C1G	-2.38	1.39	1.45
32	4	604	CLA	C3B-C4B	2.38	1.49	1.42
32	B	609	CLA	C1B-C2B	2.38	1.48	1.43
31	z	101	8CT	C33-C32	-2.38	1.43	1.50
31	Z	101	8CT	C33-C32	-2.37	1.43	1.50
32	4	606	CLA	C3B-C4B	2.37	1.49	1.42
32	4	609	CLA	C3B-C4B	2.37	1.49	1.42
32	0	606	CLA	C3B-C4B	2.36	1.49	1.42
32	7	609	CLA	C3B-C4B	2.36	1.49	1.42
31	h	102	8CT	C33-C32	-2.36	1.44	1.50
32	C	505	CLA	CMD-C2D	-2.36	1.45	1.50
32	4	601	CLA	C3B-C4B	2.35	1.49	1.42
32	0	601	CLA	C3B-C4B	2.35	1.49	1.42
32	9	604	CLA	C3B-C4B	2.35	1.49	1.42
41	d	410	PHO	CAC-C3C	-2.35	1.47	1.51
32	c	505	CLA	CMD-C2D	-2.35	1.46	1.50
33	p	311	KC2	C4B-NB	-2.35	1.34	1.37
32	7	612	CLA	C3B-C4B	2.35	1.49	1.42
38	D	410	LHG	O7-C5	-2.35	1.41	1.46
32	1	609	CLA	C3B-C4B	2.34	1.49	1.42
31	H	102	8CT	C33-C32	-2.34	1.44	1.50
32	1	612	CLA	C3B-C4B	2.34	1.49	1.42
45	A	614	DGD	O1G-C1G	-2.34	1.39	1.45
32	3	605	CLA	C3B-C4B	2.34	1.49	1.42
32	b	609	CLA	MG-NB	-2.34	2.01	2.05
32	1	601	CLA	C3B-C4B	2.34	1.49	1.42
32	0	609	CLA	C3B-C4B	2.34	1.49	1.42
32	a	405	CLA	CMD-C2D	-2.34	1.46	1.50
32	B	611	CLA	C3B-C4B	2.34	1.49	1.42
32	b	611	CLA	C3B-C4B	2.34	1.49	1.42
32	8	601	CLA	C3B-C4B	2.33	1.49	1.42
32	6	603	CLA	C3B-C4B	2.33	1.49	1.42
32	P	604	CLA	C3B-C4B	2.33	1.49	1.42
33	6	609	KC2	C4B-NB	-2.33	1.34	1.37
32	4	603	CLA	C3B-C4B	2.33	1.49	1.42
32	b	604	CLA	CMD-C2D	-2.33	1.46	1.50
32	B	604	CLA	CMD-C2D	-2.33	1.46	1.50
45	H	101	DGD	O1G-C1G	-2.33	1.40	1.45
45	h	101	DGD	O1G-C1G	-2.33	1.40	1.45
32	7	601	CLA	C3B-C4B	2.33	1.49	1.42
32	5	310	CLA	C3B-C4B	2.33	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	601	CLA	C3B-C4B	2.33	1.49	1.42
32	6	604	CLA	C3B-C4B	2.33	1.49	1.42
33	5	311	KC2	C4B-NB	-2.33	1.34	1.37
32	C	502	CLA	CMB-C2B	-2.33	1.46	1.50
32	5	303	CLA	C3B-C4B	2.33	1.49	1.42
32	P	601	CLA	C3B-C4B	2.33	1.49	1.42
32	5	312	CLA	C3B-C4B	2.33	1.49	1.42
32	8	609	CLA	C3B-C4B	2.33	1.49	1.42
32	p	310	CLA	C3B-C4B	2.33	1.49	1.42
32	b	604	CLA	CMB-C2B	-2.32	1.46	1.50
32	2	609	CLA	C3B-C4B	2.32	1.49	1.42
32	P	603	CLA	C3B-C4B	2.32	1.49	1.42
38	d	411	LHG	O7-C5	-2.32	1.41	1.46
32	6	610	CLA	C3B-C4B	2.32	1.49	1.42
41	D	402	PHO	CAC-C3C	-2.32	1.47	1.51
32	4	613	CLA	C3B-C4B	2.32	1.49	1.42
31	9	615	8CT	C33-C32	-2.32	1.44	1.50
32	p	302	CLA	C3B-C4B	2.32	1.49	1.42
32	5	303	CLA	CHC-C1C	2.32	1.43	1.38
32	8	611	CLA	C3B-C4B	2.32	1.49	1.42
32	4	613	CLA	CHC-C1C	2.32	1.43	1.38
32	4	612	CLA	C3B-C4B	2.32	1.49	1.42
32	s	303	CLA	C3B-C4B	2.32	1.49	1.42
32	P	602	CLA	CHC-C1C	2.31	1.43	1.38
43	d	404	PL9	C52-C5	-2.31	1.46	1.50
32	0	613	CLA	C3B-C4B	2.31	1.49	1.42
33	4	610	KC2	C4B-NB	-2.31	1.34	1.37
32	5	308	CLA	C3B-C4B	2.31	1.49	1.42
32	B	609	CLA	MG-NB	-2.31	2.01	2.05
32	3	601	CLA	C3B-C4B	2.31	1.49	1.42
32	P	606	CLA	C3B-C4B	2.31	1.49	1.42
32	b	608	CLA	CMD-C2D	-2.31	1.46	1.50
37	D	407	LMG	O7-C8	-2.31	1.41	1.46
32	1	612	CLA	CHC-C1C	2.31	1.43	1.38
32	3	604	CLA	C3B-C4B	2.31	1.49	1.42
45	c	516	DGD	O1G-C1G	-2.31	1.40	1.45
33	P	609	KC2	C4B-NB	-2.31	1.34	1.37
32	2	605	CLA	C3B-C4B	2.31	1.49	1.42
32	9	605	CLA	C3B-C4B	2.31	1.49	1.42
32	C	506	CLA	CMB-C2B	-2.31	1.46	1.50
32	1	607	CLA	C3B-C4B	2.31	1.49	1.42
32	6	601	CLA	C3B-C4B	2.31	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	8	602	CLA	CHC-C1C	2.30	1.43	1.38
45	C	516	DGD	O1G-C1G	-2.30	1.40	1.45
32	0	603	CLA	C3B-C4B	2.30	1.49	1.42
32	7	607	CLA	C3B-C4B	2.30	1.49	1.42
32	c	510	CLA	CMD-C2D	-2.30	1.46	1.50
32	B	613	CLA	MG-NB	-2.30	2.01	2.05
32	5	302	CLA	C3B-C4B	2.30	1.49	1.42
32	6	606	CLA	C3B-C4B	2.30	1.49	1.42
32	p	303	CLA	C3B-C4B	2.30	1.49	1.42
31	P	615	8CT	C33-C32	-2.30	1.44	1.50
31	3	615	8CT	C33-C32	-2.30	1.44	1.50
32	2	611	CLA	C3B-C4B	2.30	1.49	1.42
32	0	613	CLA	CHC-C1C	2.30	1.43	1.38
32	7	609	CLA	CHC-C1C	2.30	1.43	1.38
32	6	603	CLA	CHC-C1C	2.30	1.43	1.38
32	p	303	CLA	CHC-C1C	2.30	1.43	1.38
32	8	604	CLA	C3B-C4B	2.30	1.49	1.42
32	P	602	CLA	C3B-C4B	2.30	1.49	1.42
32	B	617	CLA	CMC-C2C	-2.30	1.46	1.50
32	0	612	CLA	C3B-C4B	2.30	1.49	1.42
32	7	601	CLA	CHC-C1C	2.30	1.43	1.38
32	0	607	CLA	C3B-C4B	2.30	1.49	1.42
39	B	601	SQD	O9-S	2.30	1.51	1.45
32	B	604	CLA	CMB-C2B	-2.29	1.46	1.50
32	3	609	CLA	CHC-C1C	2.29	1.43	1.38
32	b	613	CLA	MG-NB	-2.29	2.01	2.05
32	8	603	CLA	C3B-C4B	2.29	1.49	1.42
32	p	312	CLA	C3B-C4B	2.29	1.49	1.42
32	p	309	CLA	CHC-C1C	2.29	1.43	1.38
32	9	601	CLA	C3B-C4B	2.29	1.49	1.42
32	9	609	CLA	C3B-C4B	2.29	1.49	1.42
32	p	308	CLA	C3B-C4B	2.29	1.49	1.42
43	D	405	PL9	C52-C5	-2.29	1.46	1.50
32	5	304	CLA	C3B-C4B	2.29	1.49	1.42
32	A	603	CLA	CMD-C2D	-2.29	1.46	1.50
32	1	601	CLA	CHC-C1C	2.29	1.43	1.38
32	s	302	CLA	C3B-C4B	2.29	1.49	1.42
32	8	605	CLA	C3B-C4B	2.29	1.49	1.42
32	0	608	CLA	C3B-C4B	2.29	1.49	1.42
32	4	601	CLA	CHC-C1C	2.29	1.43	1.38
32	1	608	CLA	C3B-C4B	2.28	1.49	1.42
37	B	618	LMG	O7-C8	-2.28	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B	620	SQD	O9-S	2.28	1.51	1.45
32	b	609	CLA	CMB-C2B	-2.28	1.46	1.50
32	B	609	CLA	CMB-C2B	-2.28	1.46	1.50
32	7	612	CLA	CHC-C1C	2.28	1.43	1.38
32	A	602	CLA	MG-NB	-2.28	2.01	2.05
32	b	604	CLA	MG-NB	-2.28	2.01	2.05
32	5	312	CLA	CHC-C1C	2.28	1.43	1.38
32	5	305	CLA	C3B-C4B	2.28	1.49	1.42
32	p	309	CLA	C3B-C4B	2.28	1.49	1.42
32	8	607	CLA	C3B-C4B	2.28	1.49	1.42
31	6	615	8CT	C33-C32	-2.28	1.44	1.50
32	p	306	CLA	C3B-C4B	2.28	1.49	1.42
32	c	502	CLA	CMB-C2B	-2.28	1.46	1.50
32	2	604	CLA	C3B-C4B	2.28	1.49	1.42
32	3	609	CLA	C3B-C4B	2.28	1.49	1.42
32	4	607	CLA	C3B-C4B	2.28	1.49	1.42
32	9	611	CLA	C3B-C4B	2.28	1.49	1.42
32	A	603	CLA	MG-NB	-2.28	2.01	2.05
32	S	303	CLA	C3B-C4B	2.28	1.49	1.42
32	P	611	CLA	C3B-C4B	2.28	1.49	1.42
32	a	406	CLA	CMB-C2B	-2.28	1.46	1.50
32	0	609	CLA	CHC-C1C	2.28	1.43	1.38
32	c	502	CLA	MG-NB	-2.28	2.01	2.05
32	6	602	CLA	CHC-C1C	2.28	1.43	1.38
32	1	603	CLA	C3B-C4B	2.28	1.49	1.42
32	3	603	CLA	C3B-C4B	2.28	1.49	1.42
32	2	603	CLA	C3B-C4B	2.28	1.49	1.42
32	a	405	CLA	MG-NB	-2.28	2.01	2.05
32	9	609	CLA	CHC-C1C	2.28	1.43	1.38
32	2	612	CLA	C3B-C4B	2.28	1.49	1.42
32	B	608	CLA	CMD-C2D	-2.28	1.46	1.50
32	7	603	CLA	C3B-C4B	2.28	1.49	1.42
32	A	602	CLA	CMD-C2D	-2.28	1.46	1.50
32	a	406	CLA	CMD-C2D	-2.28	1.46	1.50
32	p	304	CLA	C3B-C4B	2.27	1.49	1.42
32	4	605	CLA	CHC-C1C	2.27	1.43	1.38
32	P	603	CLA	CHC-C1C	2.27	1.43	1.38
37	b	618	LMG	O7-C8	-2.27	1.41	1.46
37	d	406	LMG	O7-C8	-2.27	1.41	1.46
32	b	615	CLA	MG-NB	-2.27	2.01	2.05
32	0	601	CLA	CHC-C1C	2.27	1.43	1.38
39	b	601	SQD	O9-S	2.27	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1	608	CLA	CHC-C1C	2.27	1.43	1.38
32	2	607	CLA	CHC-C1C	2.27	1.43	1.38
32	C	506	CLA	C3B-C4B	2.27	1.49	1.42
32	5	309	CLA	C3B-C4B	2.27	1.49	1.42
32	0	606	CLA	CHC-C1C	2.27	1.43	1.38
32	3	610	CLA	C3B-C4B	2.27	1.49	1.42
32	4	605	CLA	C3B-C4B	2.27	1.49	1.42
32	6	611	CLA	C3B-C4B	2.27	1.49	1.42
32	C	513	CLA	C3B-C4B	2.27	1.49	1.42
32	4	608	CLA	C3B-C4B	2.27	1.49	1.42
32	5	306	CLA	C3B-C4B	2.27	1.49	1.42
32	8	611	CLA	CHC-C1C	2.27	1.43	1.38
32	b	602	CLA	C3B-C4B	2.27	1.49	1.42
32	B	615	CLA	MG-NB	-2.27	2.01	2.05
32	4	606	CLA	CHC-C1C	2.27	1.43	1.38
32	b	610	CLA	CMD-C2D	-2.27	1.46	1.50
32	1	611	CLA	C3B-C4B	2.27	1.49	1.42
32	9	603	CLA	C3B-C4B	2.27	1.49	1.42
32	p	304	CLA	CHC-C1C	2.27	1.43	1.38
32	A	603	CLA	CMB-C2B	-2.27	1.46	1.50
32	7	608	CLA	C3B-C4B	2.27	1.49	1.42
32	P	610	CLA	C3B-C4B	2.27	1.49	1.42
32	C	502	CLA	MG-NB	-2.27	2.01	2.05
32	4	611	CLA	C3B-C4B	2.27	1.49	1.42
32	b	606	CLA	MG-NB	-2.27	2.01	2.05
32	B	606	CLA	MG-NB	-2.27	2.01	2.05
32	6	602	CLA	C3B-C4B	2.27	1.49	1.42
32	0	605	CLA	C3B-C4B	2.27	1.49	1.42
32	8	612	CLA	CHC-C1C	2.27	1.43	1.38
32	c	504	CLA	C3B-C4B	2.27	1.49	1.42
32	p	305	CLA	C3B-C4B	2.27	1.49	1.42
32	5	307	CLA	C3B-C4B	2.26	1.49	1.42
32	2	602	CLA	CHC-C1C	2.26	1.43	1.38
32	4	603	CLA	CHC-C1C	2.26	1.43	1.38
32	d	402	CLA	CHC-C1C	2.26	1.43	1.38
34	2	615	II0	C13-C09	-2.26	1.32	1.35
32	P	610	CLA	CHC-C1C	2.26	1.43	1.38
32	p	307	CLA	CHC-C1C	2.26	1.43	1.38
32	5	313	CLA	C3B-C4B	2.26	1.49	1.42
39	b	620	SQD	O9-S	2.26	1.51	1.45
32	9	602	CLA	C3B-C4B	2.26	1.49	1.42
32	b	617	CLA	CMC-C2C	-2.26	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	506	CLA	CMB-C2B	-2.26	1.46	1.50
32	p	313	CLA	C3B-C4B	2.26	1.49	1.42
32	D	401	CLA	MG-NB	-2.26	2.01	2.05
32	C	502	CLA	CMC-C2C	-2.26	1.46	1.50
31	B	624	8CT	C33-C32	-2.26	1.44	1.50
32	4	602	CLA	C3B-C4B	2.26	1.49	1.42
32	0	608	CLA	CHC-C1C	2.26	1.43	1.38
32	p	307	CLA	C3B-C4B	2.26	1.49	1.42
45	c	515	DGD	O1G-C1G	-2.26	1.40	1.45
32	0	602	CLA	C3B-C4B	2.26	1.49	1.42
32	9	610	CLA	C3B-C4B	2.26	1.49	1.42
32	7	602	CLA	C3B-C4B	2.26	1.49	1.42
32	B	604	CLA	MG-NB	-2.26	2.01	2.05
32	7	611	CLA	C3B-C4B	2.26	1.49	1.42
32	6	608	CLA	C3B-C4B	2.26	1.49	1.42
32	P	607	CLA	C3B-C4B	2.26	1.49	1.42
32	0	607	CLA	CHC-C1C	2.26	1.43	1.38
32	2	607	CLA	C3B-C4B	2.26	1.49	1.42
31	k	101	8CT	C33-C32	-2.26	1.44	1.50
32	7	607	CLA	CHC-C1C	2.26	1.43	1.38
32	6	607	CLA	C3B-C4B	2.26	1.49	1.42
32	4	607	CLA	CHC-C1C	2.26	1.43	1.38
45	C	515	DGD	O1G-C1G	-2.26	1.40	1.45
32	S	302	CLA	CHC-C1C	2.26	1.43	1.38
32	P	608	CLA	CHC-C1C	2.26	1.43	1.38
32	1	602	CLA	C3B-C4B	2.25	1.49	1.42
32	4	604	CLA	CHC-C1C	2.25	1.43	1.38
32	P	608	CLA	C3B-C4B	2.25	1.49	1.42
32	0	605	CLA	CHC-C1C	2.25	1.43	1.38
32	D	403	CLA	CHC-C1C	2.25	1.43	1.38
32	C	510	CLA	CMD-C2D	-2.25	1.46	1.50
32	3	602	CLA	CHC-C1C	2.25	1.43	1.38
32	B	602	CLA	C3B-C4B	2.25	1.49	1.42
32	3	602	CLA	C3B-C4B	2.25	1.49	1.42
32	0	611	CLA	C3B-C4B	2.25	1.49	1.42
32	c	502	CLA	CMC-C2C	-2.25	1.46	1.50
32	5	304	CLA	CHC-C1C	2.25	1.43	1.38
32	6	610	CLA	CHC-C1C	2.25	1.43	1.38
32	p	308	CLA	CHC-C1C	2.25	1.43	1.38
32	B	602	CLA	CHC-C1C	2.25	1.43	1.38
32	8	608	CLA	C3B-C4B	2.25	1.49	1.42
32	8	607	CLA	CHC-C1C	2.25	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1	613	CLA	C3B-C4B	2.25	1.49	1.42
32	2	608	CLA	C3B-C4B	2.25	1.49	1.42
32	7	613	CLA	C3B-C4B	2.25	1.49	1.42
32	9	602	CLA	CHC-C1C	2.25	1.43	1.38
32	C	511	CLA	CMD-C2D	-2.25	1.46	1.50
32	1	606	CLA	CHC-C1C	2.25	1.43	1.38
32	9	605	CLA	CHC-C1C	2.25	1.43	1.38
32	2	611	CLA	CHC-C1C	2.25	1.43	1.38
32	p	312	CLA	CHC-C1C	2.25	1.43	1.38
32	3	603	CLA	CHC-C1C	2.24	1.43	1.38
32	3	605	CLA	CHC-C1C	2.24	1.43	1.38
32	8	612	CLA	C3B-C4B	2.24	1.49	1.42
32	5	309	CLA	CHC-C1C	2.24	1.43	1.38
32	5	308	CLA	CHC-C1C	2.24	1.43	1.38
32	6	601	CLA	CHC-C1C	2.24	1.43	1.38
32	P	601	CLA	CHC-C1C	2.24	1.43	1.38
32	d	402	CLA	MG-NB	-2.24	2.01	2.05
32	3	608	CLA	C3B-C4B	2.24	1.49	1.42
32	c	513	CLA	C3B-C4B	2.24	1.49	1.42
32	5	310	CLA	CHC-C1C	2.24	1.43	1.38
32	S	302	CLA	C3B-C4B	2.24	1.49	1.42
32	3	611	CLA	C3B-C4B	2.24	1.49	1.42
32	7	605	CLA	C3B-C4B	2.24	1.49	1.42
32	5	302	CLA	CHC-C1C	2.24	1.43	1.38
32	9	604	CLA	CHC-C1C	2.24	1.43	1.38
32	8	605	CLA	CMB-C2B	-2.24	1.46	1.50
32	8	602	CLA	C3B-C4B	2.24	1.49	1.42
32	B	605	CLA	CMB-C2B	-2.24	1.46	1.50
32	B	605	CLA	CMD-C2D	-2.24	1.46	1.50
32	5	307	CLA	CHC-C1C	2.24	1.43	1.38
31	K	102	8CT	C33-C32	-2.24	1.44	1.50
32	1	603	CLA	CHC-C1C	2.24	1.43	1.38
32	P	606	CLA	CHC-C1C	2.24	1.43	1.38
32	4	609	CLA	CHC-C1C	2.24	1.43	1.38
32	c	511	CLA	MG-NB	-2.24	2.01	2.05
38	B	619	LHG	O7-C5	-2.24	1.41	1.46
32	p	302	CLA	CHC-C1C	2.24	1.43	1.38
31	b	623	8CT	C33-C32	-2.24	1.44	1.50
32	1	609	CLA	CHC-C1C	2.24	1.43	1.38
32	1	607	CLA	CHC-C1C	2.23	1.43	1.38
32	3	604	CLA	CHC-C1C	2.23	1.43	1.38
32	p	313	CLA	CHC-C1C	2.23	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1	605	CLA	C3B-C4B	2.23	1.49	1.42
32	C	511	CLA	MG-NB	-2.23	2.01	2.05
32	B	610	CLA	MG-NB	-2.23	2.01	2.05
31	A	610	8CT	C33-C32	-2.23	1.44	1.50
32	9	608	CLA	C3B-C4B	2.23	1.49	1.42
32	C	508	CLA	C3B-C4B	2.23	1.49	1.42
32	s	302	CLA	CHC-C1C	2.23	1.43	1.38
32	2	612	CLA	CHC-C1C	2.23	1.43	1.38
32	B	602	CLA	MG-NB	-2.23	2.01	2.05
32	c	511	CLA	CMD-C2D	-2.23	1.46	1.50
32	0	612	CLA	CHC-C1C	2.23	1.43	1.38
32	p	306	CLA	CHC-C1C	2.23	1.43	1.38
32	b	610	CLA	MG-NB	-2.23	2.01	2.05
32	3	607	CLA	C3B-C4B	2.23	1.49	1.42
32	c	508	CLA	C3B-C4B	2.23	1.49	1.42
32	7	604	CLA	C3B-C4B	2.23	1.49	1.42
32	7	606	CLA	C3B-C4B	2.23	1.49	1.42
32	d	403	CLA	CHC-C1C	2.23	1.43	1.38
32	7	603	CLA	CHC-C1C	2.23	1.43	1.38
32	1	604	CLA	C3B-C4B	2.23	1.49	1.42
32	5	313	CLA	CHC-C1C	2.23	1.43	1.38
32	A	605	CLA	MG-NB	-2.23	2.01	2.05
32	b	615	CLA	C3B-C4B	2.23	1.49	1.42
32	b	610	CLA	CMB-C2B	-2.23	1.46	1.50
32	8	609	CLA	CHC-C1C	2.23	1.43	1.38
32	6	606	CLA	CHC-C1C	2.23	1.43	1.38
32	c	513	CLA	CHC-C1C	2.23	1.43	1.38
31	k	102	8CT	C33-C32	-2.23	1.44	1.50
32	g	102	CLA	C3B-C4B	2.23	1.49	1.42
32	D	403	CLA	MG-NB	-2.23	2.01	2.05
32	a	408	CLA	MG-NB	-2.23	2.01	2.05
32	2	602	CLA	C3B-C4B	2.23	1.49	1.42
32	C	509	CLA	C3B-C4B	2.23	1.49	1.42
38	b	619	LHG	O7-C5	-2.23	1.41	1.46
32	5	305	CLA	CHC-C1C	2.23	1.42	1.38
32	B	610	CLA	CMD-C2D	-2.22	1.46	1.50
32	c	506	CLA	C3B-C4B	2.22	1.49	1.42
32	G	101	CLA	C3B-C4B	2.22	1.49	1.42
32	2	605	CLA	CMB-C2B	-2.22	1.46	1.50
32	D	404	CLA	C3B-C4B	2.22	1.49	1.42
32	9	607	CLA	C3B-C4B	2.22	1.49	1.42
32	6	608	CLA	CHC-C1C	2.22	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	p	305	CLA	CHC-C1C	2.22	1.42	1.38
32	p	310	CLA	CHC-C1C	2.22	1.42	1.38
32	5	306	CLA	CHC-C1C	2.22	1.42	1.38
32	7	608	CLA	CHC-C1C	2.22	1.42	1.38
32	0	602	CLA	CHC-C1C	2.22	1.42	1.38
32	7	606	CLA	CHC-C1C	2.22	1.42	1.38
32	B	603	CLA	C3B-C4B	2.22	1.49	1.42
32	9	606	CLA	CHC-C1C	2.22	1.42	1.38
32	S	303	CLA	CHC-C1C	2.22	1.42	1.38
32	B	603	CLA	MG-NB	-2.22	2.01	2.05
32	s	303	CLA	CHC-C1C	2.22	1.42	1.38
32	s	303	CLA	MG-NB	-2.22	2.01	2.05
32	C	513	CLA	CHC-C1C	2.22	1.42	1.38
32	b	617	CLA	MG-NB	-2.21	2.01	2.05
32	9	610	CLA	CHC-C1C	2.21	1.42	1.38
39	5	318	SQD	O9-S	2.21	1.51	1.45
32	3	602	CLA	MG-NB	-2.21	2.01	2.05
32	b	605	CLA	CMB-C2B	-2.21	1.46	1.50
32	4	612	CLA	CHC-C1C	2.21	1.42	1.38
32	6	611	CLA	CHC-C1C	2.21	1.42	1.38
32	8	601	CLA	CHC-C1C	2.21	1.42	1.38
32	9	601	CLA	CHC-C1C	2.21	1.42	1.38
32	0	603	CLA	CHC-C1C	2.21	1.42	1.38
32	0	611	CLA	CHC-C1C	2.21	1.42	1.38
32	C	504	CLA	C3B-C4B	2.21	1.49	1.42
32	c	508	CLA	CMD-C2D	-2.21	1.46	1.50
32	6	604	CLA	CHC-C1C	2.21	1.42	1.38
41	a	407	PHO	C3D-C4D	2.21	1.44	1.41
32	d	403	CLA	C3B-C4B	2.21	1.49	1.42
32	c	506	CLA	MG-NB	-2.21	2.01	2.05
32	d	409	CLA	MG-NB	-2.21	2.01	2.05
32	c	512	CLA	MG-NB	-2.21	2.01	2.05
32	2	603	CLA	CHC-C1C	2.21	1.42	1.38
32	9	603	CLA	CHC-C1C	2.21	1.42	1.38
32	c	505	CLA	MG-NB	-2.21	2.01	2.05
32	c	509	CLA	C3B-C4B	2.21	1.49	1.42
32	3	610	CLA	CHC-C1C	2.21	1.42	1.38
32	a	408	CLA	CHC-C1C	2.21	1.42	1.38
32	2	609	CLA	CHC-C1C	2.21	1.42	1.38
32	3	611	CLA	CHC-C1C	2.21	1.42	1.38
32	8	604	CLA	CHC-C1C	2.21	1.42	1.38
32	1	606	CLA	C3B-C4B	2.21	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	505	CLA	C3B-C4B	2.21	1.49	1.42
32	C	510	CLA	MG-NB	-2.20	2.01	2.05
32	c	509	CLA	CMD-C2D	-2.20	1.46	1.50
32	P	604	CLA	CHC-C1C	2.20	1.42	1.38
32	C	511	CLA	C3B-C4B	2.20	1.49	1.42
32	C	512	CLA	C3B-C4B	2.20	1.49	1.42
32	b	611	CLA	CHC-C1C	2.20	1.42	1.38
32	B	611	CLA	CHC-C1C	2.20	1.42	1.38
32	B	609	CLA	C3B-C4B	2.20	1.49	1.42
32	9	602	CLA	MG-NB	-2.20	2.01	2.05
32	0	604	CLA	CHC-C1C	2.20	1.42	1.38
39	b	601	SQD	O7-S	2.20	1.51	1.45
32	2	604	CLA	CHC-C1C	2.20	1.42	1.38
32	3	601	CLA	CHC-C1C	2.20	1.42	1.38
32	b	602	CLA	MG-NB	-2.20	2.01	2.05
32	C	508	CLA	MG-NB	-2.20	2.01	2.05
32	C	505	CLA	C3B-C4B	2.20	1.49	1.42
32	2	608	CLA	CHC-C1C	2.20	1.42	1.38
45	A	614	DGD	C3E-C4E	2.20	1.55	1.52
32	D	404	CLA	MG-NB	-2.20	2.01	2.05
32	C	507	CLA	MG-NB	-2.20	2.01	2.05
32	c	512	CLA	C3B-C4B	2.20	1.49	1.42
32	B	615	CLA	C3B-C4B	2.20	1.49	1.42
32	c	503	CLA	MG-NB	-2.20	2.01	2.05
32	b	602	CLA	CHC-C1C	2.20	1.42	1.38
32	P	611	CLA	CHC-C1C	2.20	1.42	1.38
32	b	612	CLA	C3B-C4B	2.20	1.49	1.42
32	6	607	CLA	CHC-C1C	2.20	1.42	1.38
32	4	602	CLA	CHC-C1C	2.20	1.42	1.38
32	8	608	CLA	CHC-C1C	2.20	1.42	1.38
32	9	611	CLA	CHC-C1C	2.20	1.42	1.38
32	b	613	CLA	CMC-C2C	-2.20	1.46	1.50
32	B	613	CLA	CMC-C2C	-2.20	1.46	1.50
32	7	604	CLA	CHC-C1C	2.20	1.42	1.38
31	K	101	8CT	C33-C32	-2.20	1.44	1.50
32	C	506	CLA	MG-NB	-2.20	2.01	2.05
32	b	612	CLA	CMD-C2D	-2.20	1.46	1.50
32	D	404	CLA	CHC-C1C	2.20	1.42	1.38
32	B	612	CLA	C3B-C4B	2.20	1.49	1.42
32	1	604	CLA	CHC-C1C	2.20	1.42	1.38
37	C	517	LMG	O7-C8	-2.20	1.41	1.46
41	D	402	PHO	C3D-C4D	2.20	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	507	CLA	MG-NB	-2.20	2.01	2.05
45	a	414	DGD	C3E-C4E	2.20	1.55	1.52
37	0	619	LMG	O7-C8	-2.19	1.41	1.46
32	d	409	CLA	C3B-C4B	2.19	1.49	1.42
32	7	611	CLA	CHC-C1C	2.19	1.42	1.38
32	C	505	CLA	MG-NB	-2.19	2.01	2.05
32	b	606	CLA	CMD-C2D	-2.19	1.46	1.50
32	C	512	CLA	CMD-C2D	-2.19	1.46	1.50
32	B	606	CLA	CMD-C2D	-2.19	1.46	1.50
32	B	612	CLA	CMD-C2D	-2.19	1.46	1.50
32	c	504	CLA	CHC-C1C	2.19	1.42	1.38
32	c	502	CLA	CMD-C2D	-2.19	1.46	1.50
32	c	509	CLA	MG-NB	-2.19	2.01	2.05
32	P	607	CLA	CHC-C1C	2.19	1.42	1.38
32	B	603	CLA	CHC-C1C	2.19	1.42	1.38
32	b	603	CLA	MG-NB	-2.19	2.01	2.05
32	B	617	CLA	MG-NB	-2.19	2.01	2.05
32	4	608	CLA	CHC-C1C	2.19	1.42	1.38
32	c	508	CLA	MG-NB	-2.19	2.01	2.05
32	C	512	CLA	MG-NB	-2.19	2.01	2.05
36	0	618	IHT	C02-C07	-2.19	1.51	1.53
32	C	513	CLA	MG-NB	-2.19	2.01	2.05
32	B	602	CLA	CMD-C2D	-2.19	1.46	1.50
32	b	605	CLA	MG-NB	-2.19	2.01	2.05
32	A	605	CLA	C3B-C4B	2.19	1.49	1.42
32	c	501	CLA	MG-NB	-2.19	2.01	2.05
32	b	605	CLA	CMD-C2D	-2.19	1.46	1.50
39	p	318	SQD	O9-S	2.19	1.51	1.45
32	b	612	CLA	MG-NB	-2.19	2.01	2.05
32	d	403	CLA	MG-NB	-2.19	2.01	2.05
32	B	607	CLA	MG-NB	-2.19	2.01	2.05
32	B	612	CLA	MG-NB	-2.19	2.01	2.05
32	C	508	CLA	CMC-C2C	-2.19	1.46	1.50
32	3	609	CLA	MG-NB	-2.19	2.01	2.05
32	4	611	CLA	CHC-C1C	2.19	1.42	1.38
32	2	605	CLA	CHC-C1C	2.19	1.42	1.38
32	9	608	CLA	CHC-C1C	2.18	1.42	1.38
45	H	101	DGD	O2G-C2G	-2.18	1.41	1.46
45	h	101	DGD	O2G-C2G	-2.18	1.41	1.46
31	D	409	8CT	C33-C32	-2.18	1.44	1.50
38	S	301	LHG	O7-C5	-2.18	1.41	1.46
32	c	509	CLA	CHC-C1C	2.18	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	608	CLA	MG-NB	-2.18	2.01	2.05
39	5	318	SQD	C24-C23	2.18	1.59	1.51
32	a	408	CLA	C3B-C4B	2.18	1.49	1.42
32	b	614	CLA	MG-NB	-2.18	2.01	2.05
32	B	614	CLA	MG-NB	-2.18	2.01	2.05
32	b	607	CLA	CMD-C2D	-2.18	1.46	1.50
31	d	408	8CT	C33-C32	-2.18	1.44	1.50
32	2	605	CLA	CMD-C2D	-2.18	1.46	1.50
36	4	617	IHT	C02-C07	-2.18	1.51	1.53
32	B	607	CLA	C3B-C4B	2.18	1.49	1.42
38	s	301	LHG	O7-C5	-2.18	1.41	1.46
32	1	613	CLA	CHC-C1C	2.18	1.42	1.38
32	3	606	CLA	CHC-C1C	2.18	1.42	1.38
32	6	610	CLA	CMD-C2D	-2.18	1.46	1.50
32	D	401	CLA	CMD-C2D	-2.18	1.46	1.50
32	b	609	CLA	CMD-C2D	-2.18	1.46	1.50
32	D	401	CLA	C3B-C4B	2.18	1.49	1.42
32	3	604	CLA	MG-NB	-2.18	2.01	2.05
32	b	611	CLA	MG-NB	-2.18	2.01	2.05
32	7	602	CLA	CHC-C1C	2.18	1.42	1.38
37	c	517	LMG	O7-C8	-2.18	1.41	1.46
32	c	508	CLA	CMB-C2B	-2.18	1.46	1.50
32	A	605	CLA	CHC-C1C	2.18	1.42	1.38
39	B	601	SQD	O7-S	2.18	1.51	1.45
32	C	501	CLA	CMD-C2D	-2.18	1.46	1.50
32	C	509	CLA	CHC-C1C	2.18	1.42	1.38
39	p	318	SQD	C24-C23	2.18	1.59	1.51
32	c	511	CLA	C3B-C4B	2.18	1.49	1.42
32	b	603	CLA	C3B-C4B	2.18	1.49	1.42
32	2	602	CLA	MG-NB	-2.18	2.01	2.05
32	c	510	CLA	MG-NB	-2.18	2.01	2.05
32	C	508	CLA	CMD-C2D	-2.17	1.46	1.50
32	8	605	CLA	CHC-C1C	2.17	1.42	1.38
32	b	607	CLA	C3B-C4B	2.17	1.49	1.42
32	b	615	CLA	CMD-C2D	-2.17	1.46	1.50
32	9	607	CLA	CHC-C1C	2.17	1.42	1.38
32	B	612	CLA	CHC-C1C	2.17	1.42	1.38
32	b	616	CLA	CMD-C2D	-2.17	1.46	1.50
32	c	513	CLA	MG-NB	-2.17	2.01	2.05
32	c	512	CLA	CMD-C2D	-2.17	1.46	1.50
32	C	507	CLA	CHC-C1C	2.17	1.42	1.38
41	d	410	PHO	C3D-C4D	2.17	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	608	CLA	CMB-C2B	-2.17	1.46	1.50
32	7	613	CLA	CHC-C1C	2.17	1.42	1.38
32	3	603	CLA	MG-NB	-2.17	2.01	2.05
32	b	609	CLA	C3B-C4B	2.17	1.49	1.42
32	C	503	CLA	C3B-C4B	2.17	1.49	1.42
32	d	409	CLA	CMD-C2D	-2.17	1.46	1.50
32	9	610	CLA	MG-NB	-2.17	2.01	2.05
32	3	601	CLA	CMD-C2D	-2.17	1.46	1.50
32	c	511	CLA	CMB-C2B	-2.17	1.46	1.50
32	C	503	CLA	MG-NB	-2.17	2.01	2.05
32	b	608	CLA	C3B-C4B	2.16	1.49	1.42
32	8	608	CLA	MG-NB	-2.16	2.01	2.05
32	C	506	CLA	CMC-C2C	-2.16	1.46	1.50
32	b	607	CLA	MG-NB	-2.16	2.01	2.05
32	B	611	CLA	MG-NB	-2.16	2.01	2.05
32	1	602	CLA	CHC-C1C	2.16	1.42	1.38
32	B	609	CLA	CMD-C2D	-2.16	1.46	1.50
32	3	607	CLA	MG-NB	-2.16	2.01	2.05
32	B	607	CLA	CMD-C2D	-2.16	1.46	1.50
32	5	307	CLA	MG-NB	-2.16	2.01	2.05
32	7	602	CLA	MG-NB	-2.16	2.01	2.05
32	7	605	CLA	CMB-C2B	-2.16	1.46	1.50
37	4	618	LMG	O7-C8	-2.16	1.41	1.46
32	2	601	CLA	CHC-C1C	2.16	1.42	1.38
32	B	608	CLA	C3B-C4B	2.16	1.49	1.42
32	1	608	CLA	MG-NB	-2.16	2.01	2.05
39	b	620	SQD	O7-S	2.16	1.51	1.45
32	c	503	CLA	C3B-C4B	2.16	1.49	1.42
32	g	102	CLA	MG-NB	-2.16	2.01	2.05
32	b	603	CLA	CHC-C1C	2.16	1.42	1.38
32	3	608	CLA	MG-NB	-2.16	2.01	2.05
32	b	608	CLA	CMB-C2B	-2.16	1.46	1.50
32	b	611	CLA	CMD-C2D	-2.16	1.46	1.50
32	c	501	CLA	CMD-C2D	-2.16	1.46	1.50
32	B	611	CLA	CMD-C2D	-2.16	1.46	1.50
32	3	607	CLA	CHC-C1C	2.16	1.42	1.38
32	A	605	CLA	CMD-C2D	-2.15	1.46	1.50
32	C	509	CLA	MG-NB	-2.15	2.01	2.05
32	b	607	CLA	CMC-C2C	-2.15	1.46	1.50
32	B	607	CLA	CMC-C2C	-2.15	1.46	1.50
32	D	403	CLA	CMB-C2B	-2.15	1.46	1.50
32	7	606	CLA	MG-NB	-2.15	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	9	603	CLA	MG-NB	-2.15	2.01	2.05
39	5	318	SQD	O7-S	2.15	1.51	1.45
39	B	620	SQD	O7-S	2.15	1.51	1.45
32	C	504	CLA	MG-NB	-2.15	2.01	2.05
32	8	603	CLA	CHC-C1C	2.15	1.42	1.38
32	B	615	CLA	CMD-C2D	-2.15	1.46	1.50
32	d	402	CLA	CMB-C2B	-2.15	1.46	1.50
32	C	509	CLA	CMD-C2D	-2.15	1.46	1.50
32	C	512	CLA	CMB-C2B	-2.15	1.46	1.50
32	8	602	CLA	MG-NB	-2.15	2.01	2.05
32	b	607	CLA	CHC-C1C	2.15	1.42	1.38
32	C	504	CLA	CHC-C1C	2.15	1.42	1.38
41	A	604	PHO	C3D-C4D	2.15	1.44	1.41
32	b	612	CLA	CMB-C2B	-2.15	1.46	1.50
32	c	512	CLA	CMB-C2B	-2.15	1.46	1.50
32	3	601	CLA	MG-NB	-2.15	2.01	2.05
32	7	605	CLA	CHC-C1C	2.15	1.42	1.38
32	2	604	CLA	MG-NB	-2.15	2.01	2.05
32	7	608	CLA	MG-NB	-2.15	2.01	2.05
36	8	616	IHT	C02-C07	-2.15	1.51	1.53
32	c	504	CLA	CMD-C2D	-2.15	1.46	1.50
32	B	609	CLA	CHC-C1C	2.15	1.42	1.38
32	A	602	CLA	C3B-C4B	2.15	1.49	1.42
32	1	605	CLA	CMB-C2B	-2.15	1.46	1.50
32	c	510	CLA	C3B-C4B	2.15	1.49	1.42
32	b	614	CLA	C3B-C4B	2.15	1.49	1.42
32	b	616	CLA	C3B-C4B	2.15	1.49	1.42
32	B	614	CLA	C3B-C4B	2.15	1.49	1.42
32	B	616	CLA	C3B-C4B	2.15	1.49	1.42
32	B	615	CLA	CHC-C1C	2.15	1.42	1.38
32	9	609	CLA	MG-NB	-2.15	2.01	2.05
32	b	606	CLA	C3B-C4B	2.15	1.49	1.42
32	B	606	CLA	C3B-C4B	2.15	1.49	1.42
32	9	605	CLA	CMD-C2D	-2.15	1.46	1.50
32	9	608	CLA	MG-NB	-2.15	2.01	2.05
32	3	606	CLA	CMD-C2D	-2.15	1.46	1.50
32	C	502	CLA	CMD-C2D	-2.15	1.46	1.50
32	c	511	CLA	CHC-C1C	2.15	1.42	1.38
32	7	605	CLA	MG-NB	-2.15	2.01	2.05
32	1	611	CLA	CHC-C1C	2.14	1.42	1.38
32	g	102	CLA	CHC-C1C	2.14	1.42	1.38
32	c	503	CLA	CMD-C2D	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	507	CLA	CMD-C2D	-2.14	1.46	1.50
32	C	503	CLA	CMD-C2D	-2.14	1.46	1.50
32	p	309	CLA	MG-NB	-2.14	2.01	2.05
32	c	510	CLA	CMB-C2B	-2.14	1.46	1.50
32	2	601	CLA	MG-NB	-2.14	2.01	2.05
32	2	603	CLA	MG-NB	-2.14	2.01	2.05
32	c	506	CLA	CMD-C2D	-2.14	1.46	1.50
32	s	302	CLA	MG-NB	-2.14	2.01	2.05
32	B	616	CLA	MG-NB	-2.14	2.01	2.05
32	3	610	CLA	MG-NB	-2.14	2.01	2.05
32	1	602	CLA	MG-NB	-2.14	2.01	2.05
32	c	506	CLA	CHC-C1C	2.14	1.42	1.38
32	1	606	CLA	MG-NB	-2.14	2.01	2.05
32	2	605	CLA	MG-NB	-2.14	2.01	2.05
32	C	504	CLA	CMD-C2D	-2.14	1.46	1.50
32	B	605	CLA	MG-NB	-2.14	2.01	2.05
32	c	507	CLA	CHC-C1C	2.14	1.42	1.38
32	D	404	CLA	CMD-C2D	-2.14	1.46	1.50
32	B	613	CLA	C3B-C4B	2.14	1.49	1.42
31	b	622	8CT	C33-C32	-2.14	1.44	1.50
32	B	616	CLA	CMD-C2D	-2.14	1.46	1.50
32	b	608	CLA	MG-NB	-2.14	2.01	2.05
32	b	603	CLA	CMB-C2B	-2.14	1.46	1.50
32	B	610	CLA	CMB-C2B	-2.14	1.46	1.50
39	A	606	SQD	O9-S	2.14	1.51	1.45
32	3	608	CLA	CHC-C1C	2.14	1.42	1.38
32	b	614	CLA	CHC-C1C	2.14	1.42	1.38
32	B	614	CLA	CHC-C1C	2.14	1.42	1.38
32	9	606	CLA	CMD-C2D	-2.14	1.46	1.50
32	9	609	CLA	CMB-C2B	-2.14	1.46	1.50
32	S	303	CLA	MG-NB	-2.14	2.01	2.05
32	a	406	CLA	MG-ND	-2.14	2.01	2.05
32	B	607	CLA	CHC-C1C	2.14	1.42	1.38
32	c	501	CLA	C3B-C4B	2.14	1.49	1.42
32	B	611	CLA	CMB-C2B	-2.13	1.46	1.50
32	p	307	CLA	MG-NB	-2.13	2.01	2.05
32	C	510	CLA	C3B-C4B	2.13	1.49	1.42
32	b	617	CLA	CMB-C2B	-2.13	1.46	1.50
32	C	513	CLA	CMD-C2D	-2.13	1.46	1.50
32	8	606	CLA	CHC-C1C	2.13	1.42	1.38
32	7	604	CLA	MG-NB	-2.13	2.01	2.05
32	C	501	CLA	C3B-C4B	2.13	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	507	CLA	CMD-C2D	-2.13	1.46	1.50
32	C	508	CLA	CMB-C2B	-2.13	1.46	1.50
32	4	608	CLA	MG-NB	-2.13	2.01	2.05
37	6	616	LMG	O7-C8	-2.13	1.41	1.46
32	b	615	CLA	CHC-C1C	2.13	1.42	1.38
32	1	604	CLA	MG-NB	-2.13	2.01	2.05
32	0	608	CLA	MG-NB	-2.13	2.01	2.05
38	B	621	LHG	P-O6	2.13	1.67	1.59
32	d	402	CLA	CMC-C2C	-2.13	1.46	1.50
32	C	511	CLA	CHC-C1C	2.13	1.42	1.38
32	2	608	CLA	MG-NB	-2.13	2.01	2.05
32	b	616	CLA	MG-NB	-2.13	2.01	2.05
39	p	318	SQD	O7-S	2.13	1.51	1.45
32	C	501	CLA	MG-NB	-2.13	2.01	2.05
32	b	614	CLA	CMB-C2B	-2.13	1.46	1.50
32	c	506	CLA	CMC-C2C	-2.13	1.46	1.50
32	a	408	CLA	CMD-C2D	-2.13	1.46	1.50
32	a	405	CLA	C3B-C4B	2.13	1.48	1.42
32	b	604	CLA	C3B-C4B	2.13	1.48	1.42
32	C	503	CLA	CHC-C1C	2.13	1.42	1.38
32	8	609	CLA	MG-NB	-2.13	2.01	2.05
32	C	510	CLA	CMB-C2B	-2.13	1.46	1.50
32	P	610	CLA	CMD-C2D	-2.13	1.46	1.50
31	a	413	8CT	C33-C32	-2.13	1.44	1.50
32	b	602	CLA	CMD-C2D	-2.13	1.46	1.50
34	6	614	II0	C14-C10	-2.13	1.32	1.35
32	b	610	CLA	C3B-C4B	2.13	1.48	1.42
32	3	604	CLA	CMD-C2D	-2.13	1.46	1.50
32	c	508	CLA	CMC-C2C	-2.13	1.46	1.50
32	b	613	CLA	C3B-C4B	2.13	1.48	1.42
32	b	612	CLA	CHC-C1C	2.13	1.42	1.38
32	B	612	CLA	CMC-C2C	-2.13	1.46	1.50
32	c	510	CLA	CHC-C1C	2.12	1.42	1.38
32	C	508	CLA	CHC-C1C	2.12	1.42	1.38
32	c	503	CLA	CHC-C1C	2.12	1.42	1.38
32	c	505	CLA	CHC-C1C	2.12	1.42	1.38
32	b	615	CLA	CMB-C2B	-2.12	1.46	1.50
32	B	615	CLA	CMB-C2B	-2.12	1.46	1.50
32	6	607	CLA	MG-NB	-2.12	2.01	2.05
32	c	507	CLA	C3B-C4B	2.12	1.48	1.42
32	b	616	CLA	CMB-C2B	-2.12	1.46	1.50
32	2	609	CLA	MG-NB	-2.12	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	403	CLA	CMC-C2C	-2.12	1.46	1.50
32	5	304	CLA	MG-NB	-2.12	2.01	2.05
32	S	303	CLA	CMD-C2D	-2.12	1.46	1.50
32	b	614	CLA	CMD-C2D	-2.12	1.46	1.50
32	B	617	CLA	C3B-C4B	2.12	1.48	1.42
37	P	616	LMG	O7-C8	-2.12	1.41	1.46
32	b	603	CLA	CMD-C2D	-2.12	1.46	1.50
32	B	603	CLA	CMD-C2D	-2.12	1.46	1.50
32	0	602	CLA	MG-NB	-2.12	2.01	2.05
32	2	604	CLA	CMD-C2D	-2.12	1.46	1.50
32	3	606	CLA	CMB-C2B	-2.12	1.46	1.50
32	c	504	CLA	MG-NB	-2.12	2.01	2.05
32	c	508	CLA	CHC-C1C	2.12	1.42	1.38
32	9	601	CLA	MG-NB	-2.12	2.01	2.05
32	2	608	CLA	CMB-C2B	-2.12	1.46	1.50
32	9	601	CLA	CMD-C2D	-2.12	1.46	1.50
32	B	614	CLA	CMB-C2B	-2.12	1.46	1.50
32	1	605	CLA	CHC-C1C	2.12	1.42	1.38
32	b	617	CLA	C3B-C4B	2.12	1.48	1.42
32	C	507	CLA	C3B-C4B	2.12	1.48	1.42
32	7	607	CLA	CMD-C2D	-2.12	1.46	1.50
32	G	101	CLA	CHC-C1C	2.12	1.42	1.38
32	1	605	CLA	MG-NB	-2.12	2.01	2.05
47	v	201	HEM	CMC-C2C	2.12	1.55	1.50
32	9	611	CLA	MG-NB	-2.12	2.01	2.05
32	5	306	CLA	CMD-C2D	-2.12	1.46	1.50
32	9	606	CLA	CMB-C2B	-2.12	1.46	1.50
32	C	503	CLA	CMB-C2B	-2.12	1.46	1.50
32	4	603	CLA	MG-NB	-2.12	2.01	2.05
32	2	609	CLA	CMD-C2D	-2.12	1.46	1.50
32	5	307	CLA	CMB-C2B	-2.12	1.46	1.50
32	9	602	CLA	CMD-C2D	-2.12	1.46	1.50
32	5	309	CLA	MG-NB	-2.12	2.01	2.05
32	G	101	CLA	MG-NB	-2.12	2.01	2.05
32	8	607	CLA	CMD-C2D	-2.12	1.46	1.50
32	2	606	CLA	CHC-C1C	2.12	1.42	1.38
32	b	608	CLA	CHC-C1C	2.12	1.42	1.38
32	B	610	CLA	C3B-C4B	2.12	1.48	1.42
32	9	607	CLA	MG-NB	-2.12	2.01	2.05
32	3	607	CLA	CMD-C2D	-2.11	1.46	1.50
32	C	511	CLA	CMB-C2B	-2.11	1.46	1.50
32	b	613	CLA	CHC-C1C	2.11	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	613	CLA	CHC-C1C	2.11	1.42	1.38
32	d	403	CLA	CMD-C2D	-2.11	1.46	1.50
32	8	605	CLA	CMD-C2D	-2.11	1.46	1.50
32	S	302	CLA	MG-NB	-2.11	2.01	2.05
32	0	603	CLA	MG-NB	-2.11	2.01	2.05
32	b	617	CLA	CMD-C2D	-2.11	1.46	1.50
32	B	617	CLA	CMD-C2D	-2.11	1.46	1.50
32	5	305	CLA	MG-NB	-2.11	2.01	2.05
32	9	604	CLA	MG-NB	-2.11	2.01	2.05
32	B	617	CLA	CMB-C2B	-2.11	1.46	1.50
41	A	604	PHO	C4D-ND	-2.11	1.35	1.38
41	a	407	PHO	C4D-ND	-2.11	1.35	1.38
32	5	304	CLA	CMD-C2D	-2.11	1.46	1.50
32	7	603	CLA	CMD-C2D	-2.11	1.46	1.50
32	8	604	CLA	CMD-C2D	-2.11	1.46	1.50
38	b	621	LHG	P-O6	2.11	1.67	1.59
32	1	607	CLA	CMD-C2D	-2.11	1.46	1.50
32	b	606	CLA	CMB-C2B	-2.11	1.46	1.50
32	B	606	CLA	CMB-C2B	-2.11	1.46	1.50
32	B	614	CLA	CMD-C2D	-2.11	1.46	1.50
32	8	605	CLA	MG-NB	-2.11	2.01	2.05
32	b	602	CLA	CMB-C2B	-2.11	1.46	1.50
32	p	312	CLA	CMD-C2D	-2.11	1.46	1.50
32	B	602	CLA	CMB-C2B	-2.11	1.46	1.50
32	8	603	CLA	MG-NB	-2.11	2.01	2.05
32	C	505	CLA	CHC-C1C	2.11	1.42	1.38
32	c	513	CLA	CMD-C2D	-2.11	1.46	1.50
39	a	409	SQD	O9-S	2.11	1.51	1.45
32	B	606	CLA	CHC-C1C	2.11	1.42	1.38
32	3	602	CLA	CMD-C2D	-2.11	1.46	1.50
33	p	311	KC2	C4A-C3A	-2.11	1.40	1.44
32	0	603	CLA	CMD-C2D	-2.11	1.46	1.50
32	8	608	CLA	CMB-C2B	-2.11	1.46	1.50
32	a	406	CLA	CMC-C2C	-2.11	1.46	1.50
32	p	307	CLA	CMB-C2B	-2.11	1.46	1.50
32	9	607	CLA	CMB-C2B	-2.10	1.46	1.50
32	B	612	CLA	CMB-C2B	-2.10	1.46	1.50
32	P	607	CLA	MG-NB	-2.10	2.01	2.05
32	9	603	CLA	CMD-C2D	-2.10	1.46	1.50
32	B	604	CLA	C3B-C4B	2.10	1.48	1.42
32	2	603	CLA	CMD-C2D	-2.10	1.46	1.50
31	B	623	8CT	C33-C32	-2.10	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1	603	CLA	MG-NB	-2.10	2.01	2.05
32	8	608	CLA	CMD-C2D	-2.10	1.46	1.50
32	P	602	CLA	MG-NB	-2.10	2.01	2.05
32	b	606	CLA	CHC-C1C	2.10	1.42	1.38
32	a	405	CLA	CMB-C2B	-2.10	1.46	1.50
32	c	507	CLA	CMB-C2B	-2.10	1.46	1.50
32	C	507	CLA	CMB-C2B	-2.10	1.46	1.50
32	5	303	CLA	CMB-C2B	-2.10	1.46	1.50
32	8	606	CLA	CMB-C2B	-2.10	1.46	1.50
32	C	512	CLA	CHC-C1C	2.10	1.42	1.38
32	C	505	CLA	CMB-C2B	-2.10	1.46	1.50
32	P	610	CLA	MG-NB	-2.10	2.01	2.05
32	A	602	CLA	CHC-C1C	2.10	1.42	1.38
32	C	501	CLA	CHC-C1C	2.10	1.42	1.38
32	C	506	CLA	CHC-C1C	2.10	1.42	1.38
32	g	102	CLA	CMD-C2D	-2.10	1.46	1.50
32	9	609	CLA	CMD-C2D	-2.10	1.46	1.50
32	A	605	CLA	CMB-C2B	-2.10	1.46	1.50
32	C	506	CLA	CMD-C2D	-2.10	1.46	1.50
32	p	308	CLA	CMD-C2D	-2.10	1.46	1.50
32	3	610	CLA	CMD-C2D	-2.10	1.46	1.50
32	9	608	CLA	CMD-C2D	-2.10	1.46	1.50
32	b	609	CLA	CHC-C1C	2.10	1.42	1.38
32	5	310	CLA	MG-NB	-2.10	2.01	2.05
32	6	604	CLA	CMD-C2D	-2.10	1.46	1.50
32	7	606	CLA	CMD-C2D	-2.10	1.46	1.50
32	c	509	CLA	CMB-C2B	-2.10	1.46	1.50
37	2	617	LMG	O7-C8	-2.10	1.41	1.46
32	8	603	CLA	CMD-C2D	-2.10	1.46	1.50
32	3	603	CLA	CMD-C2D	-2.10	1.46	1.50
32	4	605	CLA	CMD-C2D	-2.10	1.46	1.50
32	P	603	CLA	CMD-C2D	-2.10	1.46	1.50
32	p	308	CLA	MG-NB	-2.10	2.01	2.05
32	3	609	CLA	CMD-C2D	-2.09	1.46	1.50
32	9	607	CLA	CMD-C2D	-2.09	1.46	1.50
32	9	610	CLA	CMB-C2B	-2.09	1.46	1.50
32	6	602	CLA	MG-NB	-2.09	2.01	2.05
32	5	312	CLA	CMD-C2D	-2.09	1.46	1.50
32	c	512	CLA	CHC-C1C	2.09	1.42	1.38
32	a	406	CLA	C3B-C4B	2.09	1.48	1.42
33	5	311	KC2	C4A-C3A	-2.09	1.40	1.44
32	b	615	CLA	CMC-C2C	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	603	CLA	CMB-C2B	-2.09	1.46	1.50
32	3	608	CLA	CMD-C2D	-2.09	1.46	1.50
32	5	308	CLA	CMD-C2D	-2.09	1.46	1.50
32	b	605	CLA	CMC-C2C	-2.09	1.46	1.50
32	b	611	CLA	CMB-C2B	-2.09	1.46	1.50
32	B	607	CLA	CMB-C2B	-2.09	1.46	1.50
32	4	602	CLA	MG-NB	-2.09	2.01	2.05
32	a	405	CLA	CHC-C1C	2.09	1.42	1.38
32	8	607	CLA	MG-NB	-2.09	2.01	2.05
32	P	603	CLA	MG-NB	-2.09	2.01	2.05
32	2	606	CLA	CMD-C2D	-2.09	1.46	1.50
47	f	101	HEM	CMB-C2B	2.09	1.55	1.50
32	D	401	CLA	CHC-C1C	2.09	1.42	1.38
32	b	616	CLA	CHC-C1C	2.09	1.42	1.38
32	8	612	CLA	MG-NB	-2.09	2.01	2.05
32	p	307	CLA	CMD-C2D	-2.09	1.46	1.50
32	s	303	CLA	CMD-C2D	-2.09	1.46	1.50
32	3	611	CLA	MG-NB	-2.09	2.01	2.05
32	3	604	CLA	CMB-C2B	-2.09	1.46	1.50
32	4	602	CLA	CMD-C2D	-2.09	1.46	1.50
32	5	306	CLA	CMB-C2B	-2.09	1.46	1.50
32	p	305	CLA	CMB-C2B	-2.09	1.46	1.50
32	8	604	CLA	MG-NB	-2.09	2.01	2.05
32	D	401	CLA	CMB-C2B	-2.09	1.46	1.50
32	p	306	CLA	CMB-C2B	-2.09	1.46	1.50
32	2	607	CLA	MG-NB	-2.09	2.01	2.05
32	8	601	CLA	MG-NB	-2.09	2.01	2.05
32	B	616	CLA	CMB-C2B	-2.09	1.46	1.50
32	0	607	CLA	CMD-C2D	-2.09	1.46	1.50
32	C	511	CLA	CMC-C2C	-2.09	1.46	1.50
32	c	513	CLA	CMC-C2C	-2.09	1.46	1.50
37	G	102	LMG	O7-C8	-2.09	1.41	1.46
32	7	603	CLA	MG-NB	-2.09	2.01	2.05
32	C	502	CLA	C3B-C4B	2.09	1.48	1.42
32	1	606	CLA	CMD-C2D	-2.09	1.46	1.50
32	3	605	CLA	CMD-C2D	-2.09	1.46	1.50
32	d	409	CLA	CMB-C2B	-2.09	1.46	1.50
32	c	509	CLA	CMC-C2C	-2.09	1.46	1.50
32	4	604	CLA	CMB-C2B	-2.09	1.46	1.50
32	p	306	CLA	CMD-C2D	-2.09	1.46	1.50
32	8	601	CLA	CMD-C2D	-2.08	1.46	1.50
32	9	604	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	s	302	CLA	CMB-C2B	-2.08	1.46	1.50
32	b	604	CLA	CHC-C1C	2.08	1.42	1.38
32	3	601	CLA	CMB-C2B	-2.08	1.46	1.50
32	P	603	CLA	CMB-C2B	-2.08	1.46	1.50
32	C	501	CLA	CMB-C2B	-2.08	1.46	1.50
32	p	303	CLA	CMD-C2D	-2.08	1.46	1.50
32	4	607	CLA	CMD-C2D	-2.08	1.46	1.50
47	V	201	HEM	CMC-C2C	2.08	1.55	1.50
32	B	617	CLA	CHC-C1C	2.08	1.42	1.38
32	2	607	CLA	CMD-C2D	-2.08	1.46	1.50
32	b	612	CLA	CMC-C2C	-2.08	1.46	1.50
32	p	312	CLA	CMB-C2B	-2.08	1.46	1.50
32	9	603	CLA	CMB-C2B	-2.08	1.46	1.50
32	B	613	CLA	CMB-C2B	-2.08	1.46	1.50
32	6	607	CLA	CMD-C2D	-2.08	1.46	1.50
32	0	611	CLA	MG-NB	-2.08	2.01	2.05
32	8	611	CLA	MG-NB	-2.08	2.01	2.05
32	C	510	CLA	CHC-C1C	2.08	1.42	1.38
32	s	303	CLA	CMB-C2B	-2.08	1.46	1.50
32	5	312	CLA	MG-NB	-2.08	2.01	2.05
32	2	608	CLA	CMD-C2D	-2.08	1.46	1.50
45	a	414	DGD	C2E-C1E	2.08	1.56	1.50
32	2	601	CLA	CMB-C2B	-2.08	1.46	1.50
32	b	616	CLA	CMC-C2C	-2.08	1.46	1.50
32	c	503	CLA	CMB-C2B	-2.08	1.46	1.50
32	8	609	CLA	CMD-C2D	-2.08	1.46	1.50
32	6	603	CLA	MG-NB	-2.08	2.01	2.05
32	6	610	CLA	MG-NB	-2.08	2.01	2.05
32	9	605	CLA	MG-NB	-2.08	2.01	2.05
32	P	611	CLA	MG-NB	-2.08	2.01	2.05
32	p	305	CLA	MG-NB	-2.08	2.01	2.05
32	2	602	CLA	CMD-C2D	-2.08	1.46	1.50
32	3	603	CLA	CMB-C2B	-2.08	1.46	1.50
32	p	304	CLA	MG-NB	-2.08	2.01	2.05
32	2	601	CLA	CMD-C2D	-2.08	1.46	1.50
32	c	501	CLA	CHC-C1C	2.08	1.42	1.38
32	a	405	CLA	CMC-C2C	-2.08	1.46	1.50
32	3	605	CLA	MG-NB	-2.08	2.01	2.05
32	b	610	CLA	CHC-C1C	2.07	1.42	1.38
32	d	409	CLA	CHC-C1C	2.07	1.42	1.38
32	B	608	CLA	CHC-C1C	2.07	1.42	1.38
32	B	610	CLA	CHC-C1C	2.07	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	6	601	CLA	MG-NB	-2.07	2.01	2.05
32	b	604	CLA	CMC-C2C	-2.07	1.46	1.50
32	B	609	CLA	CMC-C2C	-2.07	1.46	1.50
32	C	509	CLA	CMB-C2B	-2.07	1.46	1.50
32	7	607	CLA	MG-NB	-2.07	2.01	2.05
32	9	604	CLA	CMB-C2B	-2.07	1.46	1.50
32	p	303	CLA	MG-NB	-2.07	2.01	2.05
32	c	513	CLA	CMB-C2B	-2.07	1.46	1.50
47	v	201	HEM	CMB-C2B	2.07	1.55	1.50
32	A	603	CLA	CMC-C2C	-2.07	1.46	1.50
32	5	305	CLA	CMB-C2B	-2.07	1.46	1.50
32	a	408	CLA	CMB-C2B	-2.07	1.46	1.50
32	S	302	CLA	CMB-C2B	-2.07	1.46	1.50
32	4	603	CLA	CMD-C2D	-2.07	1.46	1.50
32	b	607	CLA	CMB-C2B	-2.07	1.46	1.50
32	7	609	CLA	MG-NB	-2.07	2.01	2.05
32	3	609	CLA	CMB-C2B	-2.07	1.46	1.50
32	C	510	CLA	CMC-C2C	-2.07	1.46	1.50
32	G	101	CLA	CMD-C2D	-2.07	1.46	1.50
32	1	608	CLA	CMD-C2D	-2.07	1.46	1.50
32	3	602	CLA	CMB-C2B	-2.07	1.46	1.50
32	3	608	CLA	CMB-C2B	-2.07	1.46	1.50
32	7	608	CLA	CMD-C2D	-2.07	1.46	1.50
32	8	607	CLA	CMB-C2B	-2.07	1.46	1.50
32	P	602	CLA	CMD-C2D	-2.07	1.46	1.50
32	p	310	CLA	CMB-C2B	-2.07	1.46	1.50
32	p	303	CLA	CMB-C2B	-2.07	1.46	1.50
32	1	611	CLA	MG-NB	-2.07	2.01	2.05
32	5	303	CLA	MG-NB	-2.07	2.01	2.05
32	7	608	CLA	CMB-C2B	-2.07	1.46	1.50
32	8	602	CLA	CMD-C2D	-2.07	1.46	1.50
32	P	601	CLA	CMD-C2D	-2.07	1.46	1.50
32	6	611	CLA	MG-NB	-2.07	2.01	2.05
32	3	604	CLA	CMC-C2C	-2.07	1.46	1.50
32	0	604	CLA	CMD-C2D	-2.07	1.46	1.50
32	8	602	CLA	CMC-C2C	-2.07	1.46	1.50
32	8	606	CLA	CMD-C2D	-2.07	1.46	1.50
32	6	601	CLA	CMD-C2D	-2.07	1.46	1.50
32	6	603	CLA	CMB-C2B	-2.07	1.46	1.50
47	E	101	HEM	CMB-C2B	2.07	1.55	1.50
32	C	512	CLA	CMC-C2C	-2.07	1.46	1.50
32	P	604	CLA	MG-NB	-2.07	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	5	303	CLA	CMD-C2D	-2.07	1.46	1.50
32	1	602	CLA	CMD-C2D	-2.06	1.46	1.50
32	1	604	CLA	CMD-C2D	-2.06	1.46	1.50
31	M	201	8CT	C33-C32	-2.06	1.44	1.50
31	B	622	8CT	C33-C32	-2.06	1.44	1.50
32	5	302	CLA	MG-NB	-2.06	2.01	2.05
32	P	608	CLA	MG-NB	-2.06	2.01	2.05
32	7	605	CLA	CMD-C2D	-2.06	1.46	1.50
37	g	101	LMG	O7-C8	-2.06	1.41	1.46
32	2	611	CLA	MG-NB	-2.06	2.01	2.05
32	p	306	CLA	MG-NB	-2.06	2.01	2.05
32	3	607	CLA	CMB-C2B	-2.06	1.46	1.50
32	p	302	CLA	CMD-C2D	-2.06	1.46	1.50
32	4	611	CLA	MG-NB	-2.06	2.01	2.05
32	0	606	CLA	CMB-C2B	-2.06	1.46	1.50
32	5	302	CLA	CMD-C2D	-2.06	1.46	1.50
32	C	513	CLA	CMB-C2B	-2.06	1.46	1.50
32	0	605	CLA	MG-NB	-2.06	2.01	2.05
32	b	614	CLA	CMC-C2C	-2.06	1.46	1.50
32	p	304	CLA	CMD-C2D	-2.06	1.46	1.50
39	a	409	SQD	O7-S	2.06	1.50	1.45
32	c	503	CLA	CMC-C2C	-2.06	1.46	1.50
32	C	509	CLA	CMC-C2C	-2.06	1.46	1.50
45	A	614	DGD	C2E-C1E	2.06	1.56	1.50
32	1	609	CLA	MG-NB	-2.06	2.01	2.05
32	1	609	CLA	CMB-C2B	-2.06	1.46	1.50
32	9	610	CLA	CMD-C2D	-2.06	1.46	1.50
32	2	609	CLA	CMB-C2B	-2.06	1.46	1.50
32	3	610	CLA	CMB-C2B	-2.06	1.46	1.50
32	c	510	CLA	CMC-C2C	-2.06	1.46	1.50
32	0	604	CLA	CMB-C2B	-2.06	1.46	1.50
32	9	608	CLA	CMB-C2B	-2.06	1.46	1.50
32	2	612	CLA	MG-NB	-2.06	2.01	2.05
32	9	606	CLA	MG-NB	-2.06	2.01	2.05
32	b	605	CLA	C3B-C4B	2.06	1.48	1.42
32	6	610	CLA	CMB-C2B	-2.06	1.46	1.50
32	5	308	CLA	MG-NB	-2.06	2.01	2.05
32	c	505	CLA	CMB-C2B	-2.06	1.46	1.50
32	c	511	CLA	CMC-C2C	-2.06	1.46	1.50
32	4	605	CLA	MG-NB	-2.06	2.01	2.05
32	2	612	CLA	CMB-C2B	-2.06	1.46	1.50
32	7	602	CLA	CMB-C2B	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	513	CLA	CMC-C2C	-2.06	1.46	1.50
32	A	602	CLA	CMB-C2B	-2.06	1.46	1.50
32	A	603	CLA	C3B-C4B	2.06	1.48	1.42
32	b	617	CLA	CHC-C1C	2.06	1.42	1.38
32	6	602	CLA	CMD-C2D	-2.06	1.46	1.50
32	4	601	CLA	MG-NB	-2.06	2.01	2.05
32	P	611	CLA	CMB-C2B	-2.06	1.46	1.50
32	d	409	CLA	CMC-C2C	-2.06	1.46	1.50
32	0	606	CLA	CMD-C2D	-2.06	1.46	1.50
32	2	607	CLA	CMB-C2B	-2.06	1.46	1.50
32	5	312	CLA	CMB-C2B	-2.06	1.46	1.50
32	6	603	CLA	CMD-C2D	-2.06	1.46	1.50
32	0	602	CLA	CMD-C2D	-2.06	1.46	1.50
32	1	603	CLA	CMD-C2D	-2.05	1.46	1.50
32	b	610	CLA	CMC-C2C	-2.05	1.46	1.50
32	0	601	CLA	CMD-C2D	-2.05	1.46	1.50
32	P	610	CLA	CMB-C2B	-2.05	1.46	1.50
32	p	304	CLA	CMB-C2B	-2.05	1.46	1.50
32	C	501	CLA	CMC-C2C	-2.05	1.46	1.50
32	4	601	CLA	CMD-C2D	-2.05	1.46	1.50
32	9	602	CLA	CMC-C2C	-2.05	1.46	1.50
32	B	615	CLA	CMC-C2C	-2.05	1.46	1.50
32	6	608	CLA	CMB-C2B	-2.05	1.46	1.50
32	c	501	CLA	CMB-C2B	-2.05	1.46	1.50
32	7	607	CLA	CMB-C2B	-2.05	1.46	1.50
32	P	604	CLA	CMD-C2D	-2.05	1.46	1.50
32	1	609	CLA	CMD-C2D	-2.05	1.46	1.50
32	2	602	CLA	CMB-C2B	-2.05	1.46	1.50
32	B	603	CLA	CMC-C2C	-2.05	1.46	1.50
32	2	603	CLA	CMB-C2B	-2.05	1.46	1.50
32	c	504	CLA	CMC-C2C	-2.05	1.46	1.50
32	C	502	CLA	CHC-C1C	2.05	1.42	1.38
32	3	611	CLA	CMD-C2D	-2.05	1.46	1.50
32	0	603	CLA	CMB-C2B	-2.05	1.46	1.50
32	0	605	CLA	CMD-C2D	-2.05	1.46	1.50
32	9	602	CLA	CMB-C2B	-2.05	1.46	1.50
32	9	611	CLA	CMD-C2D	-2.05	1.46	1.50
32	p	302	CLA	CMB-C2B	-2.05	1.46	1.50
32	0	611	CLA	CMD-C2D	-2.05	1.46	1.50
32	4	609	CLA	MG-NB	-2.05	2.01	2.05
32	0	609	CLA	MG-NB	-2.05	2.01	2.05
32	B	606	CLA	CMC-C2C	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	616	CLA	CMC-C2C	-2.05	1.46	1.50
32	0	608	CLA	CMD-C2D	-2.05	1.46	1.50
32	B	604	CLA	CHC-C1C	2.05	1.42	1.38
32	1	605	CLA	CMD-C2D	-2.05	1.46	1.50
32	A	602	CLA	CMC-C2C	-2.05	1.46	1.50
32	S	303	CLA	CMB-C2B	-2.05	1.46	1.50
32	b	613	CLA	CMB-C2B	-2.05	1.46	1.50
32	P	607	CLA	CMD-C2D	-2.05	1.46	1.50
32	B	604	CLA	CMC-C2C	-2.05	1.46	1.50
32	2	606	CLA	CMB-C2B	-2.05	1.46	1.50
32	4	602	CLA	CMB-C2B	-2.05	1.46	1.50
32	0	602	CLA	CMB-C2B	-2.05	1.46	1.50
32	2	608	CLA	CMC-C2C	-2.05	1.46	1.50
32	4	606	CLA	CMD-C2D	-2.05	1.46	1.50
32	c	507	CLA	CMC-C2C	-2.05	1.46	1.50
32	b	608	CLA	CMC-C2C	-2.05	1.46	1.50
32	B	608	CLA	CMC-C2C	-2.05	1.46	1.50
39	A	606	SQD	O7-S	2.05	1.50	1.45
32	5	306	CLA	MG-NB	-2.04	2.01	2.05
32	c	502	CLA	C3B-C4B	2.04	1.48	1.42
32	3	611	CLA	CMB-C2B	-2.04	1.46	1.50
32	4	612	CLA	CMB-C2B	-2.04	1.46	1.50
32	5	313	CLA	CMD-C2D	-2.04	1.46	1.50
32	6	606	CLA	CMD-C2D	-2.04	1.46	1.50
32	1	604	CLA	CMB-C2B	-2.04	1.46	1.50
32	8	611	CLA	CMD-C2D	-2.04	1.46	1.50
32	1	607	CLA	MG-NB	-2.04	2.01	2.05
47	V	201	HEM	CMB-C2B	2.04	1.55	1.50
32	1	606	CLA	CMB-C2B	-2.04	1.46	1.50
32	5	305	CLA	CMD-C2D	-2.04	1.46	1.50
32	0	605	CLA	CMB-C2B	-2.04	1.46	1.50
32	7	612	CLA	CMD-C2D	-2.04	1.46	1.50
32	8	601	CLA	CMB-C2B	-2.04	1.46	1.50
32	7	601	CLA	CMB-C2B	-2.04	1.46	1.50
32	C	504	CLA	CMC-C2C	-2.04	1.46	1.50
32	B	614	CLA	CMC-C2C	-2.04	1.46	1.50
37	8	617	LMG	O7-C8	-2.04	1.41	1.46
32	1	601	CLA	MG-NB	-2.04	2.01	2.05
32	5	307	CLA	CMD-C2D	-2.04	1.46	1.50
32	P	608	CLA	CMB-C2B	-2.04	1.46	1.50
32	p	310	CLA	MG-NB	-2.04	2.01	2.05
32	P	607	CLA	CMB-C2B	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	6	608	CLA	CMD-C2D	-2.04	1.46	1.50
32	6	608	CLA	MG-NB	-2.04	2.01	2.05
32	7	611	CLA	CMD-C2D	-2.04	1.46	1.50
32	1	607	CLA	CMB-C2B	-2.04	1.46	1.50
32	0	607	CLA	MG-NB	-2.04	2.01	2.05
32	B	605	CLA	CMC-C2C	-2.04	1.46	1.50
32	4	604	CLA	MG-NB	-2.04	2.01	2.05
32	p	312	CLA	MG-NB	-2.04	2.01	2.05
32	4	607	CLA	CMB-C2B	-2.04	1.46	1.50
32	0	612	CLA	CMB-C2B	-2.04	1.46	1.50
32	4	606	CLA	MG-NB	-2.04	2.01	2.05
32	4	601	CLA	CMB-C2B	-2.04	1.46	1.50
32	p	302	CLA	MG-NB	-2.04	2.01	2.05
32	1	601	CLA	CMB-C2B	-2.04	1.46	1.50
32	5	304	CLA	CMB-C2B	-2.04	1.46	1.50
32	9	604	CLA	CMC-C2C	-2.04	1.46	1.50
32	P	606	CLA	CMD-C2D	-2.04	1.46	1.50
32	P	608	CLA	CMD-C2D	-2.04	1.46	1.50
32	B	605	CLA	C3B-C4B	2.04	1.48	1.42
32	7	604	CLA	CMD-C2D	-2.04	1.46	1.50
32	9	606	CLA	CMC-C2C	-2.04	1.46	1.50
32	0	606	CLA	MG-NB	-2.04	2.01	2.05
32	9	605	CLA	CMB-C2B	-2.04	1.46	1.50
32	5	302	CLA	CMB-C2B	-2.04	1.46	1.50
32	9	607	CLA	CMC-C2C	-2.04	1.46	1.50
32	p	313	CLA	CMB-C2B	-2.04	1.46	1.50
37	L	102	LMG	O8-C9	-2.04	1.40	1.45
32	9	611	CLA	CMC-C2C	-2.04	1.46	1.50
32	B	610	CLA	CMC-C2C	-2.04	1.46	1.50
32	B	616	CLA	CHC-C1C	2.04	1.42	1.38
32	1	613	CLA	CMB-C2B	-2.04	1.46	1.50
32	A	605	CLA	CMC-C2C	-2.04	1.46	1.50
32	4	613	CLA	MG-NB	-2.04	2.01	2.05
32	2	612	CLA	CMD-C2D	-2.03	1.46	1.50
32	p	309	CLA	CMD-C2D	-2.03	1.46	1.50
32	6	604	CLA	MG-NB	-2.03	2.01	2.05
32	5	309	CLA	CMD-C2D	-2.03	1.46	1.50
32	9	611	CLA	CMB-C2B	-2.03	1.46	1.50
32	p	313	CLA	CMD-C2D	-2.03	1.46	1.50
32	0	601	CLA	MG-NB	-2.03	2.01	2.05
32	b	609	CLA	CMC-C2C	-2.03	1.46	1.50
32	8	608	CLA	CMC-C2C	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	602	CLA	CMC-C2C	-2.03	1.46	1.50
32	2	611	CLA	CMD-C2D	-2.03	1.46	1.50
32	4	605	CLA	CMB-C2B	-2.03	1.46	1.50
32	1	612	CLA	CMD-C2D	-2.03	1.46	1.50
32	b	603	CLA	CMC-C2C	-2.03	1.46	1.50
32	8	612	CLA	CMB-C2B	-2.03	1.46	1.50
32	4	607	CLA	MG-NB	-2.03	2.01	2.05
32	P	601	CLA	MG-NB	-2.03	2.01	2.05
32	4	603	CLA	CMB-C2B	-2.03	1.46	1.50
32	7	601	CLA	CMD-C2D	-2.03	1.46	1.50
32	7	609	CLA	CMB-C2B	-2.03	1.46	1.50
32	4	606	CLA	CMB-C2B	-2.03	1.46	1.50
32	b	606	CLA	CMC-C2C	-2.03	1.46	1.50
32	1	613	CLA	CMD-C2D	-2.03	1.46	1.50
32	4	609	CLA	CMD-C2D	-2.03	1.46	1.50
32	C	504	CLA	CMB-C2B	-2.03	1.46	1.50
32	a	408	CLA	CMC-C2C	-2.03	1.46	1.50
32	8	605	CLA	CMC-C2C	-2.03	1.46	1.50
32	7	612	CLA	MG-NB	-2.03	2.01	2.05
32	7	602	CLA	CMD-C2D	-2.03	1.46	1.50
33	1	610	KC2	C4A-C3A	-2.03	1.40	1.44
32	4	612	CLA	CMD-C2D	-2.03	1.46	1.50
32	5	308	CLA	CMC-C2C	-2.03	1.46	1.50
32	1	602	CLA	CMB-C2B	-2.03	1.46	1.50
32	3	605	CLA	CMB-C2B	-2.03	1.46	1.50
32	7	612	CLA	CMB-C2B	-2.03	1.46	1.50
32	0	613	CLA	CMB-C2B	-2.03	1.46	1.50
32	p	309	CLA	CMB-C2B	-2.03	1.46	1.50
32	4	608	CLA	CMB-C2B	-2.03	1.46	1.50
32	7	613	CLA	MG-NB	-2.03	2.01	2.05
32	2	602	CLA	CMC-C2C	-2.03	1.46	1.50
32	6	602	CLA	CMB-C2B	-2.03	1.46	1.50
32	c	501	CLA	CMC-C2C	-2.03	1.46	1.50
32	0	607	CLA	CMB-C2B	-2.03	1.46	1.50
32	8	603	CLA	CMB-C2B	-2.03	1.46	1.50
32	P	610	CLA	CMC-C2C	-2.03	1.46	1.50
32	8	604	CLA	CMB-C2B	-2.02	1.46	1.50
32	p	310	CLA	CMD-C2D	-2.02	1.46	1.50
37	l	101	LMG	O8-C9	-2.02	1.40	1.45
36	2	616	IHT	C02-C07	-2.02	1.51	1.53
47	v	201	HEM	CMD-C2D	2.02	1.54	1.50
32	1	608	CLA	CMB-C2B	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	p	308	CLA	CMC-C2C	-2.02	1.46	1.50
32	6	611	CLA	CMB-C2B	-2.02	1.46	1.50
32	0	601	CLA	CMB-C2B	-2.02	1.46	1.50
32	9	601	CLA	CMB-C2B	-2.02	1.46	1.50
32	1	603	CLA	CMB-C2B	-2.02	1.46	1.50
32	7	609	CLA	CMD-C2D	-2.02	1.46	1.50
32	0	612	CLA	CMD-C2D	-2.02	1.46	1.50
32	5	313	CLA	CMB-C2B	-2.02	1.46	1.50
32	8	609	CLA	CMB-C2B	-2.02	1.46	1.50
32	8	611	CLA	CMB-C2B	-2.02	1.46	1.50
32	1	612	CLA	CMB-C2B	-2.02	1.46	1.50
32	5	310	CLA	CMB-C2B	-2.02	1.46	1.50
32	4	611	CLA	CMD-C2D	-2.02	1.46	1.50
32	4	613	CLA	CMD-C2D	-2.02	1.46	1.50
32	7	604	CLA	CMB-C2B	-2.02	1.46	1.50
32	4	611	CLA	CMB-C2B	-2.02	1.46	1.50
32	5	308	CLA	CMB-C2B	-2.02	1.46	1.50
32	0	608	CLA	CMB-C2B	-2.02	1.46	1.50
32	7	611	CLA	CMB-C2B	-2.02	1.46	1.50
32	P	611	CLA	CMD-C2D	-2.02	1.46	1.50
32	0	613	CLA	MG-NB	-2.02	2.01	2.05
32	0	611	CLA	CMB-C2B	-2.02	1.46	1.50
32	7	611	CLA	MG-NB	-2.02	2.01	2.05
32	3	607	CLA	CMC-C2C	-2.02	1.46	1.50
32	7	601	CLA	MG-NB	-2.02	2.01	2.05
32	4	609	CLA	CMB-C2B	-2.02	1.46	1.50
32	s	302	CLA	CMD-C2D	-2.02	1.46	1.50
32	4	613	CLA	CMB-C2B	-2.02	1.46	1.50
32	6	607	CLA	CMB-C2B	-2.02	1.46	1.50
32	p	308	CLA	CMB-C2B	-2.02	1.46	1.50
32	2	606	CLA	MG-NB	-2.02	2.01	2.05
32	8	612	CLA	CMD-C2D	-2.01	1.46	1.50
32	D	404	CLA	CMC-C2C	-2.01	1.46	1.50
32	C	503	CLA	CMC-C2C	-2.01	1.46	1.50
33	2	610	KC2	C4A-C3A	-2.01	1.40	1.44
32	4	604	CLA	CMD-C2D	-2.01	1.46	1.50
32	P	602	CLA	CMB-C2B	-2.01	1.46	1.50
32	c	512	CLA	CMC-C2C	-2.01	1.46	1.50
33	8	610	KC2	C4A-C3A	-2.01	1.40	1.44
32	6	602	CLA	CMC-C2C	-2.01	1.46	1.50
32	c	504	CLA	CMB-C2B	-2.01	1.46	1.50
32	3	602	CLA	CMC-C2C	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	5	310	CLA	CMD-C2D	-2.01	1.46	1.50
32	3	606	CLA	MG-NB	-2.01	2.01	2.05
32	D	404	CLA	CMB-C2B	-2.01	1.46	1.50
32	d	403	CLA	CMB-C2B	-2.01	1.46	1.50
32	8	602	CLA	CMB-C2B	-2.01	1.46	1.50
32	p	305	CLA	CMD-C2D	-2.01	1.46	1.50
32	1	613	CLA	MG-NB	-2.01	2.01	2.05
32	1	611	CLA	CMD-C2D	-2.01	1.46	1.50
32	2	604	CLA	CMB-C2B	-2.01	1.46	1.50
32	D	401	CLA	CMC-C2C	-2.01	1.46	1.50
32	b	602	CLA	CMC-C2C	-2.01	1.46	1.50
32	C	507	CLA	CMC-C2C	-2.01	1.46	1.50
32	P	601	CLA	CMB-C2B	-2.01	1.46	1.50
41	A	604	PHO	C3B-C2B	-2.01	1.37	1.40
41	a	407	PHO	C3B-C2B	-2.01	1.37	1.40
32	3	606	CLA	CMC-C2C	-2.01	1.46	1.50
32	3	610	CLA	CMC-C2C	-2.01	1.46	1.50
32	5	303	CLA	CMC-C2C	-2.01	1.46	1.50
32	0	613	CLA	CMD-C2D	-2.01	1.46	1.50
32	B	611	CLA	CMC-C2C	-2.01	1.46	1.50
32	1	608	CLA	CMC-C2C	-2.01	1.46	1.50
32	7	613	CLA	CMD-C2D	-2.01	1.46	1.50
38	b	621	LHG	O7-C5	-2.01	1.41	1.46
38	B	621	LHG	O7-C5	-2.01	1.41	1.46
32	1	601	CLA	CMD-C2D	-2.00	1.46	1.50
32	6	611	CLA	CMD-C2D	-2.00	1.46	1.50
32	9	609	CLA	CMC-C2C	-2.00	1.46	1.50
32	8	606	CLA	MG-NB	-2.00	2.01	2.05
32	4	608	CLA	CMD-C2D	-2.00	1.46	1.50
32	6	601	CLA	CMB-C2B	-2.00	1.46	1.50
32	0	609	CLA	CMD-C2D	-2.00	1.46	1.50
32	5	309	CLA	CMB-C2B	-2.00	1.46	1.50
32	0	609	CLA	CMB-C2B	-2.00	1.46	1.50
32	9	605	CLA	CMC-C2C	-2.00	1.46	1.50
32	P	607	CLA	CMC-C2C	-2.00	1.46	1.50
32	3	603	CLA	CMC-C2C	-2.00	1.46	1.50
32	p	313	CLA	MG-NB	-2.00	2.01	2.05
45	a	414	DGD	O5D-C6D	-2.00	1.40	1.43
32	0	612	CLA	MG-NB	-2.00	2.01	2.05
32	3	611	CLA	CMC-C2C	-2.00	1.46	1.50
32	d	403	CLA	CMC-C2C	-2.00	1.46	1.50
39	5	318	SQD	C8-C7	2.00	1.56	1.50

All (2683) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	k	102	8CT	C33-C32-C31	-11.08	114.25	124.83
31	B	622	8CT	C33-C32-C31	-11.06	114.27	124.83
31	M	201	8CT	C33-C32-C31	-11.05	114.28	124.83
31	a	413	8CT	C33-C32-C31	-11.03	114.30	124.83
31	K	101	8CT	C33-C32-C31	-11.01	114.32	124.83
31	B	624	8CT	C33-C32-C31	-11.00	114.33	124.83
31	b	623	8CT	C33-C32-C31	-10.99	114.34	124.83
31	A	610	8CT	C33-C32-C31	-10.30	115.00	124.83
31	z	101	8CT	C33-C32-C31	-10.28	115.02	124.83
31	C	518	8CT	C33-C32-C31	-10.19	115.11	124.83
31	c	518	8CT	C33-C32-C31	-10.13	115.16	124.83
31	h	102	8CT	C33-C32-C31	-9.94	115.34	124.83
31	Z	101	8CT	C33-C32-C31	-9.90	115.38	124.83
31	H	102	8CT	C33-C32-C31	-9.81	115.47	124.83
31	k	101	8CT	C33-C32-C31	-9.38	115.88	124.83
31	K	102	8CT	C33-C32-C31	-9.37	115.88	124.83
31	B	623	8CT	C33-C32-C31	-8.88	116.36	124.83
31	b	622	8CT	C33-C32-C31	-8.86	116.37	124.83
31	P	615	8CT	C33-C32-C31	-8.27	116.93	124.83
31	9	615	8CT	C33-C32-C31	-8.24	116.97	124.83
31	3	615	8CT	C33-C32-C31	-8.21	117.00	124.83
31	d	408	8CT	C33-C32-C31	-8.18	117.02	124.83
31	D	409	8CT	C33-C32-C31	-8.14	117.06	124.83
31	6	615	8CT	C33-C32-C31	-8.00	117.20	124.83
31	a	413	8CT	C30-C29-C28	-7.80	112.44	124.58
31	a	413	8CT	C30-C31-C32	-7.28	112.51	121.47
31	c	518	8CT	C30-C31-C32	-7.26	112.54	121.47
31	C	518	8CT	C30-C31-C32	-7.20	112.61	121.47
32	b	605	CLA	C4A-NA-C1A	7.16	109.95	106.68
31	a	413	8CT	C14-C13-C12	-7.16	117.24	127.28
31	3	615	8CT	C04-C03-C02	-7.06	113.00	122.64
32	B	605	CLA	C4A-NA-C1A	7.05	109.89	106.68
31	9	615	8CT	C04-C03-C02	-7.03	113.03	122.64
32	C	503	CLA	C4A-NA-C1A	7.00	109.87	106.68
31	M	201	8CT	C30-C31-C32	-7.00	112.86	121.47
32	c	503	CLA	C4A-NA-C1A	6.99	109.87	106.68
31	B	622	8CT	C30-C31-C32	-6.97	112.89	121.47
32	C	502	CLA	C4A-NA-C1A	6.94	109.84	106.68
32	c	502	CLA	C4A-NA-C1A	6.92	109.84	106.68
32	b	613	CLA	C4A-NA-C1A	6.90	109.83	106.68
32	7	611	CLA	C4A-NA-C1A	6.86	109.81	106.68
32	b	617	CLA	C4A-NA-C1A	6.84	109.80	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	B	613	CLA	C4A-NA-C1A	6.84	109.80	106.68
32	B	617	CLA	C4A-NA-C1A	6.82	109.79	106.68
32	5	306	CLA	C4A-NA-C1A	6.79	109.78	106.68
32	C	511	CLA	C4A-NA-C1A	6.79	109.78	106.68
32	1	604	CLA	C4A-NA-C1A	6.78	109.77	106.68
32	D	401	CLA	C4A-NA-C1A	6.78	109.77	106.68
32	7	604	CLA	C4A-NA-C1A	6.78	109.77	106.68
32	4	612	CLA	C4A-NA-C1A	6.78	109.77	106.68
32	b	606	CLA	C4A-NA-C1A	6.78	109.77	106.68
32	c	513	CLA	C4A-NA-C1A	6.76	109.76	106.68
31	9	615	8CT	C18-C17-C16	-6.76	117.80	127.28
32	c	507	CLA	C4A-NA-C1A	6.74	109.75	106.68
32	P	611	CLA	C4A-NA-C1A	6.74	109.75	106.68
32	B	606	CLA	C4A-NA-C1A	6.74	109.75	106.68
32	0	612	CLA	C4A-NA-C1A	6.73	109.75	106.68
32	1	611	CLA	C4A-NA-C1A	6.73	109.75	106.68
32	c	501	CLA	C4A-NA-C1A	6.73	109.75	106.68
32	C	513	CLA	C4A-NA-C1A	6.73	109.75	106.68
32	7	613	CLA	C4A-NA-C1A	6.72	109.75	106.68
32	c	511	CLA	C4A-NA-C1A	6.72	109.74	106.68
31	3	615	8CT	C18-C17-C16	-6.71	117.86	127.28
32	9	607	CLA	C4A-NA-C1A	6.71	109.74	106.68
32	9	610	CLA	C4A-NA-C1A	6.70	109.74	106.68
32	D	404	CLA	C4A-NA-C1A	6.70	109.73	106.68
32	C	507	CLA	C4A-NA-C1A	6.70	109.73	106.68
32	c	512	CLA	C4A-NA-C1A	6.69	109.73	106.68
32	C	509	CLA	C4A-NA-C1A	6.68	109.73	106.68
32	2	604	CLA	C4A-NA-C1A	6.67	109.72	106.68
32	9	601	CLA	C4A-NA-C1A	6.67	109.72	106.68
32	c	509	CLA	C4A-NA-C1A	6.67	109.72	106.68
32	p	312	CLA	C4A-NA-C1A	6.66	109.72	106.68
32	5	312	CLA	C4A-NA-C1A	6.66	109.72	106.68
32	6	611	CLA	C4A-NA-C1A	6.66	109.72	106.68
32	2	611	CLA	C4A-NA-C1A	6.65	109.72	106.68
32	8	611	CLA	C4A-NA-C1A	6.65	109.72	106.68
32	d	403	CLA	C4A-NA-C1A	6.65	109.71	106.68
32	C	501	CLA	C4A-NA-C1A	6.65	109.71	106.68
32	6	610	CLA	C4A-NA-C1A	6.64	109.71	106.68
32	8	604	CLA	C4A-NA-C1A	6.64	109.71	106.68
32	P	610	CLA	C4A-NA-C1A	6.64	109.71	106.68
32	B	608	CLA	C4A-NA-C1A	6.64	109.71	106.68
32	B	616	CLA	C4A-NA-C1A	6.63	109.71	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	C	512	CLA	C4A-NA-C1A	6.63	109.70	106.68
32	p	306	CLA	C4A-NA-C1A	6.63	109.70	106.68
32	c	508	CLA	C4A-NA-C1A	6.62	109.70	106.68
32	C	508	CLA	C4A-NA-C1A	6.61	109.69	106.68
32	b	607	CLA	C4A-NA-C1A	6.61	109.69	106.68
32	2	605	CLA	C4A-NA-C1A	6.60	109.69	106.68
32	b	608	CLA	C4A-NA-C1A	6.60	109.69	106.68
32	P	607	CLA	C4A-NA-C1A	6.60	109.69	106.68
32	5	305	CLA	C4A-NA-C1A	6.59	109.69	106.68
32	b	616	CLA	C4A-NA-C1A	6.59	109.68	106.68
32	3	610	CLA	C4A-NA-C1A	6.58	109.68	106.68
32	2	608	CLA	C4A-NA-C1A	6.57	109.68	106.68
32	3	607	CLA	C4A-NA-C1A	6.57	109.67	106.68
32	d	409	CLA	C4A-NA-C1A	6.56	109.67	106.68
32	p	305	CLA	C4A-NA-C1A	6.56	109.67	106.68
32	7	606	CLA	C4A-NA-C1A	6.55	109.67	106.68
32	P	603	CLA	C4A-NA-C1A	6.55	109.67	106.68
32	a	405	CLA	C4A-NA-C1A	6.55	109.67	106.68
32	3	601	CLA	C4A-NA-C1A	6.55	109.67	106.68
32	3	608	CLA	C4A-NA-C1A	6.55	109.67	106.68
32	B	607	CLA	C4A-NA-C1A	6.54	109.66	106.68
32	C	505	CLA	C4A-NA-C1A	6.54	109.66	106.68
32	4	611	CLA	C4A-NA-C1A	6.54	109.66	106.68
32	6	607	CLA	C4A-NA-C1A	6.54	109.66	106.68
32	2	603	CLA	C4A-NA-C1A	6.53	109.66	106.68
32	A	602	CLA	C4A-NA-C1A	6.53	109.66	106.68
32	8	608	CLA	C4A-NA-C1A	6.53	109.66	106.68
32	4	605	CLA	C4A-NA-C1A	6.53	109.66	106.68
32	6	604	CLA	C4A-NA-C1A	6.52	109.66	106.68
32	5	309	CLA	C4A-NA-C1A	6.52	109.65	106.68
32	1	613	CLA	C4A-NA-C1A	6.52	109.65	106.68
32	9	608	CLA	C4A-NA-C1A	6.51	109.65	106.68
32	B	610	CLA	C4A-NA-C1A	6.51	109.65	106.68
41	D	402	PHO	C4D-CHA-CBD	-6.50	105.33	108.45
32	c	506	CLA	C4A-NA-C1A	6.49	109.64	106.68
32	c	505	CLA	C4A-NA-C1A	6.49	109.64	106.68
32	3	603	CLA	C4A-NA-C1A	6.48	109.64	106.68
31	M	201	8CT	C14-C13-C12	-6.48	118.19	127.28
32	b	610	CLA	C4A-NA-C1A	6.47	109.63	106.68
32	0	611	CLA	C4A-NA-C1A	6.47	109.63	106.68
41	d	410	PHO	C4D-CHA-CBD	-6.47	105.35	108.45
32	8	603	CLA	C4A-NA-C1A	6.46	109.63	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	C	504	CLA	C4A-NA-C1A	6.46	109.63	106.68
32	s	303	CLA	C4A-NA-C1A	6.46	109.62	106.68
32	3	611	CLA	C4A-NA-C1A	6.46	109.62	106.68
32	b	604	CLA	C4A-NA-C1A	6.45	109.62	106.68
32	G	101	CLA	C4A-NA-C1A	6.45	109.62	106.68
32	S	303	CLA	C4A-NA-C1A	6.45	109.62	106.68
32	0	602	CLA	C4A-NA-C1A	6.45	109.62	106.68
32	0	605	CLA	C4A-NA-C1A	6.45	109.62	106.68
31	B	622	8CT	C14-C13-C12	-6.44	118.24	127.28
32	b	612	CLA	C4A-NA-C1A	6.44	109.62	106.68
32	c	504	CLA	C4A-NA-C1A	6.44	109.62	106.68
32	4	602	CLA	C4A-NA-C1A	6.44	109.62	106.68
32	p	309	CLA	C4A-NA-C1A	6.44	109.62	106.68
32	9	611	CLA	C4A-NA-C1A	6.43	109.61	106.68
32	5	304	CLA	C4A-NA-C1A	6.43	109.61	106.68
32	4	609	CLA	C4A-NA-C1A	6.43	109.61	106.68
32	7	609	CLA	C4A-NA-C1A	6.42	109.61	106.68
32	9	604	CLA	C4A-NA-C1A	6.42	109.61	106.68
32	p	302	CLA	C4A-NA-C1A	6.42	109.61	106.68
32	6	601	CLA	C4A-NA-C1A	6.42	109.61	106.68
32	1	606	CLA	C4A-NA-C1A	6.41	109.61	106.68
32	9	605	CLA	C4A-NA-C1A	6.41	109.61	106.68
32	5	302	CLA	C4A-NA-C1A	6.41	109.60	106.68
32	5	313	CLA	C4A-NA-C1A	6.41	109.60	106.68
32	8	612	CLA	C4A-NA-C1A	6.41	109.60	106.68
32	C	506	CLA	C4A-NA-C1A	6.41	109.60	106.68
32	9	603	CLA	C4A-NA-C1A	6.41	109.60	106.68
32	B	612	CLA	C4A-NA-C1A	6.41	109.60	106.68
32	4	604	CLA	C4A-NA-C1A	6.41	109.60	106.68
32	c	510	CLA	C4A-NA-C1A	6.41	109.60	106.68
32	0	601	CLA	C4A-NA-C1A	6.41	109.60	106.68
32	B	615	CLA	C4A-NA-C1A	6.40	109.60	106.68
32	6	608	CLA	C4A-NA-C1A	6.40	109.60	106.68
32	b	615	CLA	C4A-NA-C1A	6.39	109.60	106.68
32	7	602	CLA	C4A-NA-C1A	6.39	109.59	106.68
32	5	310	CLA	C4A-NA-C1A	6.39	109.59	106.68
32	0	609	CLA	C4A-NA-C1A	6.39	109.59	106.68
32	3	604	CLA	C4A-NA-C1A	6.38	109.59	106.68
32	P	604	CLA	C4A-NA-C1A	6.38	109.59	106.68
32	p	313	CLA	C4A-NA-C1A	6.38	109.59	106.68
32	B	602	CLA	C4A-NA-C1A	6.38	109.59	106.68
32	8	605	CLA	C4A-NA-C1A	6.38	109.59	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	P	601	CLA	C4A-NA-C1A	6.37	109.59	106.68
32	7	612	CLA	C4A-NA-C1A	6.37	109.59	106.68
32	8	609	CLA	C4A-NA-C1A	6.37	109.58	106.68
32	7	603	CLA	C4A-NA-C1A	6.36	109.58	106.68
32	9	609	CLA	C4A-NA-C1A	6.36	109.58	106.68
32	p	310	CLA	C4A-NA-C1A	6.36	109.58	106.68
32	4	608	CLA	C4A-NA-C1A	6.35	109.58	106.68
32	C	510	CLA	C4A-NA-C1A	6.35	109.58	106.68
32	2	612	CLA	C4A-NA-C1A	6.35	109.57	106.68
32	0	608	CLA	C4A-NA-C1A	6.35	109.57	106.68
32	B	604	CLA	C4A-NA-C1A	6.34	109.57	106.68
32	6	603	CLA	C4A-NA-C1A	6.34	109.57	106.68
32	b	614	CLA	C4A-NA-C1A	6.33	109.57	106.68
32	4	601	CLA	C4A-NA-C1A	6.33	109.57	106.68
32	3	609	CLA	C4A-NA-C1A	6.33	109.57	106.68
32	7	601	CLA	C4A-NA-C1A	6.32	109.56	106.68
32	1	602	CLA	C4A-NA-C1A	6.32	109.56	106.68
32	g	102	CLA	C4A-NA-C1A	6.32	109.56	106.68
32	a	408	CLA	C4A-NA-C1A	6.32	109.56	106.68
32	b	609	CLA	C4A-NA-C1A	6.31	109.56	106.68
32	0	604	CLA	C4A-NA-C1A	6.31	109.56	106.68
32	4	613	CLA	C4A-NA-C1A	6.31	109.56	106.68
32	5	303	CLA	C4A-NA-C1A	6.31	109.56	106.68
32	5	307	CLA	C4A-NA-C1A	6.31	109.56	106.68
32	P	608	CLA	C4A-NA-C1A	6.31	109.56	106.68
32	3	605	CLA	C4A-NA-C1A	6.30	109.56	106.68
32	8	601	CLA	C4A-NA-C1A	6.30	109.55	106.68
32	p	303	CLA	C4A-NA-C1A	6.30	109.55	106.68
32	7	605	CLA	C4A-NA-C1A	6.30	109.55	106.68
32	2	601	CLA	C4A-NA-C1A	6.29	109.55	106.68
32	3	602	CLA	C4A-NA-C1A	6.29	109.55	106.68
32	p	307	CLA	C4A-NA-C1A	6.29	109.55	106.68
32	1	609	CLA	C4A-NA-C1A	6.29	109.55	106.68
31	K	101	8CT	C30-C31-C32	-6.28	113.74	121.47
32	1	601	CLA	C4A-NA-C1A	6.28	109.55	106.68
32	2	606	CLA	C4A-NA-C1A	6.28	109.55	106.68
32	1	612	CLA	C4A-NA-C1A	6.28	109.54	106.68
32	1	605	CLA	C4A-NA-C1A	6.27	109.54	106.68
32	b	602	CLA	C4A-NA-C1A	6.27	109.54	106.68
32	8	602	CLA	C4A-NA-C1A	6.26	109.54	106.68
32	8	607	CLA	C4A-NA-C1A	6.26	109.54	106.68
32	2	609	CLA	C4A-NA-C1A	6.26	109.54	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	603	CLA	C4A-NA-C1A	6.26	109.53	106.68
32	B	603	CLA	C4A-NA-C1A	6.26	109.53	106.68
32	B	614	CLA	C4A-NA-C1A	6.26	109.53	106.68
32	0	613	CLA	C4A-NA-C1A	6.25	109.53	106.68
32	s	302	CLA	C4A-NA-C1A	6.25	109.53	106.68
32	5	308	CLA	C4A-NA-C1A	6.24	109.53	106.68
32	1	603	CLA	C4A-NA-C1A	6.23	109.52	106.68
32	1	608	CLA	C4A-NA-C1A	6.23	109.52	106.68
32	2	602	CLA	C4A-NA-C1A	6.22	109.52	106.68
32	p	304	CLA	C4A-NA-C1A	6.22	109.52	106.68
32	0	603	CLA	C4A-NA-C1A	6.21	109.51	106.68
32	8	606	CLA	C4A-NA-C1A	6.21	109.51	106.68
32	P	602	CLA	C4A-NA-C1A	6.21	109.51	106.68
32	d	402	CLA	C4A-NA-C1A	6.21	109.51	106.68
31	H	102	8CT	C10-C11-C12	-6.21	117.05	126.23
32	S	302	CLA	C4A-NA-C1A	6.20	109.51	106.68
32	p	308	CLA	C4A-NA-C1A	6.20	109.51	106.68
32	B	609	CLA	C4A-NA-C1A	6.19	109.50	106.68
31	h	102	8CT	C10-C11-C12	-6.19	117.08	126.23
32	7	608	CLA	C4A-NA-C1A	6.19	109.50	106.68
32	9	602	CLA	C4A-NA-C1A	6.19	109.50	106.68
32	B	611	CLA	C4A-NA-C1A	6.17	109.49	106.68
32	b	611	CLA	C4A-NA-C1A	6.17	109.49	106.68
32	6	602	CLA	C4A-NA-C1A	6.17	109.49	106.68
32	a	406	CLA	C4A-NA-C1A	6.16	109.49	106.68
32	A	605	CLA	C4A-NA-C1A	6.15	109.48	106.68
32	9	606	CLA	C4A-NA-C1A	6.15	109.48	106.68
31	k	102	8CT	C30-C31-C32	-6.14	113.91	121.47
32	4	603	CLA	C4A-NA-C1A	6.14	109.48	106.68
32	4	607	CLA	C4A-NA-C1A	6.12	109.47	106.68
32	1	607	CLA	C4A-NA-C1A	6.12	109.47	106.68
32	D	403	CLA	C4A-NA-C1A	6.11	109.47	106.68
31	P	615	8CT	C14-C13-C12	-6.11	118.71	127.28
31	c	518	8CT	C04-C03-C02	-6.11	114.29	122.64
31	d	408	8CT	C24-C25-C26	-6.11	118.72	127.28
31	C	518	8CT	C04-C03-C02	-6.10	114.30	122.64
32	2	607	CLA	C4A-NA-C1A	6.10	109.46	106.68
32	A	603	CLA	C4A-NA-C1A	6.10	109.46	106.68
31	D	409	8CT	C24-C25-C26	-6.08	118.75	127.28
32	0	606	CLA	C4A-NA-C1A	6.06	109.45	106.68
31	6	615	8CT	C14-C13-C12	-6.06	118.78	127.28
32	6	606	CLA	C4A-NA-C1A	6.01	109.42	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	7	607	CLA	C4A-NA-C1A	6.00	109.42	106.68
32	4	606	CLA	C4A-NA-C1A	5.97	109.40	106.68
32	P	606	CLA	C4A-NA-C1A	5.97	109.40	106.68
31	k	102	8CT	C10-C11-C12	-5.96	117.42	126.23
32	0	607	CLA	C4A-NA-C1A	5.96	109.40	106.68
32	3	606	CLA	C4A-NA-C1A	5.95	109.39	106.68
31	K	101	8CT	C10-C11-C12	-5.88	117.54	126.23
41	A	604	PHO	C4D-CHA-CBD	-5.87	105.64	108.45
31	A	610	8CT	C30-C29-C28	-5.87	115.45	124.58
31	A	610	8CT	C07-C02-C03	-5.85	114.81	122.70
31	H	102	8CT	C19-C20-C21	-5.79	119.16	127.28
31	h	102	8CT	C19-C20-C21	-5.75	119.21	127.28
31	b	623	8CT	C14-C13-C12	-5.73	119.24	127.28
41	a	407	PHO	C4D-CHA-CBD	-5.73	105.71	108.45
31	6	615	8CT	C18-C17-C16	-5.70	119.29	127.28
31	B	624	8CT	C14-C13-C12	-5.68	119.31	127.28
31	P	615	8CT	C18-C17-C16	-5.68	119.31	127.28
34	p	314	II0	C41-C39-C35	-5.64	119.38	127.28
44	A	611	BCT	O2-C-O1	5.62	134.06	119.68
31	9	615	8CT	C07-C02-C03	-5.60	115.14	122.70
44	a	401	BCT	O2-C-O1	5.60	133.99	119.68
31	3	615	8CT	C07-C02-C03	-5.59	115.16	122.70
31	b	622	8CT	C01-C02-C03	-5.56	118.41	124.48
34	6	612	II0	C41-C39-C35	-5.56	119.48	127.28
31	B	623	8CT	C01-C02-C03	-5.53	118.45	124.48
31	h	102	8CT	C30-C31-C32	-5.52	114.68	121.47
36	4	617	IHT	C41-C38-C35	-5.50	119.56	127.28
36	4	617	IHT	C40-C37-C33	-5.48	119.59	127.28
31	H	102	8CT	C14-C13-C12	-5.44	119.65	127.28
36	2	616	IHT	C41-C38-C35	-5.43	119.66	127.28
31	h	102	8CT	C14-C13-C12	-5.42	119.67	127.28
34	5	314	II0	C41-C39-C35	-5.42	119.67	127.28
31	K	102	8CT	C14-C13-C12	-5.42	119.68	127.28
31	H	102	8CT	C30-C31-C32	-5.39	114.83	121.47
31	h	102	8CT	C01-C02-C03	-5.38	118.62	124.48
31	H	102	8CT	C01-C02-C03	-5.36	118.63	124.48
34	P	612	II0	C41-C39-C35	-5.36	119.76	127.28
36	p	317	IHT	C41-C38-C35	-5.32	119.82	127.28
31	B	623	8CT	C19-C20-C21	-5.31	119.83	127.28
34	3	613	II0	C42-C40-C36	-5.31	119.83	127.28
31	b	622	8CT	C19-C20-C21	-5.28	119.87	127.28
36	8	616	IHT	C41-C38-C35	-5.27	119.89	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	M	201	8CT	C18-C17-C16	-5.27	119.89	127.28
31	c	518	8CT	C14-C13-C12	-5.26	119.91	127.28
31	B	622	8CT	C18-C17-C16	-5.25	119.91	127.28
31	C	518	8CT	C14-C13-C12	-5.23	119.94	127.28
34	4	615	II0	C42-C40-C36	-5.22	119.96	127.28
36	0	618	IHT	C41-C38-C35	-5.20	119.98	127.28
31	k	101	8CT	C14-C13-C12	-5.17	120.03	127.28
34	9	613	II0	C42-C40-C36	-5.16	120.04	127.28
31	K	101	8CT	C18-C17-C16	-5.16	120.04	127.28
31	a	413	8CT	C18-C17-C16	-5.16	120.04	127.28
36	5	317	IHT	C41-C38-C35	-5.16	120.04	127.28
34	0	615	II0	C42-C40-C36	-5.16	120.05	127.28
33	p	311	KC2	O2D-CGD-CBD	5.15	120.24	111.23
36	0	618	IHT	C40-C37-C33	-5.15	120.06	127.28
33	5	311	KC2	O2D-CGD-CBD	5.14	120.22	111.23
31	k	102	8CT	C18-C17-C16	-5.14	120.07	127.28
31	k	101	8CT	C01-C02-C03	-5.12	118.89	124.48
31	d	408	8CT	C18-C17-C16	-5.12	120.10	127.28
31	K	102	8CT	C01-C02-C03	-5.11	118.91	124.48
31	D	409	8CT	C18-C17-C16	-5.08	120.15	127.28
34	p	316	II0	C42-C40-C36	-5.07	120.17	127.28
33	6	605	KC2	O2D-CGD-CBD	5.06	120.08	111.23
35	6	613	II3	C39-C36-C33	-5.04	120.21	127.28
34	2	614	II0	C42-C40-C36	-5.04	120.21	127.28
36	0	614	IHT	C41-C38-C35	-5.04	120.22	127.28
35	P	613	II3	C39-C36-C33	-5.02	120.24	127.28
31	k	101	8CT	C30-C29-C28	-5.01	116.78	124.58
31	a	413	8CT	C19-C20-C21	-4.99	120.27	127.28
31	K	102	8CT	C30-C29-C28	-4.99	116.81	124.58
31	6	615	8CT	C04-C03-C02	-4.98	115.83	122.64
36	7	618	IHT	C41-C38-C35	-4.98	120.30	127.28
34	8	615	II0	C42-C40-C36	-4.97	120.31	127.28
36	4	614	IHT	C41-C38-C35	-4.97	120.31	127.28
34	2	615	II0	C42-C40-C36	-4.96	120.32	127.28
31	B	622	8CT	C24-C25-C26	-4.95	120.33	127.28
31	3	615	8CT	C01-C02-C03	-4.95	119.08	124.48
43	D	405	PL9	C7-C3-C4	4.95	120.99	116.91
34	8	614	II0	C42-C40-C36	-4.95	120.34	127.28
43	d	404	PL9	C7-C3-C4	4.95	120.98	116.91
34	0	616	II0	C41-C39-C35	-4.94	120.35	127.28
36	1	618	IHT	C18-C22-C23	-4.93	118.94	126.23
31	9	615	8CT	C01-C02-C03	-4.93	119.11	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	M	201	8CT	C24-C25-C26	-4.92	120.38	127.28
31	3	615	8CT	C14-C13-C12	-4.91	120.39	127.28
31	P	615	8CT	C04-C03-C02	-4.91	115.92	122.64
31	9	615	8CT	C14-C13-C12	-4.90	120.41	127.28
36	1	618	IHT	C30-C27-C23	-4.89	120.42	127.28
31	B	624	8CT	C18-C17-C16	-4.87	120.45	127.28
34	4	616	II0	C41-C39-C35	-4.87	120.45	127.28
31	D	409	8CT	C10-C11-C12	-4.86	119.04	126.23
31	b	623	8CT	C18-C17-C16	-4.86	120.46	127.28
31	K	102	8CT	C18-C17-C16	-4.85	120.47	127.28
31	M	201	8CT	C01-C02-C03	-4.85	119.19	124.48
31	9	615	8CT	C24-C25-C26	-4.85	120.48	127.28
31	6	615	8CT	C07-C02-C03	-4.85	116.16	122.70
31	B	622	8CT	C01-C02-C03	-4.84	119.20	124.48
31	P	615	8CT	C07-C02-C03	-4.84	116.17	122.70
34	7	614	II0	C41-C39-C35	-4.82	120.52	127.28
31	3	615	8CT	C24-C25-C26	-4.81	120.53	127.28
31	d	408	8CT	C10-C11-C12	-4.81	119.12	126.23
31	z	101	8CT	C30-C31-C32	-4.81	115.55	121.47
31	k	101	8CT	C18-C17-C16	-4.81	120.54	127.28
33	P	605	KC2	O2D-CGD-CBD	4.81	119.63	111.23
34	5	316	II0	C42-C40-C36	-4.81	120.54	127.28
31	c	518	8CT	C07-C02-C03	-4.80	116.22	122.70
34	1	617	II0	C42-C40-C36	-4.80	120.55	127.28
34	0	617	II0	C42-C40-C36	-4.79	120.57	127.28
31	C	518	8CT	C07-C02-C03	-4.78	116.25	122.70
34	7	617	II0	C42-C40-C36	-4.75	120.62	127.28
31	b	623	8CT	C01-C02-C03	-4.74	119.31	124.48
33	7	610	KC2	O2D-CGD-CBD	4.74	119.51	111.23
34	5	319	II0	C41-C39-C35	-4.74	120.64	127.28
31	M	201	8CT	C10-C11-C12	-4.73	119.24	126.23
33	4	610	KC2	O2D-CGD-CBD	4.71	119.47	111.23
33	1	610	KC2	O2D-CGD-CBD	4.71	119.47	111.23
31	B	624	8CT	C01-C02-C03	-4.71	119.34	124.48
36	7	618	IHT	C18-C22-C23	-4.71	119.27	126.23
31	d	408	8CT	C29-C28-C26	-4.71	116.20	126.32
33	0	610	KC2	O2D-CGD-CBD	4.71	119.46	111.23
31	D	409	8CT	C29-C28-C26	-4.69	116.23	126.32
34	1	614	II0	C41-C39-C35	-4.69	120.70	127.28
36	7	618	IHT	C30-C27-C23	-4.69	120.70	127.28
31	B	622	8CT	C10-C11-C12	-4.66	119.33	126.23
31	A	610	8CT	C04-C03-C02	-4.65	116.28	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	624	8CT	C30-C31-C32	-4.65	115.75	121.47
31	c	518	8CT	C29-C28-C26	-4.64	116.34	126.32
31	b	623	8CT	C30-C31-C32	-4.64	115.76	121.47
34	5	301	II0	C42-C40-C36	-4.63	120.78	127.28
36	1	618	IHT	C41-C38-C35	-4.63	120.78	127.28
34	p	315	II0	C41-C39-C35	-4.63	120.79	127.28
34	5	315	II0	C41-C39-C35	-4.62	120.80	127.28
31	C	518	8CT	C29-C28-C26	-4.61	116.41	126.32
31	B	624	8CT	C24-C25-C26	-4.61	120.81	127.28
34	7	616	II0	C42-C40-C36	-4.58	120.85	127.28
31	b	623	8CT	C24-C25-C26	-4.58	120.85	127.28
34	1	616	II0	C42-C40-C36	-4.56	120.89	127.28
31	B	624	8CT	C19-C20-C21	-4.55	120.89	127.28
31	b	623	8CT	C19-C20-C21	-4.55	120.89	127.28
39	b	601	SQD	O47-C7-C8	4.55	121.31	111.48
36	0	618	IHT	C19-C10-C07	-4.54	119.53	124.48
31	A	610	8CT	C18-C17-C16	-4.53	120.92	127.28
39	B	601	SQD	O47-C7-C8	4.53	121.29	111.48
33	6	609	KC2	O2D-CGD-CBD	4.53	119.15	111.23
33	0	610	KC2	CHB-C1B-NB	4.53	131.18	124.80
33	p	311	KC2	CHB-C1B-NB	4.52	131.16	124.80
33	4	610	KC2	CHB-C1B-NB	4.51	131.15	124.80
36	2	616	IHT	C18-C22-C23	-4.50	119.58	126.23
33	P	609	KC2	O2D-CGD-CBD	4.50	119.09	111.23
33	7	610	KC2	CHB-C1B-NB	4.49	131.13	124.80
36	2	616	IHT	C19-C10-C07	-4.49	119.58	124.48
33	5	311	KC2	CHB-C1B-NB	4.49	131.12	124.80
45	C	514	DGD	O3G-C3G-C2G	-4.48	99.93	110.82
45	c	514	DGD	O3G-C3G-C2G	-4.47	99.95	110.82
34	p	301	II0	C41-C39-C35	-4.46	121.02	127.28
33	1	610	KC2	CHB-C1B-NB	4.46	131.08	124.80
36	4	617	IHT	C19-C10-C07	-4.46	119.62	124.48
36	2	616	IHT	C30-C27-C23	-4.45	121.03	127.28
31	M	201	8CT	C07-C02-C03	-4.45	116.69	122.70
33	P	609	KC2	CHB-C1B-NB	4.45	131.06	124.80
33	6	609	KC2	CHB-C1B-NB	4.45	131.06	124.80
36	8	616	IHT	C19-C10-C07	-4.44	119.63	124.48
38	B	619	LHG	O4-P-O5	4.44	133.10	112.44
31	k	101	8CT	C19-C18-C17	-4.44	114.43	123.52
38	L	101	LHG	O4-P-O5	4.44	133.10	112.44
38	l	102	LHG	O4-P-O5	4.44	133.09	112.44
33	8	610	KC2	CHB-C1B-NB	4.44	131.05	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	6	614	II0	C42-C40-C36	-4.44	121.06	127.28
33	2	610	KC2	CHB-C1B-NB	4.43	131.04	124.80
36	8	616	IHT	C18-C22-C23	-4.43	119.68	126.23
31	B	622	8CT	C07-C02-C03	-4.43	116.71	122.70
38	D	410	LHG	O4-P-O5	4.43	133.06	112.44
38	d	411	LHG	O4-P-O5	4.43	133.06	112.44
34	3	612	II0	C41-C39-C35	-4.43	121.06	127.28
38	b	619	LHG	O4-P-O5	4.43	133.04	112.44
38	B	621	LHG	O4-P-O5	4.43	133.04	112.44
34	p	301	II0	C42-C40-C36	-4.42	121.08	127.28
34	8	613	II0	C41-C39-C35	-4.42	121.08	127.28
38	8	618	LHG	O4-P-O5	4.42	133.00	112.44
31	Z	101	8CT	C30-C31-C32	-4.42	116.03	121.47
38	a	403	LHG	O4-P-O5	4.42	132.99	112.44
34	0	620	II0	C42-C40-C36	-4.41	121.09	127.28
38	b	621	LHG	O4-P-O5	4.41	132.97	112.44
38	S	301	LHG	O4-P-O5	4.41	132.94	112.44
38	2	618	LHG	O4-P-O5	4.40	132.93	112.44
34	2	613	II0	C41-C39-C35	-4.40	121.11	127.28
31	k	101	8CT	C10-C11-C12	-4.40	119.72	126.23
38	A	613	LHG	O4-P-O5	4.40	132.90	112.44
38	s	301	LHG	O4-P-O5	4.39	132.86	112.44
36	8	616	IHT	C30-C27-C23	-4.38	121.14	127.28
34	0	617	II0	C41-C39-C35	-4.38	121.14	127.28
38	a	402	LHG	O4-P-O5	4.38	132.81	112.44
38	A	612	LHG	O4-P-O5	4.38	132.81	112.44
36	4	614	IHT	C19-C10-C07	-4.37	119.71	124.48
31	K	101	8CT	C24-C25-C26	-4.37	121.15	127.28
34	P	614	II0	C42-C40-C36	-4.37	121.15	127.28
31	A	610	8CT	C01-C02-C03	-4.36	119.73	124.48
45	A	614	DGD	O3G-C3G-C2G	-4.36	100.21	110.82
34	9	612	II0	C41-C39-C35	-4.35	121.18	127.28
31	K	102	8CT	C19-C18-C17	-4.34	114.64	123.52
31	6	615	8CT	C01-C02-C03	-4.34	119.75	124.48
31	A	610	8CT	C19-C20-C21	-4.34	121.20	127.28
34	4	619	II0	C42-C40-C36	-4.34	121.20	127.28
35	P	613	II3	C04-C12-C21	-4.33	117.83	124.58
31	K	102	8CT	C35-C30-C29	-4.32	107.86	112.83
31	H	102	8CT	C24-C25-C26	-4.32	121.22	127.28
31	P	615	8CT	C01-C02-C03	-4.32	119.77	124.48
34	2	619	II0	C41-C39-C35	-4.32	121.22	127.28
45	c	516	DGD	O3G-C3G-C2G	-4.31	100.34	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C	516	DGD	O3G-C3G-C2G	-4.30	100.36	110.82
31	h	102	8CT	C24-C25-C26	-4.30	121.25	127.28
31	K	102	8CT	C10-C11-C12	-4.30	119.88	126.23
31	B	622	8CT	C19-C20-C21	-4.29	121.25	127.28
34	5	319	II0	C42-C40-C36	-4.29	121.26	127.28
36	0	618	IHT	C18-C22-C23	-4.28	119.90	126.23
31	B	624	8CT	C07-C02-C03	-4.28	116.92	122.70
31	k	101	8CT	C35-C30-C29	-4.27	107.91	112.83
31	k	102	8CT	C24-C25-C26	-4.27	121.29	127.28
45	a	414	DGD	O3G-C3G-C2G	-4.26	100.45	110.82
31	b	623	8CT	C07-C02-C03	-4.26	116.94	122.70
34	1	616	II0	C41-C39-C35	-4.26	121.31	127.28
31	M	201	8CT	C19-C20-C21	-4.25	121.32	127.28
45	C	515	DGD	O3G-C3G-C2G	-4.24	100.50	110.82
45	c	515	DGD	O3G-C3G-C2G	-4.24	100.51	110.82
34	9	614	II0	C42-C40-C36	-4.23	121.34	127.28
31	b	623	8CT	C10-C11-C12	-4.22	120.00	126.23
33	P	605	KC2	CHB-C1B-NB	4.21	130.73	124.80
31	6	615	8CT	C24-C25-C26	-4.21	121.38	127.28
31	b	623	8CT	C35-C30-C29	-4.20	107.99	112.83
33	6	605	KC2	CHB-C1B-NB	4.20	130.72	124.80
34	1	619	II0	C41-C39-C35	-4.20	121.39	127.28
36	4	617	IHT	C18-C22-C23	-4.20	120.02	126.23
34	5	301	II0	C41-C39-C35	-4.19	121.40	127.28
34	3	614	II0	C42-C40-C36	-4.19	121.40	127.28
31	z	101	8CT	C35-C30-C29	-4.18	108.02	112.83
35	6	613	II3	C04-C12-C21	-4.18	118.07	124.58
34	8	619	II0	C41-C39-C35	-4.18	121.42	127.28
31	B	624	8CT	C10-C11-C12	-4.18	120.06	126.23
31	Z	101	8CT	C19-C20-C21	-4.17	121.44	127.28
34	7	616	II0	C41-C39-C35	-4.16	121.44	127.28
31	P	615	8CT	C24-C25-C26	-4.15	121.45	127.28
31	z	101	8CT	C19-C20-C21	-4.14	121.47	127.28
33	2	610	KC2	CHC-C4B-NB	4.14	130.64	124.80
34	8	619	II0	C42-C40-C36	-4.14	121.47	127.28
34	1	619	II0	C42-C40-C36	-4.14	121.47	127.28
34	2	613	II0	C42-C40-C36	-4.14	121.47	127.28
31	B	624	8CT	C35-C30-C29	-4.14	108.07	112.83
31	b	623	8CT	C04-C03-C02	-4.14	116.98	122.64
31	d	408	8CT	C01-C02-C03	-4.13	119.98	124.48
31	B	623	8CT	C14-C13-C12	-4.13	121.49	127.28
33	8	610	KC2	CHC-C4B-NB	4.12	130.60	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	622	8CT	C14-C13-C12	-4.12	121.50	127.28
31	c	518	8CT	C19-C20-C21	-4.12	121.50	127.28
31	B	624	8CT	C04-C03-C02	-4.11	117.02	122.64
36	0	614	IHT	C19-C10-C07	-4.11	120.00	124.48
31	D	409	8CT	C01-C02-C03	-4.11	120.00	124.48
31	C	518	8CT	C19-C20-C21	-4.10	121.53	127.28
31	6	615	8CT	C19-C20-C21	-4.09	121.54	127.28
31	z	101	8CT	C24-C25-C26	-4.09	121.54	127.28
34	8	613	II0	C42-C40-C36	-4.08	121.56	127.28
31	a	413	8CT	C01-C02-C03	-4.07	120.05	124.48
33	6	605	KC2	C4B-CHC-C1C	-4.06	117.39	126.02
36	4	614	IHT	C18-C22-C23	-4.05	120.24	126.23
33	P	605	KC2	C4B-CHC-C1C	-4.05	117.41	126.02
31	P	615	8CT	C19-C20-C21	-4.05	121.60	127.28
31	K	101	8CT	C01-C02-C03	-4.03	120.08	124.48
31	k	102	8CT	C07-C02-C03	-4.03	117.25	122.70
34	2	619	II0	C42-C40-C36	-4.03	121.62	127.28
31	K	101	8CT	C07-C02-C03	-4.03	117.26	122.70
39	p	318	SQD	O47-C7-C8	4.02	120.18	111.48
31	c	518	8CT	C01-C02-C03	-4.01	120.11	124.48
31	Z	101	8CT	C01-C02-C03	-4.01	120.11	124.48
34	7	619	II0	C41-C39-C35	-4.01	121.66	127.28
34	5	314	II0	C42-C40-C36	-4.01	121.66	127.28
31	c	518	8CT	C18-C17-C16	-4.00	121.67	127.28
31	k	102	8CT	C01-C02-C03	-4.00	120.12	124.48
31	Z	101	8CT	C24-C25-C26	-4.00	121.67	127.28
34	7	614	II0	C42-C40-C36	-3.99	121.69	127.28
33	0	610	KC2	CHC-C4B-NB	3.99	130.41	124.80
36	0	614	IHT	C40-C37-C33	-3.98	121.69	127.28
31	C	518	8CT	C18-C17-C16	-3.98	121.69	127.28
31	C	518	8CT	C01-C02-C03	-3.98	120.14	124.48
39	B	620	SQD	O47-C7-C8	3.98	120.08	111.48
34	p	314	II0	C42-C40-C36	-3.98	121.70	127.28
39	5	318	SQD	O47-C7-C8	3.97	120.07	111.48
36	0	614	IHT	C18-C22-C23	-3.97	120.36	126.23
35	7	615	II3	C39-C36-C33	-3.97	121.72	127.28
33	2	610	KC2	C4B-CHC-C1C	-3.96	117.59	126.02
36	p	317	IHT	C18-C22-C23	-3.96	120.38	126.23
31	z	101	8CT	C18-C17-C16	-3.96	121.73	127.28
34	p	315	II0	C42-C40-C36	-3.95	121.73	127.28
33	1	610	KC2	CHC-C4B-NB	3.95	130.37	124.80
39	b	620	SQD	O47-C7-C8	3.95	120.03	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	4	610	KC2	CHC-C4B-NB	3.95	130.37	124.80
33	P	609	KC2	CHC-C4B-NB	3.94	130.35	124.80
33	6	609	KC2	CHC-C4B-NB	3.94	130.35	124.80
33	6	605	KC2	C1D-CHD-C4C	-3.94	116.98	126.25
33	7	610	KC2	CHC-C4B-NB	3.94	130.35	124.80
31	B	622	8CT	C29-C28-C26	-3.93	117.86	126.32
33	8	610	KC2	C4B-CHC-C1C	-3.93	117.66	126.02
34	7	619	II0	C42-C40-C36	-3.93	121.77	127.28
39	5	318	SQD	O9-S-O7	-3.92	101.08	113.82
36	2	616	IHT	C40-C37-C33	-3.92	121.78	127.28
36	4	614	IHT	C40-C37-C33	-3.92	121.78	127.28
33	1	610	KC2	C4B-CHC-C1C	-3.91	117.71	126.02
31	M	201	8CT	C29-C28-C26	-3.91	117.92	126.32
31	k	102	8CT	C19-C20-C21	-3.91	121.80	127.28
36	7	618	IHT	C40-C37-C33	-3.91	121.80	127.28
39	p	318	SQD	O9-S-O7	-3.90	101.13	113.82
33	P	605	KC2	C1D-CHD-C4C	-3.90	117.07	126.25
33	7	610	KC2	C4B-CHC-C1C	-3.90	117.74	126.02
39	b	620	SQD	O9-S-O7	-3.89	101.16	113.82
39	B	620	SQD	O9-S-O7	-3.89	101.17	113.82
31	Z	101	8CT	C11-C10-C03	-3.88	116.63	127.00
33	P	609	KC2	C4B-CHC-C1C	-3.88	117.77	126.02
31	K	101	8CT	C19-C20-C21	-3.88	121.84	127.28
31	Z	101	8CT	C18-C17-C16	-3.88	121.84	127.28
33	0	610	KC2	C4B-CHC-C1C	-3.87	117.79	126.02
33	6	609	KC2	C4B-CHC-C1C	-3.87	117.80	126.02
35	1	615	II3	C39-C36-C33	-3.87	121.86	127.28
33	p	311	KC2	CHC-C4B-NB	3.86	130.24	124.80
31	z	101	8CT	C11-C10-C03	-3.86	116.69	127.00
31	A	610	8CT	C30-C31-C32	-3.86	116.72	121.47
33	5	311	KC2	C4B-CHC-C1C	-3.86	117.82	126.02
33	p	311	KC2	C4B-CHC-C1C	-3.85	117.83	126.02
31	h	102	8CT	C07-C02-C03	-3.85	117.50	122.70
33	p	311	KC2	C1D-CHD-C4C	-3.85	117.19	126.25
33	4	610	KC2	C4B-CHC-C1C	-3.85	117.84	126.02
35	7	615	II3	C04-C12-C21	-3.84	118.61	124.58
33	4	610	KC2	C1D-CHD-C4C	-3.83	117.24	126.25
31	H	102	8CT	C07-C02-C03	-3.83	117.53	122.70
33	2	610	KC2	O2D-CGD-CBD	3.83	117.92	111.23
36	1	618	IHT	C40-C37-C33	-3.83	121.91	127.28
33	8	610	KC2	O2D-CGD-CBD	3.82	117.91	111.23
33	0	610	KC2	C1D-CHD-C4C	-3.82	117.26	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	5	311	KC2	C1D-CHD-C4C	-3.82	117.26	126.25
33	5	311	KC2	CHC-C4B-NB	3.82	130.18	124.80
33	P	609	KC2	C1D-CHD-C4C	-3.82	117.27	126.25
31	k	101	8CT	C25-C24-C23	-3.82	112.14	123.20
33	6	609	KC2	C1D-CHD-C4C	-3.81	117.29	126.25
31	C	518	8CT	C11-C10-C03	-3.81	116.83	127.00
36	8	616	IHT	C40-C37-C33	-3.80	121.94	127.28
31	c	518	8CT	C11-C10-C03	-3.80	116.84	127.00
34	7	617	II0	C41-C39-C35	-3.80	121.95	127.28
31	k	101	8CT	C07-C02-C03	-3.80	117.57	122.70
34	1	617	II0	C41-C39-C35	-3.80	121.95	127.28
33	P	605	KC2	CHC-C4B-NB	3.80	130.15	124.80
33	1	610	KC2	C1D-CHD-C4C	-3.79	117.32	126.25
35	1	615	II3	C04-C12-C21	-3.79	118.68	124.58
34	8	615	II0	C19-C13-C11	3.79	121.39	114.42
39	b	601	SQD	O9-S-O7	-3.79	101.50	113.82
33	7	610	KC2	C1D-CHD-C4C	-3.79	117.34	126.25
39	B	601	SQD	O9-S-O7	-3.78	101.53	113.82
36	5	317	IHT	C18-C22-C23	-3.78	120.64	126.23
33	8	610	KC2	C1D-CHD-C4C	-3.78	117.36	126.25
31	K	102	8CT	C25-C24-C23	-3.78	112.25	123.20
31	K	102	8CT	C07-C02-C03	-3.77	117.60	122.70
43	d	404	PL9	C7-C3-C2	-3.76	118.95	123.39
33	2	610	KC2	C1D-CHD-C4C	-3.76	117.40	126.25
43	A	609	PL9	C7-C3-C2	-3.76	118.96	123.39
39	A	606	SQD	O9-S-O7	-3.76	101.59	113.82
31	Z	101	8CT	C35-C30-C29	-3.76	108.51	112.83
43	a	412	PL9	C7-C3-C2	-3.75	118.97	123.39
39	a	409	SQD	O9-S-O7	-3.75	101.63	113.82
36	4	617	IHT	C30-C27-C23	-3.74	122.04	127.28
45	H	101	DGD	O3G-C3G-C2G	-3.74	101.73	110.82
43	D	405	PL9	C7-C3-C2	-3.74	118.98	123.39
33	6	605	KC2	CHC-C4B-NB	3.73	130.06	124.80
36	1	618	IHT	C19-C10-C07	-3.73	120.41	124.48
45	h	101	DGD	O3G-C3G-C2G	-3.73	101.76	110.82
31	b	622	8CT	C18-C17-C16	-3.72	122.06	127.28
31	z	101	8CT	C01-C02-C03	-3.72	120.42	124.48
36	0	618	IHT	C30-C27-C23	-3.72	122.06	127.28
31	k	102	8CT	C18-C19-C20	-3.72	115.91	123.52
31	3	615	8CT	C19-C20-C21	-3.71	122.07	127.28
32	C	503	CLA	O2D-CGD-O1D	-3.70	116.64	123.85
31	9	615	8CT	C11-C10-C03	-3.70	117.11	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	615	8CT	C19-C20-C21	-3.70	122.09	127.28
31	B	623	8CT	C18-C17-C16	-3.70	122.09	127.28
31	d	408	8CT	C19-C20-C21	-3.70	122.09	127.28
31	K	101	8CT	C18-C19-C20	-3.70	115.96	123.52
31	3	615	8CT	C11-C10-C03	-3.69	117.13	127.00
34	5	315	II0	C42-C40-C36	-3.69	122.11	127.28
31	D	409	8CT	C19-C20-C21	-3.68	122.11	127.28
36	p	317	IHT	C19-C10-C07	-3.68	120.47	124.48
32	c	503	CLA	O2D-CGD-O1D	-3.68	116.69	123.85
34	1	614	II0	C42-C40-C36	-3.68	122.12	127.28
34	9	612	II0	C42-C40-C36	-3.68	122.12	127.28
36	5	317	IHT	C40-C37-C33	-3.67	122.13	127.28
34	5	316	II0	C41-C39-C35	-3.67	122.13	127.28
34	3	612	II0	C42-C40-C36	-3.66	122.15	127.28
36	5	317	IHT	C19-C10-C07	-3.64	120.51	124.48
31	b	622	8CT	C24-C25-C26	-3.64	122.17	127.28
31	B	623	8CT	C24-C25-C26	-3.64	122.18	127.28
31	9	615	8CT	C29-C28-C26	-3.62	118.54	126.32
34	0	620	II0	C41-C39-C35	-3.61	122.22	127.28
39	a	409	SQD	O47-C7-C8	3.60	119.28	111.48
31	3	615	8CT	C29-C28-C26	-3.60	118.58	126.32
39	A	606	SQD	O47-C7-C8	3.60	119.27	111.48
34	2	615	II0	C19-C13-C11	3.60	121.04	114.42
34	P	614	II0	C41-C39-C35	-3.59	122.25	127.28
35	7	615	II3	C41-C40-C38	-3.58	122.26	127.28
32	a	406	CLA	O2D-CGD-O1D	-3.58	116.89	123.85
31	A	610	8CT	C10-C11-C12	-3.57	120.95	126.23
36	p	317	IHT	C40-C37-C33	-3.57	122.27	127.28
31	Z	101	8CT	C07-C02-C03	-3.56	117.89	122.70
35	1	615	II3	C41-C40-C38	-3.56	122.29	127.28
31	B	623	8CT	C30-C29-C28	-3.56	119.04	124.58
33	6	605	KC2	C1D-ND-C4D	3.56	108.81	106.31
31	b	622	8CT	C30-C29-C28	-3.55	119.05	124.58
36	0	614	IHT	C30-C27-C23	-3.55	122.30	127.28
31	z	101	8CT	C07-C02-C03	-3.54	117.92	122.70
34	4	619	II0	C41-C39-C35	-3.54	122.32	127.28
33	5	311	KC2	CHB-C1B-C2B	-3.53	118.14	125.49
31	a	413	8CT	C10-C11-C12	-3.53	121.02	126.23
45	c	516	DGD	O6D-C1D-O3G	-3.52	101.72	110.04
36	4	614	IHT	C30-C27-C23	-3.52	122.34	127.28
34	4	616	II0	C42-C40-C36	-3.52	122.34	127.28
31	B	623	8CT	C07-C02-C03	-3.52	117.95	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	2	610	KC2	CHC-C4B-C3B	-3.52	119.28	125.21
45	C	516	DGD	O6D-C1D-O3G	-3.52	101.74	110.04
33	p	311	KC2	CHB-C1B-C2B	-3.51	118.18	125.49
31	6	615	8CT	C10-C11-C12	-3.51	121.05	126.23
34	P	614	II0	C20-C14-C12	3.50	120.86	114.42
31	b	622	8CT	C10-C11-C12	-3.50	121.06	126.23
41	a	407	PHO	C2B-C1B-NB	-3.50	106.90	109.43
33	8	610	KC2	CHC-C4B-C3B	-3.50	119.31	125.21
31	b	622	8CT	C07-C02-C03	-3.50	117.98	122.70
31	Z	101	8CT	C13-C14-C15	-3.49	113.09	123.20
41	A	604	PHO	C2B-C1B-NB	-3.49	106.91	109.43
31	B	623	8CT	C10-C11-C12	-3.48	121.08	126.23
32	A	603	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
39	b	601	SQD	O9-S-C6	3.47	111.94	106.76
31	d	408	8CT	C14-C13-C12	-3.47	122.41	127.28
31	D	409	8CT	C14-C13-C12	-3.46	122.42	127.28
39	B	601	SQD	O9-S-C6	3.46	111.92	106.76
45	C	515	DGD	O6D-C1D-O3G	-3.46	101.87	110.04
45	c	514	DGD	O6D-C1D-O3G	-3.46	101.88	110.04
31	a	413	8CT	C05-C04-C03	3.44	115.44	110.44
31	K	101	8CT	C04-C03-C02	-3.44	117.93	122.64
45	C	514	DGD	O6D-C1D-O3G	-3.44	101.91	110.04
33	1	610	KC2	CHB-C1B-C2B	-3.44	118.34	125.49
31	k	102	8CT	C04-C03-C02	-3.44	117.94	122.64
31	C	518	8CT	C24-C25-C26	-3.43	122.47	127.28
45	c	515	DGD	O6D-C1D-O3G	-3.43	101.94	110.04
33	7	610	KC2	CHB-C1B-C2B	-3.43	118.36	125.49
31	c	518	8CT	C24-C25-C26	-3.43	122.47	127.28
39	p	318	SQD	O7-S-C6	3.42	111.86	106.76
31	P	615	8CT	C10-C11-C12	-3.41	121.18	126.23
36	7	618	IHT	C19-C10-C07	-3.41	120.76	124.48
31	B	624	8CT	C30-C29-C28	-3.41	119.27	124.58
31	K	102	8CT	C30-C31-C32	-3.41	117.28	121.47
31	b	623	8CT	C30-C29-C28	-3.41	119.28	124.58
34	6	612	II0	C42-C40-C36	-3.40	122.50	127.28
31	z	101	8CT	C13-C14-C15	-3.40	113.34	123.20
39	5	318	SQD	O7-S-C6	3.40	111.83	106.76
31	z	101	8CT	C05-C04-C03	3.40	115.37	110.44
33	0	610	KC2	CHB-C1B-C2B	-3.39	118.43	125.49
33	1	610	KC2	CHC-C4B-C3B	-3.39	119.49	125.21
31	h	102	8CT	C05-C04-C03	3.39	115.36	110.44
33	4	610	KC2	CHB-C1B-C2B	-3.39	118.44	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	0	610	KC2	CHC-C4B-C3B	-3.39	119.50	125.21
33	P	609	KC2	CHB-C1B-C2B	-3.37	118.48	125.49
31	d	408	8CT	C05-C04-C03	3.36	115.33	110.44
31	H	102	8CT	C05-C04-C03	3.36	115.33	110.44
33	6	609	KC2	CHB-C1B-C2B	-3.36	118.50	125.49
33	2	610	KC2	CHB-C1B-C2B	-3.35	118.51	125.49
33	p	311	KC2	CHD-C1D-ND	3.34	129.07	124.05
33	8	610	KC2	CHB-C1B-C2B	-3.34	118.53	125.49
33	7	610	KC2	CHC-C4B-C3B	-3.34	119.57	125.21
34	0	616	II0	C42-C40-C36	-3.34	122.60	127.28
31	D	409	8CT	C05-C04-C03	3.33	115.28	110.44
33	4	610	KC2	CHC-C4B-C3B	-3.33	119.60	125.21
34	8	615	II0	C32-C34-C36	-3.31	117.28	126.36
33	6	609	KC2	CHC-C4B-C3B	-3.31	119.62	125.21
33	5	311	KC2	CHD-C1D-ND	3.31	129.02	124.05
34	8	614	II0	C41-C39-C35	-3.31	122.64	127.28
33	P	605	KC2	C1D-ND-C4D	3.30	108.63	106.31
31	Z	101	8CT	C05-C04-C03	3.30	115.24	110.44
32	0	612	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
33	P	609	KC2	CHC-C4B-C3B	-3.30	119.65	125.21
31	k	101	8CT	C30-C31-C32	-3.30	117.41	121.47
31	a	413	8CT	C01-C02-C07	3.29	120.62	113.60
34	2	614	II0	C41-C39-C35	-3.29	122.66	127.28
41	D	402	PHO	C2B-C1B-NB	-3.29	107.05	109.43
45	a	414	DGD	O6D-C1D-O3G	-3.29	102.27	110.04
45	A	614	DGD	O6D-C1D-O3G	-3.28	102.30	110.04
32	4	612	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
31	B	623	8CT	C35-C30-C29	-3.27	109.06	112.83
32	D	404	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
32	d	403	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
32	9	604	CLA	C3B-C4B-NB	-3.27	107.61	110.53
34	2	615	II0	C32-C34-C36	-3.27	117.41	126.36
34	0	616	II0	C41-C42-C40	-3.26	116.84	123.52
31	K	102	8CT	C04-C03-C02	-3.26	118.18	122.64
33	8	610	KC2	O1D-CGD-CBD	-3.26	118.09	124.52
31	M	201	8CT	C04-C03-C02	-3.26	118.18	122.64
31	B	622	8CT	C04-C03-C02	-3.26	118.18	122.64
32	b	604	CLA	O2D-CGD-O1D	-3.25	117.51	123.85
32	B	604	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
33	4	610	KC2	CHD-C1D-ND	3.25	128.93	124.05
33	6	609	KC2	CHD-C1D-ND	3.25	128.93	124.05
41	d	410	PHO	C2B-C1B-NB	-3.25	107.08	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	2	610	KC2	O1D-CGD-CBD	-3.25	118.11	124.52
33	P	609	KC2	CHD-C1D-ND	3.25	128.92	124.05
31	b	622	8CT	C35-C30-C29	-3.24	109.10	112.83
32	a	408	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
31	k	101	8CT	C04-C03-C02	-3.24	118.21	122.64
33	8	610	KC2	CHD-C1D-ND	3.24	128.91	124.05
33	p	311	KC2	CHC-C4B-C3B	-3.24	119.75	125.21
32	D	403	CLA	O2D-CGD-O1D	-3.23	117.55	123.85
34	8	615	II0	C41-C39-C35	-3.23	122.74	127.28
34	0	616	II0	C19-C13-C11	3.23	120.36	114.42
41	d	410	PHO	O1D-CGD-CBD	3.23	129.62	124.72
31	B	623	8CT	C30-C31-C32	-3.23	117.50	121.47
32	d	402	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
34	4	616	II0	C41-C42-C40	-3.22	116.92	123.52
34	4	616	II0	C19-C13-C11	3.22	120.35	114.42
44	A	611	BCT	O3-C-O1	-3.22	111.44	119.68
33	5	311	KC2	CHC-C4B-C3B	-3.22	119.78	125.21
32	A	605	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
33	0	610	KC2	CHD-C1D-ND	3.22	128.87	124.05
32	3	604	CLA	C3B-C4B-NB	-3.21	107.66	110.53
41	D	402	PHO	O1D-CGD-CBD	3.21	129.60	124.72
33	2	610	KC2	CHD-C1D-ND	3.21	128.87	124.05
44	a	401	BCT	O3-C-O1	-3.20	111.50	119.68
33	7	610	KC2	CHD-C1D-ND	3.20	128.84	124.05
32	C	508	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
31	b	622	8CT	C30-C31-C32	-3.19	117.54	121.47
34	7	617	II0	C19-C13-C11	3.19	120.29	114.42
31	z	101	8CT	C29-C28-C26	-3.19	119.46	126.32
34	2	615	II0	C41-C39-C35	-3.19	122.81	127.28
31	h	102	8CT	C35-C30-C29	-3.18	109.16	112.83
34	1	617	II0	C19-C13-C11	3.18	120.28	114.42
31	Z	101	8CT	C29-C28-C26	-3.18	119.48	126.32
34	6	614	II0	C41-C39-C35	-3.18	122.82	127.28
33	1	610	KC2	CHD-C1D-ND	3.18	128.82	124.05
31	a	413	8CT	C11-C10-C03	-3.18	118.51	127.00
41	d	410	PHO	CMB-C2B-C3B	3.17	131.03	124.68
32	c	508	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
41	D	402	PHO	CMB-C2B-C3B	3.16	131.00	124.68
34	0	620	II0	C19-C13-C11	3.16	120.23	114.42
31	z	101	8CT	C01-C02-C07	3.15	120.32	113.60
36	7	618	IHT	C06-C09-C10	-3.15	108.43	114.06
32	b	607	CLA	O2D-CGD-O1D	-3.15	117.72	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	a	409	SQD	O9-S-C6	3.15	111.46	106.76
34	6	614	II0	C20-C14-C12	3.15	120.21	114.42
32	D	401	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
31	d	408	8CT	C01-C02-C07	3.14	120.29	113.60
32	B	607	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
31	D	409	8CT	C01-C02-C07	3.14	120.29	113.60
32	b	613	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
31	k	101	8CT	C13-C14-C15	-3.14	114.11	123.20
33	p	311	KC2	C1D-ND-C4D	3.14	108.51	106.31
32	B	613	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
39	A	606	SQD	O9-S-C6	3.12	111.42	106.76
33	p	311	KC2	C1A-NA-C4A	-3.12	105.25	106.68
34	P	612	II0	C42-C40-C36	-3.12	122.90	127.28
32	C	505	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
31	H	102	8CT	C18-C17-C16	-3.12	122.91	127.28
31	A	610	8CT	C14-C13-C12	-3.12	122.91	127.28
31	H	102	8CT	C35-C30-C29	-3.11	109.24	112.83
34	5	319	II0	C19-C13-C11	3.11	120.15	114.42
32	b	615	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
36	p	317	IHT	C30-C27-C23	-3.10	122.92	127.28
33	5	311	KC2	C1A-NA-C4A	-3.10	105.26	106.68
34	p	301	II0	C19-C13-C11	3.10	120.13	114.42
32	d	409	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
33	5	311	KC2	C1D-ND-C4D	3.10	108.49	106.31
31	h	102	8CT	C18-C17-C16	-3.09	122.94	127.28
39	B	601	SQD	O7-S-C6	3.09	111.37	106.76
32	9	604	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
32	c	505	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
31	k	102	8CT	C01-C02-C07	3.09	120.19	113.60
32	c	501	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
41	A	604	PHO	O1D-CGD-CBD	3.08	129.40	124.72
45	h	101	DGD	O6D-C1D-O3G	-3.08	102.75	110.04
31	H	102	8CT	C29-C28-C26	-3.08	119.69	126.32
31	k	102	8CT	C35-C30-C29	-3.08	109.28	112.83
31	A	610	8CT	C11-C10-C03	-3.08	118.76	127.00
39	b	601	SQD	O7-S-C6	3.08	111.36	106.76
32	c	511	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
32	C	501	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
31	K	101	8CT	C01-C02-C07	3.08	120.16	113.60
32	0	604	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
34	p	316	II0	C41-C39-C35	-3.08	122.96	127.28
43	A	609	PL9	O2-C1-C2	-3.08	117.05	121.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	602	CLA	C3B-C4B-NB	-3.08	107.78	110.53
34	5	316	II0	C20-C14-C12	3.08	120.08	114.42
32	3	609	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
31	K	102	8CT	C13-C14-C15	-3.07	114.30	123.20
32	9	602	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
33	0	610	KC2	C1A-NA-C4A	-3.07	105.28	106.68
32	b	611	CLA	C3B-C4B-NB	-3.07	107.79	110.53
32	3	604	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
32	b	616	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
32	C	511	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
33	P	609	KC2	C1D-ND-C4D	3.07	108.47	106.31
32	9	609	CLA	C3B-C4B-NB	-3.07	107.79	110.53
32	3	609	CLA	C3B-C4B-NB	-3.07	107.79	110.53
32	B	615	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
39	B	620	SQD	O7-S-C6	3.07	111.33	106.76
32	9	609	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
32	b	609	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
45	H	101	DGD	O6D-C1D-O3G	-3.06	102.80	110.04
32	9	603	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
31	h	102	8CT	C29-C28-C26	-3.06	119.74	126.32
43	a	412	PL9	O2-C1-C2	-3.06	117.07	121.43
32	3	602	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
32	B	612	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
34	4	615	II0	C41-C39-C35	-3.06	122.99	127.28
32	B	616	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
32	3	603	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
39	b	620	SQD	O7-S-C6	3.05	111.32	106.76
32	c	512	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
32	4	604	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
31	6	615	8CT	C29-C28-C26	-3.05	119.76	126.32
32	C	512	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
32	b	605	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
41	A	604	PHO	O2D-CGD-O1D	-3.05	117.92	123.85
32	c	509	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
31	Z	101	8CT	C01-C02-C07	3.04	120.09	113.60
32	B	602	CLA	C3B-C4B-NB	-3.04	107.81	110.53
34	p	316	II0	C20-C14-C12	3.04	120.02	114.42
32	p	307	CLA	C3B-C4B-NB	-3.04	107.81	110.53
33	4	610	KC2	C1A-NA-C4A	-3.04	105.29	106.68
31	B	623	8CT	C11-C10-C03	-3.04	118.87	127.00
31	P	615	8CT	C01-C02-C07	3.04	120.08	113.60
34	7	616	II0	C19-C13-C11	3.04	120.01	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1	608	CLA	C3B-C4B-NB	-3.04	107.82	110.53
32	B	605	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
32	B	609	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
39	B	620	SQD	O9-S-C6	3.03	111.28	106.76
31	b	622	8CT	C11-C10-C03	-3.03	118.90	127.00
39	5	318	SQD	O48-C23-C24	3.03	120.35	111.15
34	9	614	II0	C41-C39-C35	-3.03	123.03	127.28
31	6	615	8CT	C01-C02-C07	3.03	120.06	113.60
34	4	619	II0	C19-C13-C11	3.03	119.99	114.42
39	p	318	SQD	O48-C23-C24	3.03	120.34	111.15
32	b	612	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
32	B	611	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
32	C	509	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
41	a	407	PHO	O1D-CGD-CBD	3.03	129.31	124.72
33	P	605	KC2	CHC-C4B-C3B	-3.02	120.11	125.21
33	6	605	KC2	CHB-C1B-C2B	-3.02	119.20	125.49
31	P	615	8CT	C29-C28-C26	-3.02	119.83	126.32
34	0	615	II0	C41-C39-C35	-3.02	123.05	127.28
32	B	611	CLA	C3B-C4B-NB	-3.02	107.84	110.53
33	P	605	KC2	CHB-C1B-C2B	-3.02	119.21	125.49
41	a	407	PHO	O2D-CGD-O1D	-3.01	117.98	123.85
41	A	604	PHO	C1-C2-C3	-3.01	121.26	126.20
32	b	611	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
31	c	518	8CT	C01-C02-C07	3.01	120.02	113.60
33	8	610	KC2	C1D-ND-C4D	3.01	108.42	106.31
32	C	510	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
36	1	618	IHT	C06-C09-C10	-3.01	108.69	114.06
32	c	510	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
41	a	407	PHO	C1-C2-C3	-3.01	121.27	126.20
33	6	609	KC2	C1D-ND-C4D	3.00	108.42	106.31
32	b	614	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
32	8	607	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
34	1	616	II0	C19-C13-C11	3.00	119.93	114.42
37	A	607	LMG	O6-C1-O1	-3.00	102.97	110.04
32	C	504	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
32	B	608	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
39	b	620	SQD	O9-S-C6	2.99	111.22	106.76
31	C	518	8CT	C01-C02-C07	2.99	119.97	113.60
32	C	507	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
32	c	507	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
34	3	613	II0	C42-C41-C39	-2.98	117.42	123.52
32	a	406	CLA	C3B-C4B-NB	-2.98	107.87	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	a	410	LMG	O6-C1-O1	-2.98	103.01	110.04
33	6	605	KC2	CHC-C4B-C3B	-2.98	120.19	125.21
32	c	504	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
32	b	608	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
32	B	614	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
32	4	613	CLA	C3B-C4B-NB	-2.97	107.88	110.53
32	P	602	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
31	M	201	8CT	C35-C30-C29	2.97	116.24	112.83
33	4	610	KC2	C1D-ND-C4D	2.97	108.39	106.31
32	8	603	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
32	6	602	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
32	p	310	CLA	C3B-C4B-NB	-2.96	107.88	110.53
31	B	622	8CT	C35-C30-C29	2.96	116.23	112.83
36	5	317	IHT	C30-C27-C23	-2.96	123.13	127.28
32	7	608	CLA	C3B-C4B-NB	-2.95	107.89	110.53
33	P	609	KC2	C1A-NA-C4A	-2.95	105.33	106.68
32	c	513	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
32	s	303	CLA	C3B-C4B-NB	-2.95	107.90	110.53
31	6	615	8CT	C11-C10-C03	-2.95	119.12	127.00
32	7	602	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
32	6	610	CLA	C3B-C4B-NB	-2.95	107.90	110.53
32	2	603	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
33	2	610	KC2	C1D-ND-C4D	2.94	108.38	106.31
32	5	303	CLA	C3B-C4B-NB	-2.94	107.90	110.53
32	1	608	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
32	S	303	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
32	4	601	CLA	C3B-C4B-NB	-2.94	107.91	110.53
32	8	601	CLA	C3B-C4B-NB	-2.94	107.91	110.53
32	7	608	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
32	4	605	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
32	4	609	CLA	C3B-C4B-NB	-2.94	107.91	110.53
32	S	303	CLA	C3B-C4B-NB	-2.94	107.91	110.53
32	5	309	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
32	2	601	CLA	C3B-C4B-NB	-2.94	107.91	110.53
32	s	302	CLA	C3B-C4B-NB	-2.94	107.91	110.53
33	6	609	KC2	C1A-NA-C4A	-2.93	105.34	106.68
32	1	602	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
32	8	602	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
32	3	601	CLA	C3B-C4B-NB	-2.93	107.91	110.53
32	5	310	CLA	C3B-C4B-NB	-2.93	107.91	110.53
32	2	602	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
31	P	615	8CT	C11-C10-C03	-2.93	119.16	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	C	513	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
32	9	601	CLA	C3B-C4B-NB	-2.93	107.91	110.53
32	P	602	CLA	C3B-C4B-NB	-2.93	107.91	110.53
31	M	201	8CT	C11-C10-C03	-2.93	119.17	127.00
32	p	303	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
32	s	303	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
31	B	622	8CT	C11-C10-C03	-2.93	119.17	127.00
36	p	317	IHT	C20-C15-C12	2.93	119.81	114.42
32	3	606	CLA	C3B-C4B-NB	-2.93	107.92	110.53
32	B	606	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
32	0	609	CLA	C3B-C4B-NB	-2.92	107.92	110.53
32	5	302	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
32	7	603	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
32	2	604	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
32	b	606	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
33	0	610	KC2	C1D-ND-C4D	2.92	108.36	106.31
32	1	604	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
34	9	613	II0	C42-C41-C39	-2.92	117.54	123.52
32	9	602	CLA	C3B-C4B-NB	-2.92	107.92	110.53
31	b	622	8CT	C04-C03-C02	-2.92	118.65	122.64
32	b	615	CLA	C3B-C4B-NB	-2.91	107.93	110.53
32	6	610	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
32	c	503	CLA	O2D-CGD-CBD	2.91	116.32	111.23
32	b	617	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
32	4	603	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
32	B	602	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
32	5	303	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
33	7	610	KC2	C1D-ND-C4D	2.91	108.35	106.31
32	4	608	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
32	a	406	CLA	O2D-CGD-CBD	2.91	116.31	111.23
32	5	309	CLA	C3B-C4B-NB	-2.91	107.93	110.53
32	7	604	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
32	0	605	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
32	7	609	CLA	C3B-C4B-NB	-2.91	107.94	110.53
32	0	601	CLA	C3B-C4B-NB	-2.91	107.94	110.53
32	0	613	CLA	C3B-C4B-NB	-2.91	107.94	110.53
33	P	605	KC2	CHD-C1D-ND	2.90	128.40	124.05
32	8	607	CLA	C3B-C4B-NB	-2.90	107.94	110.53
32	p	309	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
32	5	307	CLA	C3B-C4B-NB	-2.90	107.94	110.53
32	0	601	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
36	5	317	IHT	C20-C15-C12	2.90	119.75	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2	605	CLA	C3B-C4B-NB	-2.90	107.94	110.53
32	B	617	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
35	7	615	II3	C29-C26-C24	-2.90	123.22	127.28
31	M	201	8CT	C01-C02-C07	2.90	119.77	113.60
32	1	609	CLA	C3B-C4B-NB	-2.89	107.95	110.53
32	5	306	CLA	C3B-C4B-NB	-2.89	107.95	110.53
32	b	602	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
32	8	604	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
39	A	606	SQD	O48-C23-C24	2.89	120.66	111.83
32	1	606	CLA	C3B-C4B-NB	-2.89	107.95	110.53
32	8	609	CLA	C3B-C4B-NB	-2.89	107.95	110.53
34	3	614	II0	C41-C39-C35	-2.89	123.22	127.28
32	P	610	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
32	p	303	CLA	C3B-C4B-NB	-2.89	107.95	110.53
32	9	607	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
32	2	608	CLA	C3B-C4B-NB	-2.89	107.95	110.53
32	3	602	CLA	C3B-C4B-NB	-2.89	107.95	110.53
32	3	603	CLA	C3B-C4B-NB	-2.89	107.95	110.53
32	8	608	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
32	2	609	CLA	C3B-C4B-NB	-2.88	107.95	110.53
32	p	302	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
32	4	601	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
32	9	606	CLA	C3B-C4B-NB	-2.88	107.96	110.53
31	B	623	8CT	C04-C03-C02	-2.88	118.70	122.64
32	2	609	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
32	B	612	CLA	C3B-C4B-NB	-2.88	107.96	110.53
32	7	609	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
35	P	613	II3	C39-C41-C40	-2.88	117.63	123.52
32	B	615	CLA	C3B-C4B-NB	-2.88	107.96	110.53
32	6	603	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
32	0	608	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
32	8	609	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
32	4	609	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
32	1	601	CLA	C3B-C4B-NB	-2.88	107.96	110.53
32	P	603	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
32	3	607	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
43	d	404	PL9	C7-C8-C9	-2.87	121.88	126.83
32	p	305	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
32	0	606	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
32	2	608	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
35	6	613	II3	C39-C41-C40	-2.87	117.65	123.52
39	a	409	SQD	O48-C23-C24	2.87	120.59	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	8	608	CLA	C3B-C4B-NB	-2.87	107.97	110.53
32	1	609	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
32	6	602	CLA	C3B-C4B-NB	-2.87	107.97	110.53
37	D	411	LMG	O6-C1-O1	-2.87	103.27	110.04
31	B	622	8CT	C01-C02-C07	2.87	119.71	113.60
43	D	405	PL9	C7-C8-C9	-2.87	121.89	126.83
32	A	603	CLA	C3B-C4B-NB	-2.87	107.97	110.53
32	7	605	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
32	p	304	CLA	C3B-C4B-NB	-2.86	107.97	110.53
33	1	610	KC2	C1A-NA-C4A	-2.86	105.37	106.68
32	7	601	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
32	b	612	CLA	C3B-C4B-NB	-2.86	107.97	110.53
37	d	401	LMG	O6-C1-O1	-2.86	103.28	110.04
32	P	610	CLA	C3B-C4B-NB	-2.86	107.98	110.53
32	p	310	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
32	5	304	CLA	C3B-C4B-NB	-2.86	107.98	110.53
32	5	305	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
33	6	605	KC2	CHD-C1D-ND	2.86	128.34	124.05
32	8	605	CLA	C3B-C4B-NB	-2.86	107.98	110.53
32	6	606	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
34	5	316	II0	C19-C13-C11	2.86	119.67	114.42
32	0	603	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
32	1	603	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
32	3	610	CLA	C3B-C4B-NB	-2.85	107.98	110.53
31	K	101	8CT	C35-C30-C29	-2.85	109.55	112.83
31	9	615	8CT	C35-C30-C29	-2.85	109.55	112.83
32	9	601	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
32	4	606	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
32	C	506	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
37	G	102	LMG	O6-C1-O1	-2.84	103.32	110.04
32	1	601	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
32	p	304	CLA	C1-C2-C3	-2.84	122.16	126.76
32	3	605	CLA	C3B-C4B-NB	-2.84	107.99	110.53
32	4	603	CLA	C3B-C4B-NB	-2.84	107.99	110.53
32	7	601	CLA	C3B-C4B-NB	-2.84	107.99	110.53
39	B	620	SQD	O48-C23-C24	2.84	120.50	111.83
32	5	310	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
32	9	610	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
32	8	601	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
32	P	601	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
32	3	608	CLA	CAA-C2A-C3A	-2.84	109.72	116.23
32	S	302	CLA	C3B-C4B-NB	-2.84	107.99	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	A	606	SQD	O7-S-C6	2.84	111.00	106.76
31	3	615	8CT	C35-C30-C29	-2.84	109.56	112.83
39	a	409	SQD	O7-S-C6	2.84	111.00	106.76
32	3	607	CLA	C3B-C4B-NB	-2.84	108.00	110.53
32	p	309	CLA	C3B-C4B-NB	-2.84	108.00	110.53
32	1	605	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
32	p	304	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
37	0	619	LMG	O6-C1-O1	-2.84	103.34	110.04
39	b	620	SQD	O48-C23-C24	2.84	120.48	111.83
32	5	313	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
32	p	306	CLA	C3B-C4B-NB	-2.84	108.00	110.53
32	0	609	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
32	7	613	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
32	p	302	CLA	C3B-C4B-NB	-2.83	108.00	110.53
32	5	304	CLA	C1-C2-C3	-2.83	122.18	126.76
32	c	510	CLA	C1-C2-C3	-2.83	121.55	126.20
32	3	608	CLA	C3B-C4B-NB	-2.83	108.00	110.53
32	c	506	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
32	P	607	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
32	0	602	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
32	9	610	CLA	C3B-C4B-NB	-2.83	108.00	110.53
33	1	610	KC2	C1D-ND-C4D	2.83	108.30	106.31
32	0	613	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
32	6	608	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
32	9	605	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
32	9	608	CLA	CAA-C2A-C3A	-2.83	109.75	116.23
32	3	605	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
32	p	306	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
34	p	316	II0	C32-C34-C36	-2.83	118.62	126.36
32	A	602	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
36	4	617	IHT	C20-C15-C12	2.82	119.61	114.42
32	1	607	CLA	C3B-C4B-NB	-2.82	108.01	110.53
45	a	414	DGD	CDB-CCB-CBB	-2.82	100.10	114.37
32	2	601	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
41	D	402	PHO	O2D-CGD-O1D	-2.82	118.36	123.85
41	d	410	PHO	O2D-CGD-O1D	-2.82	118.36	123.85
39	b	601	SQD	O48-C23-C24	2.82	120.43	111.83
32	1	603	CLA	C3B-C4B-NB	-2.82	108.01	110.53
36	p	317	IHT	C31-C34-C35	-2.82	118.63	126.36
32	p	313	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
32	2	612	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
32	P	604	CLA	O2D-CGD-O1D	-2.82	118.37	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	604	CLA	C3B-C4B-NB	-2.82	108.02	110.53
32	0	608	CLA	C3B-C4B-NB	-2.82	108.02	110.53
32	C	512	CLA	C3B-C4B-NB	-2.81	108.02	110.53
32	4	602	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
32	6	607	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
36	1	618	IHT	C20-C15-C12	2.81	119.59	114.42
37	4	618	LMG	O6-C1-O1	-2.81	103.40	110.04
32	P	608	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
32	1	613	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
32	6	607	CLA	C3B-C4B-NB	-2.81	108.02	110.53
32	6	608	CLA	C3B-C4B-NB	-2.81	108.02	110.53
32	P	606	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
32	5	305	CLA	C3B-C4B-NB	-2.81	108.02	110.53
34	p	316	II0	C19-C13-C11	2.81	119.59	114.42
32	6	601	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
43	d	404	PL9	C22-C23-C24	-2.81	121.20	127.62
32	4	611	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
32	5	312	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
32	9	607	CLA	C3B-C4B-NB	-2.81	108.03	110.53
32	P	603	CLA	C3B-C4B-NB	-2.81	108.03	110.53
45	c	514	DGD	CDB-CCB-CBB	-2.81	100.19	114.37
32	2	607	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
32	p	312	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
39	B	601	SQD	O48-C23-C24	2.80	120.39	111.83
32	5	306	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
32	7	607	CLA	C3B-C4B-NB	-2.80	108.03	110.53
32	5	307	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
32	c	503	CLA	C3B-C4B-NB	-2.80	108.03	110.53
32	a	408	CLA	C3B-C4B-NB	-2.80	108.03	110.53
43	D	405	PL9	C22-C23-C24	-2.80	121.21	127.62
32	9	608	CLA	C3B-C4B-NB	-2.80	108.03	110.53
32	p	312	CLA	C3B-C4B-NB	-2.80	108.03	110.53
32	9	605	CLA	C3B-C4B-NB	-2.80	108.03	110.53
45	C	514	DGD	CDB-CCB-CBB	-2.80	100.21	114.37
32	p	305	CLA	C3B-C4B-NB	-2.80	108.03	110.53
32	B	609	CLA	C3B-C4B-NB	-2.80	108.03	110.53
32	3	601	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
32	A	605	CLA	C3B-C4B-NB	-2.80	108.03	110.53
31	K	101	8CT	C14-C13-C12	-2.80	123.36	127.28
31	K	102	8CT	C24-C25-C26	-2.80	123.36	127.28
43	d	404	PL9	C40-C39-C41	2.80	120.08	115.23
32	2	611	CLA	O2D-CGD-O1D	-2.80	118.41	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	3	610	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
36	7	618	IHT	C20-C15-C12	2.80	119.56	114.42
45	A	614	DGD	CDB-CCB-CBB	-2.80	100.24	114.37
32	C	511	CLA	C3B-C4B-NB	-2.79	108.04	110.53
32	G	101	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
32	a	405	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
43	D	405	PL9	C40-C39-C41	2.79	120.08	115.23
31	B	624	8CT	C29-C28-C26	-2.79	120.32	126.32
31	b	623	8CT	C29-C28-C26	-2.79	120.32	126.32
32	9	603	CLA	C3B-C4B-NB	-2.79	108.04	110.53
33	2	610	KC2	C1A-NA-C4A	-2.79	105.41	106.68
32	6	604	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
32	1	612	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
32	p	308	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
32	g	102	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
32	8	611	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
32	4	613	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
32	c	502	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
38	A	612	LHG	O8-C23-C24	2.78	120.33	111.83
32	5	304	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
32	5	312	CLA	C3B-C4B-NB	-2.78	108.05	110.53
32	6	603	CLA	C3B-C4B-NB	-2.78	108.05	110.53
32	c	511	CLA	C3B-C4B-NB	-2.78	108.05	110.53
32	P	608	CLA	C3B-C4B-NB	-2.78	108.05	110.53
32	C	510	CLA	C1-C2-C3	-2.78	121.64	126.20
31	9	615	8CT	C13-C14-C15	-2.78	115.14	123.20
32	2	602	CLA	C3B-C4B-NB	-2.78	108.05	110.53
32	0	611	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
38	L	101	LHG	O8-C23-C24	2.78	120.32	111.83
32	8	602	CLA	C3B-C4B-NB	-2.78	108.05	110.53
32	8	612	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
31	3	615	8CT	C13-C14-C15	-2.78	115.14	123.20
32	P	601	CLA	C3B-C4B-NB	-2.78	108.05	110.53
45	C	515	DGD	CDB-CCB-CBB	-2.78	100.32	114.37
31	C	518	8CT	C35-C30-C29	2.78	116.02	112.83
45	c	515	DGD	CDB-CCB-CBB	-2.78	100.33	114.37
32	1	607	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
32	2	611	CLA	C3B-C4B-NB	-2.78	108.05	110.53
32	p	307	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
38	l	102	LHG	O8-C23-C24	2.77	120.29	111.83
32	4	605	CLA	C3B-C4B-NB	-2.77	108.06	110.53
31	A	610	8CT	C25-C24-C23	-2.77	115.17	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	0	605	CLA	C3B-C4B-NB	-2.77	108.06	110.53
32	7	606	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
31	K	101	8CT	C29-C28-C26	-2.77	120.37	126.32
32	2	607	CLA	C3B-C4B-NB	-2.77	108.06	110.53
32	4	608	CLA	C3B-C4B-NB	-2.77	108.06	110.53
32	8	603	CLA	C3B-C4B-NB	-2.77	108.06	110.53
34	2	619	II0	C19-C13-C11	2.77	119.51	114.42
32	8	611	CLA	C3B-C4B-NB	-2.76	108.06	110.53
32	B	604	CLA	C3B-C4B-NB	-2.76	108.06	110.53
31	a	413	8CT	C25-C24-C23	-2.76	115.19	123.20
32	3	608	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
32	2	605	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
32	7	611	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
32	9	611	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
33	1	610	KC2	O1D-CGD-CBD	-2.76	119.07	124.52
32	6	604	CLA	C3B-C4B-NB	-2.76	108.06	110.53
32	2	606	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
38	d	405	LHG	O8-C23-C24	2.76	120.26	111.83
32	c	512	CLA	C3B-C4B-NB	-2.76	108.06	110.53
38	a	402	LHG	O8-C23-C24	2.76	120.25	111.83
32	p	308	CLA	C3B-C4B-NB	-2.76	108.07	110.53
32	C	502	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
32	6	611	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
32	6	601	CLA	C3B-C4B-NB	-2.76	108.07	110.53
32	9	611	CLA	C3B-C4B-NB	-2.76	108.07	110.53
38	D	406	LHG	O8-C23-C24	2.76	120.25	111.83
32	7	607	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
32	8	606	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
32	7	612	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
32	B	607	CLA	C3B-C4B-NB	-2.76	108.07	110.53
34	7	616	II0	C20-C14-C10	-2.75	119.01	124.16
32	4	607	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
32	c	513	CLA	C3B-C4B-NB	-2.75	108.07	110.53
32	1	611	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
32	9	608	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
32	P	607	CLA	C3B-C4B-NB	-2.75	108.07	110.53
32	B	605	CLA	C1-C2-C3	-2.75	121.69	126.20
32	0	603	CLA	C3B-C4B-NB	-2.75	108.08	110.53
32	8	605	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
38	B	619	LHG	O8-C23-C24	2.75	120.22	111.83
31	3	615	8CT	C01-C02-C07	2.75	119.46	113.60
32	P	611	CLA	O2D-CGD-O1D	-2.75	118.50	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2	603	CLA	C3B-C4B-NB	-2.75	108.08	110.53
32	5	302	CLA	C3B-C4B-NB	-2.75	108.08	110.53
31	k	102	8CT	C29-C28-C26	-2.75	120.41	126.32
34	4	616	II0	C20-C14-C12	2.75	119.47	114.42
32	1	602	CLA	C3B-C4B-NB	-2.75	108.08	110.53
32	0	604	CLA	C3B-C4B-NB	-2.75	108.08	110.53
32	0	602	CLA	C3B-C4B-NB	-2.74	108.08	110.53
32	3	611	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
32	5	308	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
32	6	611	CLA	C3B-C4B-NB	-2.74	108.08	110.53
45	a	414	DGD	O5D-C6D-C5D	-2.74	103.24	109.42
38	b	619	LHG	O8-C23-C24	2.74	120.19	111.83
34	5	315	II0	C20-C14-C12	2.74	119.46	114.42
31	c	518	8CT	C35-C30-C29	2.74	115.97	112.83
32	b	606	CLA	C3B-C4B-NB	-2.74	108.08	110.53
37	2	617	LMG	O6-C1-O1	-2.74	103.57	110.04
32	C	503	CLA	C3B-C4B-NB	-2.74	108.09	110.53
34	0	616	II0	C20-C14-C12	2.74	119.45	114.42
32	C	503	CLA	O2D-CGD-CBD	2.74	116.01	111.23
32	1	606	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
32	P	604	CLA	C3B-C4B-NB	-2.73	108.09	110.53
33	8	610	KC2	O2D-CGD-O1D	-2.73	118.53	123.85
32	0	612	CLA	C3B-C4B-NB	-2.73	108.09	110.53
32	C	513	CLA	C3B-C4B-NB	-2.73	108.09	110.53
31	A	610	8CT	C24-C25-C26	-2.73	123.45	127.28
31	A	610	8CT	C13-C14-C15	-2.73	115.28	123.20
33	8	610	KC2	C1A-NA-C4A	-2.73	105.43	106.68
31	Z	101	8CT	C25-C24-C23	-2.73	115.29	123.20
33	7	610	KC2	O1D-CGD-CBD	-2.73	119.14	124.52
32	0	607	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
33	2	610	KC2	O2D-CGD-O1D	-2.73	118.54	123.85
34	p	301	II0	C32-C30-C26	-2.72	118.99	126.61
34	5	319	II0	C20-C14-C10	-2.72	119.07	124.16
32	B	606	CLA	C3B-C4B-NB	-2.72	108.10	110.53
38	b	621	LHG	O8-C23-C24	2.72	120.14	111.83
32	4	602	CLA	C3B-C4B-NB	-2.72	108.10	110.53
32	3	606	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
32	1	603	CLA	C1-C2-C3	-2.72	122.36	126.76
37	8	617	LMG	O6-C1-O1	-2.72	103.62	110.04
32	B	610	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
45	h	101	DGD	CDB-CCB-CBB	-2.72	100.63	114.37
32	3	611	CLA	C3B-C4B-NB	-2.72	108.11	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	610	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
45	H	101	DGD	CDB-CCB-CBB	-2.72	100.64	114.37
31	9	615	8CT	C01-C02-C07	2.72	119.39	113.60
34	2	619	II0	C20-C14-C12	2.71	119.41	114.42
31	a	413	8CT	C27-C26-C28	2.71	122.23	118.09
35	6	613	II3	C22-C18-C17	2.71	119.41	114.42
34	5	301	II0	C31-C29-C25	-2.71	119.03	126.61
38	B	621	LHG	O8-C23-C24	2.71	120.10	111.83
32	5	308	CLA	C3B-C4B-NB	-2.71	108.11	110.53
37	g	101	LMG	O6-C1-O1	-2.71	103.64	110.04
31	k	101	8CT	C24-C25-C26	-2.71	123.48	127.28
31	A	610	8CT	C35-C30-C29	-2.71	109.71	112.83
32	7	602	CLA	C3B-C4B-NB	-2.70	108.12	110.53
32	b	605	CLA	C1-C2-C3	-2.70	121.77	126.20
32	9	606	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
31	k	102	8CT	C14-C13-C12	-2.70	123.49	127.28
32	b	616	CLA	C3B-C4B-NB	-2.70	108.12	110.53
32	B	616	CLA	C3B-C4B-NB	-2.70	108.12	110.53
32	b	609	CLA	C3B-C4B-NB	-2.70	108.12	110.53
37	6	616	LMG	O6-C1-O1	-2.70	103.67	110.04
32	C	508	CLA	C3B-C4B-NB	-2.70	108.12	110.53
34	1	617	II0	C42-C41-C39	-2.69	118.01	123.52
32	P	611	CLA	C3B-C4B-NB	-2.69	108.12	110.53
38	a	403	LHG	O8-C23-C24	2.69	120.05	111.83
38	A	613	LHG	O8-C23-C24	2.69	120.04	111.83
32	c	507	CLA	C3B-C4B-NB	-2.69	108.13	110.53
31	k	101	8CT	C22-C21-C23	2.69	122.19	118.09
35	P	613	II3	C22-C18-C17	2.69	119.36	114.42
32	1	611	CLA	C3B-C4B-NB	-2.69	108.13	110.53
37	P	616	LMG	O6-C1-O1	-2.69	103.70	110.04
38	d	411	LHG	O8-C23-C24	2.68	120.02	111.83
32	C	509	CLA	C3B-C4B-NB	-2.68	108.14	110.53
32	4	604	CLA	C3B-C4B-NB	-2.68	108.14	110.53
38	D	410	LHG	O8-C23-C24	2.68	120.01	111.83
32	7	611	CLA	C3B-C4B-NB	-2.68	108.14	110.53
32	4	612	CLA	C3B-C4B-NB	-2.68	108.14	110.53
31	K	102	8CT	C11-C10-C03	-2.68	119.84	127.00
31	a	413	8CT	C14-C15-C16	-2.68	119.02	126.36
32	c	509	CLA	C3B-C4B-NB	-2.67	108.14	110.53
34	8	619	II0	C19-C13-C11	2.67	119.33	114.42
32	b	607	CLA	C3B-C4B-NB	-2.67	108.14	110.53
31	9	615	8CT	C10-C03-C02	-2.67	115.40	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	p	301	II0	C20-C14-C10	-2.67	119.17	124.16
45	A	614	DGD	O5D-C6D-C5D	-2.67	103.40	109.42
31	3	615	8CT	C10-C03-C02	-2.67	115.41	121.56
33	7	610	KC2	C1A-NA-C4A	-2.67	105.46	106.68
32	A	603	CLA	O2D-CGD-CBD	2.67	115.89	111.23
41	A	604	PHO	CMB-C2B-C3B	2.66	130.01	124.68
32	1	612	CLA	C3B-C4B-NB	-2.66	108.15	110.53
32	C	501	CLA	C3B-C4B-NB	-2.66	108.15	110.53
37	d	406	LMG	C1-C2-C3	-2.66	104.41	110.01
41	a	407	PHO	CMB-C2B-C3B	2.66	130.00	124.68
34	0	617	II0	C31-C33-C35	-2.66	119.07	126.36
32	D	404	CLA	C3B-C4B-NB	-2.65	108.16	110.53
34	1	616	II0	C20-C14-C10	-2.65	119.20	124.16
39	5	318	SQD	O9-S-C6	2.65	110.72	106.76
32	C	507	CLA	C3B-C4B-NB	-2.65	108.16	110.53
31	K	102	8CT	C22-C21-C23	2.65	122.14	118.09
34	5	319	II0	C32-C30-C26	-2.65	119.20	126.61
31	a	413	8CT	C07-C02-C03	-2.65	119.13	122.70
32	c	501	CLA	C3B-C4B-NB	-2.65	108.17	110.53
32	c	504	CLA	C3B-C4B-NB	-2.65	108.17	110.53
34	1	619	II0	C20-C14-C12	2.65	119.28	114.42
32	1	609	CLA	CAA-C2A-C3A	-2.64	110.17	116.23
31	z	101	8CT	C25-C24-C23	-2.64	115.54	123.20
37	D	407	LMG	C1-C2-C3	-2.64	104.45	110.01
32	7	604	CLA	C3B-C4B-NB	-2.64	108.17	110.53
31	3	615	8CT	C18-C19-C20	-2.64	118.12	123.52
31	Z	101	8CT	C19-C18-C17	-2.64	118.12	123.52
32	c	507	CLA	CHB-C4A-NA	2.64	128.20	124.40
32	d	403	CLA	C3B-C4B-NB	-2.63	108.18	110.53
32	S	302	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
31	k	101	8CT	C11-C10-C03	-2.63	119.98	127.00
34	4	616	II0	C31-C33-C35	-2.63	119.16	126.36
32	1	604	CLA	C3B-C4B-NB	-2.63	108.19	110.53
32	c	508	CLA	C3B-C4B-NB	-2.63	108.19	110.53
34	2	615	II0	C20-C14-C10	-2.63	119.25	124.16
38	S	301	LHG	O8-C23-C24	2.63	119.84	111.83
34	7	619	II0	C20-C14-C12	2.62	119.25	114.42
37	L	102	LMG	O6-C1-O1	-2.62	103.84	110.04
32	d	409	CLA	CHB-C4A-NA	2.62	128.19	124.40
31	9	615	8CT	C18-C19-C20	-2.62	118.16	123.52
34	0	616	II0	C31-C33-C35	-2.62	119.18	126.36
35	1	615	II3	C22-C18-C16	-2.62	119.27	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	8	615	II0	C20-C14-C10	-2.62	119.27	124.16
32	C	507	CLA	CHB-C4A-NA	2.62	128.17	124.40
32	D	401	CLA	CHB-C4A-NA	2.61	128.17	124.40
32	8	604	CLA	C3B-C4B-NB	-2.61	108.20	110.53
34	2	619	II0	C20-C14-C10	-2.61	119.28	124.16
37	l	101	LMG	O6-C1-O1	-2.61	103.87	110.04
32	7	612	CLA	C3B-C4B-NB	-2.61	108.20	110.53
38	s	301	LHG	O8-C23-C24	2.61	119.79	111.83
32	a	405	CLA	C3B-C4B-NB	-2.61	108.20	110.53
33	6	605	KC2	O1D-CGD-CBD	-2.61	119.37	124.52
32	7	609	CLA	CAA-C2A-C3A	-2.61	110.26	116.23
38	B	619	LHG	C11-C10-C9	-2.60	101.21	114.37
32	7	611	CLA	CHB-C4A-NA	2.60	128.16	124.40
43	A	609	PL9	C7-C3-C4	2.60	120.76	117.88
32	0	611	CLA	C3B-C4B-NB	-2.60	108.21	110.53
34	7	617	II0	C42-C41-C39	-2.60	118.20	123.52
34	4	616	II0	C31-C29-C25	-2.60	119.34	126.61
34	p	315	II0	C20-C14-C12	2.60	119.20	114.42
38	b	619	LHG	C11-C10-C9	-2.60	101.23	114.37
32	C	504	CLA	C3B-C4B-NB	-2.60	108.21	110.53
34	5	301	II0	C31-C33-C35	-2.60	119.24	126.36
32	9	603	CLA	C1-C2-C3	-2.60	122.56	126.76
31	K	102	8CT	C19-C20-C21	-2.60	123.64	127.28
32	0	606	CLA	C3B-C4B-NB	-2.60	108.21	110.53
32	A	602	CLA	C3B-C4B-NB	-2.60	108.21	110.53
32	2	604	CLA	C3B-C4B-NB	-2.59	108.21	110.53
32	P	610	CLA	CHB-C4A-NA	2.59	128.14	124.40
38	8	618	LHG	O8-C23-C24	2.59	119.75	111.83
31	b	622	8CT	C29-C28-C26	-2.59	120.75	126.32
32	b	607	CLA	CHB-C4A-NA	2.59	128.14	124.40
38	2	618	LHG	O8-C23-C24	2.59	119.74	111.83
32	C	510	CLA	C3B-C4B-NB	-2.59	108.22	110.53
32	b	605	CLA	CHB-C4A-NA	2.59	128.14	124.40
32	3	603	CLA	C1-C2-C3	-2.59	122.58	126.76
32	g	102	CLA	C3B-C4B-NB	-2.59	108.22	110.53
37	D	407	LMG	O6-C1-O1	-2.59	103.94	110.04
32	b	603	CLA	C3B-C4B-NB	-2.58	108.22	110.53
32	G	101	CLA	C3B-C4B-NB	-2.58	108.22	110.53
34	5	319	II0	C31-C29-C25	-2.58	119.38	126.61
32	B	603	CLA	C3B-C4B-NB	-2.58	108.22	110.53
34	7	619	II0	C27-C25-C29	-2.58	119.17	124.18
31	B	623	8CT	C29-C28-C26	-2.58	120.77	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	0	616	II0	C31-C29-C25	-2.58	119.40	126.61
35	1	615	II3	C29-C26-C24	-2.58	123.67	127.28
31	Z	101	8CT	C40-C12-C11	2.57	122.02	118.09
34	9	614	II0	C31-C29-C25	-2.57	119.41	126.61
32	3	602	CLA	C1-C2-C3	-2.57	121.98	126.20
37	d	406	LMG	O6-C1-O1	-2.57	103.96	110.04
32	4	602	CLA	CHB-C4A-NA	2.57	128.11	124.40
32	0	602	CLA	CHB-C4A-NA	2.57	128.11	124.40
33	4	610	KC2	CHD-C4C-NC	2.57	128.19	124.31
32	c	510	CLA	C3B-C4B-NB	-2.57	108.23	110.53
32	8	606	CLA	C3B-C4B-NB	-2.57	108.23	110.53
32	6	607	CLA	CHB-C4A-NA	2.57	128.11	124.40
32	7	603	CLA	C1-C2-C3	-2.57	122.60	126.76
37	C	517	LMG	O6-C1-O1	-2.57	103.97	110.04
32	4	612	CLA	CHB-C4A-NA	2.57	128.11	124.40
32	2	608	CLA	CHB-C4A-NA	2.57	128.11	124.40
32	P	611	CLA	CHB-C4A-NA	2.57	128.11	124.40
32	b	610	CLA	C3B-C4B-NB	-2.57	108.24	110.53
32	P	602	CLA	C1-C2-C3	-2.57	121.99	126.20
32	a	408	CLA	CHB-C4A-NA	2.57	128.11	124.40
32	4	606	CLA	C3B-C4B-NB	-2.57	108.24	110.53
32	B	610	CLA	C3B-C4B-NB	-2.57	108.24	110.53
32	C	503	CLA	C1-C2-C3	-2.57	121.99	126.20
34	1	619	II0	C27-C25-C29	-2.57	119.19	124.18
33	0	610	KC2	O1D-CGD-CBD	-2.57	119.46	124.52
32	1	611	CLA	CHB-C4A-NA	2.57	128.10	124.40
32	6	610	CLA	CHB-C4A-NA	2.57	128.10	124.40
34	P	614	II0	C31-C29-C25	-2.57	119.43	126.61
37	b	618	LMG	O6-C1-O1	-2.57	103.98	110.04
32	s	302	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
34	6	612	II0	C20-C14-C10	-2.56	119.37	124.16
43	a	412	PL9	C7-C3-C4	2.56	120.72	117.88
36	2	616	IHT	C20-C15-C11	-2.56	119.37	124.16
34	0	617	II0	C31-C29-C25	-2.56	119.44	126.61
37	c	517	LMG	O6-C1-O1	-2.56	103.99	110.04
32	0	612	CLA	CHB-C4A-NA	2.56	128.10	124.40
32	B	607	CLA	CHB-C4A-NA	2.56	128.09	124.40
43	d	404	PL9	C27-C28-C29	-2.56	121.77	127.62
34	8	619	II0	C20-C14-C10	-2.56	119.38	124.16
34	1	614	II0	C20-C14-C12	2.56	119.12	114.42
32	8	608	CLA	CHB-C4A-NA	2.55	128.09	124.40
43	D	405	PL9	C27-C28-C29	-2.55	121.78	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	P	607	CLA	CHB-C4A-NA	2.55	128.08	124.40
33	0	610	KC2	CHD-C4C-NC	2.55	128.15	124.31
34	4	615	II0	C42-C41-C39	-2.55	118.30	123.52
32	c	503	CLA	C1-C2-C3	-2.55	122.02	126.20
31	z	101	8CT	C19-C18-C17	-2.55	118.30	123.52
32	4	609	CLA	CAA-C2A-C3A	-2.55	110.39	116.23
38	s	301	LHG	C11-C10-C9	-2.55	101.49	114.37
33	4	610	KC2	O1D-CGD-CBD	-2.55	119.49	124.52
32	0	609	CLA	CAA-C2A-C3A	-2.55	110.39	116.23
32	2	606	CLA	C3B-C4B-NB	-2.55	108.26	110.53
32	8	603	CLA	C1-C2-C3	-2.55	122.64	126.76
36	0	618	IHT	C20-C15-C12	2.54	119.10	114.42
32	B	613	CLA	C3B-C4B-NB	-2.54	108.26	110.53
32	9	602	CLA	C1-C2-C3	-2.54	122.03	126.20
32	B	616	CLA	CHB-C4A-NA	2.54	128.07	124.40
37	B	618	LMG	O6-C1-O1	-2.54	104.03	110.04
32	b	617	CLA	C3B-C4B-NB	-2.54	108.26	110.53
34	p	301	II0	C32-C34-C36	-2.54	119.39	126.36
32	1	604	CLA	CHB-C4A-NA	2.54	128.07	124.40
34	0	617	II0	C19-C13-C09	-2.54	119.41	124.16
32	7	605	CLA	C3B-C4B-NB	-2.54	108.27	110.53
39	p	318	SQD	O9-S-C6	2.54	110.54	106.76
33	P	609	KC2	CHD-C4C-NC	2.54	128.13	124.31
32	c	505	CLA	C3B-C4B-NB	-2.54	108.27	110.53
32	b	616	CLA	CHB-C4A-NA	2.54	128.06	124.40
32	p	303	CLA	CHB-C4A-NA	2.54	128.06	124.40
32	2	603	CLA	C1-C2-C3	-2.54	122.66	126.76
31	d	408	8CT	C14-C15-C16	-2.54	119.41	126.36
38	S	301	LHG	C11-C10-C9	-2.54	101.55	114.37
34	p	314	II0	C20-C14-C10	-2.53	119.42	124.16
32	B	605	CLA	CHB-C4A-NA	2.53	128.06	124.40
31	D	409	8CT	C14-C15-C16	-2.53	119.42	126.36
31	k	101	8CT	C19-C20-C21	-2.53	123.73	127.28
37	a	410	LMG	C40-C39-C38	-2.53	101.58	114.37
34	p	316	II0	C42-C41-C39	-2.53	118.34	123.52
32	5	303	CLA	CHB-C4A-NA	2.53	128.05	124.40
32	5	310	CLA	CAA-C2A-C3A	-2.53	110.43	116.23
33	5	311	KC2	CHD-C4C-NC	2.53	128.12	124.31
37	A	607	LMG	C40-C39-C38	-2.53	101.59	114.37
34	1	619	II0	C31-C29-C25	-2.53	119.54	126.61
33	p	311	KC2	CHD-C4C-NC	2.53	128.12	124.31
32	C	505	CLA	C3B-C4B-NB	-2.53	108.27	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	B	617	CLA	C3B-C4B-NB	-2.53	108.27	110.53
36	2	616	IHT	C19-C10-C09	2.53	118.98	113.60
32	5	309	CLA	CHB-C4A-NA	2.53	128.04	124.40
45	H	101	DGD	C3G-C2G-C1G	-2.52	105.90	111.78
32	9	610	CLA	CHB-C4A-NA	2.52	128.04	124.40
34	7	619	II0	C31-C29-C25	-2.52	119.55	126.61
32	5	303	CLA	C1-C2-C3	-2.52	122.06	126.20
32	6	611	CLA	CHB-C4A-NA	2.52	128.04	124.40
45	a	414	DGD	C3G-C2G-C1G	-2.52	105.90	111.78
33	6	609	KC2	CHD-C4C-NC	2.52	128.10	124.31
32	8	611	CLA	CHB-C4A-NA	2.52	128.03	124.40
32	c	503	CLA	CHB-C4A-NA	2.52	128.03	124.40
32	7	602	CLA	CHB-C4A-NA	2.52	128.03	124.40
34	0	615	II0	C20-C14-C12	2.52	119.05	114.42
32	b	613	CLA	C3B-C4B-NB	-2.52	108.28	110.53
32	6	602	CLA	C1-C2-C3	-2.52	122.07	126.20
32	p	305	CLA	CHB-C4A-NA	2.52	128.03	124.40
32	p	303	CLA	C1-C2-C3	-2.52	122.08	126.20
32	9	607	CLA	CHB-C4A-NA	2.52	128.03	124.40
32	C	503	CLA	CHB-C4A-NA	2.52	128.03	124.40
32	0	612	CLA	O2D-CGD-CBD	2.52	115.63	111.23
45	A	614	DGD	C3G-C2G-C1G	-2.51	105.92	111.78
32	D	404	CLA	CHB-C4A-NA	2.51	128.03	124.40
32	d	403	CLA	CHB-C4A-NA	2.51	128.03	124.40
31	9	615	8CT	C10-C11-C12	-2.51	122.52	126.23
31	6	615	8CT	C35-C30-C29	-2.51	109.94	112.83
32	p	310	CLA	CAA-C2A-C3A	-2.51	110.47	116.23
34	0	617	II0	C20-C14-C12	2.51	119.04	114.42
31	P	615	8CT	C35-C30-C29	-2.51	109.94	112.83
32	2	611	CLA	CHB-C4A-NA	2.51	128.03	124.40
32	0	607	CLA	C3B-C4B-NB	-2.51	108.29	110.53
32	7	606	CLA	C3B-C4B-NB	-2.51	108.29	110.53
32	0	608	CLA	CHB-C4A-NA	2.51	128.02	124.40
45	h	101	DGD	C3G-C2G-C1G	-2.51	105.93	111.78
31	z	101	8CT	C40-C12-C11	2.51	121.92	118.09
38	D	406	LHG	C11-C10-C9	-2.51	101.68	114.37
32	2	602	CLA	CHB-C4A-NA	2.51	128.02	124.40
32	P	602	CLA	CHB-C4A-NA	2.51	128.02	124.40
32	4	608	CLA	CHB-C4A-NA	2.51	128.02	124.40
32	d	409	CLA	C3B-C4B-NB	-2.51	108.29	110.53
32	1	602	CLA	CHB-C4A-NA	2.51	128.02	124.40
32	B	617	CLA	CHB-C4A-NA	2.51	128.02	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	c	514	DGD	C3G-C2G-C1G	-2.51	105.94	111.78
36	8	616	IHT	C19-C10-C09	2.51	118.94	113.60
32	b	614	CLA	C3B-C4B-NB	-2.51	108.29	110.53
32	b	617	CLA	CHB-C4A-NA	2.51	128.02	124.40
38	d	405	LHG	C11-C10-C9	-2.51	101.69	114.37
32	1	613	CLA	C3B-C4B-NB	-2.51	108.29	110.53
32	6	602	CLA	CHB-C4A-NA	2.51	128.02	124.40
32	5	305	CLA	CHB-C4A-NA	2.50	128.01	124.40
34	4	619	II0	C20-C14-C12	2.50	119.03	114.42
32	c	509	CLA	CHB-C4A-NA	2.50	128.01	124.40
32	D	401	CLA	C3B-C4B-NB	-2.50	108.30	110.53
32	7	604	CLA	CHB-C4A-NA	2.50	128.01	124.40
33	8	610	KC2	CHD-C4C-NC	2.50	128.08	124.31
38	L	101	LHG	C11-C10-C9	-2.50	101.72	114.37
32	c	501	CLA	CHB-C4A-NA	2.50	128.01	124.40
34	4	615	II0	C20-C14-C12	2.50	119.02	114.42
34	0	615	II0	C19-C13-C09	-2.50	119.48	124.16
38	l	102	LHG	C11-C10-C9	-2.50	101.73	114.37
31	3	615	8CT	C10-C11-C12	-2.50	122.54	126.23
45	h	101	DGD	C1D-C2D-C3D	-2.50	104.75	110.01
32	9	603	CLA	CHB-C4A-NA	2.50	128.00	124.40
32	4	612	CLA	O2D-CGD-CBD	2.50	115.60	111.23
32	9	601	CLA	CHB-C4A-NA	2.50	128.00	124.40
32	1	605	CLA	C3B-C4B-NB	-2.50	108.30	110.53
34	5	301	II0	C27-C25-C29	-2.50	119.33	124.18
32	4	603	CLA	C1-C2-C3	-2.50	122.72	126.76
32	0	603	CLA	C1-C2-C3	-2.50	122.72	126.76
32	A	605	CLA	CHB-C4A-NA	2.49	128.00	124.40
45	C	514	DGD	C3G-C2G-C1G	-2.49	105.97	111.78
34	p	301	II0	C28-C26-C30	-2.49	119.34	124.18
37	B	618	LMG	C40-C39-C38	-2.49	101.76	114.37
33	P	609	KC2	O1D-CGD-CBD	-2.49	119.60	124.52
32	C	509	CLA	CHB-C4A-NA	2.49	128.00	124.40
32	8	603	CLA	CHB-C4A-NA	2.49	128.00	124.40
34	7	616	II0	C20-C14-C12	2.49	119.00	114.42
36	5	317	IHT	C31-C29-C26	-2.49	119.64	126.61
32	6	603	CLA	C1-C2-C3	-2.49	122.73	126.76
32	4	611	CLA	C3B-C4B-NB	-2.49	108.31	110.53
32	B	602	CLA	CHB-C4A-NA	2.49	127.99	124.40
36	4	617	IHT	C41-C40-C37	-2.49	118.43	123.52
32	3	607	CLA	CHB-C4A-NA	2.49	127.99	124.40
34	3	614	II0	C31-C29-C25	-2.49	119.65	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	3	610	CLA	CHB-C4A-NA	2.49	127.99	124.40
32	a	405	CLA	CHB-C4A-NA	2.49	127.99	124.40
32	B	614	CLA	C3B-C4B-NB	-2.49	108.31	110.53
32	8	602	CLA	CHB-C4A-NA	2.49	127.99	124.40
32	C	501	CLA	CHB-C4A-NA	2.49	127.99	124.40
45	H	101	DGD	C1D-C2D-C3D	-2.49	104.78	110.01
32	6	603	CLA	CHB-C4A-NA	2.48	127.99	124.40
32	p	309	CLA	CHB-C4A-NA	2.48	127.99	124.40
32	b	617	CLA	C1-C2-C3	-2.48	122.13	126.20
34	8	613	II0	C19-C13-C09	-2.48	119.52	124.16
32	3	602	CLA	CHB-C4A-NA	2.48	127.98	124.40
33	P	605	KC2	CHD-C4C-NC	2.48	128.05	124.31
32	2	612	CLA	C3B-C4B-NB	-2.48	108.31	110.53
33	6	609	KC2	O1D-CGD-CBD	-2.48	119.62	124.52
32	A	602	CLA	CHB-C4A-NA	2.48	127.98	124.40
32	c	513	CLA	CHB-C4A-NA	2.48	127.98	124.40
32	1	606	CLA	CHB-C4A-NA	2.48	127.98	124.40
32	P	603	CLA	CHB-C4A-NA	2.48	127.98	124.40
32	8	609	CLA	CAA-C2A-C3A	-2.48	110.54	116.23
39	b	620	SQD	O8-S-C6	2.48	110.76	105.97
32	2	604	CLA	CHB-C4A-NA	2.48	127.98	124.40
36	p	317	IHT	C31-C29-C26	-2.48	119.67	126.61
34	P	614	II0	C19-C13-C09	-2.48	119.53	124.16
32	2	609	CLA	CAA-C2A-C3A	-2.48	110.55	116.23
36	5	317	IHT	C31-C34-C35	-2.48	119.57	126.36
34	1	617	II0	C20-C14-C10	-2.48	119.53	124.16
34	8	613	II0	C20-C14-C10	-2.48	119.53	124.16
37	b	618	LMG	C38-C37-C36	-2.48	101.84	114.37
32	3	603	CLA	CHB-C4A-NA	2.48	127.97	124.40
32	d	402	CLA	CMB-C2B-C3B	2.47	130.11	123.53
33	5	311	KC2	CHB-C4A-C3A	-2.47	121.12	125.03
45	C	516	DGD	C3G-C2G-C1G	-2.47	106.02	111.78
45	c	516	DGD	C3G-C2G-C1G	-2.47	106.02	111.78
31	Z	101	8CT	C39-C16-C15	2.47	121.86	118.09
34	2	614	II0	C20-C14-C10	-2.47	119.54	124.16
37	b	618	LMG	C40-C39-C38	-2.47	101.88	114.37
32	2	603	CLA	CHB-C4A-NA	2.47	127.97	124.40
34	5	315	II0	C32-C30-C26	-2.47	119.70	126.61
35	7	615	II3	C22-C18-C16	-2.47	119.54	124.16
34	8	619	II0	C20-C14-C12	2.47	118.96	114.42
32	3	601	CLA	CHB-C4A-NA	2.47	127.96	124.40
39	B	620	SQD	O8-S-C6	2.47	110.74	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	8	604	CLA	CHB-C4A-NA	2.47	127.96	124.40
31	6	615	8CT	C14-C15-C16	-2.47	119.60	126.36
34	5	301	II0	C20-C14-C12	2.47	118.96	114.42
37	B	618	LMG	C38-C37-C36	-2.47	101.90	114.37
32	C	513	CLA	CHB-C4A-NA	2.46	127.96	124.40
38	a	403	LHG	C20-C19-C18	-2.46	101.91	114.37
32	4	613	CLA	CHB-C4A-NA	2.46	127.96	124.40
38	a	402	LHG	C11-C10-C9	-2.46	101.91	114.37
33	5	311	KC2	O1D-CGD-CBD	-2.46	119.66	124.52
32	B	617	CLA	C1-C2-C3	-2.46	122.16	126.20
34	7	614	II0	C19-C13-C11	2.46	118.95	114.42
32	7	608	CLA	CHB-C4A-NA	2.46	127.95	124.40
33	2	610	KC2	CHD-C4C-NC	2.46	128.02	124.31
38	A	613	LHG	C20-C19-C18	-2.46	101.92	114.37
32	c	512	CLA	CHB-C4A-NA	2.46	127.95	124.40
34	0	616	II0	C20-C14-C10	-2.46	119.56	124.16
32	2	605	CLA	CHB-C4A-NA	2.46	127.95	124.40
32	C	502	CLA	C3B-C4B-NB	-2.46	108.33	110.53
32	0	605	CLA	CHB-C4A-NA	2.46	127.95	124.40
32	p	312	CLA	CHB-C4A-NA	2.46	127.95	124.40
32	7	606	CLA	CHB-C4A-NA	2.46	127.95	124.40
31	a	413	8CT	C28-C26-C25	-2.46	115.14	119.01
32	b	602	CLA	CHB-C4A-NA	2.46	127.95	124.40
32	4	605	CLA	CHB-C4A-NA	2.46	127.94	124.40
32	b	610	CLA	CHB-C4A-NA	2.46	127.94	124.40
31	Z	101	8CT	C18-C19-C20	-2.46	118.49	123.52
32	8	612	CLA	C3B-C4B-NB	-2.45	108.34	110.53
38	B	621	LHG	C11-C10-C9	-2.45	101.97	114.37
32	b	608	CLA	CAA-C2A-C3A	-2.45	110.61	116.23
32	2	602	CLA	C1-C2-C3	-2.45	122.18	126.20
32	7	609	CLA	CHB-C4A-NA	2.45	127.94	124.40
32	p	308	CLA	CHB-C4A-NA	2.45	127.94	124.40
33	p	311	KC2	O1D-CGD-CBD	-2.45	119.69	124.52
32	C	504	CLA	CHB-C4A-NA	2.45	127.94	124.40
32	8	602	CLA	C1-C2-C3	-2.45	122.18	126.20
32	D	403	CLA	CMB-C2B-C3B	2.45	130.04	123.53
32	c	504	CLA	CHB-C4A-NA	2.45	127.94	124.40
32	C	508	CLA	CHB-C4A-NA	2.45	127.94	124.40
38	A	612	LHG	C11-C10-C9	-2.45	101.99	114.37
36	2	616	IHT	C41-C40-C37	-2.45	118.51	123.52
32	b	613	CLA	CHB-C4A-NA	2.45	127.93	124.40
32	1	608	CLA	CHB-C4A-NA	2.45	127.93	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	7	613	CLA	CHB-C4A-NA	2.45	127.93	124.40
32	C	511	CLA	CHB-C4A-NA	2.45	127.93	124.40
32	P	603	CLA	C1-C2-C3	-2.45	122.80	126.76
32	9	611	CLA	CHB-C4A-NA	2.45	127.93	124.40
38	b	621	LHG	C11-C10-C9	-2.45	102.00	114.37
32	c	505	CLA	CMB-C2B-C1B	-2.45	121.69	125.42
32	5	307	CLA	CHB-C4A-NA	2.45	127.93	124.40
32	B	615	CLA	CHB-C4A-NA	2.45	127.93	124.40
45	c	515	DGD	O5D-C6D-C5D	-2.45	103.91	109.42
45	C	515	DGD	O5D-C6D-C5D	-2.44	103.91	109.42
33	6	605	KC2	C1B-CHB-C4A	-2.44	120.82	126.02
32	3	611	CLA	CHB-C4A-NA	2.44	127.93	124.40
32	9	602	CLA	CHB-C4A-NA	2.44	127.93	124.40
32	B	608	CLA	CAA-C2A-C3A	-2.44	110.63	116.23
32	C	512	CLA	CHB-C4A-NA	2.44	127.93	124.40
34	p	314	II0	C41-C42-C40	-2.44	118.52	123.52
32	5	312	CLA	CHB-C4A-NA	2.44	127.92	124.40
36	4	617	IHT	C19-C10-C09	2.44	118.80	113.60
36	2	616	IHT	C20-C15-C12	2.44	118.91	114.42
32	b	609	CLA	CMB-C2B-C1B	-2.44	121.70	125.42
32	0	601	CLA	CHB-C4A-NA	2.44	127.92	124.40
31	b	623	8CT	C11-C10-C03	-2.44	120.48	127.00
39	A	606	SQD	O5-C5-C4	2.44	114.09	109.70
39	a	409	SQD	O5-C5-C4	2.44	114.09	109.70
32	c	508	CLA	CHB-C4A-NA	2.44	127.92	124.40
32	C	506	CLA	C3B-C4B-NB	-2.44	108.36	110.53
32	B	613	CLA	CHB-C4A-NA	2.44	127.92	124.40
34	9	612	II0	C19-C13-C09	-2.44	119.61	124.16
31	b	623	8CT	C14-C15-C16	-2.44	119.68	126.36
32	c	511	CLA	CHB-C4A-NA	2.43	127.91	124.40
32	c	502	CLA	C3B-C4B-NB	-2.43	108.36	110.53
32	C	505	CLA	CMB-C2B-C1B	-2.43	121.71	125.42
32	4	607	CLA	C3B-C4B-NB	-2.43	108.36	110.53
31	k	101	8CT	C27-C26-C28	2.43	121.80	118.09
31	B	623	8CT	C13-C14-C15	-2.43	116.15	123.20
33	p	311	KC2	CHB-C4A-C3A	-2.43	121.19	125.03
32	6	604	CLA	CHB-C4A-NA	2.43	127.91	124.40
34	7	619	II0	C20-C14-C10	-2.43	119.61	124.16
36	p	317	IHT	C41-C40-C37	-2.43	118.55	123.52
31	M	201	8CT	C14-C15-C16	-2.43	119.70	126.36
34	9	612	II0	C20-C14-C10	-2.43	119.62	124.16
35	P	613	II3	C22-C18-C16	-2.43	119.62	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	3	612	II0	C20-C14-C10	-2.43	119.62	124.16
31	B	624	8CT	C11-C10-C03	-2.43	120.52	127.00
32	1	609	CLA	CHB-C4A-NA	2.43	127.90	124.40
34	6	614	II0	C31-C33-C35	-2.43	119.71	126.36
32	8	605	CLA	CHB-C4A-NA	2.43	127.90	124.40
36	8	616	IHT	C31-C29-C26	-2.42	119.83	126.61
35	6	613	II3	C22-C18-C16	-2.42	119.63	124.16
33	6	605	KC2	CHD-C4C-NC	2.42	127.96	124.31
31	B	622	8CT	C14-C15-C16	-2.42	119.72	126.36
36	8	616	IHT	C20-C15-C11	-2.42	119.63	124.16
32	7	613	CLA	C3B-C4B-NB	-2.42	108.37	110.53
34	9	614	II0	C27-C25-C29	-2.42	119.48	124.18
34	P	612	II0	C31-C33-C35	-2.42	119.73	126.36
34	p	301	II0	C31-C29-C25	-2.42	119.84	126.61
32	1	613	CLA	CHB-C4A-NA	2.42	127.89	124.40
34	p	314	II0	C20-C14-C12	2.42	118.87	114.42
32	B	610	CLA	CHB-C4A-NA	2.42	127.89	124.40
32	B	609	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
34	P	612	II0	C28-C26-C30	-2.42	119.49	124.18
33	1	610	KC2	CHD-C4C-NC	2.42	127.95	124.31
32	4	601	CLA	CHB-C4A-NA	2.42	127.89	124.40
32	b	615	CLA	CHB-C4A-NA	2.42	127.89	124.40
36	0	618	IHT	C31-C29-C26	-2.42	119.86	126.61
32	3	608	CLA	CHB-C4A-NA	2.41	127.89	124.40
32	5	304	CLA	CHB-C4A-NA	2.41	127.89	124.40
32	p	304	CLA	CHB-C4A-NA	2.41	127.89	124.40
32	b	604	CLA	CHB-C4A-NA	2.41	127.88	124.40
32	5	306	CLA	CHB-C4A-NA	2.41	127.88	124.40
34	5	319	II0	C31-C33-C35	-2.41	119.75	126.36
34	0	620	II0	C27-C25-C29	-2.41	119.50	124.18
38	l	102	LHG	C20-C19-C18	-2.41	102.18	114.37
32	7	603	CLA	CHB-C4A-NA	2.41	127.88	124.40
35	6	613	II3	C26-C29-C32	-2.41	116.21	123.20
32	s	303	CLA	CHB-C4A-NA	2.41	127.88	124.40
32	0	613	CLA	CHB-C4A-NA	2.41	127.88	124.40
38	L	101	LHG	C20-C19-C18	-2.41	102.19	114.37
31	P	615	8CT	C14-C15-C16	-2.41	119.76	126.36
34	8	614	II0	C20-C14-C10	-2.41	119.66	124.16
32	5	308	CLA	CHB-C4A-NA	2.41	127.87	124.40
32	B	612	CLA	CHB-C4A-NA	2.41	127.87	124.40
31	B	624	8CT	C14-C15-C16	-2.41	119.77	126.36
34	6	612	II0	C31-C33-C35	-2.41	119.77	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	610	8CT	C19-C18-C17	-2.41	118.60	123.52
33	7	610	KC2	CHD-C4C-NC	2.41	127.93	124.31
32	4	609	CLA	CHB-C4A-NA	2.41	127.87	124.40
32	B	604	CLA	CHB-C4A-NA	2.40	127.87	124.40
34	6	614	II0	C31-C29-C25	-2.40	119.89	126.61
34	4	619	II0	C19-C13-C09	-2.40	119.67	124.16
32	9	608	CLA	CHB-C4A-NA	2.40	127.87	124.40
32	p	307	CLA	CHB-C4A-NA	2.40	127.87	124.40
38	d	411	LHG	C11-C10-C9	-2.40	102.22	114.37
34	3	613	II0	C19-C13-C09	-2.40	119.67	124.16
38	D	406	LHG	C20-C19-C18	-2.40	102.22	114.37
32	1	603	CLA	CHB-C4A-NA	2.40	127.87	124.40
32	6	608	CLA	CAA-C2A-C3A	-2.40	110.72	116.23
34	3	613	II0	C19-C13-C11	2.40	118.84	114.42
36	7	618	IHT	C19-C10-C09	2.40	118.72	113.60
35	6	613	II3	C41-C40-C38	-2.40	123.91	127.28
34	0	617	II0	C20-C14-C10	-2.40	119.67	124.16
32	p	302	CLA	CHB-C4A-NA	2.40	127.86	124.40
38	D	410	LHG	C11-C10-C9	-2.40	102.24	114.37
37	A	607	LMG	C38-C37-C36	-2.40	102.25	114.37
38	d	405	LHG	C20-C19-C18	-2.40	102.25	114.37
37	0	619	LMG	O1-C7-C8	-2.40	104.99	110.82
32	5	302	CLA	CHB-C4A-NA	2.40	127.86	124.40
32	a	406	CLA	CHB-C4A-NA	2.40	127.86	124.40
32	S	303	CLA	CHB-C4A-NA	2.40	127.86	124.40
32	9	605	CLA	CHB-C4A-NA	2.40	127.86	124.40
38	a	403	LHG	C11-C10-C9	-2.40	102.26	114.37
32	9	604	CLA	CHB-C4A-NA	2.40	127.86	124.40
36	0	618	IHT	C31-C34-C35	-2.39	119.80	126.36
38	A	613	LHG	C11-C10-C9	-2.39	102.27	114.37
32	p	306	CLA	CHB-C4A-NA	2.39	127.86	124.40
37	a	410	LMG	C38-C37-C36	-2.39	102.27	114.37
34	4	619	II0	C42-C41-C39	-2.39	118.62	123.52
34	2	613	II0	C19-C13-C09	-2.39	119.69	124.16
32	8	601	CLA	CHB-C4A-NA	2.39	127.85	124.40
34	1	619	II0	C20-C14-C10	-2.39	119.69	124.16
31	b	622	8CT	C13-C14-C15	-2.39	116.27	123.20
34	5	319	II0	C32-C34-C36	-2.39	119.81	126.36
34	9	614	II0	C19-C13-C09	-2.39	119.69	124.16
36	0	618	IHT	C19-C10-C09	2.39	118.69	113.60
32	5	310	CLA	CHB-C4A-NA	2.39	127.85	124.40
34	5	314	II0	C20-C14-C12	2.39	118.81	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	0	609	CLA	CHB-C4A-NA	2.39	127.84	124.40
32	2	609	CLA	CHB-C4A-NA	2.39	127.84	124.40
31	K	102	8CT	C27-C26-C28	2.39	121.73	118.09
32	b	612	CLA	CHB-C4A-NA	2.39	127.84	124.40
32	P	608	CLA	CAA-C2A-C3A	-2.38	110.76	116.23
34	3	612	II0	C19-C13-C09	-2.38	119.70	124.16
31	D	409	8CT	C11-C10-C03	-2.38	120.63	127.00
32	5	313	CLA	C3B-C4B-NB	-2.38	108.40	110.53
34	2	619	II0	C19-C13-C09	-2.38	119.70	124.16
32	b	603	CLA	CHB-C4A-NA	2.38	127.84	124.40
32	B	603	CLA	CHB-C4A-NA	2.38	127.84	124.40
31	z	101	8CT	C18-C19-C20	-2.38	118.64	123.52
32	P	604	CLA	CHB-C4A-NA	2.38	127.84	124.40
32	D	401	CLA	CMB-C2B-C1B	-2.38	121.79	125.42
37	4	618	LMG	O1-C7-C8	-2.38	105.03	110.82
36	0	614	IHT	C20-C15-C12	2.38	118.80	114.42
31	c	518	8CT	C30-C29-C28	2.38	128.28	124.58
31	C	518	8CT	C30-C29-C28	2.38	128.28	124.58
32	c	506	CLA	C3B-C4B-NB	-2.38	108.41	110.53
32	3	604	CLA	CHB-C4A-NA	2.38	127.83	124.40
32	p	313	CLA	CHB-C4A-NA	2.38	127.83	124.40
34	5	319	II0	C28-C26-C30	-2.38	119.57	124.18
32	B	606	CLA	CHB-C4A-NA	2.38	127.83	124.40
36	1	618	IHT	C19-C10-C09	2.38	118.66	113.60
31	M	201	8CT	C19-C18-C17	-2.37	118.66	123.52
34	5	314	II0	C31-C33-C35	-2.37	119.85	126.36
32	b	606	CLA	CHB-C4A-NA	2.37	127.83	124.40
32	3	605	CLA	CHB-C4A-NA	2.37	127.83	124.40
35	P	613	II3	C26-C29-C32	-2.37	116.33	123.20
31	D	409	8CT	C07-C02-C03	-2.37	119.50	122.70
32	P	601	CLA	CHB-C4A-NA	2.37	127.82	124.40
31	B	622	8CT	C19-C18-C17	-2.37	118.67	123.52
36	5	317	IHT	C20-C15-C11	-2.37	119.73	124.16
34	5	316	II0	C42-C41-C39	-2.37	118.67	123.52
34	7	617	II0	C20-C14-C10	-2.37	119.73	124.16
34	3	612	II0	C19-C13-C11	2.37	118.78	114.42
32	B	608	CLA	C3B-C4B-NB	-2.37	108.41	110.53
32	0	611	CLA	CHB-C4A-NA	2.37	127.82	124.40
34	5	315	II0	C41-C42-C40	-2.37	118.67	123.52
32	b	608	CLA	C3B-C4B-NB	-2.37	108.42	110.53
32	d	402	CLA	CHB-C4A-NA	2.37	127.82	124.40
32	D	403	CLA	CAB-C3B-C2B	2.37	129.83	123.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	609	CLA	CHB-C4A-NA	2.37	127.82	124.40
37	c	517	LMG	C40-C39-C38	-2.37	102.40	114.37
32	7	606	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
34	p	301	II0	C27-C25-C29	-2.37	119.58	124.18
34	6	612	II0	C19-C13-C11	2.37	118.77	114.42
34	p	314	II0	C19-C13-C09	-2.37	119.74	124.16
32	c	506	CLA	CHB-C4A-NA	2.37	127.81	124.40
32	c	510	CLA	CHB-C4A-NA	2.37	127.81	124.40
31	d	408	8CT	C11-C10-C03	-2.36	120.68	127.00
34	7	614	II0	C20-C14-C12	2.36	118.77	114.42
37	C	517	LMG	C40-C39-C38	-2.36	102.42	114.37
31	A	610	8CT	C27-C26-C28	2.36	121.70	118.09
32	A	603	CLA	CHB-C4A-NA	2.36	127.81	124.40
32	p	310	CLA	CHB-C4A-NA	2.36	127.81	124.40
32	b	608	CLA	CHB-C4A-NA	2.36	127.81	124.40
32	4	602	CLA	C1-C2-C3	-2.36	122.33	126.20
32	7	601	CLA	CHB-C4A-NA	2.36	127.81	124.40
34	6	612	II0	C19-C13-C09	-2.36	119.75	124.16
32	5	313	CLA	CHB-C4A-NA	2.36	127.81	124.40
37	4	618	LMG	O1-C1-C2	-2.36	104.69	108.27
32	p	313	CLA	C3B-C4B-NB	-2.36	108.42	110.53
36	4	614	IHT	C20-C15-C12	2.36	118.76	114.42
32	4	611	CLA	CHB-C4A-NA	2.36	127.80	124.40
34	5	315	II0	C28-C26-C30	-2.36	119.60	124.18
34	0	620	II0	C20-C14-C12	2.36	118.75	114.42
34	9	613	II0	C19-C13-C09	-2.36	119.75	124.16
31	D	409	8CT	C25-C24-C23	-2.36	116.37	123.20
34	5	314	II0	C19-C13-C09	-2.36	119.75	124.16
32	d	409	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
36	0	618	IHT	C20-C15-C11	-2.35	119.76	124.16
34	p	315	II0	C19-C13-C11	2.35	118.75	114.42
32	d	402	CLA	CAB-C3B-C2B	2.35	129.79	123.53
47	v	201	HEM	C4D-ND-C1D	2.35	107.99	105.21
32	9	609	CLA	CHB-C4A-NA	2.35	127.80	124.40
31	d	408	8CT	C07-C02-C03	-2.35	119.53	122.70
32	2	612	CLA	CHB-C4A-NA	2.35	127.79	124.40
32	0	603	CLA	CHB-C4A-NA	2.35	127.79	124.40
32	c	502	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
32	3	609	CLA	CHB-C4A-NA	2.35	127.79	124.40
32	D	403	CLA	CHB-C4A-NA	2.35	127.79	124.40
34	0	620	II0	C42-C41-C39	-2.35	118.71	123.52
32	1	601	CLA	CHB-C4A-NA	2.35	127.79	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	8	607	CLA	CHB-C4A-NA	2.35	127.79	124.40
32	6	608	CLA	CHB-C4A-NA	2.35	127.79	124.40
43	D	405	PL9	O1-C4-C3	-2.35	118.26	120.73
34	9	613	II0	C20-C14-C10	-2.35	119.77	124.16
32	6	601	CLA	CHB-C4A-NA	2.35	127.78	124.40
36	4	617	IHT	C31-C34-C35	-2.35	119.93	126.36
34	P	614	II0	C19-C13-C11	2.34	118.73	114.42
32	B	609	CLA	CHB-C4A-NA	2.34	127.78	124.40
34	9	614	II0	C20-C14-C12	2.34	118.73	114.42
32	8	612	CLA	CHB-C4A-NA	2.34	127.78	124.40
32	2	601	CLA	CHB-C4A-NA	2.34	127.78	124.40
34	6	614	II0	C19-C13-C09	-2.34	119.78	124.16
34	9	612	II0	C31-C29-C25	-2.34	120.06	126.61
34	5	301	II0	C20-C14-C10	-2.34	119.78	124.16
34	P	612	II0	C20-C14-C10	-2.34	119.78	124.16
32	0	602	CLA	C1-C2-C3	-2.34	122.36	126.20
32	8	609	CLA	CHB-C4A-NA	2.34	127.78	124.40
41	D	402	PHO	C1-C2-C3	-2.34	122.36	126.20
36	4	614	IHT	C20-C15-C11	-2.34	119.78	124.16
34	0	615	II0	C42-C41-C39	-2.34	118.74	123.52
32	1	612	CLA	CHB-C4A-NA	2.34	127.77	124.40
34	p	315	II0	C29-C31-C33	-2.34	116.43	123.20
34	3	614	II0	C20-C14-C12	2.34	118.72	114.42
32	C	502	CLA	CHB-C4A-NA	2.34	127.77	124.40
34	5	314	II0	C41-C42-C40	-2.34	118.74	123.52
32	2	606	CLA	CHB-C4A-NA	2.34	127.77	124.40
41	d	410	PHO	C1-C2-C3	-2.33	122.37	126.20
32	7	605	CLA	C1-C2-C3	-2.33	122.98	126.76
32	B	611	CLA	CHB-C4A-NA	2.33	127.77	124.40
33	7	610	KC2	C1B-CHB-C4A	-2.33	121.06	126.02
36	5	317	IHT	C06-C09-C10	-2.33	109.89	114.06
34	p	315	II0	C32-C30-C26	-2.33	120.08	126.61
33	P	605	KC2	O1D-CGD-CBD	-2.33	119.92	124.52
43	d	404	PL9	O2-C1-C6	2.33	124.19	120.48
32	C	510	CLA	CHB-C4A-NA	2.33	127.77	124.40
32	P	608	CLA	CHB-C4A-NA	2.33	127.77	124.40
33	P	605	KC2	C1B-CHB-C4A	-2.33	121.06	126.02
34	P	614	II0	C27-C25-C29	-2.33	119.66	124.18
34	5	301	II0	C19-C13-C09	-2.33	119.80	124.16
43	D	405	PL9	O2-C1-C6	2.33	124.19	120.48
32	1	607	CLA	CHB-C4A-NA	2.33	127.76	124.40
32	C	506	CLA	CHB-C4A-NA	2.33	127.76	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	611	CLA	CHB-C4A-NA	2.33	127.76	124.40
43	a	412	PL9	C2-C3-C4	2.33	120.31	118.66
34	3	612	II0	C32-C30-C26	-2.33	120.10	126.61
37	P	616	LMG	O2-C2-C1	-2.33	104.53	110.08
31	d	408	8CT	C25-C24-C23	-2.33	116.45	123.20
32	b	612	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
32	0	604	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
32	B	608	CLA	CHB-C4A-NA	2.33	127.76	124.40
32	d	403	CLA	CMB-C2B-C1B	-2.33	121.88	125.42
34	3	614	II0	C19-C13-C09	-2.33	119.81	124.16
34	p	315	II0	C19-C13-C09	-2.33	119.81	124.16
32	4	604	CLA	CHB-C4A-NA	2.33	127.76	124.40
37	0	619	LMG	O1-C1-C2	-2.33	104.74	108.27
32	7	612	CLA	CHB-C4A-NA	2.32	127.75	124.40
32	B	612	CLA	O2A-CGA-O1A	-2.32	117.81	123.63
34	P	614	II0	C31-C33-C35	-2.32	119.99	126.36
32	7	603	CLA	C3B-C4B-NB	-2.32	108.46	110.53
34	4	616	II0	C27-C25-C29	-2.32	119.67	124.18
32	4	603	CLA	CHB-C4A-NA	2.32	127.75	124.40
34	3	614	II0	C27-C25-C29	-2.32	119.67	124.18
34	5	315	II0	C19-C13-C09	-2.32	119.82	124.16
33	6	605	KC2	O2D-CGD-O1D	-2.32	119.33	123.85
32	D	404	CLA	CMB-C2B-C1B	-2.32	121.88	125.42
32	C	505	CLA	CHB-C4A-NA	2.32	127.75	124.40
34	9	612	II0	C28-C26-C30	-2.32	119.67	124.18
32	C	508	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
32	b	614	CLA	CHB-C4A-NA	2.32	127.75	124.40
34	3	612	II0	C28-C26-C30	-2.32	119.68	124.18
37	C	517	LMG	C38-C37-C36	-2.32	102.64	114.37
37	L	102	LMG	O2-C2-C1	-2.32	104.55	110.08
31	P	615	8CT	C04-C03-C10	2.32	121.94	115.65
36	8	616	IHT	C41-C40-C37	-2.32	118.78	123.52
34	4	615	II0	C19-C13-C11	2.32	118.68	114.42
34	0	615	II0	C19-C13-C11	2.32	118.68	114.42
34	9	612	II0	C27-C25-C29	-2.32	119.68	124.18
32	4	604	CLA	C1-C2-C3	-2.32	122.40	126.20
45	c	514	DGD	C1D-C2D-C3D	-2.32	105.14	110.01
34	5	319	II0	C27-C25-C29	-2.32	119.69	124.18
34	4	619	II0	C28-C26-C30	-2.32	119.69	124.18
34	3	613	II0	C20-C14-C12	2.31	118.68	114.42
32	0	604	CLA	CHB-C4A-NA	2.31	127.74	124.40
32	B	610	CLA	C1-C2-C3	-2.31	122.41	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	p	317	IHT	C06-C09-C10	-2.31	109.93	114.06
47	V	201	HEM	C4D-ND-C1D	2.31	107.94	105.21
37	c	517	LMG	C38-C37-C36	-2.31	102.68	114.37
33	1	610	KC2	C1B-CHB-C4A	-2.31	121.11	126.02
34	8	619	II0	C19-C13-C09	-2.31	119.84	124.16
32	8	606	CLA	CHB-C4A-NA	2.31	127.73	124.40
34	0	617	II0	C27-C25-C29	-2.31	119.69	124.18
34	1	614	II0	C20-C14-C10	-2.31	119.84	124.16
36	5	317	IHT	C41-C40-C37	-2.31	118.79	123.52
34	9	613	II0	C19-C13-C11	2.31	118.67	114.42
36	2	616	IHT	C22-C18-C07	-2.31	120.83	127.00
38	D	406	LHG	C18-C17-C16	-2.31	102.70	114.37
33	7	610	KC2	O2D-CGD-O1D	-2.31	119.36	123.85
32	C	502	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
38	d	405	LHG	C18-C17-C16	-2.31	102.70	114.37
34	3	612	II0	C31-C29-C25	-2.31	120.16	126.61
32	c	509	CLA	CMB-C2B-C1B	-2.31	121.91	125.42
34	5	315	II0	C19-C13-C11	2.31	118.66	114.42
32	B	614	CLA	CHB-C4A-NA	2.31	127.73	124.40
34	P	612	II0	C31-C29-C25	-2.31	120.16	126.61
34	1	616	II0	C19-C13-C09	-2.30	119.85	124.16
43	d	404	PL9	O1-C4-C3	-2.30	118.30	120.73
32	c	502	CLA	CHB-C4A-NA	2.30	127.72	124.40
31	k	102	8CT	C11-C10-C03	-2.30	120.84	127.00
43	d	404	PL9	C20-C19-C21	2.30	119.23	115.23
43	D	405	PL9	C20-C19-C21	2.30	119.22	115.23
32	1	605	CLA	C1-C2-C3	-2.30	123.04	126.76
37	l	101	LMG	O2-C2-C1	-2.30	104.59	110.08
32	7	607	CLA	CHB-C4A-NA	2.30	127.72	124.40
36	0	614	IHT	C20-C15-C11	-2.30	119.86	124.16
34	5	315	II0	C29-C31-C33	-2.30	116.53	123.20
31	B	623	8CT	C01-C02-C07	2.30	118.50	113.60
34	5	314	II0	C20-C14-C10	-2.30	119.86	124.16
37	G	102	LMG	O1-C1-C2	-2.30	104.78	108.27
34	9	612	II0	C32-C30-C26	-2.30	120.18	126.61
45	C	514	DGD	C1D-C2D-C3D	-2.30	105.17	110.01
32	c	505	CLA	CHB-C4A-NA	2.30	127.72	124.40
34	2	619	II0	C32-C30-C26	-2.30	120.18	126.61
32	7	603	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
34	p	314	II0	C31-C33-C35	-2.30	120.06	126.36
31	K	101	8CT	C11-C10-C03	-2.30	120.86	127.00
31	6	615	8CT	C04-C03-C10	2.30	121.88	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	622	8CT	C04-C03-C10	2.30	121.88	115.65
37	P	616	LMG	O1-C7-C8	-2.30	105.23	110.82
36	8	616	IHT	C22-C18-C07	-2.30	120.86	127.00
37	g	101	LMG	O2-C2-C1	-2.30	104.60	110.08
32	4	604	CLA	O2A-CGA-O1A	-2.30	117.89	123.63
31	M	201	8CT	C24-C23-C21	-2.30	120.07	126.36
37	6	616	LMG	O2-C2-C1	-2.30	104.61	110.08
32	D	403	CLA	C3B-C4B-NB	-2.30	107.95	110.33
32	C	509	CLA	CMB-C2B-C1B	-2.29	121.92	125.42
32	d	403	CLA	O2D-CGD-CBD	2.29	115.24	111.23
32	b	610	CLA	C1-C2-C3	-2.29	122.44	126.20
34	9	614	II0	C31-C33-C35	-2.29	120.08	126.36
34	P	612	II0	C27-C25-C29	-2.29	119.73	124.18
31	b	622	8CT	C01-C02-C07	2.29	118.48	113.60
37	G	102	LMG	O3-C3-C2	-2.29	104.97	110.38
37	G	102	LMG	O1-C7-C8	-2.29	105.25	110.82
34	2	613	II0	C19-C13-C11	2.29	118.63	114.42
37	G	102	LMG	O2-C2-C1	-2.29	104.62	110.08
37	l	101	LMG	O3-C3-C2	-2.29	104.98	110.38
31	z	101	8CT	C39-C16-C15	2.29	121.59	118.09
34	5	314	II0	C19-C13-C11	2.29	118.63	114.42
34	p	314	II0	C19-C13-C11	2.29	118.63	114.42
34	9	613	II0	C20-C14-C12	2.29	118.63	114.42
31	M	201	8CT	C04-C03-C10	2.29	121.86	115.65
34	8	613	II0	C19-C13-C11	2.29	118.63	114.42
36	8	616	IHT	C20-C15-C12	2.29	118.62	114.42
36	0	618	IHT	C28-C26-C29	-2.29	119.74	124.18
43	A	609	PL9	C2-C3-C4	2.29	120.28	118.66
34	0	620	II0	C28-C26-C30	-2.29	119.74	124.18
32	b	607	CLA	O2A-CGA-O1A	-2.28	117.91	123.63
34	2	619	II0	C28-C26-C30	-2.28	119.75	124.18
45	c	515	DGD	C3G-C2G-C1G	-2.28	106.46	111.78
32	C	509	CLA	C1-C2-C3	-2.28	122.45	126.20
36	4	614	IHT	C31-C29-C26	-2.28	120.23	126.61
34	1	614	II0	C19-C13-C11	2.28	118.62	114.42
32	2	607	CLA	CHB-C4A-NA	2.28	127.69	124.40
34	0	620	II0	C17-C04-C10	-2.28	106.43	110.52
33	1	610	KC2	O2D-CGD-O1D	-2.28	119.41	123.85
34	7	619	II0	C19-C13-C09	-2.28	119.89	124.16
32	c	508	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
37	L	102	LMG	O3-C3-C2	-2.28	105.00	110.38
37	g	101	LMG	O3-C3-C2	-2.28	105.00	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	7	618	IHT	C41-C40-C37	-2.28	118.86	123.52
34	0	616	II0	C27-C25-C29	-2.28	119.76	124.18
34	8	614	II0	C42-C41-C39	-2.28	118.86	123.52
36	0	614	IHT	C31-C34-C35	-2.28	120.12	126.36
34	5	314	II0	C32-C34-C36	-2.27	120.12	126.36
32	s	302	CLA	CHB-C4A-NA	2.27	127.68	124.40
33	p	311	KC2	C1B-CHB-C4A	-2.27	121.19	126.02
34	0	620	II0	C31-C29-C25	-2.27	120.25	126.61
36	8	616	IHT	C31-C34-C35	-2.27	120.13	126.36
45	C	515	DGD	C3G-C2G-C1G	-2.27	106.49	111.78
37	b	618	LMG	C1-C2-C3	-2.27	105.23	110.01
34	1	616	II0	C31-C33-C35	-2.27	120.13	126.36
38	A	613	LHG	C27-C26-C25	-2.27	102.89	114.37
34	8	619	II0	C32-C30-C26	-2.27	120.26	126.61
32	1	602	CLA	C1-C2-C3	-2.27	122.48	126.20
34	7	614	II0	C19-C13-C09	-2.27	119.92	124.16
34	p	315	II0	C41-C42-C40	-2.27	118.87	123.52
32	4	607	CLA	CHB-C4A-NA	2.27	127.68	124.40
34	1	617	II0	C31-C33-C35	-2.27	120.14	126.36
36	1	618	IHT	C41-C40-C37	-2.27	118.88	123.52
34	2	614	II0	C32-C34-C36	-2.27	120.14	126.36
36	p	317	IHT	C20-C15-C11	-2.27	119.92	124.16
32	c	504	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
31	B	622	8CT	C24-C23-C21	-2.27	120.14	126.36
37	6	616	LMG	O3-C3-C2	-2.27	105.03	110.38
34	4	619	II0	C32-C30-C26	-2.27	120.27	126.61
34	0	620	II0	C19-C13-C09	-2.27	119.92	124.16
32	c	509	CLA	C1-C2-C3	-2.27	122.48	126.20
32	d	409	CLA	C1-C2-C3	-2.27	122.48	126.20
34	6	612	II0	C31-C29-C25	-2.27	120.27	126.61
34	8	613	II0	C20-C14-C12	2.27	118.59	114.42
41	A	604	PHO	O2A-CGA-O1A	-2.27	117.96	123.63
34	4	619	II0	C20-C14-C10	-2.27	119.92	124.16
38	a	403	LHG	C27-C26-C25	-2.27	102.92	114.37
32	7	605	CLA	CHB-C4A-NA	2.26	127.67	124.40
32	B	607	CLA	O2A-CGA-O1A	-2.26	117.96	123.63
37	P	616	LMG	O3-C3-C2	-2.26	105.04	110.38
34	8	619	II0	C28-C26-C30	-2.26	119.79	124.18
32	D	401	CLA	C1-C2-C3	-2.26	122.49	126.20
34	8	614	II0	C19-C13-C09	-2.26	119.93	124.16
31	b	622	8CT	C19-C18-C17	-2.26	118.89	123.52
36	4	617	IHT	C22-C18-C07	-2.26	120.96	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	g	101	LMG	O1-C1-C2	-2.26	104.84	108.27
31	z	101	8CT	C14-C13-C12	-2.26	124.11	127.28
37	6	616	LMG	O1-C7-C8	-2.26	105.32	110.82
32	D	404	CLA	C1-C2-C3	-2.26	122.50	126.20
32	d	403	CLA	C1-C2-C3	-2.26	122.50	126.20
33	5	311	KC2	C1B-CHB-C4A	-2.26	121.22	126.02
34	8	614	II0	C19-C13-C11	2.26	118.57	114.42
34	7	616	II0	C42-C41-C39	-2.26	118.90	123.52
32	P	602	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
37	0	619	LMG	O2-C2-C1	-2.26	104.70	110.08
41	a	407	PHO	O2A-CGA-O1A	-2.26	117.98	123.63
32	5	303	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
33	2	610	KC2	C1B-CHB-C4A	-2.26	121.22	126.02
32	S	302	CLA	CHB-C4A-NA	2.26	127.66	124.40
37	2	617	LMG	O2-C2-C1	-2.26	104.70	110.08
34	7	616	II0	C19-C13-C09	-2.25	119.94	124.16
36	0	614	IHT	C31-C29-C26	-2.25	120.31	126.61
32	p	303	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
32	9	606	CLA	CHB-C4A-NA	2.25	127.65	124.40
32	D	404	CLA	O2D-CGD-CBD	2.25	115.17	111.23
34	3	614	II0	C42-C41-C39	-2.25	118.91	123.52
35	P	613	II3	C41-C40-C38	-2.25	124.12	127.28
31	B	623	8CT	C19-C18-C17	-2.25	118.91	123.52
34	7	616	II0	C30-C32-C34	-2.25	116.68	123.20
31	A	610	8CT	C01-C02-C07	2.25	118.39	113.60
31	C	518	8CT	C10-C11-C12	-2.25	122.91	126.23
34	5	316	II0	C19-C13-C09	-2.25	119.95	124.16
34	6	612	II0	C27-C25-C29	-2.25	119.81	124.18
31	c	518	8CT	C10-C11-C12	-2.25	122.91	126.23
32	d	402	CLA	C3B-C4B-NB	-2.25	108.00	110.33
32	p	305	CLA	C1-C2-C3	-2.25	122.52	126.20
32	1	605	CLA	CHB-C4A-NA	2.25	127.64	124.40
32	c	509	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
47	v	201	HEM	C3B-C2B-C1B	2.25	108.10	106.41
37	8	617	LMG	O2-C2-C1	-2.25	104.72	110.08
38	D	406	LHG	C27-C26-C25	-2.25	103.01	114.37
38	d	405	LHG	C27-C26-C25	-2.25	103.01	114.37
32	D	403	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
37	d	406	LMG	O3-C3-C2	-2.25	105.08	110.38
34	0	620	II0	C32-C30-C26	-2.24	120.33	126.61
34	2	615	II0	C27-C25-C29	-2.24	119.82	124.18
34	6	614	II0	C27-C25-C29	-2.24	119.82	124.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	4	618	LMG	O2-C2-C1	-2.24	104.73	110.08
31	d	408	8CT	C04-C03-C02	-2.24	119.57	122.64
31	Z	101	8CT	C14-C13-C12	-2.24	124.13	127.28
36	p	317	IHT	C28-C26-C29	-2.24	119.83	124.18
37	B	618	LMG	C1-C2-C3	-2.24	105.29	110.01
32	B	610	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
34	P	612	II0	C19-C13-C09	-2.24	119.97	124.16
34	p	301	II0	C20-C14-C12	2.24	118.54	114.42
34	8	614	II0	C32-C34-C36	-2.24	120.22	126.36
32	0	607	CLA	CHB-C4A-NA	2.24	127.63	124.40
34	3	613	II0	C20-C14-C10	-2.24	119.97	124.16
32	0	604	CLA	C1-C2-C3	-2.24	122.53	126.20
31	P	615	8CT	C40-C12-C13	-2.24	119.19	122.82
34	1	619	II0	C28-C26-C30	-2.24	119.84	124.18
34	9	612	II0	C19-C13-C11	2.24	118.53	114.42
32	B	609	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
32	6	602	CLA	O2A-CGA-O1A	-2.24	118.04	123.63
34	5	314	II0	C31-C29-C25	-2.24	120.36	126.61
32	b	613	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
34	2	614	II0	C20-C14-C12	2.23	118.53	114.42
34	7	619	II0	C19-C13-C11	2.23	118.53	114.42
36	4	614	IHT	C31-C34-C35	-2.23	120.24	126.36
32	b	609	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
32	d	402	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
34	8	613	II0	C31-C29-C25	-2.23	120.37	126.61
34	2	614	II0	C42-C41-C39	-2.23	118.96	123.52
47	E	101	HEM	C4D-ND-C1D	2.23	107.84	105.21
32	B	604	CLA	O2D-CGD-CBD	2.23	115.12	111.23
32	G	101	CLA	CHB-C4A-NA	2.23	127.61	124.40
32	B	615	CLA	C1-C2-C3	-2.23	122.55	126.20
33	0	610	KC2	C1B-CHB-C4A	-2.23	121.29	126.02
34	4	616	II0	C20-C14-C10	-2.23	120.00	124.16
32	a	408	CLA	O2D-CGD-CBD	2.23	115.12	111.23
37	A	607	LMG	O3-C3-C2	-2.23	105.13	110.38
36	8	616	IHT	C28-C26-C29	-2.23	119.86	124.18
33	4	610	KC2	C1B-CHB-C4A	-2.23	121.29	126.02
32	A	605	CLA	O2D-CGD-CBD	2.22	115.12	111.23
32	b	610	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
32	7	602	CLA	C1-C2-C3	-2.22	122.55	126.20
31	Z	101	8CT	C22-C21-C23	2.22	121.48	118.09
37	8	617	LMG	O3-C3-C2	-2.22	105.14	110.38
34	7	616	II0	C31-C33-C35	-2.22	120.27	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	8	610	KC2	C1B-CHB-C4A	-2.22	121.30	126.02
33	6	609	KC2	C1B-CHB-C4A	-2.22	121.30	126.02
31	D	409	8CT	C04-C03-C02	-2.22	119.60	122.64
33	P	609	KC2	C1B-CHB-C4A	-2.22	121.31	126.02
34	3	612	II0	C27-C25-C29	-2.22	119.88	124.18
45	c	515	DGD	O3E-C3E-C2E	-2.22	105.15	110.38
32	B	613	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
32	b	613	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
37	D	407	LMG	O3-C3-C2	-2.22	105.15	110.38
32	C	509	CLA	O2A-CGA-O1A	-2.22	118.09	123.63
37	0	619	LMG	O3-C3-C2	-2.21	105.16	110.38
32	B	611	CLA	C1-C2-C3	-2.21	122.57	126.20
32	1	602	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
31	6	615	8CT	C40-C12-C13	-2.21	119.23	122.82
37	b	618	LMG	O2-C2-C1	-2.21	104.80	110.08
31	P	615	8CT	C18-C19-C20	-2.21	118.99	123.52
34	2	614	II0	C19-C13-C11	2.21	118.49	114.42
37	a	410	LMG	O3-C3-C2	-2.21	105.16	110.38
34	p	314	II0	C28-C26-C30	-2.21	119.89	124.18
34	1	617	II0	C20-C14-C12	2.21	118.48	114.42
37	4	618	LMG	O3-C3-C2	-2.21	105.17	110.38
37	D	411	LMG	O7-C10-O9	-2.21	118.54	123.70
32	b	604	CLA	O2D-CGD-CBD	2.21	115.09	111.23
32	7	602	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
34	4	615	II0	C19-C13-C09	-2.21	120.03	124.16
37	B	618	LMG	O2-C2-C1	-2.21	104.82	110.08
32	6	604	CLA	C1-C2-C3	-2.21	122.58	126.20
34	6	614	II0	C42-C41-C39	-2.21	119.01	123.52
37	g	101	LMG	O1-C7-C8	-2.21	105.45	110.82
31	A	610	8CT	C18-C19-C20	-2.21	119.01	123.52
31	k	102	8CT	C14-C15-C16	-2.20	120.32	126.36
36	4	614	IHT	C28-C26-C29	-2.20	119.90	124.18
31	K	101	8CT	C14-C15-C16	-2.20	120.32	126.36
37	c	517	LMG	O3-C3-C2	-2.20	105.18	110.38
32	p	305	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
31	6	615	8CT	C18-C19-C20	-2.20	119.01	123.52
32	g	102	CLA	CHB-C4A-NA	2.20	127.58	124.40
32	5	305	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
32	b	611	CLA	C1-C2-C3	-2.20	122.59	126.20
45	C	515	DGD	O3E-C3E-C2E	-2.20	105.19	110.38
34	8	619	II0	C27-C25-C29	-2.20	119.91	124.18
38	L	101	LHG	C27-C26-C25	-2.20	103.24	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	9	613	II0	C41-C39-C35	-2.20	124.19	127.28
32	5	305	CLA	C1-C2-C3	-2.20	122.59	126.20
34	0	615	II0	C20-C14-C10	-2.20	120.05	124.16
36	5	317	IHT	C28-C26-C29	-2.20	119.91	124.18
34	2	614	II0	C19-C13-C09	-2.20	120.05	124.16
39	A	606	SQD	O8-S-C6	2.20	110.22	105.97
34	P	612	II0	C32-C30-C26	-2.20	120.46	126.61
32	B	612	CLA	C1-C2-C3	-2.20	122.59	126.20
36	2	616	IHT	C31-C34-C35	-2.20	120.34	126.36
32	4	605	CLA	C1-C2-C3	-2.20	123.21	126.76
32	6	606	CLA	C3B-C4B-NB	-2.20	108.57	110.53
34	P	612	II0	C41-C42-C40	-2.20	119.02	123.52
38	S	301	LHG	C27-C26-C25	-2.20	103.26	114.37
38	s	301	LHG	C27-C26-C25	-2.20	103.26	114.37
37	a	410	LMG	O2-C2-C1	-2.20	104.84	110.08
45	H	101	DGD	CAB-C9B-C8B	-2.20	103.27	114.37
39	a	409	SQD	O8-S-C6	2.20	110.21	105.97
34	6	612	II0	C28-C26-C30	-2.20	119.92	124.18
45	h	101	DGD	CAB-C9B-C8B	-2.19	103.28	114.37
31	C	518	8CT	C37-C35-C34	-2.19	104.45	109.01
37	A	607	LMG	O2-C2-C1	-2.19	104.85	110.08
34	5	314	II0	C27-C25-C29	-2.19	119.92	124.18
37	2	617	LMG	O3-C3-C2	-2.19	105.21	110.38
32	b	611	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
34	2	613	II0	C31-C29-C25	-2.19	120.48	126.61
32	A	602	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
32	C	504	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
33	0	610	KC2	O2D-CGD-O1D	-2.19	119.58	123.85
34	3	614	II0	C31-C33-C35	-2.19	120.36	126.36
39	p	318	SQD	O8-S-C6	2.19	110.20	105.97
34	7	614	II0	C20-C14-C10	-2.19	120.07	124.16
34	8	619	II0	C31-C29-C25	-2.19	120.49	126.61
34	2	614	II0	C27-C25-C29	-2.19	119.93	124.18
32	c	506	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
33	p	311	KC2	C1A-C2A-C3A	-2.19	105.27	107.28
34	8	615	II0	C27-C25-C29	-2.19	119.93	124.18
37	C	517	LMG	O3-C3-C2	-2.19	105.22	110.38
31	a	413	8CT	C18-C19-C20	-2.19	119.04	123.52
38	l	102	LHG	C27-C26-C25	-2.19	103.31	114.37
32	B	613	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
31	c	518	8CT	C37-C35-C34	-2.19	104.46	109.01
34	1	616	II0	C20-C14-C12	2.19	118.44	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	405	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
45	A	614	DGD	O2D-C2D-C1D	-2.19	104.86	110.08
34	1	619	II0	C19-C13-C11	2.19	118.44	114.42
45	c	514	DGD	CBB-CAB-C9B	-2.19	103.32	114.37
37	d	401	LMG	O7-C10-O9	-2.19	118.59	123.70
31	D	409	8CT	C27-C26-C25	-2.18	119.28	122.82
47	v	201	HEM	C1B-NB-C4B	2.18	107.79	105.21
36	0	618	IHT	C22-C18-C07	-2.18	121.17	127.00
37	P	616	LMG	O1-C1-C2	-2.18	104.96	108.27
45	C	514	DGD	CBB-CAB-C9B	-2.18	103.34	114.37
31	3	615	8CT	C39-C16-C17	-2.18	119.28	122.82
32	b	616	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
32	8	602	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
34	2	615	II0	C42-C41-C39	-2.18	119.06	123.52
32	3	603	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
36	1	618	IHT	C20-C15-C11	-2.18	120.08	124.16
34	8	613	II0	C27-C25-C29	-2.18	119.95	124.18
32	P	606	CLA	C3B-C4B-NB	-2.18	108.59	110.53
34	1	616	II0	C31-C29-C25	-2.18	120.52	126.61
32	3	602	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
32	b	615	CLA	C1-C2-C3	-2.18	122.63	126.20
34	4	619	II0	C27-C25-C29	-2.18	119.96	124.18
34	1	619	II0	C19-C13-C09	-2.18	120.09	124.16
31	A	610	8CT	C22-C21-C23	2.18	121.41	118.09
32	0	605	CLA	C1-C2-C3	-2.17	123.24	126.76
34	p	316	II0	C19-C13-C09	-2.17	120.09	124.16
33	4	610	KC2	O2D-CGD-O1D	-2.17	119.62	123.85
32	B	611	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
37	D	411	LMG	O2-C2-C1	-2.17	104.90	110.08
36	2	616	IHT	C31-C29-C26	-2.17	120.54	126.61
34	6	612	II0	C20-C14-C12	2.17	118.41	114.42
33	5	311	KC2	C1A-C2A-C3A	-2.17	105.29	107.28
35	6	613	II3	C03-C04-C12	-2.17	110.33	112.83
32	9	602	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
32	3	606	CLA	CHB-C4A-NA	2.17	127.53	124.40
37	D	411	LMG	O3-C3-C2	-2.17	105.27	110.38
34	0	615	II0	C28-C26-C30	-2.17	119.98	124.18
32	B	613	CLA	C1-C2-C3	-2.17	122.65	126.20
37	c	517	LMG	O2-C2-C1	-2.17	104.92	110.08
31	9	615	8CT	C39-C16-C17	-2.17	119.31	122.82
32	3	604	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
45	c	516	DGD	CBB-CAB-C9B	-2.16	103.43	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C	516	DGD	CBB-CAB-C9B	-2.16	103.44	114.37
32	2	602	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
34	5	319	II0	C20-C14-C12	2.16	118.40	114.42
38	b	619	LHG	C27-C26-C25	-2.16	103.44	114.37
31	d	408	8CT	C27-C26-C25	-2.16	119.31	122.82
31	Z	101	8CT	C38-C31-C32	-2.16	115.10	122.37
47	f	101	HEM	C4D-ND-C1D	2.16	107.77	105.21
32	B	605	CLA	C3B-C4B-NB	-2.16	108.60	110.53
32	B	614	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
36	7	618	IHT	C20-C15-C11	-2.16	120.12	124.16
34	8	614	II0	C20-C14-C12	2.16	118.39	114.42
32	0	606	CLA	CHB-C4A-NA	2.16	127.52	124.40
32	b	613	CLA	C1-C2-C3	-2.16	122.66	126.20
37	d	401	LMG	O1-C7-C8	-2.16	105.57	110.82
32	0	602	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
36	4	617	IHT	C20-C15-C11	-2.16	120.13	124.16
34	p	301	II0	C31-C33-C35	-2.16	120.45	126.36
34	8	614	II0	C27-C25-C29	-2.16	120.00	124.18
34	8	615	II0	C28-C26-C30	-2.16	120.00	124.18
38	B	619	LHG	C27-C26-C25	-2.16	103.47	114.37
47	V	201	HEM	C1B-NB-C4B	2.16	107.76	105.21
32	9	604	CLA	O2D-CGD-CBD	2.15	115.00	111.23
32	9	603	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
32	b	612	CLA	C1-C2-C3	-2.15	122.67	126.20
45	c	514	DGD	C5B-C4B-C3B	-2.15	103.48	114.37
45	C	514	DGD	C5B-C4B-C3B	-2.15	103.48	114.37
39	5	318	SQD	O8-S-C6	2.15	110.13	105.97
31	k	102	8CT	C25-C24-C23	-2.15	116.96	123.20
45	a	414	DGD	O2D-C2D-C1D	-2.15	104.95	110.08
32	4	602	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
34	2	613	II0	C20-C14-C10	-2.15	120.14	124.16
32	B	616	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
32	C	505	CLA	O2D-CGD-CBD	2.15	114.99	111.23
36	0	618	IHT	C41-C40-C37	-2.15	119.12	123.52
37	D	411	LMG	O1-C7-C8	-2.15	105.59	110.82
36	0	614	IHT	C28-C26-C29	-2.15	120.01	124.18
45	C	516	DGD	CAB-C9B-C8B	-2.15	103.50	114.37
32	2	605	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
45	a	414	DGD	CBB-CAB-C9B	-2.15	103.51	114.37
37	d	401	LMG	O3-C3-C2	-2.15	105.31	110.38
34	7	617	II0	C31-C33-C35	-2.15	120.48	126.36
32	3	604	CLA	O2D-CGD-CBD	2.15	114.98	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	8	604	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
32	6	604	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
31	H	102	8CT	C38-C31-C32	-2.15	115.16	122.37
32	C	506	CLA	CMB-C2B-C1B	-2.14	122.15	125.42
45	c	516	DGD	CAB-C9B-C8B	-2.14	103.53	114.37
32	P	604	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
37	D	407	LMG	O1-C7-C8	-2.14	105.60	110.82
34	p	314	II0	C32-C30-C26	-2.14	120.62	126.61
31	A	610	8CT	C40-C12-C11	2.14	121.36	118.09
34	6	612	II0	C41-C42-C40	-2.14	119.14	123.52
31	z	101	8CT	C22-C21-C23	2.14	121.36	118.09
37	C	517	LMG	O2-C2-C1	-2.14	104.97	110.08
37	L	102	LMG	O1-C7-C8	-2.14	105.61	110.82
32	b	603	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
32	8	605	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
34	5	301	II0	C19-C13-C11	2.14	118.36	114.42
32	c	505	CLA	O2D-CGD-CBD	2.14	114.97	111.23
37	b	618	LMG	O3-C3-C2	-2.14	105.33	110.38
37	d	401	LMG	O2-C2-C1	-2.14	104.98	110.08
34	2	613	II0	C27-C25-C29	-2.14	120.03	124.18
31	z	101	8CT	C38-C31-C32	-2.14	115.18	122.37
32	b	605	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
37	l	101	LMG	O1-C7-C8	-2.14	105.62	110.82
37	B	618	LMG	O3-C3-C2	-2.14	105.34	110.38
45	C	516	DGD	O5D-C6D-C5D	-2.14	104.60	109.42
32	b	614	CLA	CMB-C2B-C1B	-2.14	122.17	125.42
35	7	615	II3	C22-C18-C17	2.14	118.35	114.42
34	2	615	II0	C31-C29-C25	-2.14	120.64	126.61
32	2	604	CLA	CMB-C2B-C1B	-2.14	122.17	125.42
32	b	607	CLA	O2D-CGD-CBD	2.13	114.96	111.23
34	5	314	II0	C32-C30-C26	-2.13	120.64	126.61
34	3	613	II0	C41-C39-C35	-2.13	124.28	127.28
45	A	614	DGD	CBB-CAB-C9B	-2.13	103.58	114.37
38	L	101	LHG	C18-C17-C16	-2.13	103.58	114.37
34	7	616	II0	C31-C29-C25	-2.13	120.65	126.61
37	l	101	LMG	O7-C10-O9	-2.13	118.72	123.70
31	k	101	8CT	C23-C21-C20	-2.13	115.66	119.01
31	h	102	8CT	C38-C31-C32	-2.13	115.20	122.37
34	8	615	II0	C42-C41-C39	-2.13	119.16	123.52
34	0	617	II0	C19-C13-C11	2.13	118.34	114.42
43	d	404	PL9	O2-C1-C2	-2.13	116.99	121.83
32	B	605	CLA	O2A-CGA-O1A	-2.13	118.30	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	P	605	KC2	O2D-CGD-O1D	-2.13	119.70	123.85
32	P	604	CLA	C1-C2-C3	-2.13	122.71	126.20
45	H	101	DGD	CBB-CAB-C9B	-2.13	103.61	114.37
45	h	101	DGD	CBB-CAB-C9B	-2.13	103.61	114.37
34	p	315	II0	C20-C14-C10	-2.13	120.18	124.16
35	1	615	II3	C30-C28-C31	-2.13	120.05	124.18
34	P	612	II0	C19-C13-C11	2.13	118.33	114.42
34	5	314	II0	C28-C26-C30	-2.13	120.05	124.18
32	4	606	CLA	CHB-C4A-NA	2.13	127.47	124.40
38	l	102	LHG	C18-C17-C16	-2.13	103.62	114.37
32	9	604	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
38	A	612	LHG	C27-C26-C25	-2.12	103.64	114.37
37	d	406	LMG	O2-C2-C1	-2.12	105.02	110.08
45	c	515	DGD	CBB-CAB-C9B	-2.12	103.64	114.37
37	L	102	LMG	O7-C10-O9	-2.12	118.75	123.70
38	a	402	LHG	C27-C26-C25	-2.12	103.65	114.37
34	3	614	II0	C20-C14-C10	-2.12	120.19	124.16
34	5	315	II0	C20-C14-C10	-2.12	120.19	124.16
34	3	614	II0	C19-C13-C11	2.12	118.32	114.42
37	l	101	LMG	C1-O6-C5	-2.12	109.58	113.72
34	7	619	II0	C28-C26-C30	-2.12	120.07	124.18
34	5	319	II0	C04-C06-C08	-2.12	108.95	113.59
34	1	614	II0	C19-C13-C09	-2.12	120.20	124.16
37	D	407	LMG	O2-C2-C1	-2.12	105.03	110.08
47	E	101	HEM	C2A-C1A-NA	-2.12	107.80	110.15
34	7	617	II0	C19-C13-C09	-2.12	120.20	124.16
37	d	406	LMG	O1-C7-C8	-2.12	105.67	110.82
45	A	614	DGD	CAB-C9B-C8B	-2.12	103.67	114.37
35	7	615	II3	C26-C29-C32	-2.11	117.07	123.20
32	B	603	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
37	c	517	LMG	C1-C2-C3	-2.11	105.56	110.01
34	p	315	II0	C28-C26-C30	-2.11	120.08	124.18
32	B	607	CLA	O2D-CGD-CBD	2.11	114.92	111.23
33	6	605	KC2	C2D-C1D-ND	-2.11	108.14	110.33
35	6	613	II3	C31-C34-C37	-2.11	117.08	123.20
45	a	414	DGD	CAB-C9B-C8B	-2.11	103.69	114.37
45	A	614	DGD	C5B-C4B-C3B	-2.11	103.70	114.37
34	8	614	II0	C32-C30-C26	-2.11	120.71	126.61
34	9	612	II0	C20-C14-C12	2.11	118.30	114.42
32	s	303	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
32	S	303	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
34	p	314	II0	C32-C34-C36	-2.11	120.58	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	d	403	CLA	CMB-C2B-C3B	2.11	131.51	126.55
34	p	316	II0	C20-C14-C10	-2.11	120.22	124.16
45	C	515	DGD	CBB-CAB-C9B	-2.11	103.72	114.37
39	A	606	SQD	C46-C45-C44	-2.11	106.88	111.78
47	V	201	HEM	C3B-C2B-C1B	2.11	107.99	106.41
32	b	607	CLA	C1-C2-C3	-2.11	122.75	126.20
45	c	516	DGD	O5D-C6D-C5D	-2.10	104.67	109.42
37	L	102	LMG	C1-O6-C5	-2.10	109.61	113.72
39	a	409	SQD	C46-C45-C44	-2.10	106.88	111.78
32	B	605	CLA	O2D-CGD-CBD	2.10	114.91	111.23
34	5	316	II0	C32-C34-C36	-2.10	120.59	126.36
32	c	513	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
34	P	614	II0	C42-C41-C39	-2.10	119.21	123.52
37	C	517	LMG	C1-C2-C3	-2.10	105.58	110.01
43	D	405	PL9	O2-C1-C2	-2.10	117.05	121.83
34	1	617	II0	C19-C13-C09	-2.10	120.23	124.16
32	0	604	CLA	O2D-CGD-CBD	2.10	114.91	111.23
34	0	615	II0	C32-C30-C26	-2.10	120.73	126.61
34	2	613	II0	C41-C42-C40	-2.10	119.22	123.52
45	c	514	DGD	O5D-C6D-C5D	-2.10	104.68	109.42
35	7	615	II3	C30-C28-C31	-2.10	120.10	124.18
32	b	605	CLA	C3B-C4B-NB	-2.10	108.66	110.53
32	1	605	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
38	a	403	LHG	C18-C17-C16	-2.10	103.75	114.37
45	c	514	DGD	O3E-C3E-C2E	-2.10	105.43	110.38
35	7	615	II3	C39-C41-C40	-2.10	119.22	123.52
38	A	613	LHG	C18-C17-C16	-2.10	103.76	114.37
32	b	605	CLA	O2D-CGD-CBD	2.10	114.90	111.23
32	1	604	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
32	b	604	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
45	C	514	DGD	O5D-C6D-C5D	-2.10	104.69	109.42
32	7	606	CLA	CMB-C2B-C3B	2.10	131.48	126.55
34	4	615	II0	C28-C26-C30	-2.10	120.11	124.18
32	C	513	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
34	7	617	II0	C20-C14-C12	2.10	118.28	114.42
31	a	413	8CT	C04-C03-C02	-2.10	119.77	122.64
37	6	616	LMG	O1-C1-C2	-2.10	105.09	108.27
35	P	613	II3	C05-C06-C10	-2.09	108.07	111.18
32	7	604	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
32	C	508	CLA	O2D-CGD-CBD	2.09	114.89	111.23
34	4	619	II0	C31-C29-C25	-2.09	120.75	126.61
32	B	607	CLA	C1-C2-C3	-2.09	122.77	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	a	414	DGD	C5B-C4B-C3B	-2.09	103.79	114.37
34	2	615	II0	C20-C14-C12	2.09	118.27	114.42
34	8	613	II0	C31-C33-C35	-2.09	120.63	126.36
34	0	620	II0	C08-C12-C14	-2.09	106.97	112.18
32	c	508	CLA	O2D-CGD-CBD	2.09	114.89	111.23
32	a	408	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
36	1	618	IHT	C28-C26-C29	-2.09	120.12	124.18
32	B	604	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
34	3	612	II0	C20-C14-C12	2.09	118.26	114.42
47	E	101	HEM	C3D-C4D-ND	-2.09	107.88	110.17
34	7	617	II0	C32-C30-C26	-2.09	120.77	126.61
45	C	514	DGD	O3E-C3E-C2E	-2.09	105.45	110.38
32	D	404	CLA	CMB-C2B-C3B	2.09	131.46	126.55
32	4	604	CLA	O2D-CGD-CBD	2.09	114.88	111.23
36	4	617	IHT	C28-C26-C29	-2.09	120.13	124.18
32	6	606	CLA	CHB-C4A-NA	2.09	127.41	124.40
32	P	606	CLA	CHB-C4A-NA	2.08	127.41	124.40
36	p	317	IHT	C19-C10-C09	2.08	118.04	113.60
47	v	201	HEM	C2A-C1A-NA	-2.08	107.84	110.15
31	B	624	8CT	C01-C02-C07	2.08	118.03	113.60
32	D	401	CLA	CMB-C2B-C3B	2.08	131.44	126.55
32	C	505	CLA	CMB-C2B-C3B	2.08	131.44	126.55
34	2	615	II0	C04-C06-C08	-2.08	109.03	113.59
31	K	101	8CT	C25-C24-C23	-2.08	117.18	123.20
31	b	623	8CT	C01-C02-C07	2.08	118.03	113.60
34	3	612	II0	C31-C33-C35	-2.08	120.67	126.36
36	1	618	IHT	C31-C29-C26	-2.08	120.80	126.61
34	4	615	II0	C20-C14-C10	-2.08	120.28	124.16
34	0	617	II0	C42-C41-C39	-2.08	119.27	123.52
32	A	605	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
32	7	604	CLA	C1-C2-C3	-2.08	122.80	126.20
34	9	614	II0	C42-C41-C39	-2.08	119.27	123.52
34	2	619	II0	C27-C25-C29	-2.08	120.15	124.18
37	8	617	LMG	O7-C10-O9	-2.07	118.86	123.70
34	p	314	II0	C31-C29-C25	-2.07	120.81	126.61
36	4	617	IHT	C31-C29-C26	-2.07	120.81	126.61
37	2	617	LMG	O7-C10-O9	-2.07	118.86	123.70
32	5	304	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
34	9	614	II0	C06-C04-C10	2.07	113.57	109.49
32	C	501	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
37	2	617	LMG	O1-C7-C8	-2.07	105.78	110.82
34	1	616	II0	C28-C26-C30	-2.07	120.16	124.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	c	501	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
37	8	617	LMG	O1-C7-C8	-2.07	105.79	110.82
31	z	101	8CT	C10-C11-C12	-2.07	123.18	126.23
32	c	505	CLA	CMB-C2B-C3B	2.07	131.41	126.55
34	2	614	II0	C28-C26-C30	-2.07	120.17	124.18
35	P	613	II3	C31-C34-C37	-2.07	117.21	123.20
31	c	518	8CT	C34-C33-C32	2.07	115.54	112.07
34	1	616	II0	C42-C41-C39	-2.07	119.29	123.52
36	2	616	IHT	C28-C26-C29	-2.07	120.17	124.18
37	P	616	LMG	O7-C10-O9	-2.07	118.87	123.70
34	8	614	II0	C28-C26-C30	-2.07	120.17	124.18
31	C	518	8CT	C34-C33-C32	2.07	115.53	112.07
32	2	603	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
33	6	609	KC2	O2D-CGD-O1D	-2.06	119.83	123.85
45	c	516	DGD	C5B-C4B-C3B	-2.06	103.93	114.37
32	9	608	CLA	CMA-C3A-C2A	-2.06	111.50	116.23
34	2	619	II0	C31-C29-C25	-2.06	120.84	126.61
34	p	301	II0	C04-C06-C08	-2.06	109.07	113.59
45	C	516	DGD	C5B-C4B-C3B	-2.06	103.94	114.37
33	P	605	KC2	CAA-CBA-CGA	-2.06	116.56	127.05
34	4	615	II0	C27-C25-C29	-2.06	120.18	124.18
34	1	616	II0	C32-C30-C26	-2.06	120.85	126.61
32	3	608	CLA	CMA-C3A-C2A	-2.06	111.51	116.23
31	B	622	8CT	C40-C12-C13	-2.06	119.48	122.82
45	c	514	DGD	CAB-C9B-C8B	-2.06	103.96	114.37
34	9	614	II0	C19-C13-C11	2.06	118.21	114.42
34	1	614	II0	C27-C25-C29	-2.06	120.19	124.18
32	D	401	CLA	O2D-CGD-CBD	2.06	114.83	111.23
45	A	614	DGD	O6E-C1E-O5D	-2.06	104.91	109.40
32	B	614	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
31	K	102	8CT	C23-C21-C20	-2.06	115.78	119.01
32	9	601	CLA	O2D-CGD-CBD	2.06	114.82	111.23
34	0	615	II0	C32-C34-C36	-2.06	120.73	126.36
35	6	613	II3	C05-C06-C10	-2.06	108.13	111.18
38	b	621	LHG	C27-C26-C25	-2.06	103.98	114.37
38	B	621	LHG	C27-C26-C25	-2.05	103.98	114.37
32	9	609	CLA	O2D-CGD-CBD	2.05	114.82	111.23
32	c	501	CLA	C1-C2-C3	-2.05	122.83	126.20
32	1	604	CLA	C1-C2-C3	-2.05	122.83	126.20
32	7	605	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
45	C	514	DGD	CAB-C9B-C8B	-2.05	103.99	114.37
32	8	603	CLA	O2A-CGA-O1A	-2.05	118.49	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	p	304	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
32	c	507	CLA	C1-C2-C3	-2.05	122.83	126.20
32	b	613	CLA	CMB-C2B-C3B	2.05	131.38	126.55
32	c	509	CLA	CMB-C2B-C3B	2.05	131.38	126.55
34	5	316	II0	C31-C29-C25	-2.05	120.87	126.61
34	1	614	II0	C31-C33-C35	-2.05	120.74	126.36
34	2	614	II0	C32-C30-C26	-2.05	120.88	126.61
32	d	409	CLA	CMB-C2B-C3B	2.05	131.37	126.55
41	D	402	PHO	O2A-CGA-O1A	-2.05	118.50	123.63
34	4	615	II0	C08-C12-C14	-2.05	107.08	112.18
35	6	613	II3	C42-C38-C37	2.05	121.22	118.09
31	k	102	8CT	C05-C04-C03	2.05	113.41	110.44
32	b	602	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
34	2	613	II0	C20-C14-C12	2.05	118.18	114.42
34	P	612	II0	C20-C14-C12	2.05	118.18	114.42
45	C	515	DGD	O2D-C2D-C1D	-2.05	105.20	110.08
34	3	613	II0	C37-C35-C33	2.05	121.21	118.09
32	D	404	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
32	b	614	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
41	d	410	PHO	O2A-CGA-O1A	-2.04	118.51	123.63
32	C	503	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
34	p	314	II0	C27-C25-C29	-2.04	120.21	124.18
37	d	401	LMG	O8-C28-O10	-2.04	118.52	123.63
32	B	613	CLA	CMB-C2B-C3B	2.04	131.35	126.55
32	b	607	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
34	P	614	II0	C20-C14-C10	-2.04	120.34	124.16
31	K	101	8CT	C05-C04-C03	2.04	113.40	110.44
31	k	101	8CT	C01-C02-C07	2.04	117.94	113.60
32	3	609	CLA	O2D-CGD-CBD	2.04	114.80	111.23
34	2	615	II0	C28-C26-C30	-2.04	120.22	124.18
32	4	604	CLA	CAA-C2A-C3A	-2.04	107.49	113.00
34	0	616	II0	C32-C30-C26	-2.04	120.91	126.61
45	a	414	DGD	O6E-C1E-O5D	-2.04	104.95	109.40
37	D	411	LMG	O8-C28-O10	-2.04	118.53	123.63
34	0	620	II0	C06-C04-C10	2.04	113.50	109.49
34	4	616	II0	C32-C30-C26	-2.04	120.92	126.61
35	P	613	II3	C42-C38-C37	2.04	121.20	118.09
32	8	608	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
31	M	201	8CT	C40-C12-C13	-2.04	119.52	122.82
34	9	614	II0	C20-C14-C10	-2.04	120.35	124.16
32	B	602	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
32	C	507	CLA	C1-C2-C3	-2.03	122.86	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	615	8CT	C30-C31-C32	-2.03	118.96	121.47
34	9	612	II0	C31-C33-C35	-2.03	120.78	126.36
32	c	513	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
32	7	603	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
32	C	512	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
34	8	615	II0	C32-C30-C26	-2.03	120.92	126.61
43	d	404	PL9	C37-C38-C39	-2.03	122.97	127.62
33	4	610	KC2	O2A-CGA-O1A	-2.03	118.56	122.70
32	2	604	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
34	5	316	II0	C20-C14-C10	-2.03	120.36	124.16
32	8	604	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
45	c	515	DGD	O2D-C2D-C1D	-2.03	105.23	110.08
32	7	603	CLA	CMB-C2B-C3B	2.03	131.33	126.55
32	4	608	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
32	c	504	CLA	CMB-C2B-C3B	2.03	131.33	126.55
32	2	608	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
31	K	102	8CT	C01-C02-C07	2.03	117.93	113.60
38	D	406	LHG	C5-O7-C7	-2.03	112.94	117.80
32	C	504	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
32	d	409	CLA	O2D-CGD-CBD	2.03	114.78	111.23
32	C	509	CLA	CMB-C2B-C3B	2.03	131.32	126.55
38	L	101	LHG	C5-O7-C7	-2.03	112.94	117.80
33	6	609	KC2	O2A-CGA-O1A	-2.03	118.57	122.70
32	0	608	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
34	p	316	II0	C27-C25-C29	-2.03	120.25	124.18
32	0	605	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
43	d	404	PL9	C8-C7-C3	2.03	117.27	112.03
43	D	405	PL9	C12-C13-C14	-2.02	122.99	127.62
34	4	619	II0	C30-C32-C34	-2.02	117.34	123.20
34	3	613	II0	C27-C25-C29	-2.02	120.25	124.18
37	6	616	LMG	O7-C10-O9	-2.02	118.98	123.70
33	0	610	KC2	O2A-CGA-O1A	-2.02	118.58	122.70
33	P	609	KC2	O2A-CGA-O1A	-2.02	118.58	122.70
45	C	515	DGD	CAB-C9B-C8B	-2.02	104.15	114.37
32	4	605	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
47	V	201	HEM	C2A-C1A-NA	-2.02	107.91	110.15
32	c	512	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
45	h	101	DGD	O3E-C3E-C2E	-2.02	105.61	110.38
32	B	607	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
32	9	609	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
31	B	624	8CT	C40-C12-C13	-2.02	119.55	122.82
43	D	405	PL9	C8-C7-C3	2.02	117.25	112.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	d	403	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
32	6	602	CLA	O2D-CGD-CBD	2.02	114.76	111.23
33	P	609	KC2	O2D-CGD-O1D	-2.02	119.92	123.85
45	c	515	DGD	CAB-C9B-C8B	-2.02	104.18	114.37
34	8	615	II0	C04-C06-C08	-2.02	109.17	113.59
32	P	607	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
31	6	615	8CT	C39-C16-C17	-2.02	119.55	122.82
32	1	603	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
34	9	613	II0	C37-C35-C33	2.01	121.17	118.09
32	C	501	CLA	C1-C2-C3	-2.01	122.90	126.20
32	6	607	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
34	9	613	II0	C29-C31-C33	-2.01	117.37	123.20
34	4	616	II0	C28-C26-C30	-2.01	120.27	124.18
36	5	317	IHT	C19-C10-C09	2.01	117.89	113.60
32	c	503	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
33	P	605	KC2	C2D-C1D-ND	-2.01	108.24	110.33
33	7	610	KC2	CHB-C4A-C3A	-2.01	121.85	125.03
34	1	617	II0	C32-C30-C26	-2.01	120.99	126.61
38	d	405	LHG	C5-O7-C7	-2.01	112.98	117.80
45	H	101	DGD	O3E-C3E-C2E	-2.01	105.64	110.38
47	v	201	HEM	C3D-C4D-ND	-2.01	107.97	110.17
32	0	603	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
34	9	614	II0	C08-C12-C14	-2.01	107.18	112.18
45	C	516	DGD	O6E-C1E-O5D	-2.01	105.30	110.04
32	b	609	CLA	CMB-C2B-C3B	2.01	131.27	126.55
32	5	309	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
34	0	615	II0	C06-C04-C10	2.01	113.44	109.49
43	D	405	PL9	C37-C38-C39	-2.01	123.03	127.62
35	7	615	II3	C34-C31-C28	-2.01	121.00	126.61
32	p	309	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
34	4	619	II0	C08-C12-C14	-2.00	107.19	112.18
32	0	604	CLA	CAA-C2A-C3A	-2.00	107.58	113.00
34	0	616	II0	C19-C13-C09	-2.00	120.41	124.16
43	d	404	PL9	C12-C13-C14	-2.00	123.04	127.62
47	E	101	HEM	C1B-NB-C4B	2.00	107.58	105.21
32	4	603	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
34	0	615	II0	C27-C25-C29	-2.00	120.30	124.18

All (208) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
32	1	601	CLA	ND

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Mol	Chain	Res	Type	Atom
32	1	602	CLA	ND
32	1	603	CLA	ND
32	1	604	CLA	ND
32	1	605	CLA	ND
32	1	606	CLA	ND
32	1	607	CLA	ND
32	1	608	CLA	ND
32	1	609	CLA	ND
32	1	611	CLA	ND
32	1	612	CLA	ND
32	1	613	CLA	ND
32	2	601	CLA	ND
32	2	602	CLA	ND
32	2	603	CLA	ND
32	2	604	CLA	ND
32	2	605	CLA	ND
32	2	606	CLA	ND
32	2	607	CLA	ND
32	2	608	CLA	ND
32	2	609	CLA	ND
32	2	611	CLA	ND
32	2	612	CLA	ND
32	3	601	CLA	ND
32	3	602	CLA	ND
32	3	603	CLA	ND
32	3	604	CLA	ND
32	3	605	CLA	ND
32	3	606	CLA	ND
32	3	607	CLA	ND
32	3	608	CLA	ND
32	3	609	CLA	ND
32	3	610	CLA	ND
32	3	611	CLA	ND
32	4	601	CLA	ND
32	4	602	CLA	ND
32	4	603	CLA	ND
32	4	604	CLA	ND
32	4	605	CLA	ND
32	4	606	CLA	ND
32	4	607	CLA	ND
32	4	608	CLA	ND
32	4	609	CLA	ND

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Mol	Chain	Res	Type	Atom
32	4	611	CLA	ND
32	4	612	CLA	ND
32	4	613	CLA	ND
32	5	302	CLA	ND
32	5	303	CLA	ND
32	5	304	CLA	ND
32	5	305	CLA	ND
32	5	306	CLA	ND
32	5	307	CLA	ND
32	5	308	CLA	ND
32	5	309	CLA	ND
32	5	310	CLA	ND
32	5	312	CLA	ND
32	5	313	CLA	ND
32	6	601	CLA	ND
32	6	602	CLA	ND
32	6	603	CLA	ND
32	6	604	CLA	ND
32	6	606	CLA	ND
32	6	607	CLA	ND
32	6	608	CLA	ND
32	6	610	CLA	ND
32	6	611	CLA	ND
32	A	602	CLA	ND
32	A	603	CLA	ND
32	A	605	CLA	ND
32	D	401	CLA	ND
32	D	403	CLA	ND
32	D	404	CLA	ND
32	S	302	CLA	ND
32	S	303	CLA	ND
32	b	602	CLA	ND
32	b	603	CLA	ND
32	b	604	CLA	ND
32	b	605	CLA	ND
32	b	606	CLA	ND
32	b	607	CLA	ND
32	b	608	CLA	ND
32	b	609	CLA	ND
32	b	610	CLA	ND
32	b	611	CLA	ND
32	b	612	CLA	ND

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Mol	Chain	Res	Type	Atom
32	b	613	CLA	ND
32	b	614	CLA	ND
32	b	615	CLA	ND
32	b	616	CLA	ND
32	b	617	CLA	ND
32	c	501	CLA	ND
32	c	502	CLA	ND
32	c	503	CLA	ND
32	c	504	CLA	ND
32	c	505	CLA	ND
32	c	506	CLA	ND
32	c	507	CLA	ND
32	c	508	CLA	ND
32	c	509	CLA	ND
32	c	510	CLA	ND
32	c	511	CLA	ND
32	c	512	CLA	ND
32	c	513	CLA	ND
32	d	402	CLA	ND
32	d	403	CLA	ND
32	d	409	CLA	ND
32	g	102	CLA	ND
32	0	601	CLA	ND
32	0	602	CLA	ND
32	0	603	CLA	ND
32	0	604	CLA	ND
32	0	605	CLA	ND
32	0	606	CLA	ND
32	0	607	CLA	ND
32	0	608	CLA	ND
32	0	609	CLA	ND
32	0	611	CLA	ND
32	0	612	CLA	ND
32	0	613	CLA	ND
32	7	601	CLA	ND
32	7	602	CLA	ND
32	7	603	CLA	ND
32	7	604	CLA	ND
32	7	605	CLA	ND
32	7	606	CLA	ND
32	7	607	CLA	ND
32	7	608	CLA	ND

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Mol	Chain	Res	Type	Atom
32	7	609	CLA	ND
32	7	611	CLA	ND
32	7	612	CLA	ND
32	7	613	CLA	ND
32	8	601	CLA	ND
32	8	602	CLA	ND
32	8	603	CLA	ND
32	8	604	CLA	ND
32	8	605	CLA	ND
32	8	606	CLA	ND
32	8	607	CLA	ND
32	8	608	CLA	ND
32	8	609	CLA	ND
32	8	611	CLA	ND
32	8	612	CLA	ND
32	9	601	CLA	ND
32	9	602	CLA	ND
32	9	603	CLA	ND
32	9	604	CLA	ND
32	9	605	CLA	ND
32	9	606	CLA	ND
32	9	607	CLA	ND
32	9	608	CLA	ND
32	9	609	CLA	ND
32	9	610	CLA	ND
32	9	611	CLA	ND
32	C	501	CLA	ND
32	C	502	CLA	ND
32	C	503	CLA	ND
32	C	504	CLA	ND
32	C	505	CLA	ND
32	C	506	CLA	ND
32	C	507	CLA	ND
32	C	508	CLA	ND
32	C	509	CLA	ND
32	C	510	CLA	ND
32	C	511	CLA	ND
32	C	512	CLA	ND
32	C	513	CLA	ND
32	G	101	CLA	ND
32	P	601	CLA	ND
32	P	602	CLA	ND

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Mol	Chain	Res	Type	Atom
32	P	603	CLA	ND
32	P	604	CLA	ND
32	P	606	CLA	ND
32	P	607	CLA	ND
32	P	608	CLA	ND
32	P	610	CLA	ND
32	P	611	CLA	ND
32	a	405	CLA	ND
32	a	406	CLA	ND
32	a	408	CLA	ND
32	p	302	CLA	ND
32	p	303	CLA	ND
32	p	304	CLA	ND
32	p	305	CLA	ND
32	p	306	CLA	ND
32	p	307	CLA	ND
32	p	308	CLA	ND
32	p	309	CLA	ND
32	p	310	CLA	ND
32	p	312	CLA	ND
32	p	313	CLA	ND
32	s	302	CLA	ND
32	s	303	CLA	ND
32	B	602	CLA	ND
32	B	603	CLA	ND
32	B	604	CLA	ND
32	B	605	CLA	ND
32	B	606	CLA	ND
32	B	607	CLA	ND
32	B	608	CLA	ND
32	B	609	CLA	ND
32	B	610	CLA	ND
32	B	611	CLA	ND
32	B	612	CLA	ND
32	B	613	CLA	ND
32	B	614	CLA	ND
32	B	615	CLA	ND
32	B	616	CLA	ND
32	B	617	CLA	ND

All (3132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	M	201	8CT	C16-C17-C18-C19
31	M	201	8CT	C20-C21-C23-C24
31	M	201	8CT	C22-C21-C23-C24
31	M	201	8CT	C28-C29-C30-C31
31	M	201	8CT	C28-C29-C30-C35
31	3	615	8CT	C12-C13-C14-C15
31	3	615	8CT	C20-C21-C23-C24
31	3	615	8CT	C22-C21-C23-C24
31	3	615	8CT	C28-C29-C30-C31
31	6	615	8CT	C28-C29-C30-C31
31	D	409	8CT	C02-C03-C10-C11
31	D	409	8CT	C12-C13-C14-C15
31	D	409	8CT	C14-C15-C16-C17
31	D	409	8CT	C14-C15-C16-C39
31	D	409	8CT	C25-C26-C28-C29
31	D	409	8CT	C28-C29-C30-C31
31	D	409	8CT	C28-C29-C30-C35
31	H	102	8CT	C10-C11-C12-C13
31	H	102	8CT	C10-C11-C12-C40
31	H	102	8CT	C14-C15-C16-C17
31	H	102	8CT	C28-C29-C30-C31
31	K	101	8CT	C14-C15-C16-C17
31	K	101	8CT	C14-C15-C16-C39
31	K	101	8CT	C18-C19-C20-C21
31	K	101	8CT	C28-C29-C30-C31
31	K	102	8CT	C14-C15-C16-C17
31	K	102	8CT	C14-C15-C16-C39
31	K	102	8CT	C16-C17-C18-C19
31	Z	101	8CT	C10-C11-C12-C13
31	Z	101	8CT	C10-C11-C12-C40
31	Z	101	8CT	C14-C15-C16-C17
31	Z	101	8CT	C14-C15-C16-C39
31	Z	101	8CT	C20-C21-C23-C24
31	Z	101	8CT	C22-C21-C23-C24
31	Z	101	8CT	C28-C29-C30-C31
31	b	622	8CT	C28-C29-C30-C31
31	b	622	8CT	C28-C29-C30-C35
31	b	623	8CT	C25-C26-C28-C29
31	b	623	8CT	C27-C26-C28-C29
31	c	518	8CT	C28-C29-C30-C31
31	c	518	8CT	C28-C29-C30-C35
31	d	408	8CT	C02-C03-C10-C11
31	d	408	8CT	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
31	d	408	8CT	C14-C15-C16-C17
31	d	408	8CT	C14-C15-C16-C39
31	d	408	8CT	C25-C26-C28-C29
31	d	408	8CT	C28-C29-C30-C31
31	d	408	8CT	C28-C29-C30-C35
31	k	101	8CT	C14-C15-C16-C17
31	k	101	8CT	C14-C15-C16-C39
31	k	101	8CT	C16-C17-C18-C19
31	k	102	8CT	C14-C15-C16-C17
31	k	102	8CT	C14-C15-C16-C39
31	k	102	8CT	C18-C19-C20-C21
31	k	102	8CT	C28-C29-C30-C31
31	z	101	8CT	C10-C11-C12-C13
31	z	101	8CT	C10-C11-C12-C40
31	z	101	8CT	C14-C15-C16-C17
31	z	101	8CT	C14-C15-C16-C39
31	z	101	8CT	C20-C21-C23-C24
31	z	101	8CT	C22-C21-C23-C24
31	z	101	8CT	C28-C29-C30-C31
31	9	615	8CT	C12-C13-C14-C15
31	9	615	8CT	C20-C21-C23-C24
31	9	615	8CT	C22-C21-C23-C24
31	9	615	8CT	C28-C29-C30-C31
31	C	518	8CT	C28-C29-C30-C31
31	C	518	8CT	C28-C29-C30-C35
31	P	615	8CT	C28-C29-C30-C31
31	h	102	8CT	C10-C11-C12-C13
31	h	102	8CT	C10-C11-C12-C40
31	h	102	8CT	C14-C15-C16-C17
31	h	102	8CT	C28-C29-C30-C31
31	B	622	8CT	C16-C17-C18-C19
31	B	622	8CT	C20-C21-C23-C24
31	B	622	8CT	C22-C21-C23-C24
31	B	622	8CT	C28-C29-C30-C31
31	B	622	8CT	C28-C29-C30-C35
31	B	623	8CT	C28-C29-C30-C31
31	B	623	8CT	C28-C29-C30-C35
31	B	624	8CT	C25-C26-C28-C29
31	B	624	8CT	C27-C26-C28-C29
32	1	601	CLA	C4B-C3B-CAB-CBB
32	1	602	CLA	C1A-C2A-CAA-CBA
32	1	602	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	1	603	CLA	C1A-C2A-CAA-CBA
32	1	603	CLA	C3A-C2A-CAA-CBA
32	1	605	CLA	C1A-C2A-CAA-CBA
32	1	605	CLA	C3A-C2A-CAA-CBA
32	1	605	CLA	CBD-CGD-O2D-CED
32	1	606	CLA	C1A-C2A-CAA-CBA
32	1	606	CLA	C3A-C2A-CAA-CBA
32	1	607	CLA	C1A-C2A-CAA-CBA
32	1	607	CLA	C3A-C2A-CAA-CBA
32	1	607	CLA	C4B-C3B-CAB-CBB
32	1	608	CLA	C2B-C3B-CAB-CBB
32	1	608	CLA	C4B-C3B-CAB-CBB
32	1	609	CLA	C2B-C3B-CAB-CBB
32	1	609	CLA	C4B-C3B-CAB-CBB
32	1	611	CLA	CBD-CGD-O2D-CED
32	1	612	CLA	C2B-C3B-CAB-CBB
32	1	612	CLA	C4B-C3B-CAB-CBB
32	1	612	CLA	CBD-CGD-O2D-CED
32	1	613	CLA	CBD-CGD-O2D-CED
32	2	602	CLA	C1A-C2A-CAA-CBA
32	2	602	CLA	C3A-C2A-CAA-CBA
32	2	603	CLA	C1A-C2A-CAA-CBA
32	2	603	CLA	C3A-C2A-CAA-CBA
32	2	609	CLA	C2B-C3B-CAB-CBB
32	2	609	CLA	C4B-C3B-CAB-CBB
32	2	611	CLA	C1A-C2A-CAA-CBA
32	2	611	CLA	C3A-C2A-CAA-CBA
32	2	612	CLA	CBD-CGD-O2D-CED
32	3	601	CLA	CBD-CGD-O2D-CED
32	3	601	CLA	O1D-CGD-O2D-CED
32	3	602	CLA	C1A-C2A-CAA-CBA
32	3	602	CLA	C3A-C2A-CAA-CBA
32	3	605	CLA	C3A-C2A-CAA-CBA
32	3	605	CLA	C4B-C3B-CAB-CBB
32	3	607	CLA	CBD-CGD-O2D-CED
32	3	609	CLA	C4B-C3B-CAB-CBB
32	4	601	CLA	C4B-C3B-CAB-CBB
32	4	602	CLA	C1A-C2A-CAA-CBA
32	4	602	CLA	C3A-C2A-CAA-CBA
32	4	603	CLA	C1A-C2A-CAA-CBA
32	4	603	CLA	C3A-C2A-CAA-CBA
32	4	605	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	4	607	CLA	C4B-C3B-CAB-CBB
32	4	609	CLA	C4B-C3B-CAB-CBB
32	4	611	CLA	CBD-CGD-O2D-CED
32	4	612	CLA	C4B-C3B-CAB-CBB
32	4	612	CLA	CBD-CGD-O2D-CED
32	4	613	CLA	C2B-C3B-CAB-CBB
32	4	613	CLA	C4B-C3B-CAB-CBB
32	4	613	CLA	CBD-CGD-O2D-CED
32	5	302	CLA	C4B-C3B-CAB-CBB
32	5	303	CLA	C1A-C2A-CAA-CBA
32	5	303	CLA	C3A-C2A-CAA-CBA
32	5	303	CLA	C2B-C3B-CAB-CBB
32	5	303	CLA	C4B-C3B-CAB-CBB
32	5	306	CLA	C1A-C2A-CAA-CBA
32	5	306	CLA	C3A-C2A-CAA-CBA
32	5	307	CLA	C2B-C3B-CAB-CBB
32	5	307	CLA	C4B-C3B-CAB-CBB
32	5	307	CLA	CHA-CBD-CGD-O2D
32	5	308	CLA	C1A-C2A-CAA-CBA
32	5	308	CLA	C3A-C2A-CAA-CBA
32	5	310	CLA	C4B-C3B-CAB-CBB
32	5	312	CLA	C1A-C2A-CAA-CBA
32	5	312	CLA	C3A-C2A-CAA-CBA
32	5	313	CLA	CHA-CBD-CGD-O2D
32	6	602	CLA	C1A-C2A-CAA-CBA
32	6	602	CLA	C3A-C2A-CAA-CBA
32	6	611	CLA	CHA-CBD-CGD-O2D
32	A	602	CLA	C1A-C2A-CAA-CBA
32	A	602	CLA	C3A-C2A-CAA-CBA
32	A	605	CLA	C1A-C2A-CAA-CBA
32	A	605	CLA	C3A-C2A-CAA-CBA
32	D	404	CLA	C2-C3-C5-C6
32	D	404	CLA	C4-C3-C5-C6
32	S	302	CLA	C3A-C2A-CAA-CBA
32	S	302	CLA	CBD-CGD-O2D-CED
32	S	303	CLA	C2B-C3B-CAB-CBB
32	S	303	CLA	C4B-C3B-CAB-CBB
32	S	303	CLA	CHA-CBD-CGD-O1D
32	S	303	CLA	CHA-CBD-CGD-O2D
32	b	602	CLA	CAD-CBD-CGD-O1D
32	b	602	CLA	CAD-CBD-CGD-O2D
32	b	603	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	b	613	CLA	C1A-C2A-CAA-CBA
32	b	614	CLA	CBD-CGD-O2D-CED
32	b	614	CLA	C14-C13-C15-C16
32	b	615	CLA	CAD-CBD-CGD-O1D
32	b	615	CLA	CAD-CBD-CGD-O2D
32	b	616	CLA	C4B-C3B-CAB-CBB
32	c	507	CLA	CHA-CBD-CGD-O2D
32	c	508	CLA	CHA-CBD-CGD-O1D
32	c	508	CLA	CHA-CBD-CGD-O2D
32	c	513	CLA	C1A-C2A-CAA-CBA
32	c	513	CLA	C3A-C2A-CAA-CBA
32	d	403	CLA	C2-C3-C5-C6
32	d	403	CLA	C4-C3-C5-C6
32	g	102	CLA	C1A-C2A-CAA-CBA
32	0	601	CLA	C4B-C3B-CAB-CBB
32	0	602	CLA	C1A-C2A-CAA-CBA
32	0	602	CLA	C3A-C2A-CAA-CBA
32	0	603	CLA	C1A-C2A-CAA-CBA
32	0	603	CLA	C3A-C2A-CAA-CBA
32	0	605	CLA	CBD-CGD-O2D-CED
32	0	607	CLA	C4B-C3B-CAB-CBB
32	0	609	CLA	C4B-C3B-CAB-CBB
32	0	611	CLA	CBD-CGD-O2D-CED
32	0	612	CLA	C4B-C3B-CAB-CBB
32	0	612	CLA	CBD-CGD-O2D-CED
32	0	613	CLA	C2B-C3B-CAB-CBB
32	0	613	CLA	C4B-C3B-CAB-CBB
32	7	601	CLA	C4B-C3B-CAB-CBB
32	7	602	CLA	C1A-C2A-CAA-CBA
32	7	602	CLA	C3A-C2A-CAA-CBA
32	7	603	CLA	C1A-C2A-CAA-CBA
32	7	603	CLA	C3A-C2A-CAA-CBA
32	7	605	CLA	C1A-C2A-CAA-CBA
32	7	605	CLA	C3A-C2A-CAA-CBA
32	7	606	CLA	C1A-C2A-CAA-CBA
32	7	606	CLA	C3A-C2A-CAA-CBA
32	7	607	CLA	C1A-C2A-CAA-CBA
32	7	607	CLA	C3A-C2A-CAA-CBA
32	7	607	CLA	C4B-C3B-CAB-CBB
32	7	608	CLA	C2B-C3B-CAB-CBB
32	7	608	CLA	C4B-C3B-CAB-CBB
32	7	609	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	7	609	CLA	C4B-C3B-CAB-CBB
32	7	611	CLA	CBD-CGD-O2D-CED
32	7	612	CLA	C2B-C3B-CAB-CBB
32	7	612	CLA	C4B-C3B-CAB-CBB
32	7	612	CLA	CBD-CGD-O2D-CED
32	7	613	CLA	CBD-CGD-O2D-CED
32	8	602	CLA	C1A-C2A-CAA-CBA
32	8	602	CLA	C3A-C2A-CAA-CBA
32	8	603	CLA	C1A-C2A-CAA-CBA
32	8	603	CLA	C3A-C2A-CAA-CBA
32	8	609	CLA	C2B-C3B-CAB-CBB
32	8	609	CLA	C4B-C3B-CAB-CBB
32	8	611	CLA	C1A-C2A-CAA-CBA
32	8	611	CLA	C3A-C2A-CAA-CBA
32	8	612	CLA	CBD-CGD-O2D-CED
32	9	601	CLA	CBD-CGD-O2D-CED
32	9	602	CLA	C1A-C2A-CAA-CBA
32	9	602	CLA	C3A-C2A-CAA-CBA
32	9	605	CLA	C3A-C2A-CAA-CBA
32	9	605	CLA	C4B-C3B-CAB-CBB
32	9	607	CLA	CBD-CGD-O2D-CED
32	9	609	CLA	C4B-C3B-CAB-CBB
32	C	507	CLA	CHA-CBD-CGD-O2D
32	C	508	CLA	CHA-CBD-CGD-O1D
32	C	508	CLA	CHA-CBD-CGD-O2D
32	C	513	CLA	C1A-C2A-CAA-CBA
32	C	513	CLA	C3A-C2A-CAA-CBA
32	G	101	CLA	C1A-C2A-CAA-CBA
32	P	602	CLA	C1A-C2A-CAA-CBA
32	P	602	CLA	C3A-C2A-CAA-CBA
32	P	611	CLA	CHA-CBD-CGD-O1D
32	P	611	CLA	CHA-CBD-CGD-O2D
32	a	405	CLA	C1A-C2A-CAA-CBA
32	a	405	CLA	C3A-C2A-CAA-CBA
32	a	408	CLA	C1A-C2A-CAA-CBA
32	a	408	CLA	C3A-C2A-CAA-CBA
32	p	302	CLA	C4B-C3B-CAB-CBB
32	p	303	CLA	C1A-C2A-CAA-CBA
32	p	303	CLA	C3A-C2A-CAA-CBA
32	p	303	CLA	C2B-C3B-CAB-CBB
32	p	303	CLA	C4B-C3B-CAB-CBB
32	p	306	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	p	306	CLA	C3A-C2A-CAA-CBA
32	p	307	CLA	C2B-C3B-CAB-CBB
32	p	307	CLA	C4B-C3B-CAB-CBB
32	p	307	CLA	CHA-CBD-CGD-O2D
32	p	308	CLA	C1A-C2A-CAA-CBA
32	p	308	CLA	C3A-C2A-CAA-CBA
32	p	310	CLA	C4B-C3B-CAB-CBB
32	p	312	CLA	C1A-C2A-CAA-CBA
32	p	312	CLA	C3A-C2A-CAA-CBA
32	p	312	CLA	CBD-CGD-O2D-CED
32	p	313	CLA	CHA-CBD-CGD-O2D
32	s	302	CLA	C3A-C2A-CAA-CBA
32	s	302	CLA	CBD-CGD-O2D-CED
32	s	303	CLA	C2B-C3B-CAB-CBB
32	s	303	CLA	C4B-C3B-CAB-CBB
32	s	303	CLA	CHA-CBD-CGD-O1D
32	s	303	CLA	CHA-CBD-CGD-O2D
32	B	602	CLA	CAD-CBD-CGD-O1D
32	B	602	CLA	CAD-CBD-CGD-O2D
32	B	603	CLA	C1A-C2A-CAA-CBA
32	B	613	CLA	C1A-C2A-CAA-CBA
32	B	614	CLA	CBD-CGD-O2D-CED
32	B	614	CLA	C14-C13-C15-C16
32	B	615	CLA	CAD-CBD-CGD-O1D
32	B	615	CLA	CAD-CBD-CGD-O2D
32	B	616	CLA	C4B-C3B-CAB-CBB
33	1	610	KC2	C1A-C2A-CAA-CBA
33	1	610	KC2	C2B-C3B-CAB-CBB
33	1	610	KC2	C4B-C3B-CAB-CBB
33	1	610	KC2	CHA-CBD-CGD-O2D
33	1	610	KC2	CBD-CGD-O2D-CED
33	2	610	KC2	C3A-C2A-CAA-CBA
33	2	610	KC2	C2B-C3B-CAB-CBB
33	2	610	KC2	C4B-C3B-CAB-CBB
33	4	610	KC2	C1A-C2A-CAA-CBA
33	4	610	KC2	C3A-C2A-CAA-CBA
33	4	610	KC2	C2B-C3B-CAB-CBB
33	4	610	KC2	C2C-C3C-CAC-CBC
33	4	610	KC2	C2A-CAA-CBA-CGA
33	4	610	KC2	CHA-CBD-CGD-O1D
33	5	311	KC2	C2B-C3B-CAB-CBB
33	5	311	KC2	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
33	5	311	KC2	C2C-C3C-CAC-CBC
33	5	311	KC2	C4C-C3C-CAC-CBC
33	5	311	KC2	CHA-CBD-CGD-O1D
33	5	311	KC2	CHA-CBD-CGD-O2D
33	6	605	KC2	C3A-C2A-CAA-CBA
33	6	605	KC2	C2B-C3B-CAB-CBB
33	6	605	KC2	C4B-C3B-CAB-CBB
33	6	605	KC2	C2C-C3C-CAC-CBC
33	6	605	KC2	C4C-C3C-CAC-CBC
33	6	605	KC2	CBD-CGD-O2D-CED
33	6	609	KC2	C1A-C2A-CAA-CBA
33	6	609	KC2	C3A-C2A-CAA-CBA
33	6	609	KC2	C2B-C3B-CAB-CBB
33	6	609	KC2	C4B-C3B-CAB-CBB
33	6	609	KC2	C2C-C3C-CAC-CBC
33	6	609	KC2	C2A-CAA-CBA-CGA
33	6	609	KC2	CHA-CBD-CGD-O1D
33	0	610	KC2	C1A-C2A-CAA-CBA
33	0	610	KC2	C3A-C2A-CAA-CBA
33	0	610	KC2	C2B-C3B-CAB-CBB
33	0	610	KC2	C2C-C3C-CAC-CBC
33	0	610	KC2	C2A-CAA-CBA-CGA
33	0	610	KC2	CHA-CBD-CGD-O1D
33	7	610	KC2	C1A-C2A-CAA-CBA
33	7	610	KC2	C2B-C3B-CAB-CBB
33	7	610	KC2	C4B-C3B-CAB-CBB
33	7	610	KC2	CHA-CBD-CGD-O2D
33	7	610	KC2	CBD-CGD-O2D-CED
33	8	610	KC2	C3A-C2A-CAA-CBA
33	8	610	KC2	C2B-C3B-CAB-CBB
33	8	610	KC2	C4B-C3B-CAB-CBB
33	P	605	KC2	C1A-C2A-CAA-CBA
33	P	605	KC2	C2B-C3B-CAB-CBB
33	P	605	KC2	C4B-C3B-CAB-CBB
33	P	605	KC2	C2C-C3C-CAC-CBC
33	P	605	KC2	C4C-C3C-CAC-CBC
33	P	605	KC2	CBD-CGD-O2D-CED
33	P	609	KC2	C1A-C2A-CAA-CBA
33	P	609	KC2	C3A-C2A-CAA-CBA
33	P	609	KC2	C2B-C3B-CAB-CBB
33	P	609	KC2	C4B-C3B-CAB-CBB
33	P	609	KC2	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
33	P	609	KC2	C2A-CAA-CBA-CGA
33	P	609	KC2	CHA-CBD-CGD-O1D
33	p	311	KC2	C2B-C3B-CAB-CBB
33	p	311	KC2	C4B-C3B-CAB-CBB
33	p	311	KC2	C2C-C3C-CAC-CBC
33	p	311	KC2	C4C-C3C-CAC-CBC
33	p	311	KC2	CHA-CBD-CGD-O1D
33	p	311	KC2	CHA-CBD-CGD-O2D
34	1	616	II0	C31-C33-C35-C39
34	1	617	II0	C31-C33-C35-C39
34	2	615	II0	C32-C34-C36-C40
34	3	614	II0	C31-C33-C35-C37
34	3	614	II0	C31-C33-C35-C39
34	5	301	II0	C31-C33-C35-C37
34	5	301	II0	C31-C33-C35-C39
34	6	614	II0	C31-C33-C35-C37
34	6	614	II0	C31-C33-C35-C39
34	0	617	II0	C31-C33-C35-C37
34	0	617	II0	C31-C33-C35-C39
34	7	616	II0	C31-C33-C35-C39
34	7	617	II0	C31-C33-C35-C39
34	8	615	II0	C32-C34-C36-C40
34	9	614	II0	C31-C33-C35-C37
34	9	614	II0	C31-C33-C35-C39
34	P	614	II0	C31-C33-C35-C39
34	p	316	II0	C32-C34-C36-C38
34	p	316	II0	C32-C34-C36-C40
35	1	615	II3	C03-C04-C12-C21
35	1	615	II3	C07-C04-C12-C21
35	P	613	II3	C12-C21-C24-C26
36	4	614	IHT	C30-C32-C33-C36
36	4	614	IHT	C30-C32-C33-C37
36	4	617	IHT	C30-C32-C33-C36
36	4	617	IHT	C30-C32-C33-C37
36	0	614	IHT	C30-C32-C33-C36
36	0	614	IHT	C30-C32-C33-C37
36	0	618	IHT	C30-C32-C33-C36
36	0	618	IHT	C30-C32-C33-C37
37	D	411	LMG	C2-C1-O1-C7
37	d	401	LMG	C2-C1-O1-C7
37	l	101	LMG	O7-C8-C9-O8
37	l	101	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
37	L	102	LMG	O7-C8-C9-O8
37	L	102	LMG	C11-C10-O7-C8
37	P	616	LMG	C11-C10-O7-C8
38	2	618	LHG	O1-C1-C2-C3
38	2	618	LHG	O2-C2-C3-O3
38	2	618	LHG	C3-O3-P-O4
38	2	618	LHG	C4-O6-P-O3
38	A	613	LHG	C8-C7-O7-C5
38	D	410	LHG	C3-O3-P-O4
38	D	410	LHG	C3-O3-P-O5
38	D	410	LHG	C3-O3-P-O6
38	S	301	LHG	C3-O3-P-O4
38	S	301	LHG	C3-O3-P-O6
38	S	301	LHG	O9-C7-O7-C5
38	S	301	LHG	C8-C7-O7-C5
38	b	619	LHG	C3-O3-P-O6
38	b	619	LHG	C4-O6-P-O3
38	b	619	LHG	C4-O6-P-O5
38	b	619	LHG	O6-C4-C5-O7
38	b	619	LHG	O9-C7-O7-C5
38	d	411	LHG	C3-O3-P-O4
38	d	411	LHG	C3-O3-P-O5
38	d	411	LHG	C3-O3-P-O6
38	l	102	LHG	C3-O3-P-O5
38	l	102	LHG	C3-O3-P-O6
38	8	618	LHG	O1-C1-C2-C3
38	8	618	LHG	O2-C2-C3-O3
38	8	618	LHG	C3-O3-P-O4
38	8	618	LHG	C4-O6-P-O3
38	L	101	LHG	C3-O3-P-O5
38	L	101	LHG	C3-O3-P-O6
38	a	403	LHG	C8-C7-O7-C5
38	s	301	LHG	C3-O3-P-O4
38	s	301	LHG	C3-O3-P-O6
38	s	301	LHG	O9-C7-O7-C5
38	s	301	LHG	C8-C7-O7-C5
38	B	619	LHG	C3-O3-P-O6
38	B	619	LHG	C4-O6-P-O3
38	B	619	LHG	C4-O6-P-O5
38	B	619	LHG	O6-C4-C5-O7
38	B	619	LHG	O9-C7-O7-C5
39	5	318	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
39	5	318	SQD	C8-C7-O47-C45
39	5	318	SQD	C5-C6-S-O7
39	5	318	SQD	C5-C6-S-O8
39	5	318	SQD	C5-C6-S-O9
39	b	601	SQD	O6-C44-C45-O47
39	b	601	SQD	O49-C7-O47-C45
39	b	601	SQD	C8-C7-O47-C45
39	b	601	SQD	O10-C23-O48-C46
39	b	601	SQD	C24-C23-O48-C46
39	b	601	SQD	O5-C5-C6-S
39	b	620	SQD	C8-C7-O47-C45
39	b	620	SQD	O5-C5-C6-S
39	p	318	SQD	O5-C1-O6-C44
39	p	318	SQD	C8-C7-O47-C45
39	p	318	SQD	C5-C6-S-O7
39	p	318	SQD	C5-C6-S-O8
39	p	318	SQD	C5-C6-S-O9
39	B	601	SQD	O6-C44-C45-O47
39	B	601	SQD	O49-C7-O47-C45
39	B	601	SQD	C8-C7-O47-C45
39	B	601	SQD	O10-C23-O48-C46
39	B	601	SQD	C24-C23-O48-C46
39	B	601	SQD	O5-C5-C6-S
39	B	620	SQD	C8-C7-O47-C45
39	B	620	SQD	O5-C5-C6-S
32	1	611	CLA	O1D-CGD-O2D-CED
32	1	613	CLA	O1D-CGD-O2D-CED
32	3	607	CLA	O1D-CGD-O2D-CED
32	4	611	CLA	O1D-CGD-O2D-CED
32	A	602	CLA	O1D-CGD-O2D-CED
32	0	611	CLA	O1D-CGD-O2D-CED
32	7	611	CLA	O1D-CGD-O2D-CED
32	7	613	CLA	O1D-CGD-O2D-CED
32	9	601	CLA	O1D-CGD-O2D-CED
32	9	607	CLA	O1D-CGD-O2D-CED
32	a	405	CLA	O1D-CGD-O2D-CED
33	P	605	KC2	O1D-CGD-O2D-CED
32	1	601	CLA	O1D-CGD-O2D-CED
32	4	605	CLA	O1D-CGD-O2D-CED
32	S	302	CLA	O1D-CGD-O2D-CED
32	0	605	CLA	O1D-CGD-O2D-CED
32	7	601	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	s	302	CLA	O1D-CGD-O2D-CED
33	1	610	KC2	O1D-CGD-O2D-CED
33	7	610	KC2	O1D-CGD-O2D-CED
32	1	601	CLA	CBD-CGD-O2D-CED
32	1	602	CLA	CBD-CGD-O2D-CED
32	1	604	CLA	CBD-CGD-O2D-CED
32	2	609	CLA	CBD-CGD-O2D-CED
32	2	611	CLA	CBD-CGD-O2D-CED
32	4	608	CLA	CBD-CGD-O2D-CED
32	5	306	CLA	CBD-CGD-O2D-CED
32	5	310	CLA	CBD-CGD-O2D-CED
32	5	312	CLA	CBD-CGD-O2D-CED
32	6	610	CLA	CBD-CGD-O2D-CED
32	A	602	CLA	CBD-CGD-O2D-CED
32	b	606	CLA	CBD-CGD-O2D-CED
32	b	608	CLA	CBD-CGD-O2D-CED
32	b	611	CLA	CBD-CGD-O2D-CED
32	b	613	CLA	CBD-CGD-O2D-CED
32	c	506	CLA	CBD-CGD-O2D-CED
32	0	608	CLA	CBD-CGD-O2D-CED
32	0	613	CLA	CBD-CGD-O2D-CED
32	7	601	CLA	CBD-CGD-O2D-CED
32	7	602	CLA	CBD-CGD-O2D-CED
32	7	604	CLA	CBD-CGD-O2D-CED
32	7	605	CLA	CBD-CGD-O2D-CED
32	8	609	CLA	CBD-CGD-O2D-CED
32	8	611	CLA	CBD-CGD-O2D-CED
32	C	501	CLA	CBD-CGD-O2D-CED
32	C	506	CLA	CBD-CGD-O2D-CED
32	P	610	CLA	CBD-CGD-O2D-CED
32	a	405	CLA	CBD-CGD-O2D-CED
32	p	306	CLA	CBD-CGD-O2D-CED
32	p	310	CLA	CBD-CGD-O2D-CED
32	B	606	CLA	CBD-CGD-O2D-CED
32	B	608	CLA	CBD-CGD-O2D-CED
32	B	611	CLA	CBD-CGD-O2D-CED
32	B	613	CLA	CBD-CGD-O2D-CED
33	2	610	KC2	CBD-CGD-O2D-CED
33	8	610	KC2	CBD-CGD-O2D-CED
39	b	620	SQD	O10-C23-O48-C46
39	B	620	SQD	O10-C23-O48-C46
32	2	611	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	7	605	CLA	O1D-CGD-O2D-CED
32	8	611	CLA	O1D-CGD-O2D-CED
33	6	605	KC2	O1D-CGD-O2D-CED
39	b	620	SQD	C24-C23-O48-C46
39	B	620	SQD	C24-C23-O48-C46
32	A	602	CLA	O1A-CGA-O2A-C1
32	a	405	CLA	O1A-CGA-O2A-C1
37	D	411	LMG	O10-C28-O8-C9
37	d	401	LMG	O10-C28-O8-C9
38	A	613	LHG	O10-C23-O8-C6
38	a	403	LHG	O10-C23-O8-C6
39	5	318	SQD	O10-C23-O48-C46
39	p	318	SQD	O10-C23-O48-C46
41	A	604	PHO	O1A-CGA-O2A-C1
41	a	407	PHO	O1A-CGA-O2A-C1
32	1	602	CLA	O1D-CGD-O2D-CED
32	1	605	CLA	O1D-CGD-O2D-CED
32	4	612	CLA	O1D-CGD-O2D-CED
32	b	614	CLA	O1D-CGD-O2D-CED
32	7	602	CLA	O1D-CGD-O2D-CED
32	B	614	CLA	O1D-CGD-O2D-CED
33	1	610	KC2	CAA-CBA-CGA-O1A
33	4	610	KC2	CAA-CBA-CGA-O2A
33	0	610	KC2	CAA-CBA-CGA-O2A
33	7	610	KC2	CAA-CBA-CGA-O1A
32	2	612	CLA	O1D-CGD-O2D-CED
32	8	612	CLA	O1D-CGD-O2D-CED
32	6	611	CLA	CBD-CGD-O2D-CED
32	7	608	CLA	CBD-CGD-O2D-CED
37	6	616	LMG	O9-C10-O7-C8
37	l	101	LMG	O9-C10-O7-C8
37	L	102	LMG	O9-C10-O7-C8
37	P	616	LMG	O9-C10-O7-C8
38	A	613	LHG	O9-C7-O7-C5
38	b	621	LHG	O9-C7-O7-C5
38	a	403	LHG	O9-C7-O7-C5
38	B	621	LHG	O9-C7-O7-C5
39	5	318	SQD	O49-C7-O47-C45
39	b	620	SQD	O49-C7-O47-C45
39	p	318	SQD	O49-C7-O47-C45
39	B	620	SQD	O49-C7-O47-C45
32	3	609	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
32	b	607	CLA	C3-C5-C6-C7
32	b	612	CLA	C3-C5-C6-C7
32	c	503	CLA	C3-C5-C6-C7
32	0	602	CLA	C3-C5-C6-C7
32	9	609	CLA	C3-C5-C6-C7
32	C	503	CLA	C3-C5-C6-C7
32	B	607	CLA	C3-C5-C6-C7
32	B	612	CLA	C3-C5-C6-C7
41	A	604	PHO	C3-C5-C6-C7
41	a	407	PHO	C3-C5-C6-C7
32	C	503	CLA	CBA-CGA-O2A-C1
37	D	411	LMG	C29-C28-O8-C9
37	d	401	LMG	C29-C28-O8-C9
41	A	604	PHO	CBA-CGA-O2A-C1
41	a	407	PHO	CBA-CGA-O2A-C1
32	1	608	CLA	CBD-CGD-O2D-CED
32	2	608	CLA	CBD-CGD-O2D-CED
32	4	601	CLA	CBD-CGD-O2D-CED
32	5	303	CLA	CBD-CGD-O2D-CED
32	5	309	CLA	CBD-CGD-O2D-CED
32	6	602	CLA	CBD-CGD-O2D-CED
32	b	605	CLA	CBD-CGD-O2D-CED
32	c	501	CLA	CBD-CGD-O2D-CED
32	0	601	CLA	CBD-CGD-O2D-CED
32	7	606	CLA	CBD-CGD-O2D-CED
32	8	608	CLA	CBD-CGD-O2D-CED
32	P	602	CLA	CBD-CGD-O2D-CED
32	P	611	CLA	CBD-CGD-O2D-CED
32	p	309	CLA	CBD-CGD-O2D-CED
32	B	605	CLA	CBD-CGD-O2D-CED
37	6	616	LMG	C11-C10-O7-C8
37	D	411	LMG	C11-C10-O7-C8
37	d	401	LMG	C11-C10-O7-C8
38	b	619	LHG	C8-C7-O7-C5
38	B	619	LHG	C8-C7-O7-C5
32	1	612	CLA	O1D-CGD-O2D-CED
32	4	613	CLA	O1D-CGD-O2D-CED
32	0	612	CLA	O1D-CGD-O2D-CED
32	7	612	CLA	O1D-CGD-O2D-CED
32	p	312	CLA	O1D-CGD-O2D-CED
33	1	610	KC2	CAA-CBA-CGA-O2A
33	4	610	KC2	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
33	6	609	KC2	CAA-CBA-CGA-O1A
33	6	609	KC2	CAA-CBA-CGA-O2A
33	0	610	KC2	CAA-CBA-CGA-O1A
33	7	610	KC2	CAA-CBA-CGA-O2A
33	P	609	KC2	CAA-CBA-CGA-O1A
33	P	609	KC2	CAA-CBA-CGA-O2A
32	b	604	CLA	C4-C3-C5-C6
32	b	612	CLA	C4-C3-C5-C6
32	c	504	CLA	C4-C3-C5-C6
32	C	504	CLA	C4-C3-C5-C6
32	B	604	CLA	C4-C3-C5-C6
32	B	612	CLA	C4-C3-C5-C6
32	b	604	CLA	C2-C3-C5-C6
32	b	612	CLA	C2-C3-C5-C6
32	c	504	CLA	C2-C3-C5-C6
32	C	504	CLA	C2-C3-C5-C6
32	B	604	CLA	C2-C3-C5-C6
32	B	612	CLA	C2-C3-C5-C6
32	6	606	CLA	CBD-CGD-O2D-CED
32	8	602	CLA	CBD-CGD-O2D-CED
32	P	606	CLA	CBD-CGD-O2D-CED
32	4	613	CLA	C2A-CAA-CBA-CGA
32	b	603	CLA	C2A-CAA-CBA-CGA
32	B	603	CLA	C2A-CAA-CBA-CGA
32	S	303	CLA	C3-C5-C6-C7
32	b	605	CLA	C3-C5-C6-C7
32	s	303	CLA	C3-C5-C6-C7
32	B	605	CLA	C3-C5-C6-C7
32	A	602	CLA	CBA-CGA-O2A-C1
32	c	503	CLA	CBA-CGA-O2A-C1
32	a	405	CLA	CBA-CGA-O2A-C1
37	l	101	LMG	C29-C28-O8-C9
37	L	102	LMG	C29-C28-O8-C9
38	A	613	LHG	C24-C23-O8-C6
38	a	403	LHG	C24-C23-O8-C6
39	5	318	SQD	C24-C23-O48-C46
39	p	318	SQD	C24-C23-O48-C46
45	c	515	DGD	C2A-C1A-O1G-C1G
45	C	515	DGD	C2A-C1A-O1G-C1G
31	M	201	8CT	C12-C13-C14-C15
31	M	201	8CT	C18-C19-C20-C21
31	K	102	8CT	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
31	Z	101	8CT	C12-C13-C14-C15
31	k	101	8CT	C12-C13-C14-C15
31	z	101	8CT	C12-C13-C14-C15
31	B	622	8CT	C18-C19-C20-C21
34	4	619	II0	C26-C30-C32-C34
34	5	315	II0	C36-C40-C42-C41
34	0	620	II0	C26-C30-C32-C34
34	p	315	II0	C36-C40-C42-C41
36	4	617	IHT	C33-C37-C40-C41
32	b	602	CLA	O1A-CGA-O2A-C1
32	B	602	CLA	O1A-CGA-O2A-C1
37	l	101	LMG	O10-C28-O8-C9
37	D	411	LMG	O9-C10-O7-C8
37	d	401	LMG	O9-C10-O7-C8
32	5	312	CLA	O1D-CGD-O2D-CED
32	p	306	CLA	O1D-CGD-O2D-CED
32	4	602	CLA	C3-C5-C6-C7
32	4	604	CLA	C3-C5-C6-C7
32	c	504	CLA	C3-C5-C6-C7
32	0	604	CLA	C3-C5-C6-C7
32	C	504	CLA	C3-C5-C6-C7
32	2	602	CLA	CBD-CGD-O2D-CED
32	5	302	CLA	CBD-CGD-O2D-CED
32	p	302	CLA	CBD-CGD-O2D-CED
32	p	303	CLA	CBD-CGD-O2D-CED
32	4	608	CLA	O1D-CGD-O2D-CED
32	b	613	CLA	O1D-CGD-O2D-CED
32	0	608	CLA	O1D-CGD-O2D-CED
32	0	613	CLA	O1D-CGD-O2D-CED
32	C	501	CLA	O1D-CGD-O2D-CED
32	B	613	CLA	O1D-CGD-O2D-CED
32	4	605	CLA	CBA-CGA-O2A-C1
37	b	618	LMG	O6-C5-C6-O5
37	B	618	LMG	O6-C5-C6-O5
32	c	503	CLA	O1A-CGA-O2A-C1
32	C	503	CLA	O1A-CGA-O2A-C1
37	L	102	LMG	O10-C28-O8-C9
45	c	515	DGD	O1A-C1A-O1G-C1G
45	C	515	DGD	O1A-C1A-O1G-C1G
32	6	610	CLA	O1D-CGD-O2D-CED
32	P	610	CLA	O1D-CGD-O2D-CED
37	D	411	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
32	4	604	CLA	CBD-CGD-O2D-CED
32	p	313	CLA	CBD-CGD-O2D-CED
38	b	621	LHG	C8-C7-O7-C5
38	B	621	LHG	C8-C7-O7-C5
45	A	614	DGD	C2B-C1B-O2G-C2G
45	a	414	DGD	C2B-C1B-O2G-C2G
32	5	310	CLA	O1D-CGD-O2D-CED
37	d	401	LMG	O6-C5-C6-O5
32	b	608	CLA	O1D-CGD-O2D-CED
32	7	604	CLA	O1D-CGD-O2D-CED
32	p	310	CLA	O1D-CGD-O2D-CED
32	B	608	CLA	O1D-CGD-O2D-CED
32	3	603	CLA	CBD-CGD-O2D-CED
32	5	304	CLA	CBD-CGD-O2D-CED
32	5	313	CLA	CBD-CGD-O2D-CED
32	b	610	CLA	CBD-CGD-O2D-CED
32	0	604	CLA	CBD-CGD-O2D-CED
32	9	603	CLA	CBD-CGD-O2D-CED
32	9	610	CLA	CBD-CGD-O2D-CED
32	p	304	CLA	CBD-CGD-O2D-CED
32	5	306	CLA	O1D-CGD-O2D-CED
32	b	606	CLA	O1D-CGD-O2D-CED
32	b	611	CLA	O1D-CGD-O2D-CED
32	B	606	CLA	O1D-CGD-O2D-CED
32	B	611	CLA	O1D-CGD-O2D-CED
32	b	602	CLA	CBA-CGA-O2A-C1
32	B	602	CLA	CBA-CGA-O2A-C1
33	2	610	KC2	CAA-CBA-CGA-O2A
33	8	610	KC2	CAA-CBA-CGA-O2A
33	P	605	KC2	CAA-CBA-CGA-O1A
32	4	602	CLA	C4-C3-C5-C6
37	l	101	LMG	O6-C5-C6-O5
37	L	102	LMG	O6-C5-C6-O5
32	3	610	CLA	CBD-CGD-O2D-CED
32	8	601	CLA	CBD-CGD-O2D-CED
32	B	610	CLA	CBD-CGD-O2D-CED
41	D	402	PHO	CBD-CGD-O2D-CED
41	d	410	PHO	CBD-CGD-O2D-CED
32	1	604	CLA	O1D-CGD-O2D-CED
32	c	506	CLA	O1D-CGD-O2D-CED
32	C	506	CLA	O1D-CGD-O2D-CED
37	D	411	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
37	d	401	LMG	O6-C1-O1-C7
45	c	516	DGD	O6D-C1D-O3G-C3G
45	C	516	DGD	O6D-C1D-O3G-C3G
32	2	609	CLA	O1D-CGD-O2D-CED
32	8	609	CLA	O1D-CGD-O2D-CED
32	5	304	CLA	CBA-CGA-O2A-C1
32	b	617	CLA	CBA-CGA-O2A-C1
32	C	512	CLA	CBA-CGA-O2A-C1
32	p	304	CLA	CBA-CGA-O2A-C1
32	B	617	CLA	CBA-CGA-O2A-C1
32	1	606	CLA	CBD-CGD-O2D-CED
32	2	601	CLA	CBD-CGD-O2D-CED
32	b	615	CLA	CBD-CGD-O2D-CED
32	c	504	CLA	CBD-CGD-O2D-CED
32	c	508	CLA	CBD-CGD-O2D-CED
32	7	603	CLA	CBD-CGD-O2D-CED
32	C	504	CLA	CBD-CGD-O2D-CED
32	C	508	CLA	CBD-CGD-O2D-CED
32	B	615	CLA	CBD-CGD-O2D-CED
33	6	609	KC2	CBD-CGD-O2D-CED
33	P	609	KC2	CBD-CGD-O2D-CED
33	5	311	KC2	CAA-CBA-CGA-O2A
33	p	311	KC2	CAA-CBA-CGA-O2A
32	4	605	CLA	O1A-CGA-O2A-C1
37	b	618	LMG	C4-C5-C6-O5
37	B	618	LMG	C4-C5-C6-O5
31	K	102	8CT	C18-C19-C20-C21
31	k	101	8CT	C18-C19-C20-C21
31	B	622	8CT	C12-C13-C14-C15
34	4	616	II0	C36-C40-C42-C41
36	0	618	IHT	C33-C37-C40-C41
32	5	304	CLA	O1A-CGA-O2A-C1
32	b	617	CLA	O1A-CGA-O2A-C1
32	p	304	CLA	O1A-CGA-O2A-C1
32	B	617	CLA	O1A-CGA-O2A-C1
38	2	618	LHG	C1-C2-C3-O3
38	D	406	LHG	C1-C2-C3-O3
38	b	619	LHG	C1-C2-C3-O3
38	d	405	LHG	C1-C2-C3-O3
38	B	619	LHG	C1-C2-C3-O3
32	6	611	CLA	O1D-CGD-O2D-CED
32	2	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	S	303	CLA	CBA-CGA-O2A-C1
32	c	512	CLA	CBA-CGA-O2A-C1
32	0	605	CLA	CBA-CGA-O2A-C1
32	8	603	CLA	CBA-CGA-O2A-C1
32	s	303	CLA	CBA-CGA-O2A-C1
41	D	402	PHO	CBA-CGA-O2A-C1
41	d	410	PHO	CBA-CGA-O2A-C1
45	c	516	DGD	C2A-C1A-O1G-C1G
45	C	516	DGD	C2A-C1A-O1G-C1G
37	D	407	LMG	O6-C5-C6-O5
37	d	406	LMG	O6-C5-C6-O5
32	8	607	CLA	CBD-CGD-O2D-CED
38	S	301	LHG	C28-C29-C30-C31
38	a	403	LHG	C28-C29-C30-C31
38	s	301	LHG	C28-C29-C30-C31
32	1	608	CLA	O1D-CGD-O2D-CED
32	7	608	CLA	O1D-CGD-O2D-CED
33	2	610	KC2	O1D-CGD-O2D-CED
33	8	610	KC2	O1D-CGD-O2D-CED
33	2	610	KC2	CAA-CBA-CGA-O1A
33	8	610	KC2	CAA-CBA-CGA-O1A
32	1	607	CLA	CBD-CGD-O2D-CED
32	b	606	CLA	C6-C7-C8-C9
32	b	606	CLA	C14-C13-C15-C16
32	b	607	CLA	C11-C10-C8-C9
32	c	507	CLA	C11-C12-C13-C14
32	c	509	CLA	C6-C7-C8-C9
32	C	507	CLA	C11-C12-C13-C14
32	C	509	CLA	C6-C7-C8-C9
32	B	606	CLA	C6-C7-C8-C9
32	B	606	CLA	C14-C13-C15-C16
32	B	607	CLA	C11-C10-C8-C9
37	l	101	LMG	C4-C5-C6-O5
32	4	601	CLA	O1D-CGD-O2D-CED
32	0	601	CLA	O1D-CGD-O2D-CED
32	7	606	CLA	O1D-CGD-O2D-CED
32	P	611	CLA	O1D-CGD-O2D-CED
45	c	516	DGD	C2D-C1D-O3G-C3G
45	C	516	DGD	C2D-C1D-O3G-C3G
38	D	406	LHG	O2-C2-C3-O3
38	d	405	LHG	O2-C2-C3-O3
37	L	102	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
32	c	512	CLA	CBD-CGD-O2D-CED
31	M	201	8CT	C10-C11-C12-C40
31	D	409	8CT	C10-C11-C12-C40
31	D	409	8CT	C27-C26-C28-C29
31	H	102	8CT	C14-C15-C16-C39
31	c	518	8CT	C27-C26-C28-C29
31	d	408	8CT	C10-C11-C12-C40
31	d	408	8CT	C27-C26-C28-C29
31	C	518	8CT	C27-C26-C28-C29
31	a	413	8CT	C10-C11-C12-C40
31	h	102	8CT	C14-C15-C16-C39
31	B	622	8CT	C10-C11-C12-C40
34	1	616	II0	C31-C33-C35-C37
34	1	617	II0	C31-C33-C35-C37
34	2	615	II0	C32-C34-C36-C38
34	7	616	II0	C31-C33-C35-C37
34	7	617	II0	C31-C33-C35-C37
34	8	615	II0	C32-C34-C36-C38
34	P	614	II0	C31-C33-C35-C37
35	P	613	II3	C12-C21-C24-C25
31	D	409	8CT	C10-C11-C12-C13
31	K	101	8CT	C10-C11-C12-C13
31	c	518	8CT	C25-C26-C28-C29
31	d	408	8CT	C10-C11-C12-C13
31	k	102	8CT	C10-C11-C12-C13
31	C	518	8CT	C25-C26-C28-C29
31	a	413	8CT	C10-C11-C12-C13
45	c	514	DGD	C1A-C2A-C3A-C4A
32	2	603	CLA	O1A-CGA-O2A-C1
32	0	605	CLA	O1A-CGA-O2A-C1
32	8	603	CLA	O1A-CGA-O2A-C1
37	6	616	LMG	O7-C8-C9-O8
32	b	605	CLA	O1D-CGD-O2D-CED
32	c	501	CLA	O1D-CGD-O2D-CED
32	7	603	CLA	CBA-CGA-O2A-C1
38	D	406	LHG	C23-C24-C25-C26
38	d	405	LHG	C23-C24-C25-C26
45	C	514	DGD	C1A-C2A-C3A-C4A
32	B	605	CLA	O1D-CGD-O2D-CED
32	7	607	CLA	CBD-CGD-O2D-CED
32	b	612	CLA	C5-C6-C7-C8
32	b	613	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	b	615	CLA	C15-C16-C17-C18
32	C	503	CLA	C8-C10-C11-C12
32	B	612	CLA	C5-C6-C7-C8
32	B	613	CLA	C15-C16-C17-C18
32	B	615	CLA	C15-C16-C17-C18
37	A	607	LMG	C28-C29-C30-C31
37	a	410	LMG	C28-C29-C30-C31
32	S	303	CLA	O1A-CGA-O2A-C1
32	s	303	CLA	O1A-CGA-O2A-C1
32	D	404	CLA	C5-C6-C7-C8
32	c	503	CLA	C8-C10-C11-C12
32	2	607	CLA	CBD-CGD-O2D-CED
32	1	603	CLA	CBA-CGA-O2A-C1
32	b	605	CLA	C4-C3-C5-C6
32	B	605	CLA	C4-C3-C5-C6
32	d	403	CLA	C5-C6-C7-C8
38	A	612	LHG	C23-C24-C25-C26
38	a	402	LHG	C23-C24-C25-C26
31	A	610	8CT	C18-C19-C20-C21
31	H	102	8CT	C18-C19-C20-C21
31	b	622	8CT	C18-C19-C20-C21
31	c	518	8CT	C12-C13-C14-C15
31	C	518	8CT	C12-C13-C14-C15
31	h	102	8CT	C18-C19-C20-C21
31	B	623	8CT	C18-C19-C20-C21
36	4	614	IHT	C23-C27-C30-C32
36	4	617	IHT	C23-C27-C30-C32
36	0	614	IHT	C23-C27-C30-C32
36	0	618	IHT	C23-C27-C30-C32
36	0	618	IHT	C35-C38-C41-C40
38	A	613	LHG	C28-C29-C30-C31
38	b	619	LHG	C7-C8-C9-C10
38	B	619	LHG	C7-C8-C9-C10
39	b	620	SQD	C7-C8-C9-C10
39	B	620	SQD	C7-C8-C9-C10
45	A	614	DGD	C1A-C2A-C3A-C4A
45	a	414	DGD	C1A-C2A-C3A-C4A
32	c	503	CLA	C10-C11-C12-C13
32	S	303	CLA	C2A-CAA-CBA-CGA
32	b	607	CLA	C2A-CAA-CBA-CGA
32	b	611	CLA	C2A-CAA-CBA-CGA
32	0	613	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
32	s	303	CLA	C2A-CAA-CBA-CGA
32	B	607	CLA	C2A-CAA-CBA-CGA
32	B	611	CLA	C2A-CAA-CBA-CGA
32	B	612	CLA	C2A-CAA-CBA-CGA
32	6	607	CLA	C8-C10-C11-C12
32	b	614	CLA	C13-C15-C16-C17
32	b	617	CLA	C5-C6-C7-C8
32	C	503	CLA	C10-C11-C12-C13
32	B	614	CLA	C13-C15-C16-C17
32	B	617	CLA	C5-C6-C7-C8
37	D	411	LMG	C4-C5-C6-O5
37	d	401	LMG	C4-C5-C6-O5
37	D	411	LMG	C10-C11-C12-C13
37	d	401	LMG	C10-C11-C12-C13
38	2	618	LHG	C23-C24-C25-C26
38	D	406	LHG	C7-C8-C9-C10
38	b	621	LHG	C23-C24-C25-C26
38	d	405	LHG	C7-C8-C9-C10
38	l	102	LHG	C23-C24-C25-C26
38	8	618	LHG	C23-C24-C25-C26
38	L	101	LHG	C23-C24-C25-C26
38	B	621	LHG	C23-C24-C25-C26
32	P	602	CLA	O1D-CGD-O2D-CED
41	D	402	PHO	O1A-CGA-O2A-C1
41	d	410	PHO	O1A-CGA-O2A-C1
37	6	616	LMG	O6-C1-O1-C7
37	c	517	LMG	O6-C1-O1-C7
37	0	619	LMG	O6-C1-O1-C7
37	C	517	LMG	O6-C1-O1-C7
37	P	616	LMG	O6-C1-O1-C7
45	c	515	DGD	O6E-C1E-O5D-C6D
45	C	515	DGD	O6E-C1E-O5D-C6D
32	2	608	CLA	O1D-CGD-O2D-CED
32	5	309	CLA	O1D-CGD-O2D-CED
32	p	309	CLA	O1D-CGD-O2D-CED
32	P	607	CLA	C8-C10-C11-C12
38	b	619	LHG	O2-C2-C3-O3
38	B	619	LHG	O2-C2-C3-O3
32	8	608	CLA	O1D-CGD-O2D-CED
32	b	612	CLA	CBA-CGA-O2A-C1
32	c	505	CLA	CBA-CGA-O2A-C1
32	B	612	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	c	512	CLA	O1A-CGA-O2A-C1
32	C	512	CLA	O1A-CGA-O2A-C1
32	5	305	CLA	C5-C6-C7-C8
32	p	305	CLA	C5-C6-C7-C8
32	5	302	CLA	O1D-CGD-O2D-CED
32	5	303	CLA	O1D-CGD-O2D-CED
32	6	602	CLA	O1D-CGD-O2D-CED
32	6	606	CLA	O1D-CGD-O2D-CED
32	8	602	CLA	O1D-CGD-O2D-CED
32	P	606	CLA	O1D-CGD-O2D-CED
32	1	608	CLA	C8-C10-C11-C12
32	2	608	CLA	C8-C10-C11-C12
32	3	604	CLA	C5-C6-C7-C8
32	8	608	CLA	C8-C10-C11-C12
32	C	508	CLA	C13-C15-C16-C17
32	p	309	CLA	C8-C10-C11-C12
32	7	603	CLA	O1A-CGA-O2A-C1
45	H	101	DGD	C1A-C2A-C3A-C4A
45	h	101	DGD	C1A-C2A-C3A-C4A
32	2	602	CLA	O1D-CGD-O2D-CED
32	p	302	CLA	O1D-CGD-O2D-CED
45	c	515	DGD	O6E-C5E-C6E-O5E
45	C	515	DGD	O6E-C5E-C6E-O5E
32	4	602	CLA	C5-C6-C7-C8
32	5	309	CLA	C8-C10-C11-C12
32	c	508	CLA	C13-C15-C16-C17
32	b	615	CLA	CBA-CGA-O2A-C1
32	0	603	CLA	CBA-CGA-O2A-C1
32	C	505	CLA	CBA-CGA-O2A-C1
32	B	615	CLA	CBA-CGA-O2A-C1
33	5	311	KC2	C2A-CAA-CBA-CGA
33	p	311	KC2	C2A-CAA-CBA-CGA
32	p	303	CLA	O1D-CGD-O2D-CED
32	A	602	CLA	C3-C5-C6-C7
32	a	405	CLA	C3-C5-C6-C7
32	3	611	CLA	CBD-CGD-O2D-CED
32	B	604	CLA	CBD-CGD-O2D-CED
31	D	409	8CT	C23-C24-C25-C26
31	Z	101	8CT	C18-C19-C20-C21
31	b	623	8CT	C18-C19-C20-C21
31	d	408	8CT	C23-C24-C25-C26
31	z	101	8CT	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
31	B	624	8CT	C18-C19-C20-C21
34	4	616	II0	C35-C39-C41-C42
34	0	616	II0	C35-C39-C41-C42
34	0	616	II0	C36-C40-C42-C41
34	p	316	II0	C26-C30-C32-C34
32	B	607	CLA	C10-C11-C12-C13
32	1	603	CLA	O1A-CGA-O2A-C1
38	8	618	LHG	C1-C2-C3-O3
32	6	611	CLA	C2A-CAA-CBA-CGA
32	b	612	CLA	C2A-CAA-CBA-CGA
32	P	611	CLA	C2A-CAA-CBA-CGA
32	c	513	CLA	CBA-CGA-O2A-C1
32	7	605	CLA	CBA-CGA-O2A-C1
32	C	513	CLA	CBA-CGA-O2A-C1
32	S	303	CLA	C13-C15-C16-C17
32	b	606	CLA	C5-C6-C7-C8
32	b	607	CLA	C10-C11-C12-C13
32	b	614	CLA	C15-C16-C17-C18
32	c	507	CLA	C10-C11-C12-C13
32	7	608	CLA	C8-C10-C11-C12
32	C	507	CLA	C10-C11-C12-C13
32	P	607	CLA	C10-C11-C12-C13
32	B	606	CLA	C5-C6-C7-C8
32	B	614	CLA	C15-C16-C17-C18
32	b	604	CLA	CBD-CGD-O2D-CED
32	p	313	CLA	O1D-CGD-O2D-CED
32	6	607	CLA	C10-C11-C12-C13
38	A	612	LHG	C32-C33-C34-C35
38	a	402	LHG	C32-C33-C34-C35
32	b	611	CLA	C15-C16-C17-C18
32	9	604	CLA	C5-C6-C7-C8
32	s	303	CLA	C13-C15-C16-C17
32	B	611	CLA	C15-C16-C17-C18
32	B	614	CLA	C8-C10-C11-C12
32	0	602	CLA	C4-C3-C5-C6
32	4	602	CLA	C2-C3-C5-C6
32	4	604	CLA	O1D-CGD-O2D-CED
32	0	602	CLA	C5-C6-C7-C8
32	C	502	CLA	CBD-CGD-O2D-CED
32	5	313	CLA	O1D-CGD-O2D-CED
37	4	618	LMG	C2-C1-O1-C7
37	c	517	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
37	g	101	LMG	C2-C1-O1-C7
37	0	619	LMG	C2-C1-O1-C7
37	C	517	LMG	C2-C1-O1-C7
39	5	318	SQD	C2-C1-O6-C44
39	p	318	SQD	C2-C1-O6-C44
45	c	515	DGD	C2E-C1E-O5D-C6D
45	C	515	DGD	C2E-C1E-O5D-C6D
32	b	614	CLA	C8-C10-C11-C12
37	0	619	LMG	C10-C11-C12-C13
37	c	517	LMG	C4-C5-C6-O5
37	C	517	LMG	C4-C5-C6-O5
32	1	608	CLA	C11-C12-C13-C14
32	7	608	CLA	C11-C12-C13-C14
32	9	607	CLA	C10-C11-C12-C13
32	b	612	CLA	O1A-CGA-O2A-C1
32	B	612	CLA	O1A-CGA-O2A-C1
38	A	613	LHG	C23-C24-C25-C26
31	3	615	8CT	C14-C15-C16-C39
31	6	615	8CT	C10-C11-C12-C40
31	A	610	8CT	C10-C11-C12-C40
31	K	101	8CT	C27-C26-C28-C29
31	b	622	8CT	C27-C26-C28-C29
31	b	623	8CT	C10-C11-C12-C40
31	k	102	8CT	C27-C26-C28-C29
31	9	615	8CT	C14-C15-C16-C39
31	P	615	8CT	C10-C11-C12-C40
31	a	413	8CT	C27-C26-C28-C29
31	B	623	8CT	C27-C26-C28-C29
31	B	624	8CT	C10-C11-C12-C40
34	5	319	II0	C32-C34-C36-C38
31	M	201	8CT	C10-C11-C12-C13
31	3	615	8CT	C14-C15-C16-C17
31	6	615	8CT	C10-C11-C12-C13
31	K	101	8CT	C25-C26-C28-C29
31	b	622	8CT	C25-C26-C28-C29
31	b	623	8CT	C10-C11-C12-C13
31	k	102	8CT	C25-C26-C28-C29
31	9	615	8CT	C14-C15-C16-C17
31	P	615	8CT	C10-C11-C12-C13
31	B	622	8CT	C10-C11-C12-C13
31	B	623	8CT	C25-C26-C28-C29
31	B	624	8CT	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
47	f	101	HEM	C2A-CAA-CBA-CGA
32	b	615	CLA	O1A-CGA-O2A-C1
32	B	615	CLA	O1A-CGA-O2A-C1
32	4	611	CLA	C2A-CAA-CBA-CGA
32	5	312	CLA	C2A-CAA-CBA-CGA
32	c	507	CLA	C2A-CAA-CBA-CGA
32	0	611	CLA	C2A-CAA-CBA-CGA
32	C	507	CLA	C2A-CAA-CBA-CGA
32	p	312	CLA	C2A-CAA-CBA-CGA
38	D	410	LHG	O1-C1-C2-C3
38	d	411	LHG	O1-C1-C2-C3
37	4	618	LMG	C10-C11-C12-C13
32	9	610	CLA	O1D-CGD-O2D-CED
39	5	318	SQD	C44-C45-O47-C7
39	p	318	SQD	C44-C45-O47-C7
32	4	608	CLA	C11-C12-C13-C14
32	0	608	CLA	C11-C12-C13-C14
32	5	304	CLA	O1D-CGD-O2D-CED
32	0	604	CLA	O1D-CGD-O2D-CED
32	p	304	CLA	O1D-CGD-O2D-CED
32	1	604	CLA	C5-C6-C7-C8
32	b	610	CLA	C15-C16-C17-C18
32	c	509	CLA	C10-C11-C12-C13
37	4	618	LMG	O6-C1-O1-C7
37	g	101	LMG	O6-C1-O1-C7
37	D	407	LMG	C11-C10-O7-C8
37	d	406	LMG	C11-C10-O7-C8
38	a	402	LHG	C29-C30-C31-C32
32	3	603	CLA	O1D-CGD-O2D-CED
32	3	610	CLA	O1D-CGD-O2D-CED
32	b	610	CLA	O1D-CGD-O2D-CED
32	9	603	CLA	O1D-CGD-O2D-CED
32	B	610	CLA	O1D-CGD-O2D-CED
38	A	612	LHG	C29-C30-C31-C32
37	P	616	LMG	O7-C8-C9-O8
41	D	402	PHO	O1D-CGD-O2D-CED
41	d	410	PHO	O1D-CGD-O2D-CED
32	C	510	CLA	CBA-CGA-O2A-C1
32	p	306	CLA	CBA-CGA-O2A-C1
32	5	306	CLA	C8-C10-C11-C12
32	b	612	CLA	C8-C10-C11-C12
32	c	507	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
32	C	507	CLA	C13-C15-C16-C17
32	B	610	CLA	C15-C16-C17-C18
32	B	612	CLA	C8-C10-C11-C12
32	3	607	CLA	C11-C12-C13-C15
32	4	608	CLA	C11-C12-C13-C15
32	5	309	CLA	C11-C12-C13-C14
32	0	608	CLA	C11-C12-C13-C15
32	p	309	CLA	C11-C12-C13-C14
32	0	603	CLA	O1A-CGA-O2A-C1
32	C	505	CLA	O1A-CGA-O2A-C1
32	7	604	CLA	C5-C6-C7-C8
32	1	606	CLA	O1D-CGD-O2D-CED
45	C	514	DGD	O6E-C5E-C6E-O5E
32	b	612	CLA	C13-C15-C16-C17
32	B	612	CLA	C13-C15-C16-C17
38	A	613	LHG	C17-C18-C19-C20
32	c	502	CLA	CBD-CGD-O2D-CED
32	7	609	CLA	CBD-CGD-O2D-CED
37	D	407	LMG	C16-C17-C18-C19
37	D	411	LMG	C12-C13-C14-C15
37	d	401	LMG	C12-C13-C14-C15
38	A	612	LHG	C24-C25-C26-C27
38	l	102	LHG	C12-C13-C14-C15
38	a	403	LHG	C17-C18-C19-C20
38	a	403	LHG	C29-C30-C31-C32
39	a	409	SQD	C31-C32-C33-C34
32	2	601	CLA	O1D-CGD-O2D-CED
32	8	601	CLA	O1D-CGD-O2D-CED
45	c	514	DGD	O6E-C5E-C6E-O5E
32	c	505	CLA	C5-C6-C7-C8
32	C	505	CLA	C5-C6-C7-C8
37	d	406	LMG	C16-C17-C18-C19
38	D	406	LHG	C13-C14-C15-C16
38	d	405	LHG	C13-C14-C15-C16
38	L	101	LHG	C12-C13-C14-C15
38	s	301	LHG	C24-C25-C26-C27
38	B	619	LHG	C24-C25-C26-C27
39	A	606	SQD	C31-C32-C33-C34
39	b	620	SQD	C29-C30-C31-C32
39	B	620	SQD	C29-C30-C31-C32
32	c	505	CLA	O1A-CGA-O2A-C1
32	5	306	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	c	510	CLA	CBA-CGA-O2A-C1
37	l	101	LMG	C31-C32-C33-C34
38	2	618	LHG	C24-C25-C26-C27
38	S	301	LHG	C24-C25-C26-C27
38	b	619	LHG	C24-C25-C26-C27
38	a	402	LHG	C24-C25-C26-C27
39	b	601	SQD	C33-C34-C35-C36
45	A	614	DGD	C6B-C7B-C8B-C9B
45	H	101	DGD	C4A-C5A-C6A-C7A
45	a	414	DGD	C6B-C7B-C8B-C9B
45	h	101	DGD	C4A-C5A-C6A-C7A
34	2	613	II0	C10-C22-C24-C26
34	p	315	II0	C09-C21-C23-C25
34	p	315	II0	C10-C22-C24-C26
36	2	616	IHT	C11-C21-C24-C26
38	2	618	LHG	O1-C1-C2-O2
38	8	618	LHG	O1-C1-C2-O2
38	b	621	LHG	C10-C11-C12-C13
38	B	621	LHG	C10-C11-C12-C13
39	b	601	SQD	C27-C28-C29-C30
39	B	601	SQD	C33-C34-C35-C36
32	c	504	CLA	O1D-CGD-O2D-CED
32	c	508	CLA	O1D-CGD-O2D-CED
32	C	508	CLA	O1D-CGD-O2D-CED
32	1	605	CLA	C4B-C3B-CAB-CBB
32	3	601	CLA	C4B-C3B-CAB-CBB
32	3	608	CLA	C4B-C3B-CAB-CBB
32	4	611	CLA	C4B-C3B-CAB-CBB
32	5	304	CLA	C4B-C3B-CAB-CBB
32	5	305	CLA	C4B-C3B-CAB-CBB
32	6	608	CLA	C4B-C3B-CAB-CBB
32	6	610	CLA	C4B-C3B-CAB-CBB
32	b	602	CLA	C4B-C3B-CAB-CBB
32	c	502	CLA	C4B-C3B-CAB-CBB
32	g	102	CLA	C4B-C3B-CAB-CBB
32	0	611	CLA	C4B-C3B-CAB-CBB
32	7	605	CLA	C4B-C3B-CAB-CBB
32	9	601	CLA	C4B-C3B-CAB-CBB
32	9	608	CLA	C4B-C3B-CAB-CBB
32	C	502	CLA	C4B-C3B-CAB-CBB
32	G	101	CLA	C4B-C3B-CAB-CBB
32	P	608	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	P	610	CLA	C4B-C3B-CAB-CBB
32	p	304	CLA	C4B-C3B-CAB-CBB
32	p	305	CLA	C4B-C3B-CAB-CBB
32	p	306	CLA	C4B-C3B-CAB-CBB
32	B	602	CLA	C4B-C3B-CAB-CBB
39	A	606	SQD	C23-C24-C25-C26
39	a	409	SQD	C23-C24-C25-C26
37	L	102	LMG	C31-C32-C33-C34
38	8	618	LHG	C24-C25-C26-C27
32	2	608	CLA	C11-C12-C13-C15
32	1	608	CLA	C10-C11-C12-C13
32	7	608	CLA	C10-C11-C12-C13
32	p	306	CLA	C8-C10-C11-C12
37	D	407	LMG	C17-C18-C19-C20
45	H	101	DGD	C6A-C7A-C8A-C9A
45	h	101	DGD	C6A-C7A-C8A-C9A
32	c	503	CLA	C6-C7-C8-C10
32	C	503	CLA	C6-C7-C8-C10
37	D	407	LMG	C32-C33-C34-C35
37	d	406	LMG	C17-C18-C19-C20
39	b	620	SQD	C10-C11-C12-C13
39	B	601	SQD	C27-C28-C29-C30
39	B	620	SQD	C10-C11-C12-C13
37	b	618	LMG	C28-C29-C30-C31
37	0	619	LMG	C28-C29-C30-C31
37	B	618	LMG	C28-C29-C30-C31
32	C	509	CLA	C10-C11-C12-C13
32	b	615	CLA	C11-C12-C13-C15
32	c	502	CLA	C6-C7-C8-C10
32	C	502	CLA	C6-C7-C8-C10
32	B	615	CLA	C11-C12-C13-C15
37	A	607	LMG	C33-C34-C35-C36
37	D	407	LMG	C15-C16-C17-C18
37	d	401	LMG	C35-C36-C37-C38
37	d	406	LMG	C15-C16-C17-C18
37	d	406	LMG	C32-C33-C34-C35
45	c	514	DGD	C4B-C5B-C6B-C7B
45	a	414	DGD	C3A-C4A-C5A-C6A
32	c	513	CLA	O1A-CGA-O2A-C1
32	7	605	CLA	O1A-CGA-O2A-C1
32	3	603	CLA	C3A-C2A-CAA-CBA
32	5	304	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	6	603	CLA	C3A-C2A-CAA-CBA
32	D	403	CLA	C3A-C2A-CAA-CBA
32	b	603	CLA	C3A-C2A-CAA-CBA
32	b	613	CLA	C3A-C2A-CAA-CBA
32	b	617	CLA	C3A-C2A-CAA-CBA
32	d	402	CLA	C3A-C2A-CAA-CBA
32	9	603	CLA	C3A-C2A-CAA-CBA
32	P	603	CLA	C3A-C2A-CAA-CBA
32	p	304	CLA	C3A-C2A-CAA-CBA
32	B	603	CLA	C3A-C2A-CAA-CBA
32	B	613	CLA	C3A-C2A-CAA-CBA
32	B	617	CLA	C3A-C2A-CAA-CBA
37	D	411	LMG	C35-C36-C37-C38
37	c	517	LMG	C29-C30-C31-C32
39	b	620	SQD	C17-C18-C19-C20
32	6	604	CLA	C5-C6-C7-C8
38	D	410	LHG	C23-C24-C25-C26
38	d	411	LHG	C23-C24-C25-C26
32	7	603	CLA	O1D-CGD-O2D-CED
32	C	504	CLA	O1D-CGD-O2D-CED
38	a	403	LHG	C32-C33-C34-C35
32	b	616	CLA	C16-C17-C18-C19
32	8	608	CLA	C11-C12-C13-C15
32	9	607	CLA	C11-C12-C13-C15
32	B	616	CLA	C16-C17-C18-C19
32	C	513	CLA	O1A-CGA-O2A-C1
37	a	410	LMG	C33-C34-C35-C36
38	L	101	LHG	C34-C35-C36-C37
45	H	101	DGD	CAB-CBB-CCB-CDB
45	C	514	DGD	C4B-C5B-C6B-C7B
32	1	609	CLA	CBD-CGD-O2D-CED
32	b	607	CLA	CBD-CGD-O2D-CED
45	A	614	DGD	C7B-C8B-C9B-CAB
45	c	516	DGD	C5B-C6B-C7B-C8B
45	C	516	DGD	C5B-C6B-C7B-C8B
45	h	101	DGD	CAB-CBB-CCB-CDB
32	1	605	CLA	CBA-CGA-O2A-C1
32	2	602	CLA	CBA-CGA-O2A-C1
32	4	603	CLA	CBA-CGA-O2A-C1
32	8	602	CLA	CBA-CGA-O2A-C1
32	c	502	CLA	C11-C10-C8-C7
32	C	502	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
37	c	517	LMG	C11-C12-C13-C14
37	c	517	LMG	C32-C33-C34-C35
37	d	401	LMG	C34-C35-C36-C37
37	C	517	LMG	C29-C30-C31-C32
37	a	410	LMG	C31-C32-C33-C34
38	D	406	LHG	C32-C33-C34-C35
38	L	101	LHG	C31-C32-C33-C34
39	b	601	SQD	C9-C10-C11-C12
39	B	601	SQD	C9-C10-C11-C12
39	B	620	SQD	C17-C18-C19-C20
39	5	318	SQD	C7-C8-C9-C10
39	b	601	SQD	C23-C24-C25-C26
39	p	318	SQD	C7-C8-C9-C10
37	A	607	LMG	C31-C32-C33-C34
37	D	411	LMG	C30-C31-C32-C33
37	D	411	LMG	C34-C35-C36-C37
37	d	401	LMG	C30-C31-C32-C33
37	C	517	LMG	C11-C12-C13-C14
37	C	517	LMG	C32-C33-C34-C35
37	a	410	LMG	C29-C30-C31-C32
38	A	613	LHG	C32-C33-C34-C35
38	d	405	LHG	C32-C33-C34-C35
39	A	606	SQD	C9-C10-C11-C12
39	b	601	SQD	C29-C30-C31-C32
39	a	409	SQD	C9-C10-C11-C12
39	B	601	SQD	C29-C30-C31-C32
39	B	620	SQD	C9-C10-C11-C12
45	H	101	DGD	C3B-C4B-C5B-C6B
45	c	514	DGD	C9B-CAB-CBB-CCB
45	c	515	DGD	C6A-C7A-C8A-C9A
45	C	514	DGD	C9B-CAB-CBB-CCB
45	C	515	DGD	C6A-C7A-C8A-C9A
37	l	101	LMG	C12-C13-C14-C15
38	b	619	LHG	C11-C10-C9-C8
39	A	606	SQD	C12-C13-C14-C15
39	a	409	SQD	C12-C13-C14-C15
45	h	101	DGD	C3B-C4B-C5B-C6B
32	b	615	CLA	O1D-CGD-O2D-CED
37	A	607	LMG	C29-C30-C31-C32
45	c	514	DGD	C2A-C3A-C4A-C5A
45	C	516	DGD	C6A-C7A-C8A-C9A
32	B	615	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
37	b	618	LMG	C16-C17-C18-C19
37	l	101	LMG	C32-C33-C34-C35
37	L	102	LMG	C32-C33-C34-C35
37	a	410	LMG	C15-C16-C17-C18
37	B	618	LMG	C35-C36-C37-C38
38	A	613	LHG	C29-C30-C31-C32
38	D	406	LHG	C14-C15-C16-C17
38	B	619	LHG	C11-C10-C9-C8
39	B	620	SQD	C30-C31-C32-C33
45	C	514	DGD	C2A-C3A-C4A-C5A
32	5	309	CLA	C11-C12-C13-C15
32	p	309	CLA	C11-C12-C13-C15
38	D	410	LHG	C7-C8-C9-C10
38	d	411	LHG	C7-C8-C9-C10
39	B	601	SQD	C23-C24-C25-C26
32	p	306	CLA	O1A-CGA-O2A-C1
31	M	201	8CT	C02-C03-C10-C11
31	M	201	8CT	C04-C03-C10-C11
31	3	615	8CT	C04-C03-C10-C11
31	D	409	8CT	C04-C03-C10-C11
31	K	101	8CT	C02-C03-C10-C11
31	d	408	8CT	C04-C03-C10-C11
31	k	102	8CT	C02-C03-C10-C11
31	9	615	8CT	C04-C03-C10-C11
31	a	413	8CT	C02-C03-C10-C11
31	B	622	8CT	C02-C03-C10-C11
31	B	622	8CT	C04-C03-C10-C11
32	1	601	CLA	C2B-C3B-CAB-CBB
32	1	607	CLA	C2B-C3B-CAB-CBB
32	3	601	CLA	C2B-C3B-CAB-CBB
32	3	605	CLA	C2B-C3B-CAB-CBB
32	3	609	CLA	C2B-C3B-CAB-CBB
32	4	601	CLA	C2B-C3B-CAB-CBB
32	4	607	CLA	C2B-C3B-CAB-CBB
32	4	609	CLA	C2B-C3B-CAB-CBB
32	4	612	CLA	C2B-C3B-CAB-CBB
32	5	302	CLA	C2B-C3B-CAB-CBB
32	5	310	CLA	C2B-C3B-CAB-CBB
32	b	602	CLA	C2B-C3B-CAB-CBB
32	b	616	CLA	C2B-C3B-CAB-CBB
32	0	601	CLA	C2B-C3B-CAB-CBB
32	0	607	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	0	609	CLA	C2B-C3B-CAB-CBB
32	0	612	CLA	C2B-C3B-CAB-CBB
32	7	601	CLA	C2B-C3B-CAB-CBB
32	7	607	CLA	C2B-C3B-CAB-CBB
32	9	601	CLA	C2B-C3B-CAB-CBB
32	9	605	CLA	C2B-C3B-CAB-CBB
32	9	609	CLA	C2B-C3B-CAB-CBB
32	p	302	CLA	C2B-C3B-CAB-CBB
32	p	305	CLA	C2B-C3B-CAB-CBB
32	p	310	CLA	C2B-C3B-CAB-CBB
32	B	602	CLA	C2B-C3B-CAB-CBB
32	B	616	CLA	C2B-C3B-CAB-CBB
36	1	618	IHT	C02-C07-C18-C22
36	1	618	IHT	C10-C07-C18-C22
36	7	618	IHT	C02-C07-C18-C22
36	7	618	IHT	C10-C07-C18-C22
37	b	618	LMG	C35-C36-C37-C38
39	b	620	SQD	C9-C10-C11-C12
39	b	620	SQD	C30-C31-C32-C33
32	5	303	CLA	CBA-CGA-O2A-C1
32	6	602	CLA	CBA-CGA-O2A-C1
38	b	621	LHG	C24-C23-O8-C6
32	2	608	CLA	C10-C11-C12-C13
37	A	607	LMG	C15-C16-C17-C18
37	B	618	LMG	C16-C17-C18-C19
38	d	405	LHG	C14-C15-C16-C17
45	c	514	DGD	C5B-C6B-C7B-C8B
45	c	516	DGD	C6A-C7A-C8A-C9A
47	E	101	HEM	C2A-CAA-CBA-CGA
38	b	621	LHG	C11-C12-C13-C14
38	B	621	LHG	C11-C12-C13-C14
45	C	514	DGD	C5B-C6B-C7B-C8B
41	D	402	PHO	C2A-CAA-CBA-CGA
41	d	410	PHO	C2A-CAA-CBA-CGA
38	B	619	LHG	C23-C24-C25-C26
32	8	608	CLA	C10-C11-C12-C13
38	l	102	LHG	C31-C32-C33-C34
32	4	603	CLA	O1A-CGA-O2A-C1
32	5	306	CLA	O1A-CGA-O2A-C1
32	c	510	CLA	O1A-CGA-O2A-C1
32	C	510	CLA	O1A-CGA-O2A-C1
37	a	410	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
37	8	617	LMG	C14-C15-C16-C17
38	b	621	LHG	C25-C26-C27-C28
38	B	621	LHG	C25-C26-C27-C28
39	B	601	SQD	C10-C11-C12-C13
45	A	614	DGD	C5B-C6B-C7B-C8B
33	5	311	KC2	CAA-CBA-CGA-O1A
37	2	617	LMG	C14-C15-C16-C17
37	B	618	LMG	C31-C32-C33-C34
39	b	601	SQD	C10-C11-C12-C13
32	b	605	CLA	C2-C3-C5-C6
32	0	602	CLA	C2-C3-C5-C6
32	B	605	CLA	C2-C3-C5-C6
37	A	607	LMG	O6-C5-C6-O5
37	b	618	LMG	C31-C32-C33-C34
38	S	301	LHG	C11-C10-C9-C8
38	s	301	LHG	C11-C10-C9-C8
39	B	601	SQD	C32-C33-C34-C35
38	a	403	LHG	C23-C24-C25-C26
32	1	602	CLA	CBA-CGA-O2A-C1
32	3	602	CLA	CBA-CGA-O2A-C1
32	D	404	CLA	CBA-CGA-O2A-C1
32	c	502	CLA	CBA-CGA-O2A-C1
32	d	403	CLA	CBA-CGA-O2A-C1
32	9	602	CLA	CBA-CGA-O2A-C1
32	C	502	CLA	CBA-CGA-O2A-C1
32	P	602	CLA	CBA-CGA-O2A-C1
32	p	303	CLA	CBA-CGA-O2A-C1
38	B	621	LHG	C24-C23-O8-C6
32	c	507	CLA	C11-C10-C8-C9
32	C	507	CLA	C11-C10-C8-C9
37	D	411	LMG	C31-C32-C33-C34
37	d	401	LMG	C31-C32-C33-C34
38	a	402	LHG	C10-C11-C12-C13
39	b	601	SQD	C32-C33-C34-C35
32	b	615	CLA	C12-C13-C15-C16
38	a	403	LHG	C11-C10-C9-C8
39	B	620	SQD	C16-C17-C18-C19
45	H	101	DGD	C4B-C5B-C6B-C7B
45	h	101	DGD	C4B-C5B-C6B-C7B
32	B	615	CLA	C12-C13-C15-C16
32	b	613	CLA	C8-C10-C11-C12
32	B	613	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
38	d	405	LHG	C15-C16-C17-C18
39	b	620	SQD	C16-C17-C18-C19
38	b	619	LHG	C23-C24-C25-C26
37	D	411	LMG	C13-C14-C15-C16
38	A	612	LHG	C10-C11-C12-C13
38	D	406	LHG	C15-C16-C17-C18
39	b	601	SQD	C11-C10-C9-C8
39	b	620	SQD	C33-C34-C35-C36
33	p	311	KC2	CAA-CBA-CGA-O1A
38	A	612	LHG	O2-C2-C3-O3
37	C	517	LMG	C16-C17-C18-C19
38	A	612	LHG	C27-C28-C29-C30
38	A	613	LHG	C11-C10-C9-C8
38	a	402	LHG	C27-C28-C29-C30
39	B	601	SQD	C11-C10-C9-C8
39	B	620	SQD	C33-C34-C35-C36
45	A	614	DGD	C8B-C9B-CAB-CBB
45	a	414	DGD	C5B-C6B-C7B-C8B
32	b	605	CLA	C8-C10-C11-C12
32	B	605	CLA	C8-C10-C11-C12
32	7	602	CLA	CBA-CGA-O2A-C1
31	K	101	8CT	C16-C17-C18-C19
31	Z	101	8CT	C23-C24-C25-C26
31	k	102	8CT	C16-C17-C18-C19
37	d	401	LMG	C13-C14-C15-C16
38	A	612	LHG	C8-C7-O7-C5
38	a	402	LHG	C8-C7-O7-C5
39	A	606	SQD	C8-C7-O47-C45
39	a	409	SQD	C8-C7-O47-C45
38	s	301	LHG	C30-C31-C32-C33
32	3	607	CLA	C10-C11-C12-C13
32	7	602	CLA	C5-C6-C7-C8
37	c	517	LMG	O9-C10-O7-C8
37	C	517	LMG	O9-C10-O7-C8
39	a	409	SQD	O49-C7-O47-C45
45	A	614	DGD	O1B-C1B-O2G-C2G
38	S	301	LHG	C30-C31-C32-C33
37	c	517	LMG	C16-C17-C18-C19
45	c	516	DGD	C6B-C7B-C8B-C9B
32	0	608	CLA	C8-C10-C11-C12
32	P	604	CLA	C5-C6-C7-C8
31	M	201	8CT	C14-C15-C16-C39

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Mol	Chain	Res	Type	Atoms
31	K	101	8CT	C10-C11-C12-C40
31	k	102	8CT	C10-C11-C12-C40
31	k	102	8CT	C22-C21-C23-C24
34	p	301	II0	C32-C34-C36-C38
38	L	101	LHG	C7-C8-C9-C10
37	2	617	LMG	C30-C31-C32-C33
45	C	516	DGD	C6B-C7B-C8B-C9B
37	D	411	LMG	C8-C7-O1-C1
37	d	401	LMG	C8-C7-O1-C1
32	A	605	CLA	C2A-CAA-CBA-CGA
32	a	408	CLA	C2A-CAA-CBA-CGA
32	2	608	CLA	C11-C12-C13-C14
32	7	608	CLA	C11-C12-C13-C15
32	8	608	CLA	C11-C12-C13-C14
41	A	604	PHO	C16-C17-C18-C20
41	a	407	PHO	C16-C17-C18-C20
45	c	516	DGD	C2B-C3B-C4B-C5B
45	C	516	DGD	C2B-C3B-C4B-C5B
38	b	621	LHG	C28-C29-C30-C31
38	B	621	LHG	C28-C29-C30-C31
33	1	610	KC2	C2C-C3C-CAC-CBC
33	7	610	KC2	C2C-C3C-CAC-CBC
38	S	301	LHG	C27-C28-C29-C30
38	s	301	LHG	C27-C28-C29-C30
37	c	517	LMG	C30-C31-C32-C33
32	9	611	CLA	CBD-CGD-O2D-CED
38	l	102	LHG	C24-C25-C26-C27
38	l	102	LHG	C34-C35-C36-C37
32	1	605	CLA	O1A-CGA-O2A-C1
32	2	602	CLA	O1A-CGA-O2A-C1
32	6	602	CLA	O1A-CGA-O2A-C1
32	8	602	CLA	O1A-CGA-O2A-C1
45	c	516	DGD	O1A-C1A-O1G-C1G
32	4	608	CLA	C8-C10-C11-C12
32	b	609	CLA	C13-C15-C16-C17
32	B	609	CLA	C13-C15-C16-C17
37	C	517	LMG	C30-C31-C32-C33
38	S	301	LHG	C25-C26-C27-C28
38	L	101	LHG	C24-C25-C26-C27
38	l	102	LHG	C7-C8-C9-C10
37	d	406	LMG	C18-C19-C20-C21
38	s	301	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
39	A	606	SQD	O49-C7-O47-C45
37	D	407	LMG	C18-C19-C20-C21
39	p	318	SQD	C11-C12-C13-C14
45	c	514	DGD	C7B-C8B-C9B-CAB
43	D	405	PL9	C34-C36-C37-C38
43	d	404	PL9	C34-C36-C37-C38
32	C	513	CLA	CBD-CGD-O2D-CED
32	b	614	CLA	C10-C11-C12-C13
32	b	617	CLA	C10-C11-C12-C13
32	B	614	CLA	C10-C11-C12-C13
32	B	617	CLA	C10-C11-C12-C13
33	2	610	KC2	C2A-CAA-CBA-CGA
33	4	610	KC2	C4B-C3B-CAB-CBB
33	4	610	KC2	C4C-C3C-CAC-CBC
33	0	610	KC2	C4B-C3B-CAB-CBB
33	0	610	KC2	C4C-C3C-CAC-CBC
33	8	610	KC2	C2A-CAA-CBA-CGA
32	1	608	CLA	C11-C12-C13-C15
32	B	603	CLA	C5-C6-C7-C8
45	c	516	DGD	C5A-C6A-C7A-C8A
32	5	303	CLA	O1A-CGA-O2A-C1
45	C	516	DGD	O1A-C1A-O1G-C1G
37	b	618	LMG	C30-C31-C32-C33
38	D	406	LHG	C27-C28-C29-C30
38	d	405	LHG	C27-C28-C29-C30
45	C	514	DGD	C7B-C8B-C9B-CAB
32	b	603	CLA	C5-C6-C7-C8
37	B	618	LMG	C30-C31-C32-C33
38	l	102	LHG	C30-C31-C32-C33
39	5	318	SQD	C11-C12-C13-C14
45	C	516	DGD	C5A-C6A-C7A-C8A
32	D	404	CLA	C3-C5-C6-C7
32	d	403	CLA	C3-C5-C6-C7
39	5	318	SQD	O47-C45-C46-O48
39	b	601	SQD	O47-C45-C46-O48
39	p	318	SQD	O47-C45-C46-O48
39	B	601	SQD	O47-C45-C46-O48
32	B	612	CLA	C11-C12-C13-C15
37	c	517	LMG	C31-C32-C33-C34
37	C	517	LMG	C31-C32-C33-C34
37	a	410	LMG	C18-C19-C20-C21
39	p	318	SQD	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
39	B	620	SQD	C11-C12-C13-C14
45	c	515	DGD	C2B-C3B-C4B-C5B
45	C	515	DGD	C3A-C4A-C5A-C6A
45	C	515	DGD	C2B-C3B-C4B-C5B
32	b	613	CLA	CBA-CGA-O2A-C1
32	0	602	CLA	CBA-CGA-O2A-C1
32	B	613	CLA	CBA-CGA-O2A-C1
32	P	602	CLA	O1A-CGA-O2A-C1
32	b	612	CLA	C11-C12-C13-C15
32	C	504	CLA	C11-C10-C8-C7
37	D	407	LMG	C30-C31-C32-C33
37	d	406	LMG	C30-C31-C32-C33
37	8	617	LMG	C30-C31-C32-C33
37	C	517	LMG	C34-C35-C36-C37
39	b	601	SQD	C25-C26-C27-C28
39	b	620	SQD	C11-C12-C13-C14
45	C	514	DGD	C4A-C5A-C6A-C7A
37	A	607	LMG	C18-C19-C20-C21
37	c	517	LMG	C34-C35-C36-C37
38	B	619	LHG	C9-C10-C11-C12
45	c	515	DGD	C3A-C4A-C5A-C6A
38	b	619	LHG	C9-C10-C11-C12
39	5	318	SQD	C11-C10-C9-C8
32	b	616	CLA	C16-C17-C18-C20
32	B	616	CLA	C16-C17-C18-C20
32	1	602	CLA	C5-C6-C7-C8
39	A	606	SQD	C15-C16-C17-C18
39	a	409	SQD	C15-C16-C17-C18
45	c	514	DGD	C4A-C5A-C6A-C7A
32	c	504	CLA	C11-C10-C8-C7
45	a	414	DGD	O1B-C1B-O2G-C2G
38	a	402	LHG	O2-C2-C3-O3
37	B	618	LMG	C37-C38-C39-C40
38	L	101	LHG	C30-C31-C32-C33
32	c	501	CLA	C2A-CAA-CBA-CGA
32	C	501	CLA	C2A-CAA-CBA-CGA
38	D	410	LHG	C13-C14-C15-C16
39	a	409	SQD	C28-C29-C30-C31
32	5	309	CLA	C10-C11-C12-C13
32	p	309	CLA	C10-C11-C12-C13
38	d	411	LHG	C13-C14-C15-C16
37	c	517	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
37	C	517	LMG	C38-C39-C40-C41
39	A	606	SQD	C28-C29-C30-C31
32	1	602	CLA	O1A-CGA-O2A-C1
32	9	602	CLA	O1A-CGA-O2A-C1
32	p	303	CLA	O1A-CGA-O2A-C1
38	L	101	LHG	C33-C34-C35-C36
39	B	601	SQD	C25-C26-C27-C28
45	c	516	DGD	C8A-C9A-CAA-CBA
32	1	612	CLA	C1A-C2A-CAA-CBA
32	2	612	CLA	C1A-C2A-CAA-CBA
32	3	603	CLA	C1A-C2A-CAA-CBA
32	3	605	CLA	C1A-C2A-CAA-CBA
32	3	610	CLA	C1A-C2A-CAA-CBA
32	3	611	CLA	C1A-C2A-CAA-CBA
32	4	612	CLA	C1A-C2A-CAA-CBA
32	5	304	CLA	C1A-C2A-CAA-CBA
32	5	313	CLA	C1A-C2A-CAA-CBA
32	6	603	CLA	C1A-C2A-CAA-CBA
32	A	603	CLA	C1A-C2A-CAA-CBA
32	D	401	CLA	C1A-C2A-CAA-CBA
32	S	302	CLA	C1A-C2A-CAA-CBA
32	b	617	CLA	C1A-C2A-CAA-CBA
32	c	501	CLA	C1A-C2A-CAA-CBA
32	c	503	CLA	C1A-C2A-CAA-CBA
32	d	409	CLA	C1A-C2A-CAA-CBA
32	0	612	CLA	C1A-C2A-CAA-CBA
32	7	612	CLA	C1A-C2A-CAA-CBA
32	8	612	CLA	C1A-C2A-CAA-CBA
32	9	603	CLA	C1A-C2A-CAA-CBA
32	9	605	CLA	C1A-C2A-CAA-CBA
32	9	610	CLA	C1A-C2A-CAA-CBA
32	9	611	CLA	C1A-C2A-CAA-CBA
32	C	501	CLA	C1A-C2A-CAA-CBA
32	P	603	CLA	C1A-C2A-CAA-CBA
32	a	406	CLA	C1A-C2A-CAA-CBA
32	p	304	CLA	C1A-C2A-CAA-CBA
32	p	313	CLA	C1A-C2A-CAA-CBA
32	s	302	CLA	C1A-C2A-CAA-CBA
32	B	617	CLA	C1A-C2A-CAA-CBA
37	C	517	LMG	O6-C5-C6-O5
32	0	608	CLA	C5-C6-C7-C8
32	C	507	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
38	L	101	LHG	C28-C29-C30-C31
38	l	102	LHG	C28-C29-C30-C31
38	l	102	LHG	C33-C34-C35-C36
39	a	409	SQD	C10-C11-C12-C13
45	C	516	DGD	C8A-C9A-CAA-CBA
37	c	517	LMG	O6-C5-C6-O5
32	7	602	CLA	O1A-CGA-O2A-C1
38	b	619	LHG	O6-C4-C5-C6
38	B	619	LHG	O6-C4-C5-C6
45	A	614	DGD	C3A-C4A-C5A-C6A
32	6	602	CLA	C11-C10-C8-C7
32	S	303	CLA	C6-C7-C8-C10
32	b	604	CLA	C6-C7-C8-C10
32	c	505	CLA	C12-C13-C15-C16
32	c	511	CLA	C12-C13-C15-C16
32	C	505	CLA	C12-C13-C15-C16
32	C	511	CLA	C12-C13-C15-C16
32	P	602	CLA	C11-C10-C8-C7
32	s	303	CLA	C6-C7-C8-C10
32	B	604	CLA	C6-C7-C8-C10
39	A	606	SQD	C11-C12-C13-C14
39	a	409	SQD	C11-C12-C13-C14
32	3	602	CLA	O1A-CGA-O2A-C1
32	D	404	CLA	O1A-CGA-O2A-C1
32	d	403	CLA	O1A-CGA-O2A-C1
32	C	502	CLA	O1A-CGA-O2A-C1
32	4	608	CLA	C5-C6-C7-C8
32	c	507	CLA	C15-C16-C17-C18
32	c	511	CLA	C15-C16-C17-C18
37	d	406	LMG	C4-C5-C6-O5
37	A	607	LMG	C32-C33-C34-C35
37	a	410	LMG	C32-C33-C34-C35
39	A	606	SQD	C10-C11-C12-C13
32	c	502	CLA	O1A-CGA-O2A-C1
37	2	617	LMG	O6-C5-C6-O5
32	c	512	CLA	O1D-CGD-O2D-CED
32	5	313	CLA	C2A-CAA-CBA-CGA
32	5	306	CLA	C11-C10-C8-C9
32	S	303	CLA	C11-C12-C13-C14
32	c	505	CLA	C11-C12-C13-C14
32	c	507	CLA	C14-C13-C15-C16
32	9	609	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	C	505	CLA	C11-C12-C13-C14
32	C	507	CLA	C14-C13-C15-C16
32	C	511	CLA	C14-C13-C15-C16
32	s	303	CLA	C11-C12-C13-C14
37	A	607	LMG	C14-C15-C16-C17
37	a	410	LMG	C14-C15-C16-C17
45	H	101	DGD	C9A-CAA-CBA-CCA
45	h	101	DGD	C9A-CAA-CBA-CCA
37	8	617	LMG	O6-C5-C6-O5
31	B	623	8CT	C12-C13-C14-C15
38	a	403	LHG	C25-C26-C27-C28
37	D	407	LMG	C4-C5-C6-O5
32	4	602	CLA	CBA-CGA-O2A-C1
32	C	501	CLA	CBA-CGA-O2A-C1
37	2	617	LMG	C29-C28-O8-C9
37	c	517	LMG	C37-C38-C39-C40
37	4	618	LMG	O6-C5-C6-O5
37	C	517	LMG	C37-C38-C39-C40
37	B	618	LMG	C34-C35-C36-C37
37	g	101	LMG	O6-C5-C6-O5
45	H	101	DGD	O6E-C5E-C6E-O5E
37	2	617	LMG	O1-C7-C8-C9
37	c	517	LMG	O1-C7-C8-C9
37	g	101	LMG	O1-C7-C8-C9
37	C	517	LMG	O1-C7-C8-C9
37	G	102	LMG	O1-C7-C8-C9
38	D	410	LHG	C4-C5-C6-O8
38	b	621	LHG	C4-C5-C6-O8
38	d	411	LHG	C4-C5-C6-O8
38	B	621	LHG	C4-C5-C6-O8
39	5	318	SQD	C44-C45-C46-O48
39	A	606	SQD	O6-C44-C45-C46
39	b	601	SQD	O6-C44-C45-C46
39	a	409	SQD	O6-C44-C45-C46
39	B	601	SQD	O6-C44-C45-C46
45	c	516	DGD	C1G-C2G-C3G-O3G
45	C	516	DGD	C1G-C2G-C3G-O3G
32	8	607	CLA	O1D-CGD-O2D-CED
45	h	101	DGD	O6E-C5E-C6E-O5E
33	0	610	KC2	CBD-CGD-O2D-CED
37	d	406	LMG	C14-C15-C16-C17
37	D	407	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
37	b	618	LMG	C34-C35-C36-C37
37	b	618	LMG	C37-C38-C39-C40
32	1	607	CLA	O1D-CGD-O2D-CED
32	c	501	CLA	CBA-CGA-O2A-C1
37	G	102	LMG	C29-C28-O8-C9
37	g	101	LMG	C28-C29-C30-C31
37	0	619	LMG	O6-C5-C6-O5
45	c	516	DGD	O6E-C5E-C6E-O5E
45	C	516	DGD	O6E-C5E-C6E-O5E
37	D	411	LMG	C32-C33-C34-C35
37	d	401	LMG	C32-C33-C34-C35
37	G	102	LMG	C28-C29-C30-C31
32	b	613	CLA	O1A-CGA-O2A-C1
32	0	602	CLA	O1A-CGA-O2A-C1
32	B	613	CLA	O1A-CGA-O2A-C1
32	B	607	CLA	CBD-CGD-O2D-CED
32	b	606	CLA	C8-C10-C11-C12
32	B	606	CLA	C8-C10-C11-C12
31	3	615	8CT	C10-C11-C12-C40
31	H	102	8CT	C27-C26-C28-C29
31	9	615	8CT	C10-C11-C12-C40
31	h	102	8CT	C27-C26-C28-C29
37	G	102	LMG	O6-C5-C6-O5
31	3	615	8CT	C10-C11-C12-C13
31	H	102	8CT	C25-C26-C28-C29
31	9	615	8CT	C10-C11-C12-C13
31	h	102	8CT	C25-C26-C28-C29
32	b	609	CLA	C15-C16-C17-C18
32	B	609	CLA	C15-C16-C17-C18
37	c	517	LMG	C13-C14-C15-C16
32	c	501	CLA	C10-C11-C12-C13
32	C	501	CLA	C10-C11-C12-C13
32	b	609	CLA	CBA-CGA-O2A-C1
32	B	609	CLA	CBA-CGA-O2A-C1
45	a	414	DGD	C7B-C8B-C9B-CAB
31	b	622	8CT	C12-C13-C14-C15
31	b	622	8CT	C16-C17-C18-C19
31	c	518	8CT	C18-C19-C20-C21
31	z	101	8CT	C16-C17-C18-C19
31	z	101	8CT	C23-C24-C25-C26
31	C	518	8CT	C18-C19-C20-C21
31	B	623	8CT	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
36	4	617	IHT	C35-C38-C41-C40
32	7	607	CLA	O1D-CGD-O2D-CED
32	4	602	CLA	O1A-CGA-O2A-C1
37	6	616	LMG	O10-C28-O8-C9
37	C	517	LMG	C13-C14-C15-C16
45	A	614	DGD	C3B-C4B-C5B-C6B
39	A	606	SQD	C24-C23-O48-C46
39	a	409	SQD	C24-C23-O48-C46
32	2	607	CLA	O1D-CGD-O2D-CED
38	A	613	LHG	C25-C26-C27-C28
45	c	516	DGD	C4A-C5A-C6A-C7A
45	C	516	DGD	C4A-C5A-C6A-C7A
32	3	607	CLA	C11-C12-C13-C14
32	0	602	CLA	C11-C12-C13-C14
37	b	618	LMG	O7-C8-C9-O8
37	P	616	LMG	O1-C7-C8-O7
37	B	618	LMG	O7-C8-C9-O8
39	b	601	SQD	C24-C25-C26-C27
39	B	620	SQD	C14-C15-C16-C17
39	b	620	SQD	C14-C15-C16-C17
32	C	504	CLA	C6-C7-C8-C10
37	l	101	LMG	C30-C31-C32-C33
32	1	602	CLA	C3-C5-C6-C7
32	B	614	CLA	C3-C5-C6-C7
45	a	414	DGD	C8B-C9B-CAB-CBB
45	A	614	DGD	C6A-C7A-C8A-C9A
32	c	504	CLA	C6-C7-C8-C10
37	A	607	LMG	C34-C35-C36-C37
37	a	410	LMG	C38-C39-C40-C41
45	a	414	DGD	C9B-CAB-CBB-CCB
32	C	504	CLA	CBA-CGA-O2A-C1
37	A	607	LMG	C38-C39-C40-C41
32	c	513	CLA	CBD-CGD-O2D-CED
37	a	410	LMG	C34-C35-C36-C37
41	D	402	PHO	C15-C16-C17-C18
32	b	614	CLA	C3-C5-C6-C7
32	4	602	CLA	C11-C12-C13-C14
32	c	504	CLA	C10-C11-C12-C13
32	C	504	CLA	C10-C11-C12-C13
41	d	410	PHO	C15-C16-C17-C18
32	1	602	CLA	C4-C3-C5-C6
32	c	507	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
32	C	507	CLA	C4-C3-C5-C6
32	C	511	CLA	CBA-CGA-O2A-C1
37	8	617	LMG	C29-C28-O8-C9
39	B	620	SQD	C23-C24-C25-C26
37	d	406	LMG	O9-C10-O7-C8
34	5	301	II0	C09-C21-C23-C25
34	5	315	II0	C09-C21-C23-C25
34	6	612	II0	C10-C22-C24-C26
34	6	614	II0	C09-C21-C23-C25
34	7	614	II0	C09-C21-C23-C25
34	7	619	II0	C10-C22-C24-C26
34	9	612	II0	C09-C21-C23-C25
34	9	613	II0	C10-C22-C24-C26
35	6	613	II3	C16-C23-C27-C28
36	4	617	IHT	C11-C21-C24-C26
32	2	605	CLA	C6-C7-C8-C9
32	2	605	CLA	C11-C10-C8-C9
32	3	609	CLA	C6-C7-C8-C9
32	6	602	CLA	C11-C10-C8-C9
32	b	604	CLA	C6-C7-C8-C9
32	b	609	CLA	C11-C12-C13-C14
32	c	501	CLA	C11-C12-C13-C14
32	c	502	CLA	C11-C12-C13-C14
32	c	505	CLA	C14-C13-C15-C16
32	8	605	CLA	C6-C7-C8-C9
32	8	605	CLA	C11-C10-C8-C9
32	C	501	CLA	C11-C12-C13-C14
32	C	502	CLA	C11-C12-C13-C14
32	C	505	CLA	C14-C13-C15-C16
32	P	602	CLA	C11-C10-C8-C9
32	p	306	CLA	C11-C10-C8-C9
32	B	604	CLA	C6-C7-C8-C9
32	B	609	CLA	C11-C12-C13-C14
38	D	406	LHG	C28-C29-C30-C31
38	d	405	LHG	C28-C29-C30-C31
32	3	611	CLA	O1D-CGD-O2D-CED
32	1	603	CLA	C4B-C3B-CAB-CBB
32	1	611	CLA	C4B-C3B-CAB-CBB
32	2	603	CLA	C4B-C3B-CAB-CBB
32	2	605	CLA	C4B-C3B-CAB-CBB
32	2	607	CLA	C4B-C3B-CAB-CBB
32	2	608	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	2	612	CLA	C4B-C3B-CAB-CBB
32	3	610	CLA	C4B-C3B-CAB-CBB
32	3	611	CLA	C4B-C3B-CAB-CBB
32	4	605	CLA	C4B-C3B-CAB-CBB
32	5	306	CLA	C4B-C3B-CAB-CBB
32	6	601	CLA	C4B-C3B-CAB-CBB
32	6	602	CLA	C4B-C3B-CAB-CBB
32	6	606	CLA	C4B-C3B-CAB-CBB
32	6	611	CLA	C4B-C3B-CAB-CBB
32	A	603	CLA	C4B-C3B-CAB-CBB
32	b	617	CLA	C4B-C3B-CAB-CBB
32	0	605	CLA	C4B-C3B-CAB-CBB
32	7	611	CLA	C4B-C3B-CAB-CBB
32	8	603	CLA	C4B-C3B-CAB-CBB
32	8	605	CLA	C4B-C3B-CAB-CBB
32	8	607	CLA	C4B-C3B-CAB-CBB
32	8	608	CLA	C4B-C3B-CAB-CBB
32	8	612	CLA	C4B-C3B-CAB-CBB
32	9	610	CLA	C4B-C3B-CAB-CBB
32	9	611	CLA	C4B-C3B-CAB-CBB
32	C	512	CLA	C4B-C3B-CAB-CBB
32	P	601	CLA	C4B-C3B-CAB-CBB
32	P	602	CLA	C4B-C3B-CAB-CBB
32	P	606	CLA	C4B-C3B-CAB-CBB
32	P	611	CLA	C4B-C3B-CAB-CBB
32	a	406	CLA	C4B-C3B-CAB-CBB
32	p	313	CLA	C4B-C3B-CAB-CBB
32	B	617	CLA	C4B-C3B-CAB-CBB
37	d	401	LMG	C29-C30-C31-C32
39	b	620	SQD	C23-C24-C25-C26
37	D	411	LMG	C29-C30-C31-C32
37	d	401	LMG	C14-C15-C16-C17
45	A	614	DGD	CAB-CBB-CCB-CDB
32	c	504	CLA	CBA-CGA-O2A-C1
32	p	305	CLA	C2A-CAA-CBA-CGA
32	p	313	CLA	C2A-CAA-CBA-CGA
37	D	411	LMG	C14-C15-C16-C17
37	B	618	LMG	C17-C18-C19-C20
39	b	601	SQD	C2-C1-O6-C44
39	B	601	SQD	C2-C1-O6-C44
37	b	618	LMG	C17-C18-C19-C20
37	L	102	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
45	H	101	DGD	C8B-C9B-CAB-CBB
45	h	101	DGD	C8B-C9B-CAB-CBB
38	D	406	LHG	O6-C4-C5-C6
38	d	405	LHG	O6-C4-C5-C6
38	b	619	LHG	C27-C28-C29-C30
38	b	621	LHG	C9-C10-C11-C12
38	B	621	LHG	C9-C10-C11-C12
32	2	605	CLA	C6-C7-C8-C10
32	2	605	CLA	C11-C10-C8-C7
32	3	609	CLA	C6-C7-C8-C10
32	5	306	CLA	C11-C10-C8-C7
32	S	303	CLA	C11-C12-C13-C15
32	b	609	CLA	C11-C12-C13-C15
32	b	614	CLA	C12-C13-C15-C16
32	b	617	CLA	C11-C12-C13-C15
32	c	501	CLA	C6-C7-C8-C10
32	c	501	CLA	C11-C12-C13-C15
32	c	502	CLA	C11-C12-C13-C15
32	c	502	CLA	C12-C13-C15-C16
32	c	505	CLA	C11-C12-C13-C15
32	c	507	CLA	C12-C13-C15-C16
32	8	605	CLA	C6-C7-C8-C10
32	8	605	CLA	C11-C10-C8-C7
32	9	609	CLA	C6-C7-C8-C10
32	C	501	CLA	C6-C7-C8-C10
32	C	501	CLA	C11-C12-C13-C15
32	C	502	CLA	C11-C12-C13-C15
32	C	502	CLA	C12-C13-C15-C16
32	C	505	CLA	C11-C12-C13-C15
32	C	507	CLA	C12-C13-C15-C16
32	s	303	CLA	C11-C12-C13-C15
32	B	609	CLA	C11-C12-C13-C15
32	B	614	CLA	C12-C13-C15-C16
32	B	617	CLA	C11-C12-C13-C15
37	2	617	LMG	C32-C33-C34-C35
39	b	601	SQD	C7-C8-C9-C10
39	B	601	SQD	C7-C8-C9-C10
45	A	614	DGD	CCB-CDB-CEB-CFB
37	D	407	LMG	O9-C10-O7-C8
32	C	504	CLA	C15-C16-C17-C18
37	0	619	LMG	C32-C33-C34-C35
37	8	617	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
37	G	102	LMG	C29-C30-C31-C32
32	3	610	CLA	C3A-C2A-CAA-CBA
32	g	102	CLA	C3A-C2A-CAA-CBA
32	9	610	CLA	C3A-C2A-CAA-CBA
32	G	101	CLA	C3A-C2A-CAA-CBA
38	B	619	LHG	C27-C28-C29-C30
37	g	101	LMG	C29-C30-C31-C32
37	L	102	LMG	C30-C31-C32-C33
32	b	609	CLA	O1A-CGA-O2A-C1
32	c	501	CLA	O1A-CGA-O2A-C1
32	C	501	CLA	O1A-CGA-O2A-C1
32	B	609	CLA	O1A-CGA-O2A-C1
32	b	616	CLA	C10-C11-C12-C13
37	B	618	LMG	C39-C40-C41-C42
32	9	603	CLA	CBA-CGA-O2A-C1
31	A	610	8CT	C16-C17-C18-C19
31	K	102	8CT	C23-C24-C25-C26
31	Z	101	8CT	C16-C17-C18-C19
31	k	101	8CT	C23-C24-C25-C26
31	B	622	8CT	C14-C15-C16-C39
45	c	514	DGD	O1A-C1A-O1G-C1G
37	b	618	LMG	C39-C40-C41-C42
37	L	102	LMG	C14-C15-C16-C17
39	B	601	SQD	C24-C25-C26-C27
32	c	504	CLA	C15-C16-C17-C18
31	A	610	8CT	C10-C11-C12-C13
38	s	301	LHG	C23-C24-C25-C26
37	4	618	LMG	C32-C33-C34-C35
37	4	618	LMG	O1-C7-C8-C9
37	6	616	LMG	O1-C7-C8-C9
37	6	616	LMG	C7-C8-C9-O8
37	b	618	LMG	C7-C8-C9-O8
37	0	619	LMG	O1-C7-C8-C9
37	8	617	LMG	O1-C7-C8-C9
37	L	102	LMG	C7-C8-C9-O8
37	P	616	LMG	O1-C7-C8-C9
37	P	616	LMG	C7-C8-C9-O8
37	B	618	LMG	C7-C8-C9-O8
38	S	301	LHG	C4-C5-C6-O8
38	l	102	LHG	C4-C5-C6-O8
38	L	101	LHG	C4-C5-C6-O8
38	s	301	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
39	b	601	SQD	C44-C45-C46-O48
39	p	318	SQD	C44-C45-C46-O48
39	B	601	SQD	C44-C45-C46-O48
32	C	512	CLA	CBD-CGD-O2D-CED
32	B	616	CLA	C10-C11-C12-C13
45	A	614	DGD	C4A-C5A-C6A-C7A
45	C	514	DGD	O1A-C1A-O1G-C1G
32	7	602	CLA	C4-C3-C5-C6
43	D	405	PL9	C15-C14-C16-C17
43	d	404	PL9	C15-C14-C16-C17
38	S	301	LHG	C23-C24-C25-C26
32	3	603	CLA	CBA-CGA-O2A-C1
32	C	502	CLA	O1D-CGD-O2D-CED
45	C	515	DGD	C4E-C5E-C6E-O5E
31	b	622	8CT	C04-C03-C10-C11
31	B	623	8CT	C04-C03-C10-C11
32	2	605	CLA	C2B-C3B-CAB-CBB
32	6	601	CLA	C2B-C3B-CAB-CBB
32	8	605	CLA	C2B-C3B-CAB-CBB
32	P	601	CLA	C2B-C3B-CAB-CBB
36	4	614	IHT	C02-C07-C18-C22
36	0	614	IHT	C02-C07-C18-C22
45	c	515	DGD	C4E-C5E-C6E-O5E
37	6	616	LMG	C29-C28-O8-C9
37	l	101	LMG	C34-C35-C36-C37
37	L	102	LMG	C34-C35-C36-C37
39	b	601	SQD	C31-C32-C33-C34
47	V	201	HEM	C3D-CAD-CBD-CGD
32	b	603	CLA	C6-C7-C8-C10
32	B	603	CLA	C6-C7-C8-C10
32	8	604	CLA	C2A-CAA-CBA-CGA
37	2	617	LMG	O7-C8-C9-O8
37	8	617	LMG	O7-C8-C9-O8
38	D	410	LHG	O7-C5-C6-O8
38	d	411	LHG	O7-C5-C6-O8
32	B	615	CLA	C4-C3-C5-C6
39	B	601	SQD	C31-C32-C33-C34
32	C	511	CLA	C15-C16-C17-C18
38	L	101	LHG	C29-C30-C31-C32
45	c	515	DGD	C1B-C2B-C3B-C4B
32	c	502	CLA	O1D-CGD-O2D-CED
32	S	303	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	c	511	CLA	C14-C13-C15-C16
32	s	303	CLA	C6-C7-C8-C9
45	a	414	DGD	C3B-C4B-C5B-C6B
32	7	609	CLA	O1D-CGD-O2D-CED
32	1	609	CLA	O1D-CGD-O2D-CED
32	b	604	CLA	O1D-CGD-O2D-CED
32	B	604	CLA	O1D-CGD-O2D-CED
32	p	305	CLA	C3-C5-C6-C7
38	s	301	LHG	C26-C27-C28-C29
32	c	513	CLA	O2A-C1-C2-C3
32	C	513	CLA	O2A-C1-C2-C3
32	b	606	CLA	C13-C15-C16-C17
38	S	301	LHG	C26-C27-C28-C29
38	l	102	LHG	C29-C30-C31-C32
32	B	606	CLA	C13-C15-C16-C17
39	a	409	SQD	O10-C23-O48-C46
39	b	620	SQD	C19-C20-C21-C22
39	B	620	SQD	C19-C20-C21-C22
32	9	607	CLA	C11-C12-C13-C14
39	A	606	SQD	O10-C23-O48-C46
32	c	502	CLA	C8-C10-C11-C12
32	C	502	CLA	C8-C10-C11-C12
37	a	410	LMG	C36-C37-C38-C39
45	C	515	DGD	C1B-C2B-C3B-C4B
37	A	607	LMG	C36-C37-C38-C39
38	d	405	LHG	C30-C31-C32-C33
41	A	604	PHO	C16-C17-C18-C19
41	a	407	PHO	C16-C17-C18-C19
32	c	504	CLA	O1A-CGA-O2A-C1
32	9	603	CLA	O1A-CGA-O2A-C1
32	4	604	CLA	C5-C6-C7-C8
31	c	518	8CT	C10-C11-C12-C40
31	C	518	8CT	C10-C11-C12-C40
32	7	602	CLA	C11-C12-C13-C14
32	5	303	CLA	C11-C10-C8-C7
32	D	401	CLA	C11-C10-C8-C7
32	b	607	CLA	C11-C10-C8-C7
32	c	507	CLA	C6-C7-C8-C10
32	c	509	CLA	C6-C7-C8-C10
32	d	409	CLA	C11-C10-C8-C7
32	C	507	CLA	C6-C7-C8-C10
32	C	509	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
32	p	303	CLA	C11-C10-C8-C7
32	p	306	CLA	C11-C10-C8-C7
32	B	607	CLA	C11-C10-C8-C7
38	D	406	LHG	C30-C31-C32-C33
38	D	410	LHG	C9-C10-C11-C12
38	d	411	LHG	C9-C10-C11-C12
39	A	606	SQD	C24-C25-C26-C27
31	M	201	8CT	C14-C15-C16-C17
31	c	518	8CT	C10-C11-C12-C13
31	C	518	8CT	C10-C11-C12-C13
31	a	413	8CT	C25-C26-C28-C29
34	5	319	II0	C32-C34-C36-C40
34	p	301	II0	C32-C34-C36-C40
32	B	610	CLA	CBA-CGA-O2A-C1
47	v	201	HEM	C3D-CAD-CBD-CGD
32	C	504	CLA	O1A-CGA-O2A-C1
39	A	606	SQD	C45-C44-O6-C1
39	a	409	SQD	C45-C44-O6-C1
32	2	604	CLA	C2A-CAA-CBA-CGA
32	3	604	CLA	C2A-CAA-CBA-CGA
32	3	605	CLA	C2A-CAA-CBA-CGA
32	5	305	CLA	C2A-CAA-CBA-CGA
32	c	513	CLA	C2A-CAA-CBA-CGA
32	9	604	CLA	C2A-CAA-CBA-CGA
32	9	605	CLA	C2A-CAA-CBA-CGA
32	C	513	CLA	C2A-CAA-CBA-CGA
43	a	412	PL9	C7-C8-C9-C11
32	9	611	CLA	O1D-CGD-O2D-CED
32	b	615	CLA	C4-C3-C5-C6
32	C	503	CLA	C4-C3-C5-C6
45	C	514	DGD	C6A-C7A-C8A-C9A
32	B	615	CLA	C2-C3-C5-C6
33	2	610	KC2	C2C-C3C-CAC-CBC
33	8	610	KC2	C2C-C3C-CAC-CBC
45	c	514	DGD	C5A-C6A-C7A-C8A
32	6	602	CLA	C11-C12-C13-C14
45	c	514	DGD	C6A-C7A-C8A-C9A
32	b	610	CLA	CBA-CGA-O2A-C1
37	D	411	LMG	C9-C8-O7-C10
37	d	401	LMG	C9-C8-O7-C10
39	A	606	SQD	C44-C45-O47-C7
39	a	409	SQD	C44-C45-O47-C7

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Mol	Chain	Res	Type	Atoms
37	d	406	LMG	C19-C20-C21-C22
39	a	409	SQD	C24-C25-C26-C27
31	b	623	8CT	C16-C17-C18-C19
37	D	407	LMG	C19-C20-C21-C22
45	C	514	DGD	C5A-C6A-C7A-C8A
39	b	620	SQD	C24-C25-C26-C27
32	3	603	CLA	O1A-CGA-O2A-C1
32	C	511	CLA	O1A-CGA-O2A-C1
45	H	101	DGD	C7B-C8B-C9B-CAB
45	h	101	DGD	C7B-C8B-C9B-CAB
38	D	406	LHG	O6-C4-C5-O7
39	B	620	SQD	C24-C25-C26-C27
32	P	602	CLA	C11-C12-C13-C14
32	b	607	CLA	O1D-CGD-O2D-CED
37	2	617	LMG	C7-C8-C9-O8
37	l	101	LMG	C7-C8-C9-O8
45	c	514	DGD	C1G-C2G-C3G-O3G
45	c	516	DGD	O1G-C1G-C2G-C3G
45	C	514	DGD	C1G-C2G-C3G-O3G
45	C	516	DGD	O1G-C1G-C2G-C3G
33	2	610	KC2	C4C-C3C-CAC-CBC
33	6	609	KC2	C4C-C3C-CAC-CBC
33	8	610	KC2	C4C-C3C-CAC-CBC
33	P	609	KC2	C4C-C3C-CAC-CBC
47	E	101	HEM	C4C-C3C-CAC-CBC
47	f	101	HEM	C4C-C3C-CAC-CBC
33	6	605	KC2	CAA-CBA-CGA-O1A
38	D	406	LHG	C11-C12-C13-C14
32	0	604	CLA	C5-C6-C7-C8
37	2	617	LMG	O1-C7-C8-O7
37	6	616	LMG	O1-C7-C8-O7
37	8	617	LMG	O1-C7-C8-O7
37	C	517	LMG	O7-C8-C9-O8
38	S	301	LHG	O7-C5-C6-O8
38	s	301	LHG	O7-C5-C6-O8
32	d	409	CLA	C11-C10-C8-C9
38	d	405	LHG	C11-C12-C13-C14
45	C	515	DGD	CAB-CBB-CCB-CDB
38	B	621	LHG	C12-C13-C14-C15
37	d	406	LMG	C10-C11-C12-C13
38	b	621	LHG	C12-C13-C14-C15
45	A	614	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
31	B	624	8CT	C16-C17-C18-C19
34	5	315	II0	C25-C29-C31-C33
32	C	513	CLA	O1D-CGD-O2D-CED
32	C	505	CLA	C15-C16-C17-C18
38	a	403	LHG	C10-C11-C12-C13
32	c	503	CLA	C4-C3-C5-C6
37	D	407	LMG	C10-C11-C12-C13
38	2	618	LHG	O6-C4-C5-C6
38	8	618	LHG	O6-C4-C5-C6
32	0	604	CLA	C2A-CAA-CBA-CGA
33	4	610	KC2	CBD-CGD-O2D-CED
45	c	515	DGD	CAB-CBB-CCB-CDB
45	H	101	DGD	C1B-C2B-C3B-C4B
45	h	101	DGD	C1B-C2B-C3B-C4B
32	c	505	CLA	C15-C16-C17-C18
39	b	601	SQD	C4-C5-C6-S
39	B	601	SQD	C4-C5-C6-S
37	C	517	LMG	C11-C10-O7-C8
39	a	409	SQD	C30-C31-C32-C33
37	D	411	LMG	C15-C16-C17-C18
37	d	401	LMG	C15-C16-C17-C18
34	4	616	II0	C09-C21-C23-C25
34	0	616	II0	C09-C21-C23-C25
35	7	615	II3	C16-C23-C27-C28
32	1	608	CLA	C1A-C2A-CAA-CBA
32	2	601	CLA	C4B-C3B-CAB-CBB
32	3	604	CLA	C4B-C3B-CAB-CBB
32	4	606	CLA	C4B-C3B-CAB-CBB
32	6	604	CLA	C4B-C3B-CAB-CBB
32	d	402	CLA	C1A-C2A-CAA-CBA
32	0	604	CLA	C4B-C3B-CAB-CBB
32	0	606	CLA	C4B-C3B-CAB-CBB
32	7	608	CLA	C1A-C2A-CAA-CBA
32	8	601	CLA	C4B-C3B-CAB-CBB
32	9	604	CLA	C4B-C3B-CAB-CBB
32	P	604	CLA	C4B-C3B-CAB-CBB
32	b	613	CLA	C4-C3-C5-C6
32	c	501	CLA	C4-C3-C5-C6
32	C	501	CLA	C4-C3-C5-C6
32	B	613	CLA	C4-C3-C5-C6
31	B	622	8CT	C14-C15-C16-C17
32	4	604	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
37	C	517	LMG	C17-C18-C19-C20
38	s	301	LHG	C31-C32-C33-C34
32	S	303	CLA	C10-C11-C12-C13
38	a	403	LHG	O6-C4-C5-C6
39	A	606	SQD	C30-C31-C32-C33
38	S	301	LHG	C31-C32-C33-C34
32	2	602	CLA	C11-C10-C8-C7
32	3	609	CLA	C11-C10-C8-C7
32	D	403	CLA	C11-C10-C8-C7
32	b	616	CLA	C12-C13-C15-C16
32	c	505	CLA	C6-C7-C8-C10
32	c	507	CLA	C11-C12-C13-C15
32	c	508	CLA	C12-C13-C15-C16
32	c	509	CLA	C11-C10-C8-C7
32	d	402	CLA	C11-C10-C8-C7
32	8	602	CLA	C11-C10-C8-C7
32	9	609	CLA	C11-C10-C8-C7
32	C	505	CLA	C6-C7-C8-C10
32	C	507	CLA	C11-C12-C13-C15
32	C	508	CLA	C12-C13-C15-C16
32	C	509	CLA	C11-C10-C8-C7
32	B	616	CLA	C12-C13-C15-C16
37	c	517	LMG	C17-C18-C19-C20
32	0	606	CLA	CBD-CGD-O2D-CED
37	P	616	LMG	O10-C28-O8-C9
32	7	601	CLA	C3A-C2A-CAA-CBA
32	3	607	CLA	CBA-CGA-O2A-C1
32	c	511	CLA	CBA-CGA-O2A-C1
32	9	607	CLA	CBA-CGA-O2A-C1
32	b	612	CLA	C10-C11-C12-C13
32	B	612	CLA	C10-C11-C12-C13
37	A	607	LMG	C12-C13-C14-C15
32	b	610	CLA	O1A-CGA-O2A-C1
32	B	610	CLA	O1A-CGA-O2A-C1
32	s	303	CLA	C10-C11-C12-C13
32	B	603	CLA	C15-C16-C17-C18
37	a	410	LMG	C12-C13-C14-C15
41	A	604	PHO	C4-C3-C5-C6
41	a	407	PHO	C4-C3-C5-C6
38	D	410	LHG	C10-C11-C12-C13
32	b	615	CLA	C2-C3-C5-C6
38	d	411	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
38	A	613	LHG	O6-C4-C5-O7
38	d	405	LHG	O6-C4-C5-O7
38	a	403	LHG	O6-C4-C5-O7
37	c	517	LMG	C11-C10-O7-C8
32	6	604	CLA	C2A-CAA-CBA-CGA
32	C	503	CLA	C2A-CAA-CBA-CGA
32	C	505	CLA	C2A-CAA-CBA-CGA
32	5	303	CLA	C11-C10-C8-C9
32	D	401	CLA	C11-C10-C8-C9
32	b	617	CLA	C11-C12-C13-C14
32	c	501	CLA	C6-C7-C8-C9
32	c	507	CLA	C6-C7-C8-C9
32	C	501	CLA	C6-C7-C8-C9
32	C	502	CLA	C14-C13-C15-C16
32	C	507	CLA	C6-C7-C8-C9
32	p	303	CLA	C11-C10-C8-C9
32	B	617	CLA	C11-C12-C13-C14
38	a	403	LHG	C27-C28-C29-C30
31	H	102	8CT	C16-C17-C18-C19
31	P	615	8CT	C18-C19-C20-C21
31	h	102	8CT	C16-C17-C18-C19
34	2	619	II0	C26-C30-C32-C34
34	8	619	II0	C26-C30-C32-C34
45	c	514	DGD	C8B-C9B-CAB-CBB
32	c	513	CLA	O1D-CGD-O2D-CED
32	c	505	CLA	C13-C15-C16-C17
32	C	505	CLA	C13-C15-C16-C17
32	A	603	CLA	C1-C2-C3-C4
32	c	513	CLA	C1-C2-C3-C4
32	C	513	CLA	C1-C2-C3-C4
32	a	406	CLA	C1-C2-C3-C4
33	1	610	KC2	C3A-C2A-CAA-CBA
33	6	605	KC2	C1A-C2A-CAA-CBA
33	7	610	KC2	C3A-C2A-CAA-CBA
33	P	605	KC2	C3A-C2A-CAA-CBA
33	p	311	KC2	C3A-C2A-CAA-CBA
35	7	615	II3	C03-C04-C12-C21
38	A	613	LHG	C10-C11-C12-C13
38	a	403	LHG	C31-C32-C33-C34
45	C	514	DGD	C8B-C9B-CAB-CBB
32	5	305	CLA	C3-C5-C6-C7
37	4	618	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
37	D	411	LMG	O7-C8-C9-O8
37	c	517	LMG	O1-C7-C8-O7
37	c	517	LMG	O7-C8-C9-O8
37	d	401	LMG	O7-C8-C9-O8
37	g	101	LMG	O1-C7-C8-O7
37	0	619	LMG	O1-C7-C8-O7
37	C	517	LMG	O1-C7-C8-O7
37	G	102	LMG	O1-C7-C8-O7
38	A	613	LHG	O7-C5-C6-O8
38	b	621	LHG	O7-C5-C6-O8
38	l	102	LHG	O7-C5-C6-O8
38	L	101	LHG	O7-C5-C6-O8
38	a	403	LHG	O7-C5-C6-O8
38	B	621	LHG	O7-C5-C6-O8
39	A	606	SQD	O6-C44-C45-O47
39	a	409	SQD	O6-C44-C45-O47
45	c	514	DGD	O2G-C2G-C3G-O3G
45	C	514	DGD	O2G-C2G-C3G-O3G
45	C	516	DGD	O2G-C2G-C3G-O3G
32	C	512	CLA	O1D-CGD-O2D-CED
32	C	508	CLA	C15-C16-C17-C18
37	D	411	LMG	C7-C8-C9-O8
37	c	517	LMG	C7-C8-C9-O8
37	d	401	LMG	C7-C8-C9-O8
37	8	617	LMG	C7-C8-C9-O8
37	C	517	LMG	C7-C8-C9-O8
38	A	613	LHG	C4-C5-C6-O8
38	a	403	LHG	C4-C5-C6-O8
45	a	414	DGD	C4B-C5B-C6B-C7B
32	2	605	CLA	C8-C10-C11-C12
32	c	508	CLA	C15-C16-C17-C18
32	8	605	CLA	C8-C10-C11-C12
32	5	304	CLA	CAD-CBD-CGD-O2D
32	b	606	CLA	CAD-CBD-CGD-O2D
32	b	610	CLA	CAD-CBD-CGD-O2D
32	c	502	CLA	CAD-CBD-CGD-O2D
32	c	506	CLA	CAD-CBD-CGD-O2D
32	C	502	CLA	CAD-CBD-CGD-O2D
32	C	506	CLA	CAD-CBD-CGD-O2D
32	p	304	CLA	CAD-CBD-CGD-O2D
32	B	606	CLA	CAD-CBD-CGD-O2D
32	B	610	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	3	607	CLA	O1A-CGA-O2A-C1
32	9	607	CLA	O1A-CGA-O2A-C1
41	D	402	PHO	C3-C5-C6-C7
32	c	503	CLA	C2A-CAA-CBA-CGA
32	c	505	CLA	C2A-CAA-CBA-CGA
32	P	604	CLA	C2A-CAA-CBA-CGA
32	c	511	CLA	O1A-CGA-O2A-C1
37	C	517	LMG	C35-C36-C37-C38
38	a	403	LHG	C24-C25-C26-C27
31	M	201	8CT	C23-C24-C25-C26
31	a	413	8CT	C18-C19-C20-C21
32	1	606	CLA	CHA-CBD-CGD-O1D
32	1	606	CLA	CHA-CBD-CGD-O2D
32	2	606	CLA	CHA-CBD-CGD-O1D
32	2	606	CLA	CHA-CBD-CGD-O2D
32	3	603	CLA	CHA-CBD-CGD-O1D
32	3	603	CLA	CHA-CBD-CGD-O2D
32	3	605	CLA	CHA-CBD-CGD-O1D
32	3	605	CLA	CHA-CBD-CGD-O2D
32	3	611	CLA	CHA-CBD-CGD-O1D
32	3	611	CLA	CHA-CBD-CGD-O2D
32	4	612	CLA	CHA-CBD-CGD-O1D
32	4	612	CLA	CHA-CBD-CGD-O2D
32	5	304	CLA	CAD-CBD-CGD-O1D
32	5	307	CLA	CHA-CBD-CGD-O1D
32	5	313	CLA	CHA-CBD-CGD-O1D
32	6	611	CLA	CHA-CBD-CGD-O1D
32	S	302	CLA	CHA-CBD-CGD-O1D
32	S	302	CLA	CHA-CBD-CGD-O2D
32	b	606	CLA	CAD-CBD-CGD-O1D
32	b	610	CLA	CAD-CBD-CGD-O1D
32	c	502	CLA	CAD-CBD-CGD-O1D
32	c	506	CLA	CAD-CBD-CGD-O1D
32	c	507	CLA	CHA-CBD-CGD-O1D
32	c	510	CLA	CHA-CBD-CGD-O1D
32	c	510	CLA	CHA-CBD-CGD-O2D
32	0	612	CLA	CHA-CBD-CGD-O1D
32	0	612	CLA	CHA-CBD-CGD-O2D
32	7	606	CLA	CHA-CBD-CGD-O1D
32	7	606	CLA	CHA-CBD-CGD-O2D
32	8	606	CLA	CHA-CBD-CGD-O1D
32	8	606	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	9	603	CLA	CHA-CBD-CGD-O1D
32	9	603	CLA	CHA-CBD-CGD-O2D
32	9	605	CLA	CHA-CBD-CGD-O1D
32	9	605	CLA	CHA-CBD-CGD-O2D
32	9	611	CLA	CHA-CBD-CGD-O1D
32	9	611	CLA	CHA-CBD-CGD-O2D
32	C	502	CLA	CAD-CBD-CGD-O1D
32	C	506	CLA	CAD-CBD-CGD-O1D
32	C	507	CLA	CHA-CBD-CGD-O1D
32	C	510	CLA	CHA-CBD-CGD-O1D
32	C	510	CLA	CHA-CBD-CGD-O2D
32	p	304	CLA	CAD-CBD-CGD-O1D
32	p	307	CLA	CHA-CBD-CGD-O1D
32	p	313	CLA	CHA-CBD-CGD-O1D
32	s	302	CLA	CHA-CBD-CGD-O1D
32	s	302	CLA	CHA-CBD-CGD-O2D
32	B	606	CLA	CAD-CBD-CGD-O1D
32	B	610	CLA	CAD-CBD-CGD-O1D
33	1	610	KC2	CHA-CBD-CGD-O1D
33	4	610	KC2	CHA-CBD-CGD-O2D
33	6	609	KC2	CHA-CBD-CGD-O2D
33	0	610	KC2	CHA-CBD-CGD-O2D
33	7	610	KC2	CHA-CBD-CGD-O1D
33	P	605	KC2	CHA-CBD-CGD-O1D
33	P	609	KC2	CHA-CBD-CGD-O2D
34	p	315	II0	C25-C29-C31-C33
38	2	618	LHG	C4-O6-P-O5
38	D	410	LHG	C4-O6-P-O3
38	D	410	LHG	C4-O6-P-O4
38	D	410	LHG	C4-O6-P-O5
38	S	301	LHG	C4-O6-P-O5
38	b	619	LHG	C3-O3-P-O5
38	d	411	LHG	C4-O6-P-O3
38	d	411	LHG	C4-O6-P-O4
38	d	411	LHG	C4-O6-P-O5
38	8	618	LHG	C4-O6-P-O5
38	s	301	LHG	C4-O6-P-O5
38	B	619	LHG	C3-O3-P-O5
32	C	511	CLA	C3-C5-C6-C7
45	c	516	DGD	C2A-C3A-C4A-C5A
45	C	516	DGD	C2A-C3A-C4A-C5A
37	D	411	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
38	B	621	LHG	C27-C28-C29-C30
31	A	610	8CT	C04-C03-C10-C11
31	K	101	8CT	C04-C03-C10-C11
31	k	102	8CT	C04-C03-C10-C11
32	1	605	CLA	C2B-C3B-CAB-CBB
32	3	604	CLA	C2B-C3B-CAB-CBB
32	3	608	CLA	C2B-C3B-CAB-CBB
32	4	606	CLA	C2B-C3B-CAB-CBB
32	4	611	CLA	C2B-C3B-CAB-CBB
32	5	304	CLA	C2B-C3B-CAB-CBB
32	5	305	CLA	C2B-C3B-CAB-CBB
32	6	604	CLA	C2B-C3B-CAB-CBB
32	6	608	CLA	C2B-C3B-CAB-CBB
32	6	610	CLA	C2B-C3B-CAB-CBB
32	c	502	CLA	C2B-C3B-CAB-CBB
32	g	102	CLA	C2B-C3B-CAB-CBB
32	0	606	CLA	C2B-C3B-CAB-CBB
32	0	611	CLA	C2B-C3B-CAB-CBB
32	7	605	CLA	C2B-C3B-CAB-CBB
32	9	608	CLA	C2B-C3B-CAB-CBB
32	C	502	CLA	C2B-C3B-CAB-CBB
32	G	101	CLA	C2B-C3B-CAB-CBB
32	P	604	CLA	C2B-C3B-CAB-CBB
32	P	608	CLA	C2B-C3B-CAB-CBB
32	P	610	CLA	C2B-C3B-CAB-CBB
32	p	304	CLA	C2B-C3B-CAB-CBB
32	p	306	CLA	C2B-C3B-CAB-CBB
37	c	517	LMG	C35-C36-C37-C38
37	d	401	LMG	C33-C34-C35-C36
38	b	621	LHG	C27-C28-C29-C30
45	H	101	DGD	O2G-C1B-C2B-C3B
45	h	101	DGD	O2G-C1B-C2B-C3B
32	C	503	CLA	C2-C3-C5-C6
31	M	201	8CT	C27-C26-C28-C29
31	B	622	8CT	C27-C26-C28-C29
34	5	316	II0	C31-C33-C35-C37
45	c	514	DGD	C4D-C5D-C6D-O5D
45	C	514	DGD	C4D-C5D-C6D-O5D
38	l	102	LHG	C15-C16-C17-C18
45	c	515	DGD	C2A-C3A-C4A-C5A
32	4	604	CLA	C6-C7-C8-C10
37	B	618	LMG	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
41	d	410	PHO	C3-C5-C6-C7
37	D	407	LMG	C34-C35-C36-C37
38	L	101	LHG	C15-C16-C17-C18
32	b	603	CLA	C15-C16-C17-C18
37	d	406	LMG	C34-C35-C36-C37
45	C	515	DGD	C2A-C3A-C4A-C5A
45	H	101	DGD	CDA-CEA-CFA-CGA
31	B	622	8CT	C23-C24-C25-C26
32	5	303	CLA	C11-C12-C13-C14
32	B	606	CLA	C15-C16-C17-C18
32	D	403	CLA	C11-C12-C13-C15
32	d	402	CLA	C11-C12-C13-C15
45	h	101	DGD	CDA-CEA-CFA-CGA
38	A	613	LHG	O6-C4-C5-C6
45	H	101	DGD	C9B-CAB-CBB-CCB
32	2	605	CLA	CBA-CGA-O2A-C1
45	H	101	DGD	C4D-C5D-C6D-O5D
32	b	606	CLA	C15-C16-C17-C18
32	c	502	CLA	C14-C13-C15-C16
32	8	602	CLA	C11-C10-C8-C9
38	S	301	LHG	C32-C33-C34-C35
32	b	613	CLA	C6-C7-C8-C10
32	s	303	CLA	C12-C13-C15-C16
32	B	613	CLA	C6-C7-C8-C10
38	s	301	LHG	C32-C33-C34-C35
38	L	101	LHG	C27-C28-C29-C30
38	a	402	LHG	C28-C29-C30-C31
39	b	620	SQD	C32-C33-C34-C35
39	B	620	SQD	C32-C33-C34-C35
45	H	101	DGD	C6B-C7B-C8B-C9B
45	h	101	DGD	C4D-C5D-C6D-O5D
32	2	605	CLA	O1A-CGA-O2A-C1
32	B	607	CLA	O1D-CGD-O2D-CED
38	l	102	LHG	C27-C28-C29-C30
45	h	101	DGD	C6B-C7B-C8B-C9B
32	1	602	CLA	C2-C3-C5-C6
32	c	507	CLA	C2-C3-C5-C6
32	C	507	CLA	C2-C3-C5-C6
38	A	612	LHG	C28-C29-C30-C31
38	S	301	LHG	C24-C23-O8-C6
43	A	609	PL9	C7-C8-C9-C11
38	A	613	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
45	c	516	DGD	O1G-C1G-C2G-O2G
45	c	516	DGD	O2G-C2G-C3G-O3G
45	C	516	DGD	O1G-C1G-C2G-O2G
45	c	515	DGD	C6B-C7B-C8B-C9B
32	3	605	CLA	CAA-CBA-CGA-O2A
38	b	619	LHG	C25-C26-C27-C28
38	B	619	LHG	C28-C29-C30-C31
32	9	602	CLA	C4-C3-C5-C6
39	A	606	SQD	O48-C23-C24-C25
32	4	606	CLA	CBD-CGD-O2D-CED
37	L	102	LMG	O1-C7-C8-C9
45	h	101	DGD	C9B-CAB-CBB-CCB
38	b	619	LHG	C28-C29-C30-C31
32	9	605	CLA	CAA-CBA-CGA-O2A
39	a	409	SQD	O48-C23-C24-C25
34	5	314	II0	C32-C34-C36-C38
37	B	618	LMG	C13-C14-C15-C16
37	b	618	LMG	C13-C14-C15-C16
32	c	501	CLA	C16-C17-C18-C20
32	C	501	CLA	C16-C17-C18-C20
38	A	613	LHG	C31-C32-C33-C34
32	8	605	CLA	CBA-CGA-O2A-C1
39	5	318	SQD	C45-C44-O6-C1
32	1	604	CLA	C2A-CAA-CBA-CGA
32	3	607	CLA	C2A-CAA-CBA-CGA
32	7	604	CLA	C2A-CAA-CBA-CGA
32	9	607	CLA	C2A-CAA-CBA-CGA
31	6	615	8CT	C18-C19-C20-C21
31	c	518	8CT	C16-C17-C18-C19
31	C	518	8CT	C16-C17-C18-C19
45	c	515	DGD	C7B-C8B-C9B-CAB
45	C	515	DGD	C7B-C8B-C9B-CAB
32	3	602	CLA	C4-C3-C5-C6
32	c	503	CLA	C2-C3-C5-C6
41	A	604	PHO	C2-C3-C5-C6
41	a	407	PHO	C2-C3-C5-C6
34	1	616	II0	C10-C22-C24-C26
34	3	612	II0	C10-C22-C24-C26
34	4	619	II0	C09-C21-C23-C25
34	9	612	II0	C10-C22-C24-C26
35	P	613	II3	C16-C23-C27-C28
36	1	618	IHT	C11-C21-C24-C26

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Mol	Chain	Res	Type	Atoms
32	0	606	CLA	O1D-CGD-O2D-CED
32	b	615	CLA	C16-C17-C18-C20
32	0	604	CLA	C6-C7-C8-C10
32	B	603	CLA	C16-C17-C18-C20
32	B	615	CLA	C16-C17-C18-C20
32	2	602	CLA	C11-C10-C8-C9
32	D	403	CLA	C11-C10-C8-C9
32	d	402	CLA	C11-C10-C8-C9
32	9	609	CLA	C11-C10-C8-C9
45	C	515	DGD	C6B-C7B-C8B-C9B
37	P	616	LMG	C29-C28-O8-C9
32	1	613	CLA	C4B-C3B-CAB-CBB
32	4	604	CLA	C4B-C3B-CAB-CBB
32	5	312	CLA	C4B-C3B-CAB-CBB
32	5	313	CLA	C4B-C3B-CAB-CBB
32	6	607	CLA	C4B-C3B-CAB-CBB
32	b	610	CLA	C4B-C3B-CAB-CBB
32	c	512	CLA	C4B-C3B-CAB-CBB
32	0	602	CLA	C4B-C3B-CAB-CBB
32	7	613	CLA	C4B-C3B-CAB-CBB
32	P	607	CLA	C4B-C3B-CAB-CBB
32	p	312	CLA	C4B-C3B-CAB-CBB
32	B	610	CLA	C4B-C3B-CAB-CBB
32	b	603	CLA	C16-C17-C18-C20
38	s	301	LHG	C24-C23-O8-C6
32	5	308	CLA	C2A-CAA-CBA-CGA
38	B	619	LHG	C25-C26-C27-C28
32	7	602	CLA	C2-C3-C5-C6
32	C	512	CLA	O2A-C1-C2-C3
45	c	514	DGD	O6D-C5D-C6D-O5D
45	C	514	DGD	O6D-C5D-C6D-O5D
45	a	414	DGD	C5A-C6A-C7A-C8A
32	8	605	CLA	O1A-CGA-O2A-C1
33	1	610	KC2	C4C-C3C-CAC-CBC
33	7	610	KC2	C4C-C3C-CAC-CBC
32	S	303	CLA	C12-C13-C15-C16
32	b	605	CLA	C11-C10-C8-C7
32	b	617	CLA	C6-C7-C8-C10
32	P	602	CLA	C6-C7-C8-C10
32	B	605	CLA	C11-C10-C8-C7
32	B	617	CLA	C6-C7-C8-C10
32	c	502	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
37	D	407	LMG	C33-C34-C35-C36
38	a	403	LHG	C34-C35-C36-C37
37	d	406	LMG	C33-C34-C35-C36
32	5	305	CLA	C3A-C2A-CAA-CBA
32	D	404	CLA	C3A-C2A-CAA-CBA
32	b	612	CLA	C3A-C2A-CAA-CBA
32	c	503	CLA	C3A-C2A-CAA-CBA
32	d	403	CLA	C3A-C2A-CAA-CBA
32	C	503	CLA	C3A-C2A-CAA-CBA
32	p	305	CLA	C3A-C2A-CAA-CBA
32	B	612	CLA	C3A-C2A-CAA-CBA
32	7	613	CLA	CAA-CBA-CGA-O1A
39	A	606	SQD	C34-C35-C36-C37
32	C	502	CLA	C10-C11-C12-C13
32	1	613	CLA	CAA-CBA-CGA-O1A
32	P	610	CLA	CAA-CBA-CGA-O2A
34	7	616	II0	C26-C30-C32-C34
36	1	618	IHT	C26-C29-C31-C34
32	c	503	CLA	C5-C6-C7-C8
32	C	503	CLA	C5-C6-C7-C8
32	4	606	CLA	O1D-CGD-O2D-CED
31	k	102	8CT	C20-C21-C23-C24
39	a	409	SQD	C34-C35-C36-C37
32	c	511	CLA	C4-C3-C5-C6
32	C	511	CLA	C4-C3-C5-C6
32	b	613	CLA	C2-C3-C5-C6
32	B	613	CLA	C2-C3-C5-C6
32	3	610	CLA	C2A-CAA-CBA-CGA
32	9	610	CLA	C2A-CAA-CBA-CGA
32	G	101	CLA	C2A-CAA-CBA-CGA
32	6	610	CLA	CAA-CBA-CGA-O2A
32	P	610	CLA	CAA-CBA-CGA-O1A
32	7	602	CLA	C3-C5-C6-C7
32	B	617	CLA	C8-C10-C11-C12
32	5	306	CLA	C6-C7-C8-C9
32	6	602	CLA	C6-C7-C8-C9
32	b	605	CLA	C11-C10-C8-C9
32	b	611	CLA	C11-C12-C13-C14
32	b	612	CLA	C6-C7-C8-C9
32	b	617	CLA	C14-C13-C15-C16
32	P	602	CLA	C6-C7-C8-C9
32	p	306	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	B	605	CLA	C11-C10-C8-C9
32	B	611	CLA	C11-C12-C13-C14
32	B	612	CLA	C6-C7-C8-C9
32	B	617	CLA	C14-C13-C15-C16
32	1	606	CLA	C4C-C3C-CAC-CBC
32	P	607	CLA	C11-C12-C13-C15
45	H	101	DGD	CCB-CDB-CEB-CFB
32	b	617	CLA	C8-C10-C11-C12
32	p	303	CLA	C11-C12-C13-C14
41	D	402	PHO	C1A-C2A-CAA-CBA
41	d	410	PHO	C1A-C2A-CAA-CBA
32	6	607	CLA	C11-C12-C13-C15
32	D	404	CLA	CBD-CGD-O2D-CED
32	d	403	CLA	CBD-CGD-O2D-CED
32	c	511	CLA	C2-C3-C5-C6
37	a	410	LMG	C16-C17-C18-C19
38	D	410	LHG	O1-C1-C2-O2
38	d	411	LHG	O1-C1-C2-O2
32	6	610	CLA	CAA-CBA-CGA-O1A
32	0	611	CLA	CAA-CBA-CGA-O1A
37	0	619	LMG	C29-C30-C31-C32
32	5	309	CLA	C2A-CAA-CBA-CGA
32	g	102	CLA	C2A-CAA-CBA-CGA
32	p	309	CLA	C2A-CAA-CBA-CGA
39	B	620	SQD	C26-C27-C28-C29
32	2	608	CLA	C1A-C2A-CAA-CBA
32	D	403	CLA	C1A-C2A-CAA-CBA
32	c	502	CLA	C1A-C2A-CAA-CBA
32	8	608	CLA	C1A-C2A-CAA-CBA
32	C	502	CLA	C1A-C2A-CAA-CBA
32	C	503	CLA	C1A-C2A-CAA-CBA
37	c	517	LMG	C36-C37-C38-C39
37	C	517	LMG	C36-C37-C38-C39
32	b	613	CLA	C16-C17-C18-C19
32	B	613	CLA	C16-C17-C18-C19
39	b	620	SQD	C26-C27-C28-C29
38	A	613	LHG	C34-C35-C36-C37
31	Z	101	8CT	C02-C03-C10-C11
31	z	101	8CT	C02-C03-C10-C11
32	1	606	CLA	C2B-C3B-CAB-CBB
32	2	601	CLA	C2B-C3B-CAB-CBB
32	2	603	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	2	607	CLA	C2B-C3B-CAB-CBB
32	3	610	CLA	C2B-C3B-CAB-CBB
32	4	602	CLA	C2B-C3B-CAB-CBB
32	4	604	CLA	C2B-C3B-CAB-CBB
32	4	605	CLA	C2B-C3B-CAB-CBB
32	5	306	CLA	C2B-C3B-CAB-CBB
32	5	309	CLA	C2B-C3B-CAB-CBB
32	5	312	CLA	C2B-C3B-CAB-CBB
32	5	313	CLA	C2B-C3B-CAB-CBB
32	6	606	CLA	C2B-C3B-CAB-CBB
32	6	607	CLA	C2B-C3B-CAB-CBB
32	6	611	CLA	C2B-C3B-CAB-CBB
32	A	603	CLA	C2B-C3B-CAB-CBB
32	c	512	CLA	C2B-C3B-CAB-CBB
32	0	602	CLA	C2B-C3B-CAB-CBB
32	0	604	CLA	C2B-C3B-CAB-CBB
32	0	605	CLA	C2B-C3B-CAB-CBB
32	8	601	CLA	C2B-C3B-CAB-CBB
32	8	603	CLA	C2B-C3B-CAB-CBB
32	9	604	CLA	C2B-C3B-CAB-CBB
32	9	610	CLA	C2B-C3B-CAB-CBB
32	C	512	CLA	C2B-C3B-CAB-CBB
32	P	602	CLA	C2B-C3B-CAB-CBB
32	P	606	CLA	C2B-C3B-CAB-CBB
32	P	607	CLA	C2B-C3B-CAB-CBB
32	P	611	CLA	C2B-C3B-CAB-CBB
32	a	406	CLA	C2B-C3B-CAB-CBB
32	p	312	CLA	C2B-C3B-CAB-CBB
36	4	614	IHT	C10-C07-C18-C22
36	0	614	IHT	C10-C07-C18-C22
38	D	410	LHG	O2-C2-C3-O3
38	d	411	LHG	O2-C2-C3-O3
32	1	606	CLA	C2C-C3C-CAC-CBC
37	g	101	LMG	C29-C28-O8-C9
37	A	607	LMG	C16-C17-C18-C19
32	c	511	CLA	C3-C5-C6-C7
32	4	611	CLA	CAA-CBA-CGA-O1A
32	b	603	CLA	O2A-C1-C2-C3
32	c	512	CLA	O2A-C1-C2-C3
32	B	603	CLA	O2A-C1-C2-C3
32	b	606	CLA	C6-C7-C8-C10
32	c	510	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
32	C	512	CLA	C11-C10-C8-C7
32	B	606	CLA	C6-C7-C8-C10
38	b	619	LHG	C15-C16-C17-C18
38	a	403	LHG	C9-C10-C11-C12
32	2	608	CLA	C2A-CAA-CBA-CGA
32	6	602	CLA	C2A-CAA-CBA-CGA
32	b	604	CLA	C2A-CAA-CBA-CGA
32	b	609	CLA	C2A-CAA-CBA-CGA
32	8	608	CLA	C2A-CAA-CBA-CGA
32	P	602	CLA	C2A-CAA-CBA-CGA
32	B	604	CLA	C2A-CAA-CBA-CGA
32	B	609	CLA	C2A-CAA-CBA-CGA
32	1	613	CLA	CAA-CBA-CGA-O2A
38	A	613	LHG	C9-C10-C11-C12
38	A	612	LHG	C12-C13-C14-C15
38	B	619	LHG	C15-C16-C17-C18
39	A	606	SQD	C25-C26-C27-C28
32	1	611	CLA	CAA-CBA-CGA-O2A
32	7	613	CLA	CAA-CBA-CGA-O2A
38	A	613	LHG	C33-C34-C35-C36
31	K	101	8CT	C22-C21-C23-C24
32	1	602	CLA	C11-C12-C13-C14
32	7	611	CLA	CAA-CBA-CGA-O2A
32	C	511	CLA	C2-C3-C5-C6
32	4	608	CLA	C10-C11-C12-C13
32	0	608	CLA	C10-C11-C12-C13
45	C	516	DGD	CAB-CBB-CCB-CDB
37	d	406	LMG	C11-C12-C13-C14
38	a	402	LHG	C12-C13-C14-C15
32	c	501	CLA	C15-C16-C17-C18
32	B	603	CLA	C16-C17-C18-C19
37	D	407	LMG	C11-C12-C13-C14
39	a	409	SQD	C25-C26-C27-C28
32	4	611	CLA	CAA-CBA-CGA-O2A
32	0	611	CLA	CAA-CBA-CGA-O2A
45	c	516	DGD	CAB-CBB-CCB-CDB
32	C	501	CLA	C15-C16-C17-C18
32	c	509	CLA	C13-C15-C16-C17
32	b	603	CLA	C16-C17-C18-C19
32	1	612	CLA	CAA-CBA-CGA-O2A
32	7	611	CLA	CAA-CBA-CGA-O1A
32	c	508	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	C	509	CLA	C13-C15-C16-C17
38	A	613	LHG	C7-C8-C9-C10
38	a	403	LHG	C7-C8-C9-C10
32	8	605	CLA	CAA-CBA-CGA-O2A
37	B	618	LMG	O1-C7-C8-C9
32	7	612	CLA	CAA-CBA-CGA-O2A
32	3	601	CLA	C1A-C2A-CAA-CBA
32	9	601	CLA	C1A-C2A-CAA-CBA
32	7	606	CLA	C4C-C3C-CAC-CBC
32	2	602	CLA	C2A-CAA-CBA-CGA
32	8	602	CLA	C2A-CAA-CBA-CGA
32	C	508	CLA	C8-C10-C11-C12
32	b	613	CLA	C16-C17-C18-C20
32	3	602	CLA	C11-C12-C13-C14
34	1	617	II0	C09-C21-C23-C25
34	1	619	II0	C09-C21-C23-C25
34	1	619	II0	C10-C22-C24-C26
34	2	619	II0	C09-C21-C23-C25
34	4	616	II0	C10-C22-C24-C26
34	0	615	II0	C09-C21-C23-C25
34	0	616	II0	C10-C22-C24-C26
34	7	617	II0	C09-C21-C23-C25
34	7	617	II0	C10-C22-C24-C26
34	9	614	II0	C10-C22-C24-C26
36	5	317	IHT	C11-C21-C24-C26
32	9	602	CLA	C11-C12-C13-C14
37	B	618	LMG	C38-C39-C40-C41
32	B	613	CLA	C16-C17-C18-C20
32	B	615	CLA	C16-C17-C18-C19
32	1	606	CLA	C4B-C3B-CAB-CBB
32	4	602	CLA	C4B-C3B-CAB-CBB
32	5	309	CLA	C4B-C3B-CAB-CBB
32	8	602	CLA	C4B-C3B-CAB-CBB
32	p	309	CLA	C4B-C3B-CAB-CBB
32	1	611	CLA	CAA-CBA-CGA-O1A
32	2	612	CLA	CAA-CBA-CGA-O2A
32	8	612	CLA	CAA-CBA-CGA-O2A
32	2	605	CLA	CAA-CBA-CGA-O2A
32	b	615	CLA	C16-C17-C18-C19
47	E	101	HEM	CAA-CBA-CGA-O2A
37	a	410	LMG	C37-C38-C39-C40
45	c	514	DGD	CCB-CDB-CEB-CFB

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Mol	Chain	Res	Type	Atoms
45	C	514	DGD	CCB-CDB-CEB-CFB
37	A	607	LMG	C37-C38-C39-C40
32	4	613	CLA	CAA-CBA-CGA-O2A
32	0	605	CLA	CAA-CBA-CGA-O2A
32	p	303	CLA	C8-C10-C11-C12
37	c	517	LMG	C14-C15-C16-C17
37	L	102	LMG	C29-C30-C31-C32
32	c	512	CLA	C11-C10-C8-C7
32	C	510	CLA	C11-C10-C8-C7
39	A	606	SQD	C33-C34-C35-C36
45	h	101	DGD	CCB-CDB-CEB-CFB
32	0	612	CLA	CAA-CBA-CGA-O2A
32	7	607	CLA	CAA-CBA-CGA-O2A
37	C	517	LMG	C28-C29-C30-C31
32	2	612	CLA	CAA-CBA-CGA-O1A
32	8	612	CLA	CAA-CBA-CGA-O1A
31	M	201	8CT	C25-C26-C28-C29
37	D	407	LMG	C8-C7-O1-C1
37	d	406	LMG	C8-C7-O1-C1
37	P	616	LMG	C8-C7-O1-C1
39	p	318	SQD	C45-C44-O6-C1
45	c	515	DGD	C2G-C3G-O3G-C1D
45	C	515	DGD	C2G-C3G-O3G-C1D
32	d	403	CLA	O1D-CGD-O2D-CED
37	a	410	LMG	C13-C14-C15-C16
32	1	607	CLA	CAA-CBA-CGA-O2A
32	p	308	CLA	CAA-CBA-CGA-O2A
32	C	512	CLA	C2-C3-C5-C6
32	b	611	CLA	C2-C1-O2A-CGA
32	B	611	CLA	C2-C1-O2A-CGA
37	A	607	LMG	C13-C14-C15-C16
37	c	517	LMG	C28-C29-C30-C31
32	4	604	CLA	C3A-C2A-CAA-CBA
32	b	609	CLA	C3A-C2A-CAA-CBA
32	0	604	CLA	C3A-C2A-CAA-CBA
32	B	609	CLA	C3A-C2A-CAA-CBA
32	4	606	CLA	CAA-CBA-CGA-O2A
32	7	606	CLA	CAA-CBA-CGA-O2A
32	c	501	CLA	C2-C3-C5-C6
32	C	501	CLA	C2-C3-C5-C6
37	L	102	LMG	C35-C36-C37-C38
32	4	612	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
32	D	404	CLA	O1D-CGD-O2D-CED
45	c	514	DGD	CBB-CCB-CDB-CEB
38	l	102	LHG	C11-C10-C9-C8
32	c	512	CLA	C2-C3-C5-C6
32	5	308	CLA	CAA-CBA-CGA-O2A
37	C	517	LMG	C14-C15-C16-C17
38	a	403	LHG	C33-C34-C35-C36
45	C	514	DGD	CBB-CCB-CDB-CEB
32	0	606	CLA	CAA-CBA-CGA-O2A
37	l	101	LMG	C35-C36-C37-C38
32	1	607	CLA	CAA-CBA-CGA-O1A
32	4	613	CLA	CAA-CBA-CGA-O1A
32	0	613	CLA	CAA-CBA-CGA-O2A
38	a	403	LHG	C1-C2-C3-O3
38	L	101	LHG	C11-C10-C9-C8
32	1	612	CLA	CAA-CBA-CGA-O1A
32	5	308	CLA	CAA-CBA-CGA-O1A
32	7	607	CLA	CAA-CBA-CGA-O1A
32	7	612	CLA	CAA-CBA-CGA-O1A
37	b	618	LMG	O1-C7-C8-C9
37	l	101	LMG	O1-C7-C8-C9
32	4	612	CLA	CAA-CBA-CGA-O1A
32	p	308	CLA	CAA-CBA-CGA-O1A
32	p	308	CLA	C2A-CAA-CBA-CGA
31	9	615	8CT	C23-C24-C25-C26
34	1	616	II0	C26-C30-C32-C34
32	4	606	CLA	CAA-CBA-CGA-O1A
47	E	101	HEM	CAA-CBA-CGA-O1A
37	4	618	LMG	C28-C29-C30-C31
32	0	606	CLA	CAA-CBA-CGA-O1A
32	0	612	CLA	CAA-CBA-CGA-O1A
32	3	609	CLA	C11-C10-C8-C9
32	b	613	CLA	C6-C7-C8-C9
32	b	616	CLA	C14-C13-C15-C16
32	c	505	CLA	C6-C7-C8-C9
32	c	508	CLA	C14-C13-C15-C16
32	C	505	CLA	C6-C7-C8-C9
32	C	508	CLA	C14-C13-C15-C16
32	B	613	CLA	C6-C7-C8-C9
32	B	616	CLA	C14-C13-C15-C16
32	6	607	CLA	C11-C12-C13-C14
32	P	607	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	0	613	CLA	CAA-CBA-CGA-O1A
31	B	622	8CT	C25-C26-C28-C29
34	5	314	II0	C32-C34-C36-C40
34	5	316	II0	C31-C33-C35-C39
32	2	611	CLA	C2A-CAA-CBA-CGA
32	8	611	CLA	C2A-CAA-CBA-CGA
32	6	602	CLA	C6-C7-C8-C10
32	b	606	CLA	C12-C13-C15-C16
32	9	602	CLA	C11-C10-C8-C7
32	B	606	CLA	C12-C13-C15-C16
32	7	604	CLA	C3-C5-C6-C7
32	7	606	CLA	C2C-C3C-CAC-CBC
31	b	623	8CT	C04-C03-C10-C11
31	c	518	8CT	C04-C03-C10-C11
31	C	518	8CT	C04-C03-C10-C11
31	B	624	8CT	C04-C03-C10-C11
32	1	603	CLA	C2B-C3B-CAB-CBB
32	1	611	CLA	C2B-C3B-CAB-CBB
32	1	613	CLA	C2B-C3B-CAB-CBB
32	2	608	CLA	C2B-C3B-CAB-CBB
32	2	612	CLA	C2B-C3B-CAB-CBB
32	3	611	CLA	C2B-C3B-CAB-CBB
32	4	608	CLA	C2B-C3B-CAB-CBB
32	6	602	CLA	C2B-C3B-CAB-CBB
32	D	404	CLA	C2B-C3B-CAB-CBB
32	b	610	CLA	C2B-C3B-CAB-CBB
32	b	617	CLA	C2B-C3B-CAB-CBB
32	c	503	CLA	C2B-C3B-CAB-CBB
32	0	608	CLA	C2B-C3B-CAB-CBB
32	7	606	CLA	C2B-C3B-CAB-CBB
32	7	611	CLA	C2B-C3B-CAB-CBB
32	7	613	CLA	C2B-C3B-CAB-CBB
32	8	607	CLA	C2B-C3B-CAB-CBB
32	8	608	CLA	C2B-C3B-CAB-CBB
32	8	612	CLA	C2B-C3B-CAB-CBB
32	9	611	CLA	C2B-C3B-CAB-CBB
32	p	309	CLA	C2B-C3B-CAB-CBB
32	p	313	CLA	C2B-C3B-CAB-CBB
32	B	610	CLA	C2B-C3B-CAB-CBB
32	B	617	CLA	C2B-C3B-CAB-CBB
39	p	318	SQD	O48-C23-C24-C25
32	8	605	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
45	H	101	DGD	CCA-CDA-CEA-CFA
37	l	101	LMG	C14-C15-C16-C17
45	h	101	DGD	CCA-CDA-CEA-CFA
32	d	402	CLA	CAA-CBA-CGA-O2A
37	G	102	LMG	O6-C1-O1-C7
37	b	618	LMG	C38-C39-C40-C41
39	a	409	SQD	C19-C20-C21-C22
32	4	605	CLA	CAA-CBA-CGA-O2A
39	A	606	SQD	O47-C7-C8-C9
45	A	614	DGD	O2G-C1B-C2B-C3B
43	D	405	PL9	C13-C14-C16-C17
43	d	404	PL9	C13-C14-C16-C17
32	7	606	CLA	CAA-CBA-CGA-O1A
45	c	515	DGD	O1B-C1B-O2G-C2G
45	C	515	DGD	O1B-C1B-O2G-C2G
32	1	608	CLA	C2A-CAA-CBA-CGA
32	7	602	CLA	C2A-CAA-CBA-CGA
32	7	608	CLA	C2A-CAA-CBA-CGA
37	G	102	LMG	C11-C10-O7-C8
39	A	606	SQD	C19-C20-C21-C22
39	p	318	SQD	C13-C14-C15-C16
32	1	606	CLA	CAA-CBA-CGA-O2A
32	c	501	CLA	CAA-CBA-CGA-O2A
32	C	510	CLA	CAA-CBA-CGA-O2A
39	5	318	SQD	C12-C13-C14-C15
32	5	305	CLA	CAA-CBA-CGA-O2A
32	b	614	CLA	CAA-CBA-CGA-O2A
32	c	510	CLA	CAA-CBA-CGA-O2A
32	C	501	CLA	CAA-CBA-CGA-O2A
32	B	614	CLA	CAA-CBA-CGA-O2A
45	a	414	DGD	O2G-C1B-C2B-C3B
39	a	409	SQD	C33-C34-C35-C36
47	f	101	HEM	CAA-CBA-CGA-O2A
32	p	305	CLA	CAA-CBA-CGA-O2A
39	a	409	SQD	O47-C7-C8-C9
32	3	602	CLA	C2-C3-C5-C6
32	9	602	CLA	C2-C3-C5-C6
45	C	515	DGD	C5A-C6A-C7A-C8A
32	4	607	CLA	CAA-CBA-CGA-O2A
32	6	611	CLA	CAA-CBA-CGA-O2A
32	8	606	CLA	CAA-CBA-CGA-O2A
45	c	515	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
39	b	620	SQD	O47-C7-C8-C9
38	d	405	LHG	C16-C17-C18-C19
39	p	318	SQD	C12-C13-C14-C15
34	3	614	II0	C09-C21-C23-C25
34	3	614	II0	C10-C22-C24-C26
32	5	313	CLA	CAA-CBA-CGA-O2A
32	c	510	CLA	C11-C10-C8-C9
32	C	510	CLA	C11-C10-C8-C9
32	C	512	CLA	C11-C10-C8-C9
32	4	604	CLA	CAA-CBA-CGA-O2A
32	S	303	CLA	CAA-CBA-CGA-O2A
32	p	306	CLA	CAA-CBA-CGA-O2A
32	s	303	CLA	CAA-CBA-CGA-O2A
45	H	101	DGD	CBB-CCB-CDB-CEB
38	2	618	LHG	O6-C4-C5-O7
32	4	608	CLA	C4B-C3B-CAB-CBB
32	5	309	CLA	C1A-C2A-CAA-CBA
32	D	404	CLA	C1A-C2A-CAA-CBA
32	b	604	CLA	C4B-C3B-CAB-CBB
32	b	611	CLA	C4B-C3B-CAB-CBB
32	b	612	CLA	C1A-C2A-CAA-CBA
32	c	503	CLA	C4B-C3B-CAB-CBB
32	d	403	CLA	C1A-C2A-CAA-CBA
32	0	608	CLA	C4B-C3B-CAB-CBB
32	C	503	CLA	C4B-C3B-CAB-CBB
32	p	309	CLA	C1A-C2A-CAA-CBA
32	B	604	CLA	C4B-C3B-CAB-CBB
32	B	611	CLA	C4B-C3B-CAB-CBB
32	B	612	CLA	C1A-C2A-CAA-CBA
32	P	611	CLA	CAA-CBA-CGA-O1A
37	4	618	LMG	C29-C30-C31-C32
38	D	406	LHG	C16-C17-C18-C19
32	5	306	CLA	CAA-CBA-CGA-O2A
32	B	603	CLA	CAA-CBA-CGA-O2A
37	l	101	LMG	O7-C10-C11-C12
37	G	102	LMG	O8-C28-C29-C30
39	b	620	SQD	O47-C45-C46-O48
39	B	620	SQD	O47-C45-C46-O48
31	3	615	8CT	C23-C24-C25-C26
31	D	409	8CT	C16-C17-C18-C19
31	d	408	8CT	C16-C17-C18-C19
34	9	612	II0	C26-C30-C32-C34

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Mol	Chain	Res	Type	Atoms
32	2	606	CLA	CAA-CBA-CGA-O2A
32	6	611	CLA	CAA-CBA-CGA-O1A
32	6	604	CLA	CAA-CBA-CGA-O2A
37	g	101	LMG	O8-C28-C29-C30
32	3	602	CLA	C2A-CAA-CBA-CGA
32	9	602	CLA	C2A-CAA-CBA-CGA
32	b	603	CLA	CAA-CBA-CGA-O2A
32	c	503	CLA	CAA-CBA-CGA-O2A
32	0	604	CLA	CAA-CBA-CGA-O2A
39	B	620	SQD	O47-C7-C8-C9
39	A	606	SQD	C17-C18-C19-C20
39	5	318	SQD	C13-C14-C15-C16
38	A	613	LHG	C1-C2-C3-O3
39	A	606	SQD	C5-C6-S-O9
39	a	409	SQD	C5-C6-S-O9
37	d	406	LMG	C28-C29-C30-C31
39	a	409	SQD	C17-C18-C19-C20
32	1	603	CLA	C2-C1-O2A-CGA
32	5	304	CLA	C2-C1-O2A-CGA
32	D	403	CLA	C2-C1-O2A-CGA
32	d	402	CLA	C2-C1-O2A-CGA
32	7	603	CLA	C2-C1-O2A-CGA
32	p	304	CLA	C2-C1-O2A-CGA
32	D	403	CLA	CAA-CBA-CGA-O2A
32	C	503	CLA	CAA-CBA-CGA-O2A
32	3	602	CLA	C11-C10-C8-C7
38	D	410	LHG	C24-C23-O8-C6
38	l	102	LHG	C17-C18-C19-C20
32	P	611	CLA	CAA-CBA-CGA-O2A
37	D	407	LMG	C28-C29-C30-C31
37	b	618	LMG	C12-C13-C14-C15
38	D	406	LHG	O8-C23-C24-C25
38	S	301	LHG	C29-C30-C31-C32
38	s	301	LHG	C29-C30-C31-C32
32	6	607	CLA	C2A-CAA-CBA-CGA
32	P	607	CLA	C2A-CAA-CBA-CGA
32	p	313	CLA	CAA-CBA-CGA-O2A
45	c	515	DGD	C8B-C9B-CAB-CBB
39	5	318	SQD	O48-C23-C24-C25
32	b	614	CLA	C5-C6-C7-C8
32	P	604	CLA	CAA-CBA-CGA-O2A
38	d	405	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
45	h	101	DGD	CBB-CCB-CDB-CEB
32	B	614	CLA	C5-C6-C7-C8
37	4	618	LMG	C15-C16-C17-C18
37	D	411	LMG	O10-C28-C29-C30
32	b	614	CLA	C16-C17-C18-C20
32	B	614	CLA	C16-C17-C18-C20
38	L	101	LHG	C17-C18-C19-C20
47	f	101	HEM	CAA-CBA-CGA-O1A
37	d	401	LMG	O10-C28-C29-C30
37	B	618	LMG	C12-C13-C14-C15
45	C	515	DGD	C8B-C9B-CAB-CBB
37	0	619	LMG	C15-C16-C17-C18
32	1	606	CLA	CAA-CBA-CGA-O1A
38	b	621	LHG	C24-C25-C26-C27
38	B	621	LHG	C24-C25-C26-C27
38	d	411	LHG	C24-C23-O8-C6
32	c	509	CLA	C11-C10-C8-C9
32	c	512	CLA	C11-C10-C8-C9
32	C	509	CLA	C11-C10-C8-C9
32	b	614	CLA	CAA-CBA-CGA-O1A
32	c	501	CLA	CAA-CBA-CGA-O1A
32	B	614	CLA	CAA-CBA-CGA-O1A
38	D	406	LHG	O9-C7-C8-C9
34	3	612	II0	C26-C30-C32-C34
32	8	606	CLA	CAA-CBA-CGA-O1A
32	b	612	CLA	C15-C16-C17-C18
32	B	612	CLA	C15-C16-C17-C18
32	C	501	CLA	CAA-CBA-CGA-O1A
38	d	405	LHG	O9-C7-C8-C9
33	2	610	KC2	C1A-C2A-CAA-CBA
33	5	311	KC2	C3A-C2A-CAA-CBA
33	8	610	KC2	C1A-C2A-CAA-CBA
32	b	603	CLA	O1A-CGA-O2A-C1
32	5	313	CLA	CAA-CBA-CGA-O1A
32	p	307	CLA	CAA-CBA-CGA-O2A
39	b	620	SQD	C31-C32-C33-C34
32	5	306	CLA	CAA-CBA-CGA-O1A
32	S	303	CLA	CAA-CBA-CGA-O1A
32	b	603	CLA	CAA-CBA-CGA-O1A
32	C	510	CLA	CAA-CBA-CGA-O1A
32	1	604	CLA	C3-C5-C6-C7
39	B	620	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
32	B	603	CLA	O1A-CGA-O2A-C1
32	4	607	CLA	CAA-CBA-CGA-O1A
32	5	307	CLA	CAA-CBA-CGA-O2A
32	d	402	CLA	CAA-CBA-CGA-O1A
32	B	603	CLA	CAA-CBA-CGA-O1A
37	6	616	LMG	C8-C7-O1-C1
37	g	101	LMG	C8-C7-O1-C1
45	c	514	DGD	C5D-C6D-O5D-C1E
45	C	514	DGD	C5D-C6D-O5D-C1E
37	L	102	LMG	O1-C7-C8-O7
37	B	618	LMG	O1-C7-C8-O7
32	D	403	CLA	CAA-CBA-CGA-O1A
32	s	303	CLA	CAA-CBA-CGA-O1A
37	2	617	LMG	O9-C10-C11-C12
32	c	505	CLA	C10-C11-C12-C13
32	1	602	CLA	C2A-CAA-CBA-CGA
38	l	102	LHG	C26-C27-C28-C29
32	4	604	CLA	CAA-CBA-CGA-O1A
32	p	306	CLA	CAA-CBA-CGA-O1A
37	8	617	LMG	O9-C10-C11-C12
39	A	606	SQD	O49-C7-C8-C9
39	a	409	SQD	O49-C7-C8-C9
32	b	603	CLA	C13-C15-C16-C17
32	C	505	CLA	C10-C11-C12-C13
38	D	410	LHG	C2-C3-O3-P
38	d	411	LHG	C2-C3-O3-P
32	1	604	CLA	CAA-CBA-CGA-O2A
32	2	604	CLA	CAA-CBA-CGA-O2A
32	7	604	CLA	CAA-CBA-CGA-O2A
32	p	313	CLA	CAA-CBA-CGA-O1A
32	c	510	CLA	CAA-CBA-CGA-O1A
32	0	604	CLA	CAA-CBA-CGA-O1A
32	1	605	CLA	CAD-CBD-CGD-O2D
32	4	613	CLA	CAD-CBD-CGD-O2D
32	b	608	CLA	CAD-CBD-CGD-O2D
32	0	613	CLA	CAD-CBD-CGD-O2D
41	A	604	PHO	CAD-CBD-CGD-O2D
41	a	407	PHO	CAD-CBD-CGD-O2D
32	3	604	CLA	CAA-CBA-CGA-O2A
32	8	604	CLA	CAA-CBA-CGA-O2A
32	2	606	CLA	CAA-CBA-CGA-O1A
32	2	605	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
32	5	306	CLA	C2-C1-O2A-CGA
32	c	504	CLA	C2-C1-O2A-CGA
32	C	504	CLA	C2-C1-O2A-CGA
32	6	604	CLA	CAA-CBA-CGA-O1A
37	d	401	LMG	O8-C28-C29-C30
37	L	102	LMG	O7-C10-C11-C12
38	L	101	LHG	C26-C27-C28-C29
32	S	302	CLA	CAA-CBA-CGA-O2A
32	5	305	CLA	CAA-CBA-CGA-O1A
32	p	305	CLA	CAA-CBA-CGA-O1A
32	B	603	CLA	C13-C15-C16-C17
32	b	613	CLA	CAA-CBA-CGA-O2A
32	c	513	CLA	CAA-CBA-CGA-O2A
32	9	604	CLA	CAA-CBA-CGA-O2A
32	C	513	CLA	CAA-CBA-CGA-O2A
32	B	613	CLA	CAA-CBA-CGA-O2A
37	D	411	LMG	O8-C28-C29-C30
32	P	604	CLA	CAA-CBA-CGA-O1A
37	4	618	LMG	O10-C28-C29-C30
45	c	516	DGD	C4B-C5B-C6B-C7B
32	c	503	CLA	CAA-CBA-CGA-O1A
38	S	301	LHG	O10-C23-C24-C25
39	b	620	SQD	O49-C7-C8-C9

There are no ring outliers.

202 monomers are involved in 390 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	L	101	LHG	2	0
37	c	517	LMG	3	0
32	c	502	CLA	1	0
32	B	610	CLA	3	0
32	7	607	CLA	2	0
32	d	403	CLA	1	0
32	1	612	CLA	2	0
32	P	611	CLA	1	0
32	c	505	CLA	3	0
38	d	405	LHG	1	0
32	4	613	CLA	1	0
47	v	201	HEM	3	0
45	H	101	DGD	6	0
32	0	608	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	a	402	LHG	4	0
32	p	304	CLA	1	0
32	B	603	CLA	4	0
32	c	501	CLA	1	0
32	g	102	CLA	2	0
32	4	607	CLA	4	0
32	5	304	CLA	1	0
32	c	506	CLA	1	0
32	0	603	CLA	1	0
32	1	603	CLA	1	0
45	c	514	DGD	1	0
32	2	605	CLA	2	0
32	c	507	CLA	1	0
32	B	609	CLA	4	0
38	l	102	LHG	2	0
32	4	604	CLA	1	0
32	8	603	CLA	2	0
32	7	603	CLA	1	0
32	8	607	CLA	1	0
39	A	606	SQD	5	0
32	b	611	CLA	2	0
32	8	608	CLA	3	0
32	b	614	CLA	1	0
32	s	303	CLA	1	0
38	D	406	LHG	1	0
32	0	601	CLA	1	0
47	E	101	HEM	2	0
32	B	613	CLA	2	0
32	4	606	CLA	1	0
32	8	609	CLA	1	0
32	C	501	CLA	1	0
38	a	403	LHG	6	0
32	C	502	CLA	2	0
32	C	504	CLA	4	0
32	P	607	CLA	1	0
32	7	612	CLA	2	0
32	p	305	CLA	2	0
32	p	308	CLA	1	0
34	0	616	II0	1	0
32	b	615	CLA	1	0
39	p	318	SQD	3	0
32	D	404	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1	607	CLA	3	0
32	3	607	CLA	3	0
41	a	407	PHO	1	0
32	S	303	CLA	1	0
32	C	505	CLA	2	0
45	c	515	DGD	4	0
36	1	618	IHT	1	0
32	a	406	CLA	3	0
32	3	606	CLA	2	0
32	B	612	CLA	3	0
34	7	614	II0	1	0
32	0	602	CLA	3	0
32	2	603	CLA	2	0
37	A	607	LMG	2	0
32	2	609	CLA	1	0
32	C	506	CLA	1	0
32	5	307	CLA	2	0
32	P	610	CLA	1	0
32	4	612	CLA	1	0
32	4	602	CLA	3	0
32	3	609	CLA	3	0
32	B	616	CLA	3	0
37	2	617	LMG	1	0
32	8	605	CLA	1	0
32	B	617	CLA	4	0
32	P	604	CLA	1	0
47	f	101	HEM	3	0
32	p	303	CLA	2	0
32	C	503	CLA	4	0
37	D	411	LMG	1	0
32	9	602	CLA	1	0
32	b	616	CLA	2	0
31	Z	101	8CT	1	0
32	S	302	CLA	4	0
32	4	608	CLA	3	0
32	7	605	CLA	2	0
45	C	514	DGD	2	0
32	P	602	CLA	3	0
32	b	604	CLA	2	0
32	9	606	CLA	2	0
41	d	410	PHO	3	0
32	C	507	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	C	516	DGD	5	0
32	b	607	CLA	2	0
45	C	515	DGD	4	0
32	b	605	CLA	3	0
32	b	606	CLA	4	0
32	C	512	CLA	1	0
32	G	101	CLA	1	0
32	6	610	CLA	1	0
32	p	306	CLA	1	0
39	B	620	SQD	1	0
32	c	510	CLA	2	0
32	C	509	CLA	1	0
34	1	614	II0	1	0
32	5	306	CLA	2	0
38	b	621	LHG	3	0
32	C	508	CLA	1	0
45	A	614	DGD	1	0
32	a	408	CLA	2	0
32	9	609	CLA	3	0
32	b	610	CLA	2	0
34	4	616	II0	1	0
37	a	410	LMG	3	0
32	1	602	CLA	4	0
32	B	615	CLA	1	0
32	9	607	CLA	4	0
32	c	512	CLA	2	0
39	b	601	SQD	1	0
32	b	603	CLA	4	0
32	4	603	CLA	2	0
32	0	607	CLA	4	0
32	D	403	CLA	3	0
32	3	604	CLA	1	0
32	c	509	CLA	1	0
32	0	613	CLA	1	0
32	9	604	CLA	1	0
32	6	602	CLA	3	0
38	A	612	LHG	5	0
32	1	606	CLA	3	0
32	0	604	CLA	1	0
32	a	405	CLA	4	0
32	A	602	CLA	5	0
41	D	402	PHO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	B	604	CLA	2	0
32	c	504	CLA	4	0
31	z	101	8CT	1	0
45	a	414	DGD	1	0
32	B	607	CLA	3	0
32	5	305	CLA	2	0
32	c	513	CLA	2	0
32	7	606	CLA	2	0
32	b	612	CLA	3	0
32	5	303	CLA	2	0
32	C	511	CLA	3	0
32	4	601	CLA	1	0
33	P	605	KC2	3	0
32	7	608	CLA	1	0
32	C	510	CLA	2	0
32	c	511	CLA	4	0
32	b	613	CLA	2	0
38	A	613	LHG	5	0
39	a	409	SQD	6	0
32	0	612	CLA	1	0
32	2	602	CLA	1	0
47	V	201	HEM	3	0
32	8	606	CLA	5	0
32	B	606	CLA	6	0
32	1	605	CLA	1	0
37	d	401	LMG	1	0
41	A	604	PHO	1	0
32	1	613	CLA	1	0
32	b	617	CLA	2	0
32	B	614	CLA	1	0
32	6	611	CLA	1	0
38	B	621	LHG	3	0
37	b	618	LMG	1	0
32	6	607	CLA	1	0
37	8	617	LMG	2	0
32	7	602	CLA	4	0
32	C	513	CLA	2	0
32	d	402	CLA	1	0
32	2	607	CLA	1	0
32	9	605	CLA	1	0
39	5	318	SQD	4	0
32	2	608	CLA	3	0

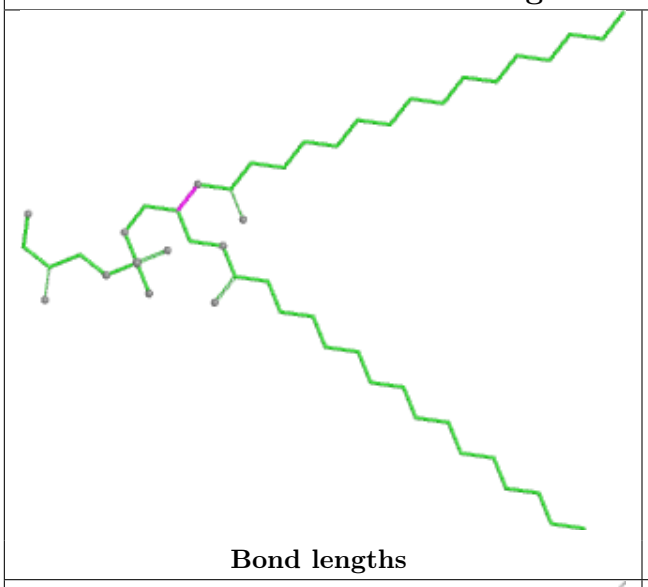
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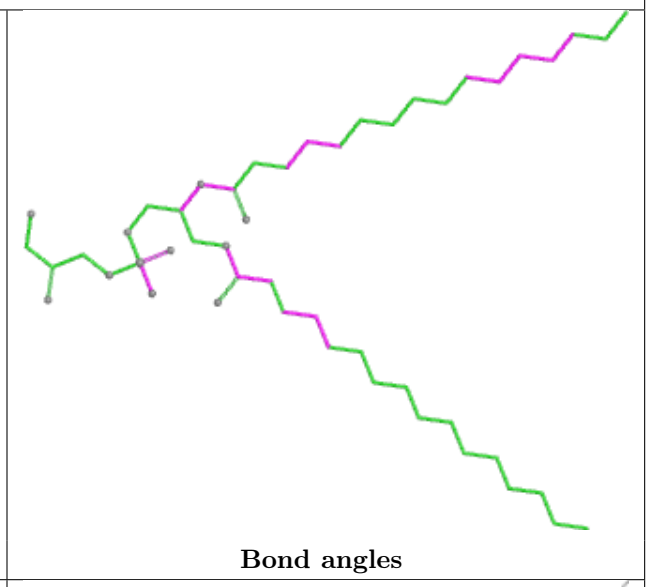
Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	B	601	SQD	2	0
32	B	611	CLA	2	0
32	A	605	CLA	3	0
37	L	102	LMG	1	0
39	b	620	SQD	1	0
32	p	307	CLA	2	0
32	2	606	CLA	5	0
37	C	517	LMG	3	0
38	s	301	LHG	1	0
32	s	302	CLA	3	0
38	S	301	LHG	1	0
45	c	516	DGD	3	0
32	3	605	CLA	1	0
32	b	609	CLA	4	0
32	B	605	CLA	3	0
32	8	602	CLA	1	0
32	A	603	CLA	3	0
32	3	602	CLA	1	0
32	1	608	CLA	1	0
45	h	101	DGD	5	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.

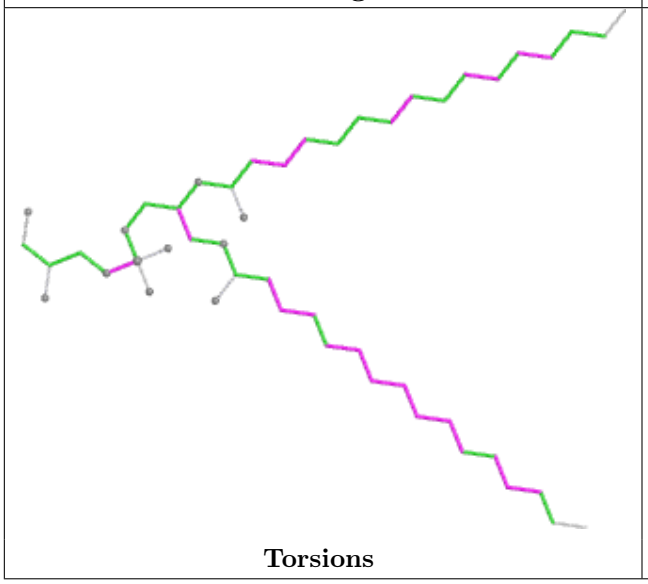
Ligand LHG L 101



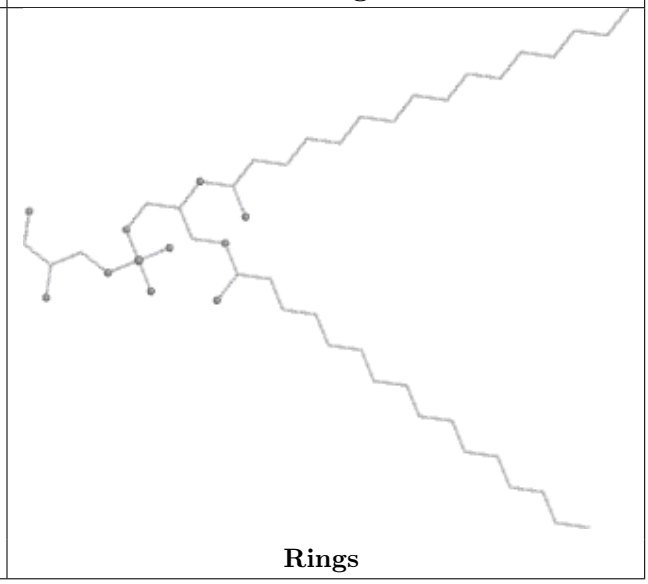
Bond lengths



Bond angles

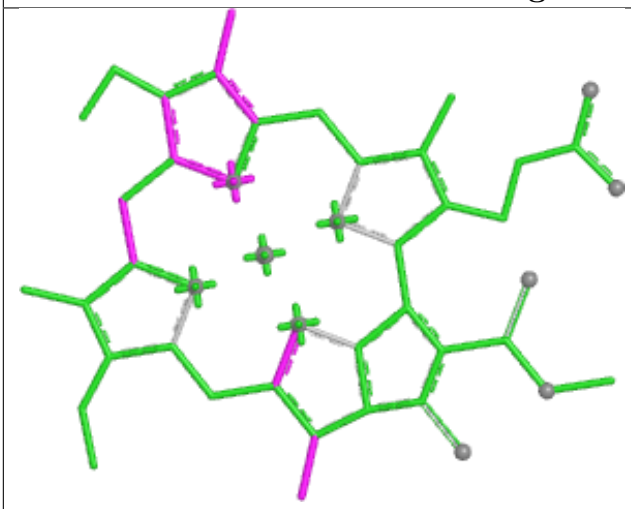


Torsions

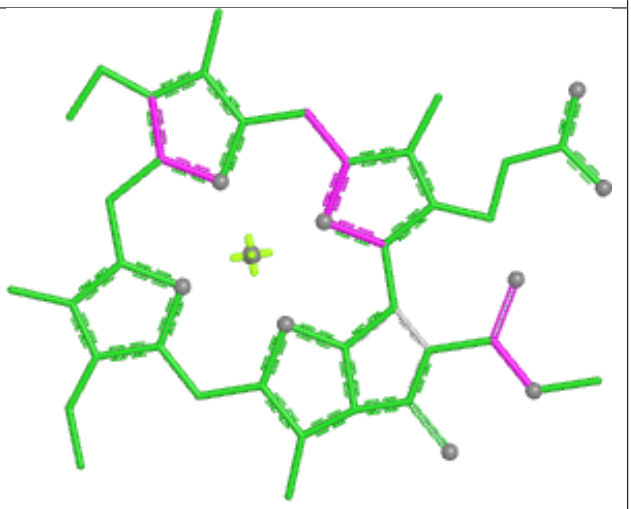


Rings

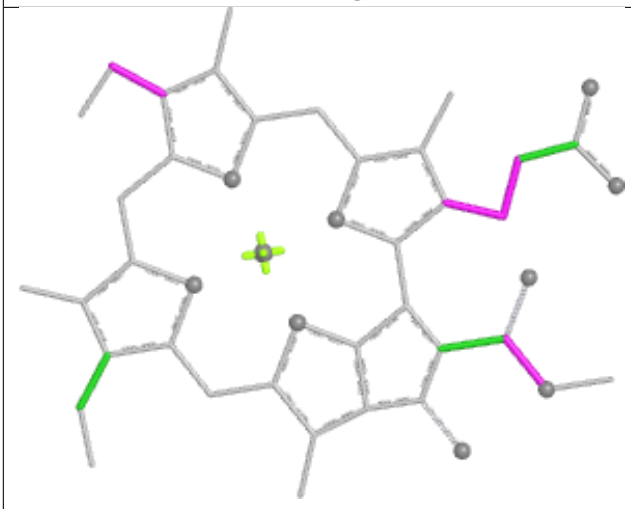
Ligand CLA 5 312



Bond lengths



Bond angles

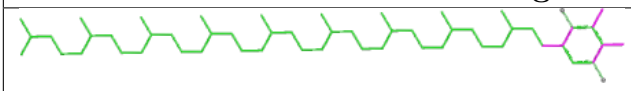


Torsions

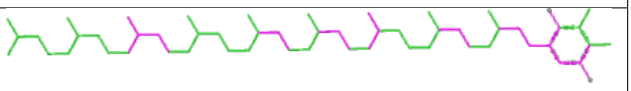


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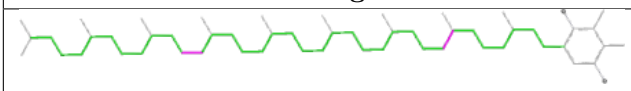
Ligand PL9 d 404



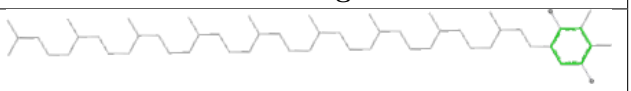
Bond lengths



Bond angles

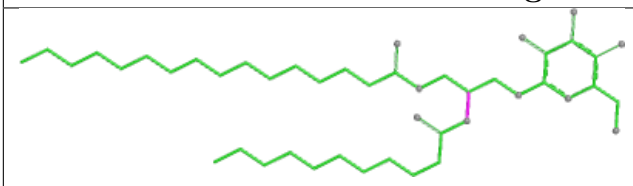


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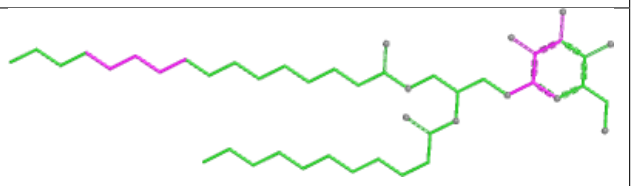


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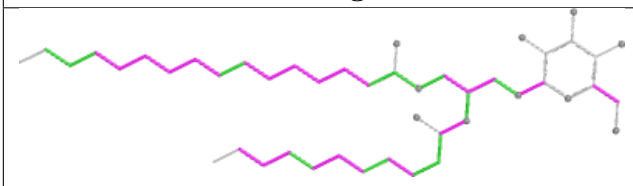
Ligand LMG c 517



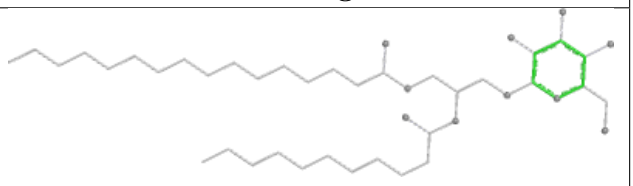
Bond lengths



Bond angles

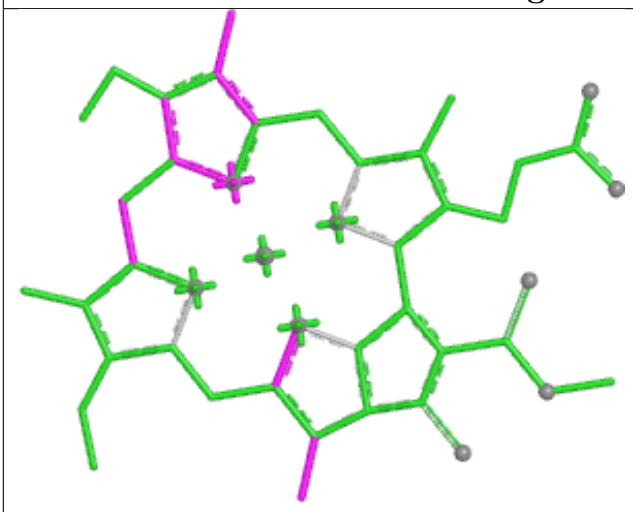


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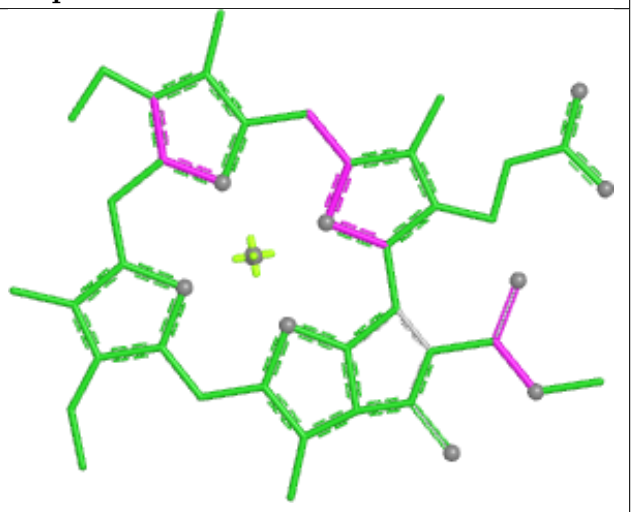


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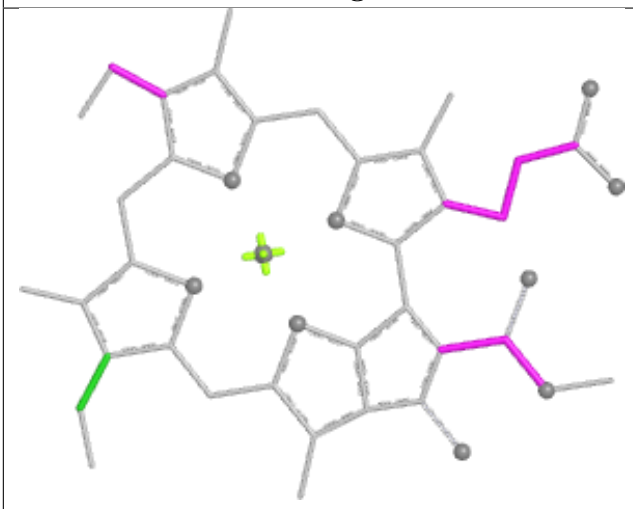
Ligand CLA p 313



Bond lengths



Bond angles

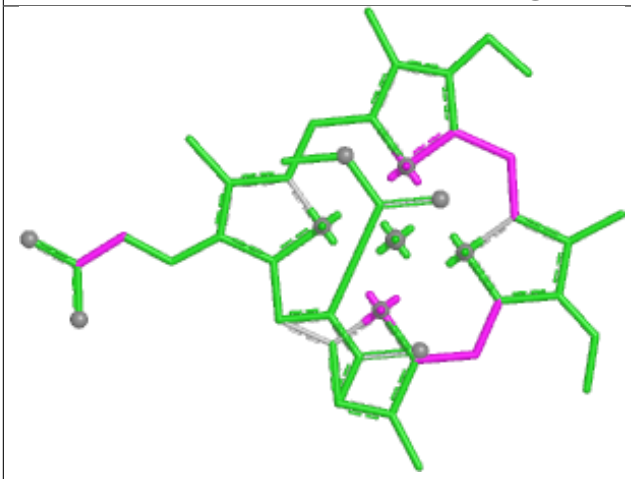


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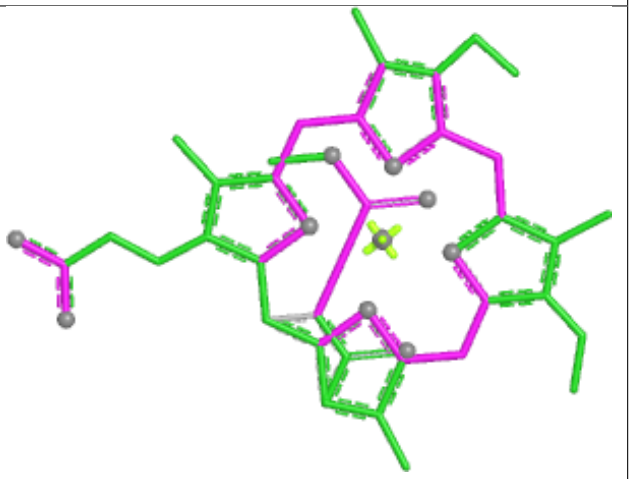


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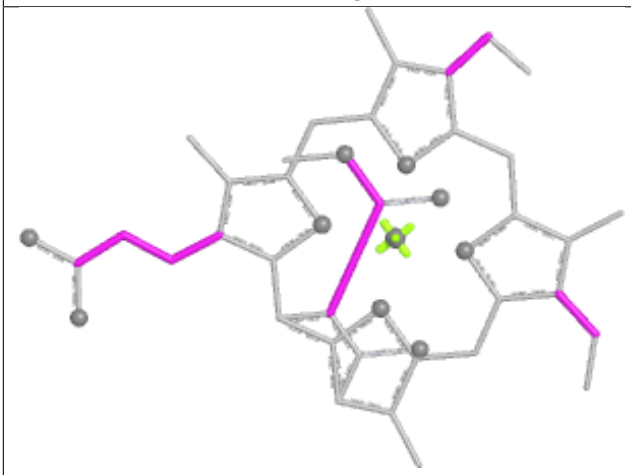
Ligand KC2 P 609



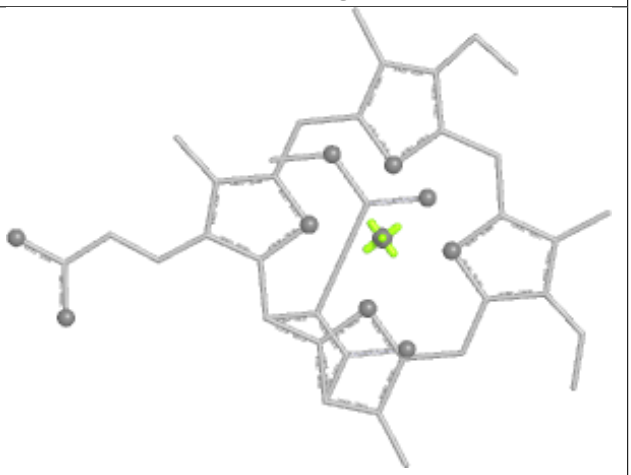
Bond lengths



Bond angles

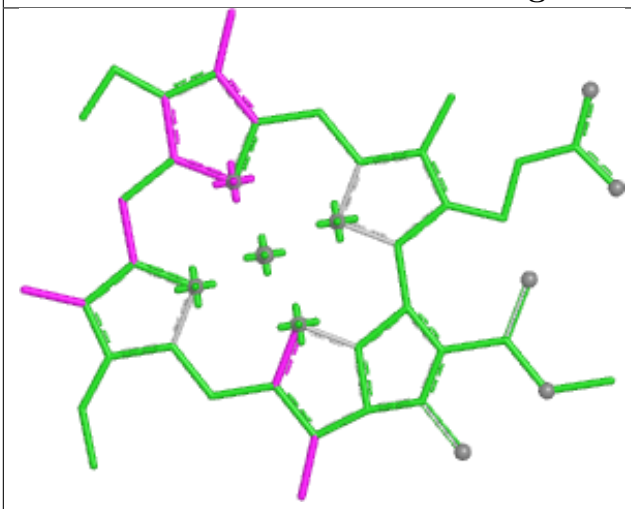


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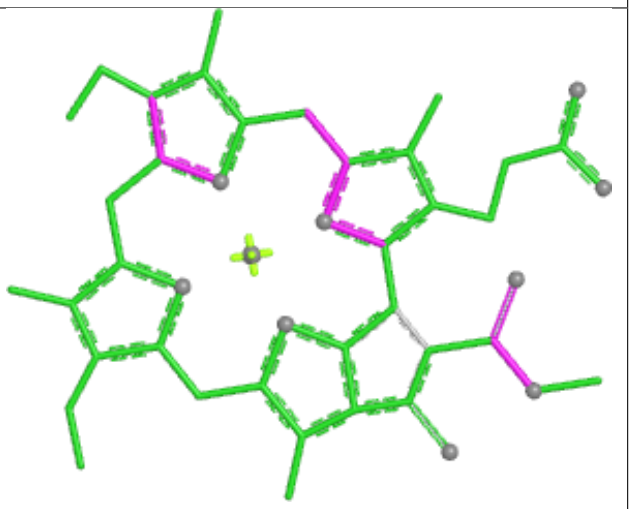


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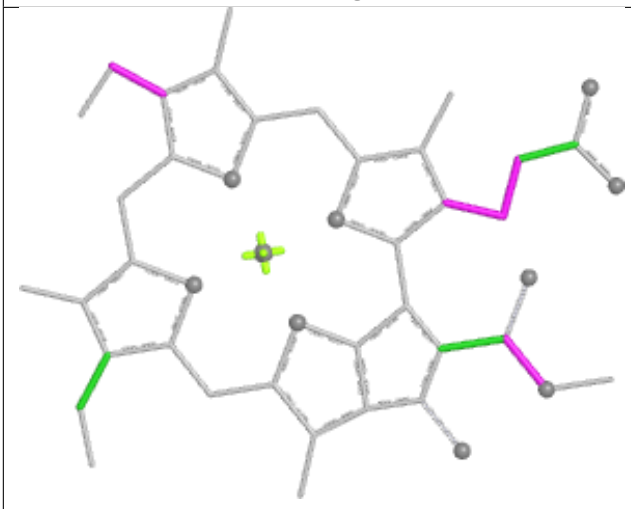
Ligand CLA 3 610



Bond lengths



Bond angles

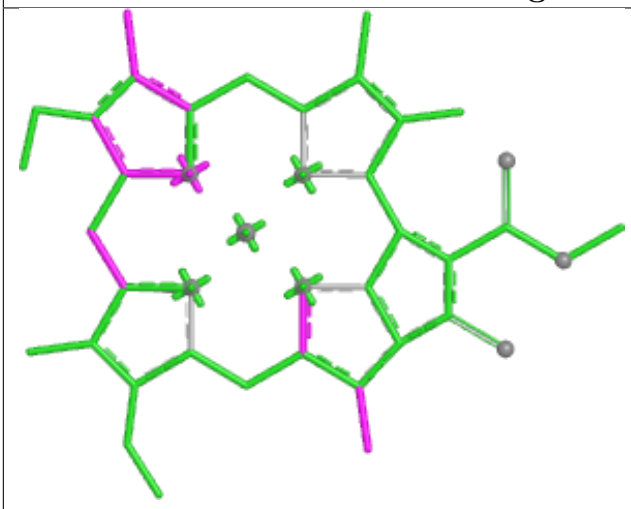


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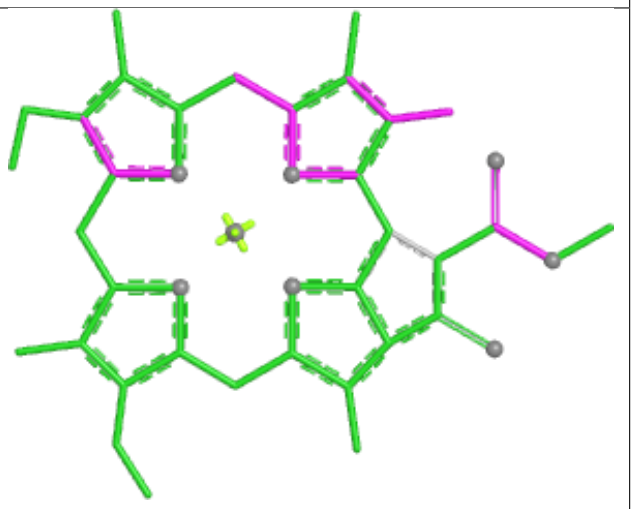


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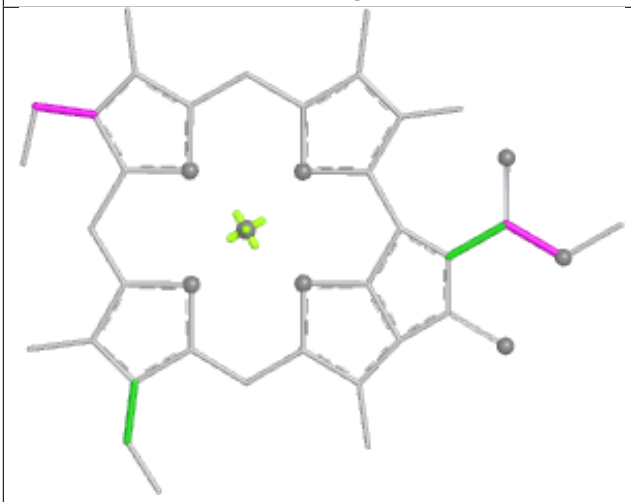
Ligand CLA 1 609



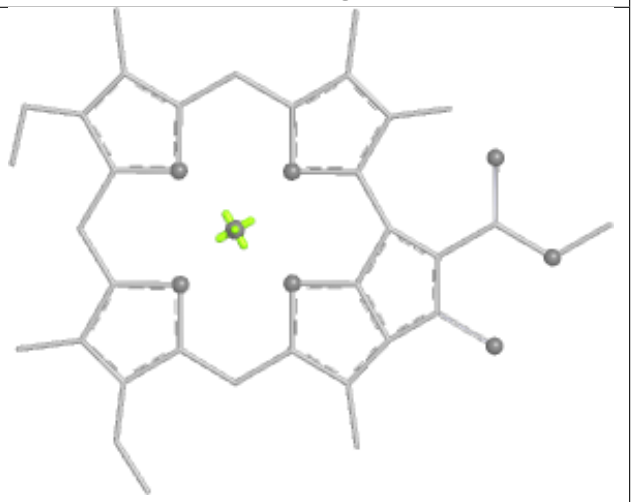
Bond lengths



Bond angles

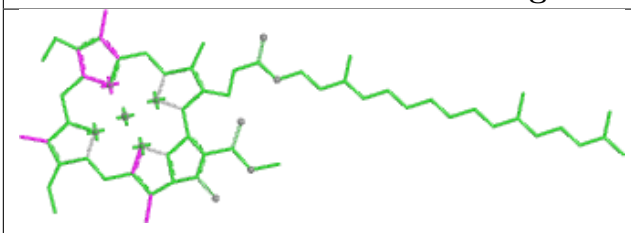


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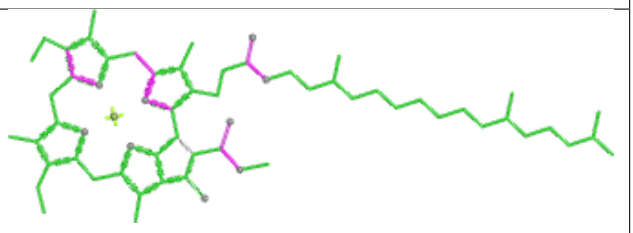


Rings

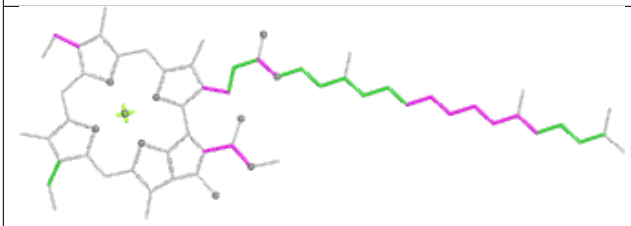
Ligand CLA c 502



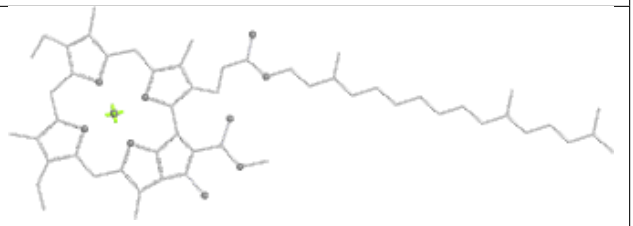
Bond lengths



Bond angles

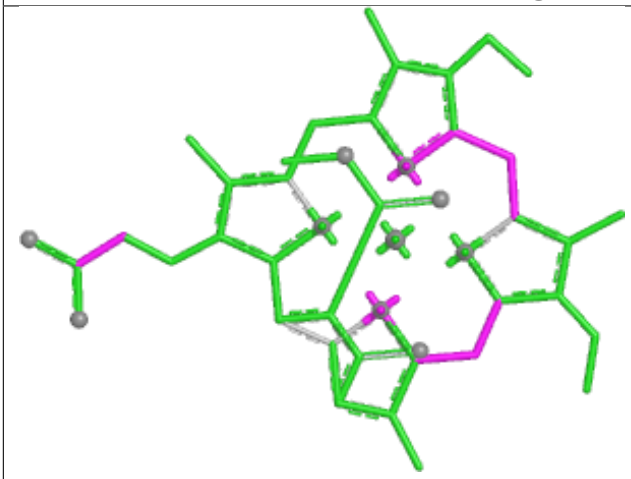


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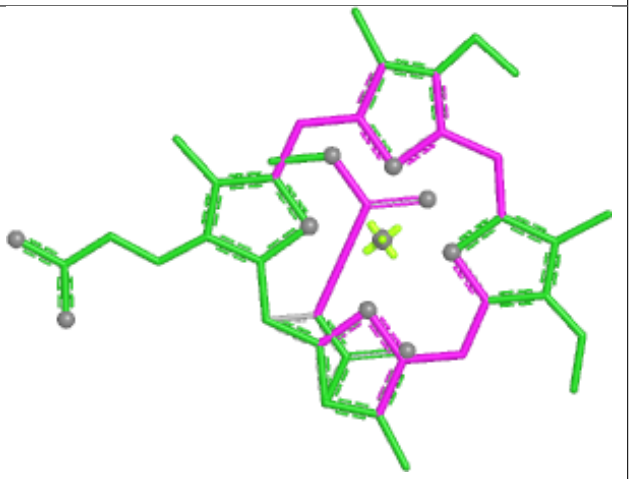


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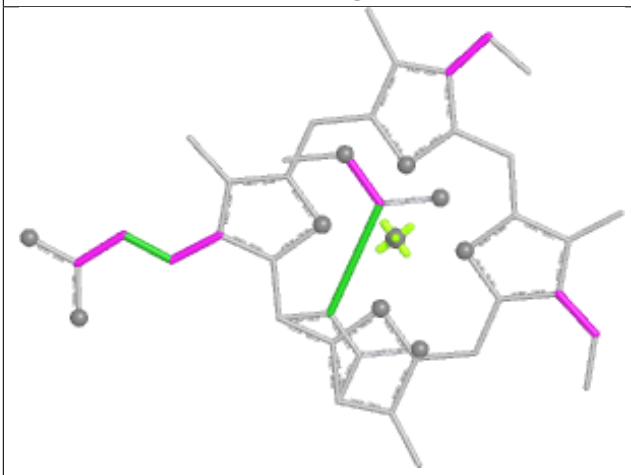
Ligand KC2 6 605



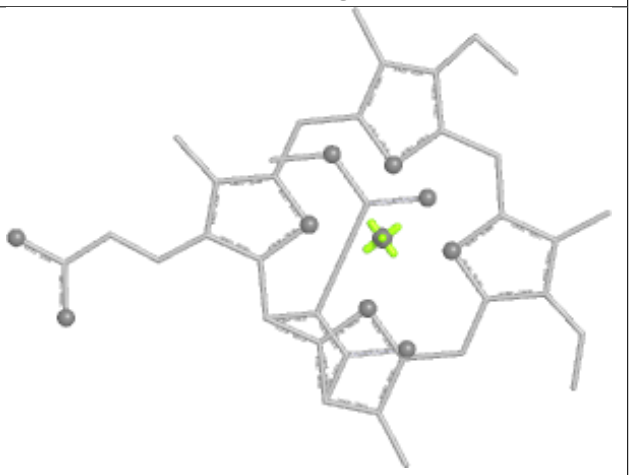
Bond lengths



Bond angles

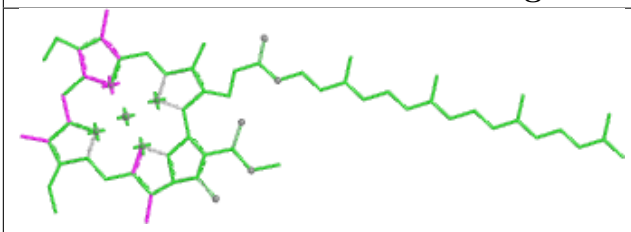


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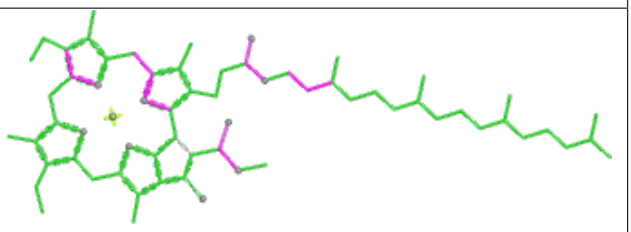


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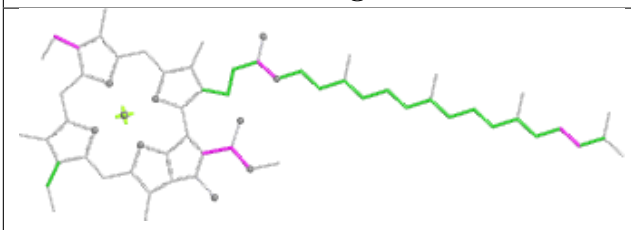
Ligand CLA B 610



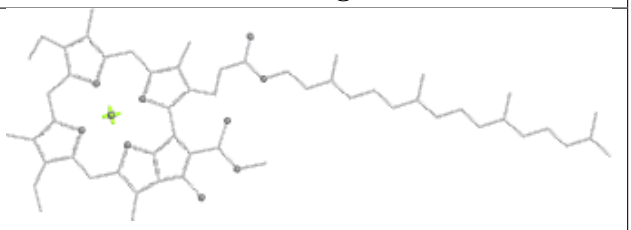
Bond lengths



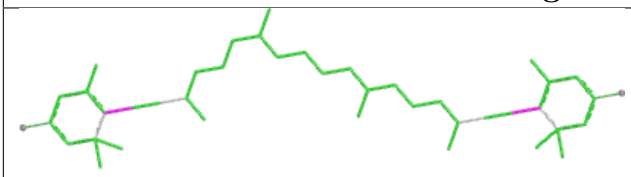
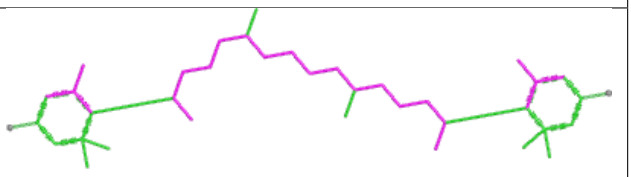
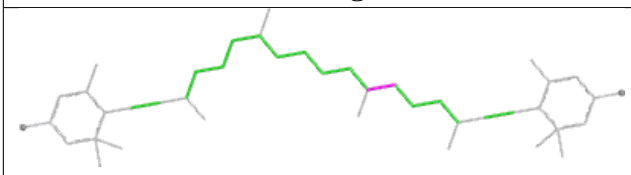
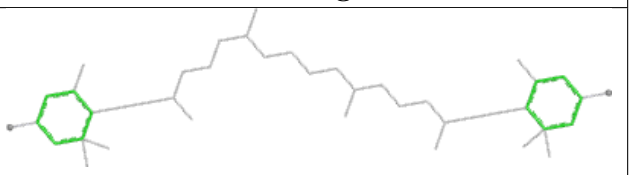
Bond angles

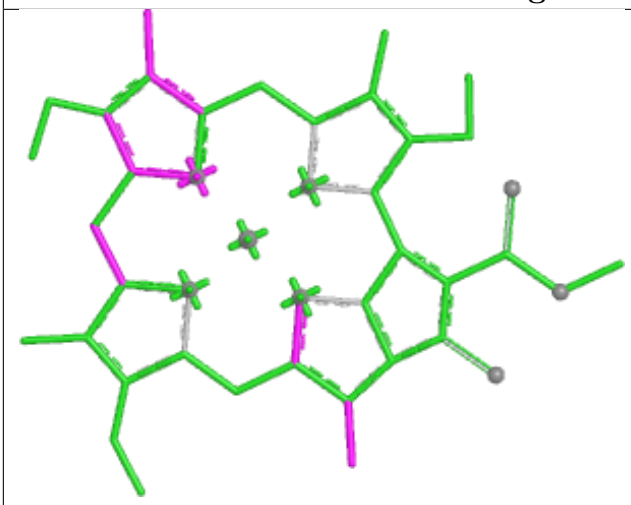
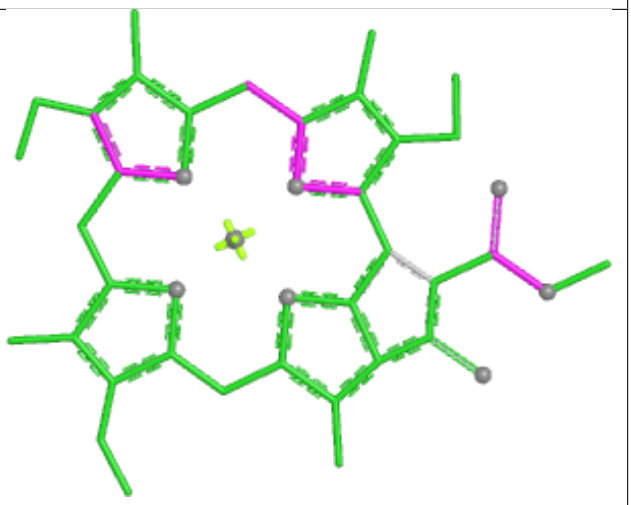
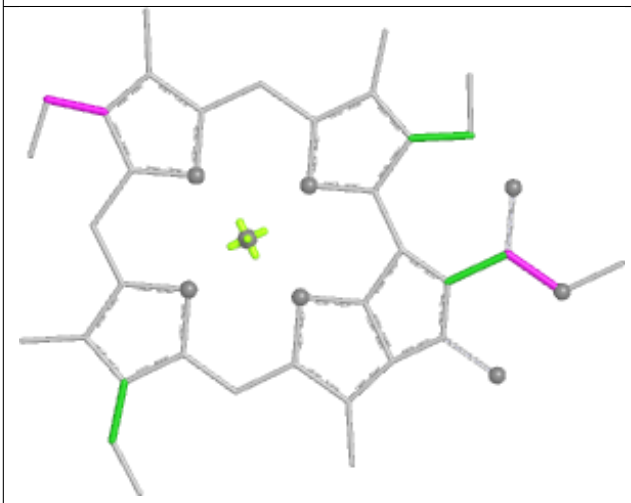


Torsions

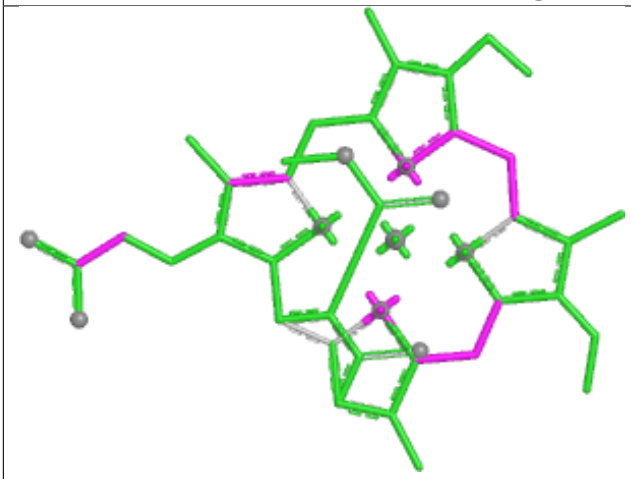


Rings

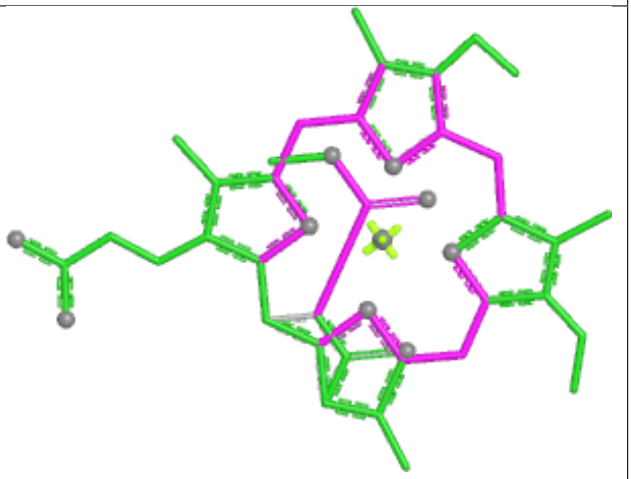
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 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

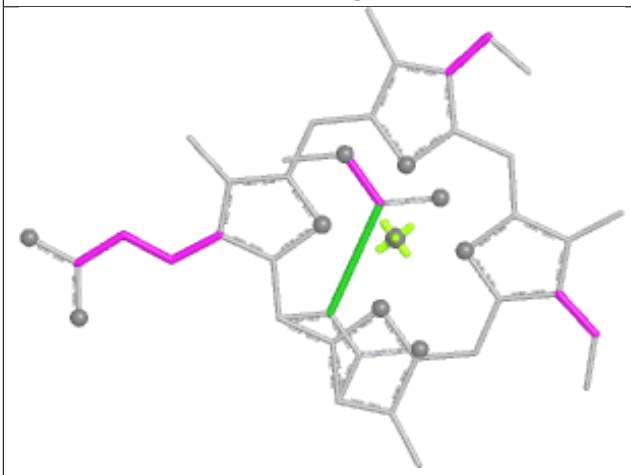
Ligand KC2 8 610



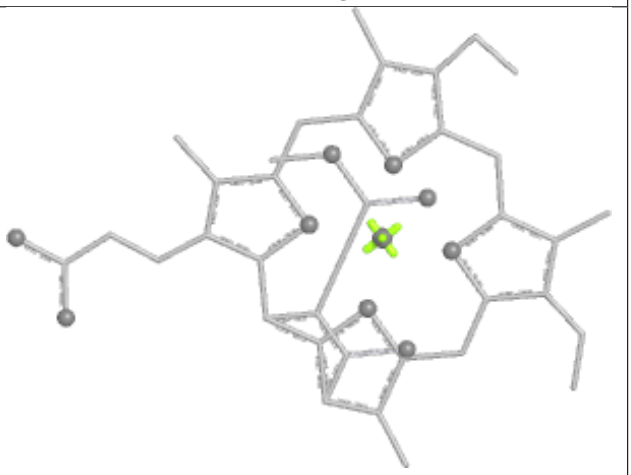
Bond lengths



Bond angles

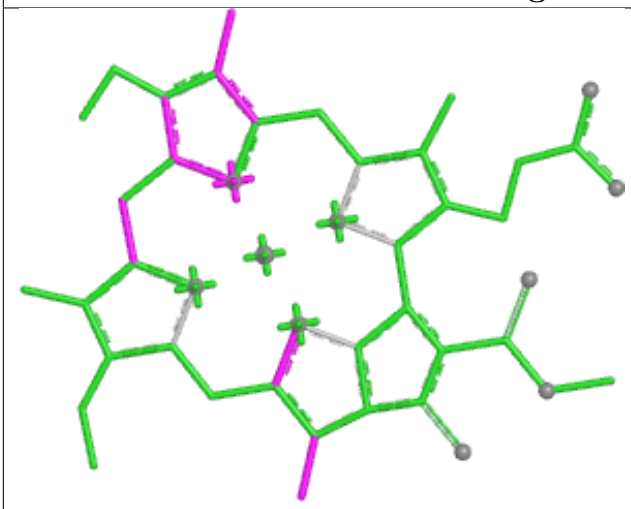


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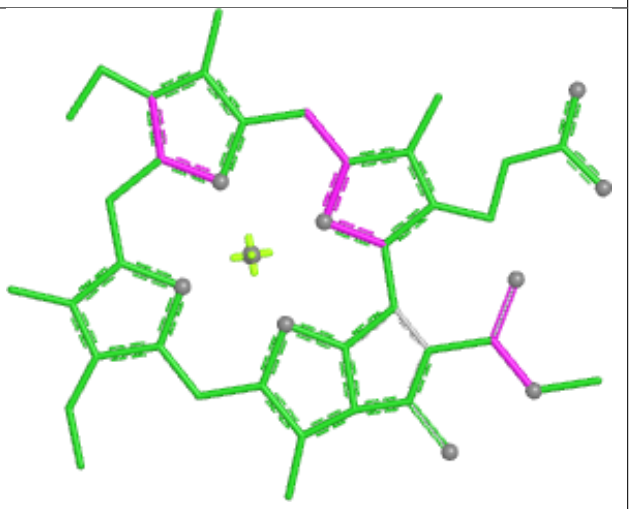


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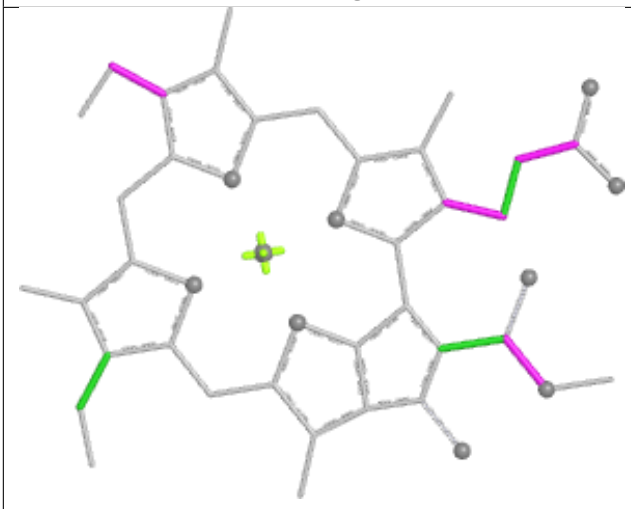
Ligand CLA 7 607



Bond lengths



Bond angles

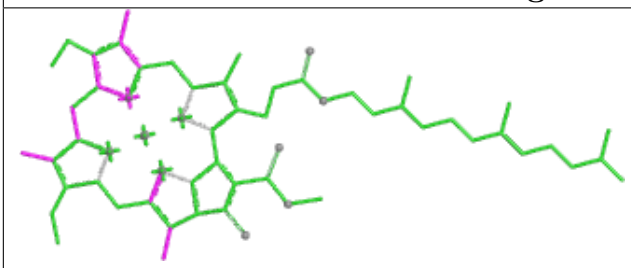


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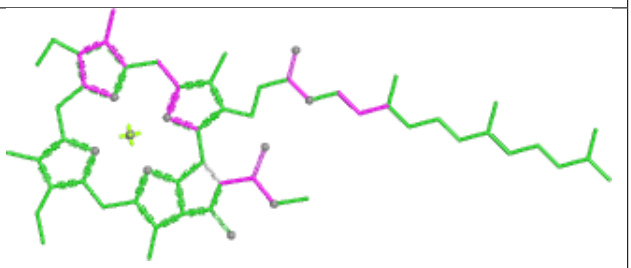


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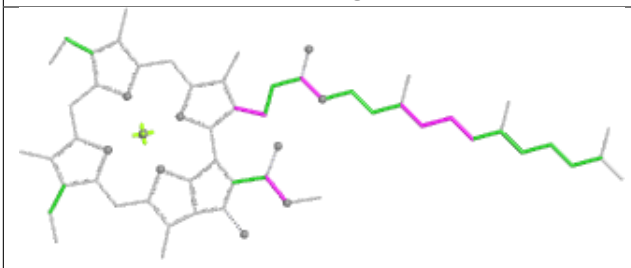
Ligand CLA d 403



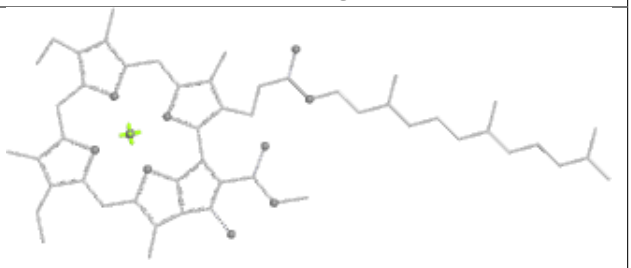
Bond lengths



Bond angles

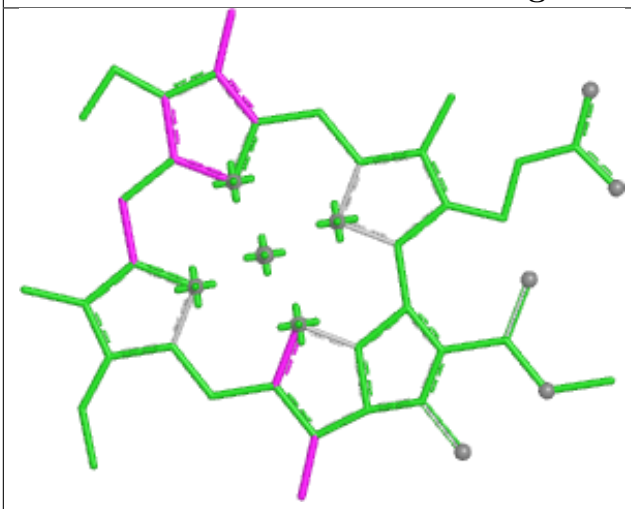


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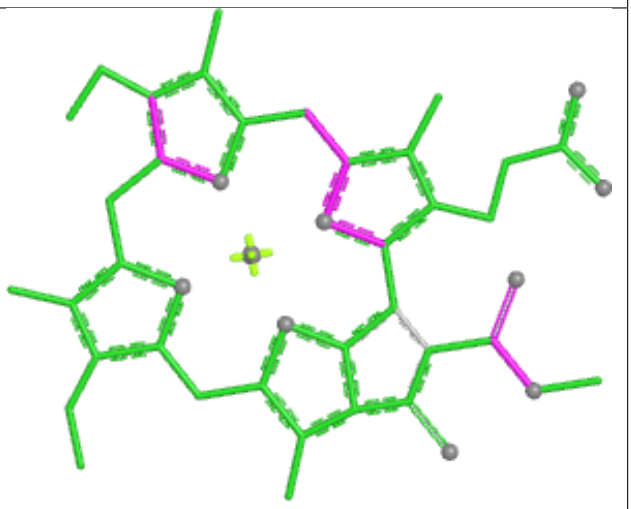


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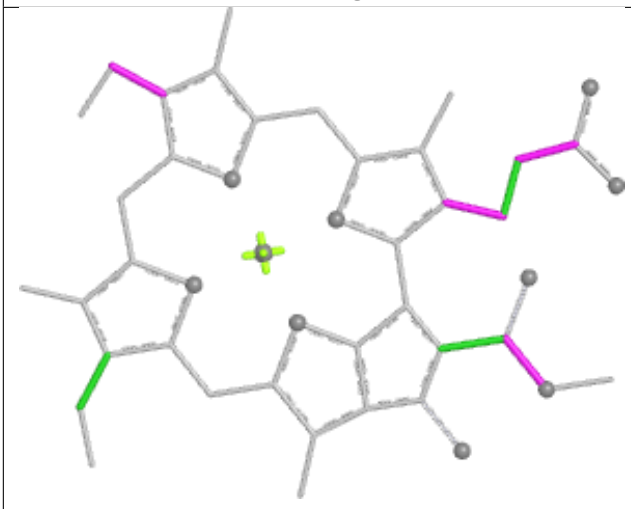
Ligand CLA 1 612



Bond lengths



Bond angles

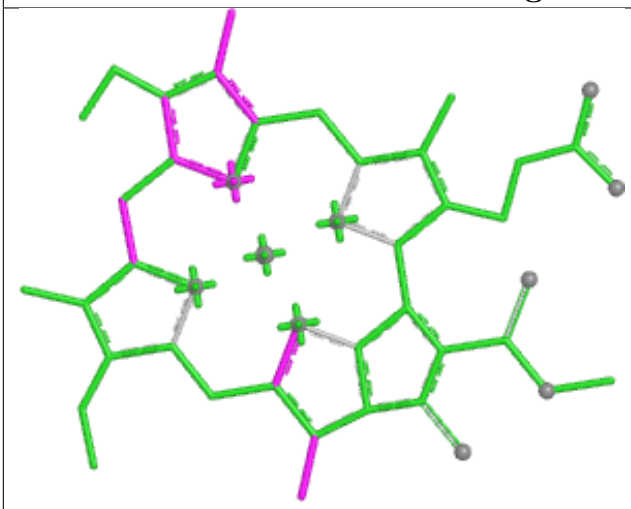


Torsions

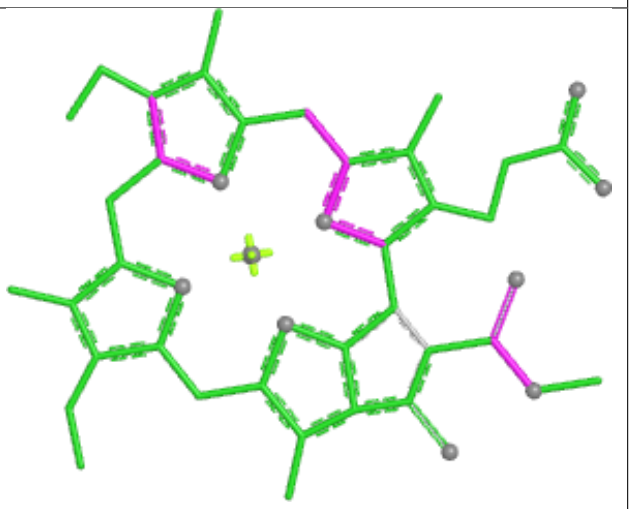


Rings

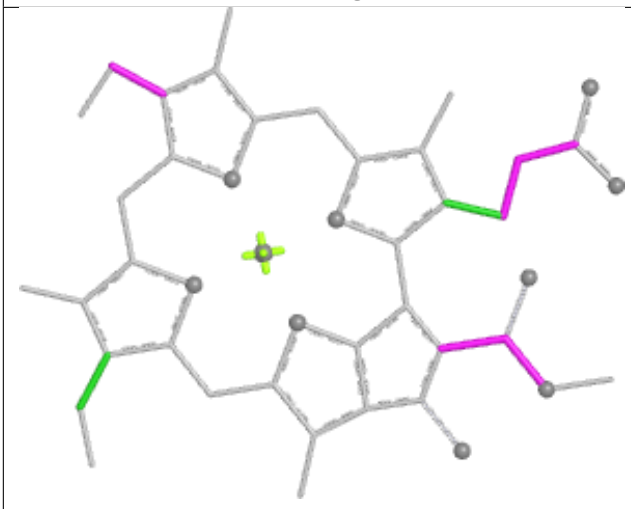
Ligand CLA P 611



Bond lengths



Bond angles

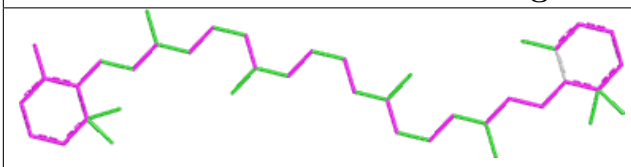


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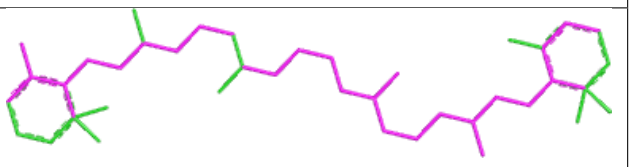


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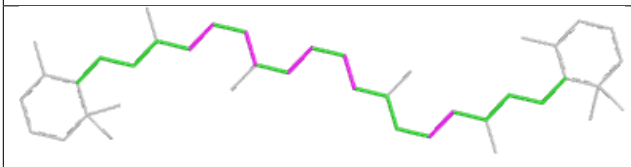
Ligand 8CT k 101



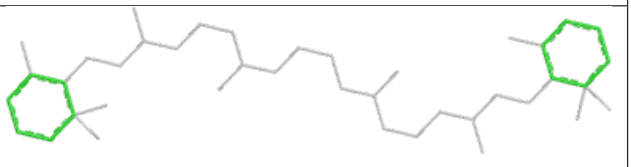
Bond lengths



Bond angles

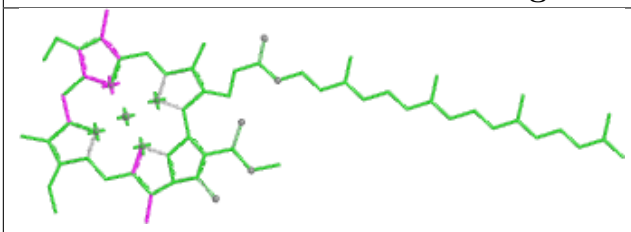


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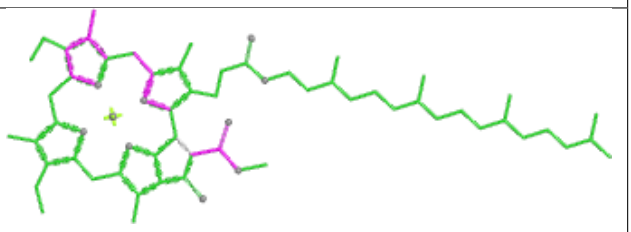


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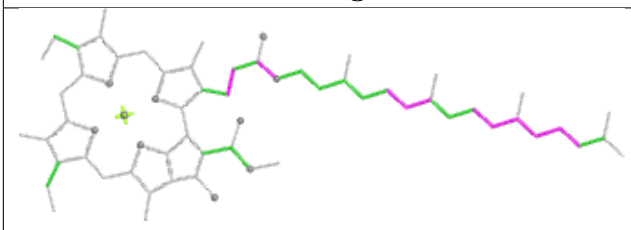
Ligand CLA c 505



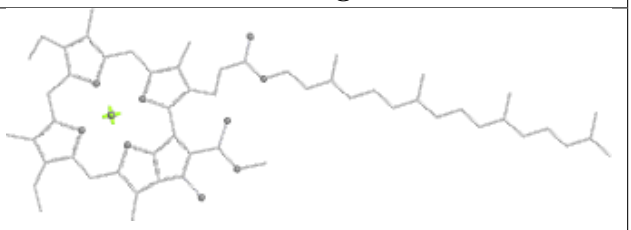
Bond lengths



Bond angles

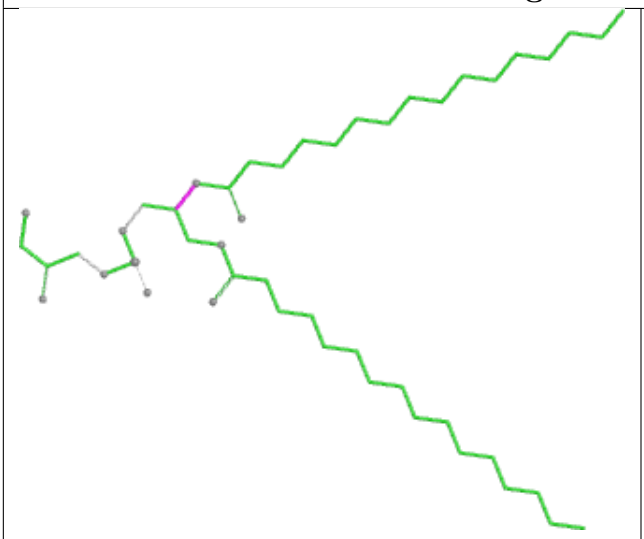


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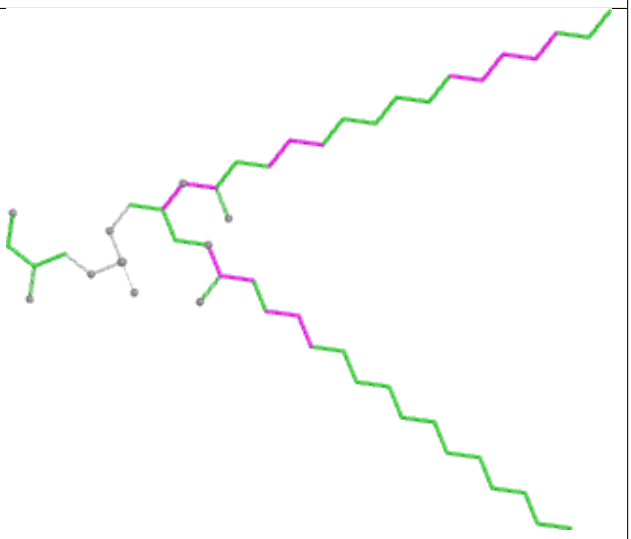


Rings

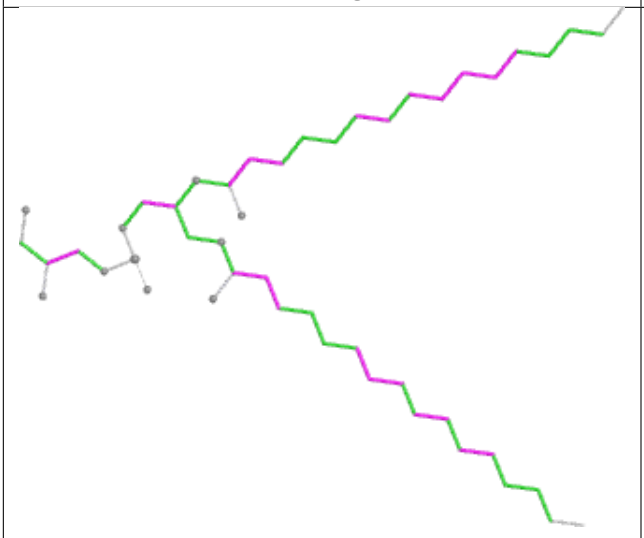
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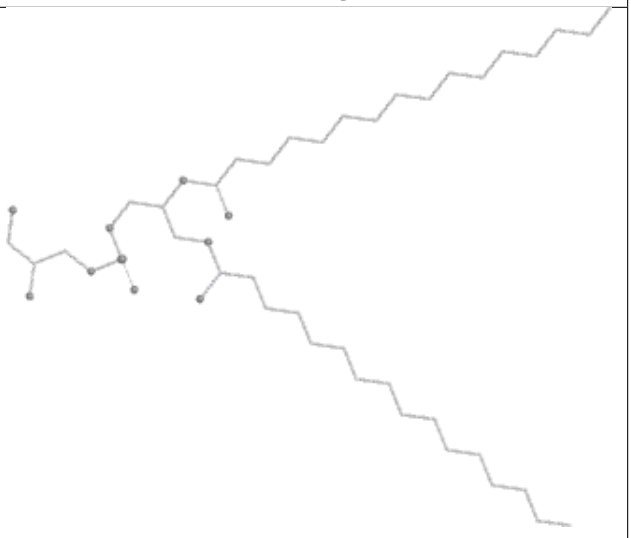
Bond lengths



Bond angles

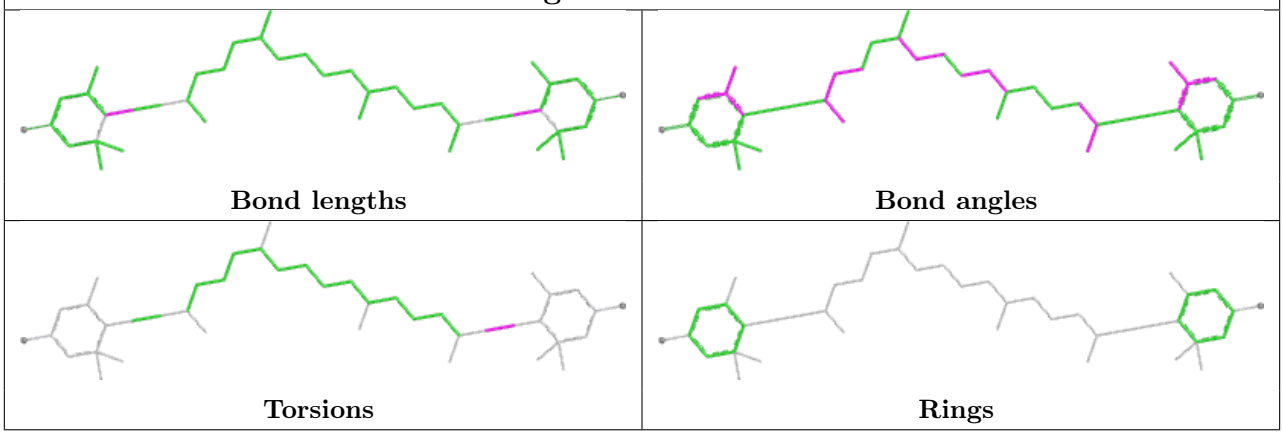


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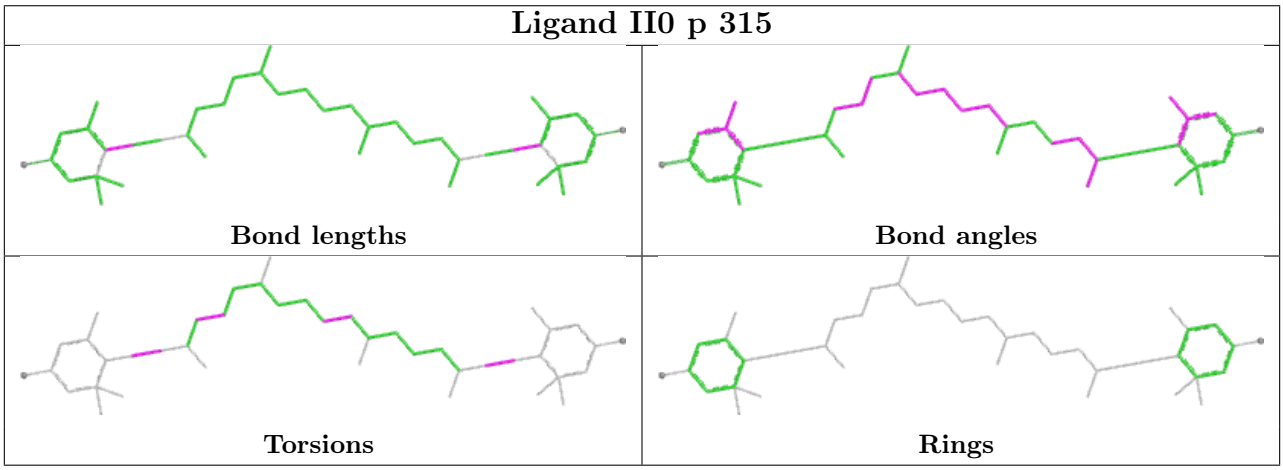


Rings

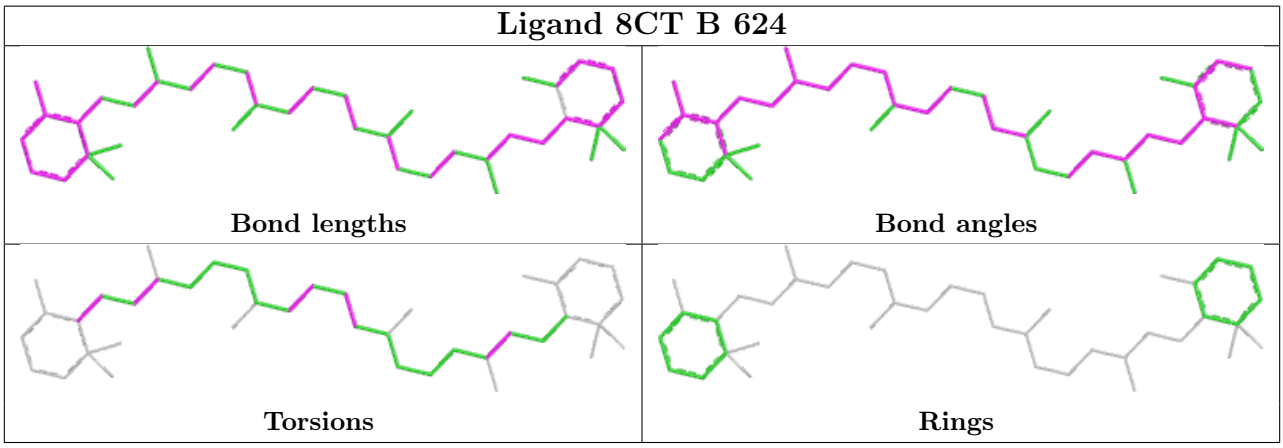
Ligand II0 7 619



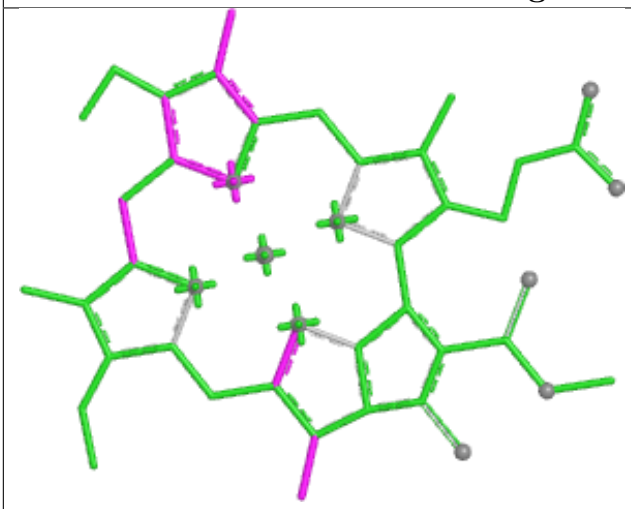
Ligand II0 p 315



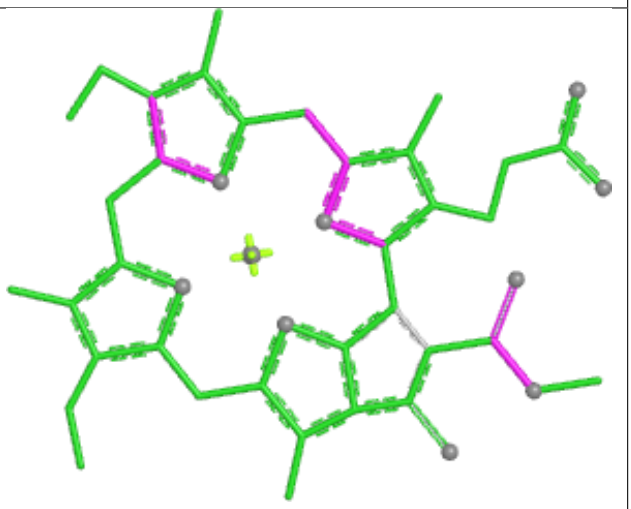
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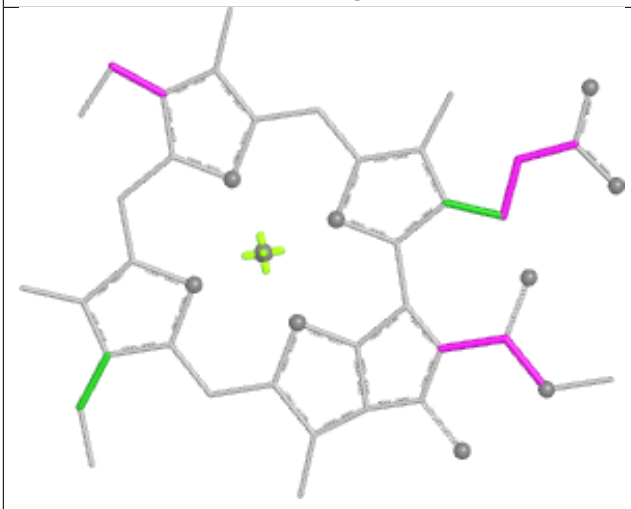
Ligand CLA 4 613



Bond lengths



Bond angles

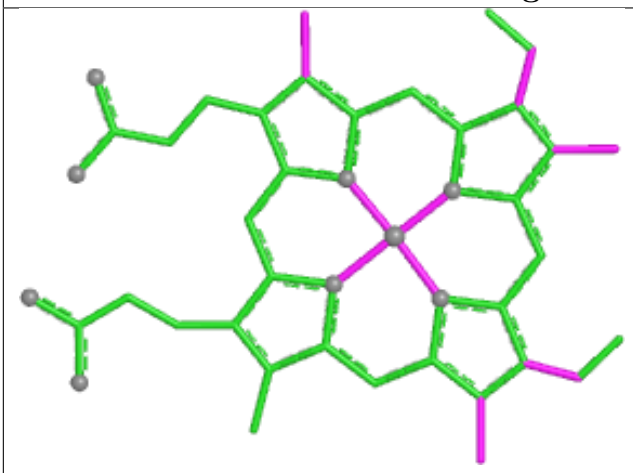


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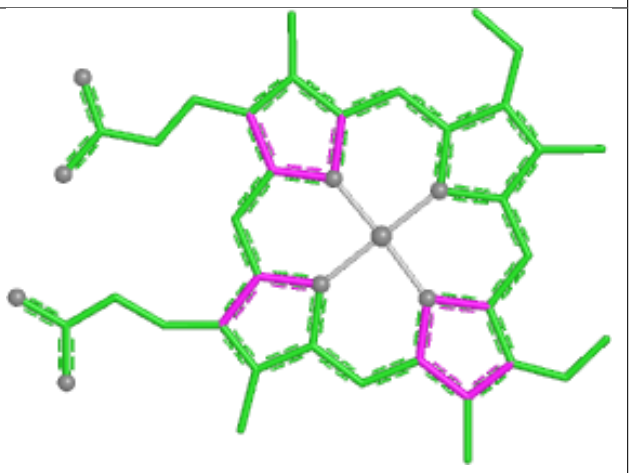


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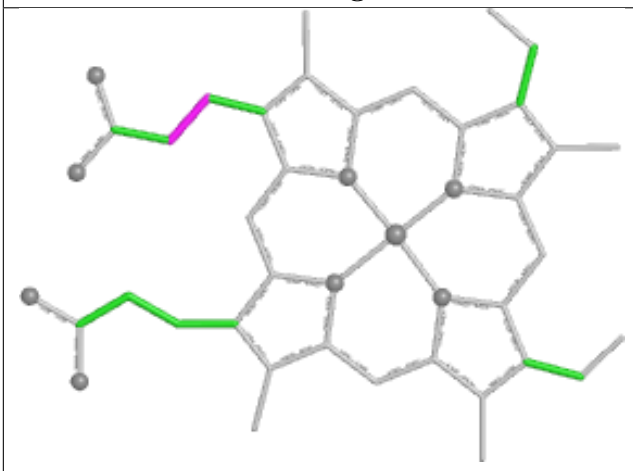
Ligand HEM v 201



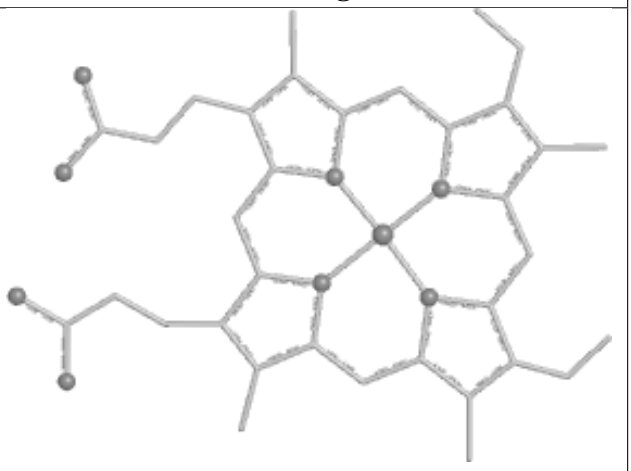
Bond lengths



Bond angles

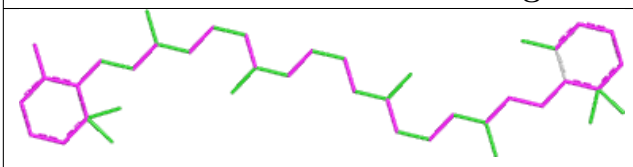


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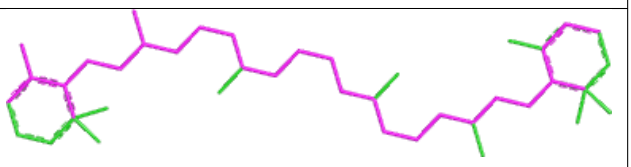


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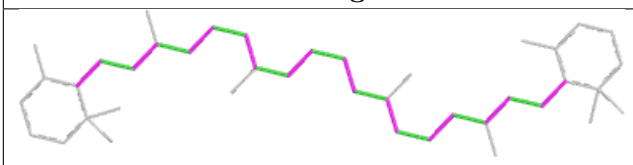
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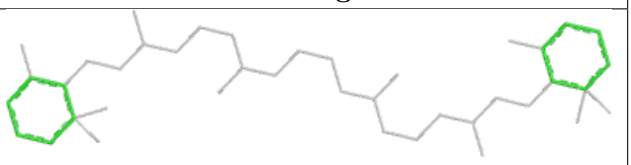
Bond lengths



Bond angles

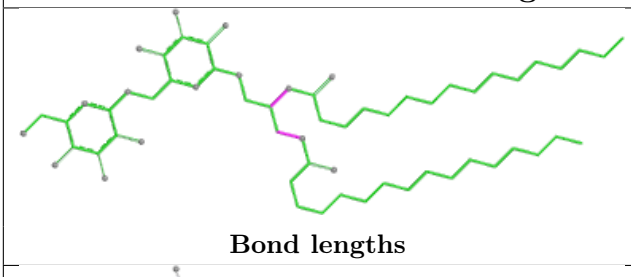


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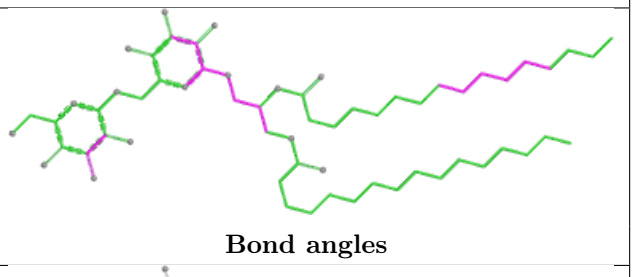


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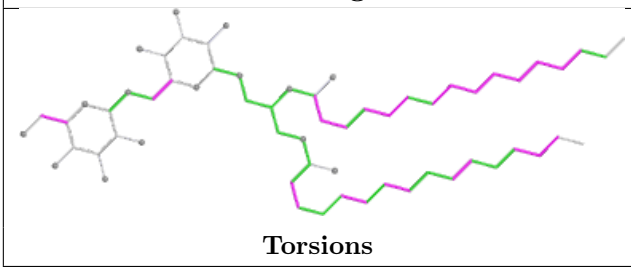
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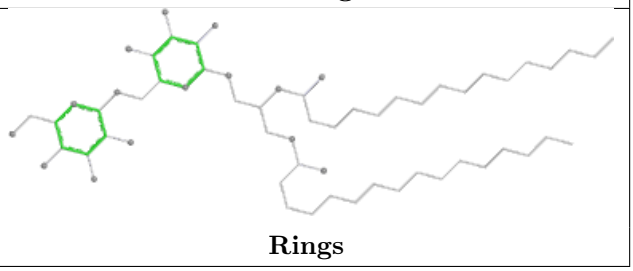
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Bond angles

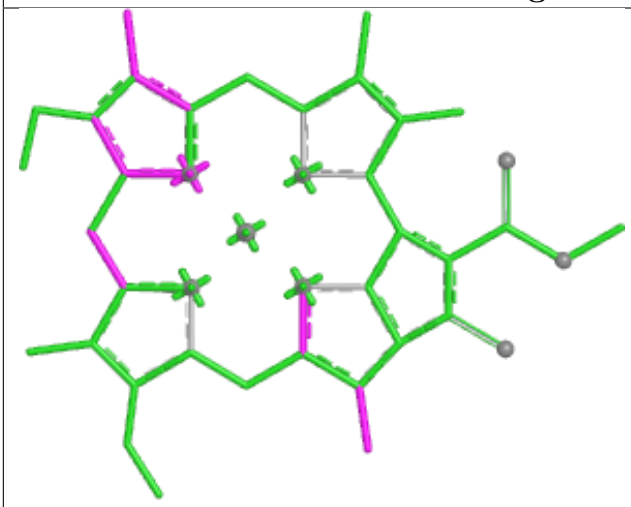


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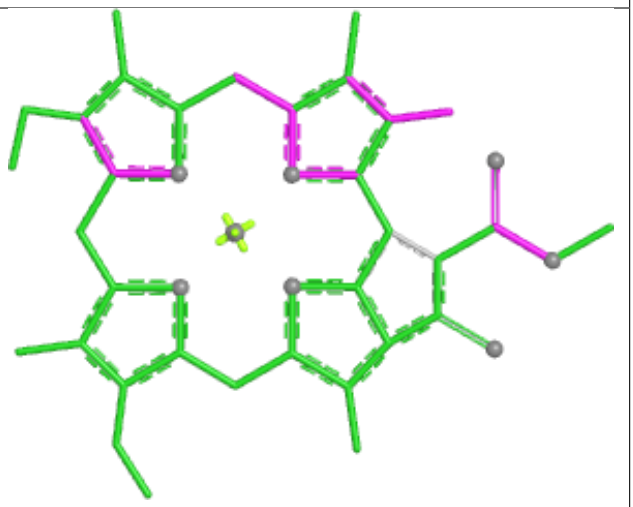


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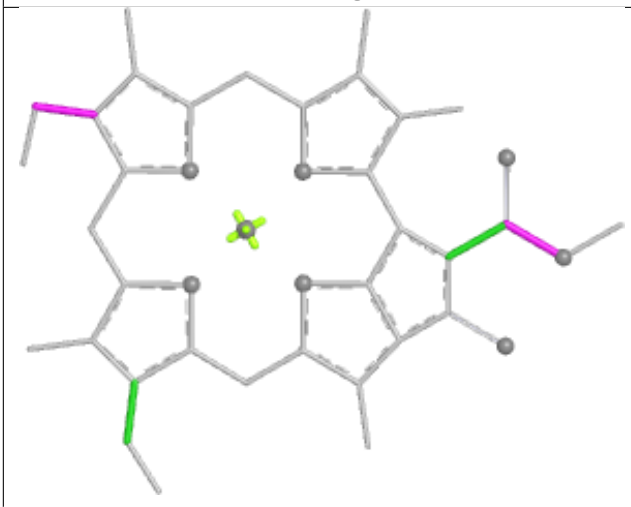
Ligand CLA 5 310



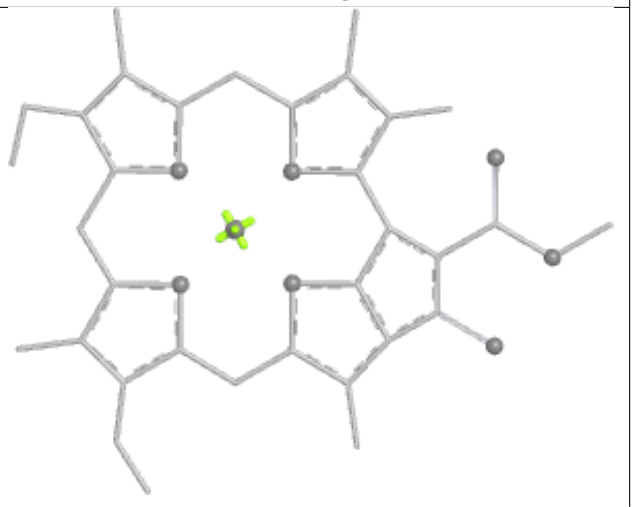
Bond lengths



Bond angles

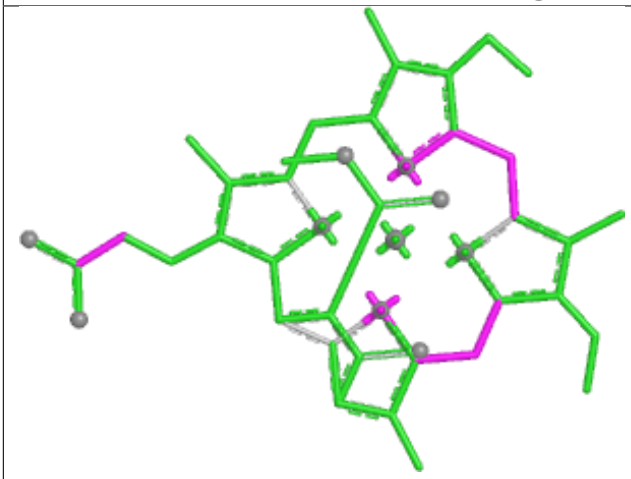


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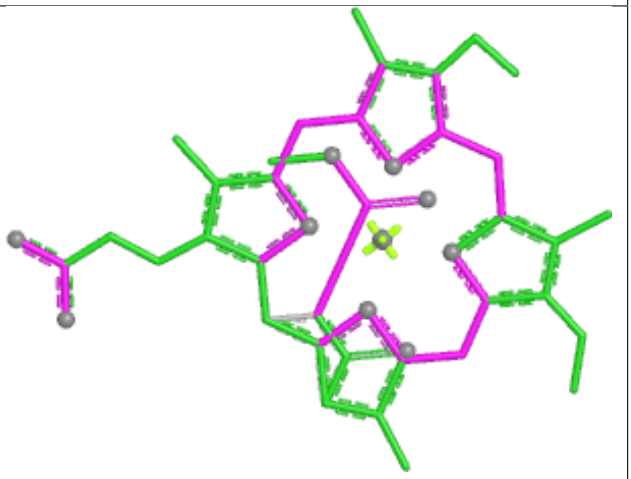


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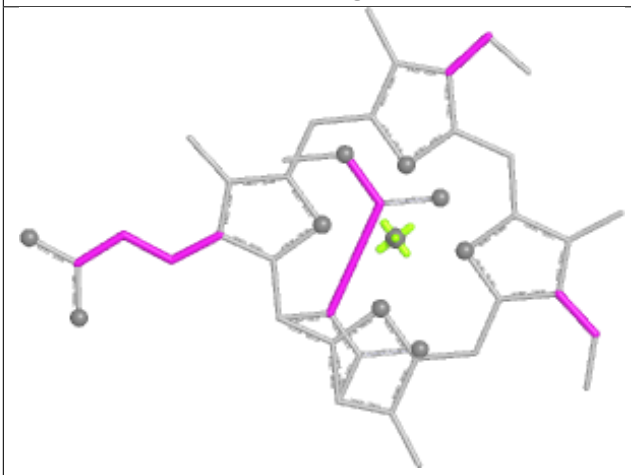
Ligand KC2 0 610



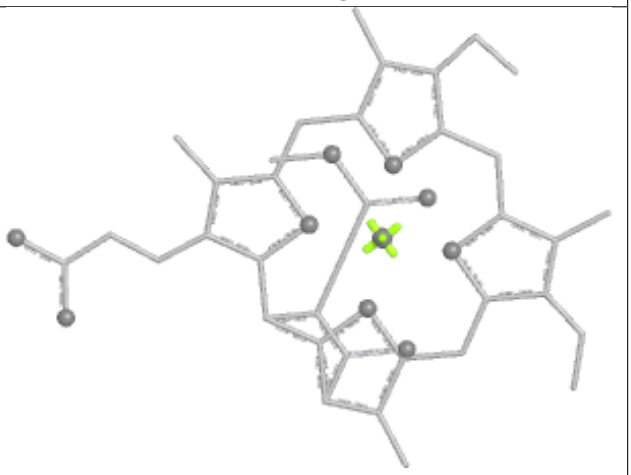
Bond lengths



Bond angles

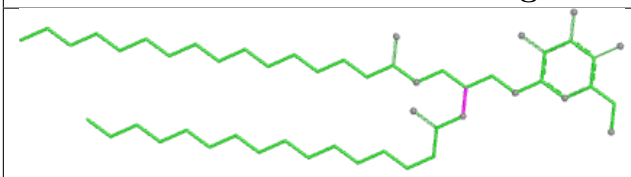


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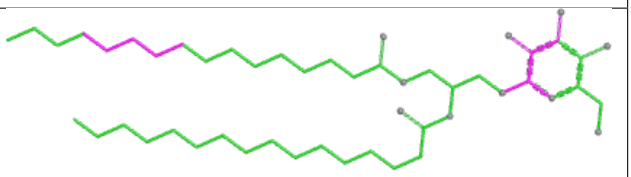


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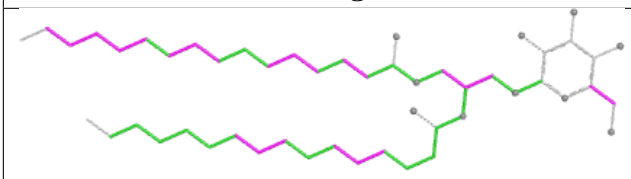
Ligand LMG B 618



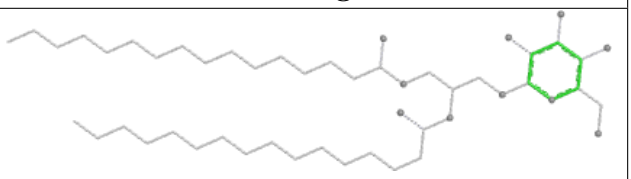
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Bond angles

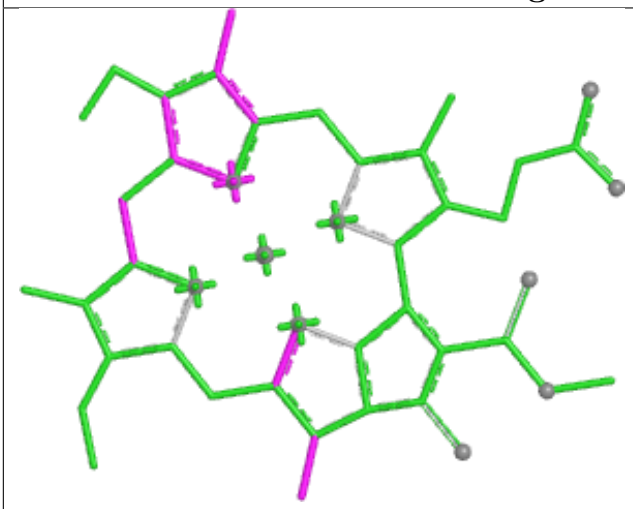


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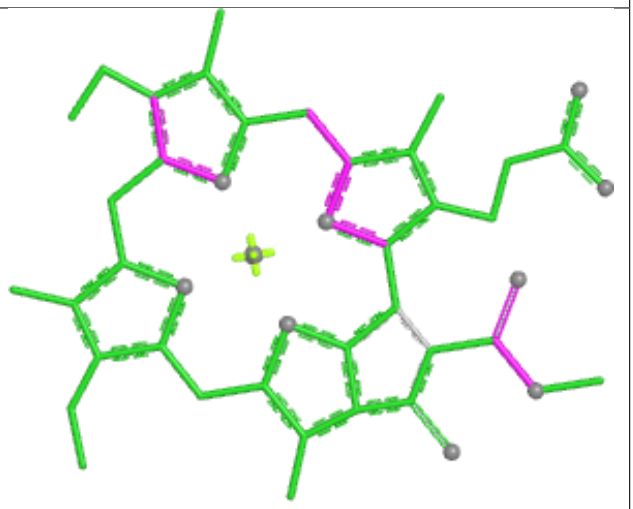


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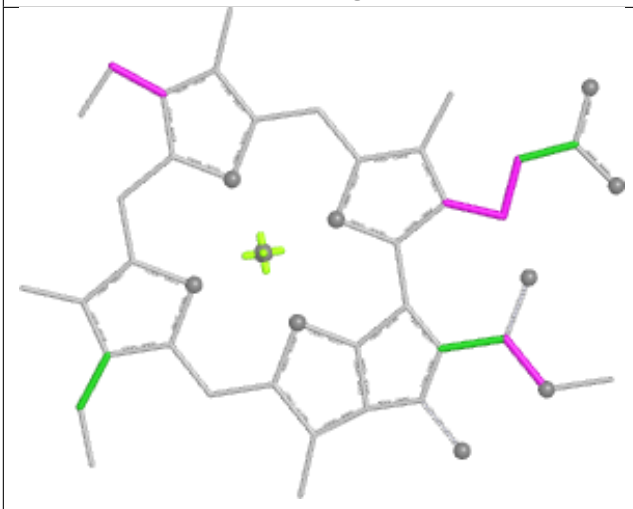
Ligand CLA 9 610



Bond lengths



Bond angles

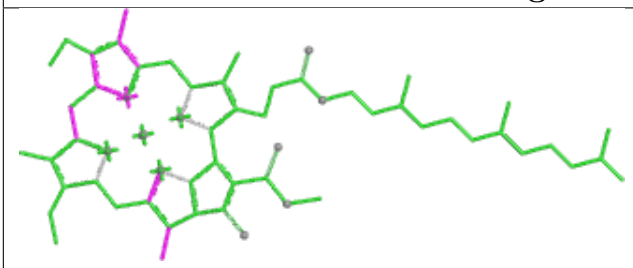


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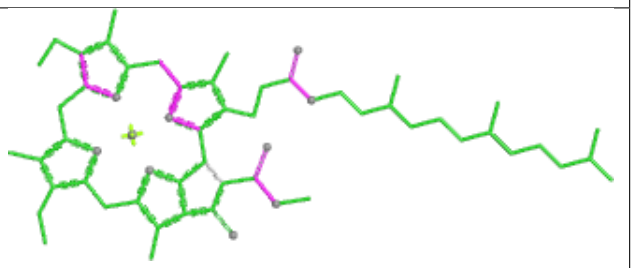


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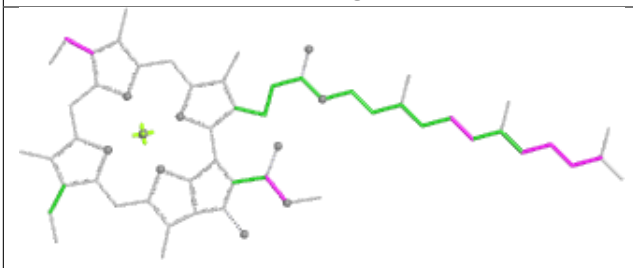
Ligand CLA 0 608



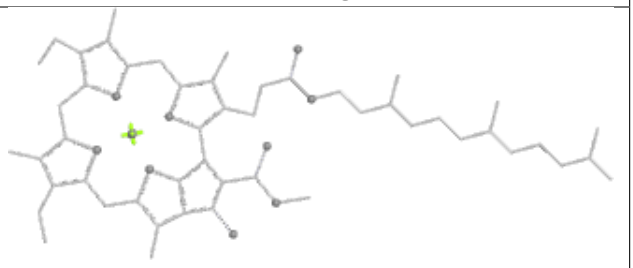
Bond lengths



Bond angles

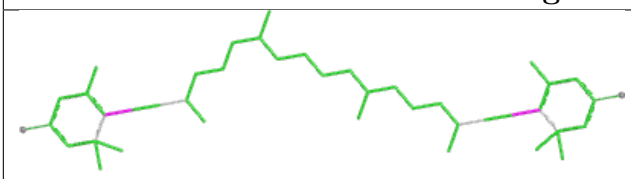


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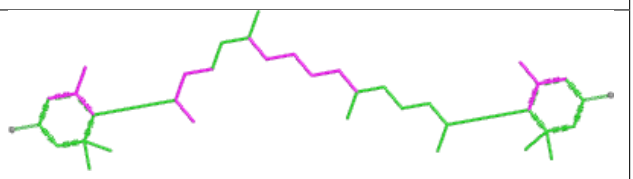


Rings

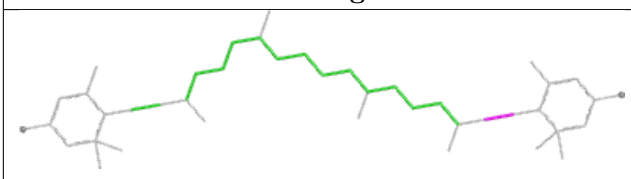
Ligand II0 2 613



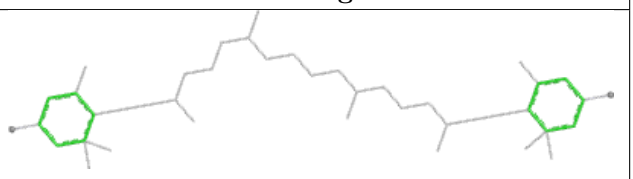
Bond lengths



Bond angles

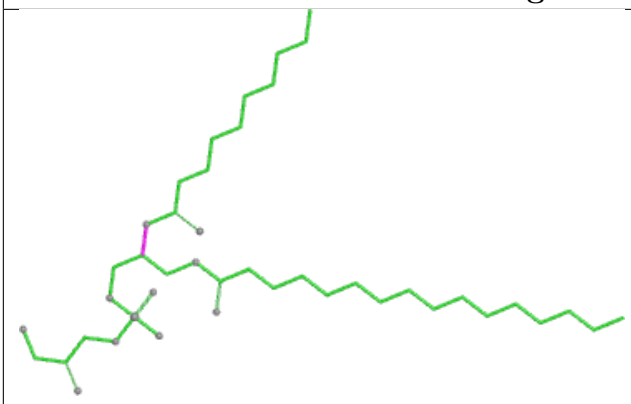


Torsions

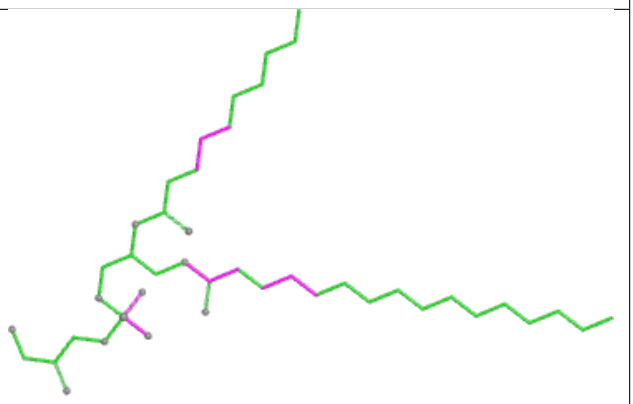


Rings

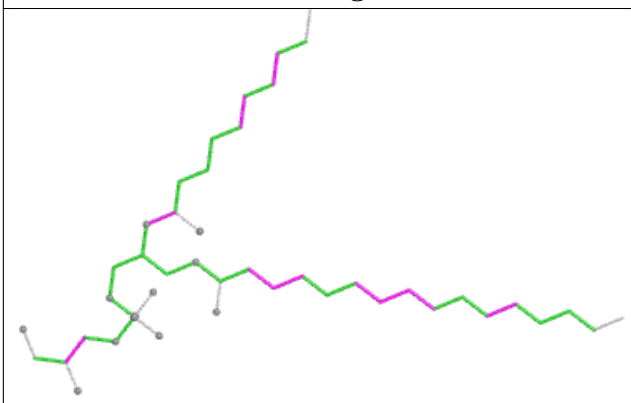
Ligand LHG a 402



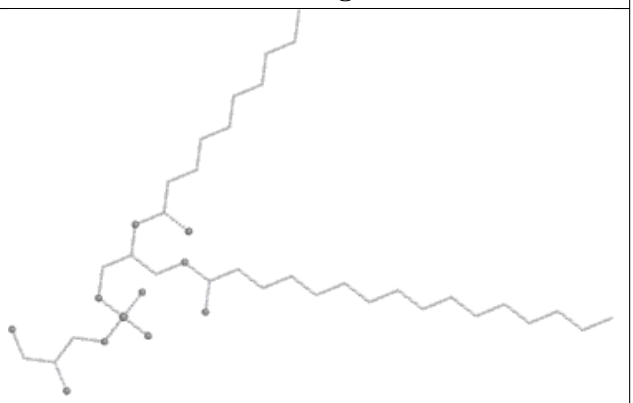
Bond lengths



Bond angles

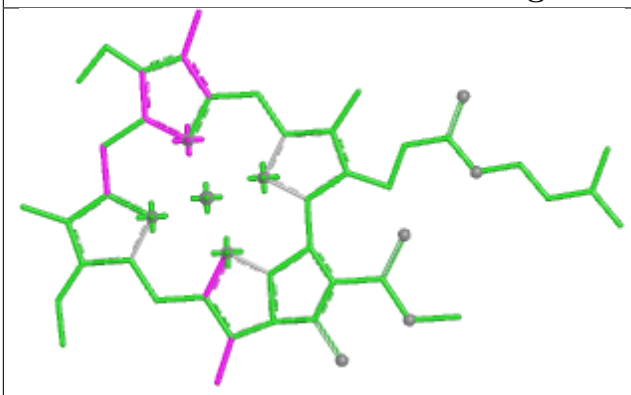


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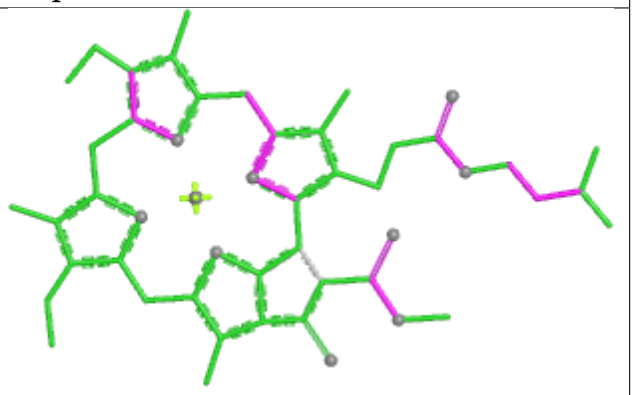


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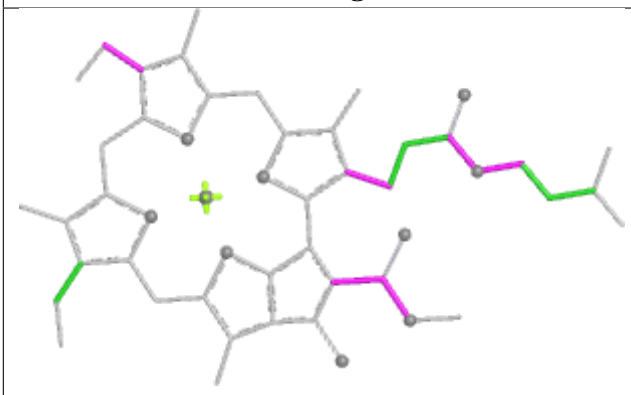
Ligand CLA p 304



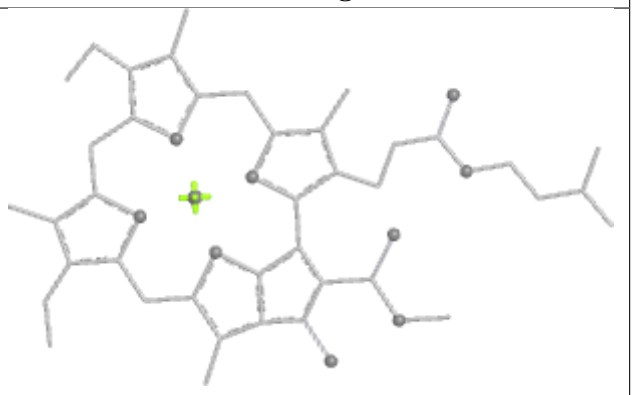
Bond lengths



Bond angles

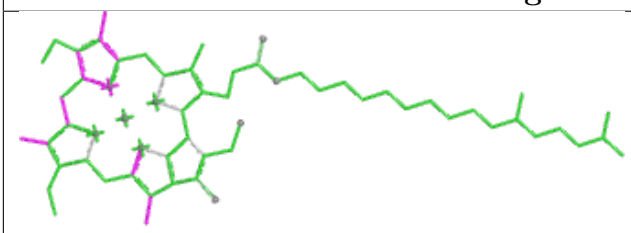


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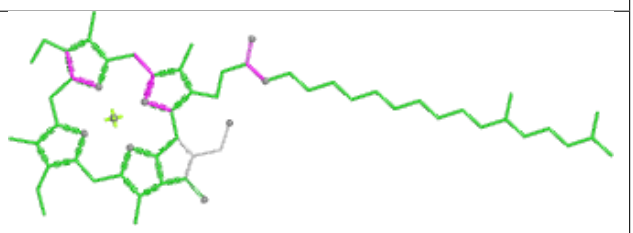


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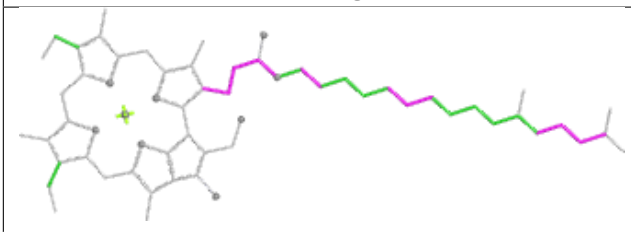
Ligand CLA B 603



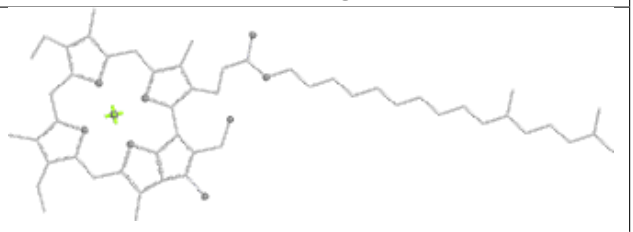
Bond lengths



Bond angles

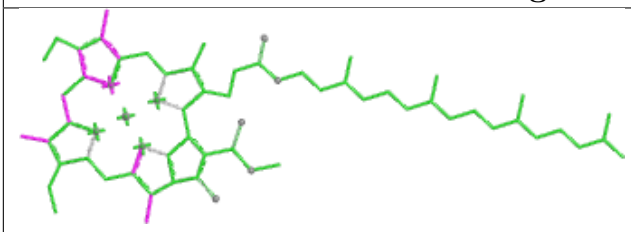


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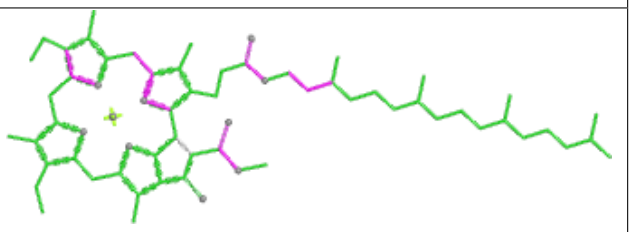


Rings

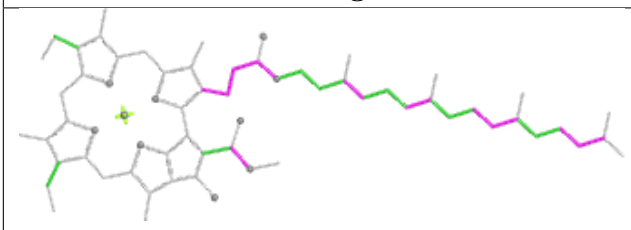
Ligand CLA c 501



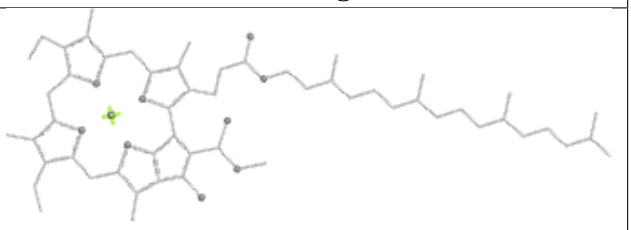
Bond lengths



Bond angles

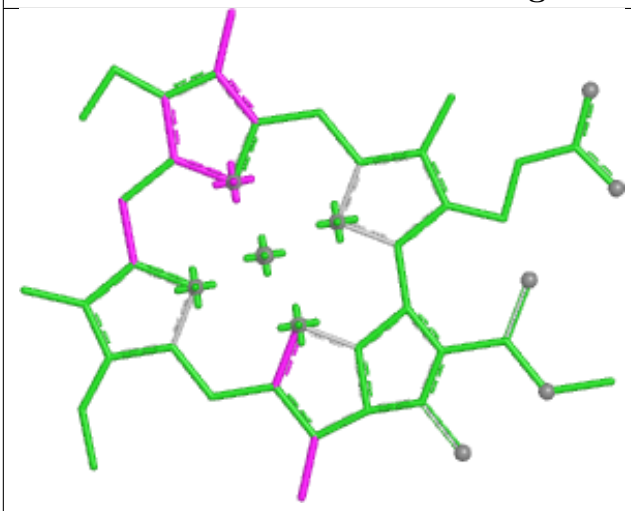


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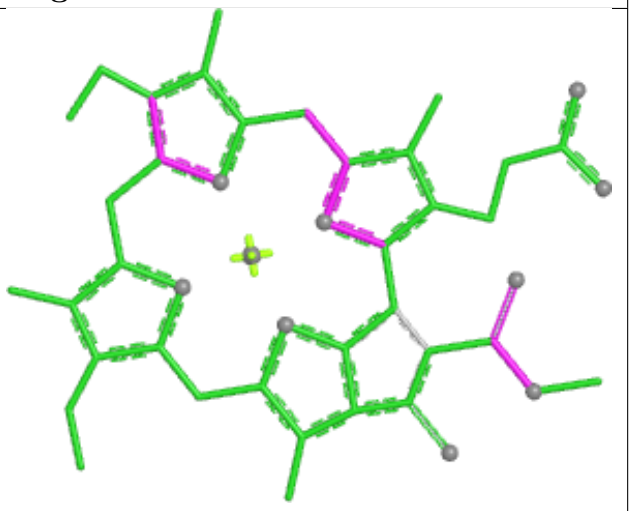


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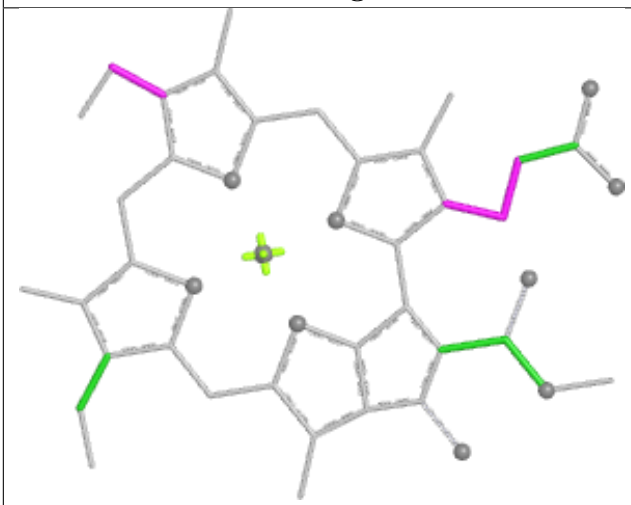
Ligand CLA g 102



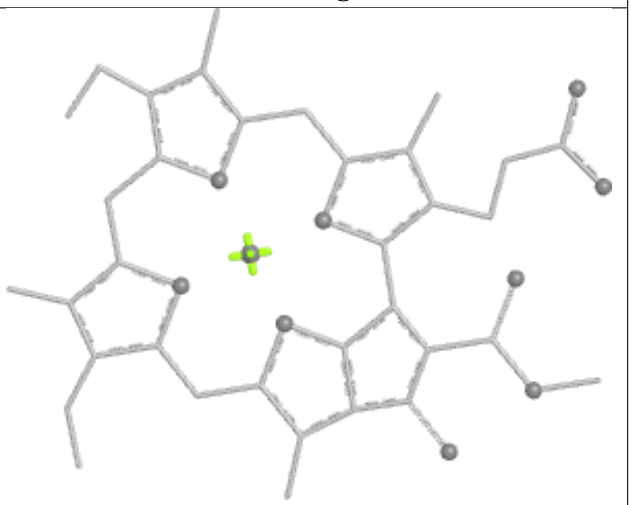
Bond lengths



Bond angles

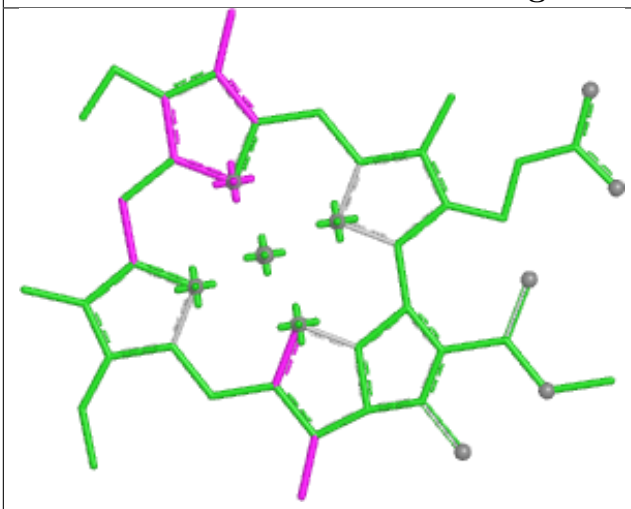


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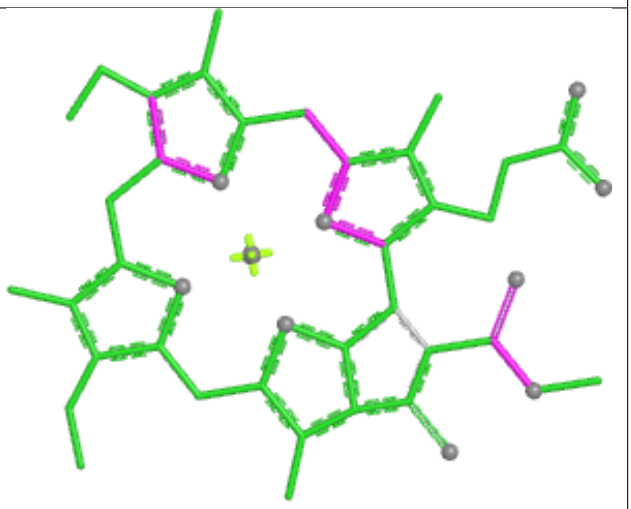


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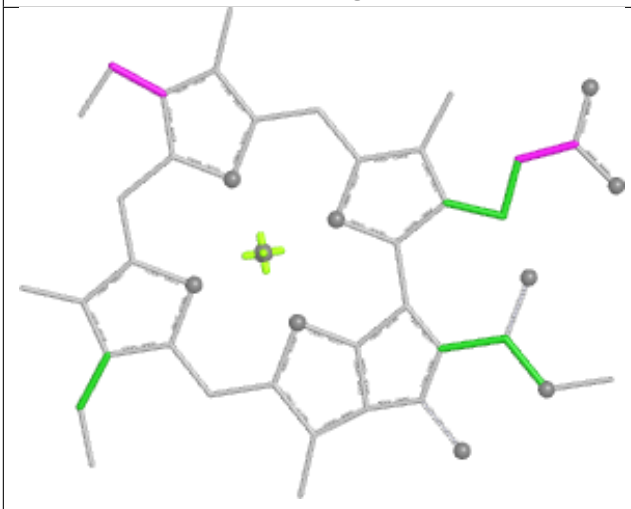
Ligand CLA 4 607



Bond lengths



Bond angles

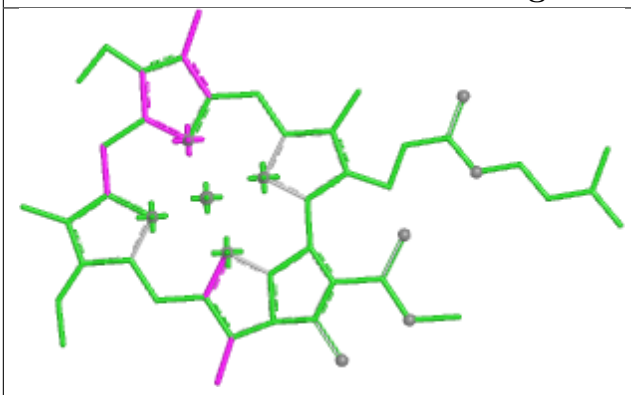


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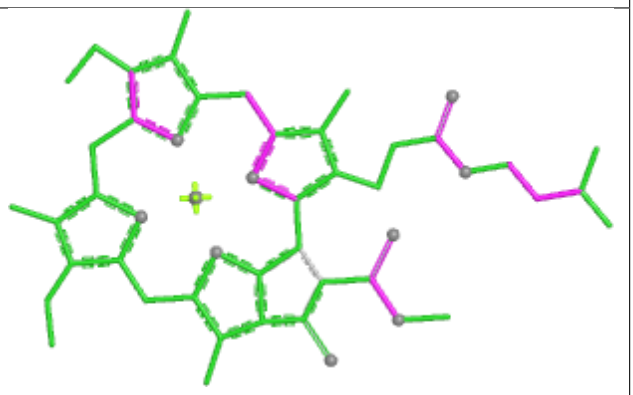


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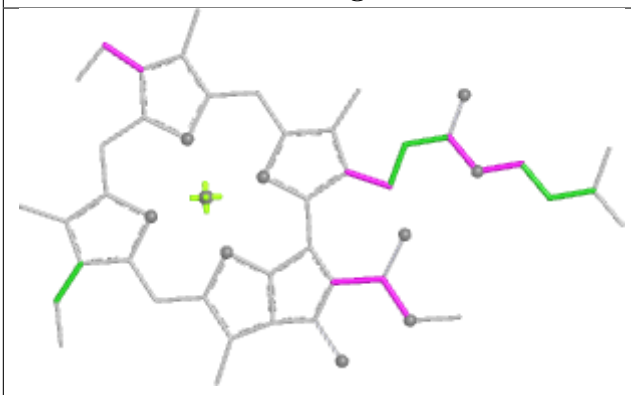
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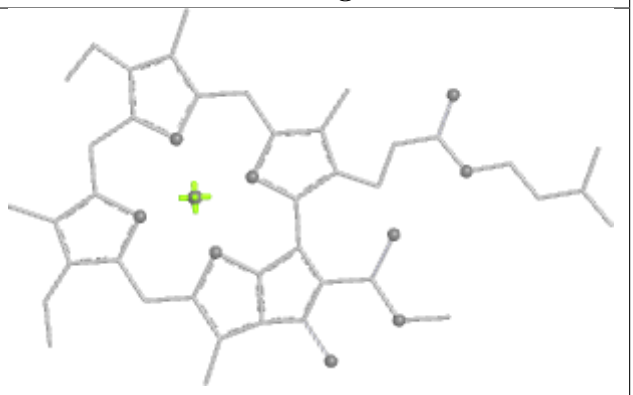
Bond lengths



Bond angles

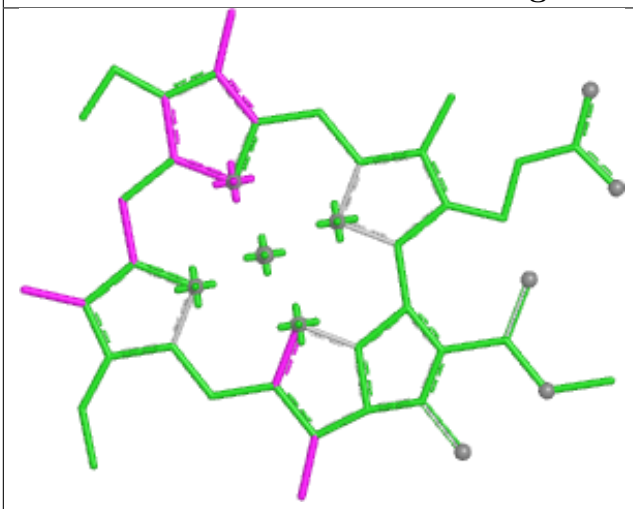


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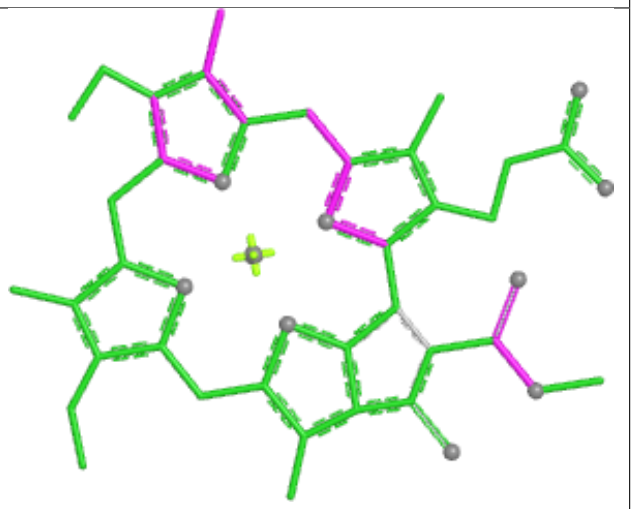


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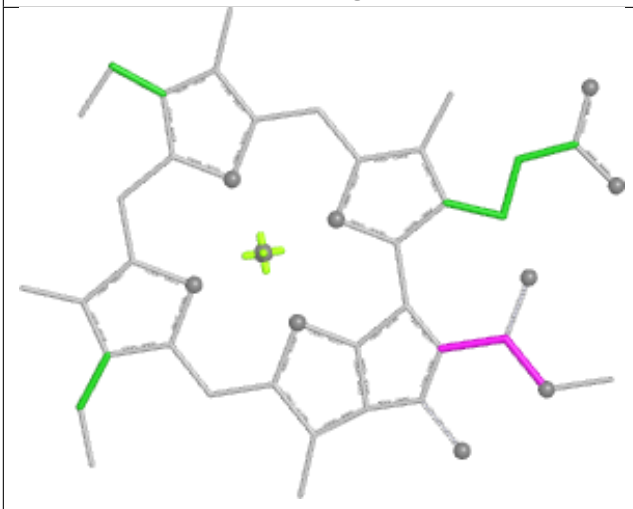
Ligand CLA c 506



Bond lengths



Bond angles

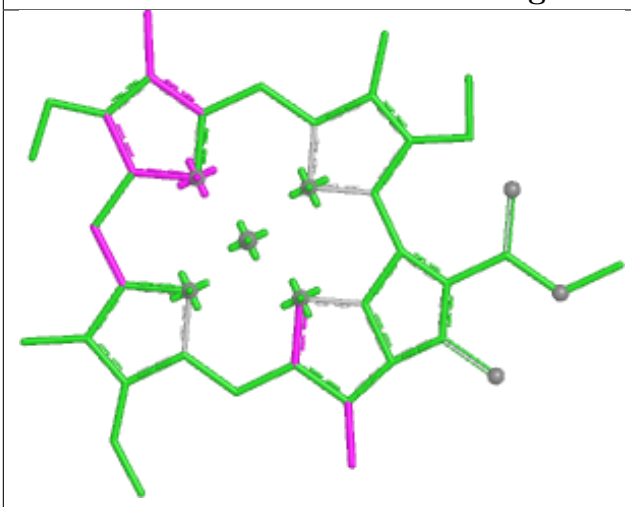


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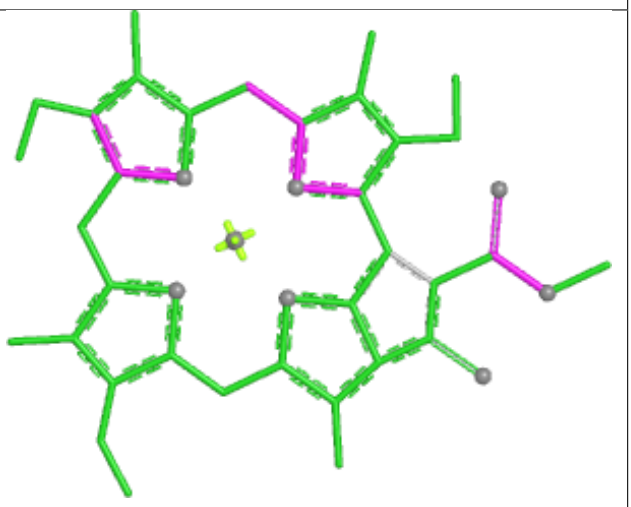


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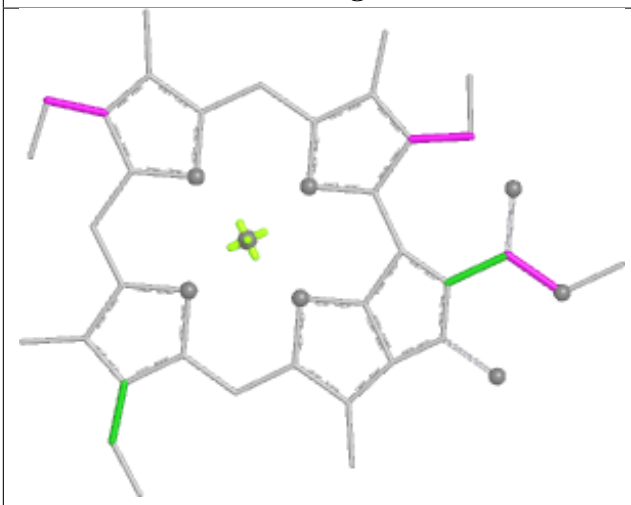
Ligand CLA 7 601



Bond lengths



Bond angles

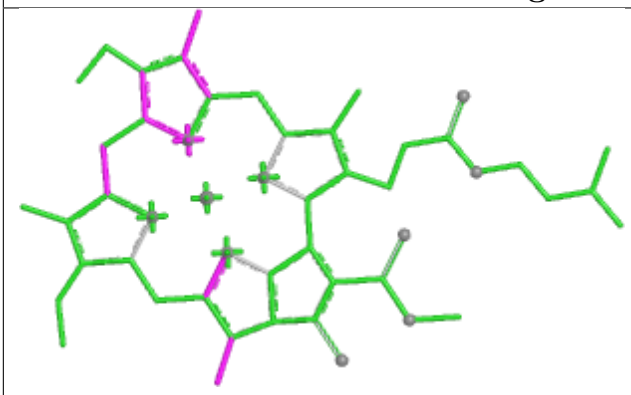


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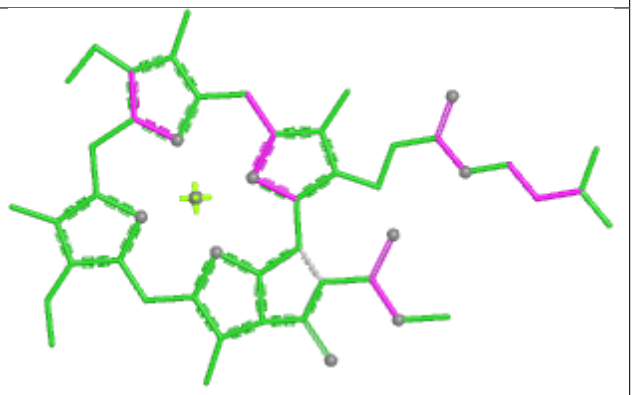


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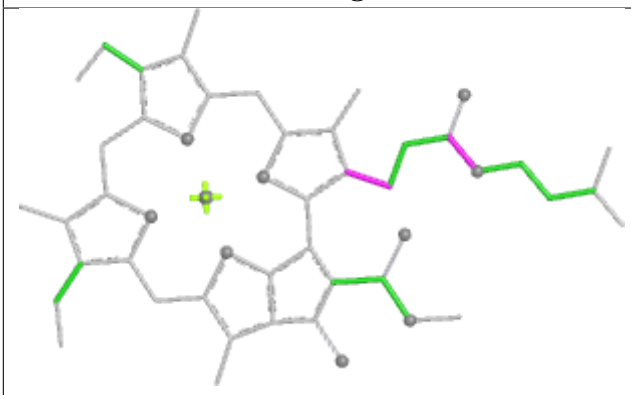
Ligand CLA 0 603



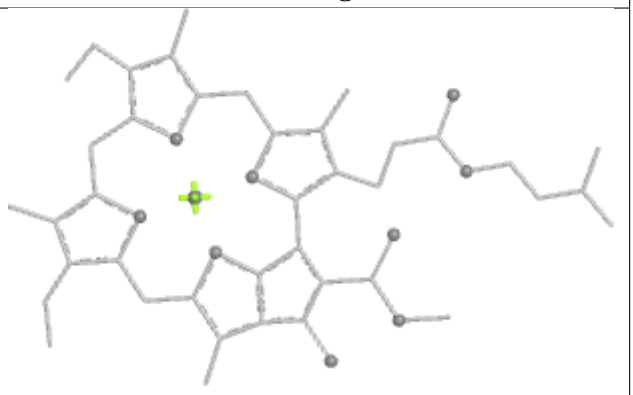
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Bond angles

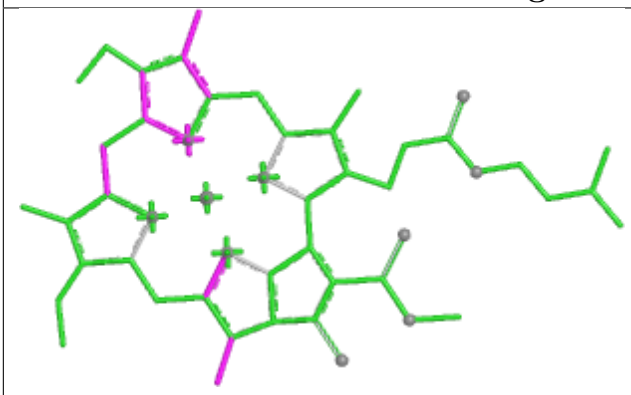


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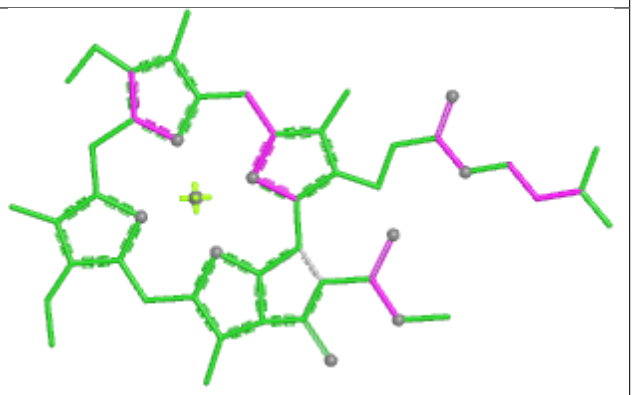


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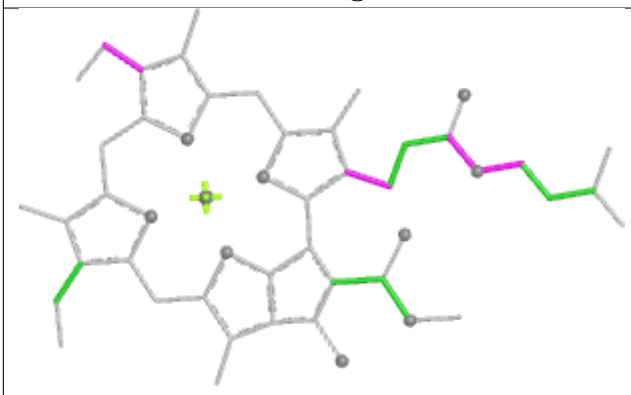
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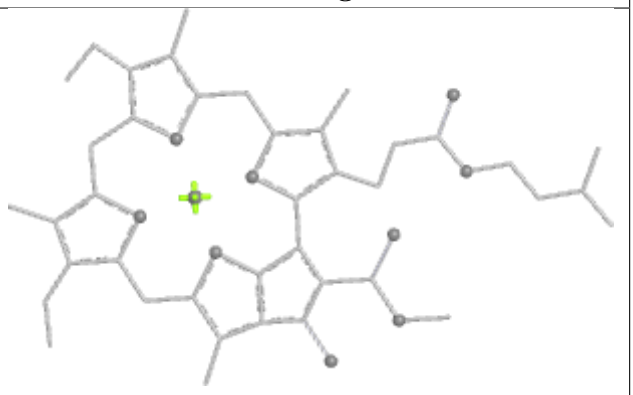
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Bond angles

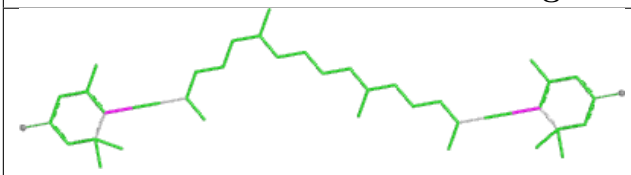


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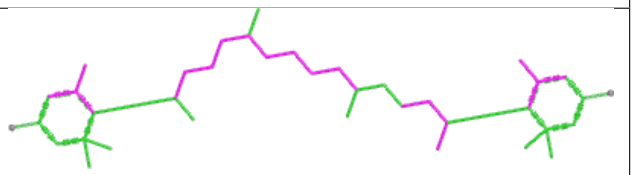


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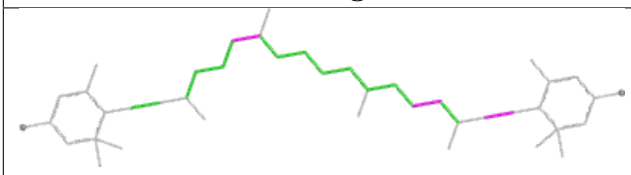
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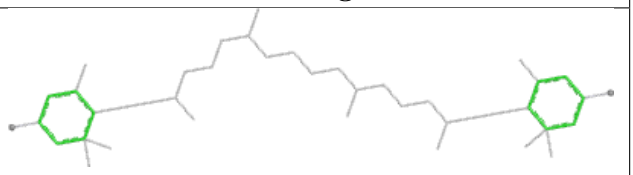
Bond lengths



Bond angles

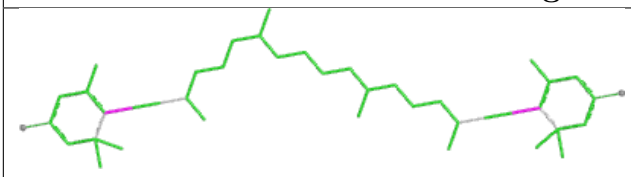


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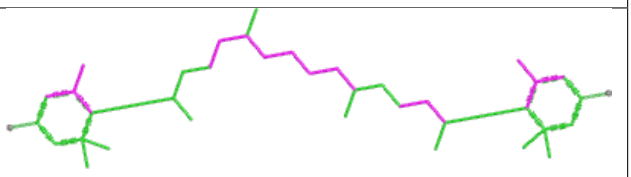


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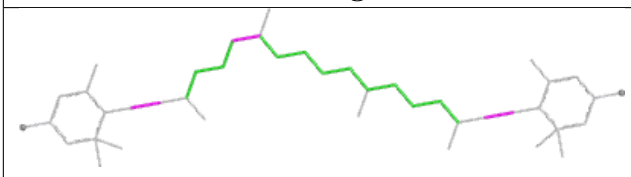
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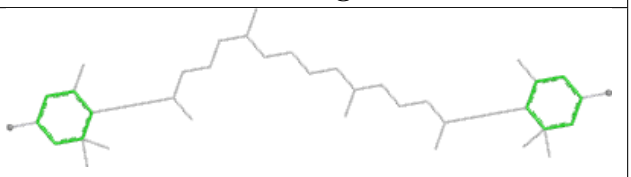
Bond lengths



Bond angles

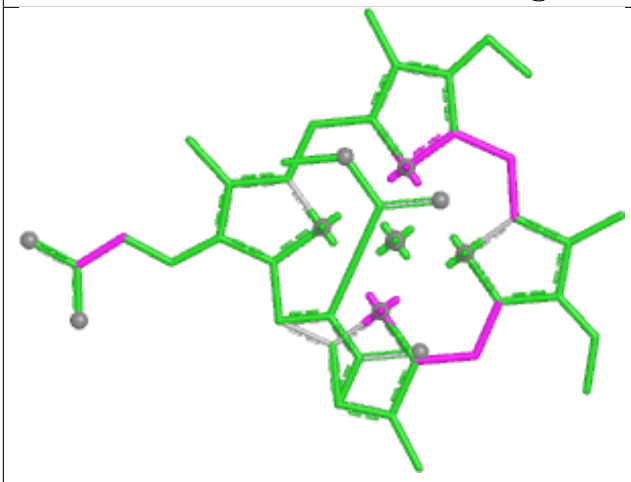


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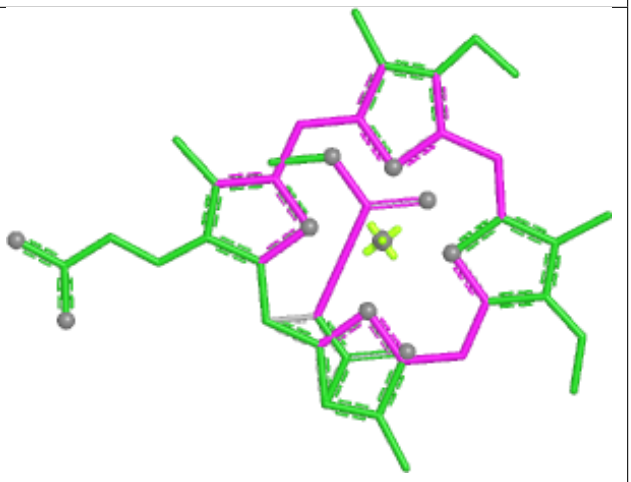


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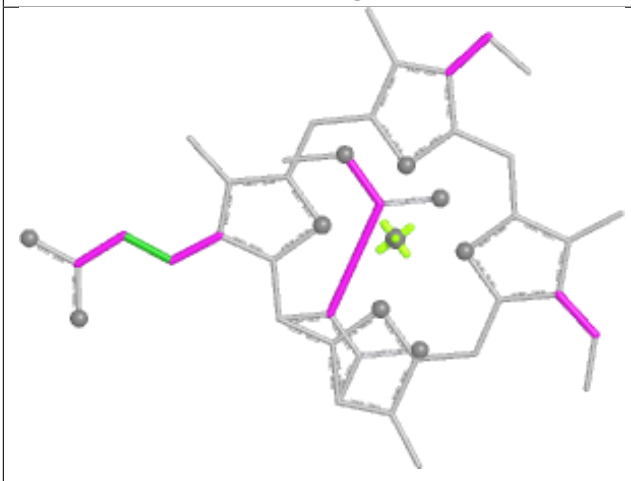
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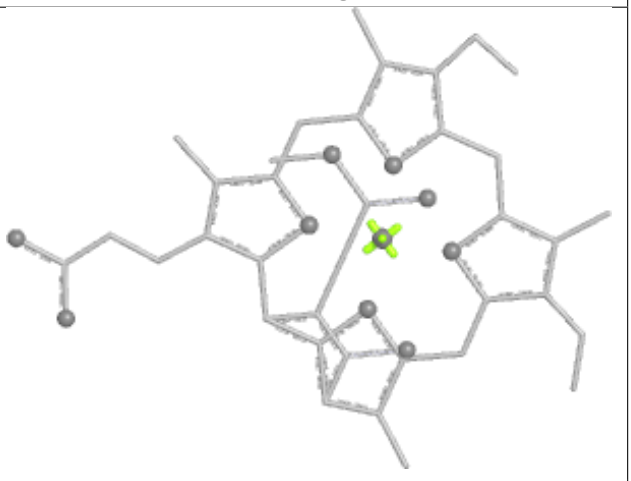
Bond lengths



Bond angles

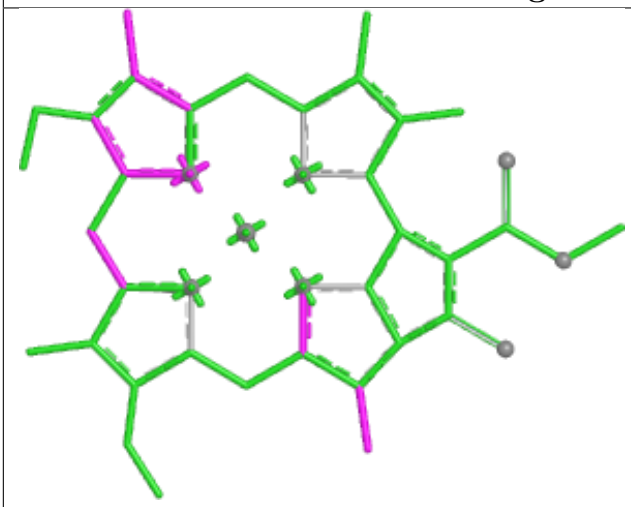


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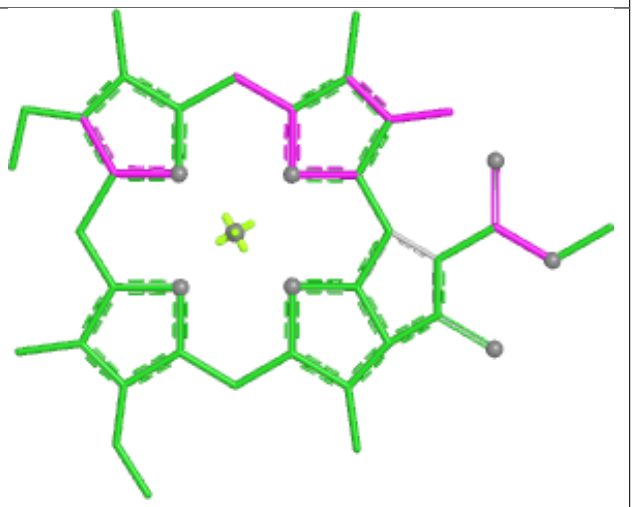


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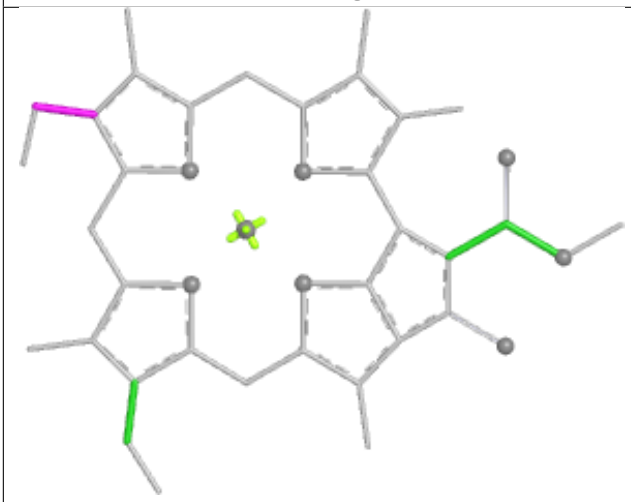
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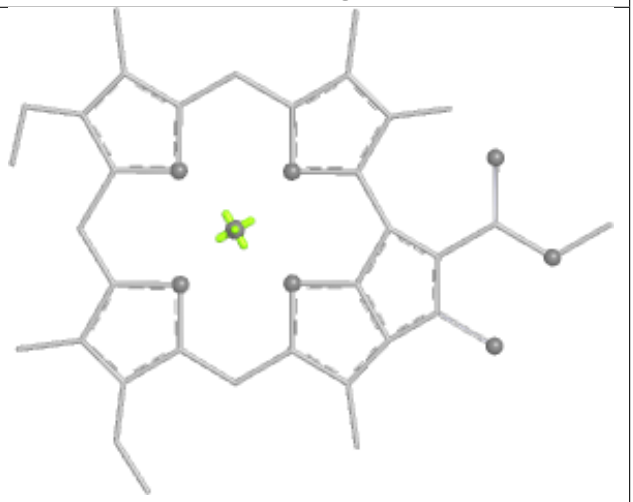
Bond lengths



Bond angles

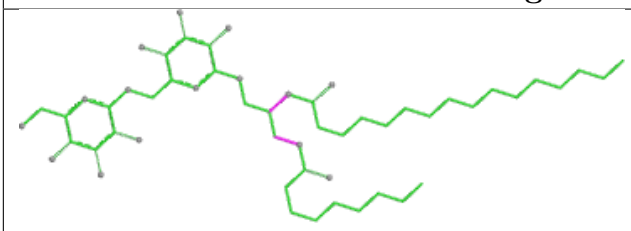


Torsions

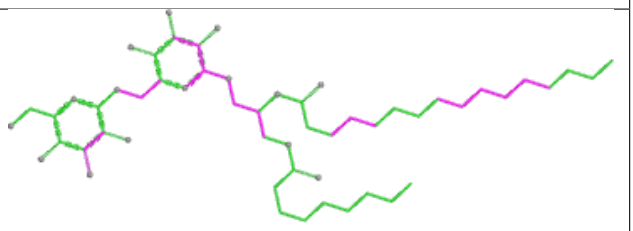


Rings

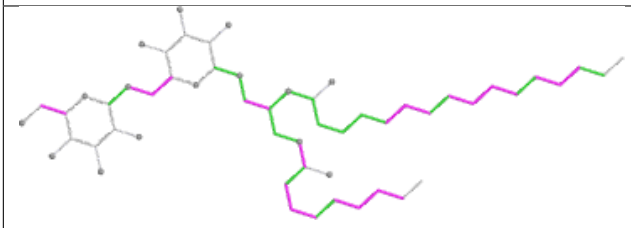
Ligand DGD c 514



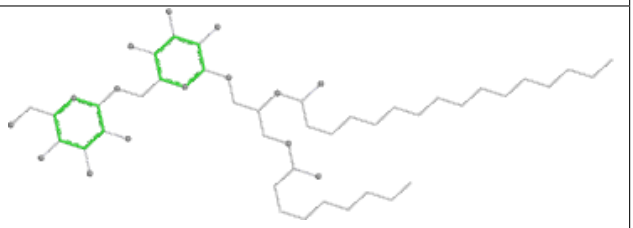
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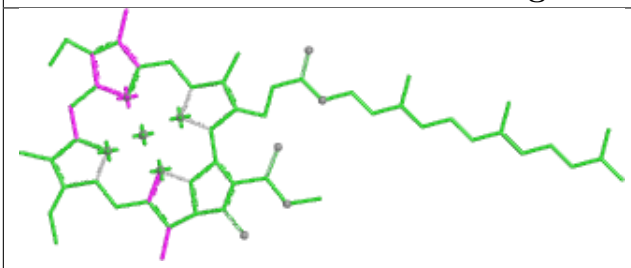
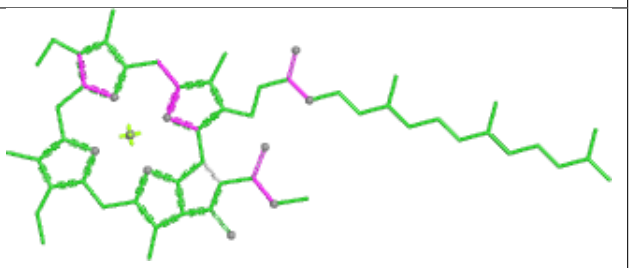
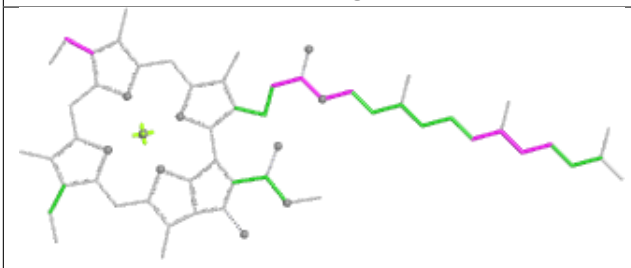
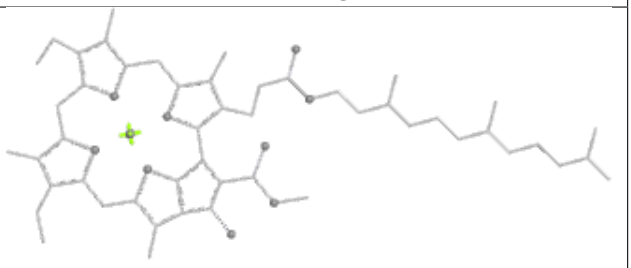
Bond angles

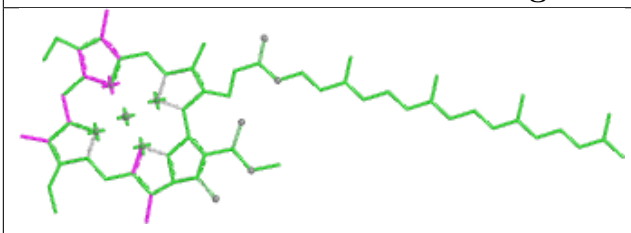
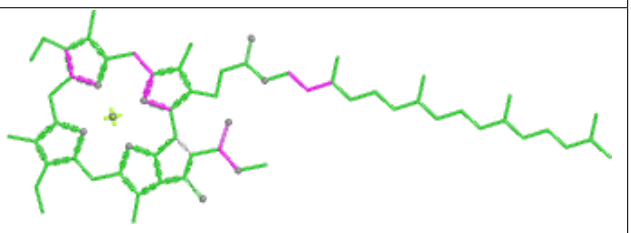
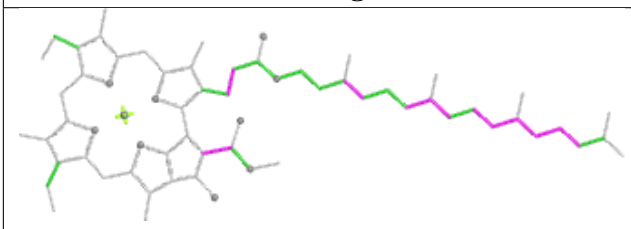
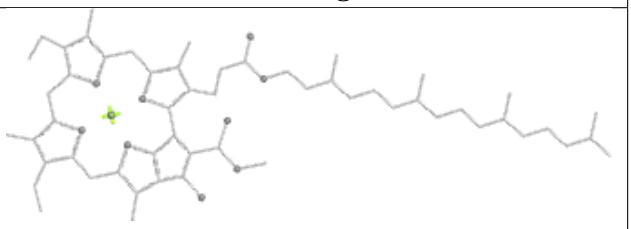


Torsions

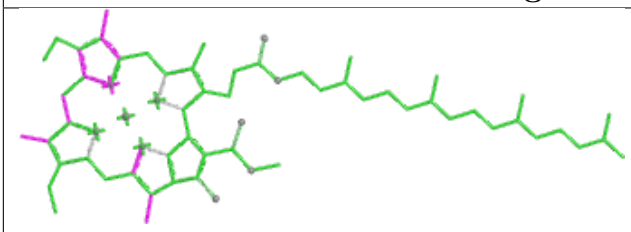


Rings

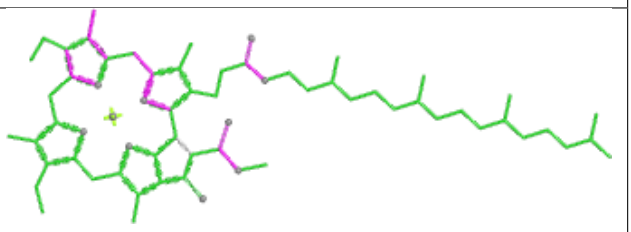
Ligand CLA 2 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

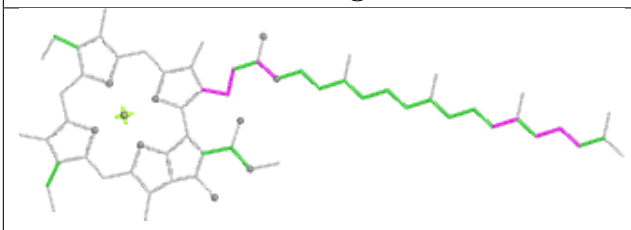
Ligand CLA B 609



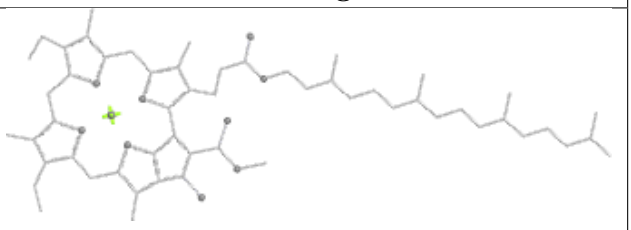
Bond lengths



Bond angles

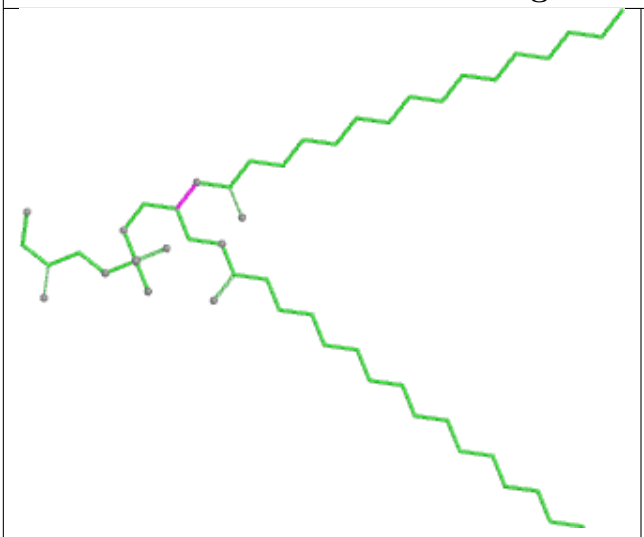


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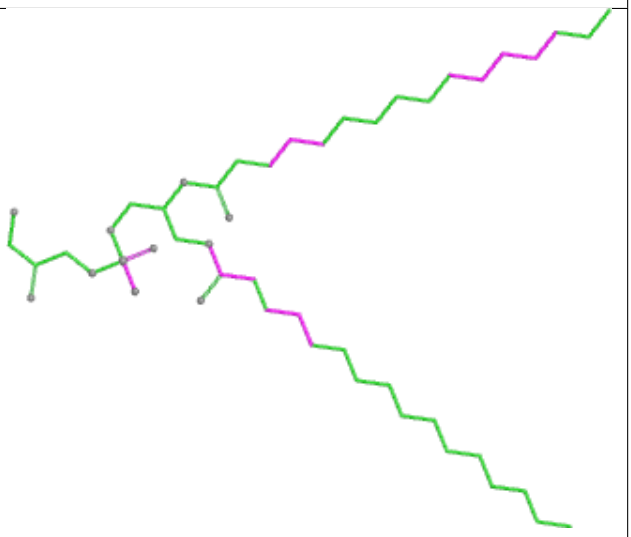


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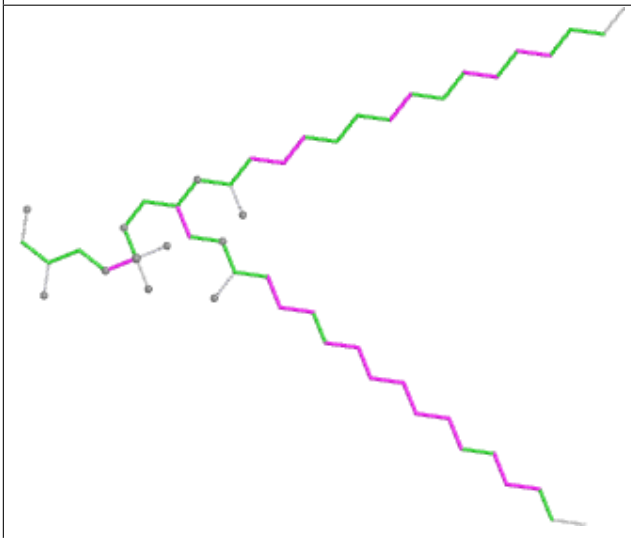
Ligand LHG l 102



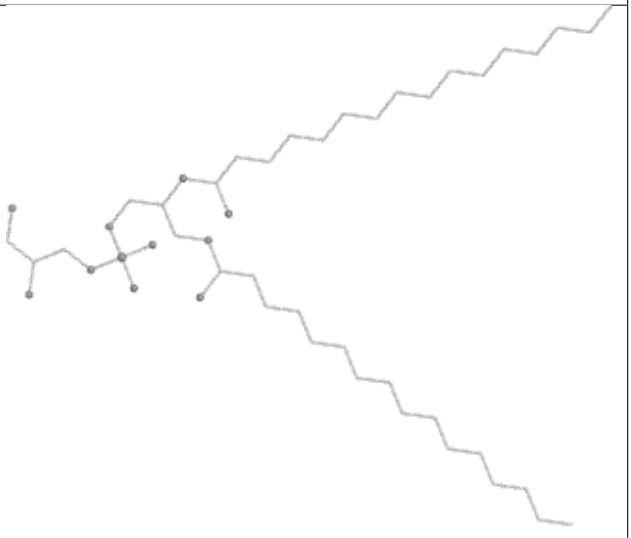
Bond lengths



Bond angles

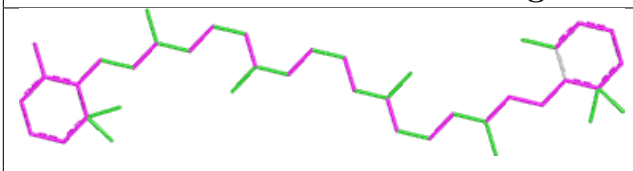


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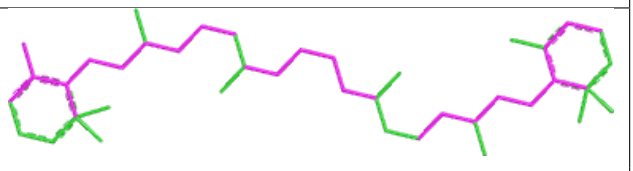


Rings

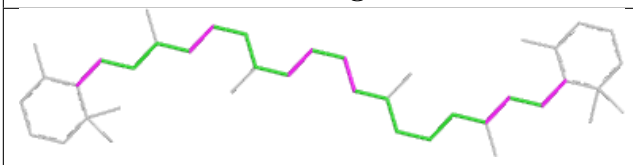
Ligand 8CT B 623



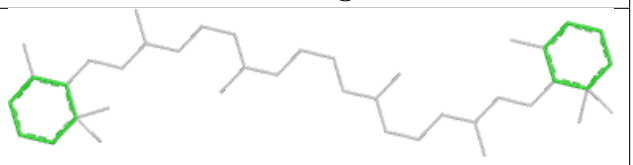
Bond lengths



Bond angles

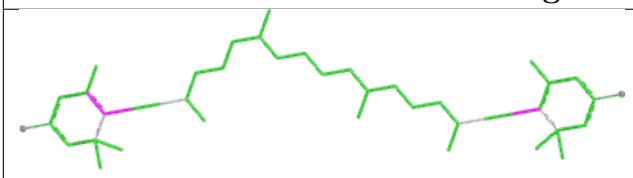


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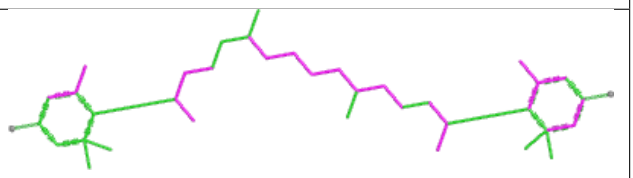


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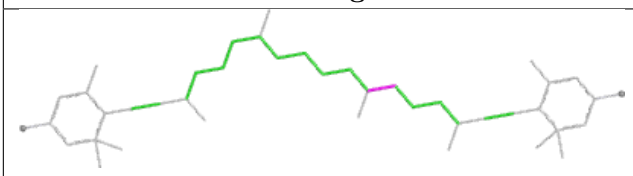
Ligand II0 2 615



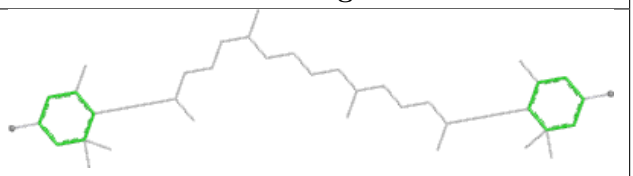
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Bond angles

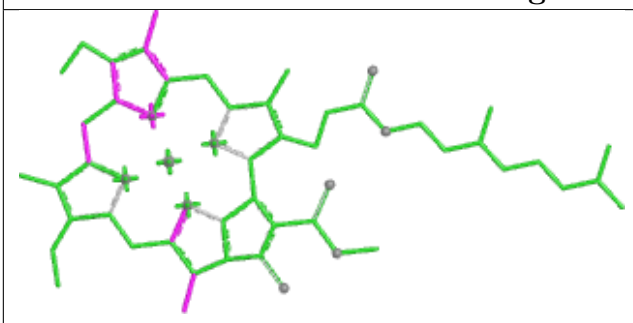


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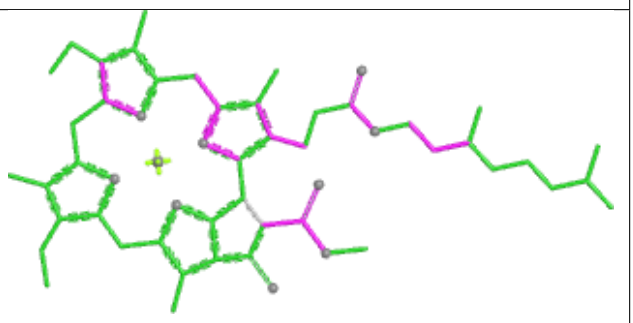


Rings

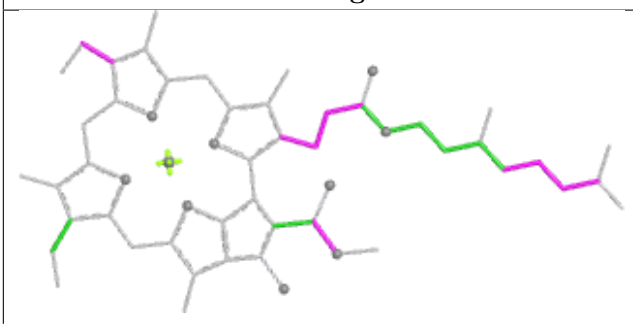
Ligand CLA 4 604



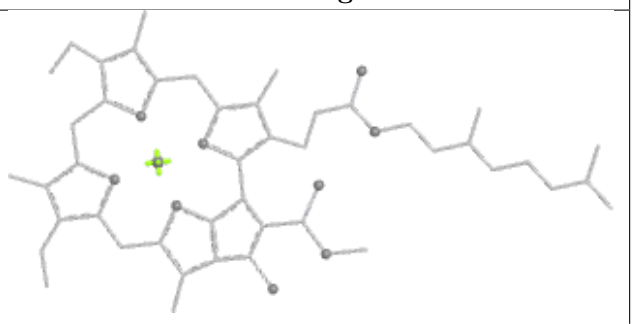
Bond lengths



Bond angles

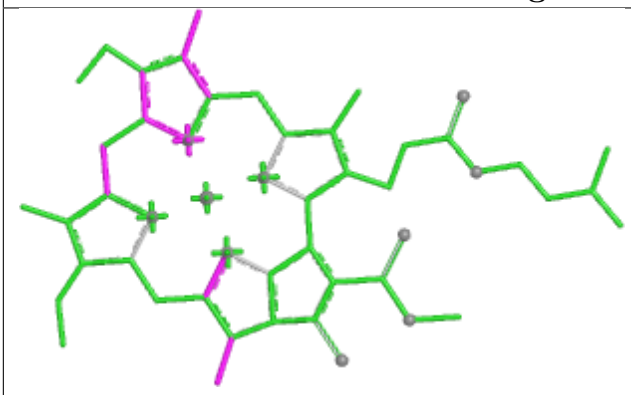


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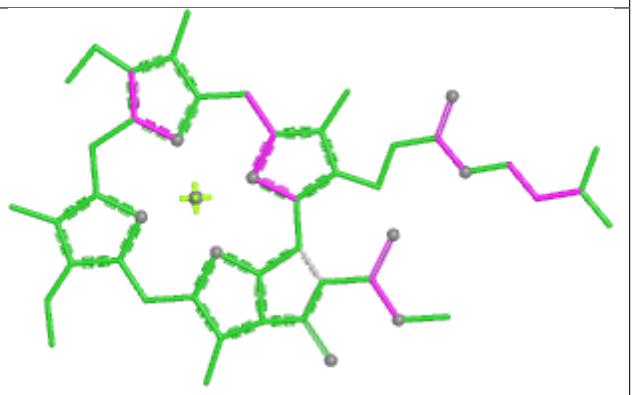


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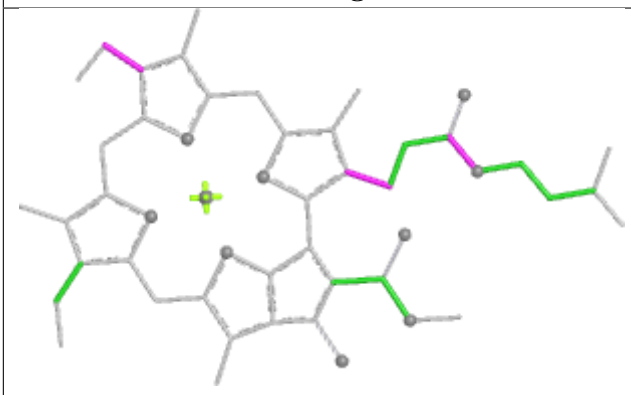
Ligand CLA 8 603



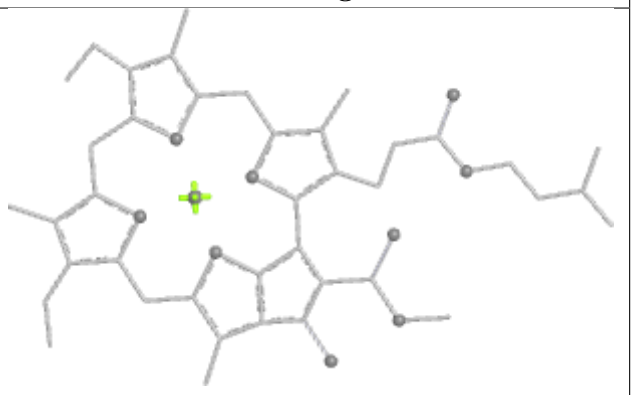
Bond lengths



Bond angles

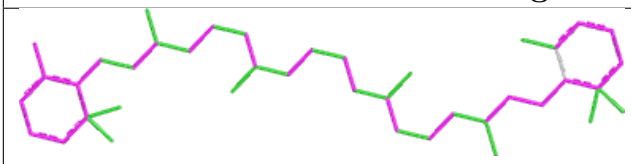


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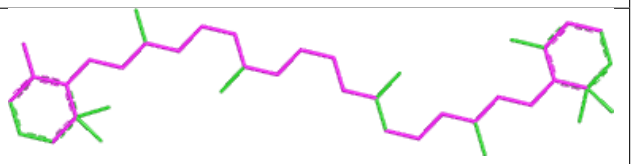


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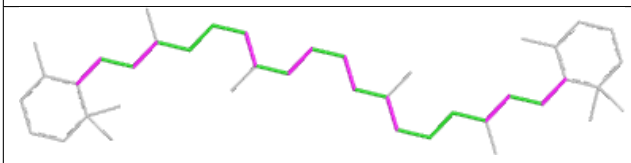
Ligand 8CT k 102



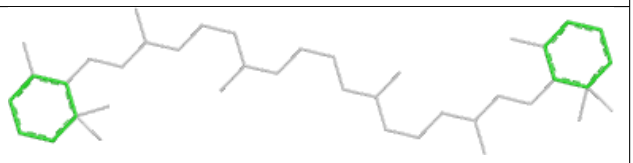
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Bond angles

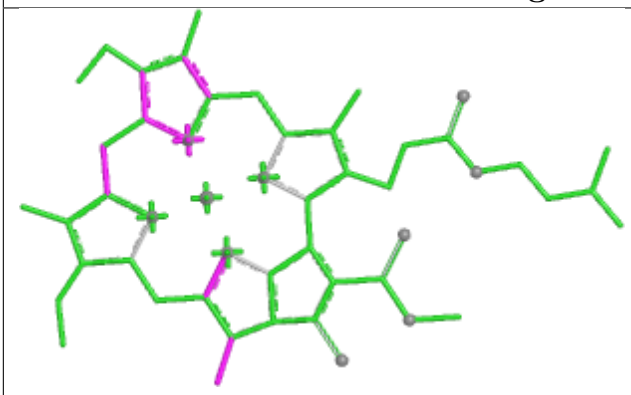


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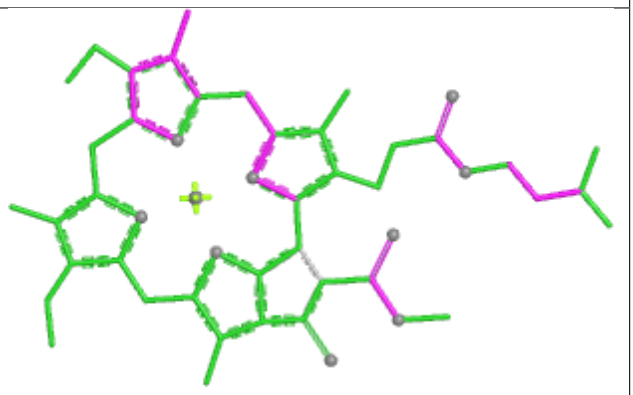


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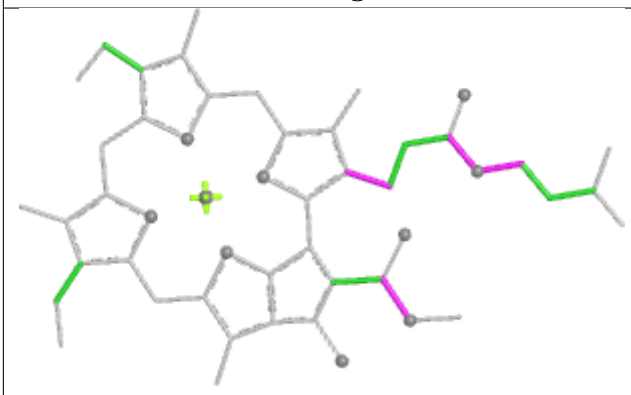
Ligand CLA 7 603



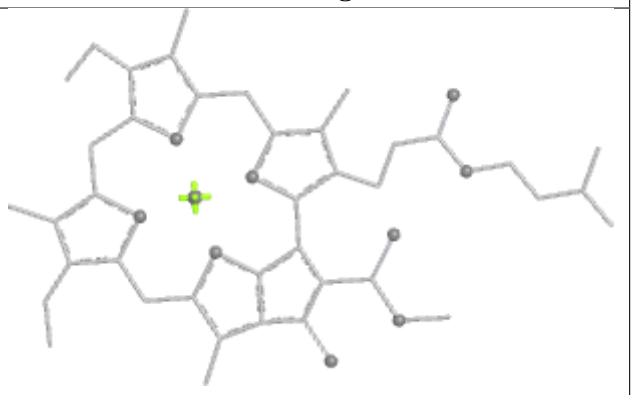
Bond lengths



Bond angles

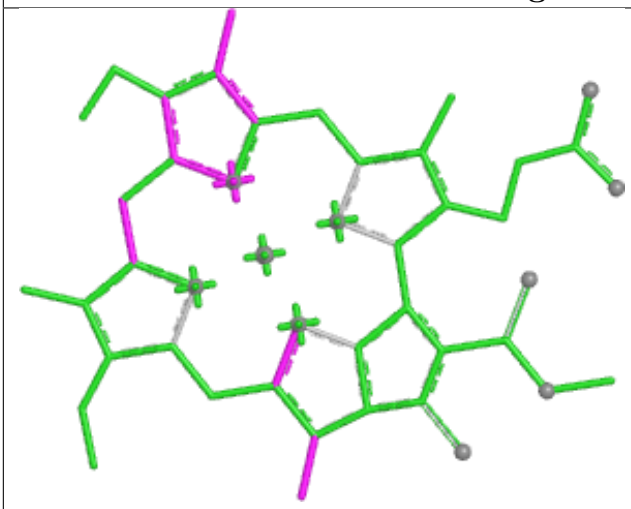


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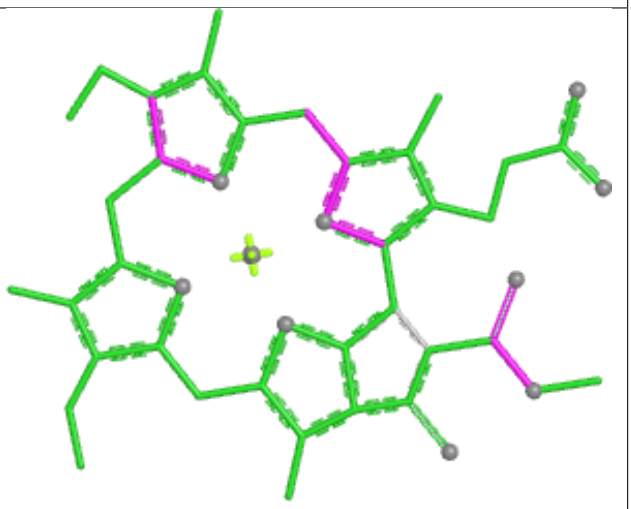


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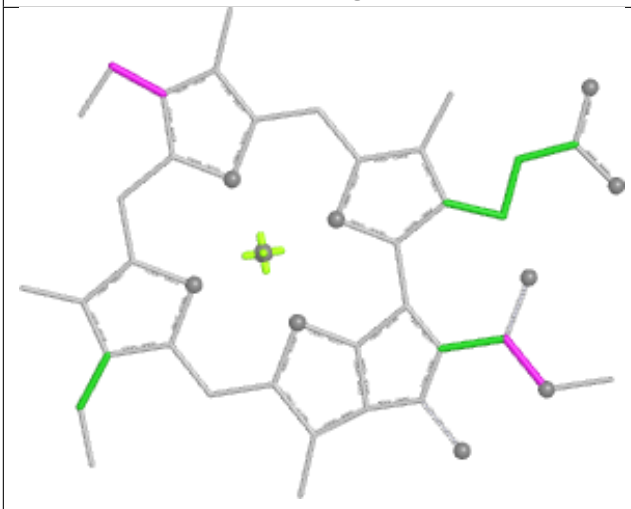
Ligand CLA 8 607



Bond lengths



Bond angles

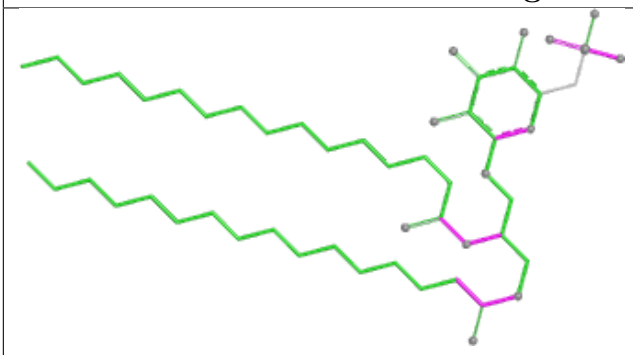


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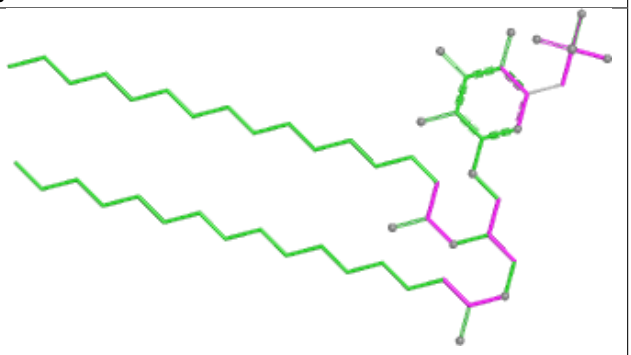


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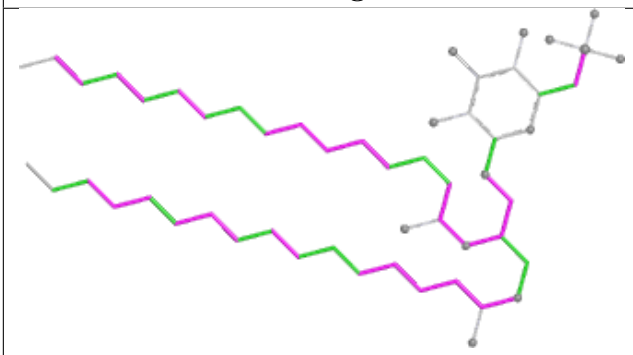
Ligand SQD A 606



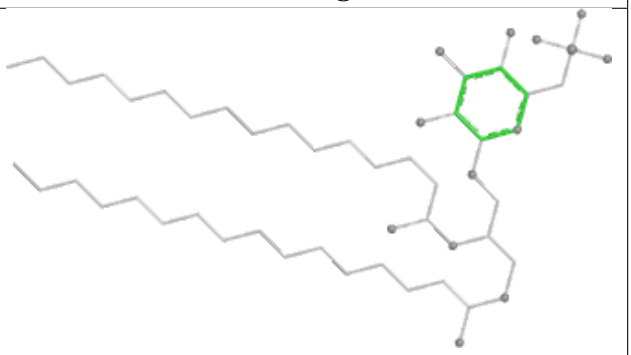
Bond lengths



Bond angles

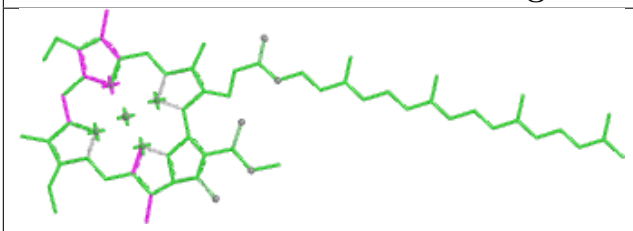


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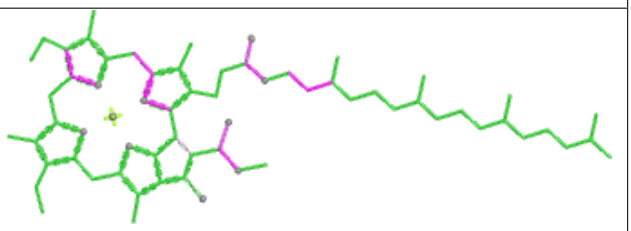


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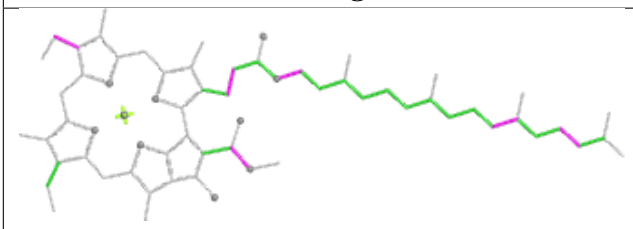
Ligand CLA b 611



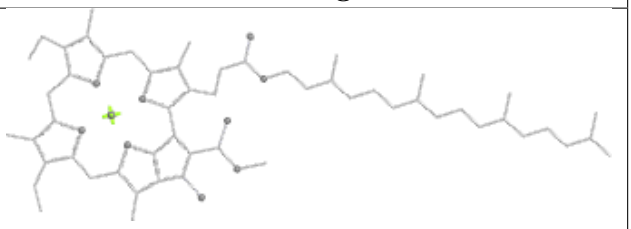
Bond lengths



Bond angles

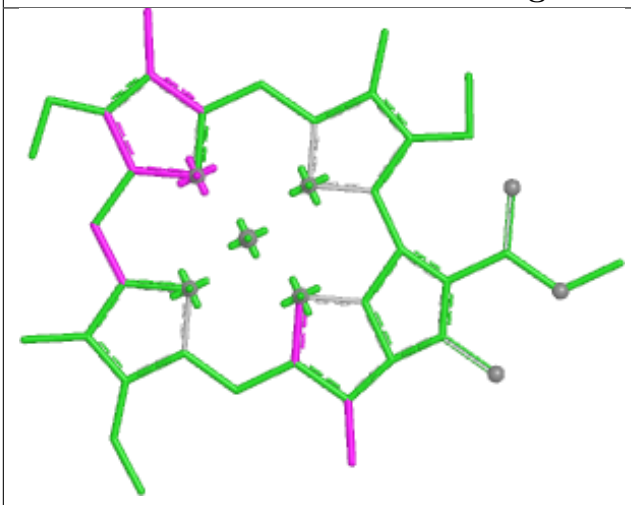


Torsions

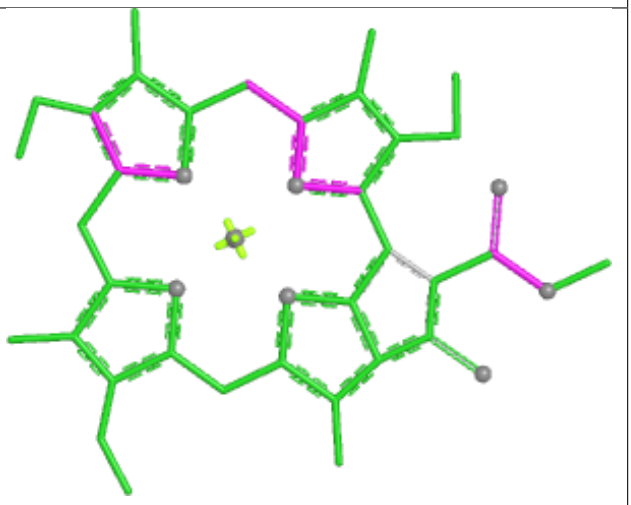


Rings

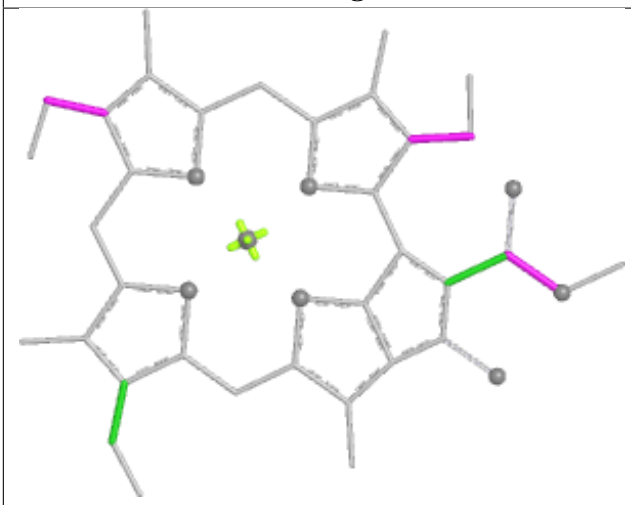
Ligand CLA 3 601



Bond lengths



Bond angles

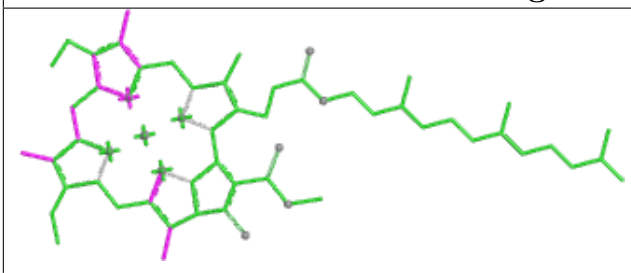


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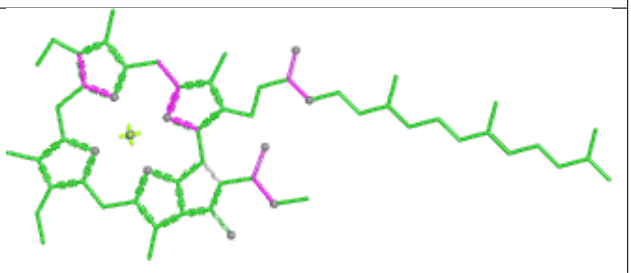


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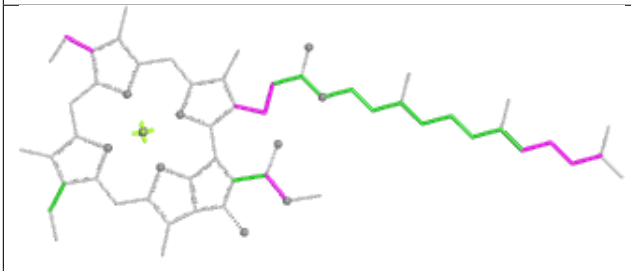
Ligand CLA 8 608



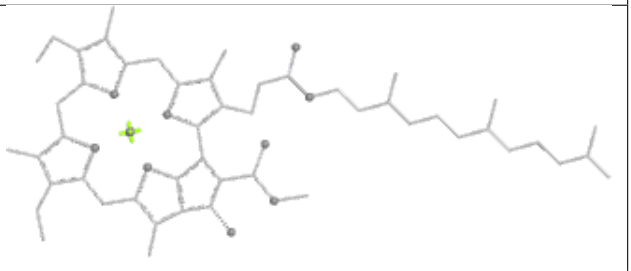
Bond lengths



Bond angles

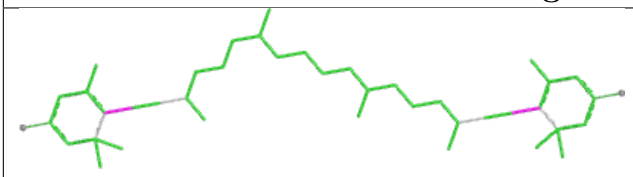


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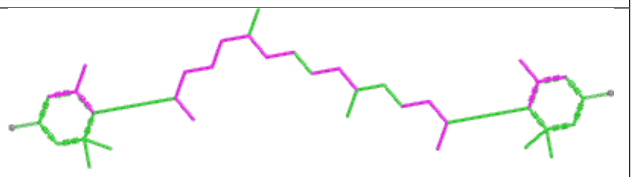


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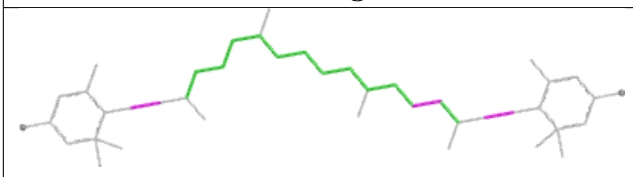
Ligand II0 9 612



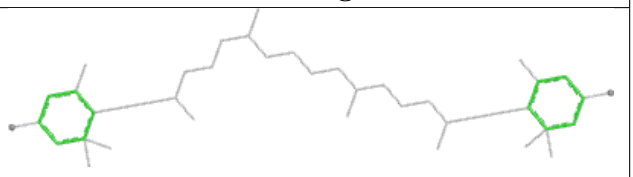
Bond lengths



Bond angles

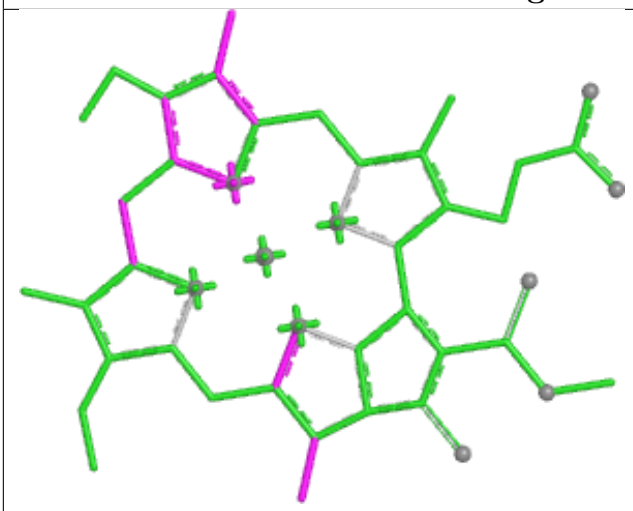


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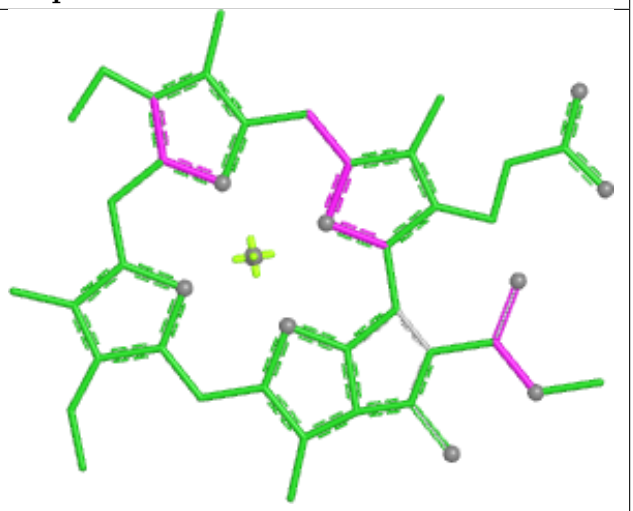


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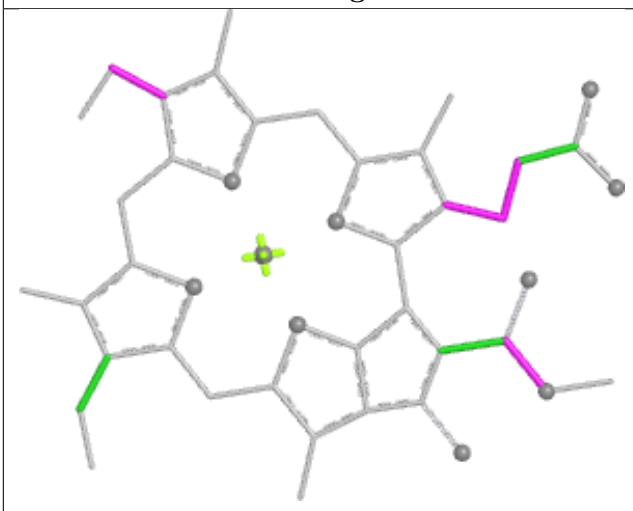
Ligand CLA p 312



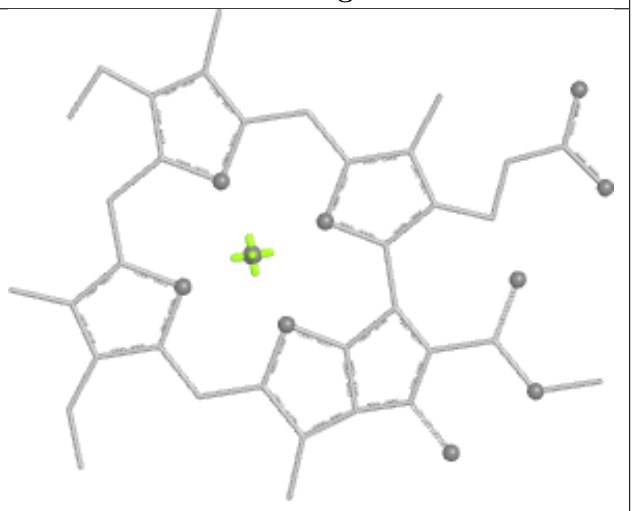
Bond lengths



Bond angles

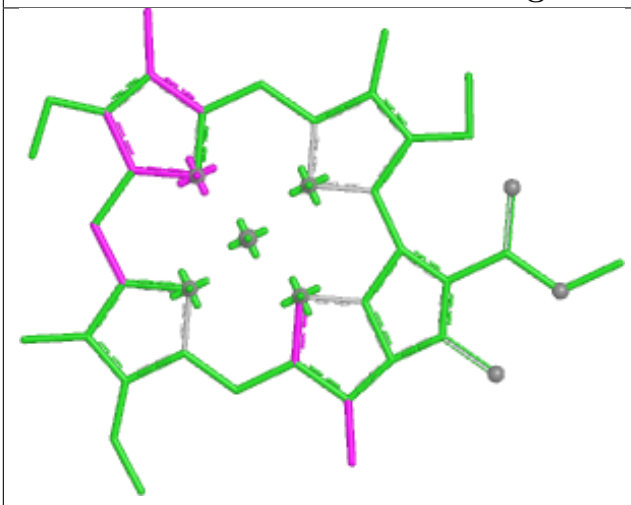


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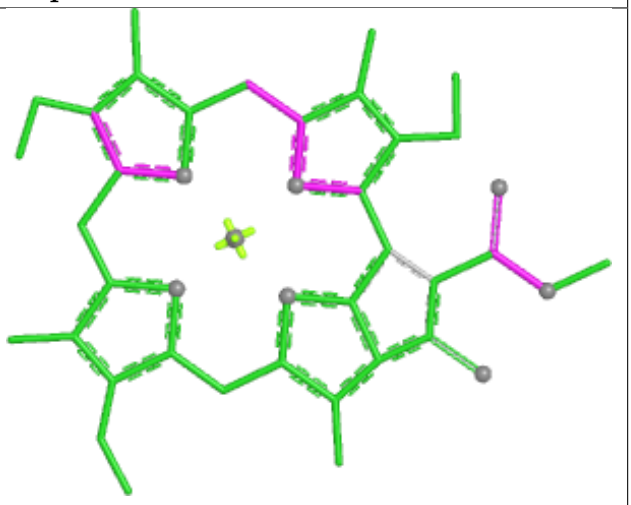


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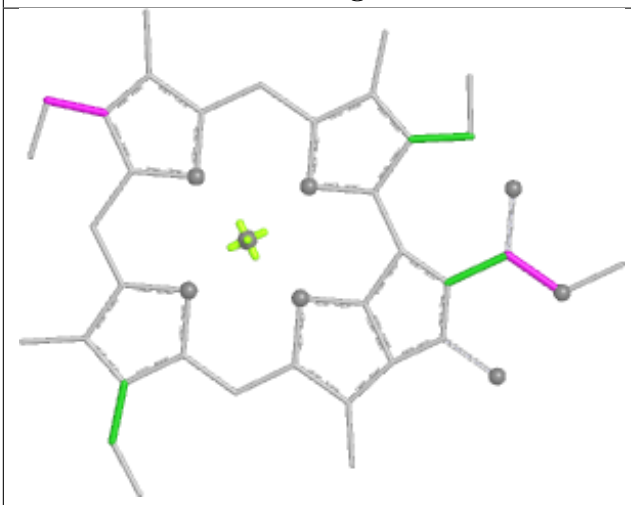
Ligand CLA p 302



Bond lengths



Bond angles

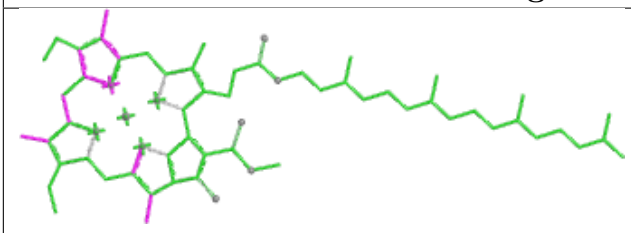


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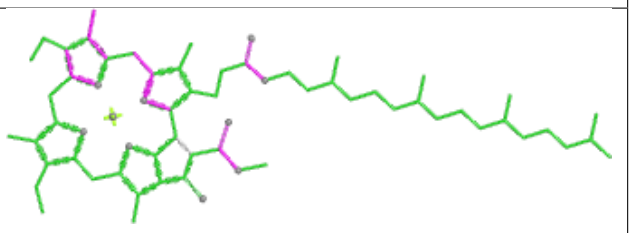


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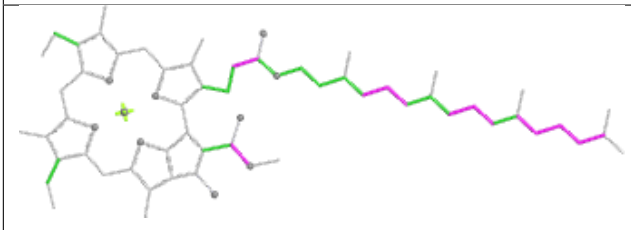
Ligand CLA b 614



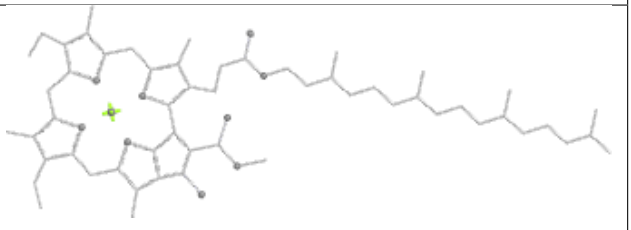
Bond lengths



Bond angles

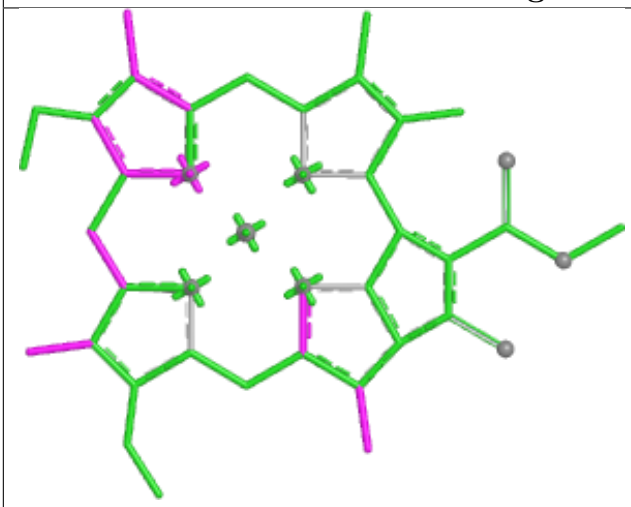


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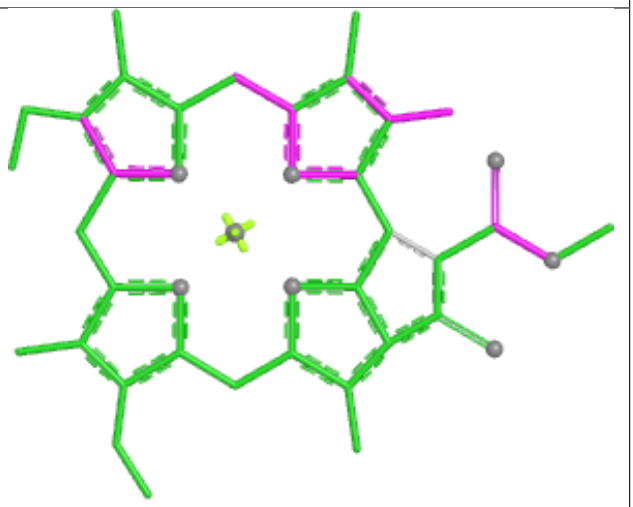


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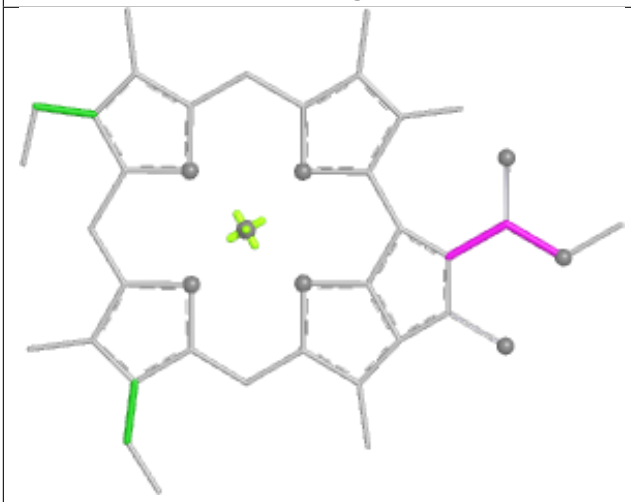
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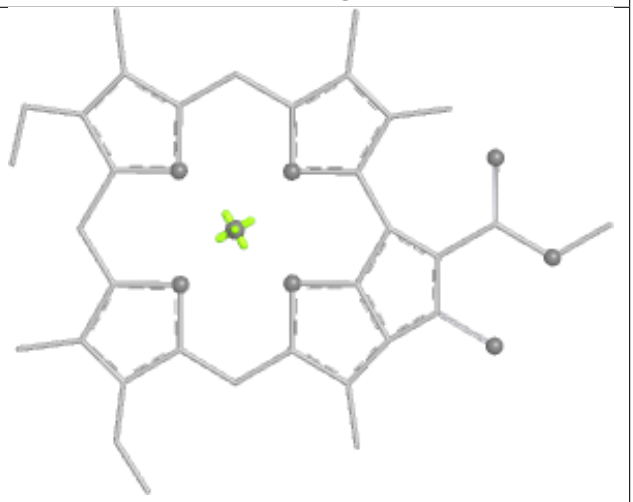
Bond lengths



Bond angles

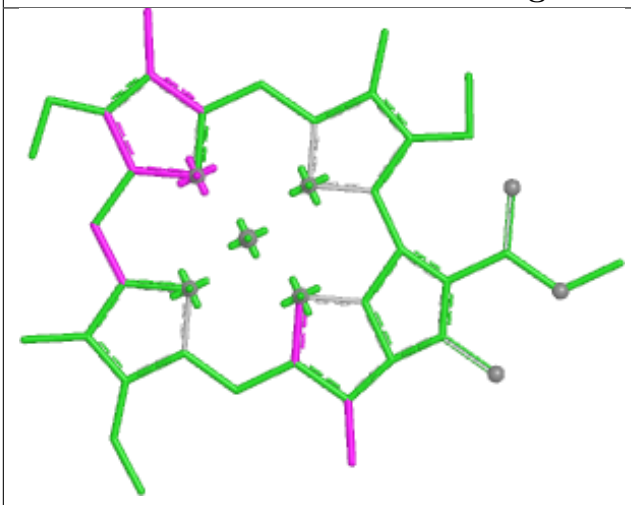


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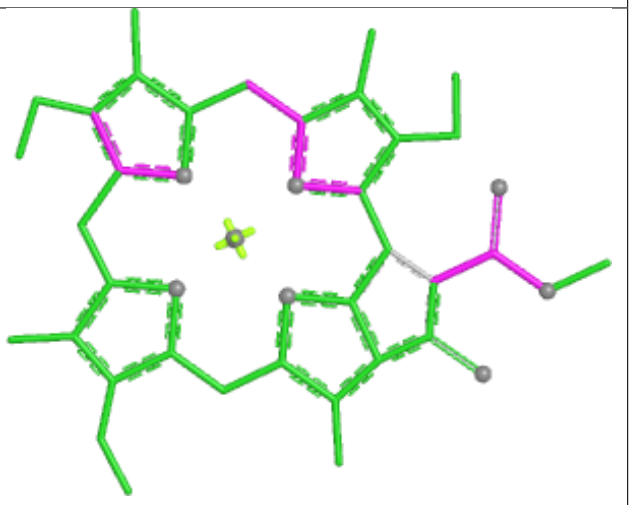


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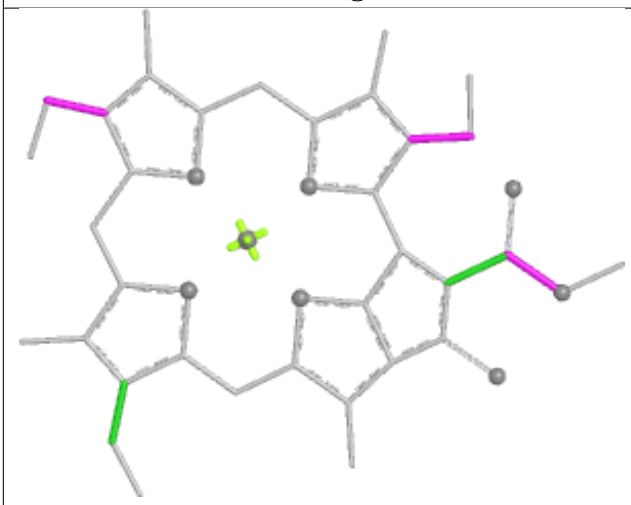
Ligand CLA 9 601



Bond lengths



Bond angles

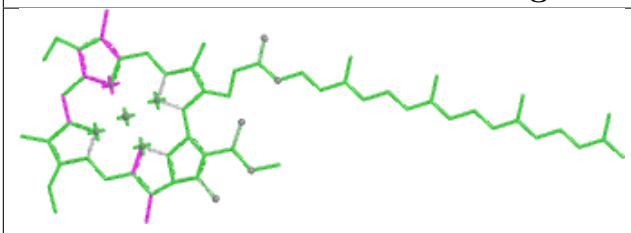


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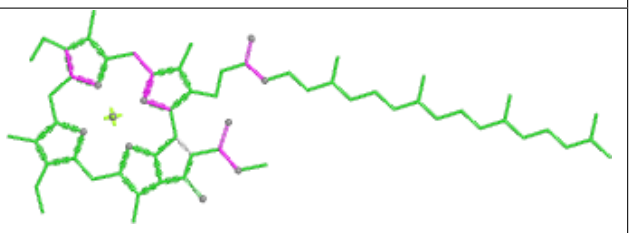


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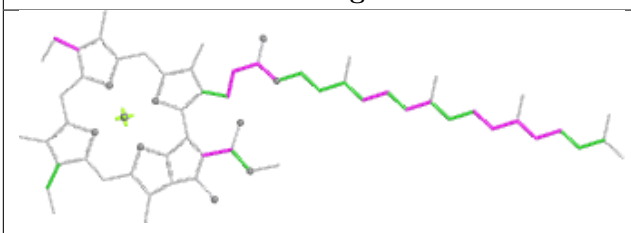
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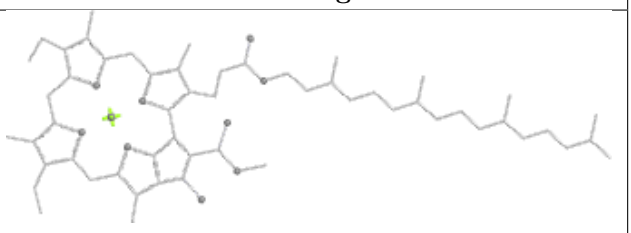
Bond lengths



Bond angles

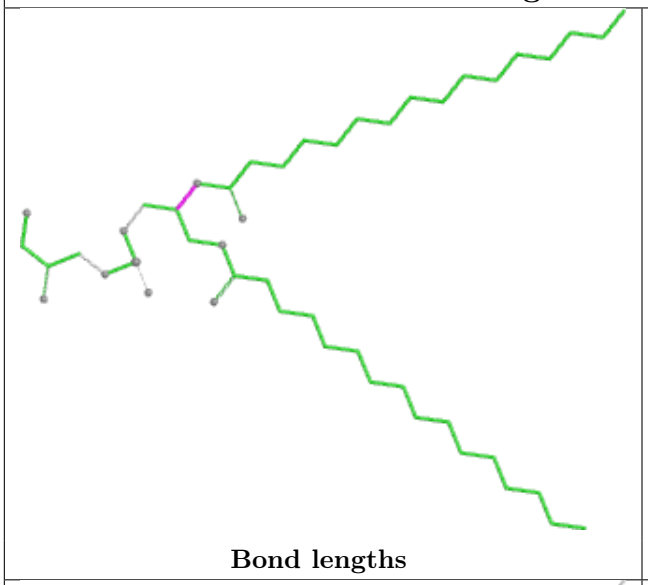


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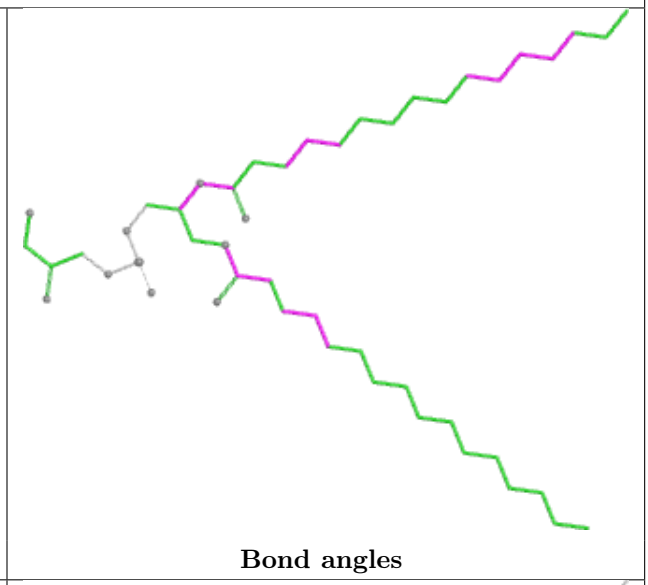


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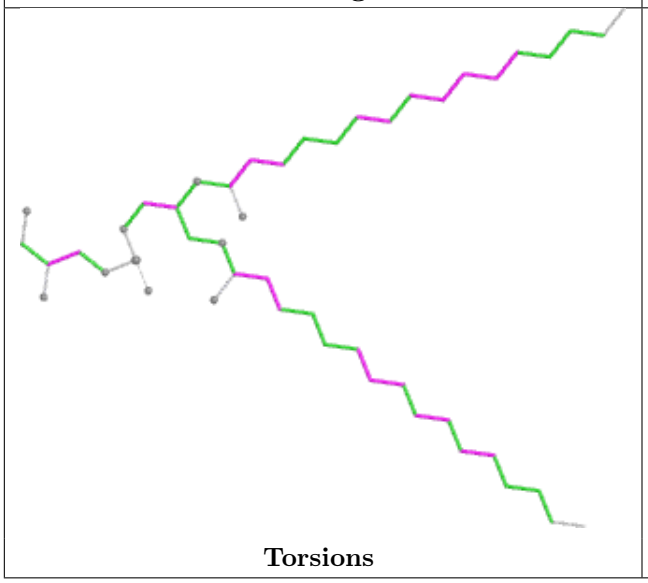
Ligand LHG D 406



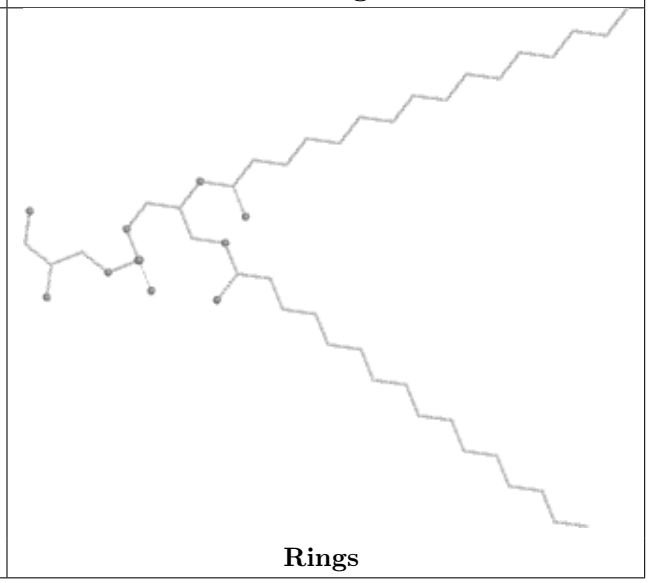
Bond lengths



Bond angles

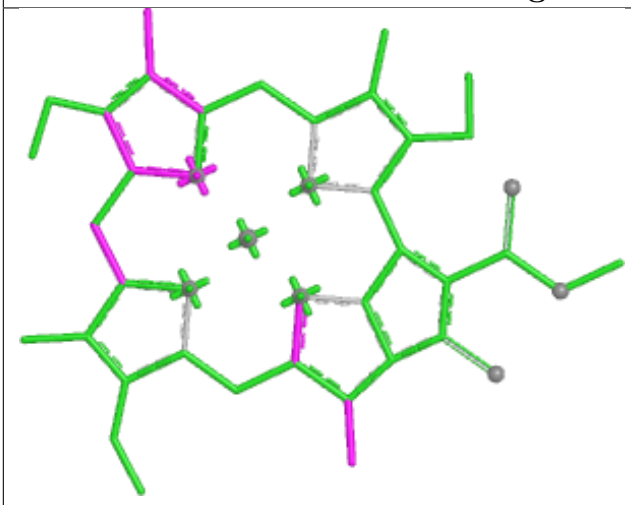


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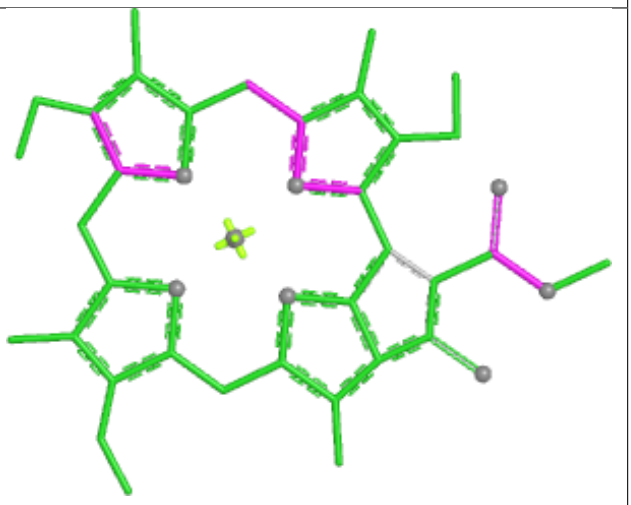


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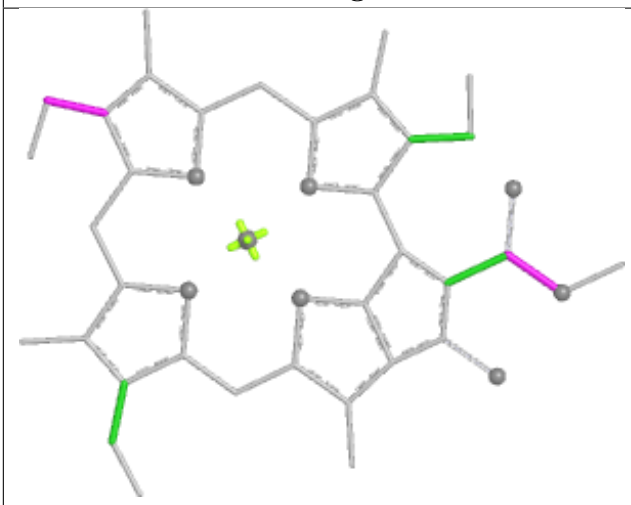
Ligand CLA 5 302



Bond lengths



Bond angles

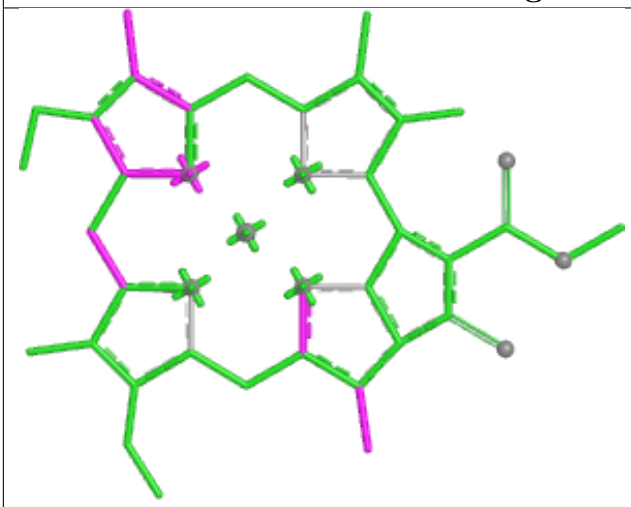


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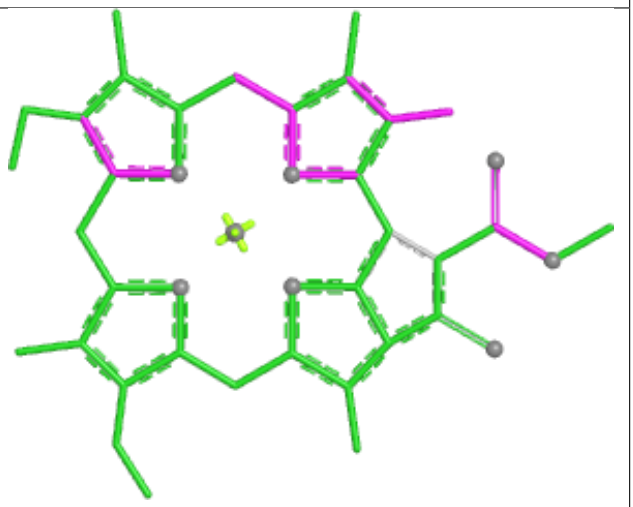


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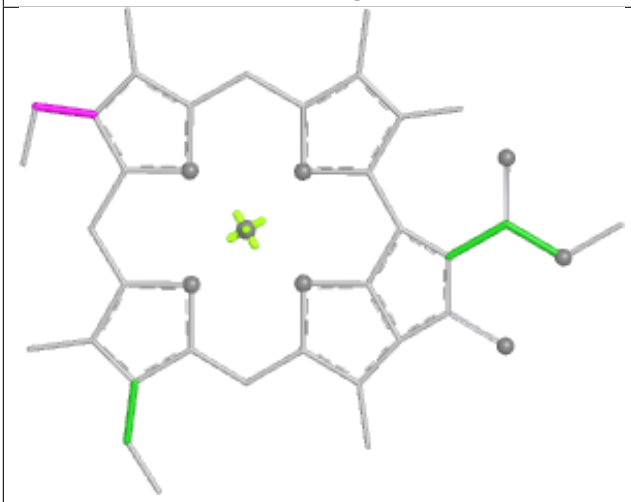
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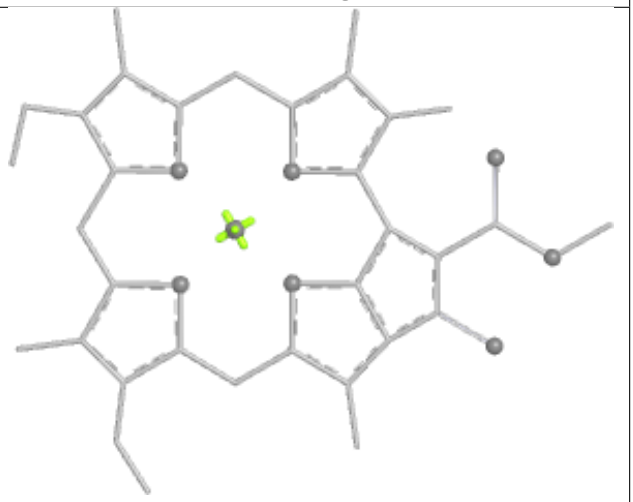
Bond lengths



Bond angles

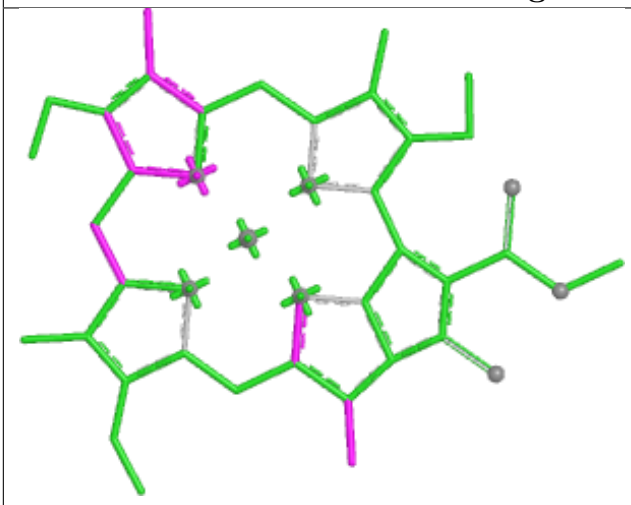


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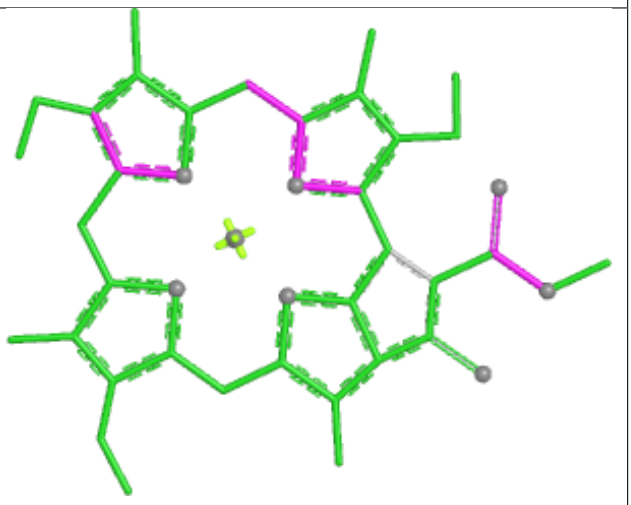


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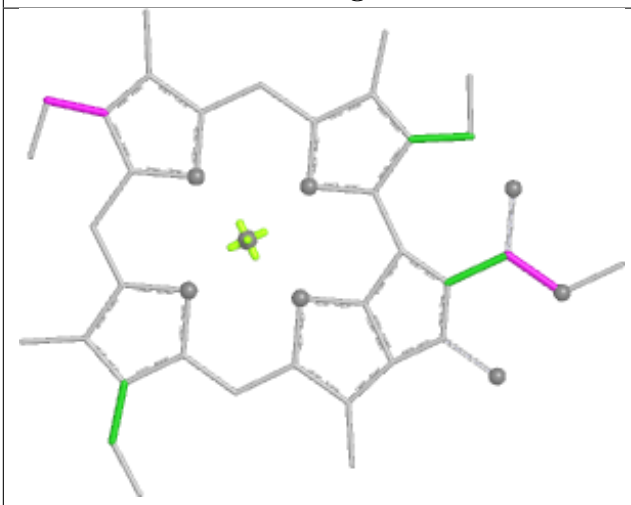
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Bond lengths



Bond angles

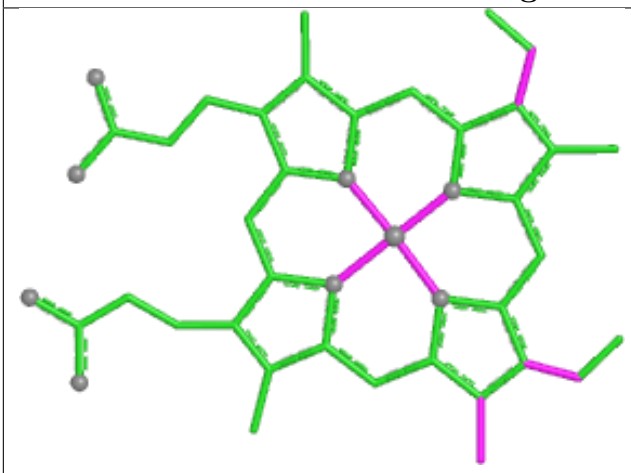


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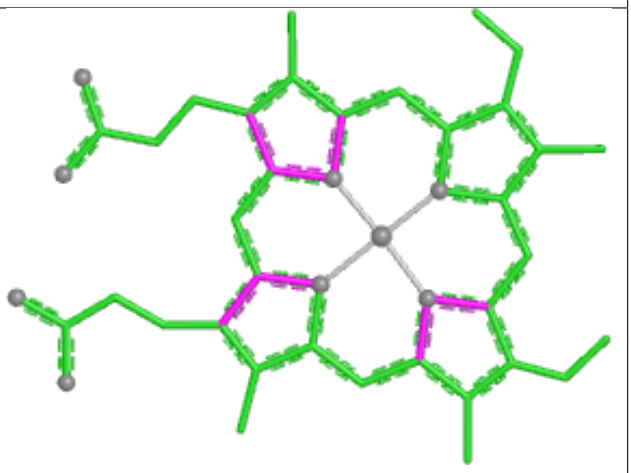


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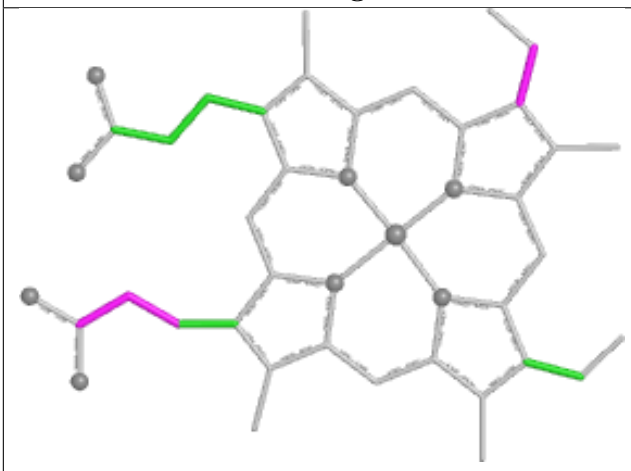
Ligand HEM E 101



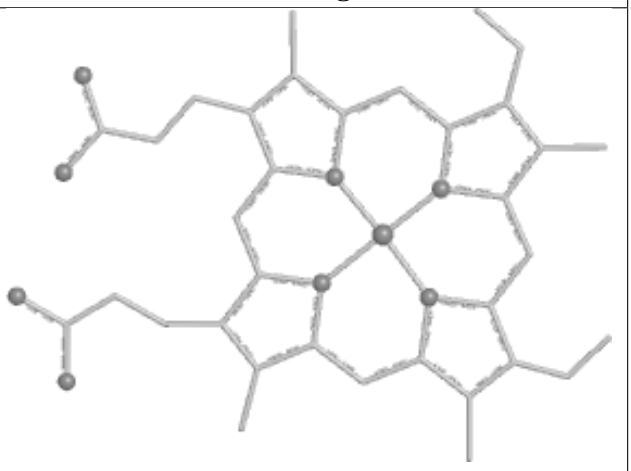
Bond lengths



Bond angles

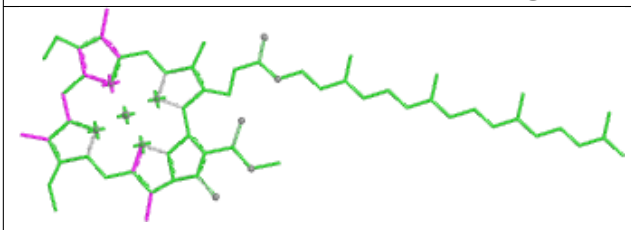


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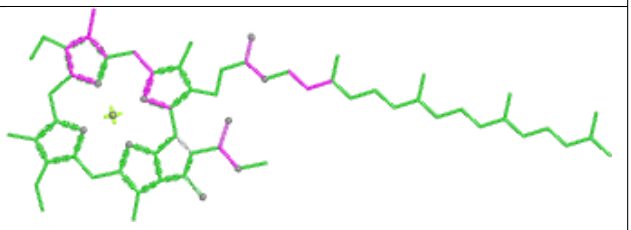


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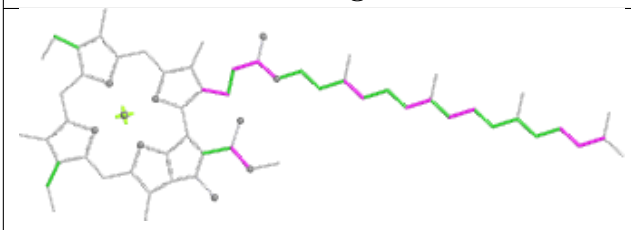
Ligand CLA B 613



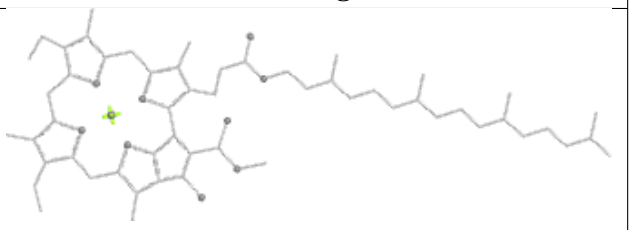
Bond lengths



Bond angles

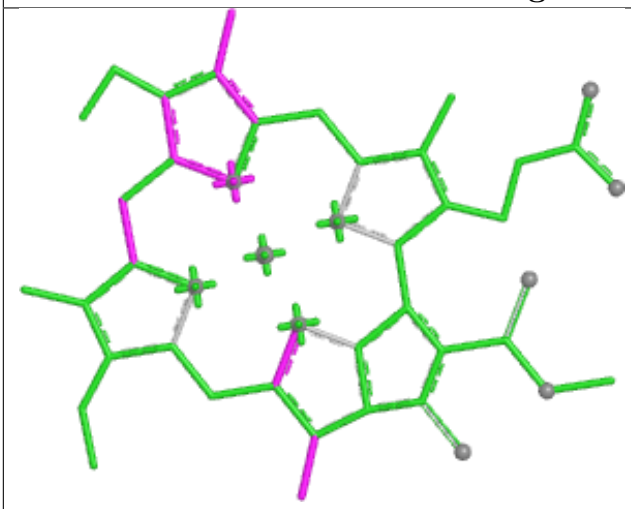


Torsions

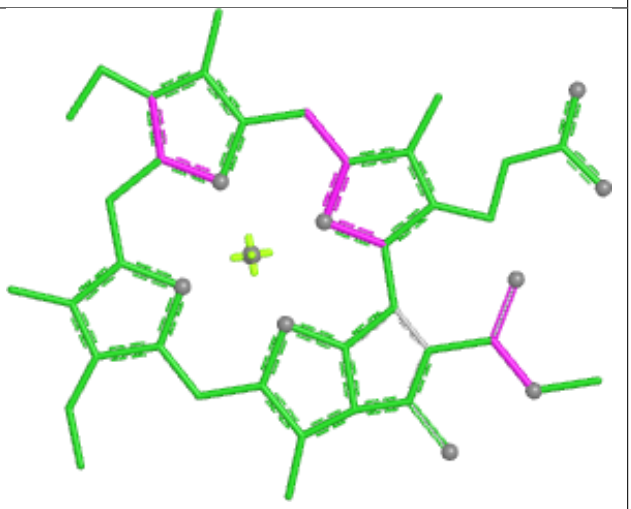


Rings

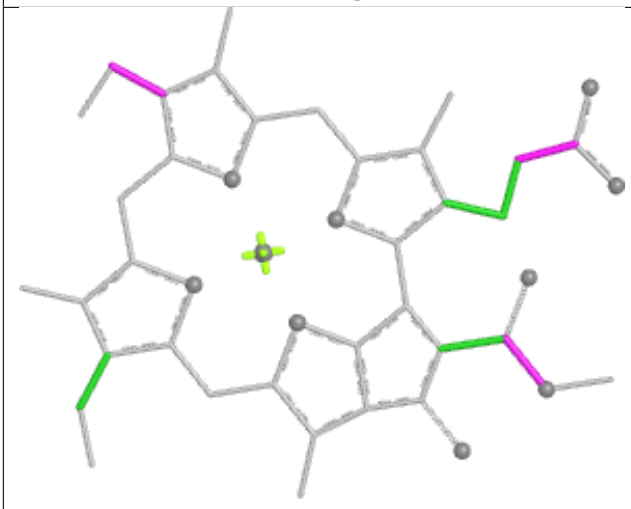
Ligand CLA 4 606



Bond lengths



Bond angles

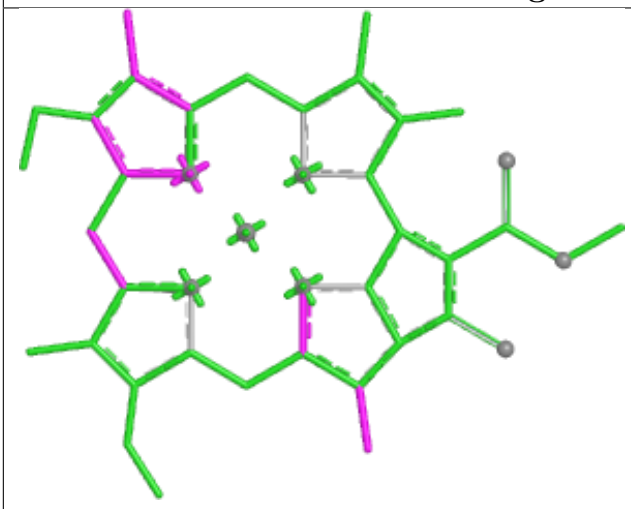


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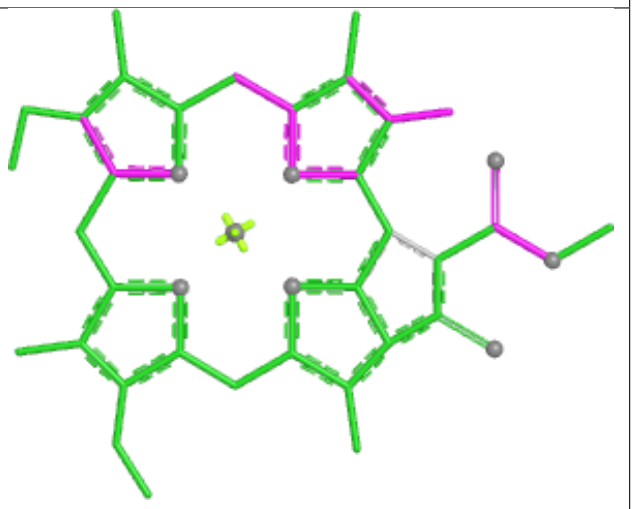


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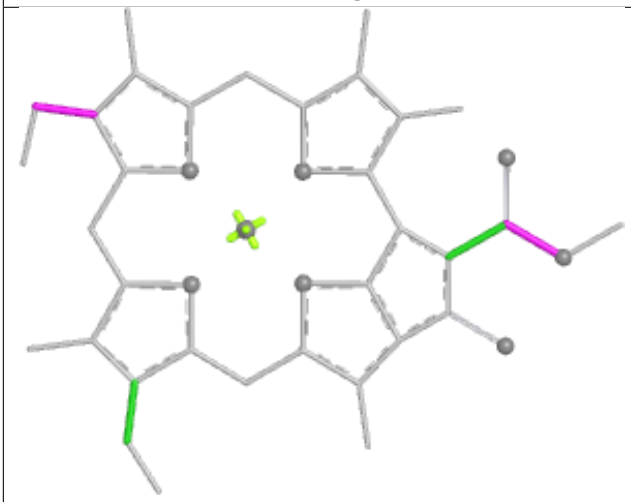
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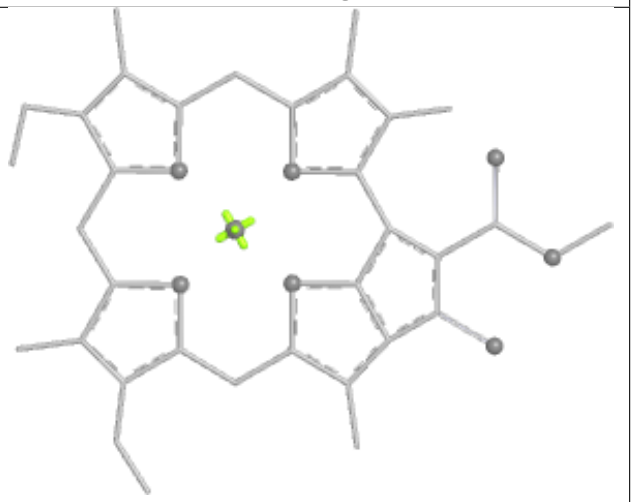
Bond lengths



Bond angles

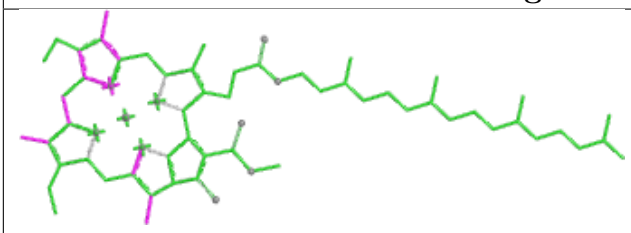


Torsions

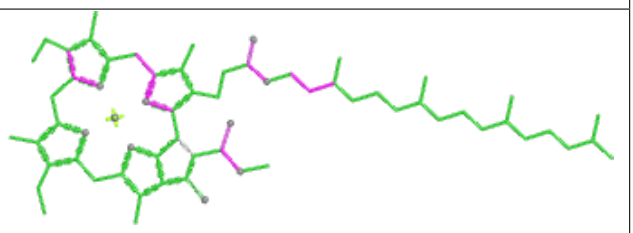


Rings

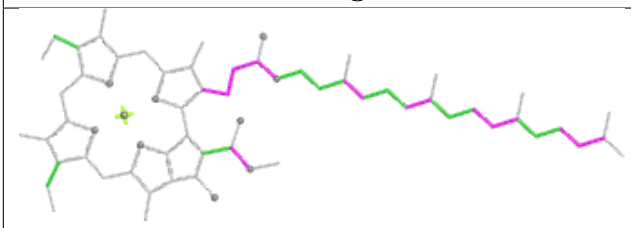
Ligand CLA C 501



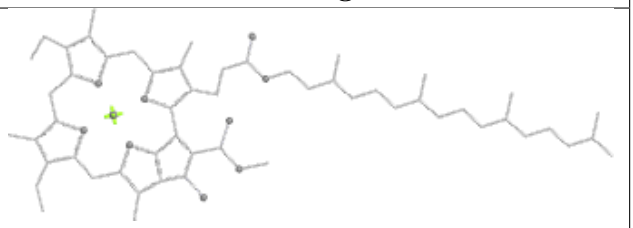
Bond lengths



Bond angles

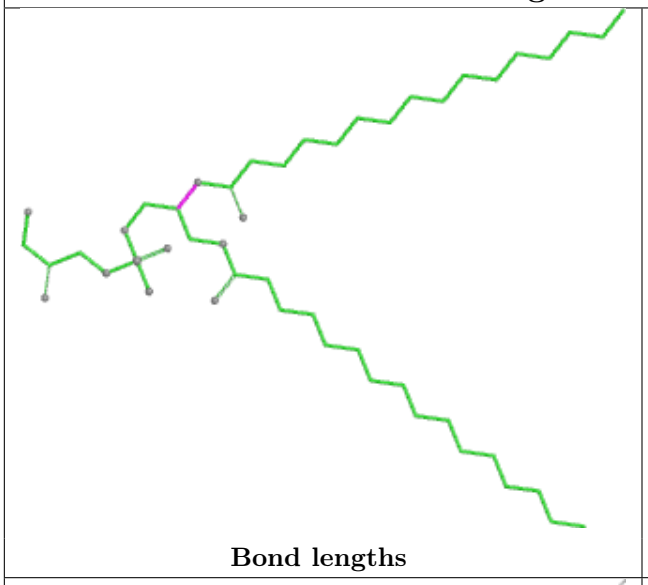


Torsions

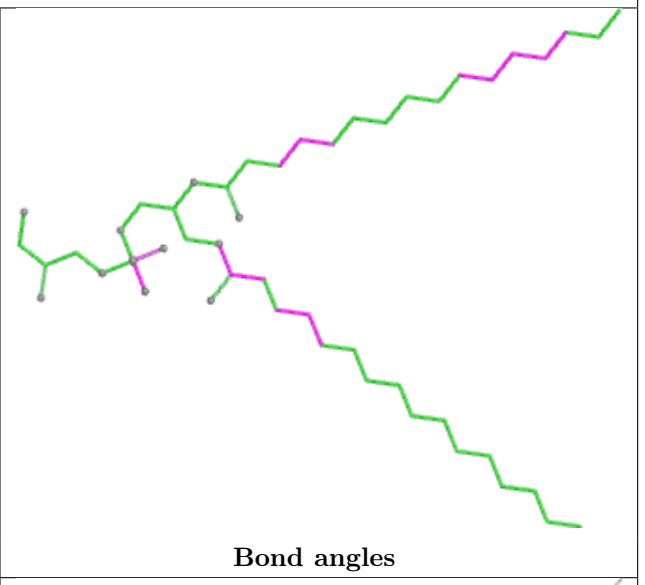


Rings

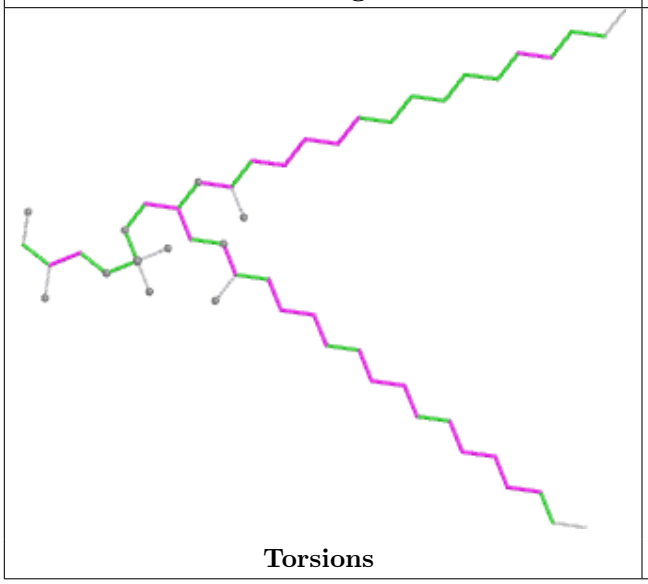
Ligand LHG a 403



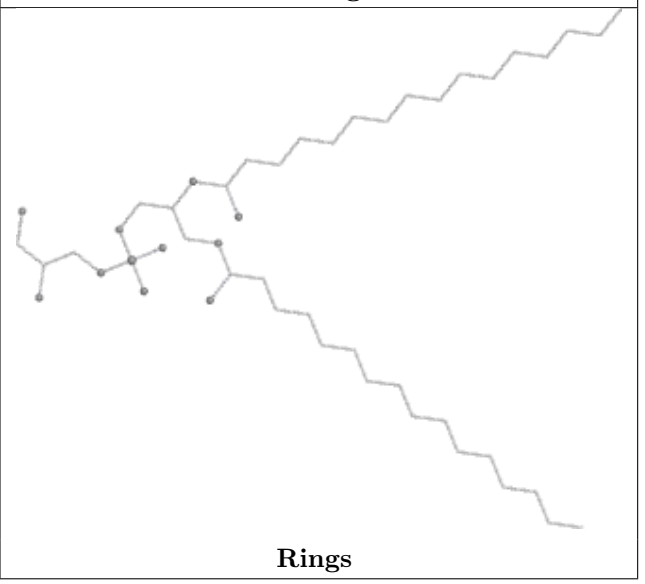
Bond lengths



Bond angles

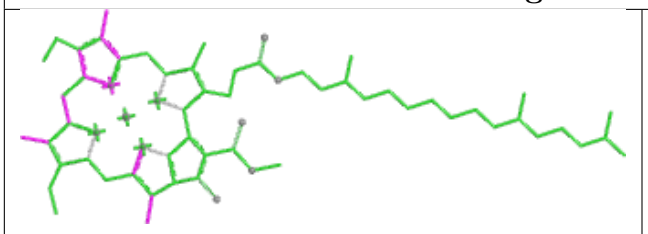


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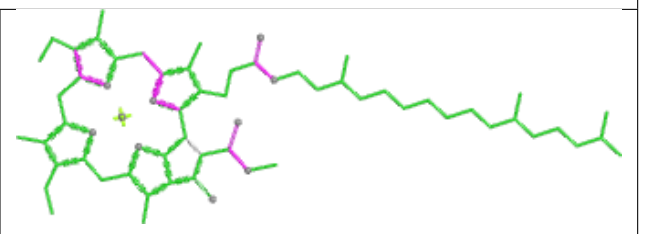


Rings

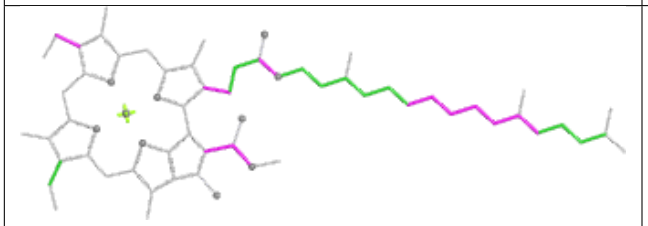
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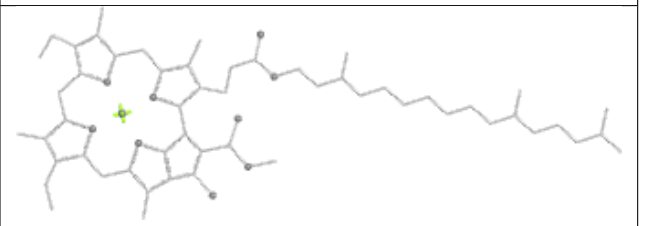
Bond lengths



Bond angles

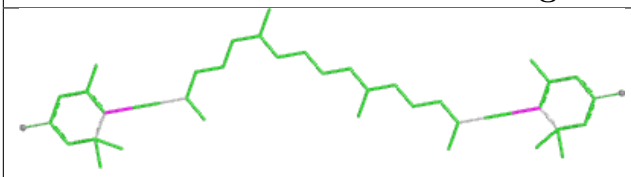


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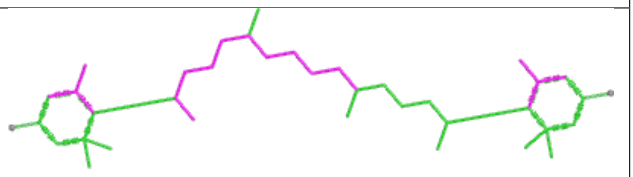


Rings

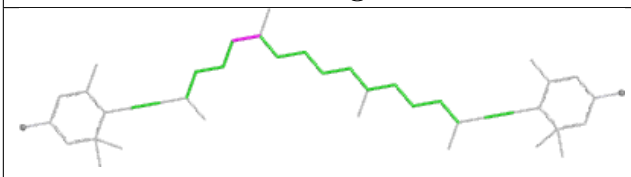
Ligand II0 P 614



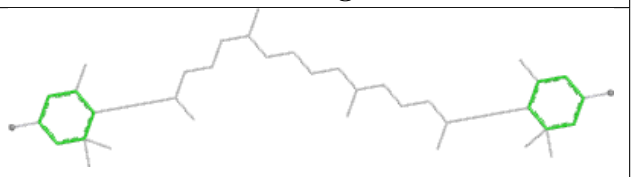
Bond lengths



Bond angles

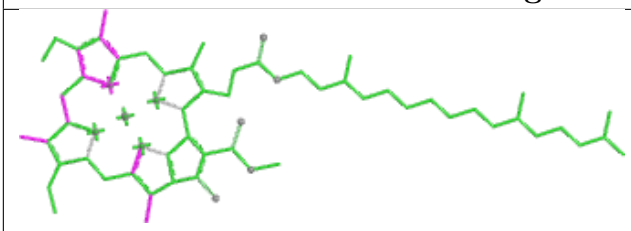


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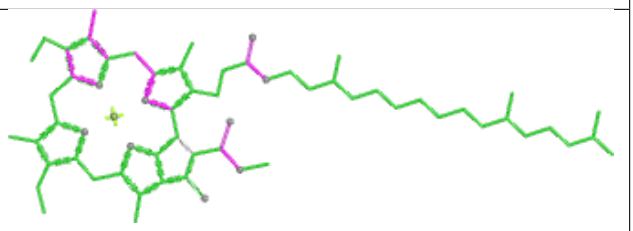


Rings

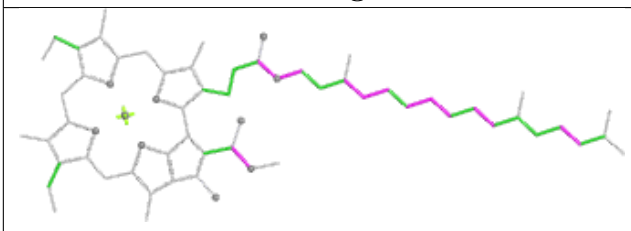
Ligand CLA C 504



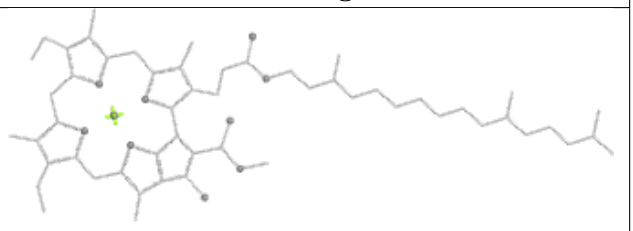
Bond lengths



Bond angles

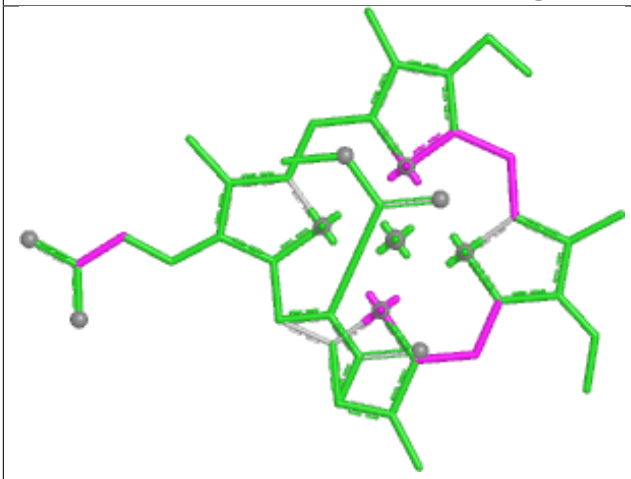


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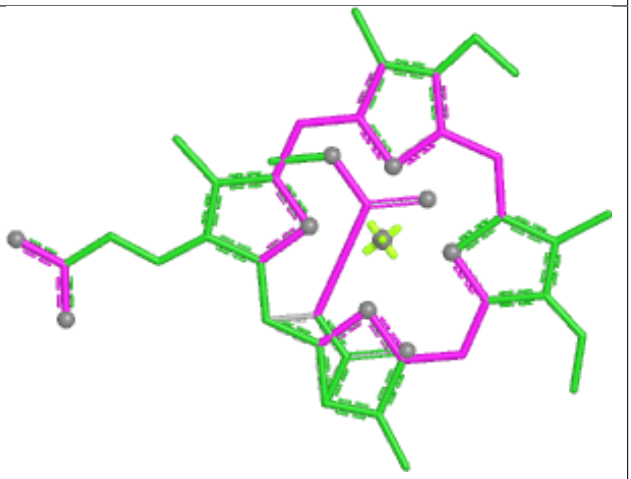


Rings

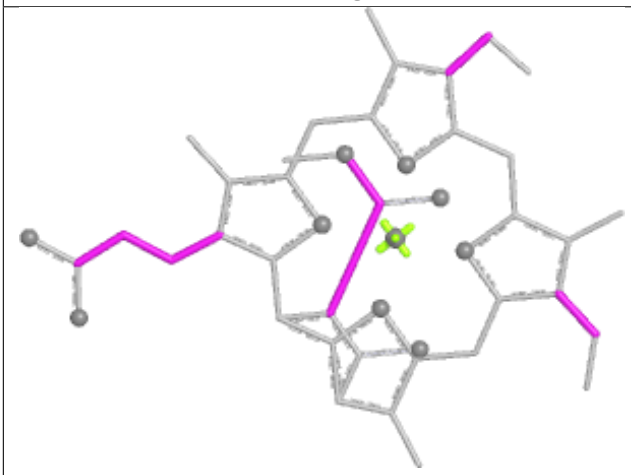
Ligand KC2 6 609



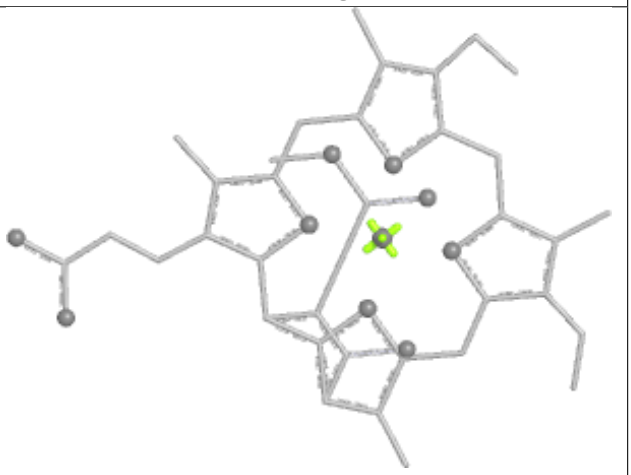
Bond lengths



Bond angles



Torsions

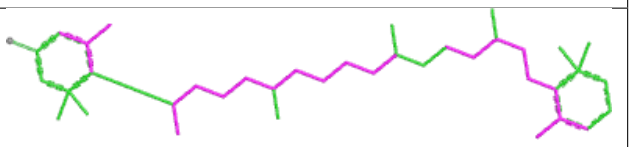


Rings

Ligand IHT 2 616



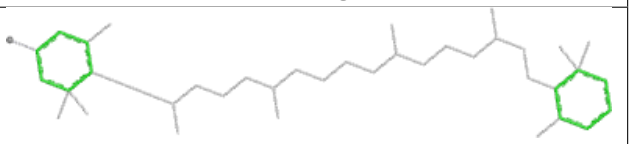
Bond lengths



Bond angles

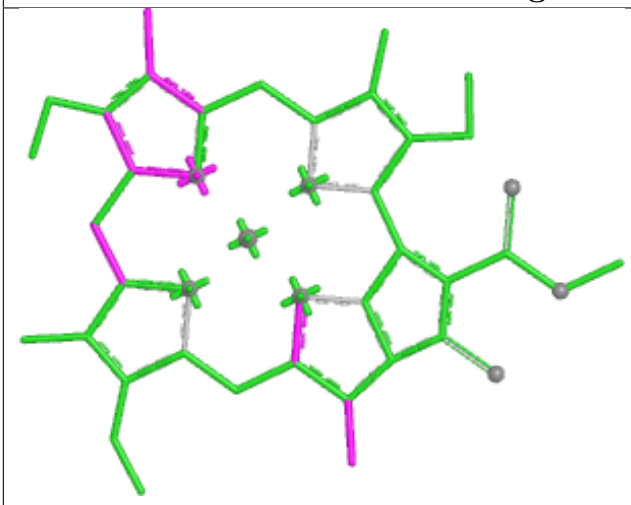


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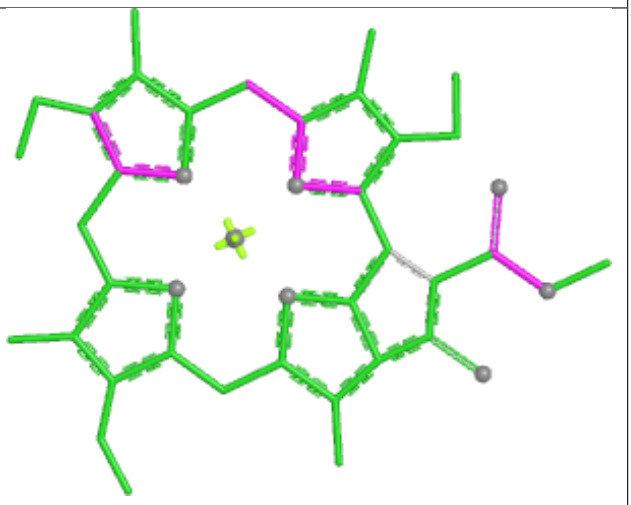


Rings

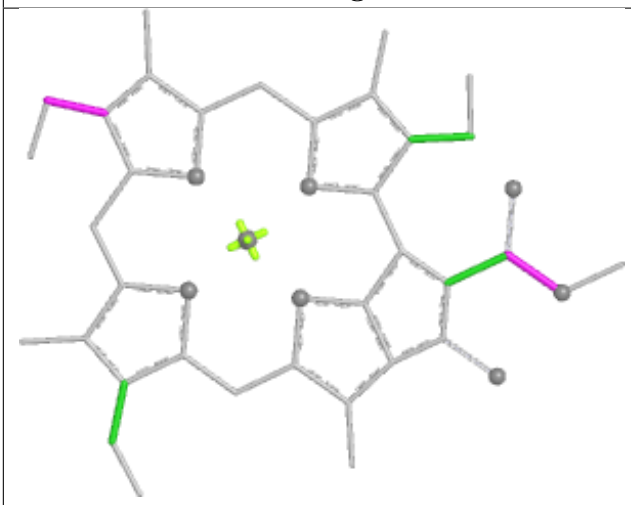
Ligand CLA 8 601



Bond lengths



Bond angles

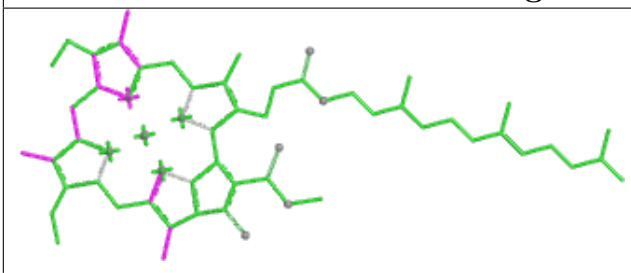


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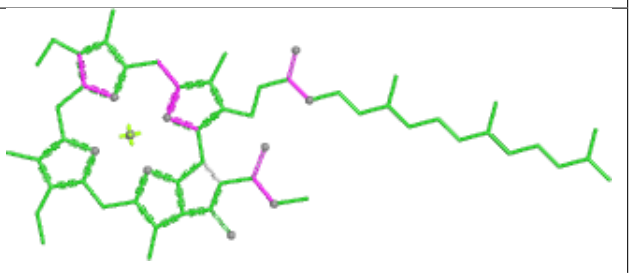


Rings

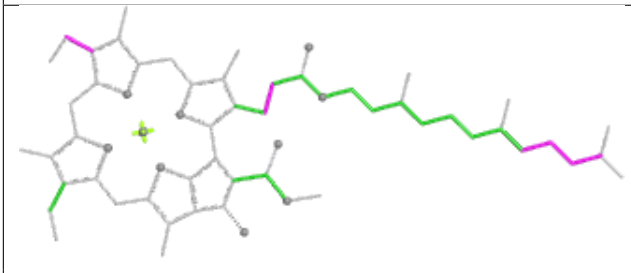
Ligand CLA P 607



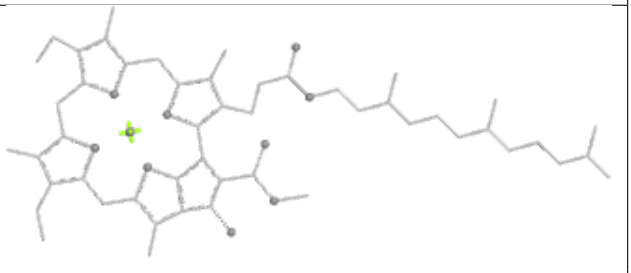
Bond lengths



Bond angles

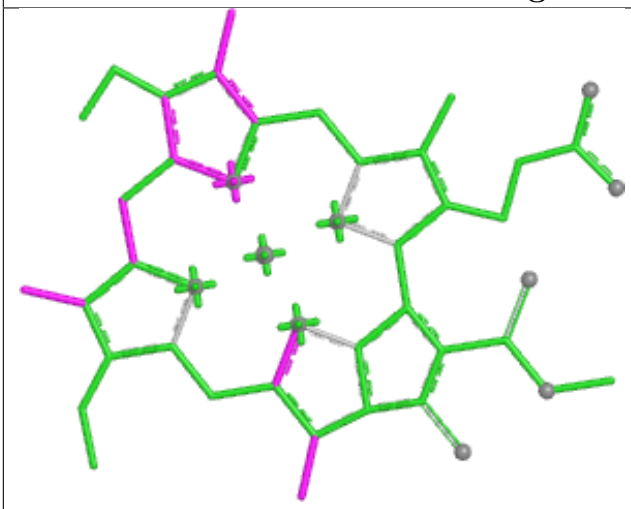


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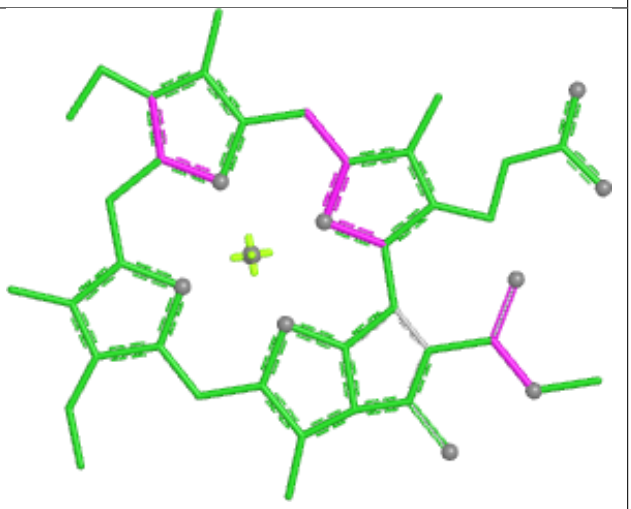


Rings

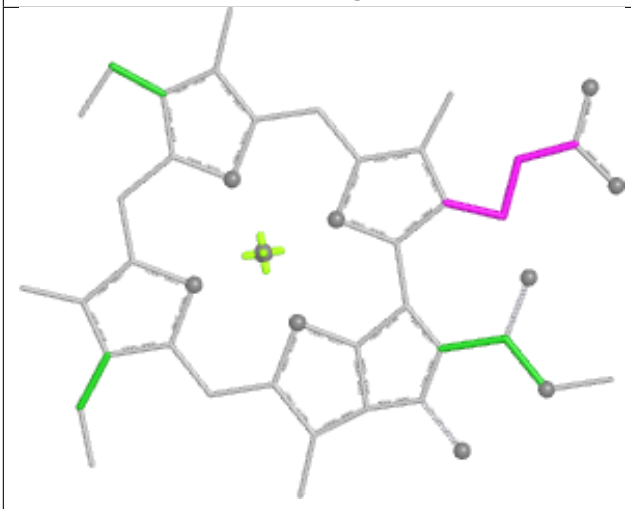
Ligand CLA 5 308



Bond lengths



Bond angles

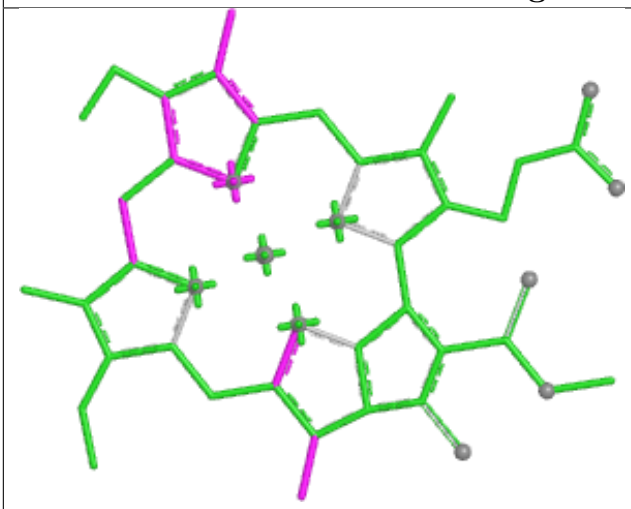


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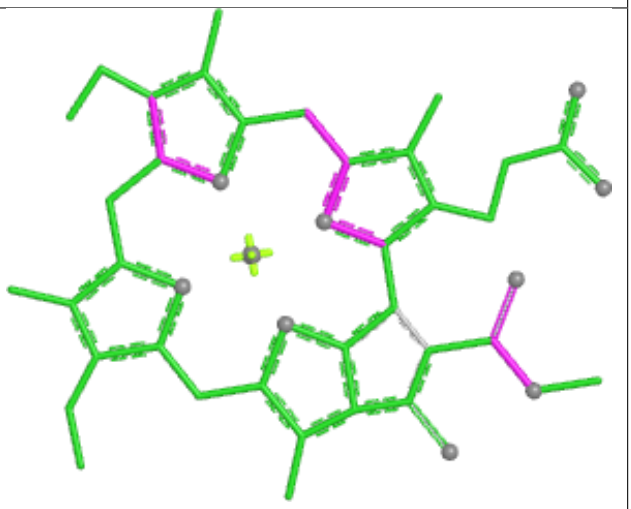


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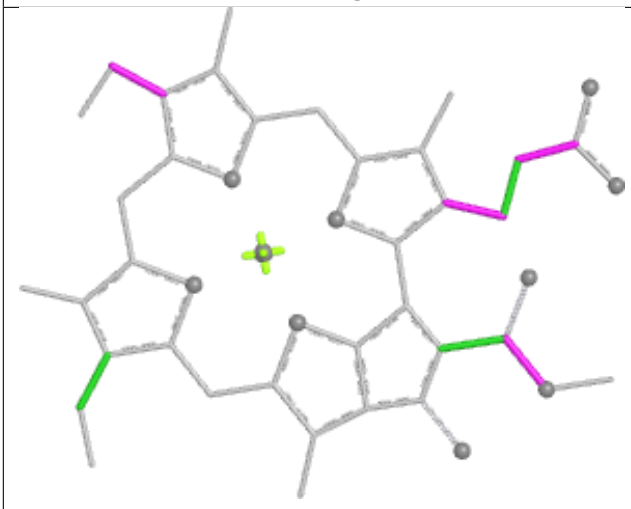
Ligand CLA 7 612



Bond lengths



Bond angles

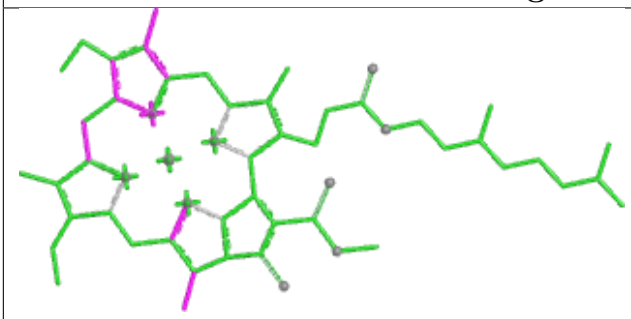


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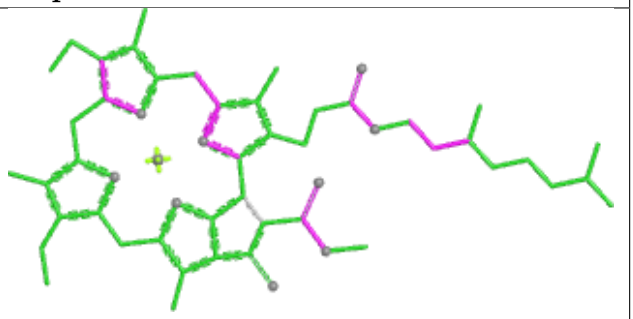


Rings

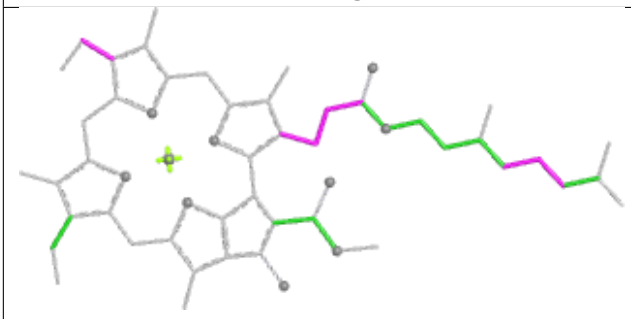
Ligand CLA p 305



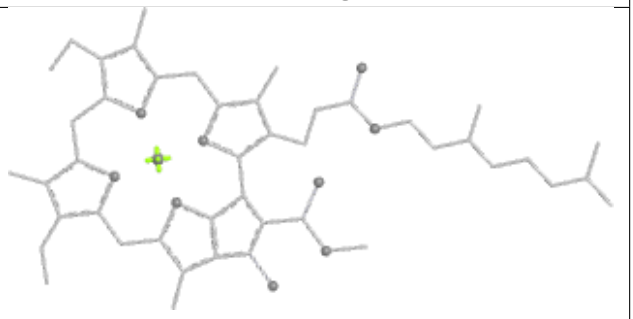
Bond lengths



Bond angles

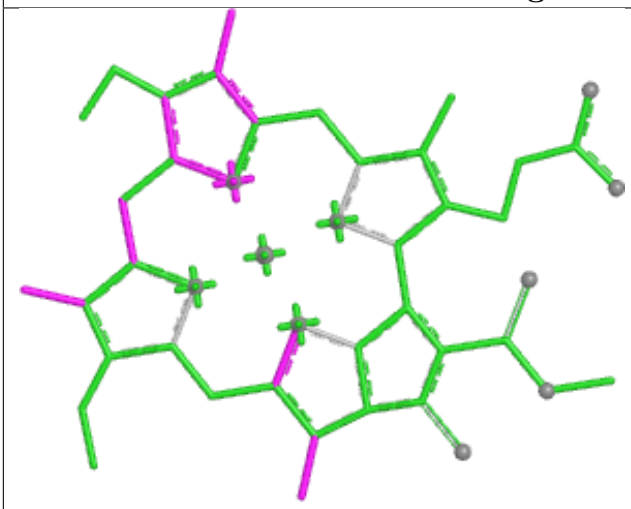


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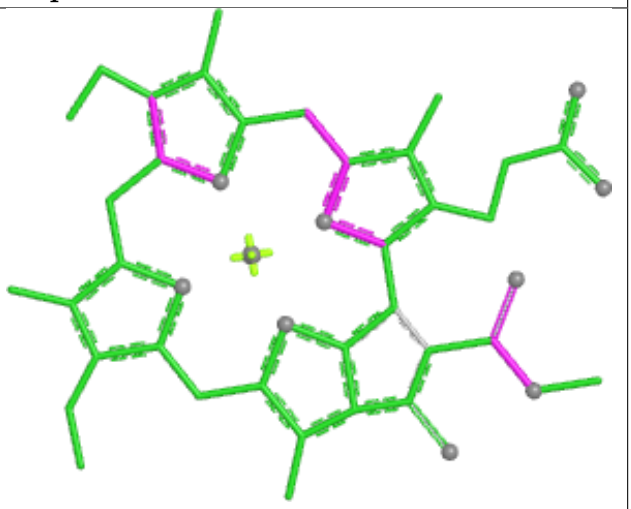


Rings

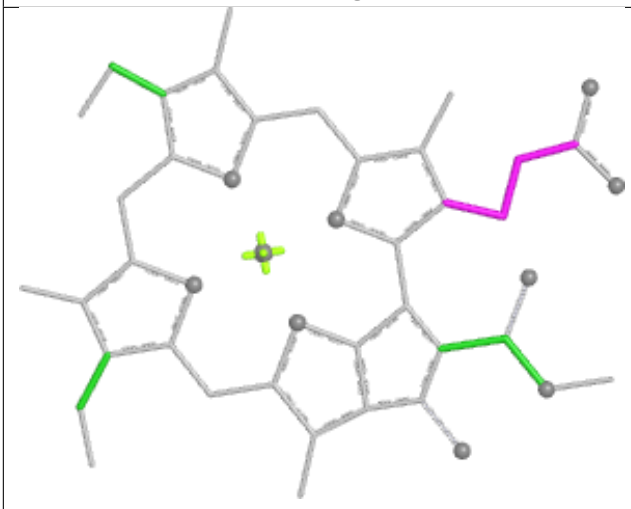
Ligand CLA p 308



Bond lengths



Bond angles

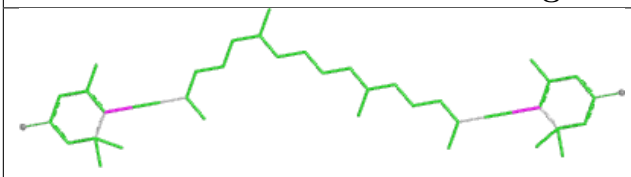


Torsions

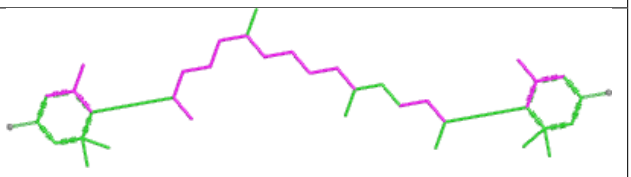


Rings

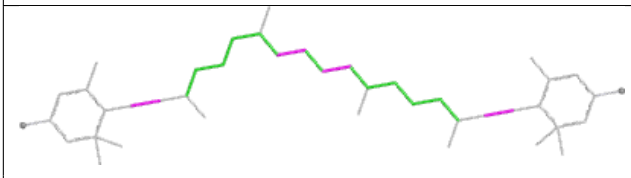
Ligand II0 0 616



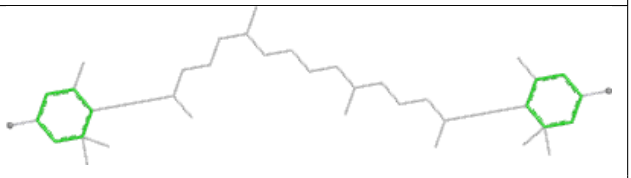
Bond lengths



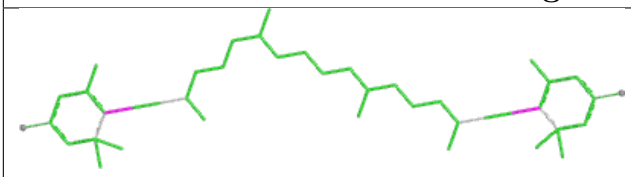
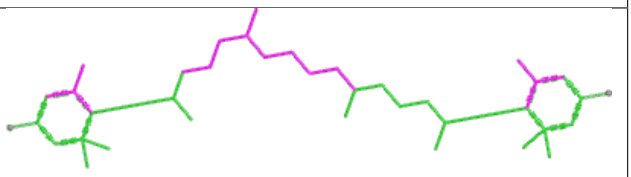
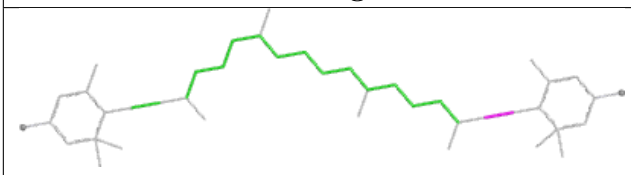
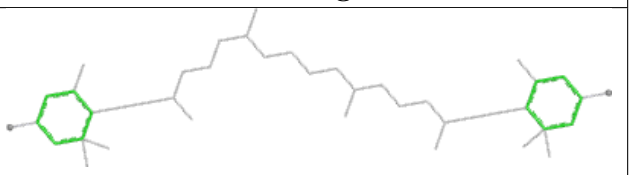
Bond angles

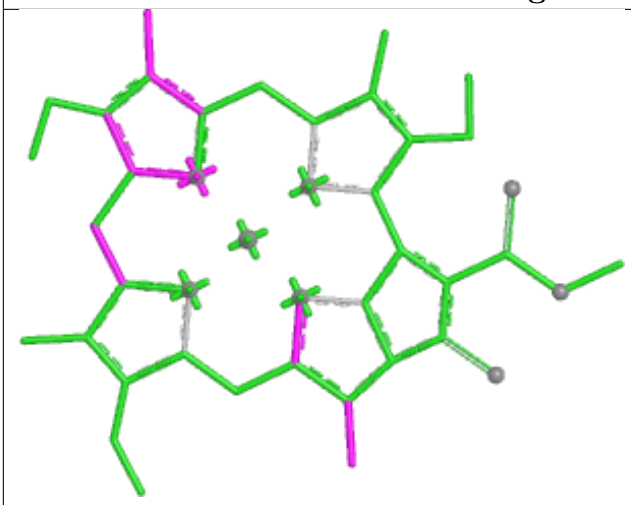
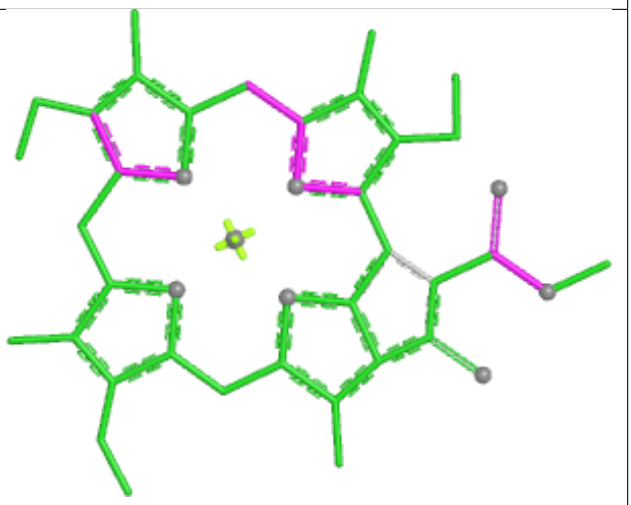
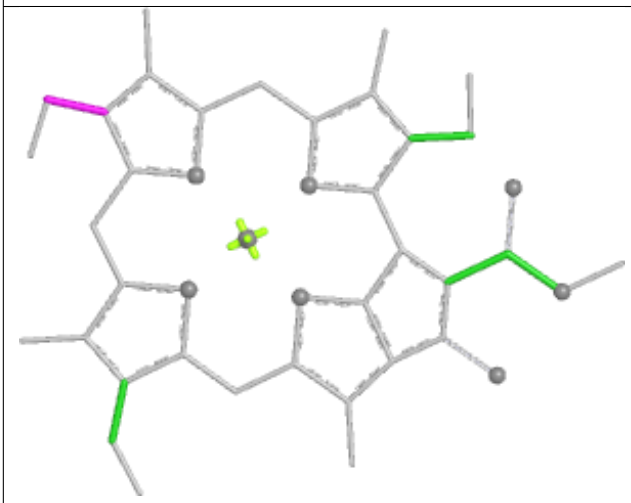


Torsions

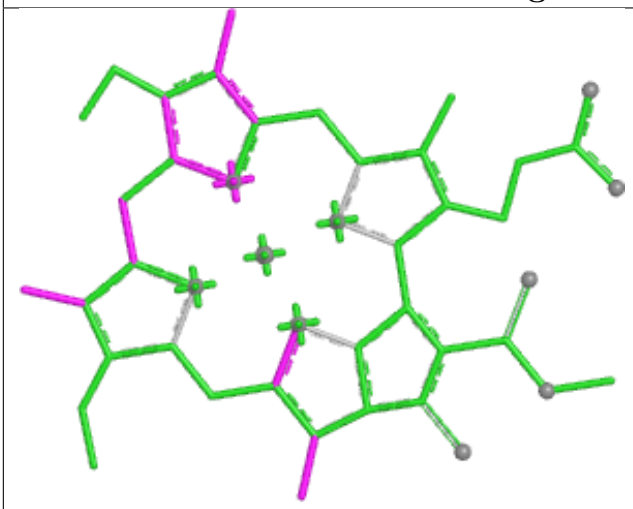


Rings

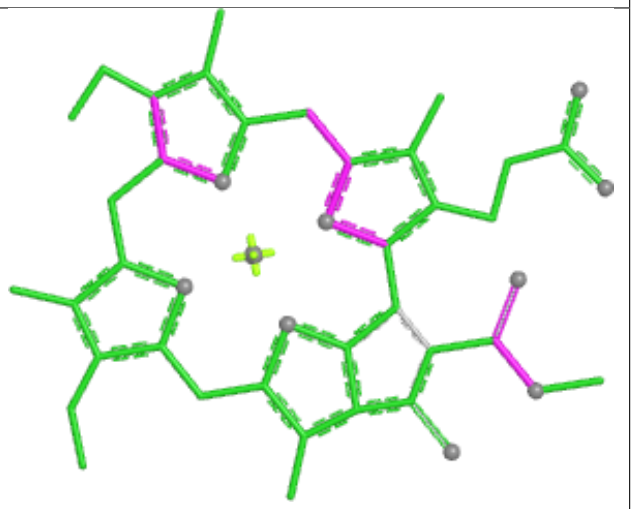
Ligand II0 9 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

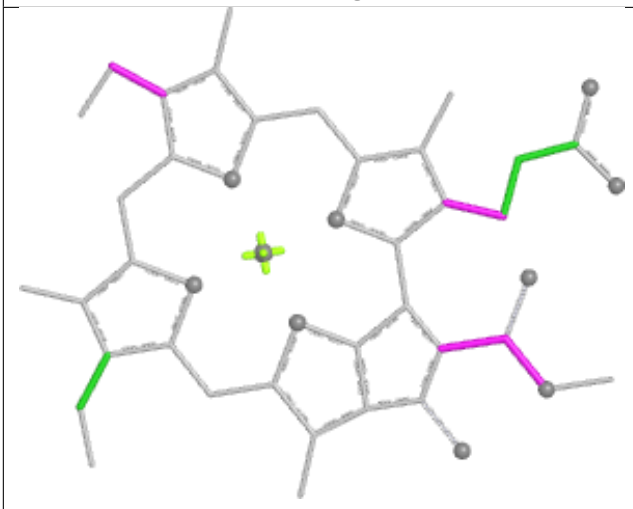
Ligand CLA 3 611



Bond lengths



Bond angles

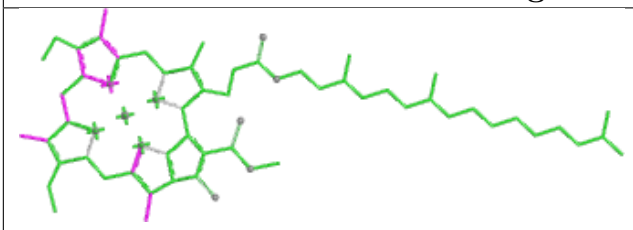


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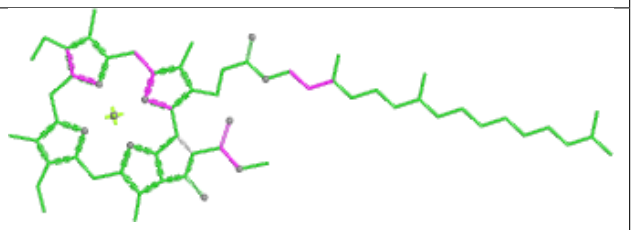


Rings

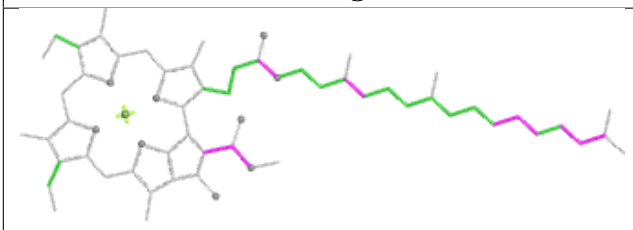
Ligand CLA b 615



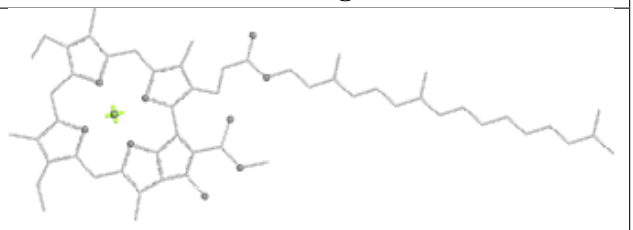
Bond lengths



Bond angles

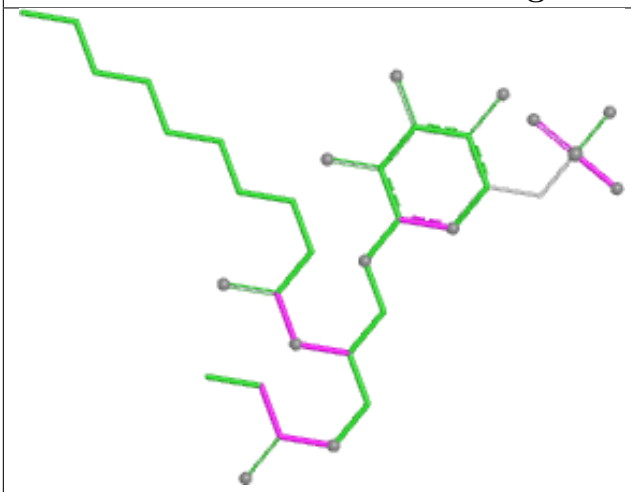


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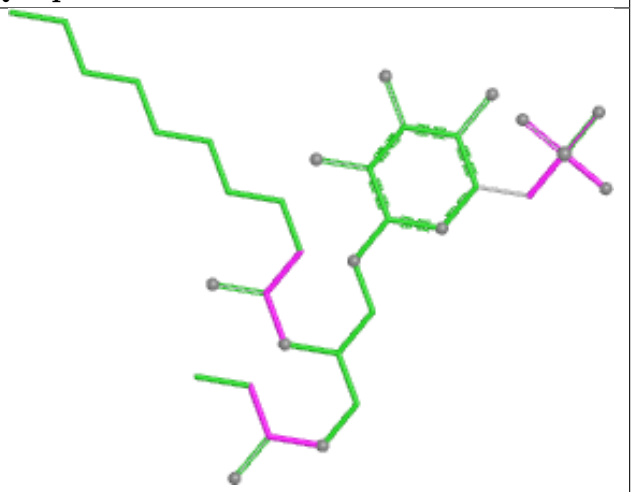


Rings

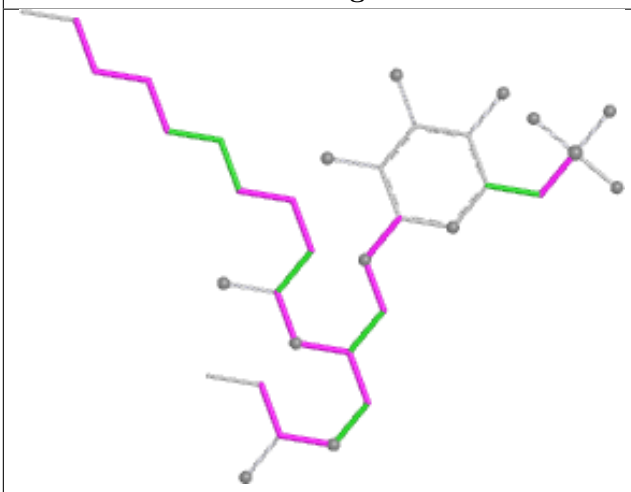
Ligand SQD p 318



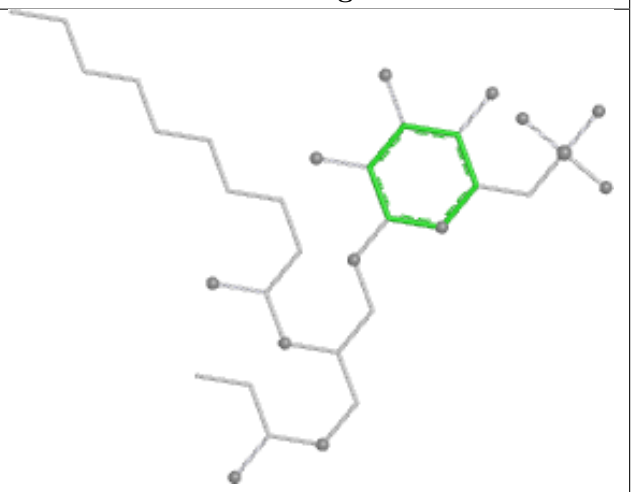
Bond lengths



Bond angles

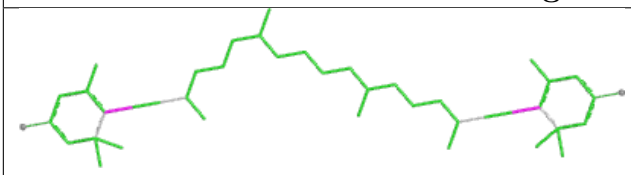


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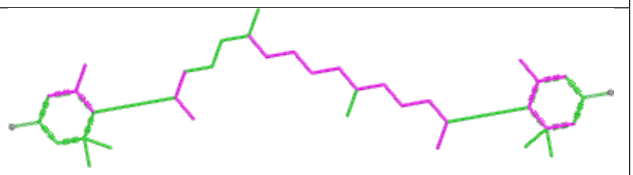


Rings

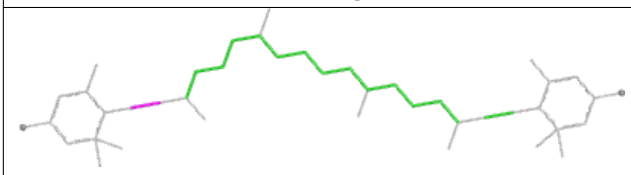
Ligand II0 0 615



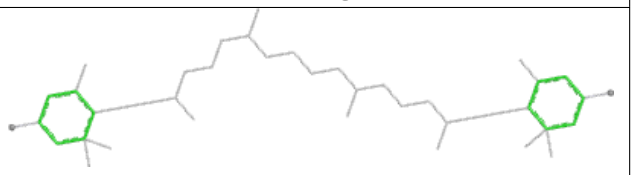
Bond lengths



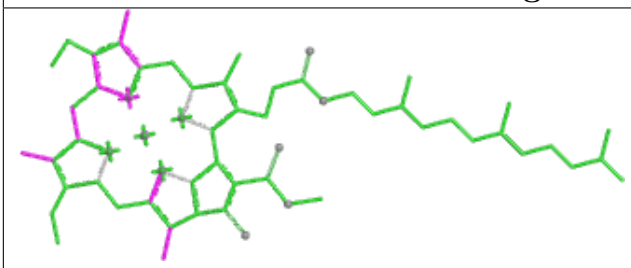
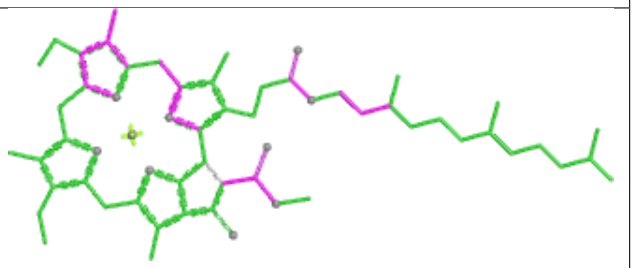
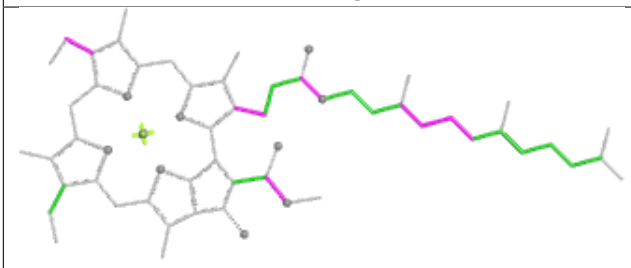
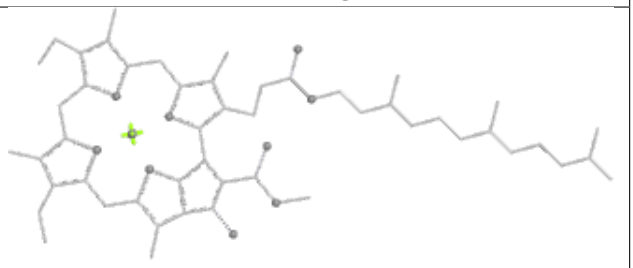
Bond angles

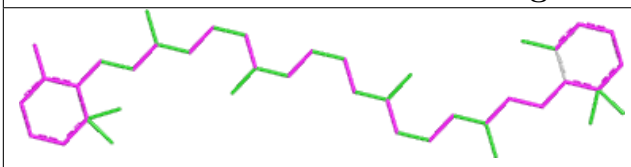
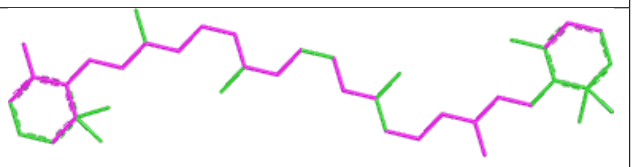
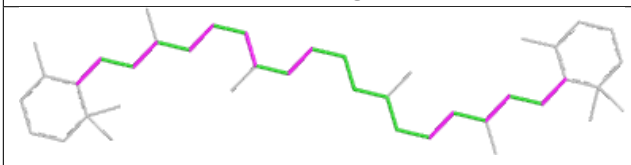
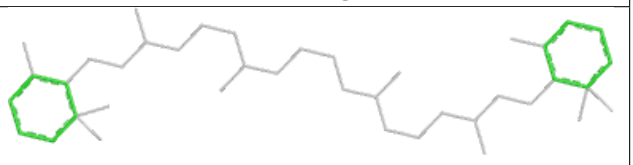


Torsions

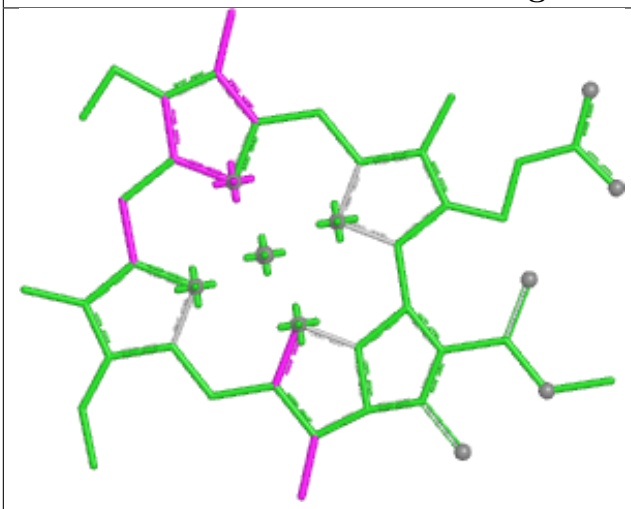


Rings

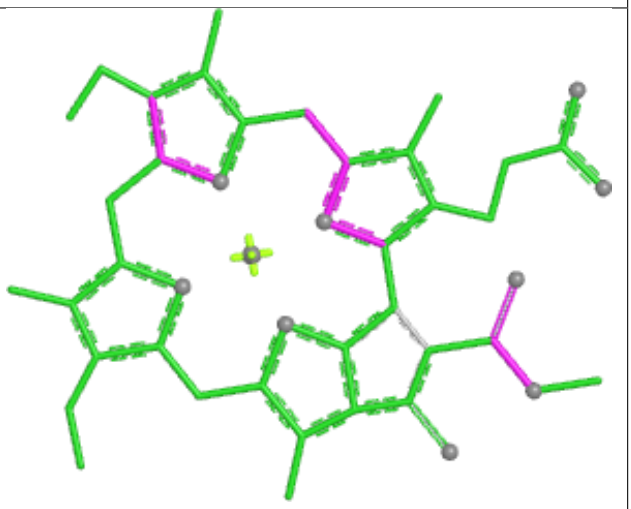
Ligand CLA D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 8CT d 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

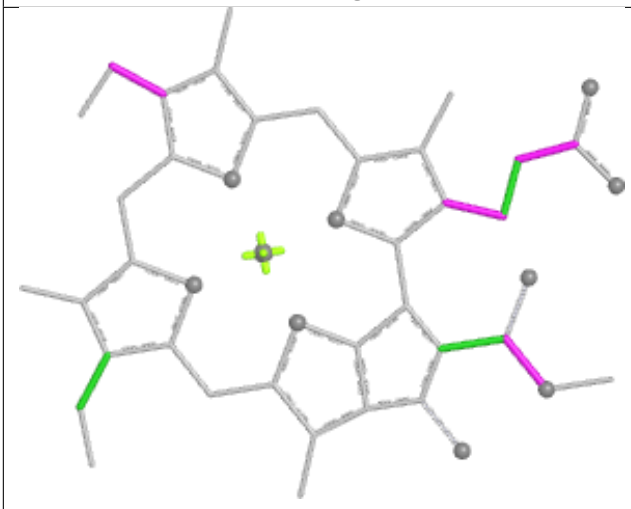
Ligand CLA 1 607



Bond lengths



Bond angles

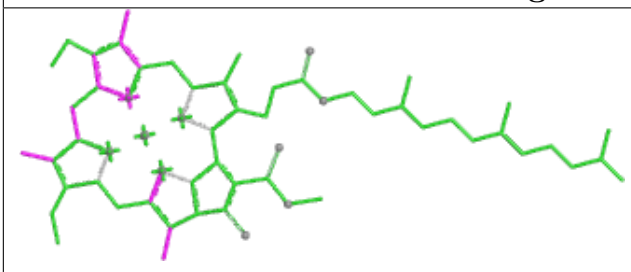


Torsions

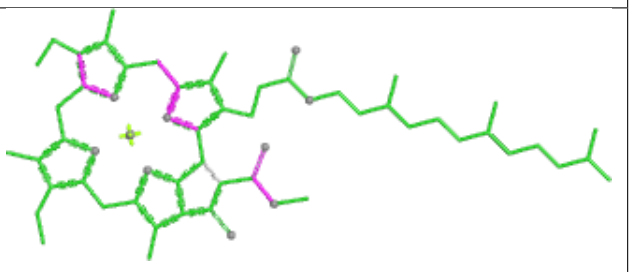


Rings

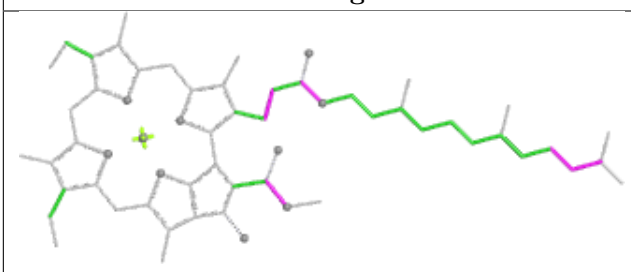
Ligand CLA 3 607



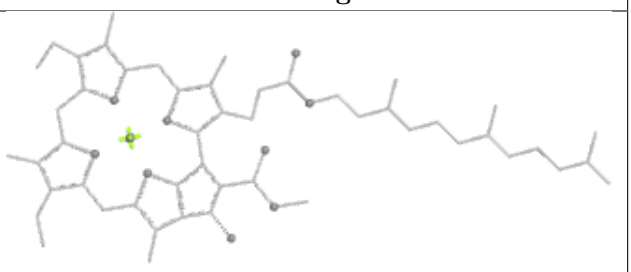
Bond lengths



Bond angles

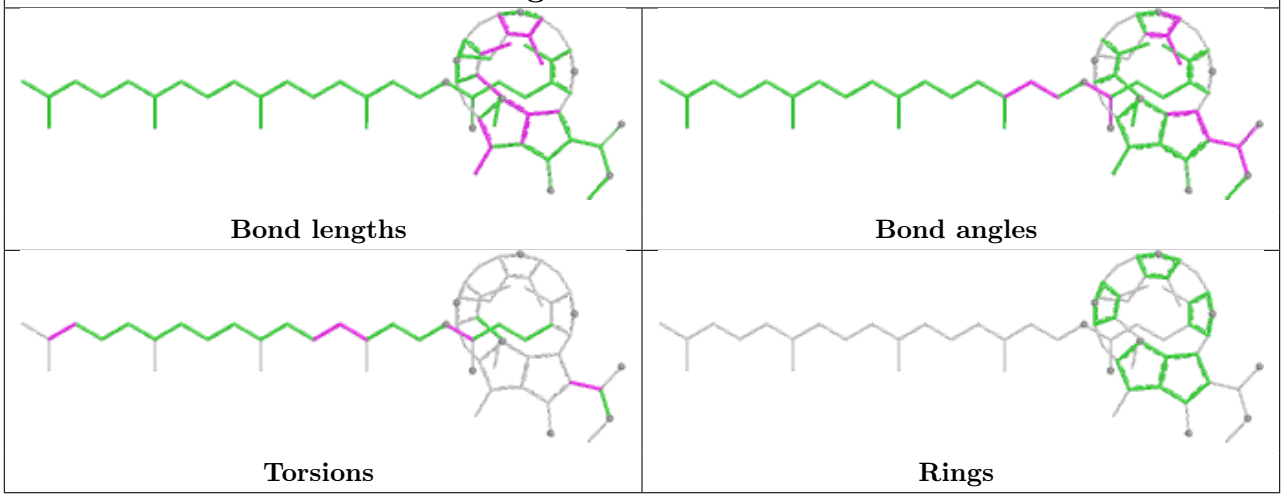


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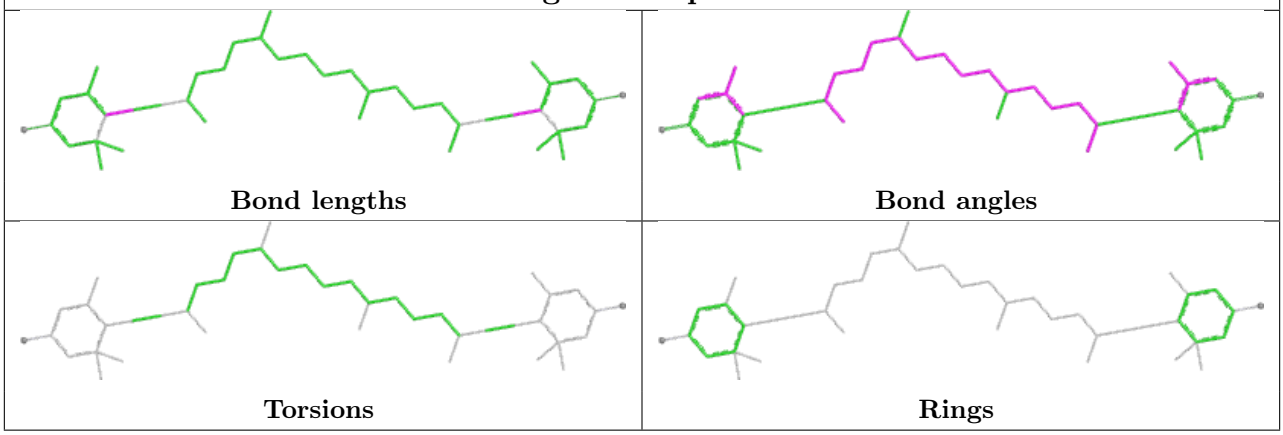


Rings

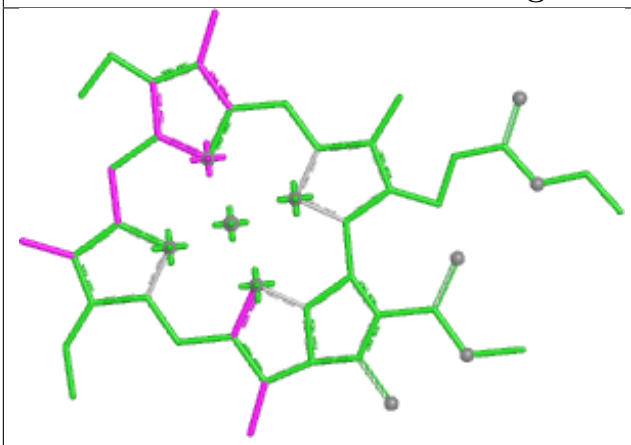
Ligand PHO a 407



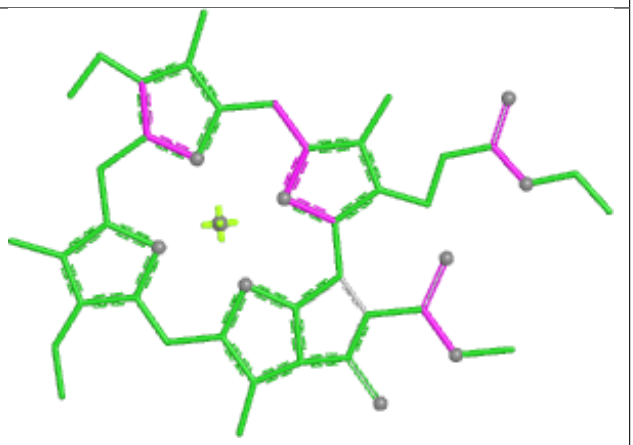
Ligand II0 p 314



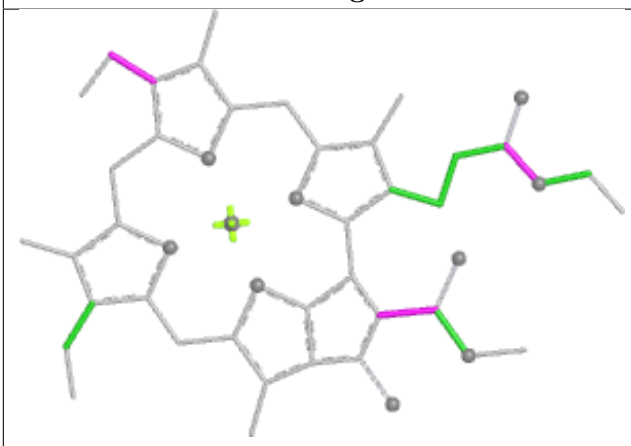
Ligand CLA b 602



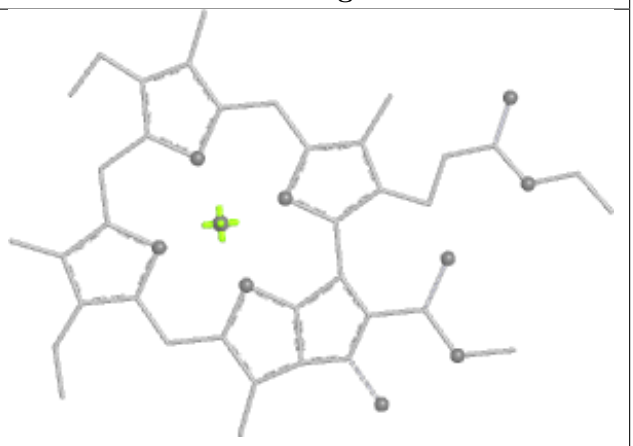
Bond lengths



Bond angles

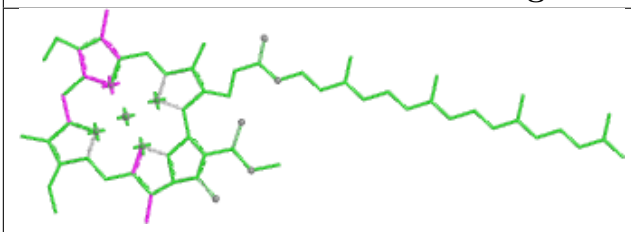


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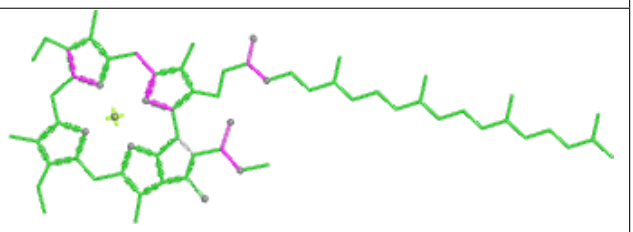


Rings

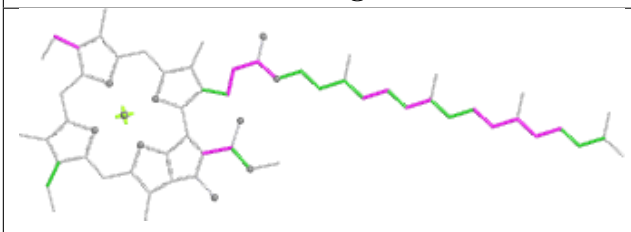
Ligand CLA S 303



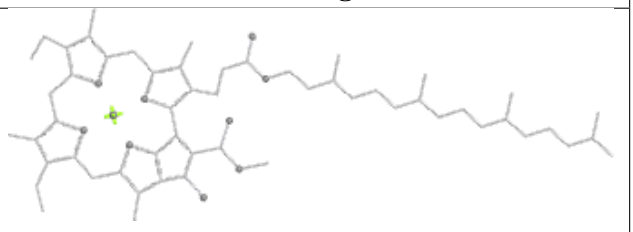
Bond lengths



Bond angles

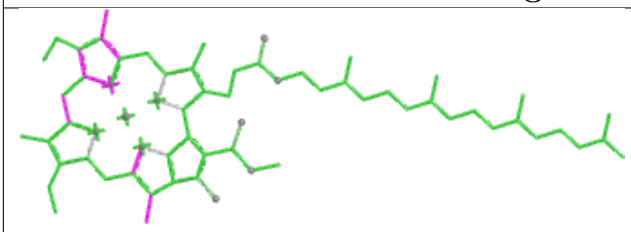


Torsions

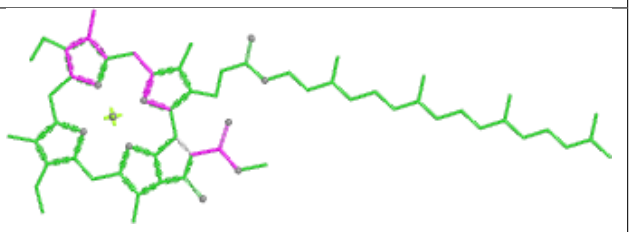


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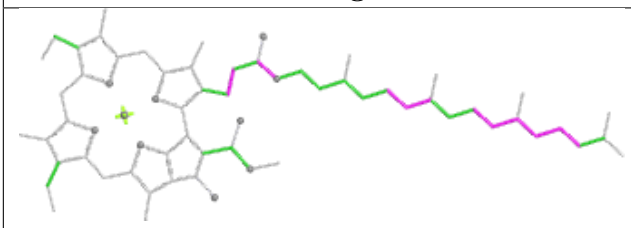
Ligand CLA C 505



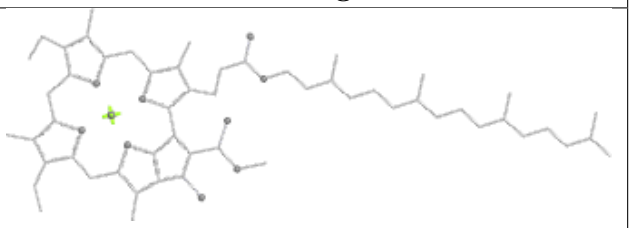
Bond lengths



Bond angles

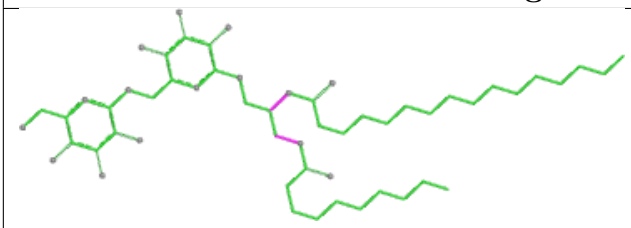


Torsions

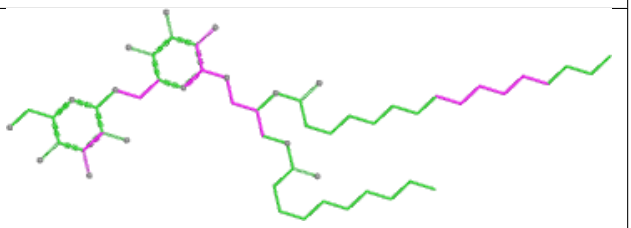


Rings

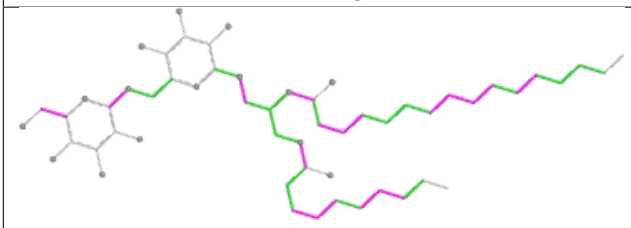
Ligand DGD c 515



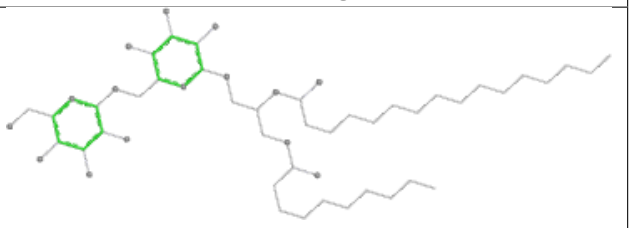
Bond lengths



Bond angles



Torsions

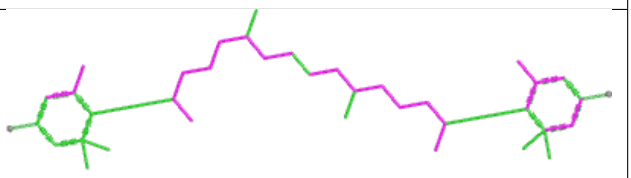


Rings

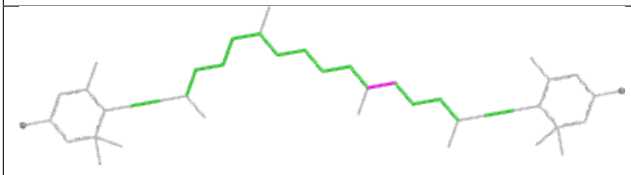
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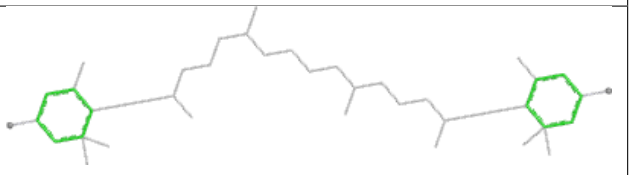
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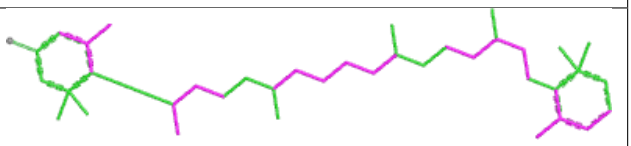
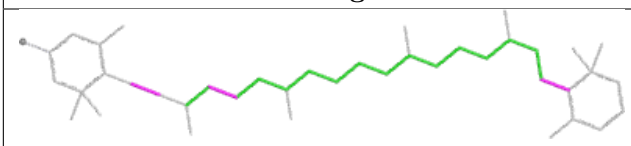
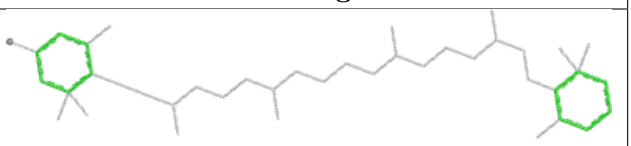
Bond angles

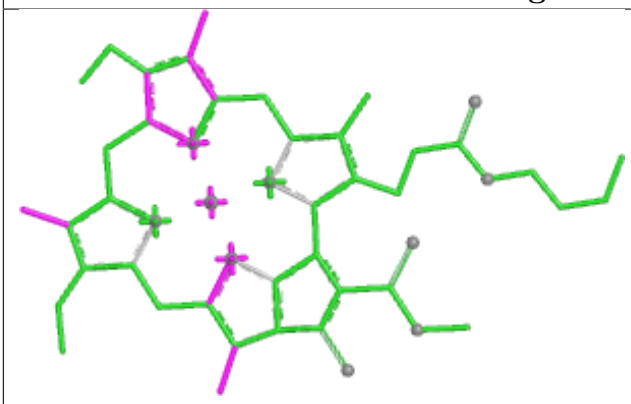
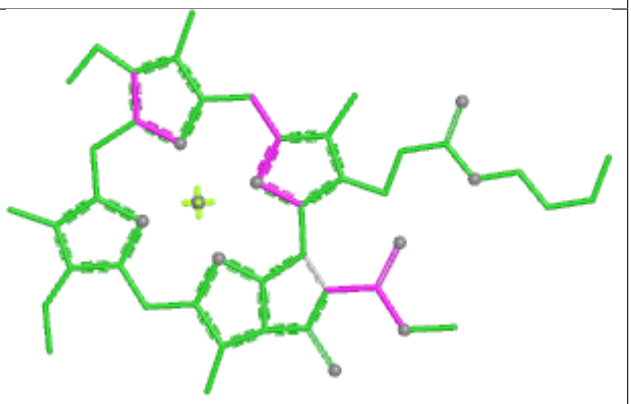
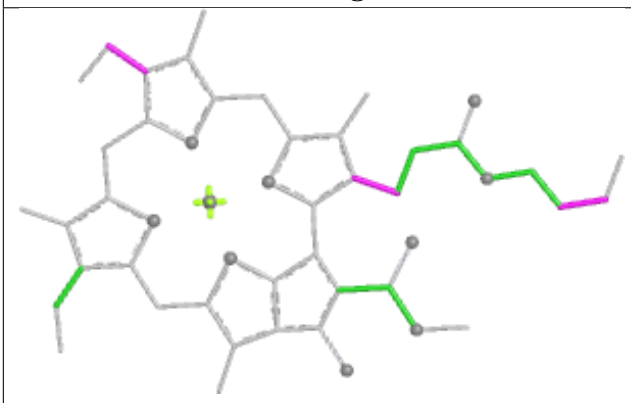
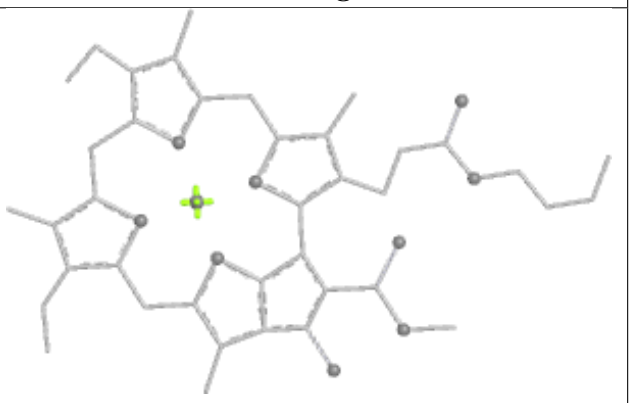


Torsions

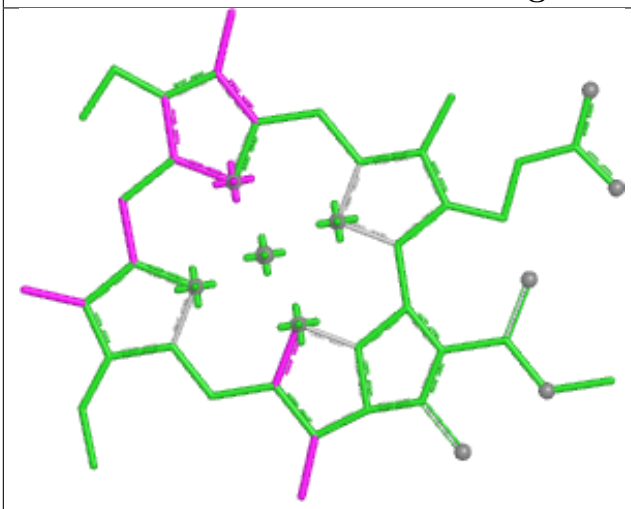


Rings

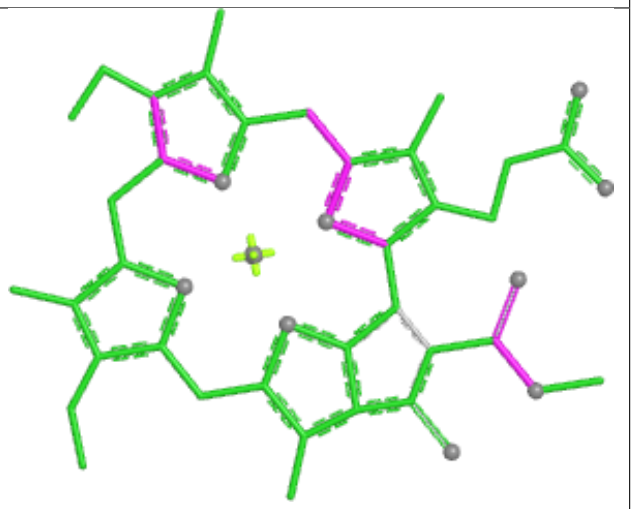
Ligand IHT 1 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

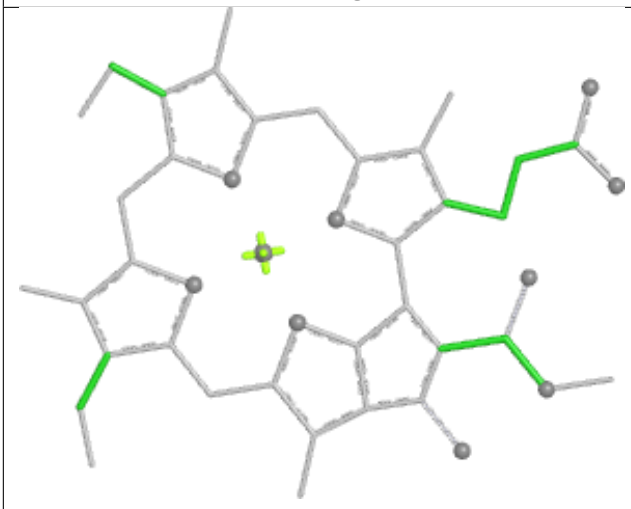
Ligand CLA 3 606



Bond lengths



Bond angles

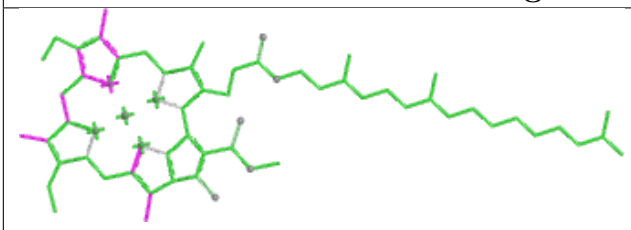


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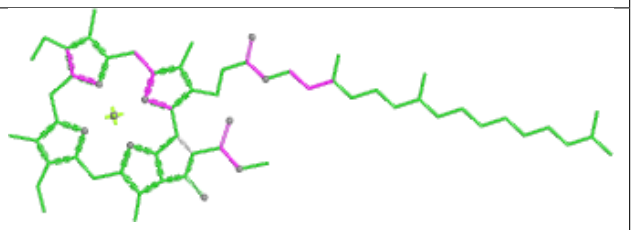


Rings

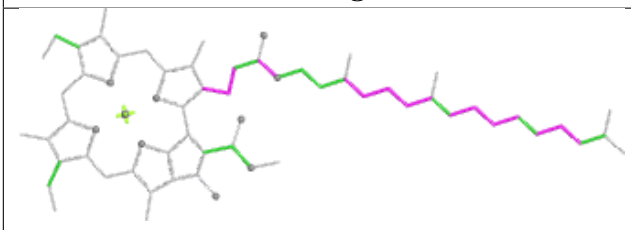
Ligand CLA B 612



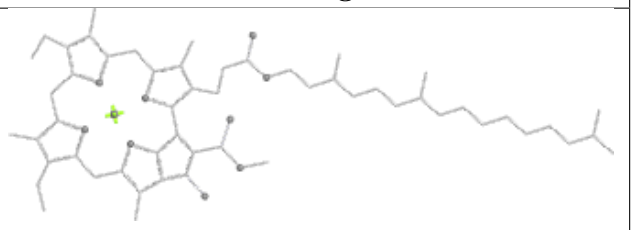
Bond lengths



Bond angles

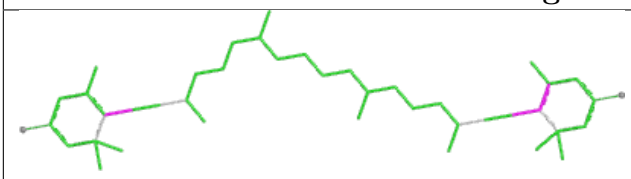


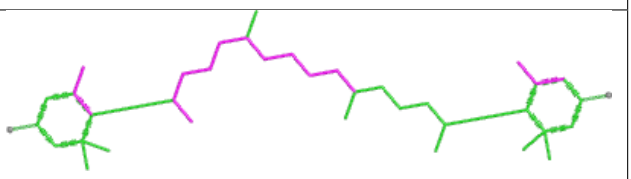
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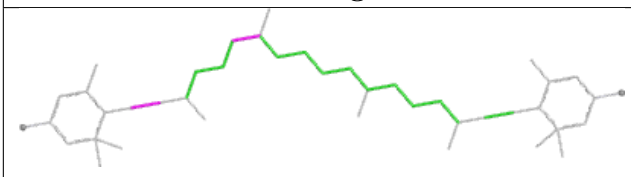


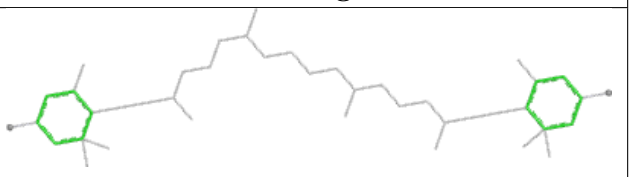
Rings

Ligand II0 6 614

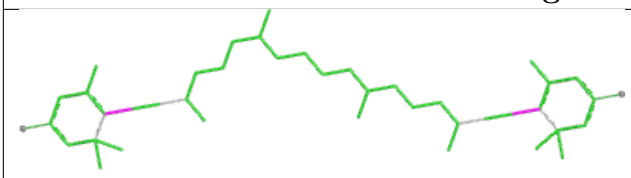

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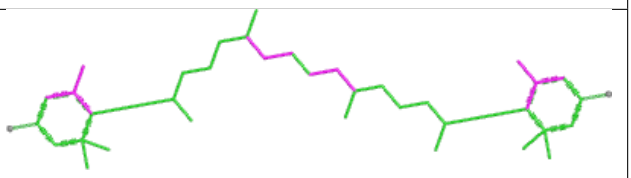

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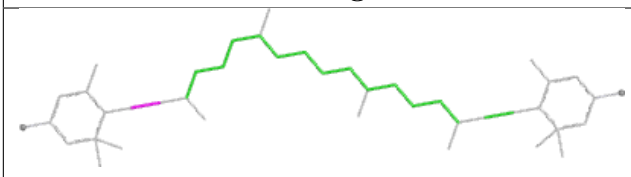

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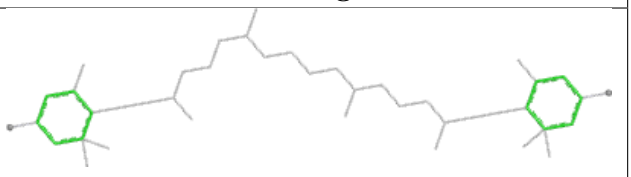

Rings

Ligand II0 7 614

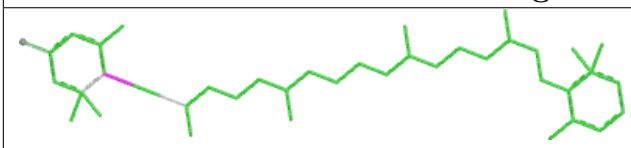

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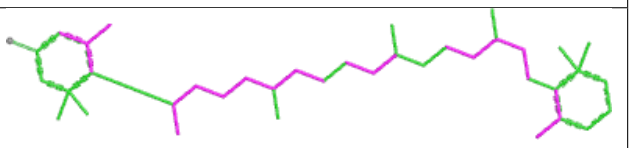

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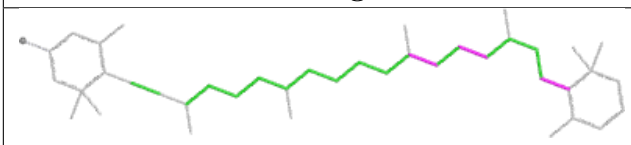

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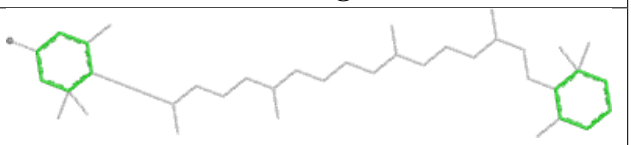

Rings

Ligand IHT 4 614

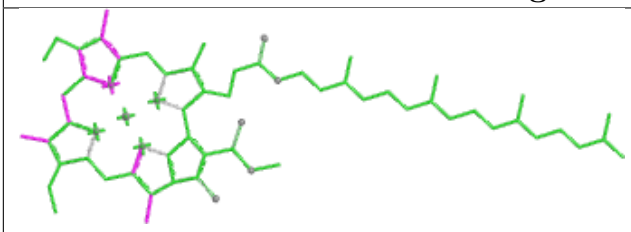

Bond lengths


Bond angles

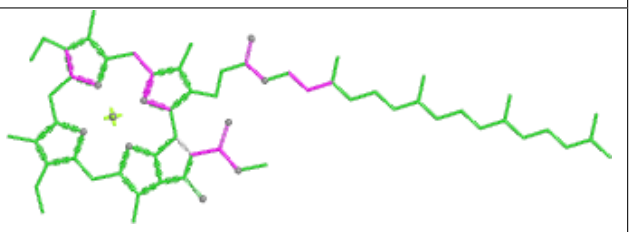

Torsions


Rings

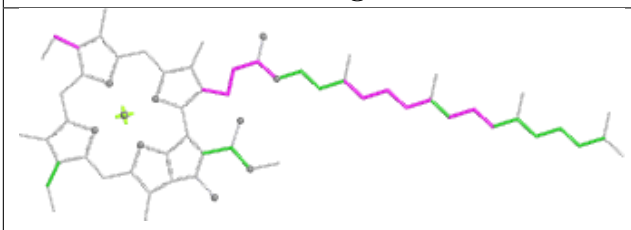
Ligand CLA c 503



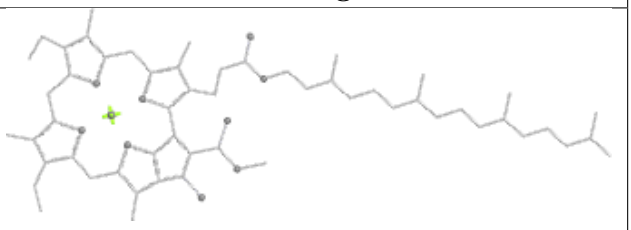
Bond lengths



Bond angles

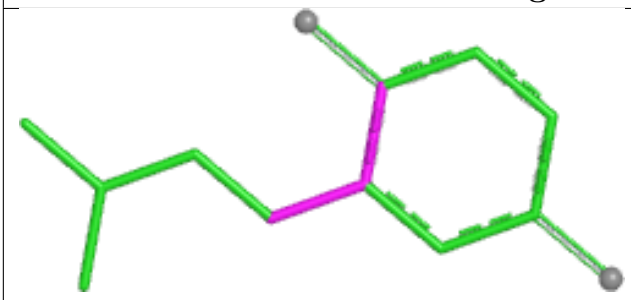


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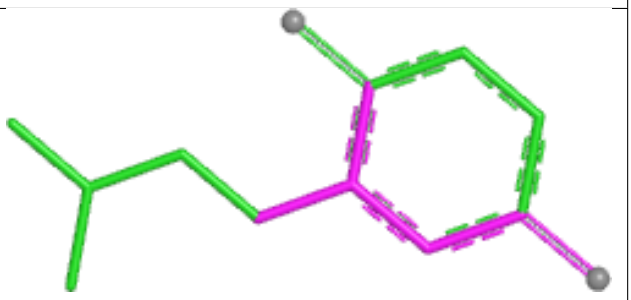


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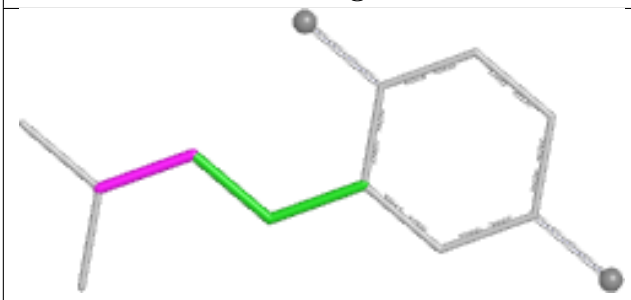
Ligand PL9 A 609



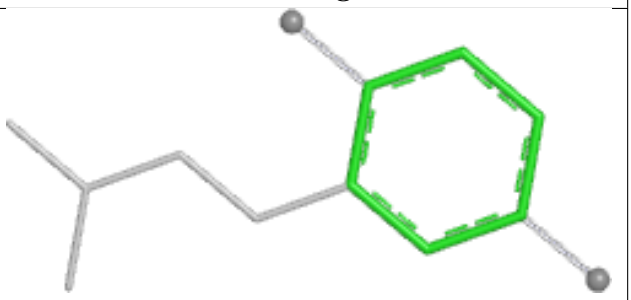
Bond lengths



Bond angles

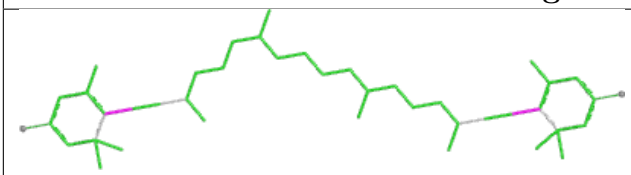


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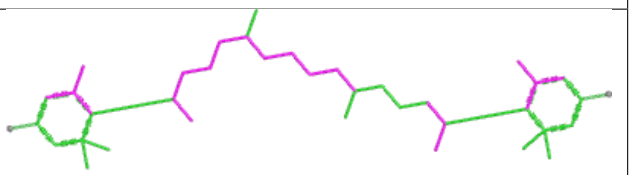


Rings

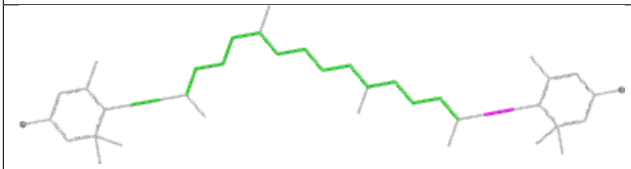
Ligand II0 6 612



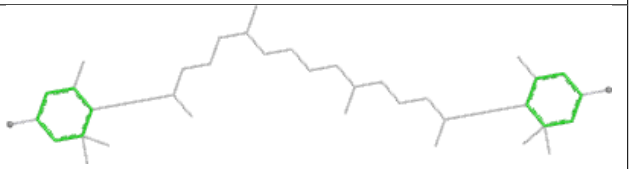
Bond lengths



Bond angles

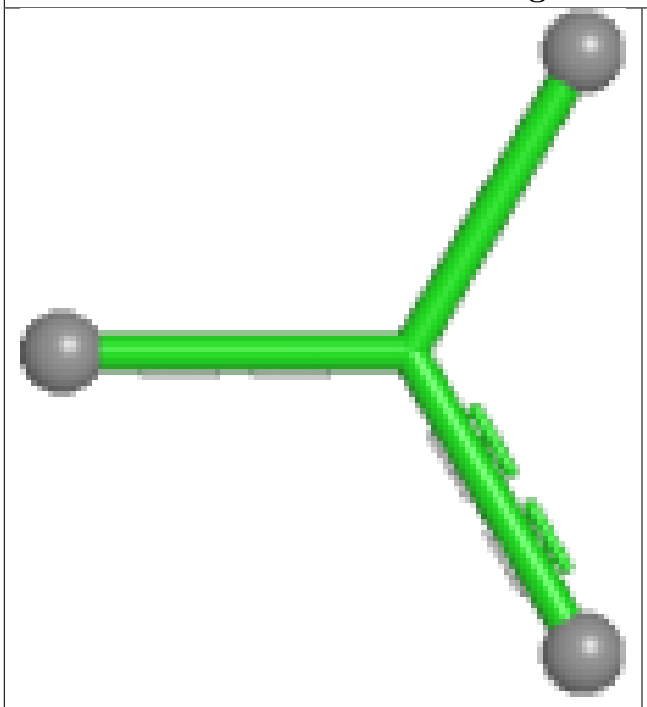


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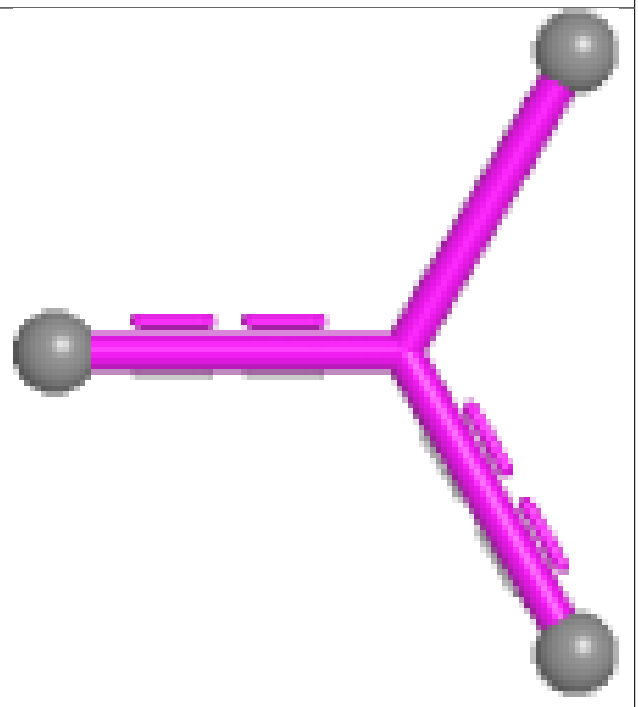


Rings

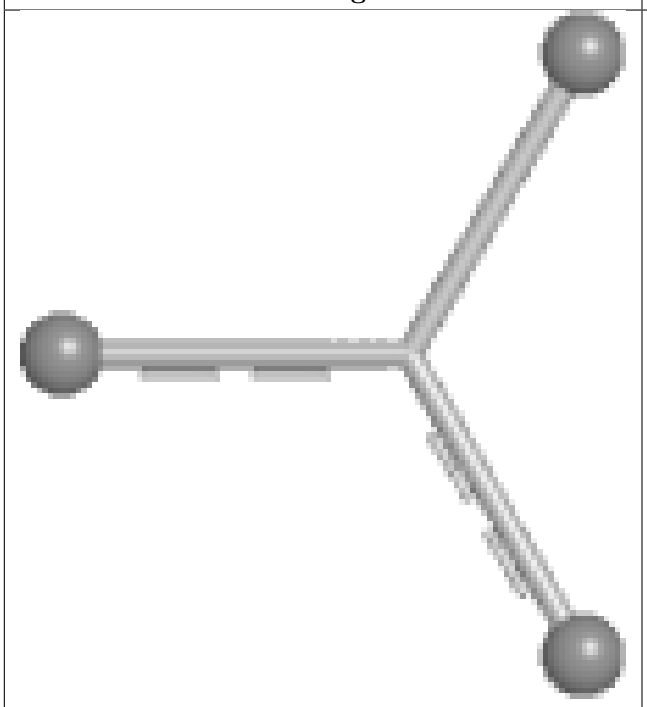
Ligand BCT a 401



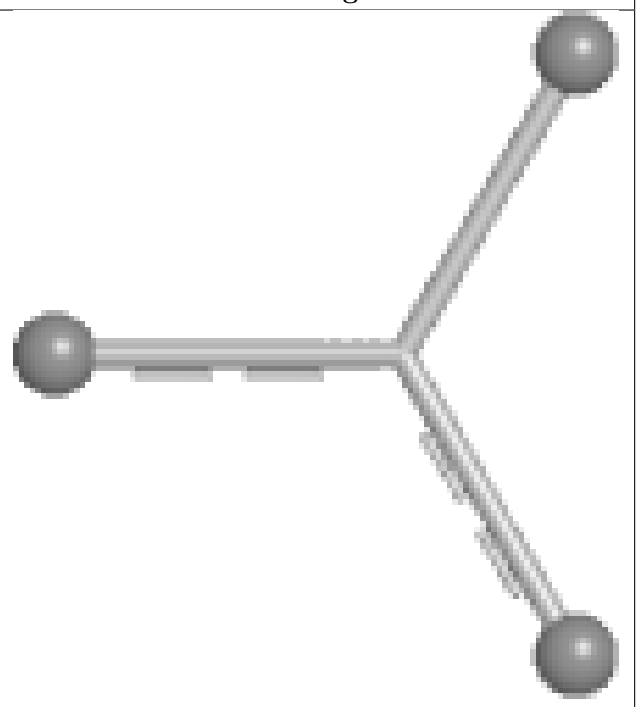
Bond lengths



Bond angles

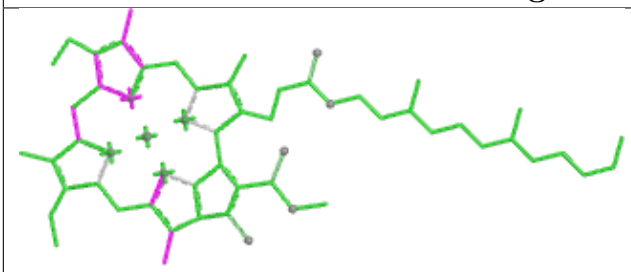


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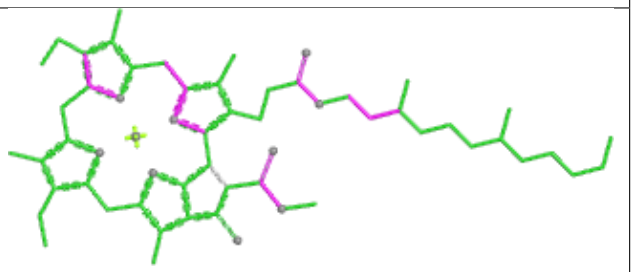


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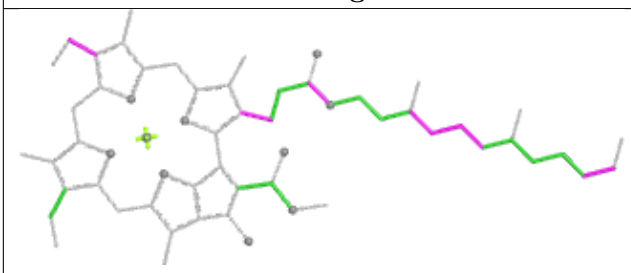
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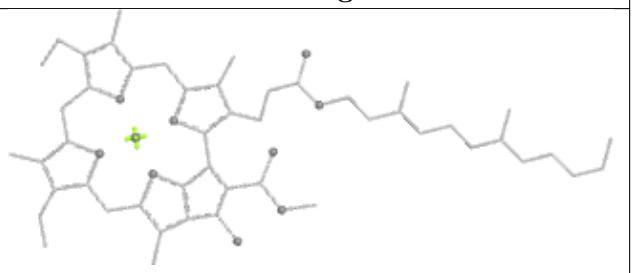
Bond lengths



Bond angles

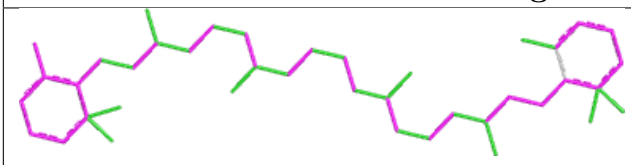


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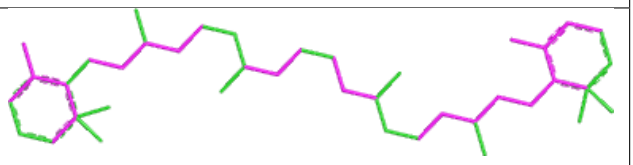


Rings

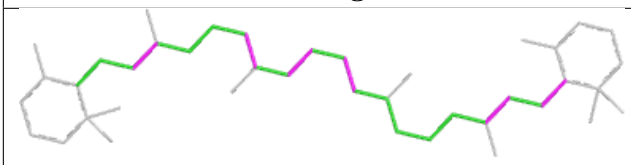
Ligand 8CT h 102



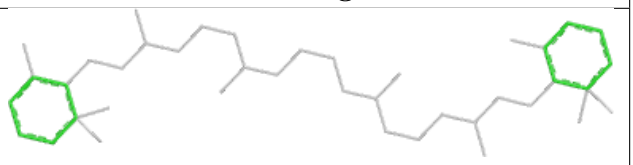
Bond lengths



Bond angles

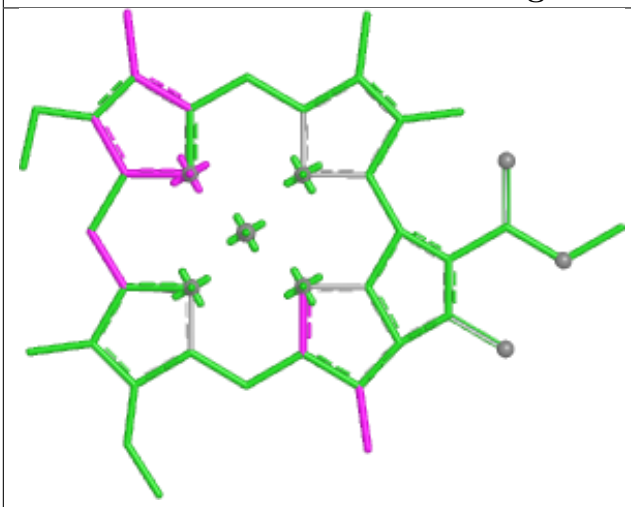


Torsions

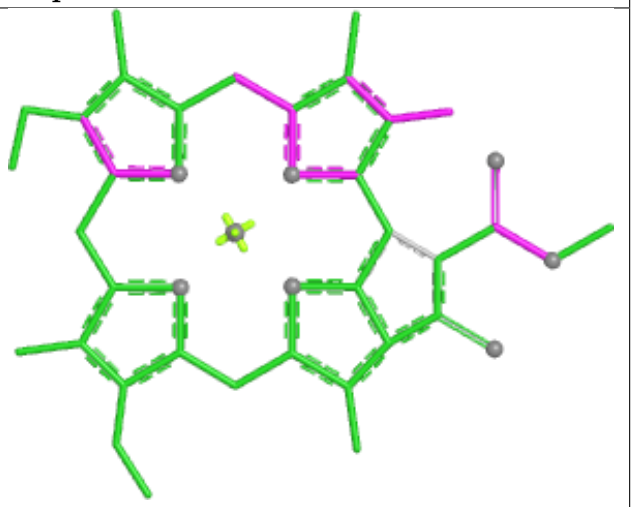


Rings

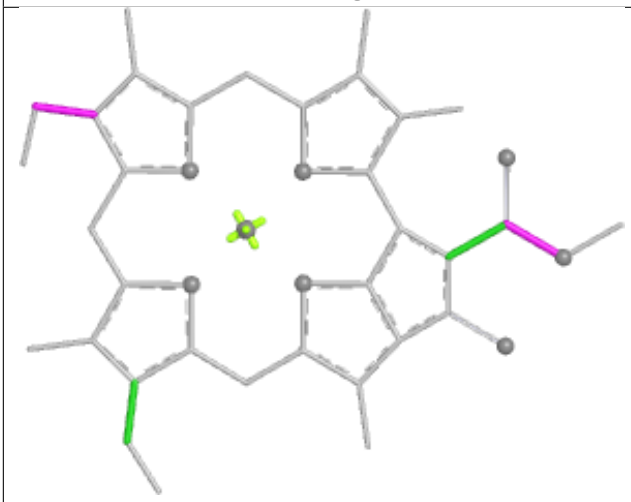
Ligand CLA p 310



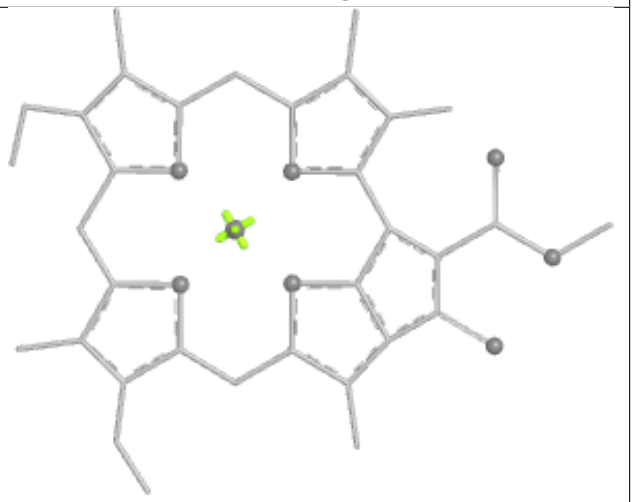
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Bond angles

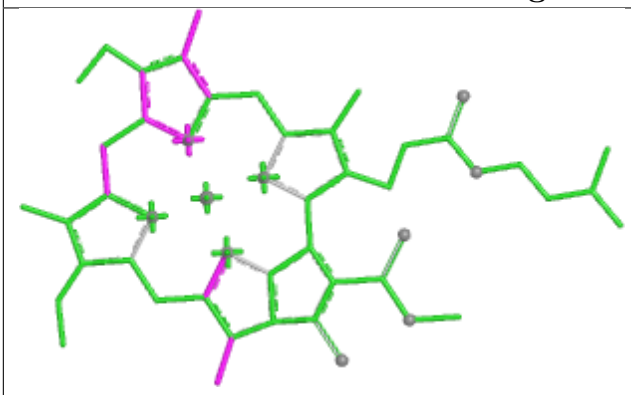


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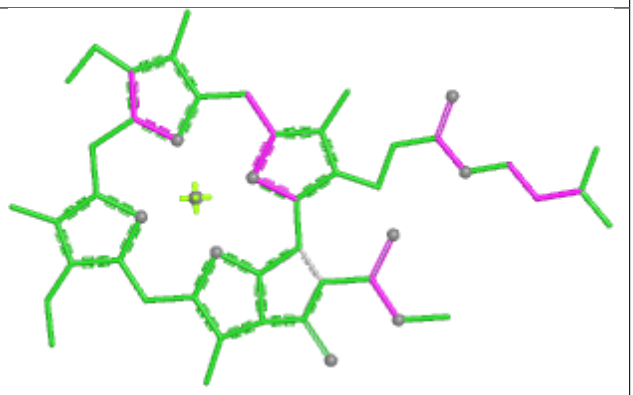


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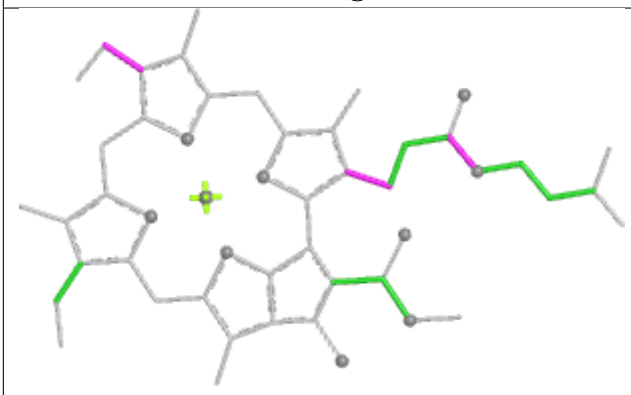
Ligand CLA 2 603



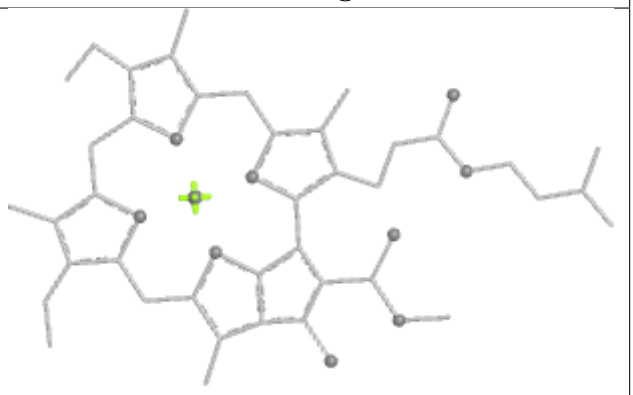
Bond lengths



Bond angles

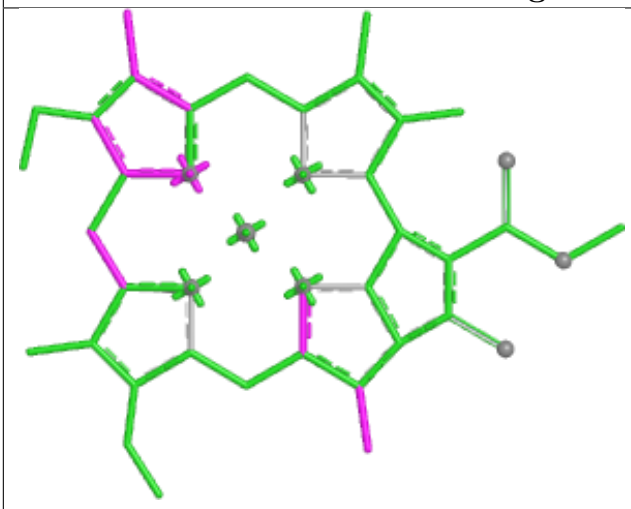


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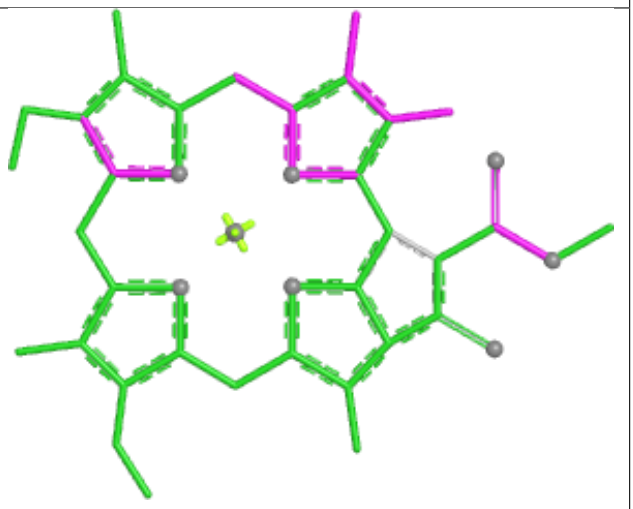


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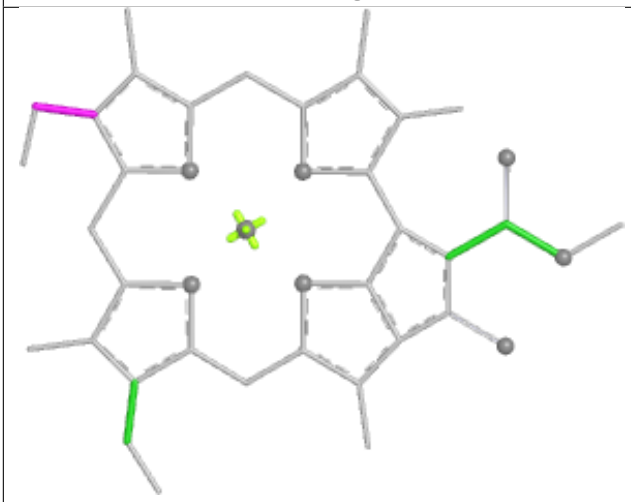
Ligand CLA 9 608



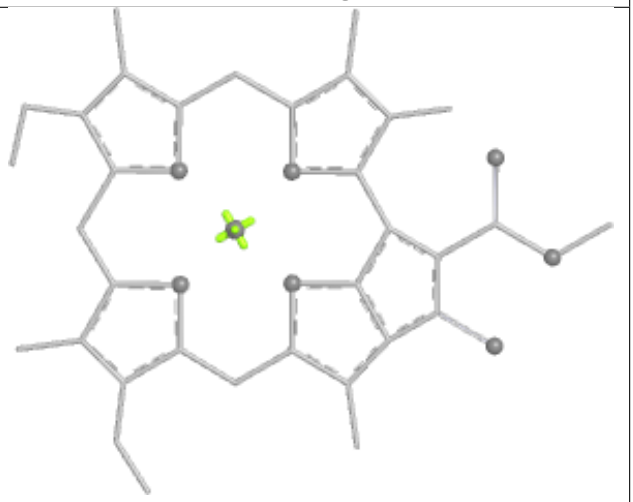
Bond lengths



Bond angles



Torsions

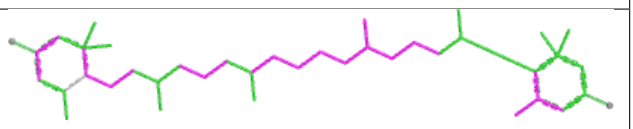


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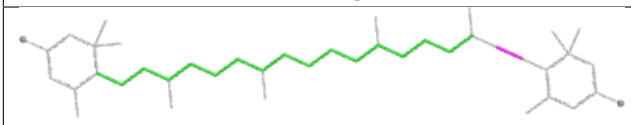
Ligand II3 6 613



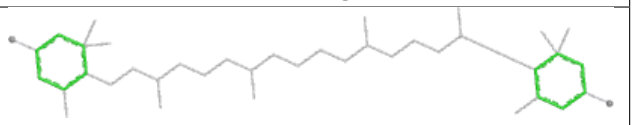
Bond lengths



Bond angles

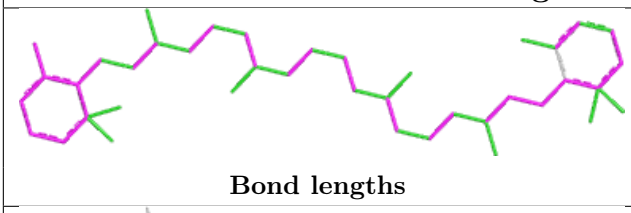


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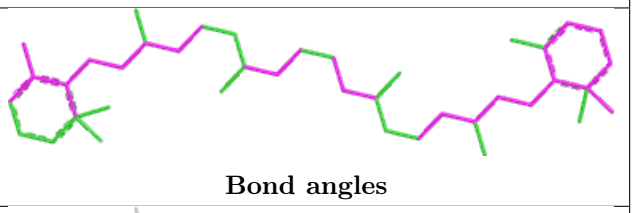


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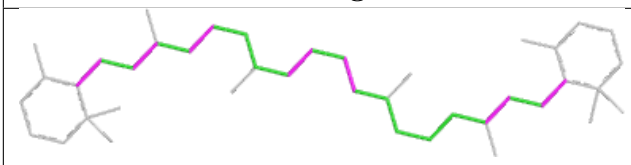
Ligand 8CT c 518



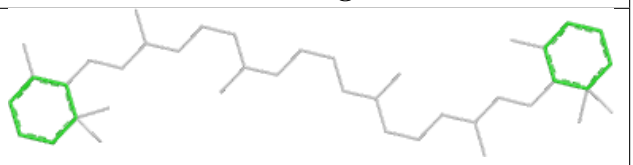
Bond lengths



Bond angles

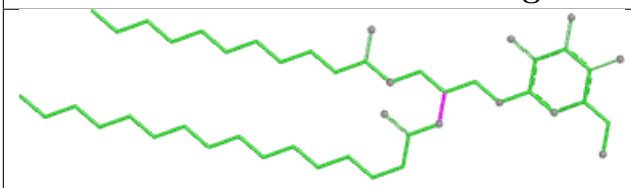


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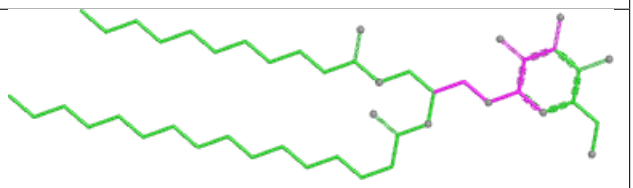


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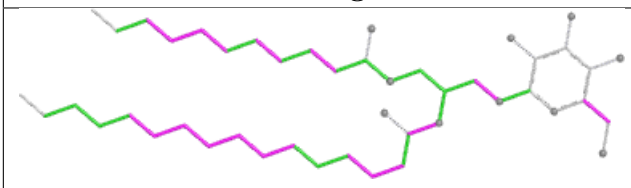
Ligand LMG d 406



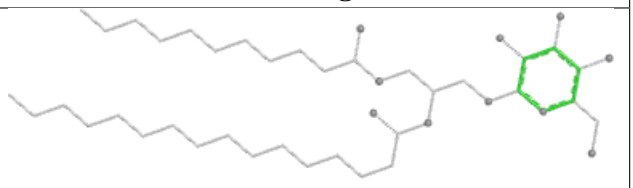
Bond lengths



Bond angles

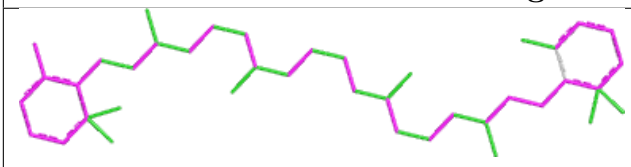


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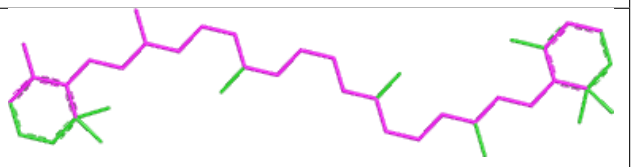


Rings

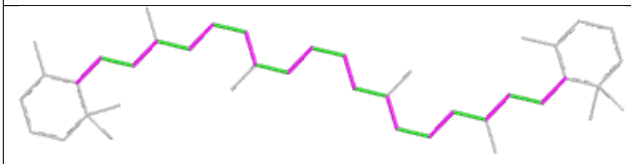
Ligand 8CT B 622



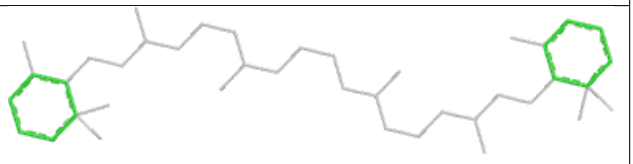
Bond lengths



Bond angles

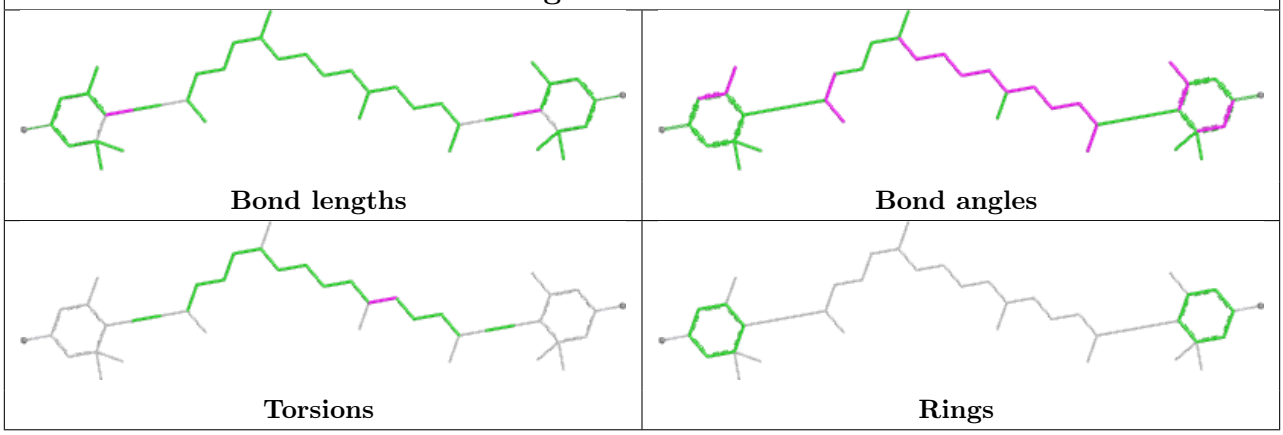


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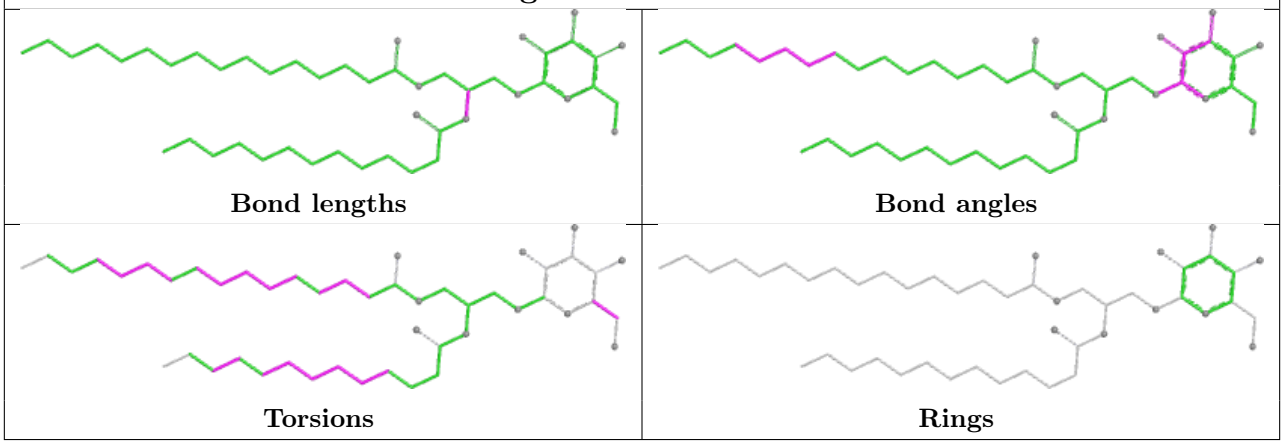


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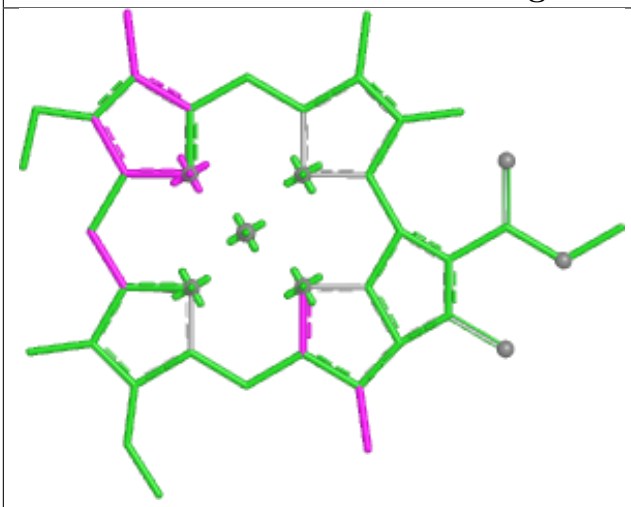
Ligand II0 8 615



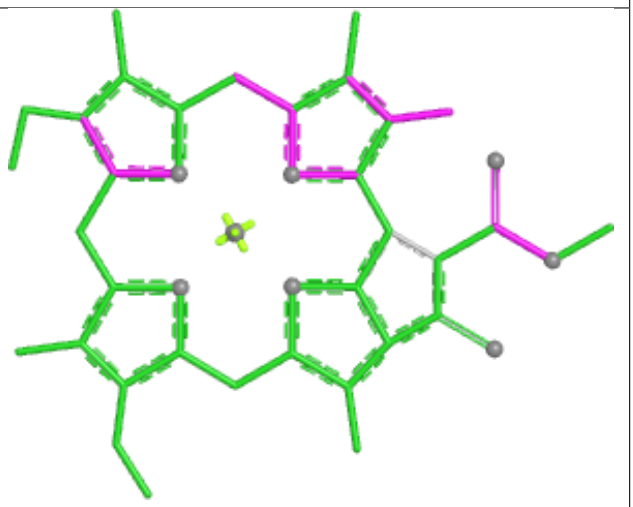
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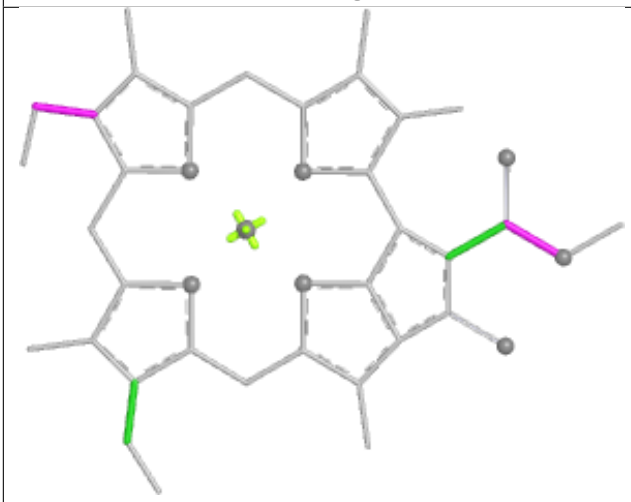
Ligand CLA 2 609



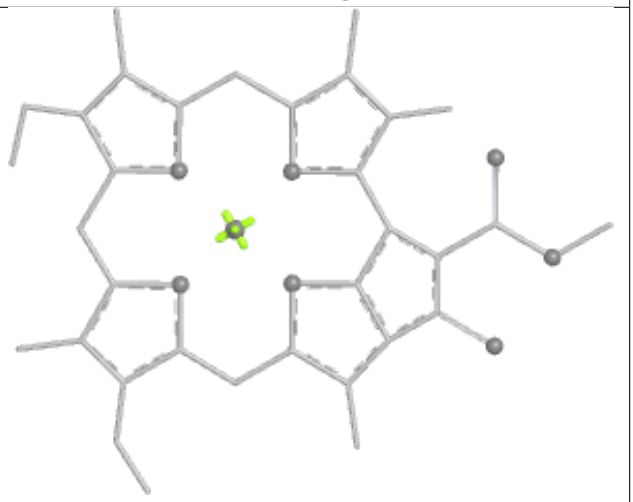
Bond lengths



Bond angles

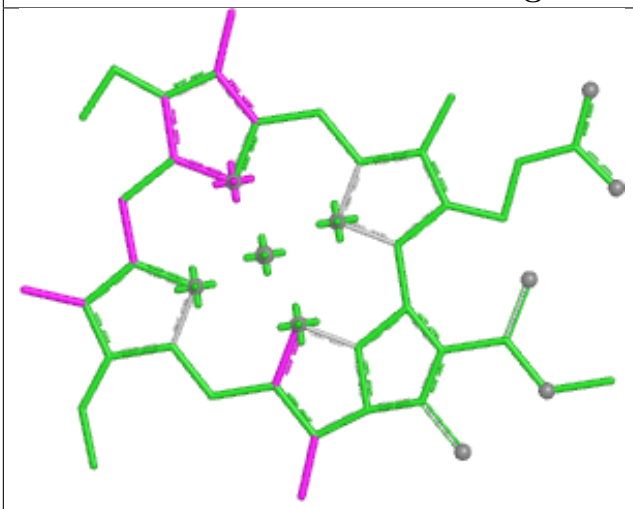


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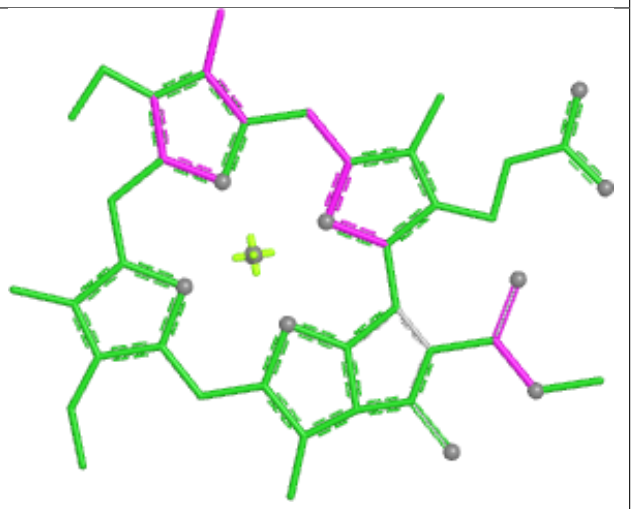


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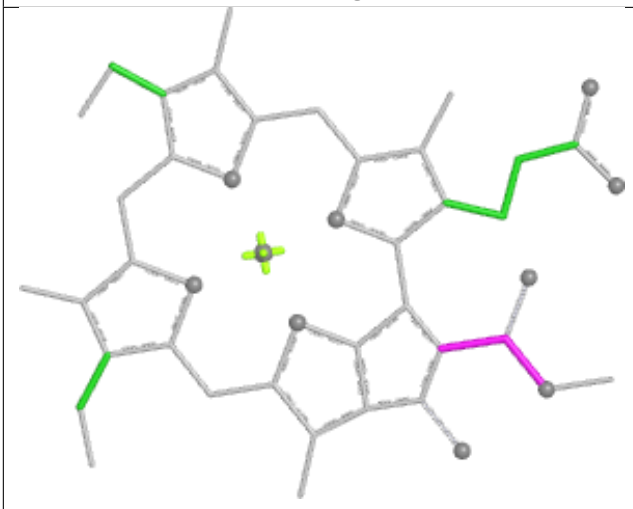
Ligand CLA C 506



Bond lengths



Bond angles

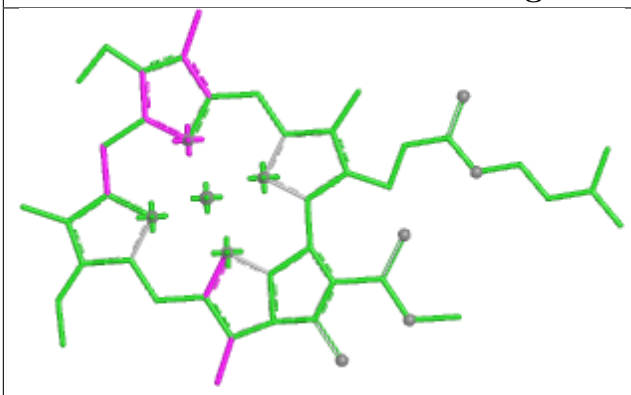


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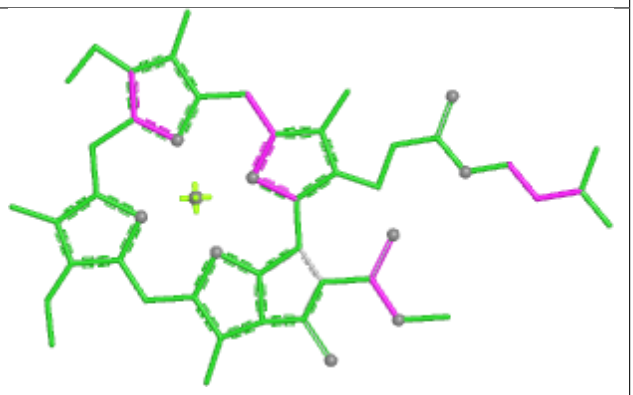


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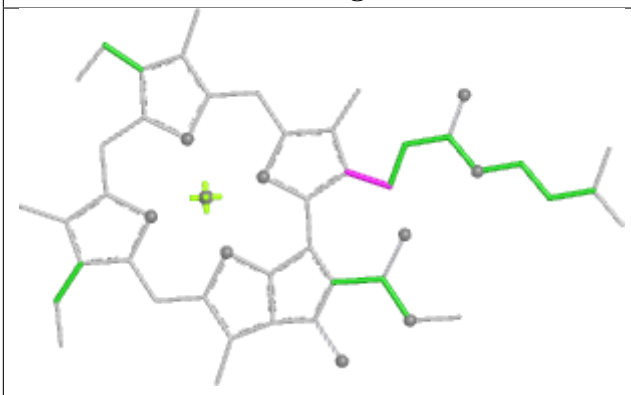
Ligand CLA P 603



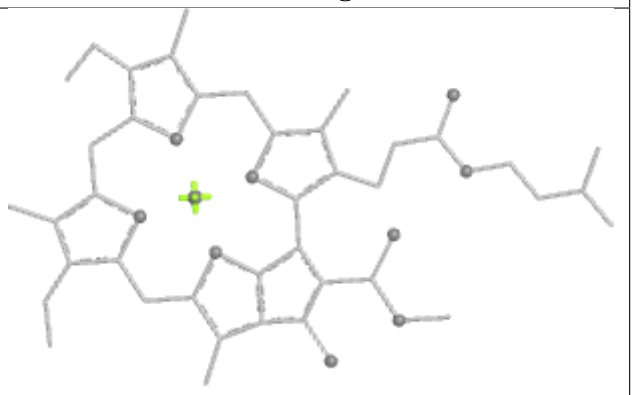
Bond lengths



Bond angles

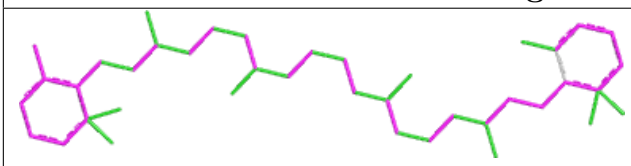


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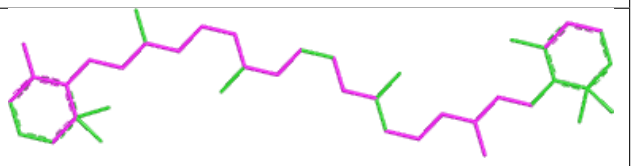


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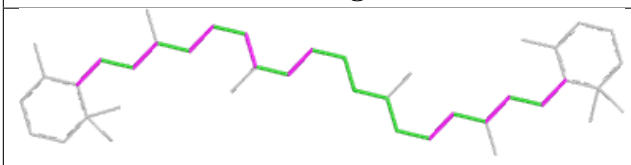
Ligand 8CT D 409



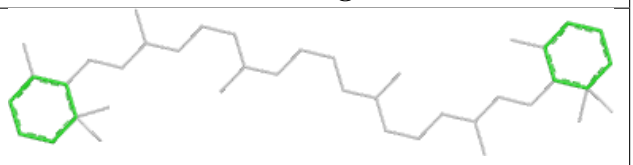
Bond lengths



Bond angles

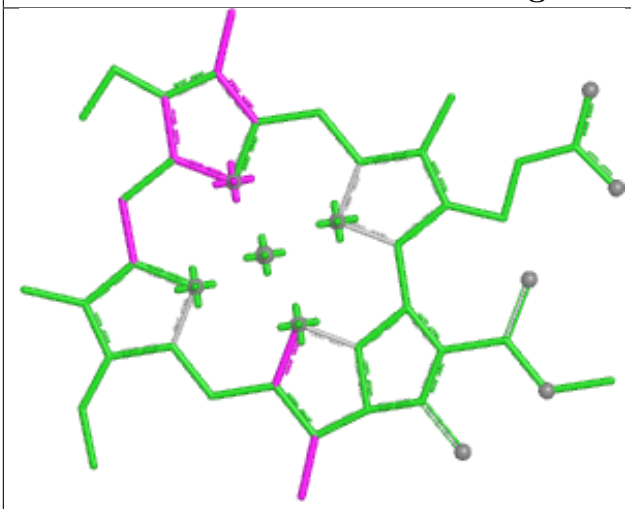


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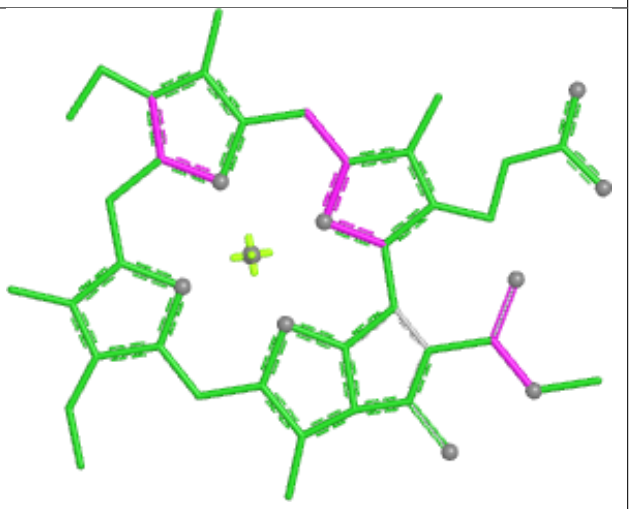


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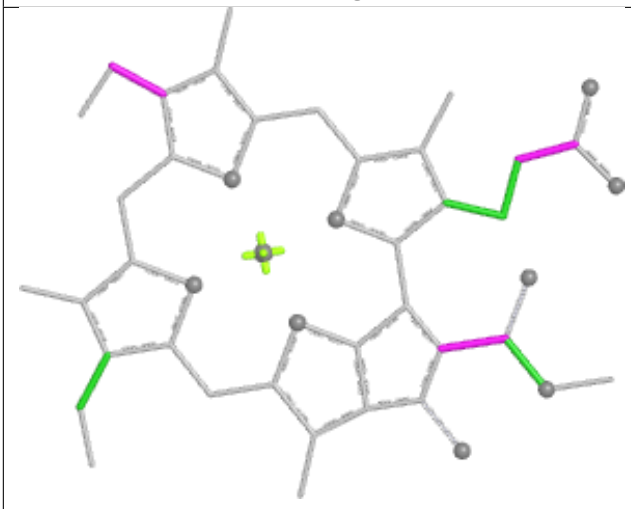
Ligand CLA 5 307



Bond lengths



Bond angles

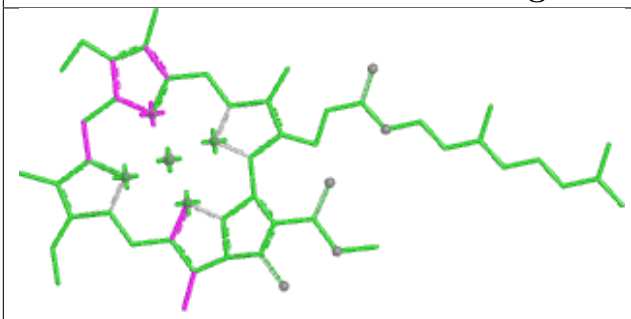


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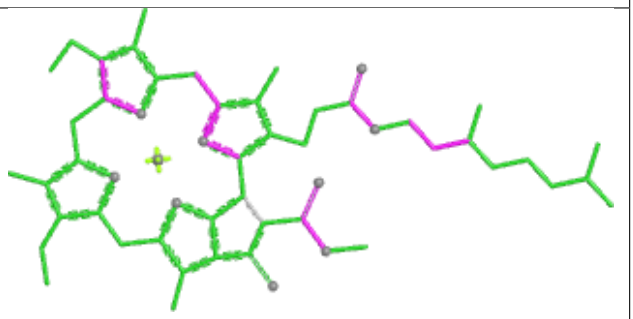


Rings

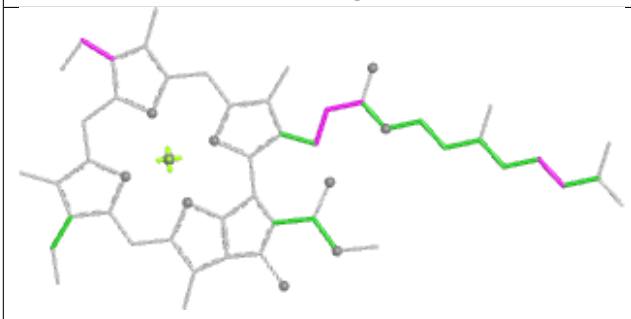
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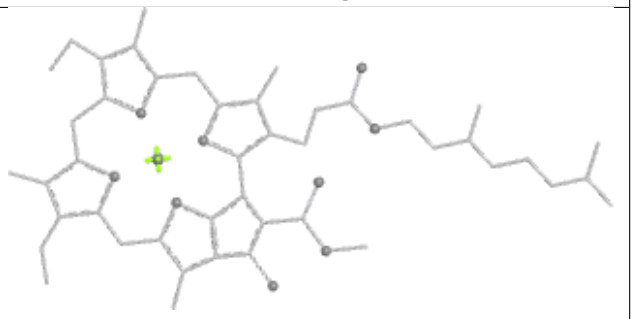
Bond lengths



Bond angles

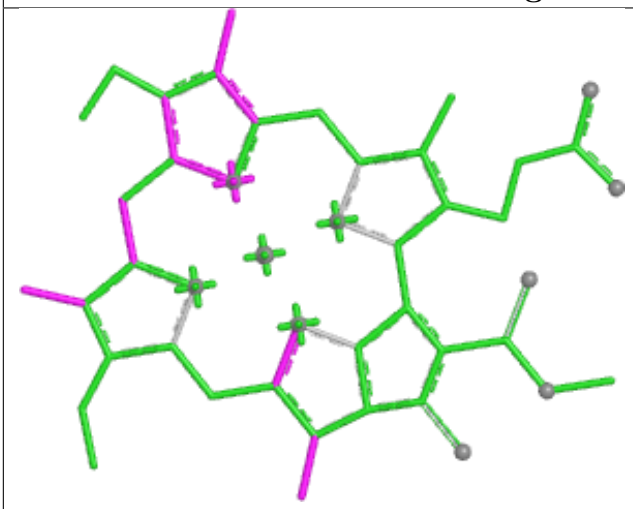


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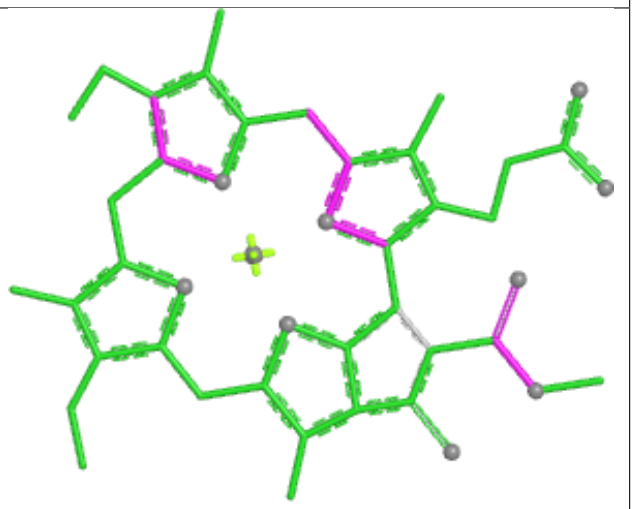


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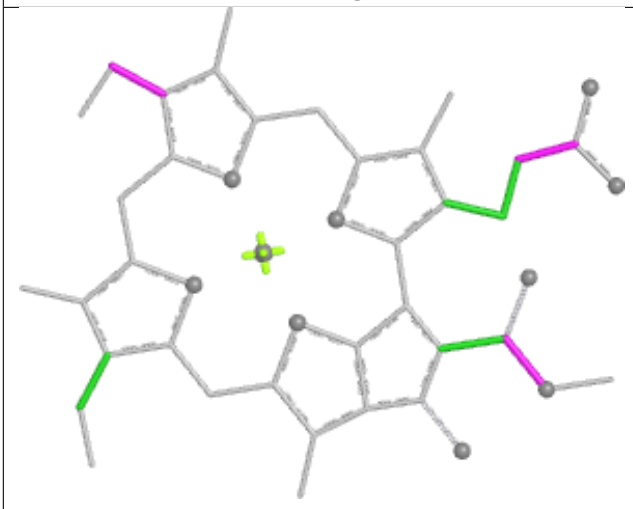
Ligand CLA P 610



Bond lengths



Bond angles

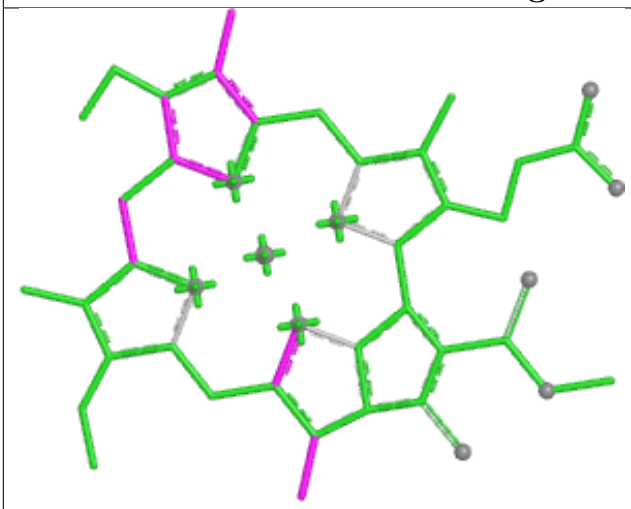


Torsions

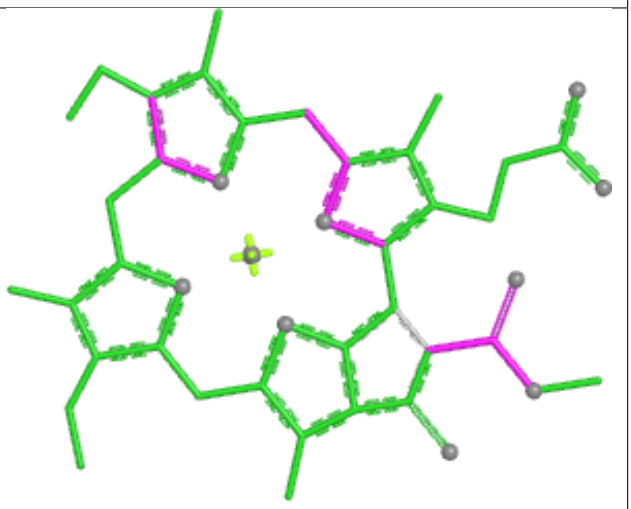


Rings

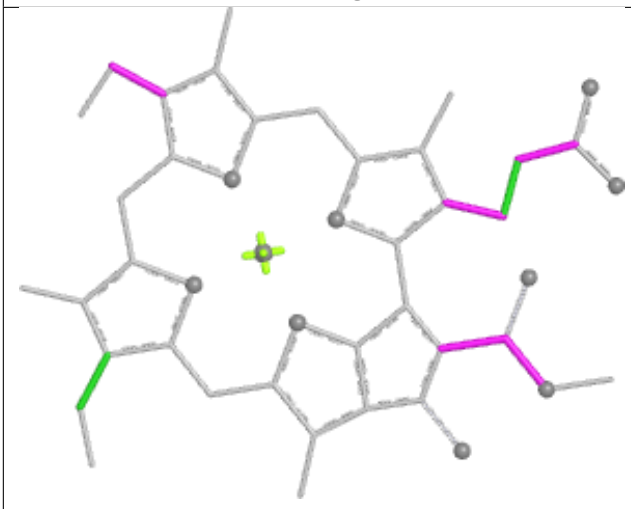
Ligand CLA 4 612



Bond lengths



Bond angles

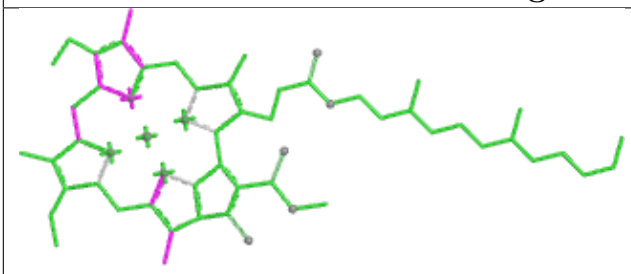


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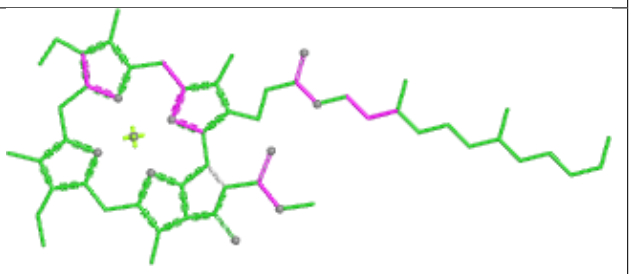


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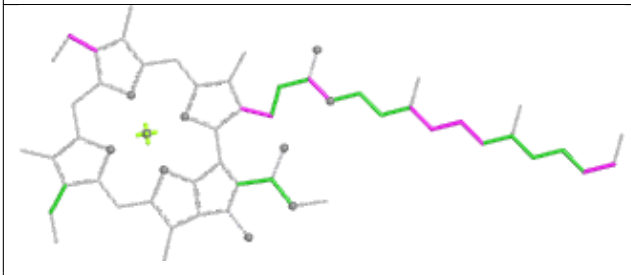
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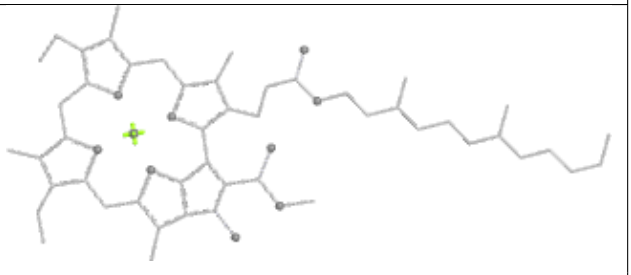
Bond lengths



Bond angles

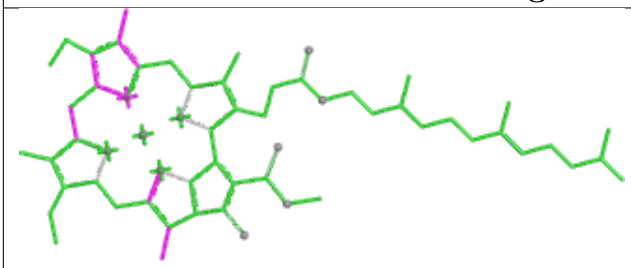


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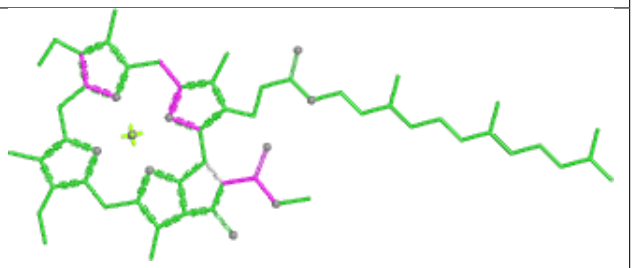


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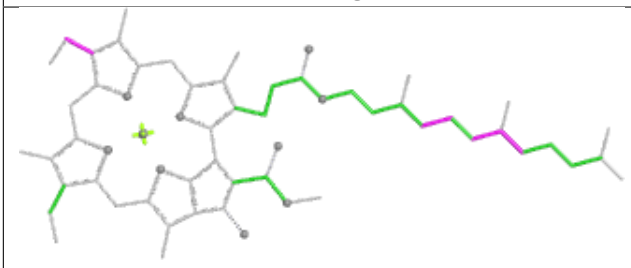
Ligand CLA 3 609



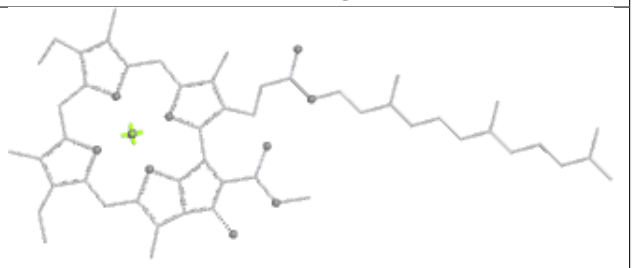
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Bond angles

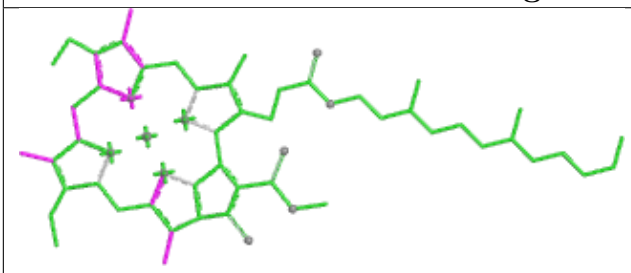


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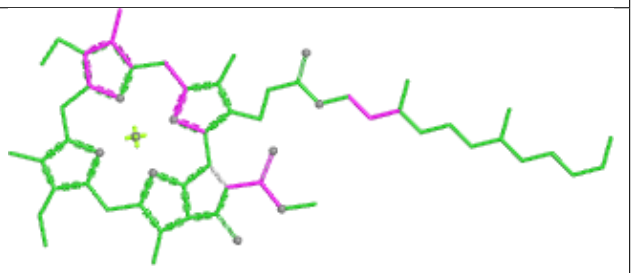


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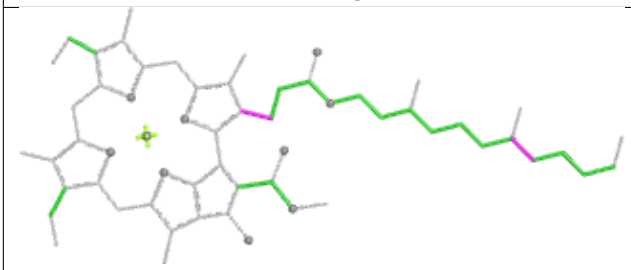
Ligand CLA D 401



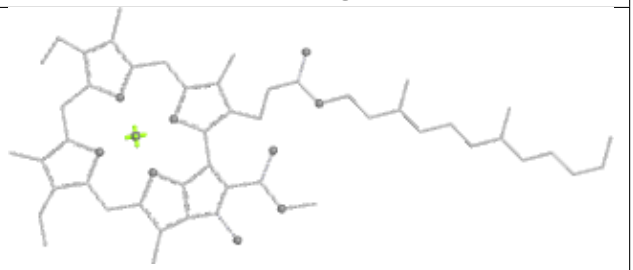
Bond lengths



Bond angles

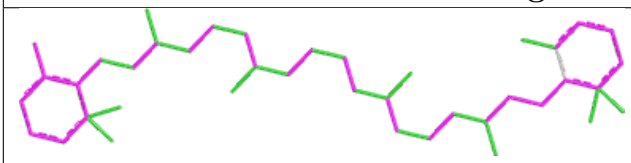


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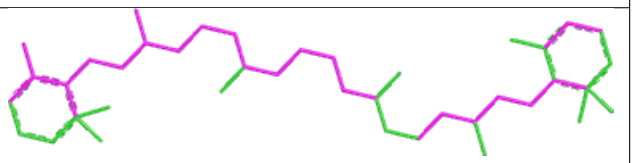


Rings

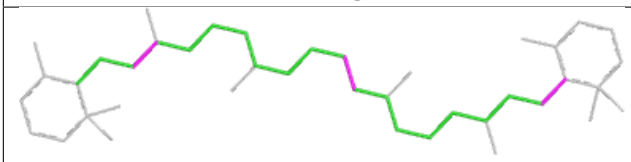
Ligand 8CT P 615



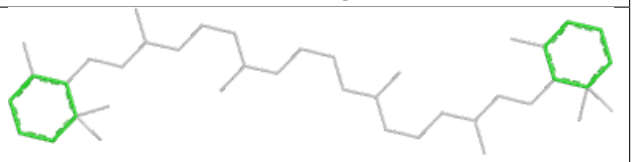
Bond lengths



Bond angles

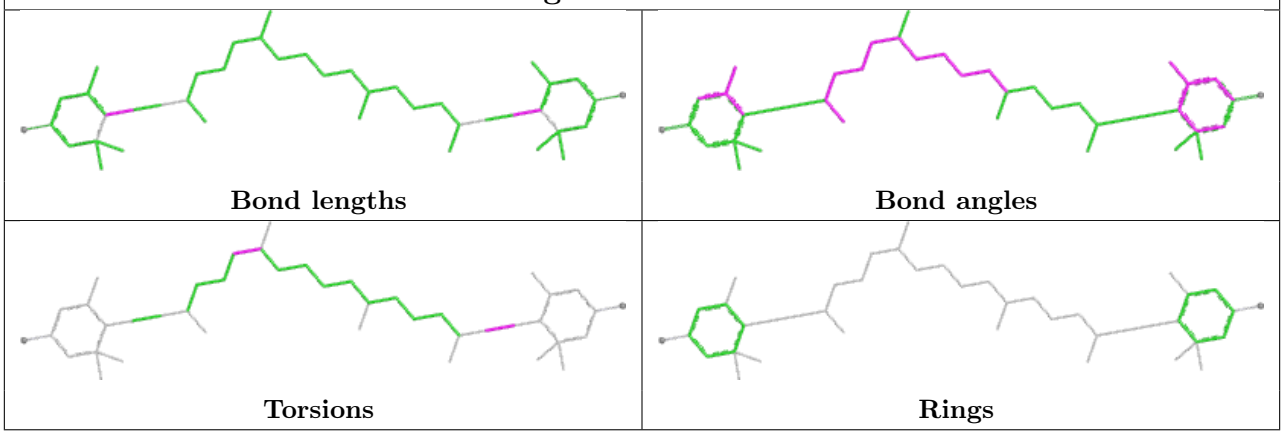


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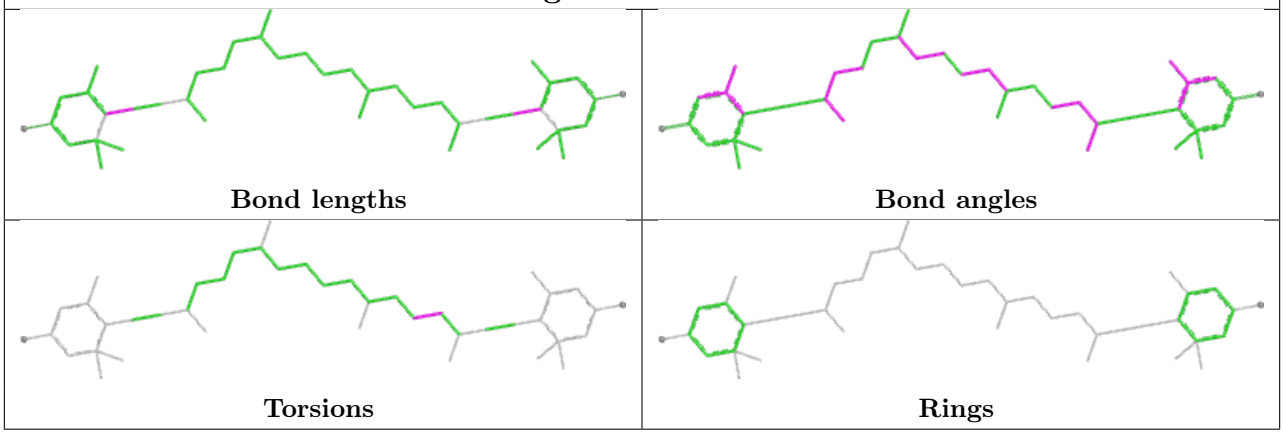


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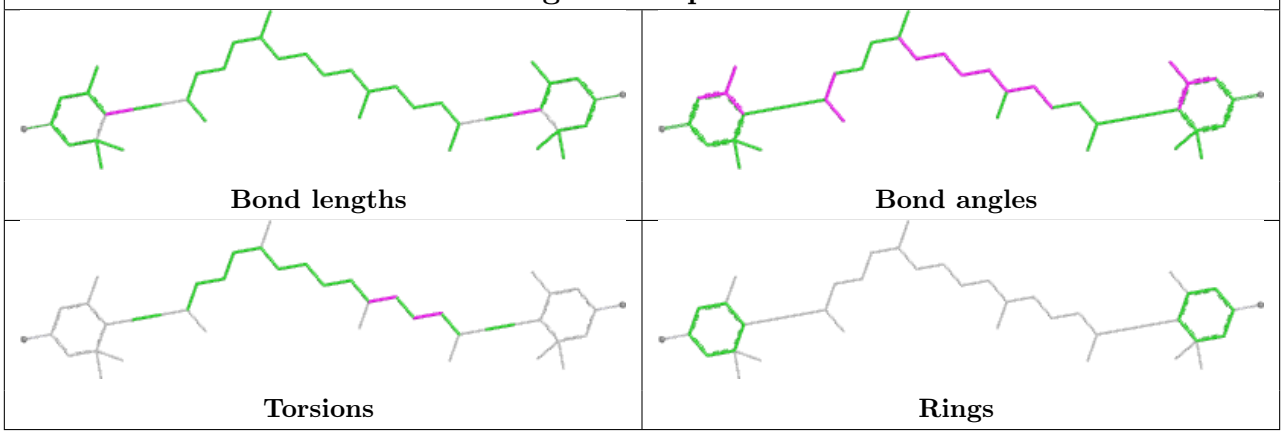
Ligand II0 9 614



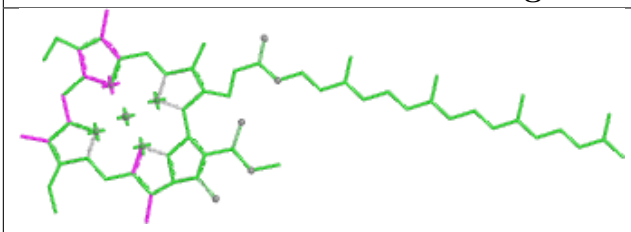
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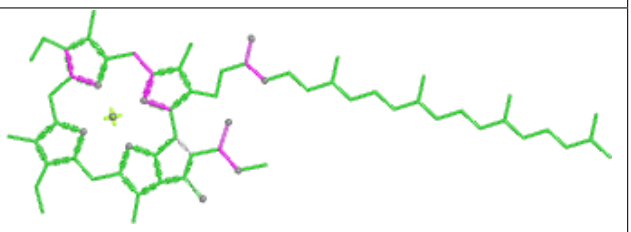
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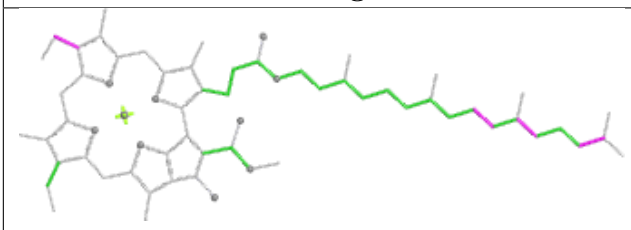
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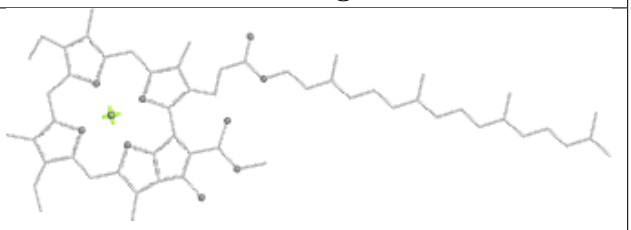
Bond lengths



Bond angles

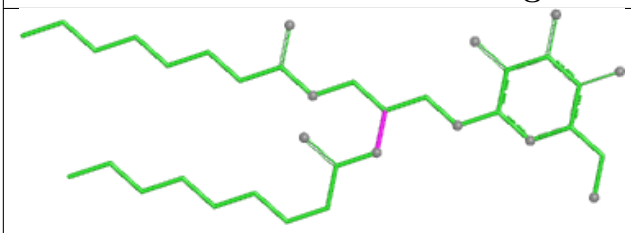


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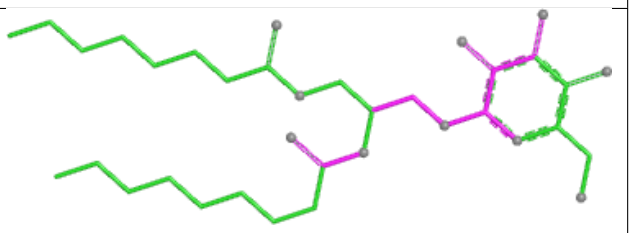


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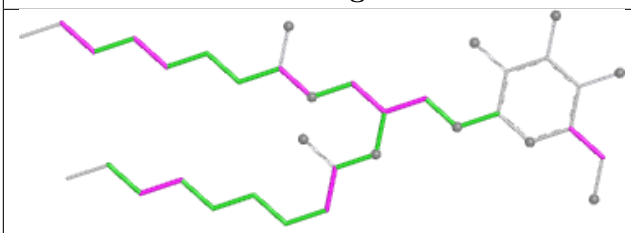
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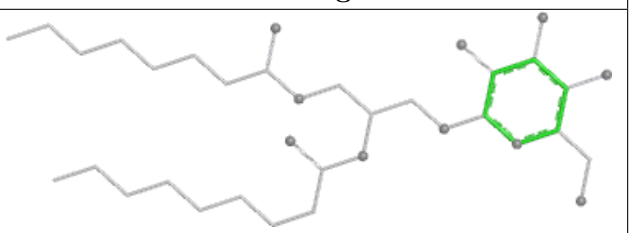
Bond lengths



Bond angles

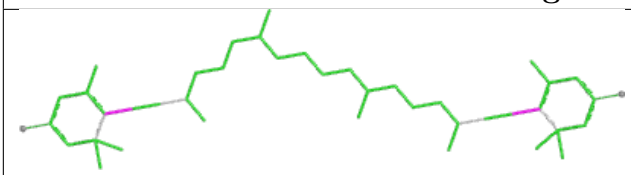


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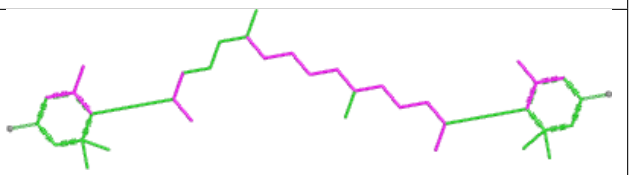


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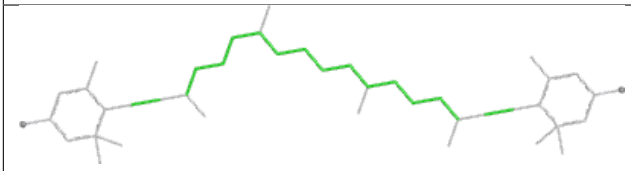
Ligand II0 2 614



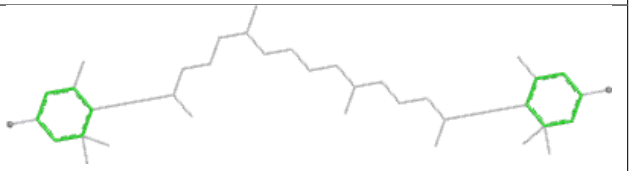
Bond lengths



Bond angles

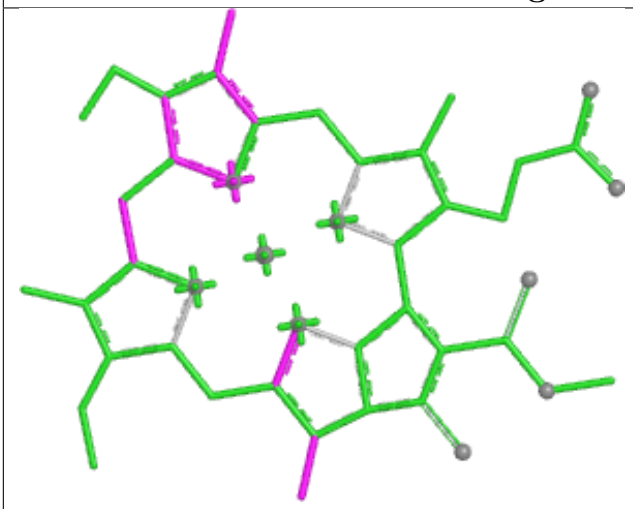


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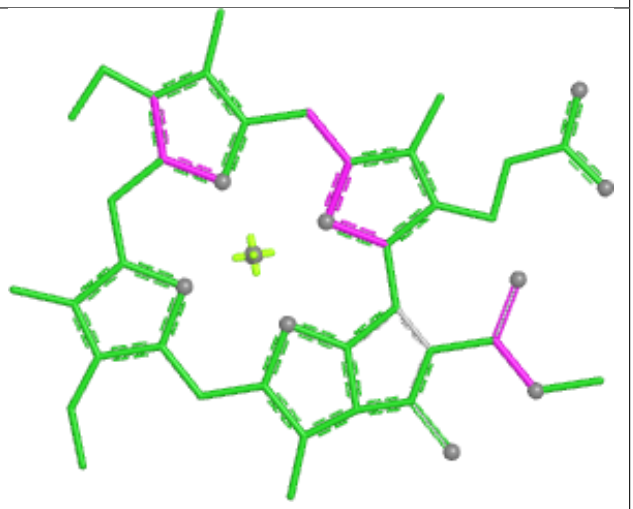


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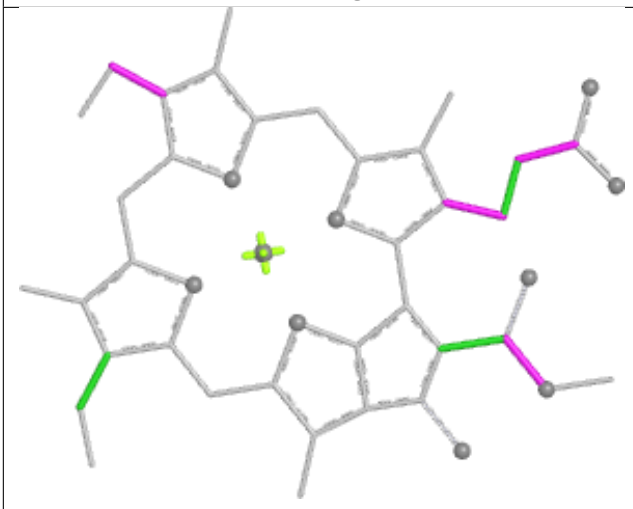
Ligand CLA 8 612



Bond lengths



Bond angles

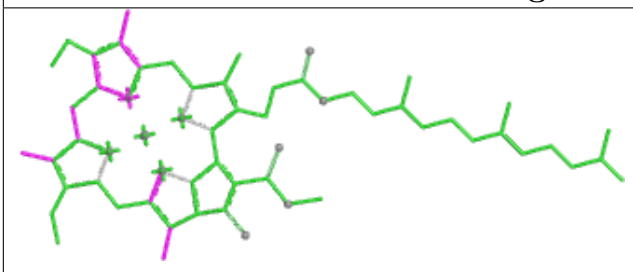


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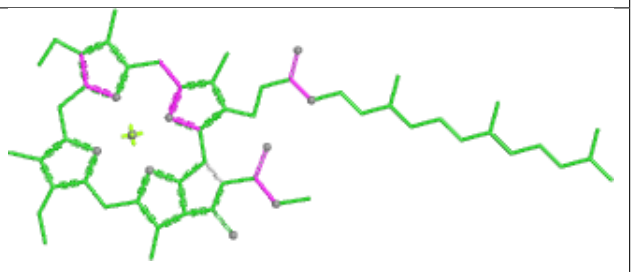


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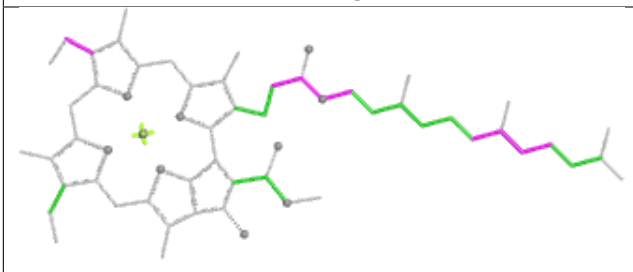
Ligand CLA 8 605



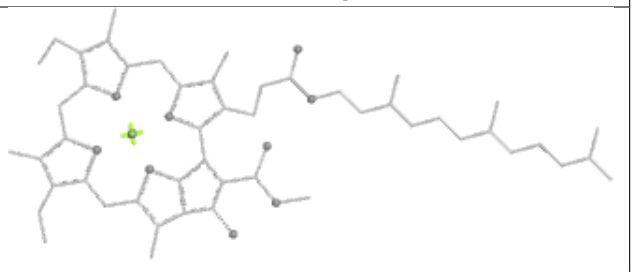
Bond lengths



Bond angles

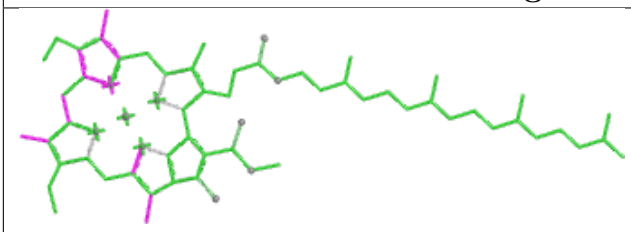


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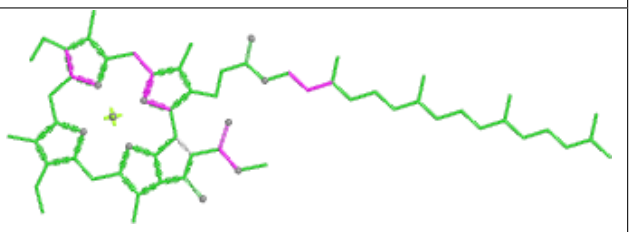


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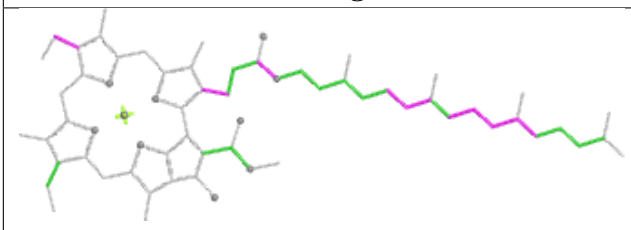
Ligand CLA B 617



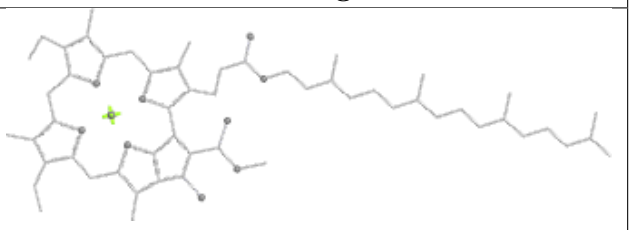
Bond lengths



Bond angles

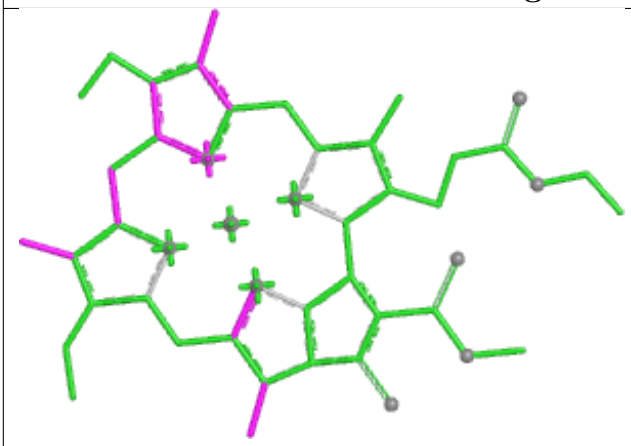


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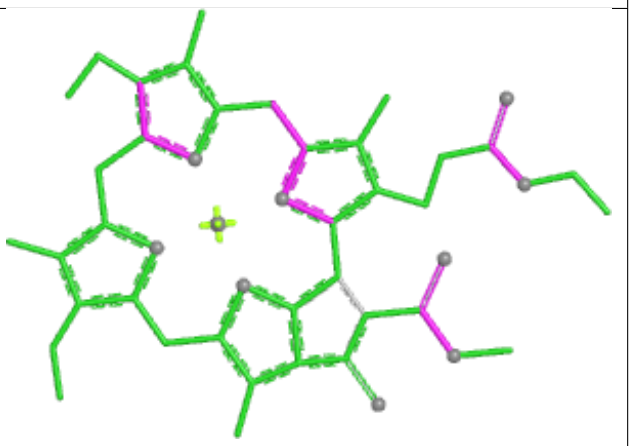


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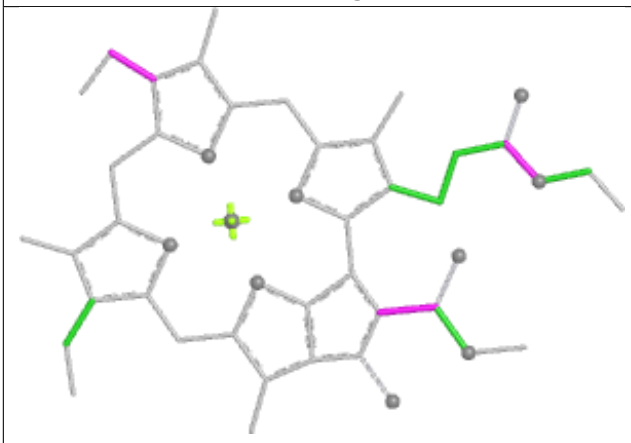
Ligand CLA B 602



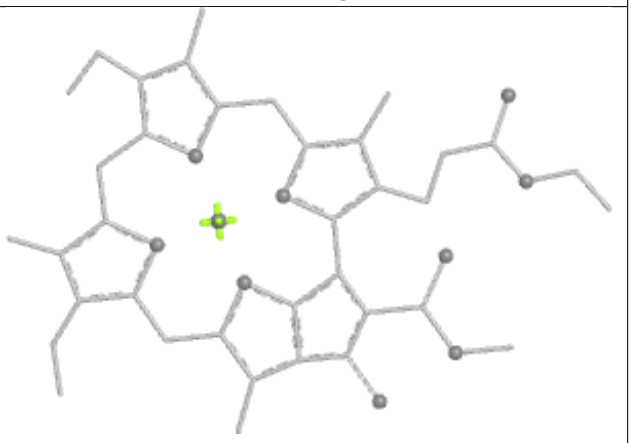
Bond lengths



Bond angles

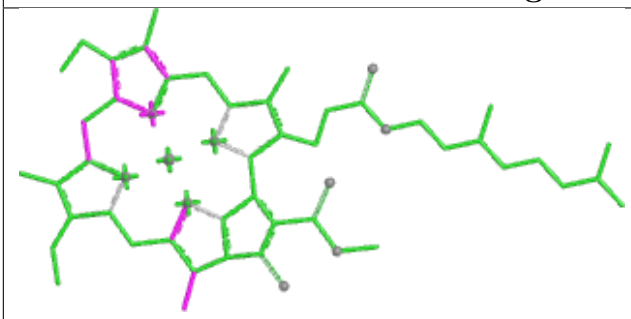


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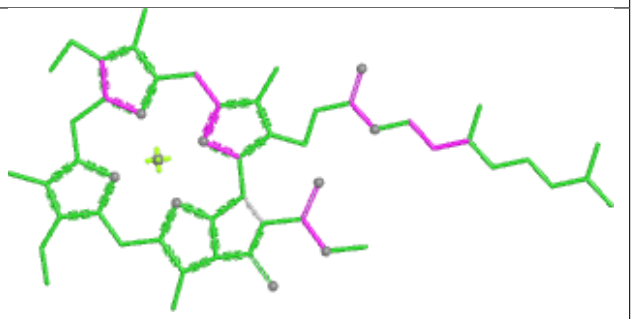


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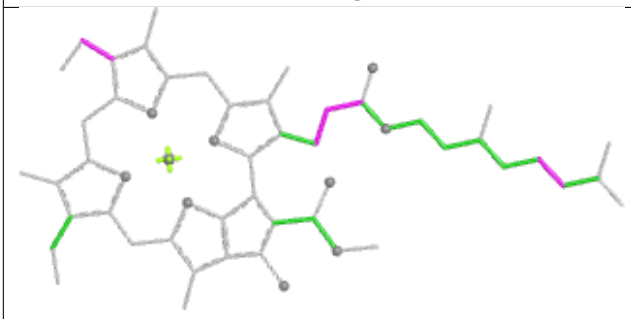
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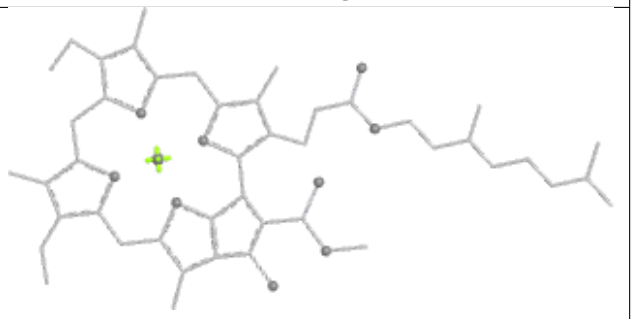
Bond lengths



Bond angles

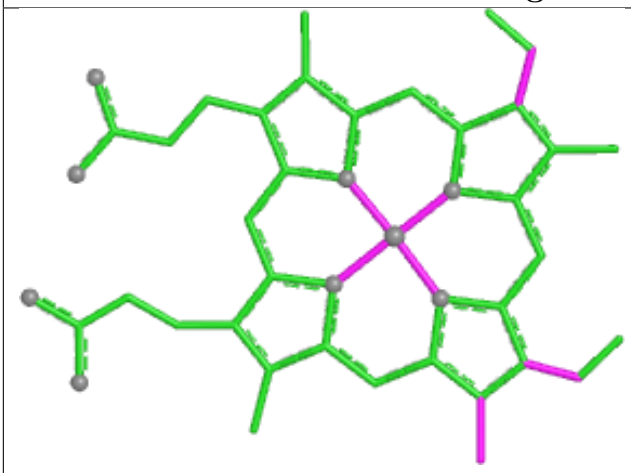


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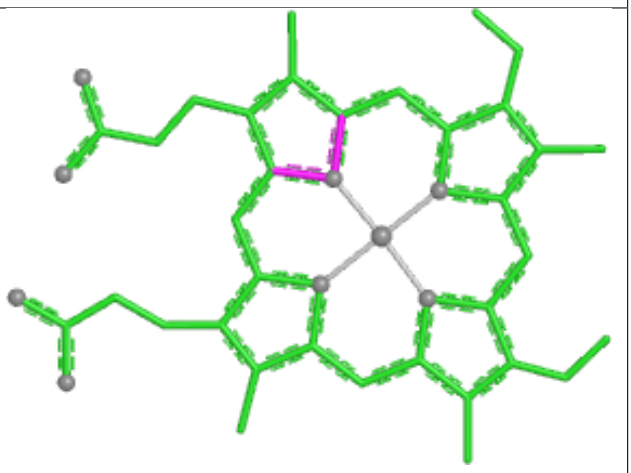


Rings

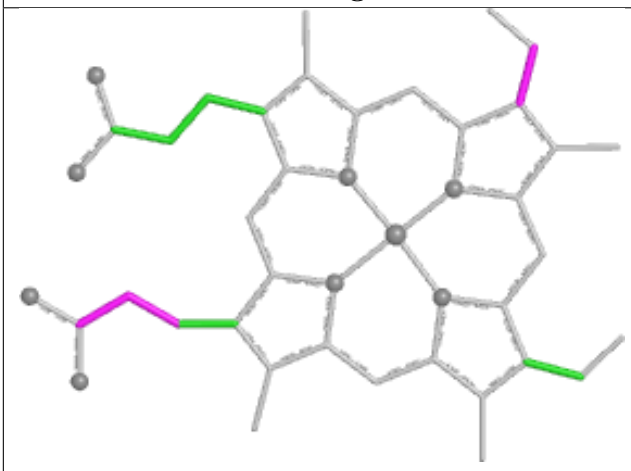
Ligand HEM f 101



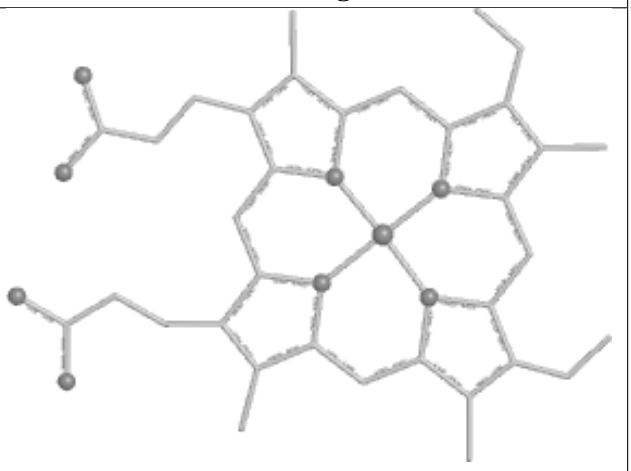
Bond lengths



Bond angles

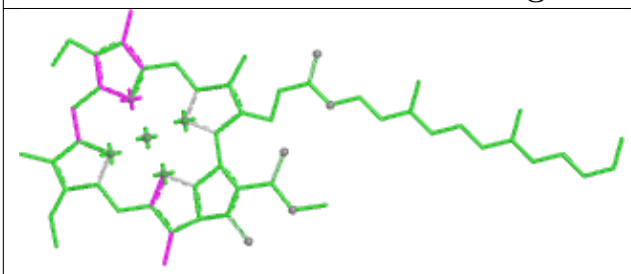


Torsions

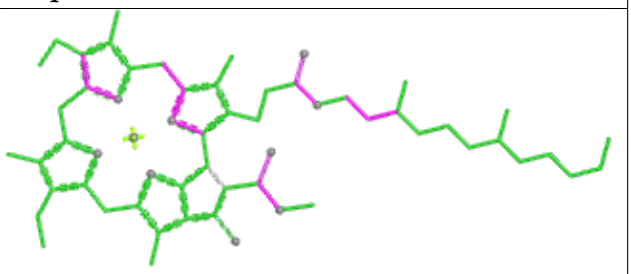


Rings

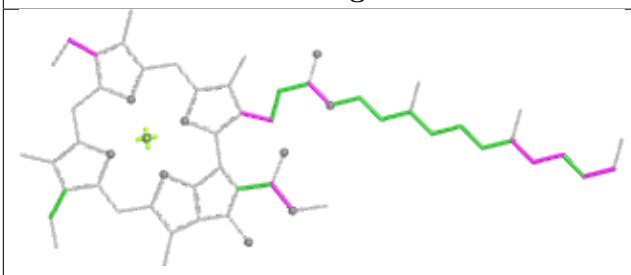
Ligand CLA p 303



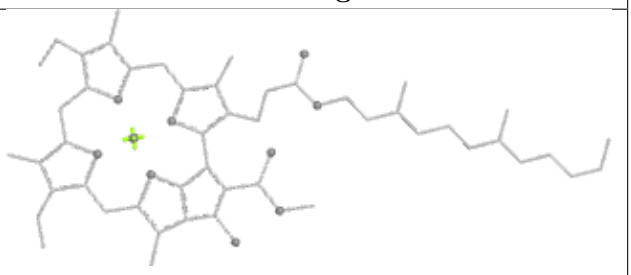
Bond lengths



Bond angles

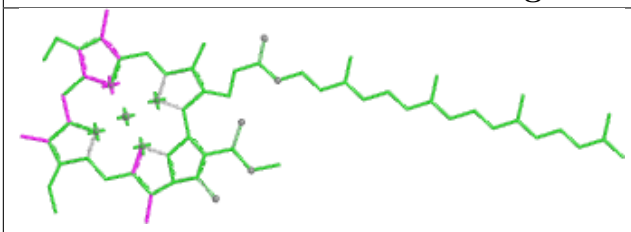


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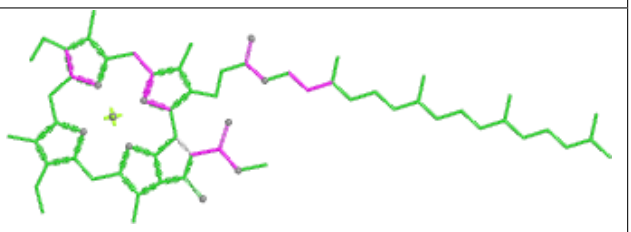


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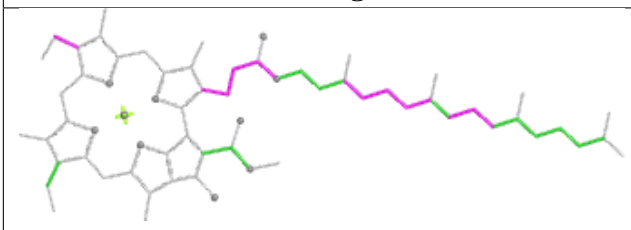
Ligand CLA C 503



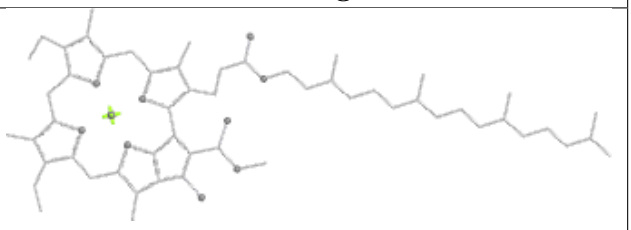
Bond lengths



Bond angles

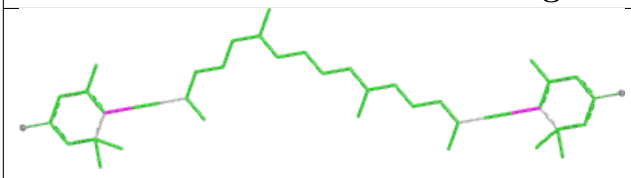


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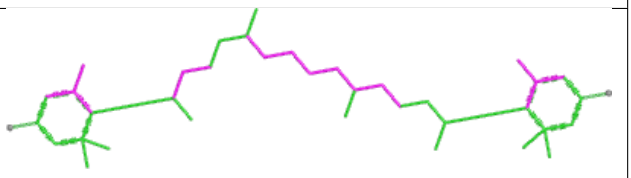


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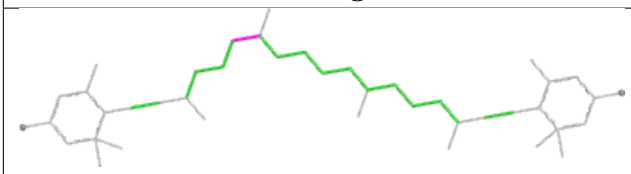
Ligand II0 5 316



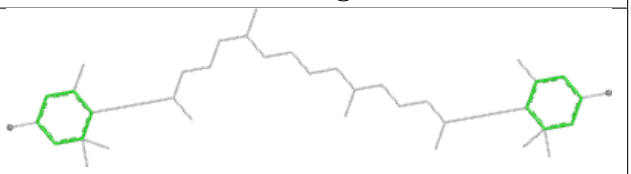
Bond lengths



Bond angles

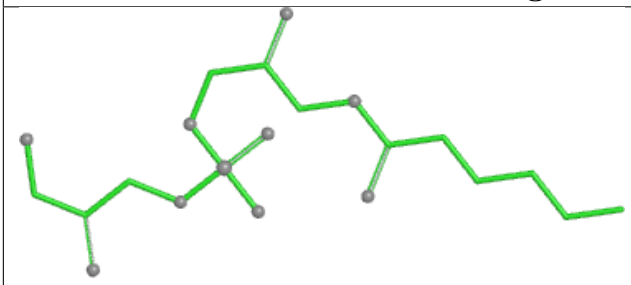


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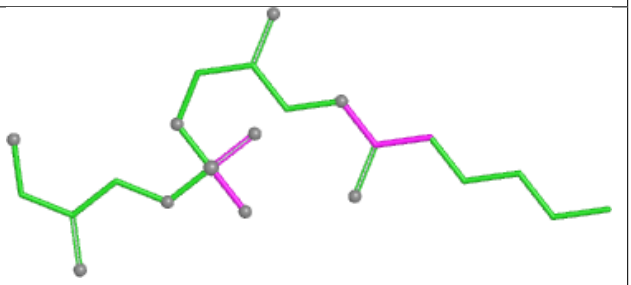


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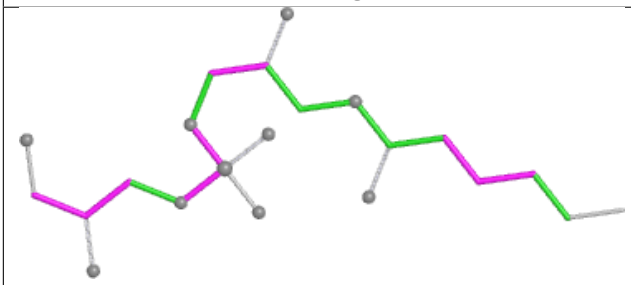
Ligand LHG 8 618



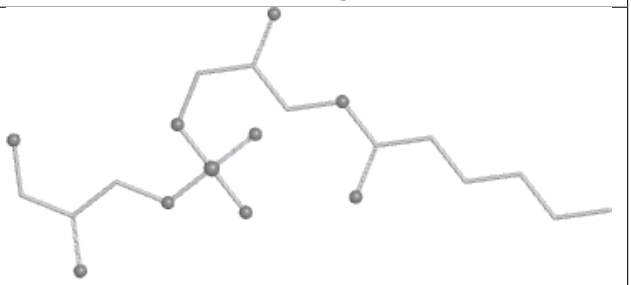
Bond lengths



Bond angles

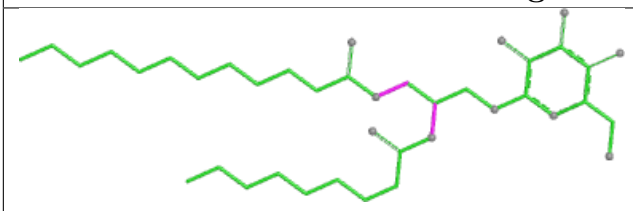


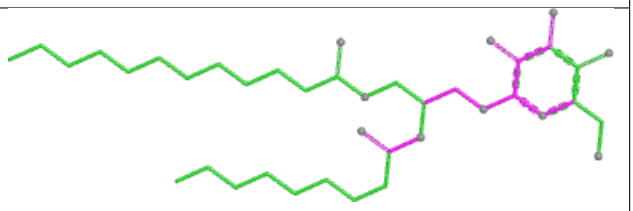
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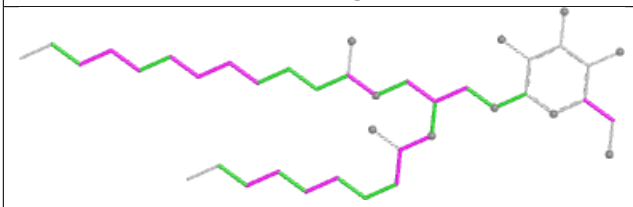


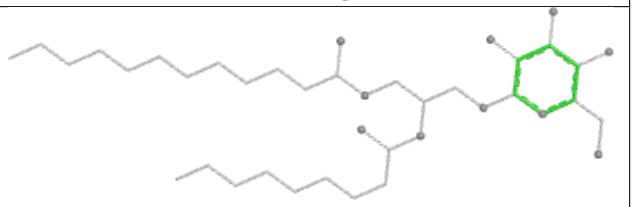
Rings

Ligand LMG l 101

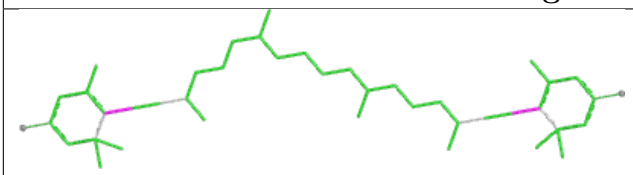

Bond lengths

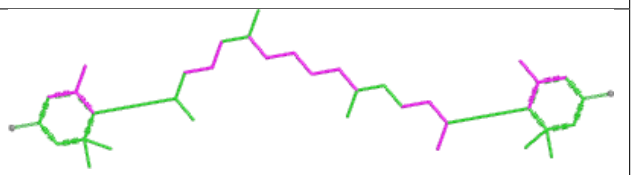

Bond angles

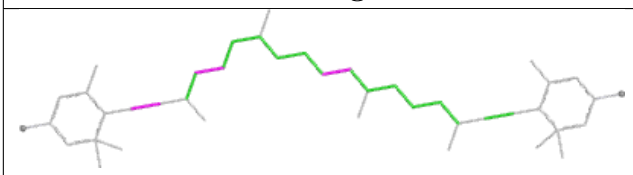

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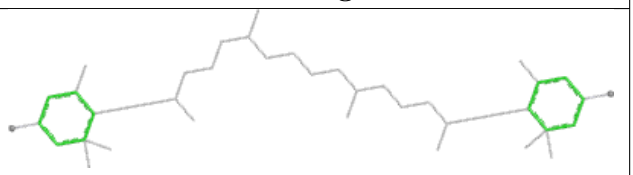

Rings

Ligand II0 5 315

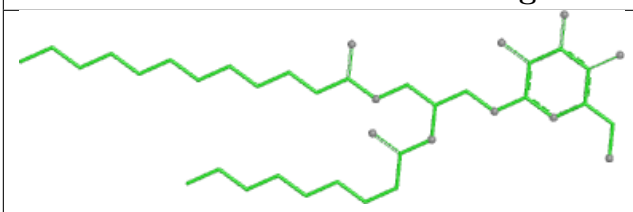

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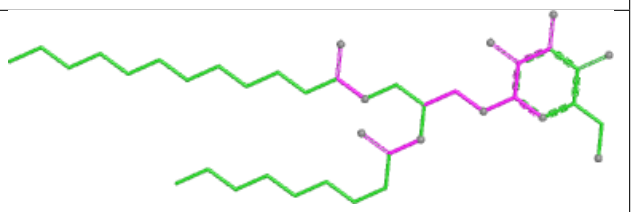

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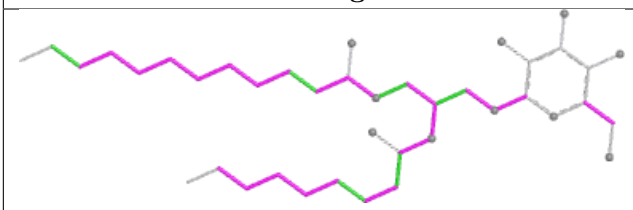

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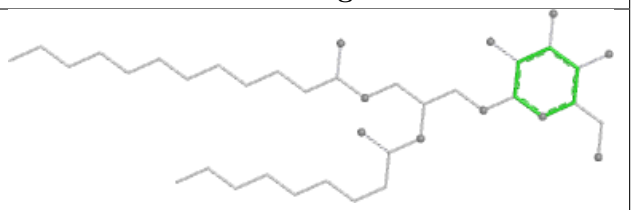

Rings

Ligand LMG D 411

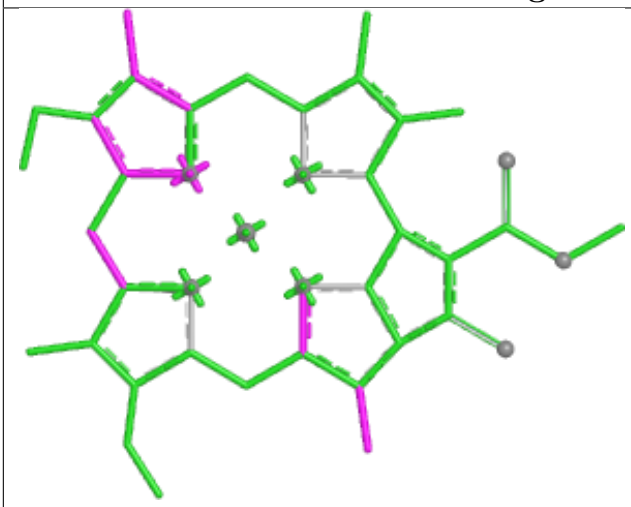

Bond lengths


Bond angles

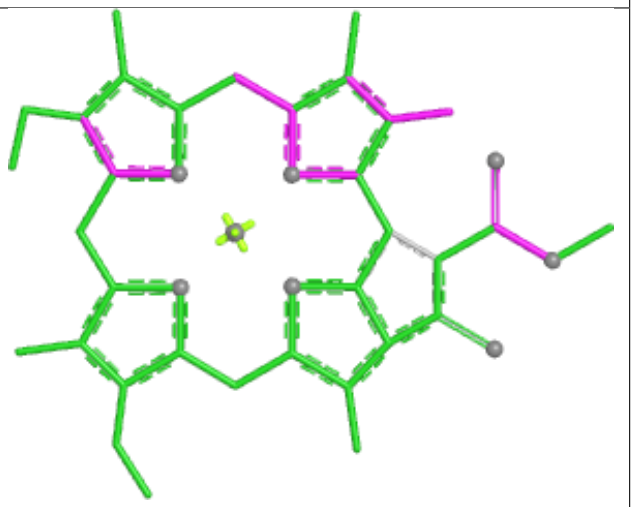

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Rings

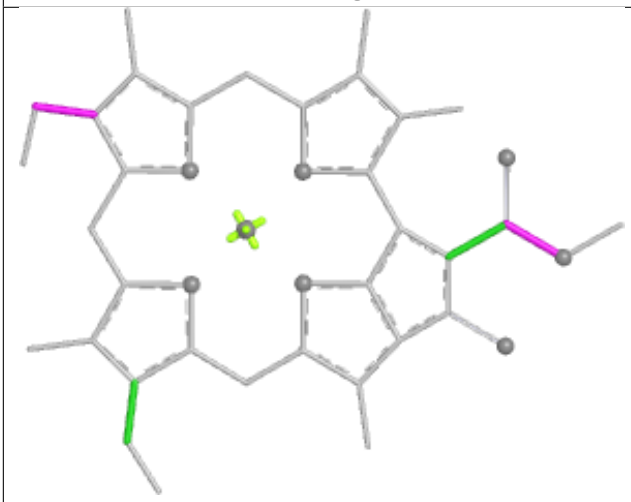
Ligand CLA 7 609



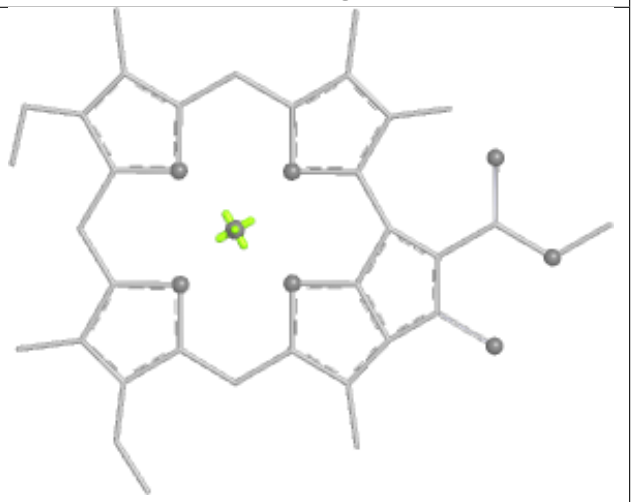
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Bond angles

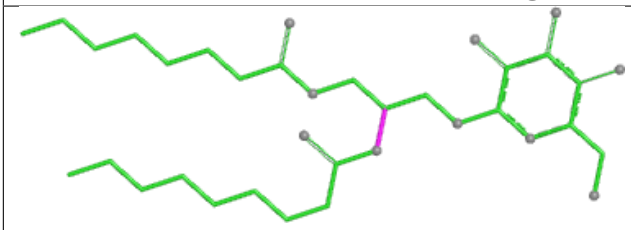


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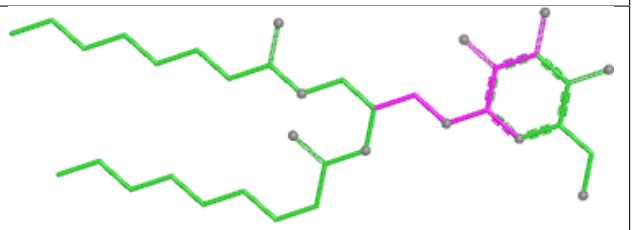


Rings

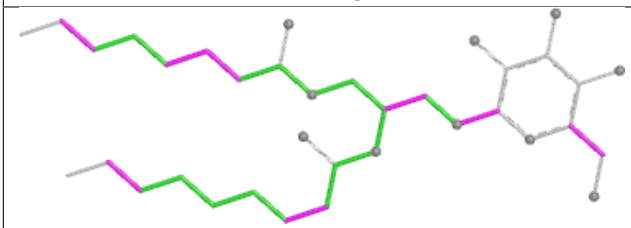
Ligand LMG 0 619



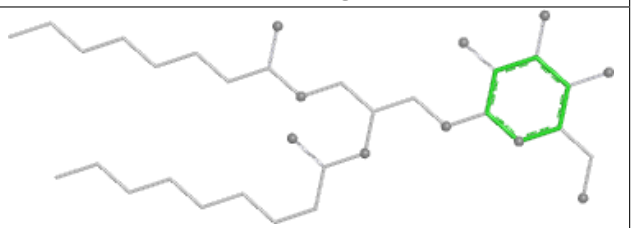
Bond lengths



Bond angles

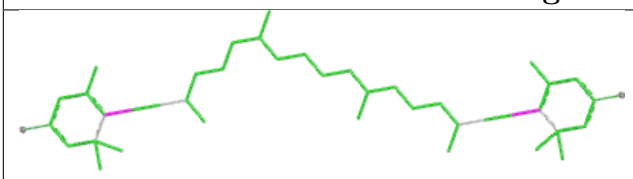


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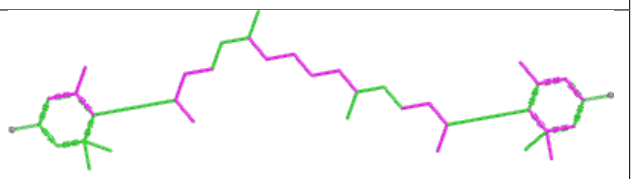


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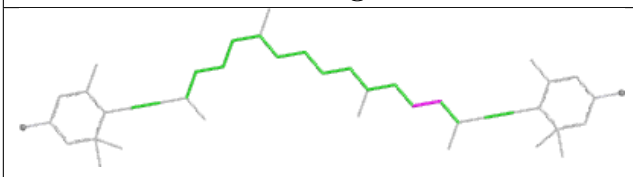
Ligand II0 0 620



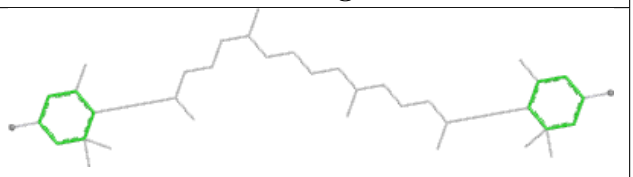
Bond lengths



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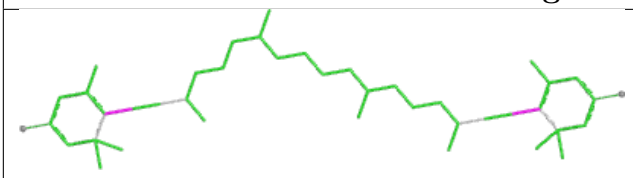


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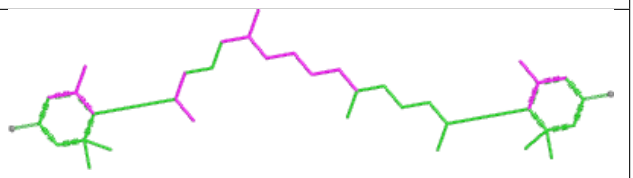


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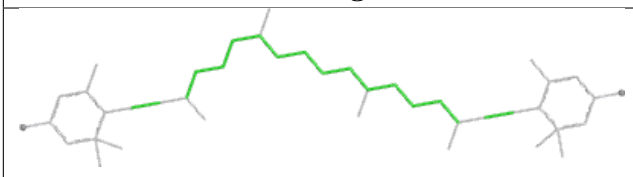
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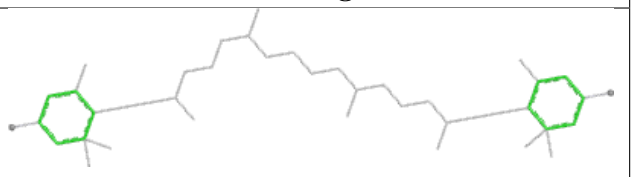
Bond lengths



Bond angles

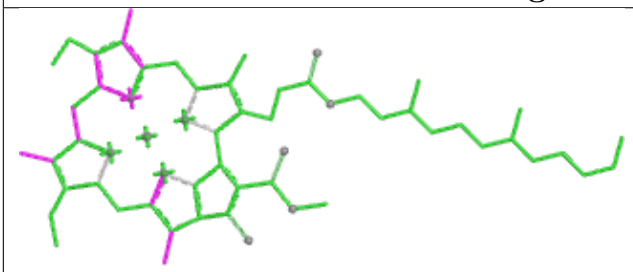


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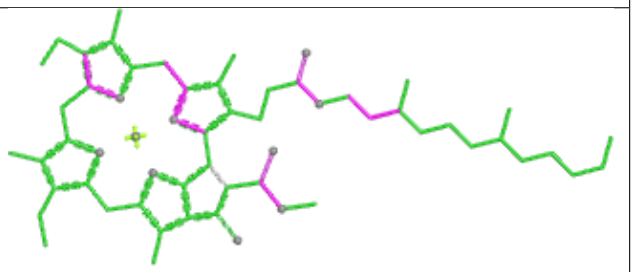


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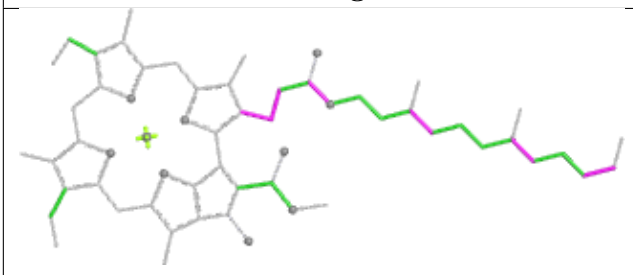
Ligand CLA 9 602



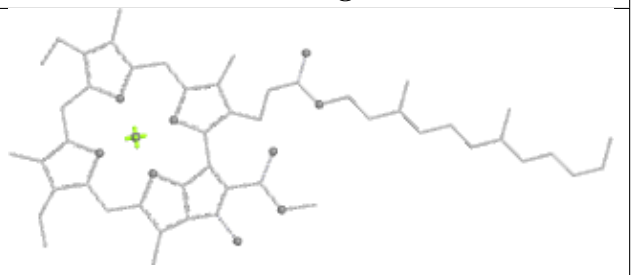
Bond lengths



Bond angles

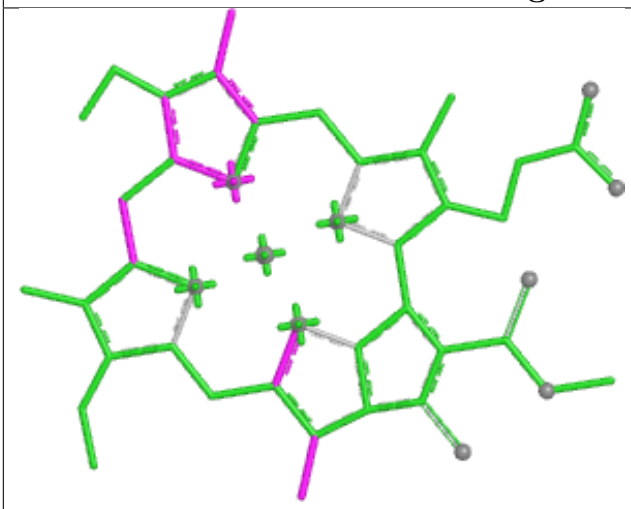


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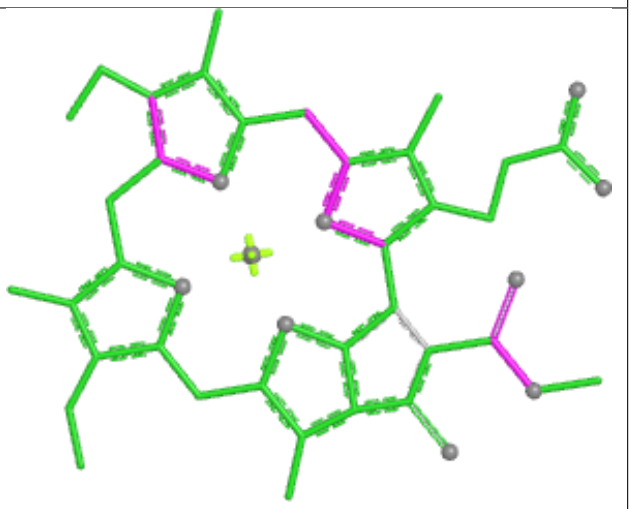


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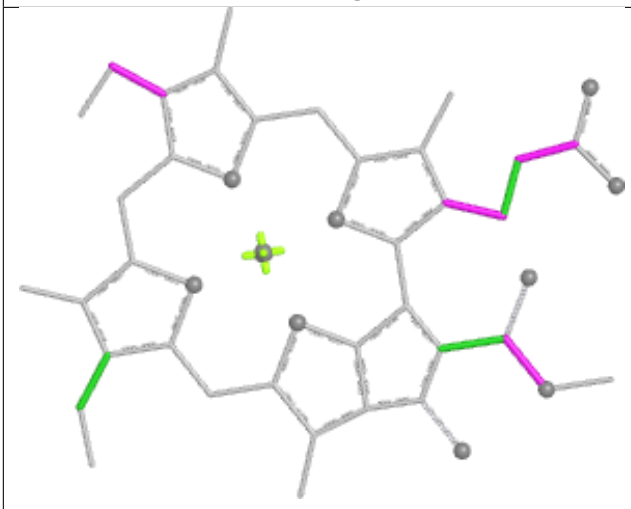
Ligand CLA 2 612



Bond lengths



Bond angles

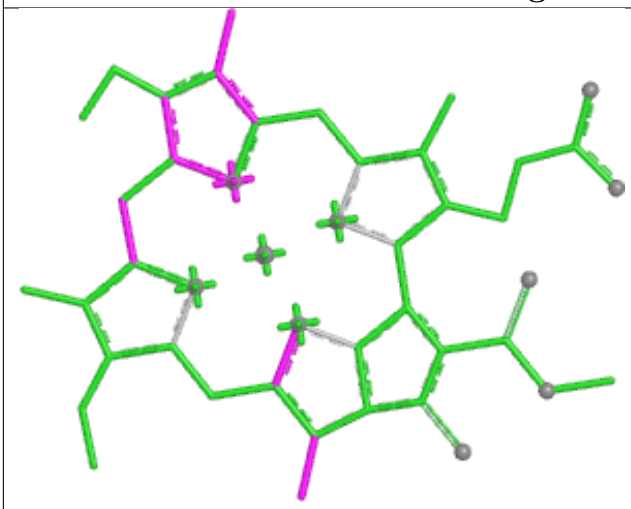


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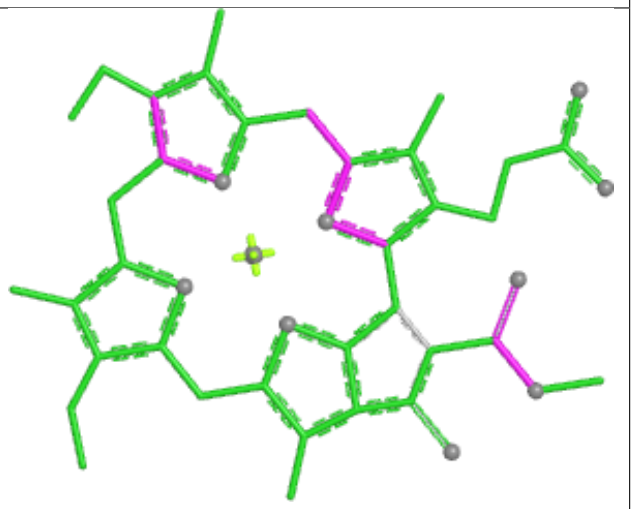


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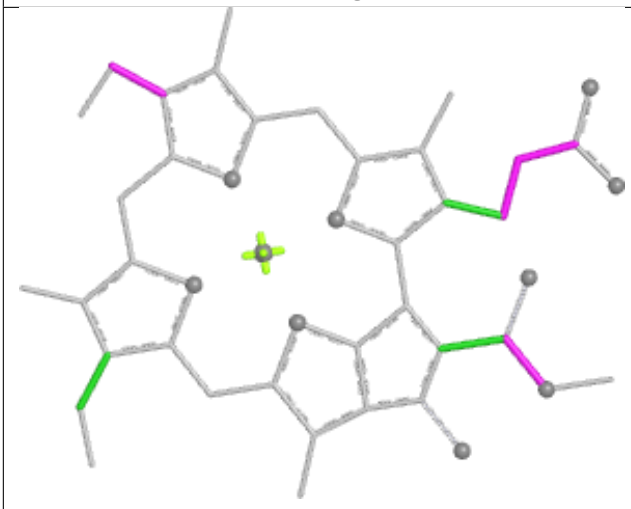
Ligand CLA 4 611



Bond lengths



Bond angles

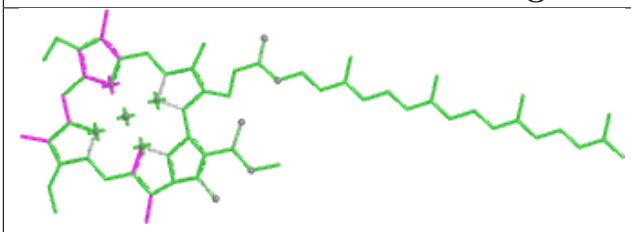


Torsions

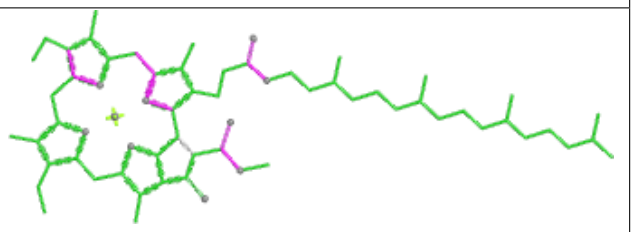


Rings

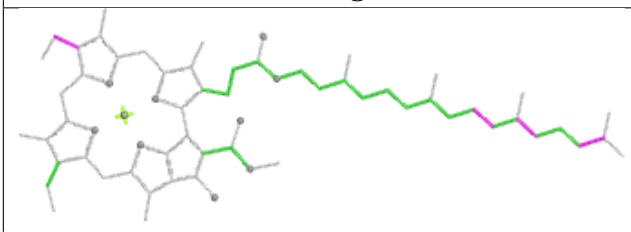
Ligand CLA b 616



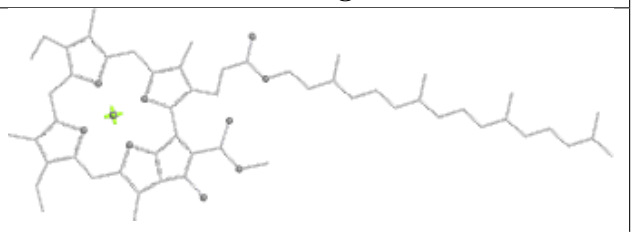
Bond lengths



Bond angles

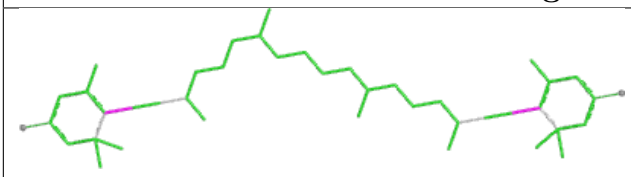


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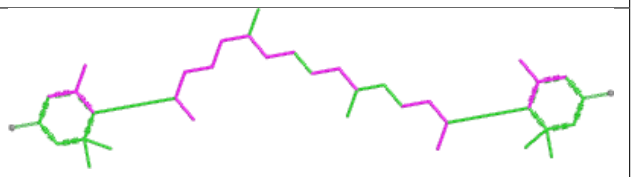


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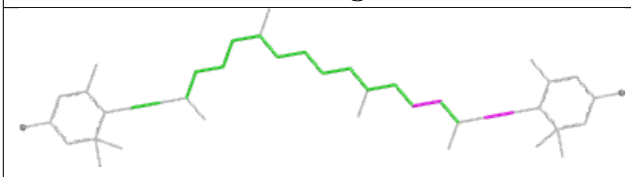
Ligand II0 3 612



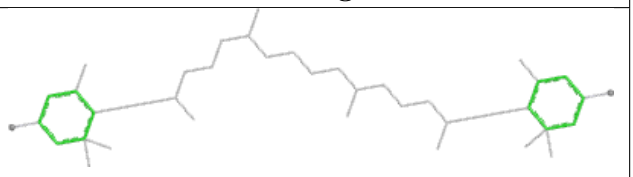
Bond lengths



Bond angles

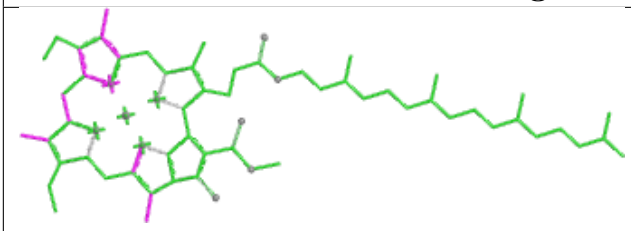


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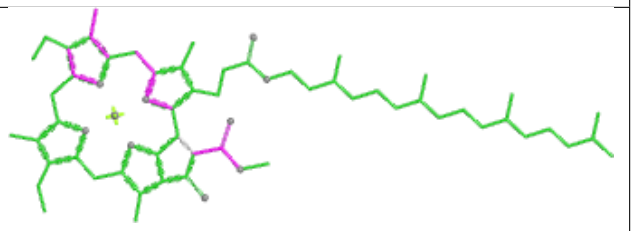


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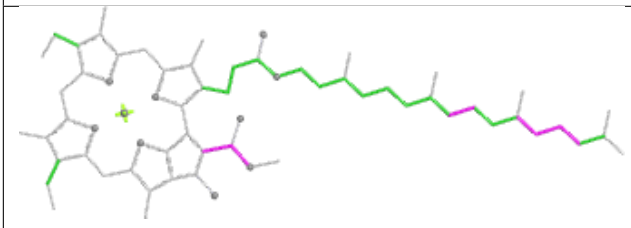
Ligand CLA c 508



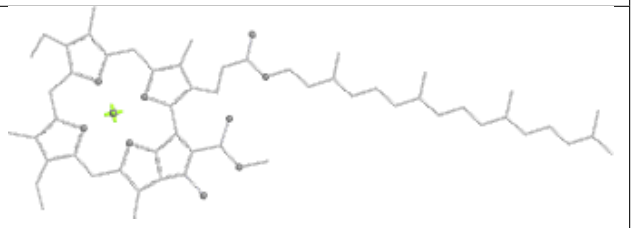
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Bond angles

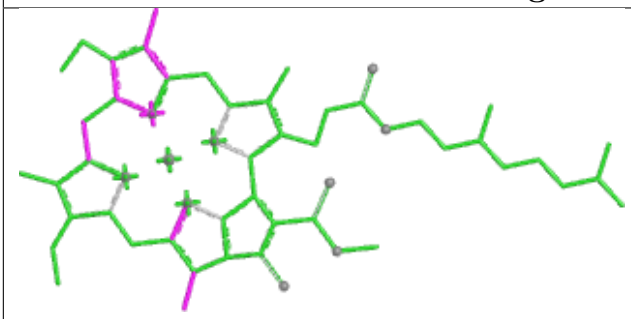


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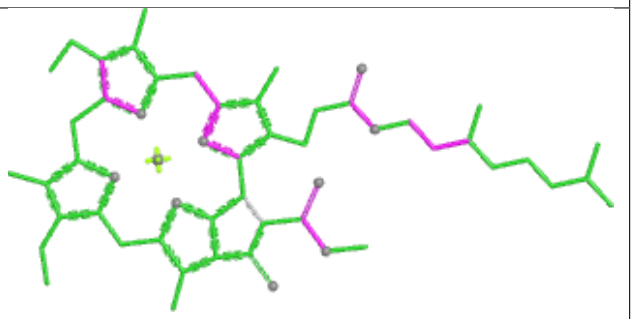


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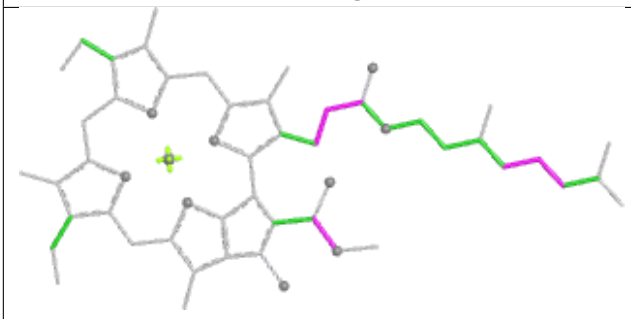
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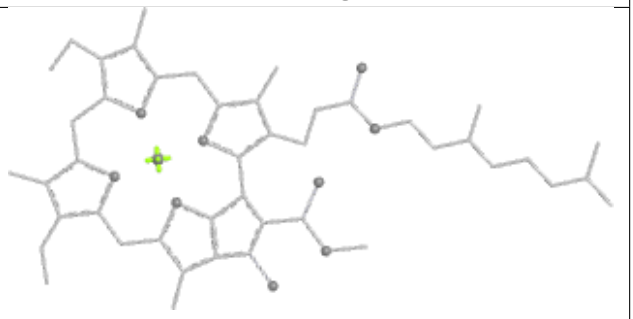
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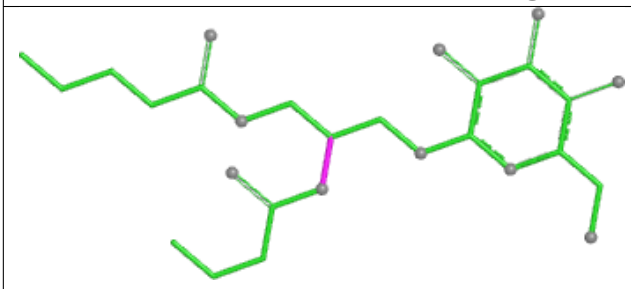


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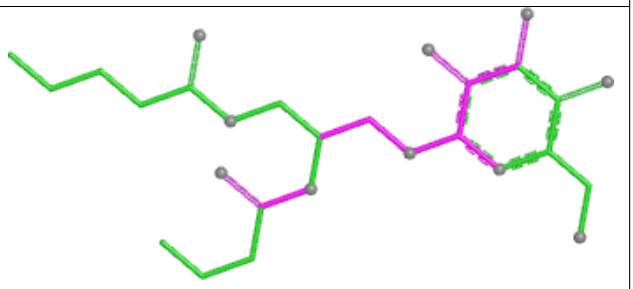


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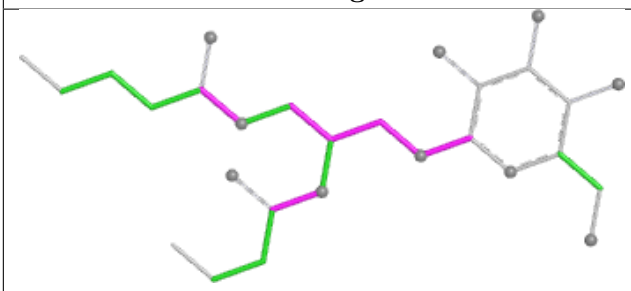
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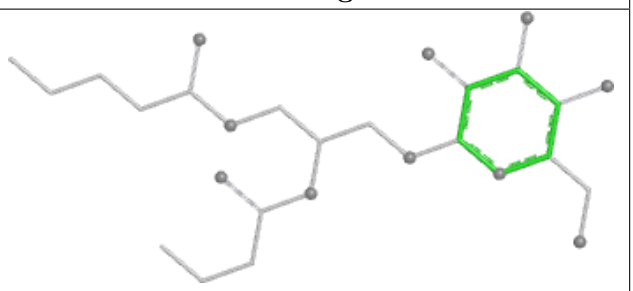
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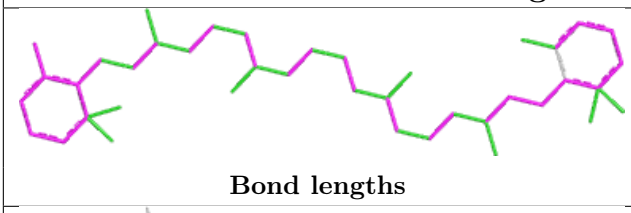


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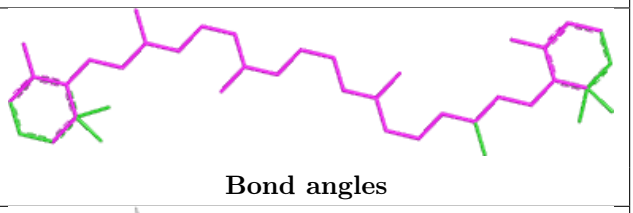


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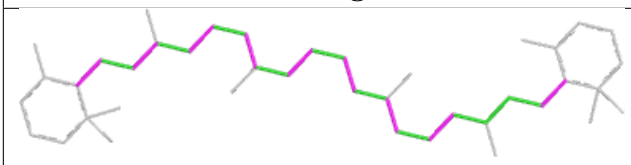
Ligand 8CT Z 101



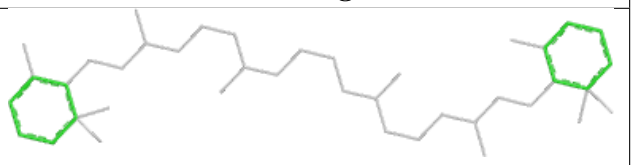
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Bond angles

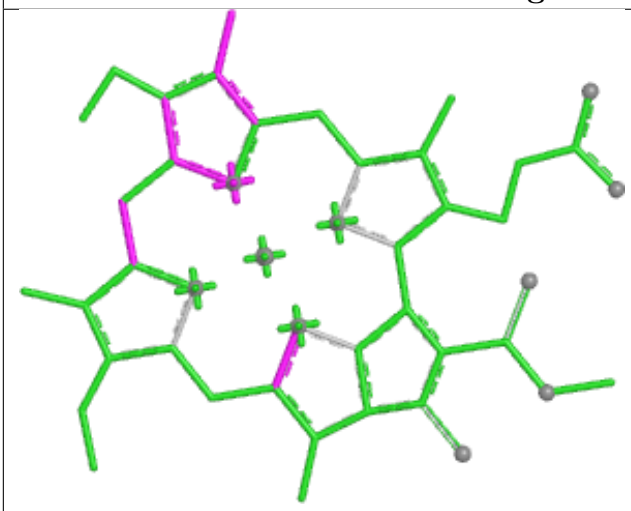


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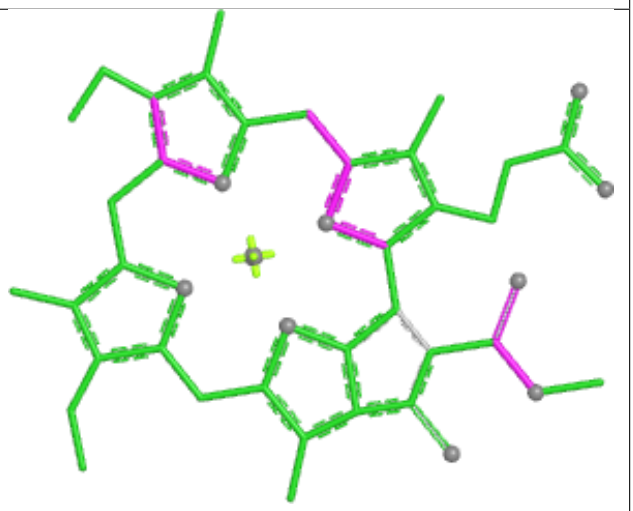


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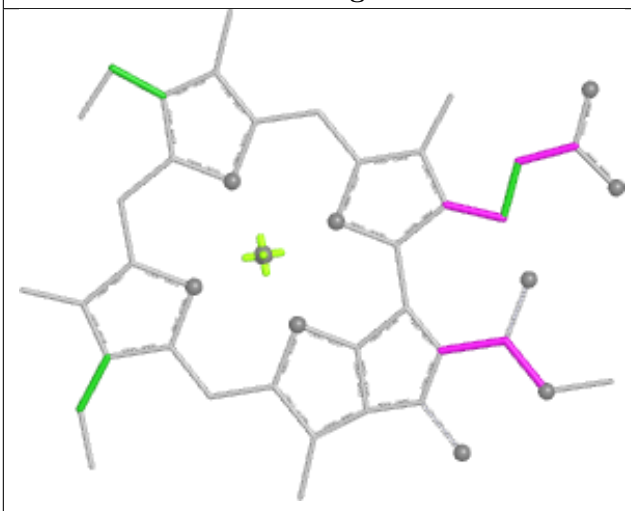
Ligand CLA S 302



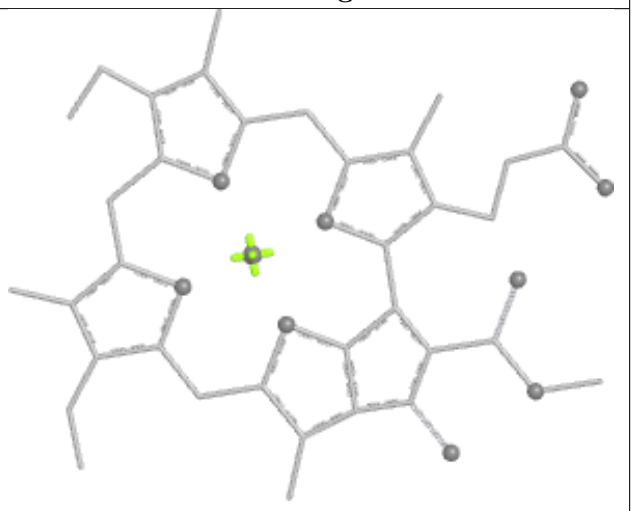
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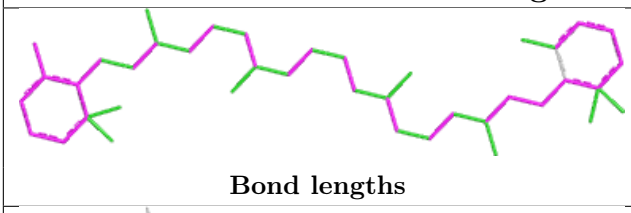


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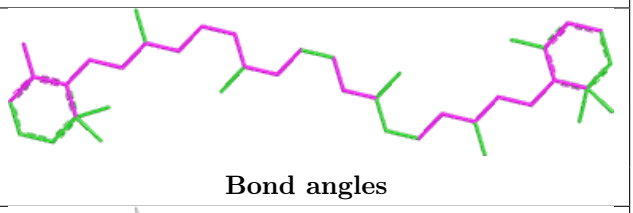


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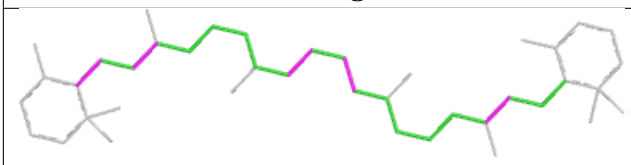
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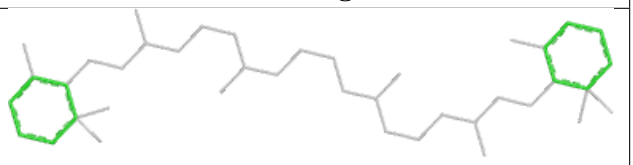
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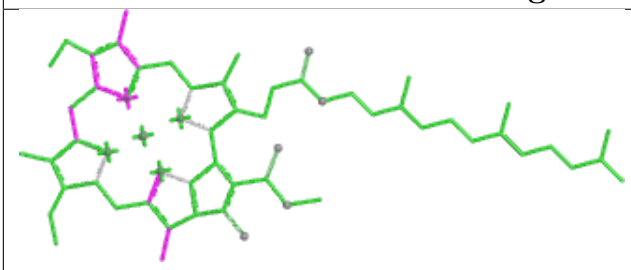


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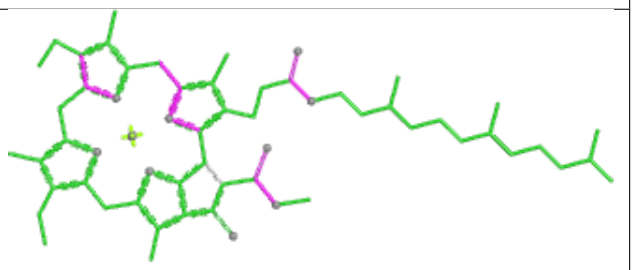


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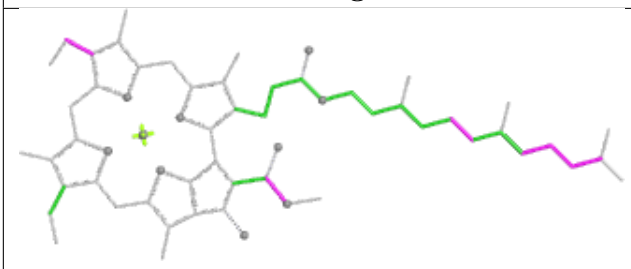
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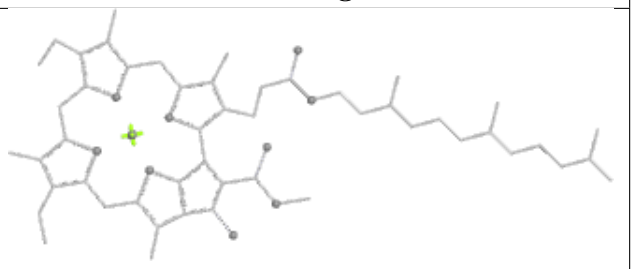
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Bond angles



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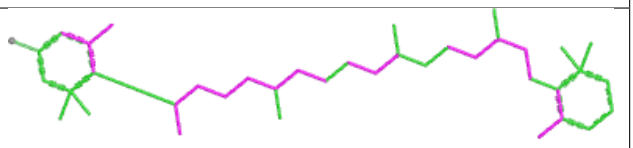


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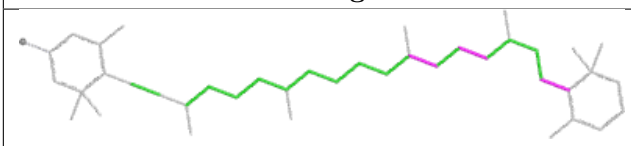
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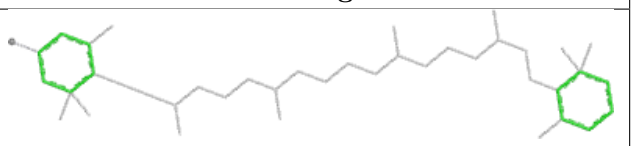
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Bond angles

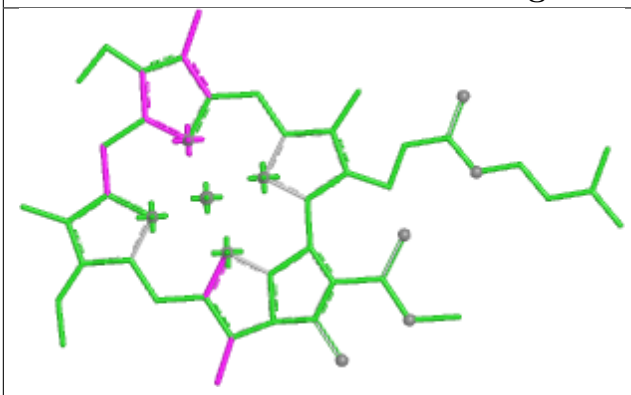


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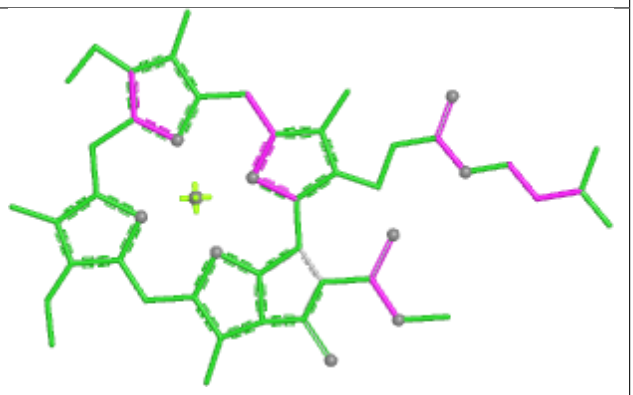


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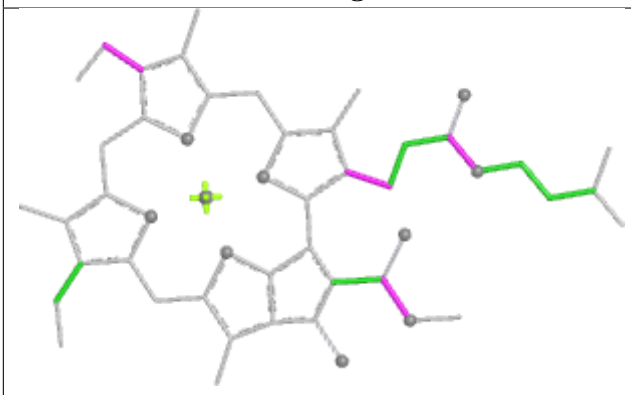
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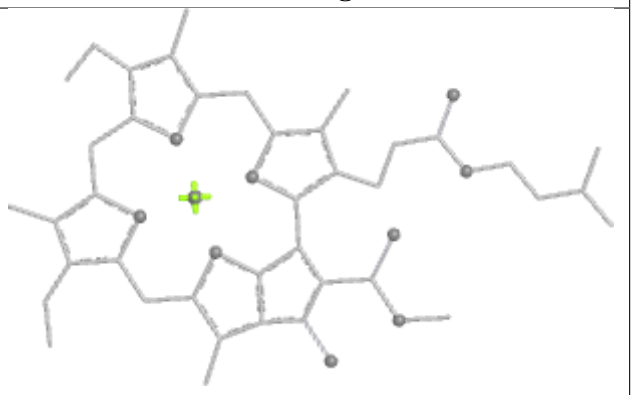
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Bond angles

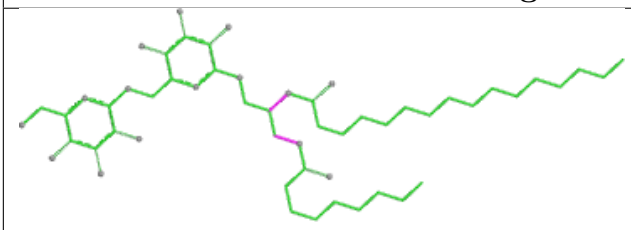


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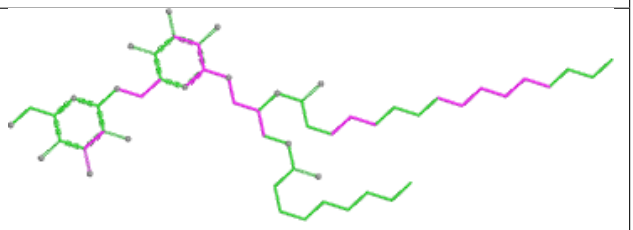


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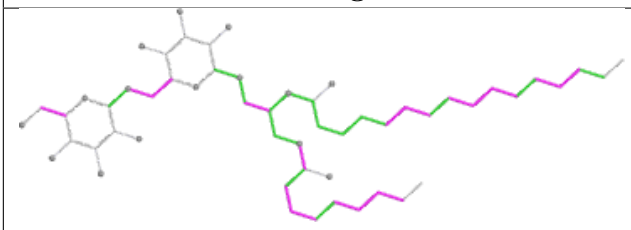
Ligand DGD C 514



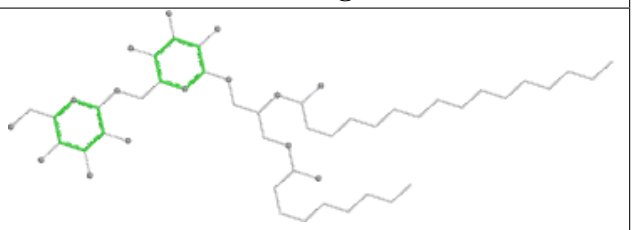
Bond lengths



Bond angles

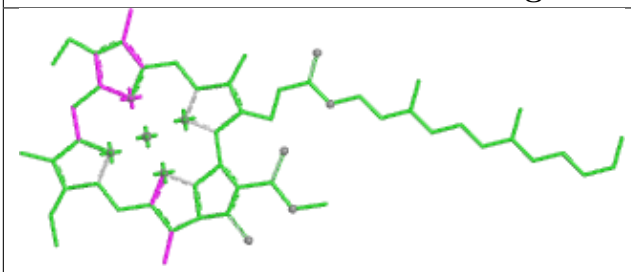


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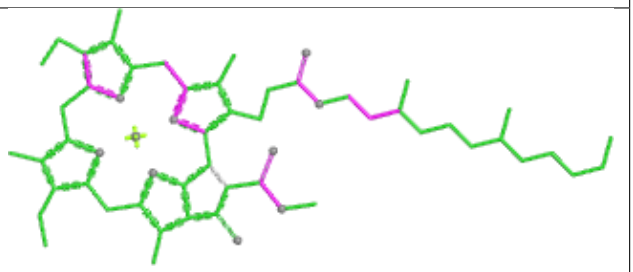


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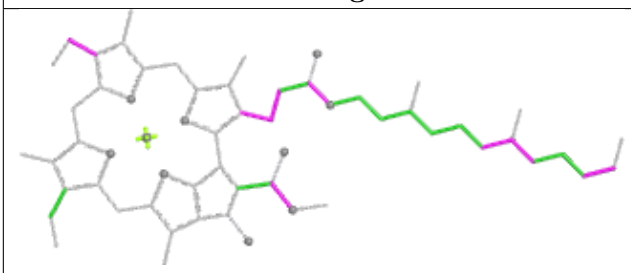
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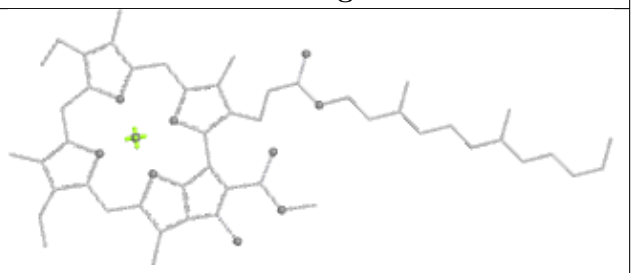
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Bond angles

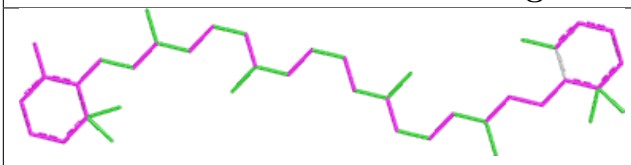


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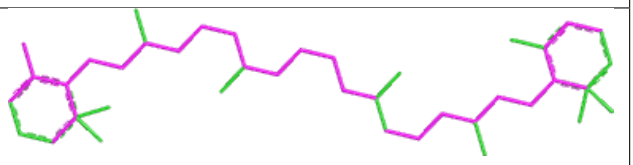


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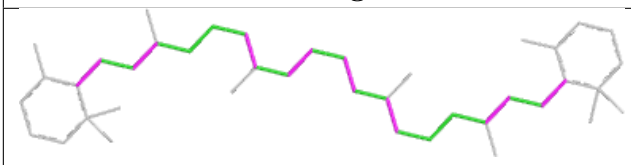
Ligand 8CT K 101



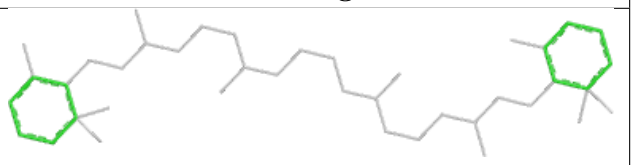
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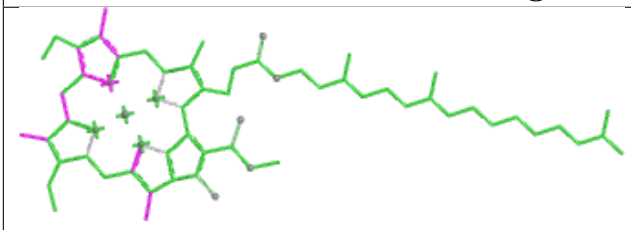


Torsions

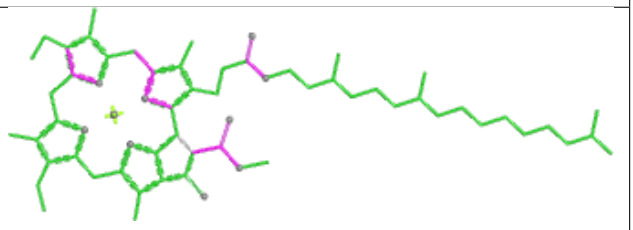


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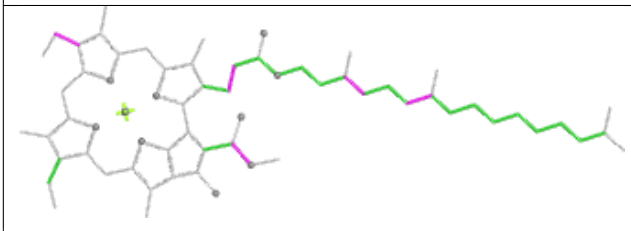
Ligand CLA b 604



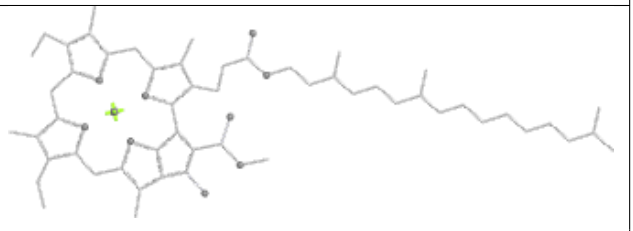
Bond lengths



Bond angles

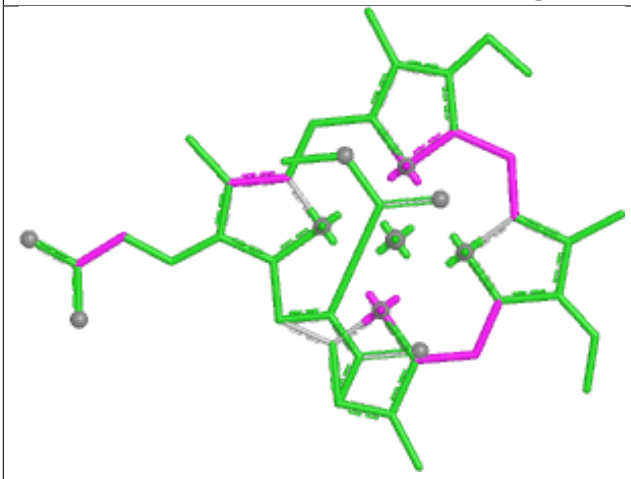


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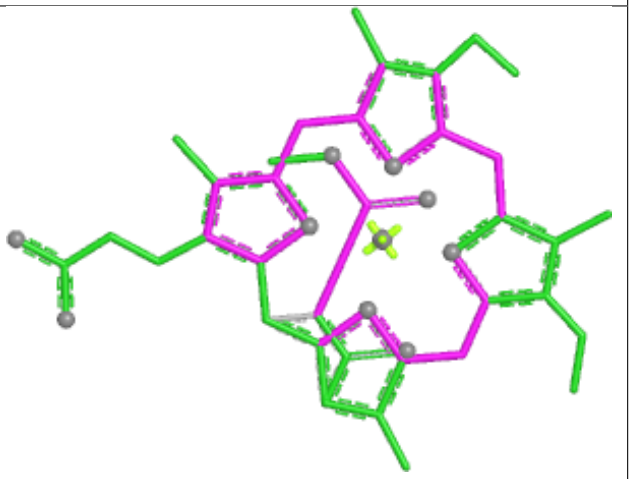


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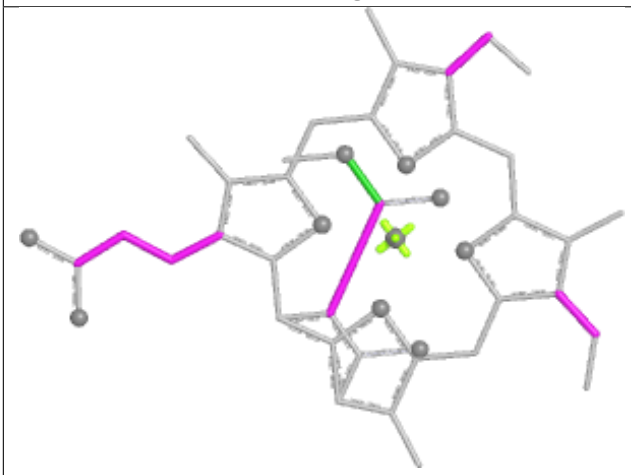
Ligand KC2 5 311



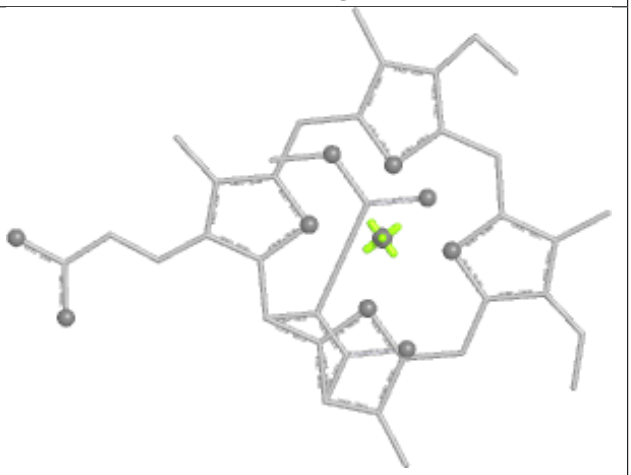
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Bond angles

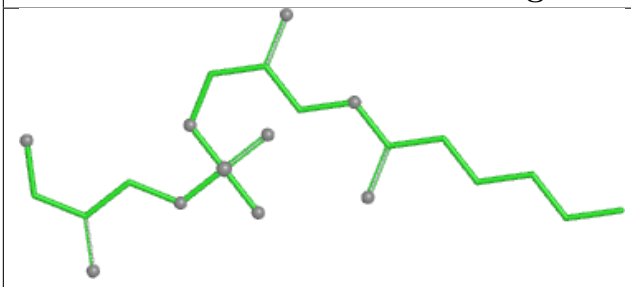


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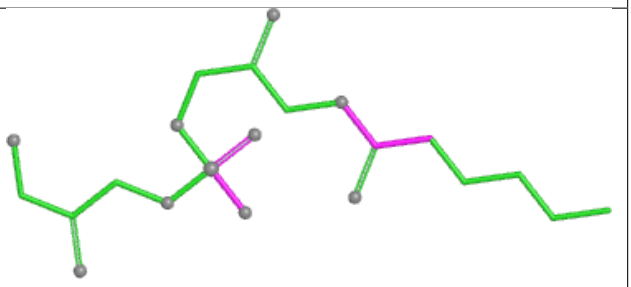


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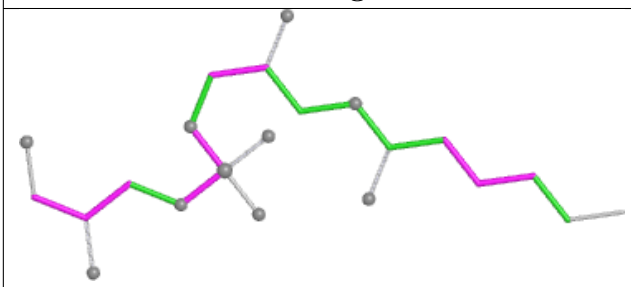
Ligand LHG 2 618



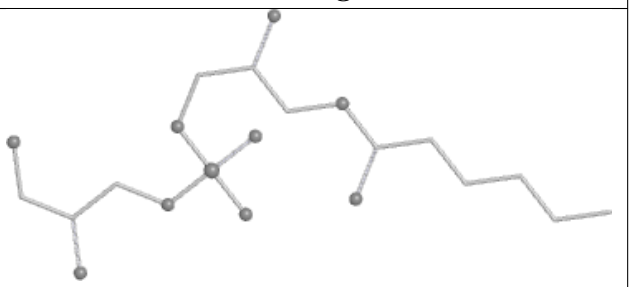
Bond lengths



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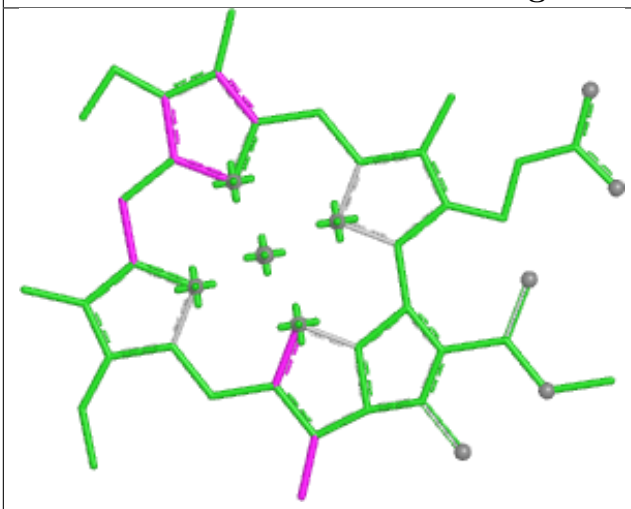


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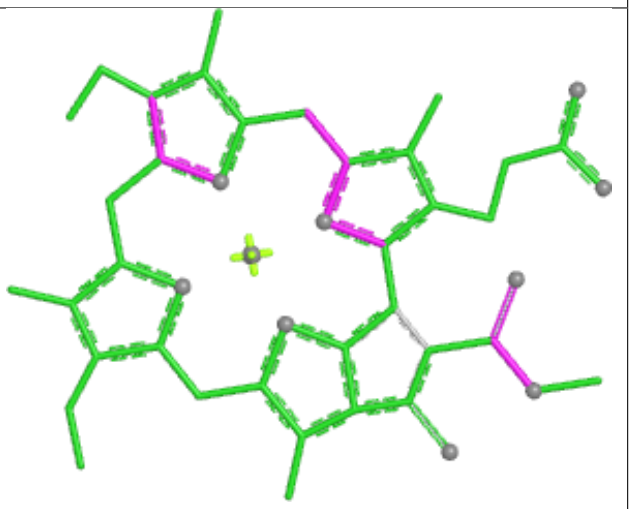


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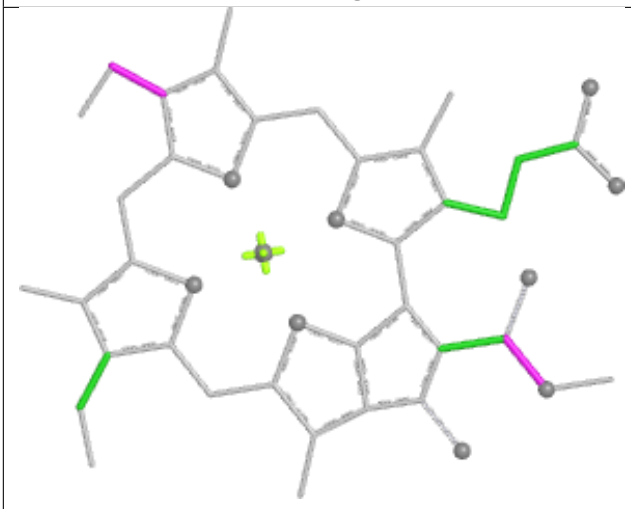
Ligand CLA 6 606



Bond lengths



Bond angles

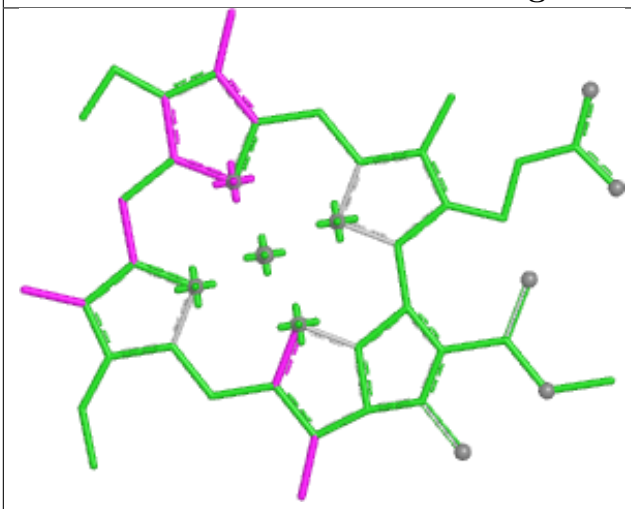


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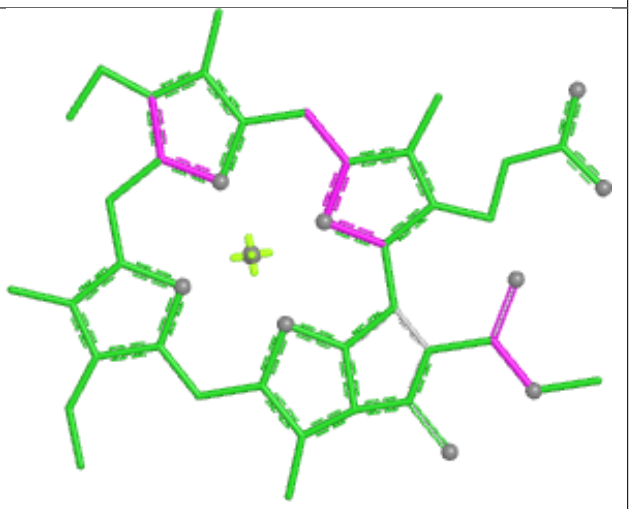


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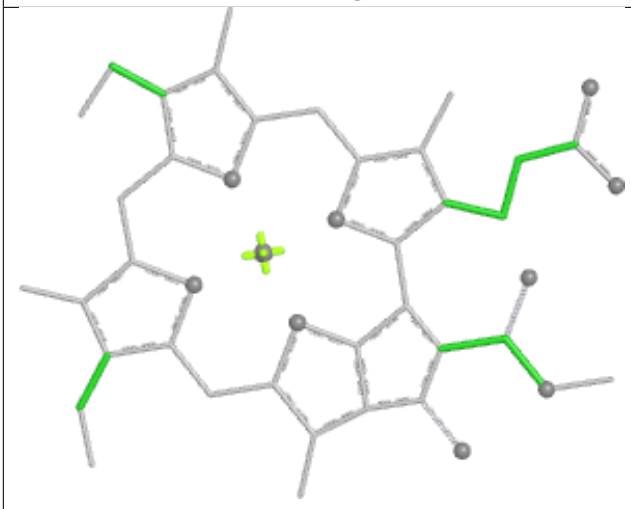
Ligand CLA 9 606



Bond lengths



Bond angles

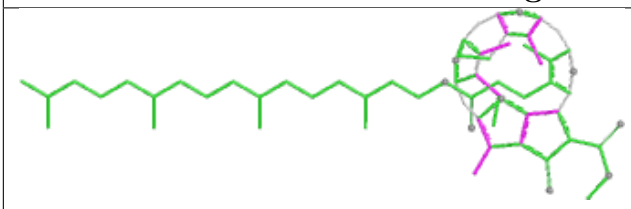


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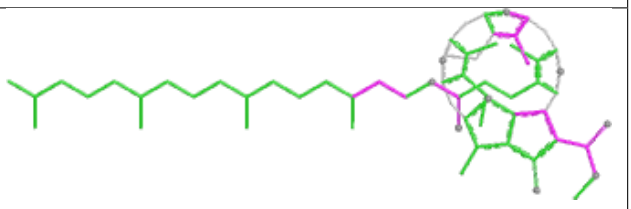


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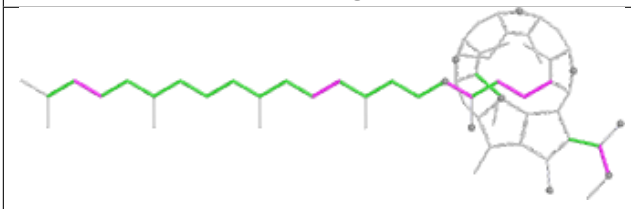
Ligand PHO d 410



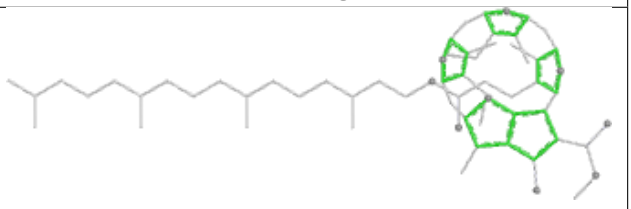
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Bond angles

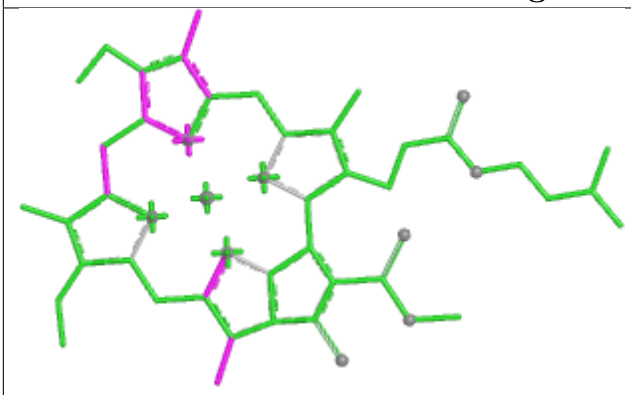


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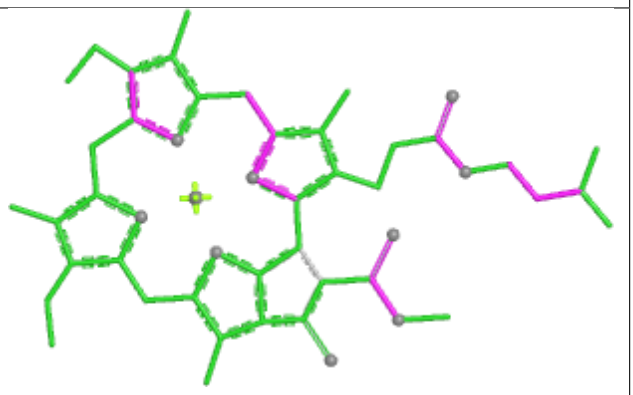


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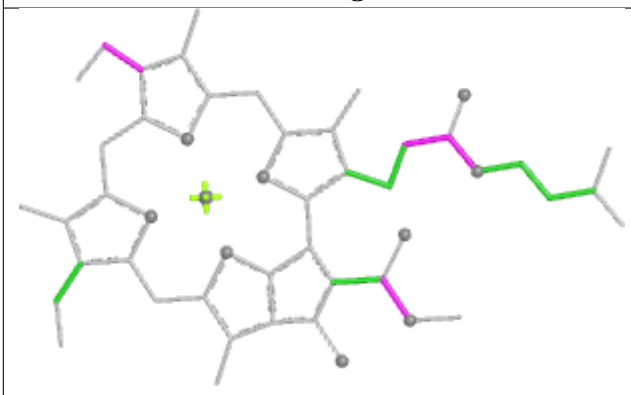
Ligand CLA 4 605



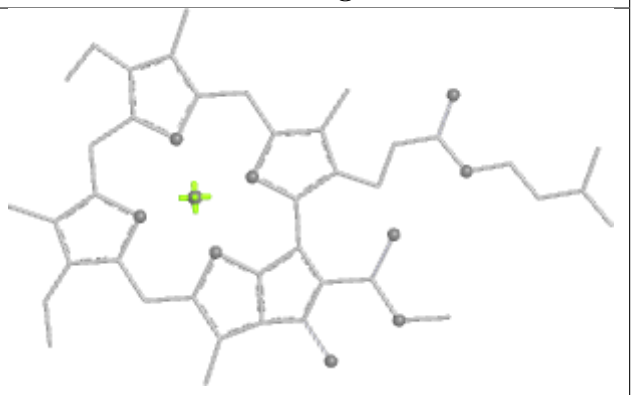
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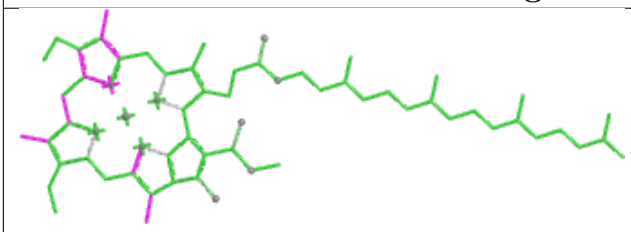


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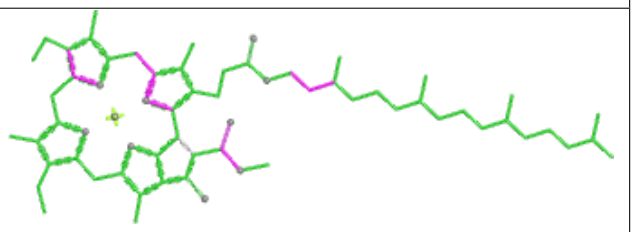


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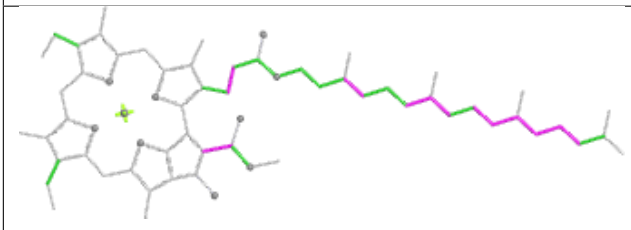
Ligand CLA C 507



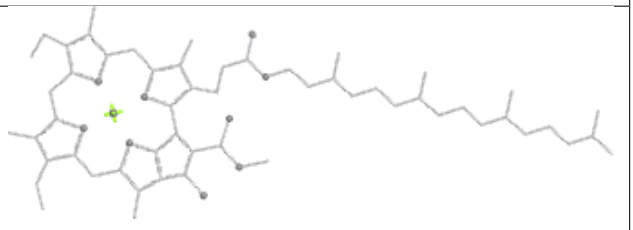
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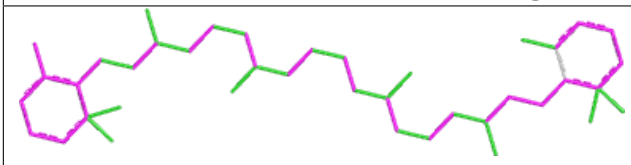


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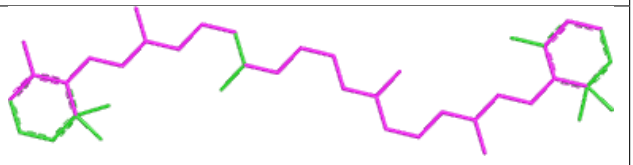


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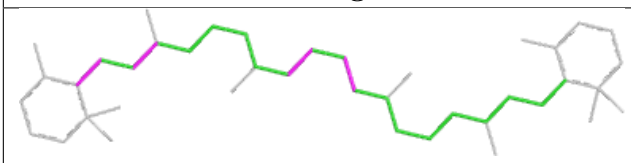
Ligand 8CT A 610



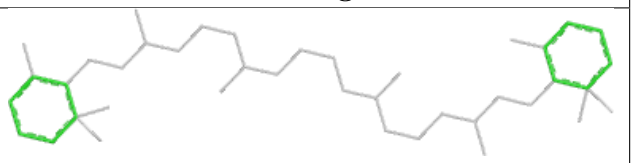
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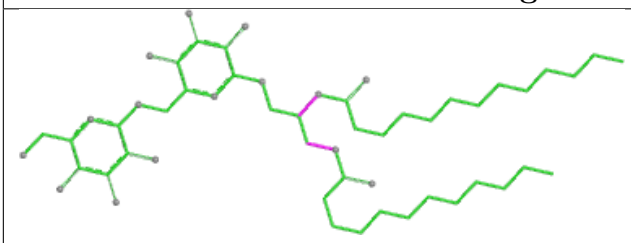


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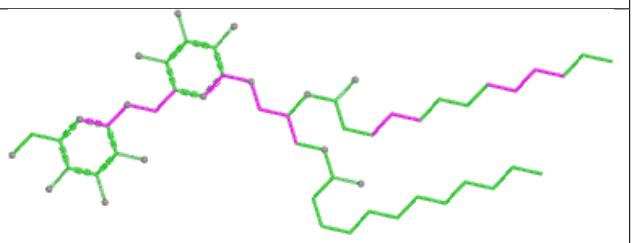


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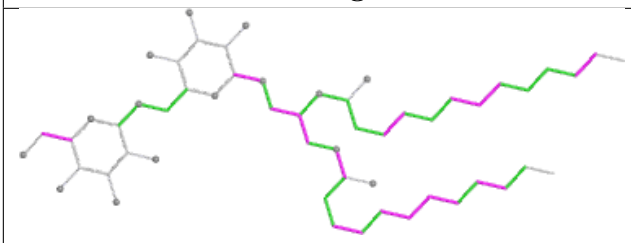
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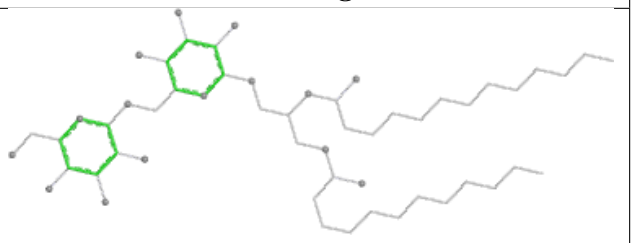
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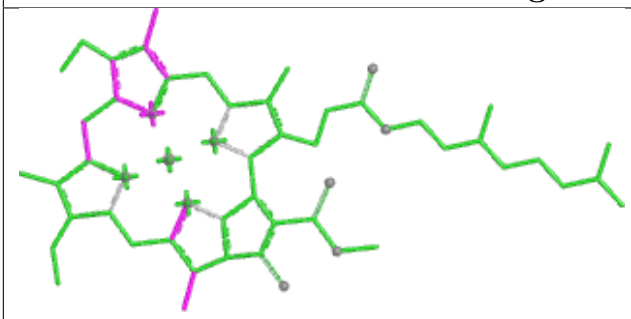


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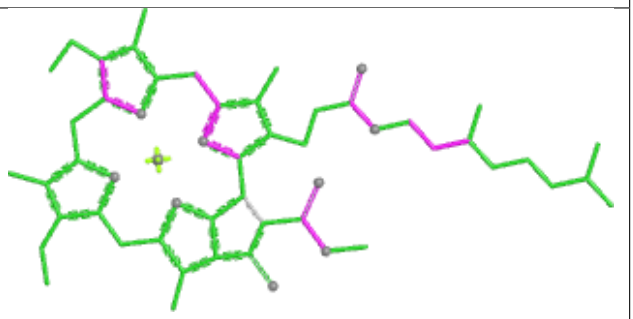


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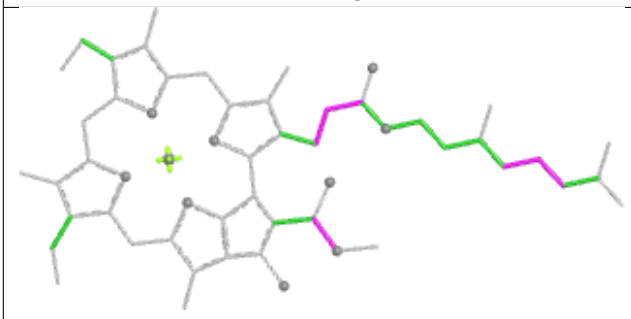
Ligand CLA 1 604



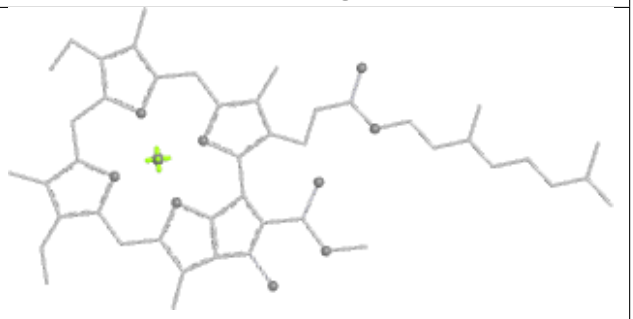
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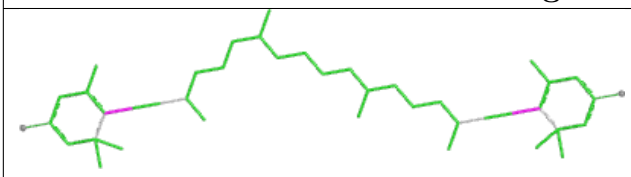


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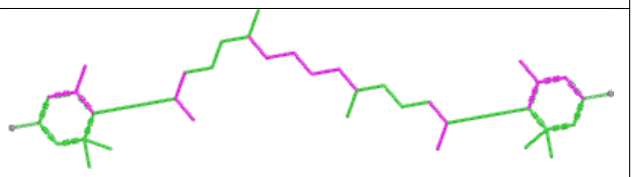


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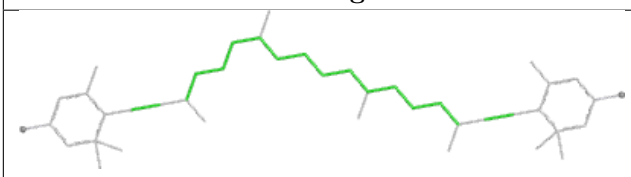
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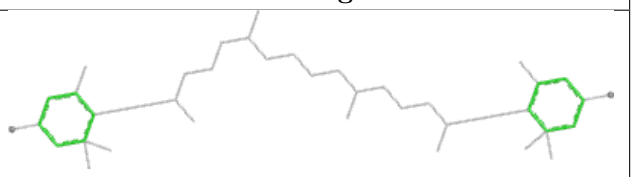
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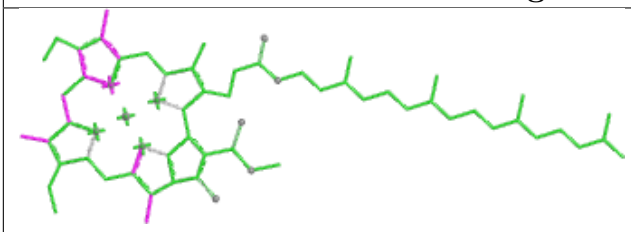


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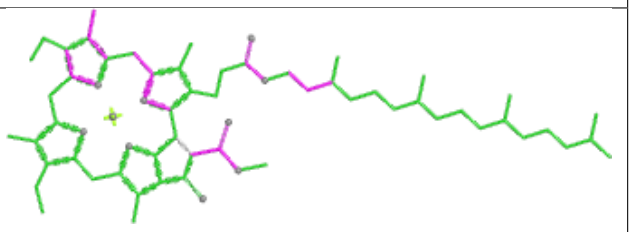


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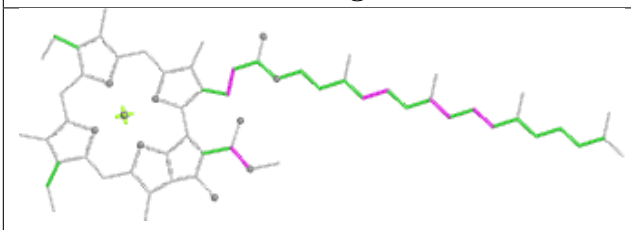
Ligand CLA b 607



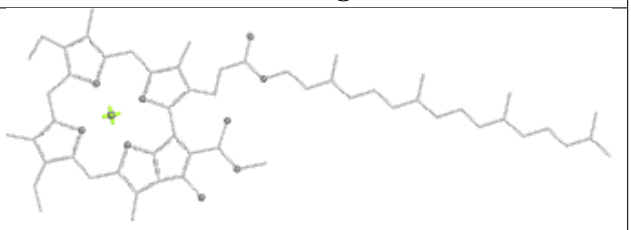
Bond lengths



Bond angles

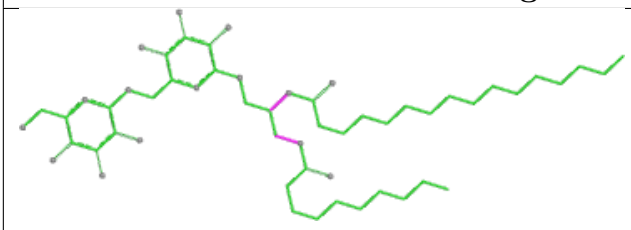


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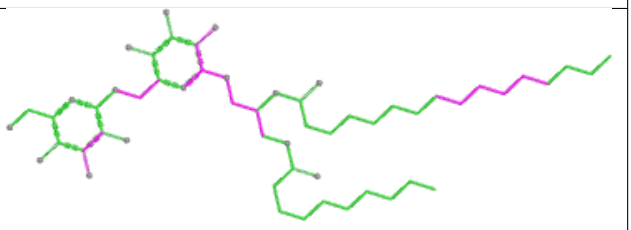


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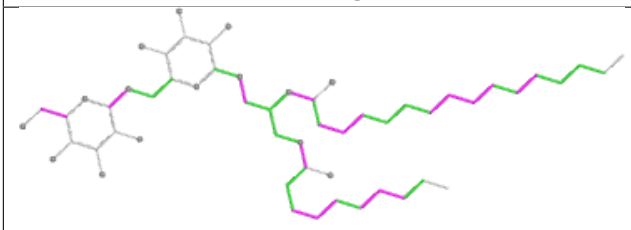
Ligand DGD C 515



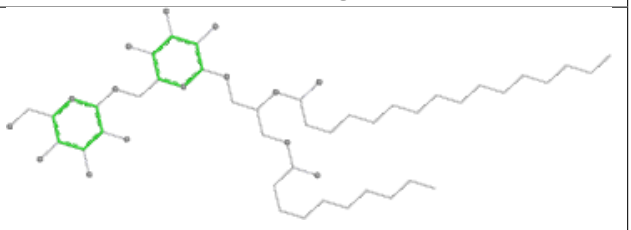
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Bond angles

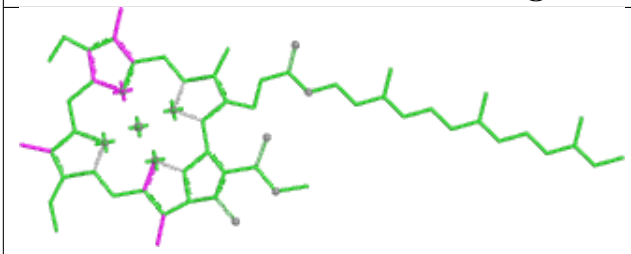


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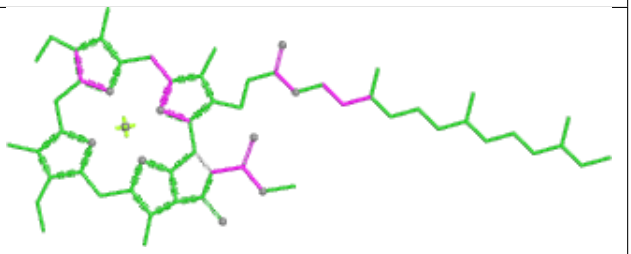


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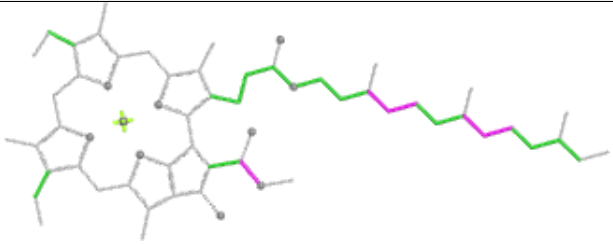
Ligand CLA b 605



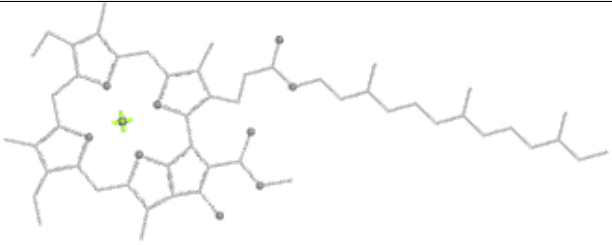
Bond lengths



Bond angles

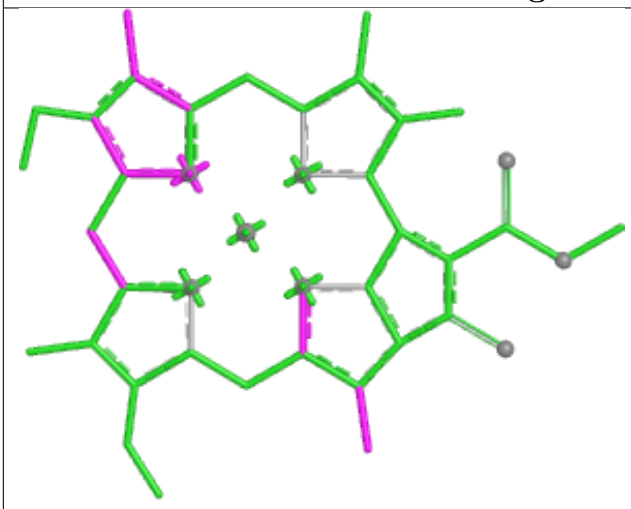


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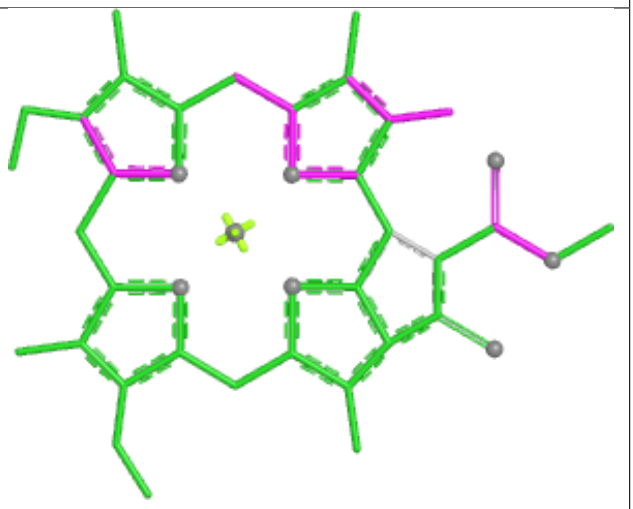


Rings

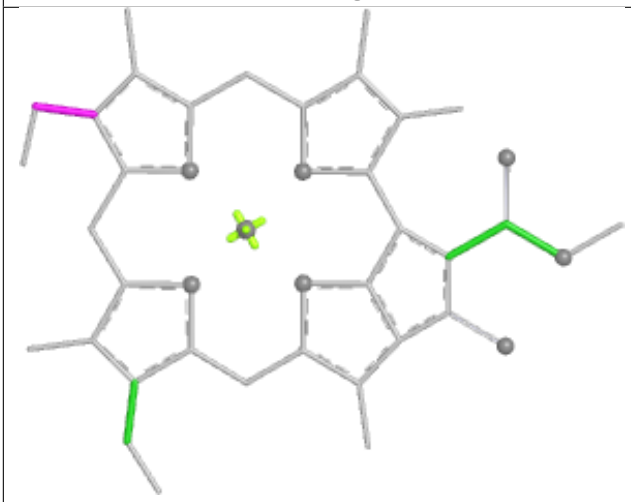
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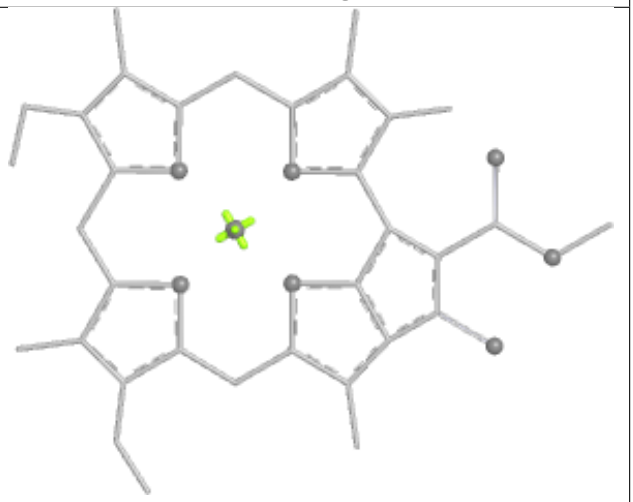
Bond lengths



Bond angles



Torsions

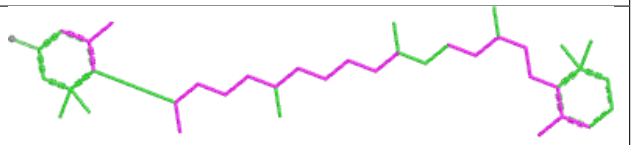


Rings

Ligand IHT 8 616



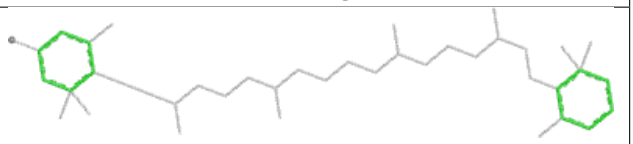
Bond lengths



Bond angles



Torsions

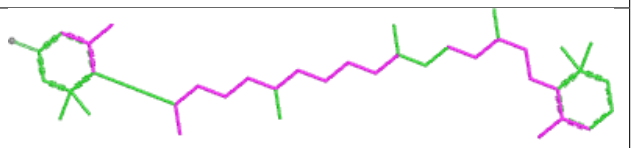


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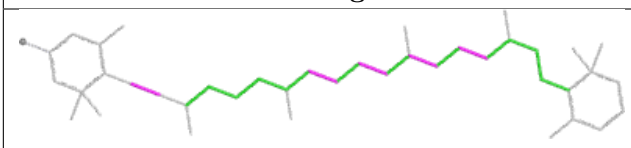
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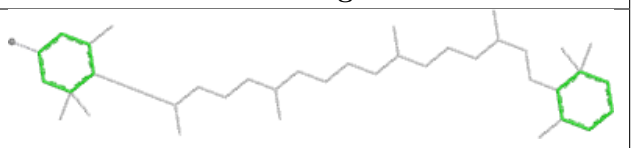
Bond lengths



Bond angles

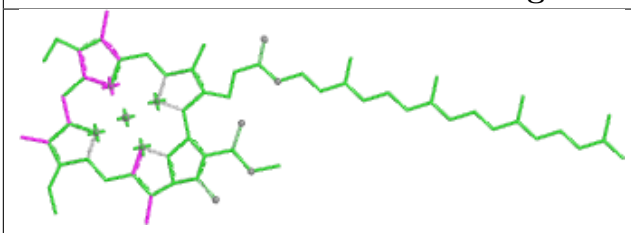


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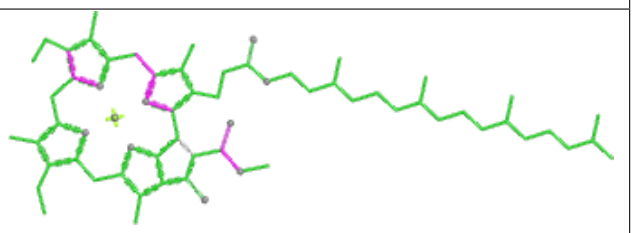


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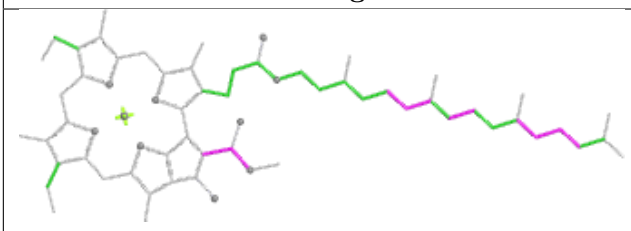
Ligand CLA b 606



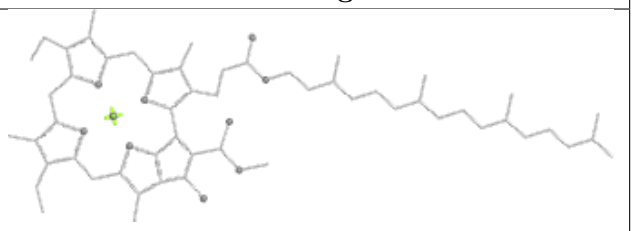
Bond lengths



Bond angles

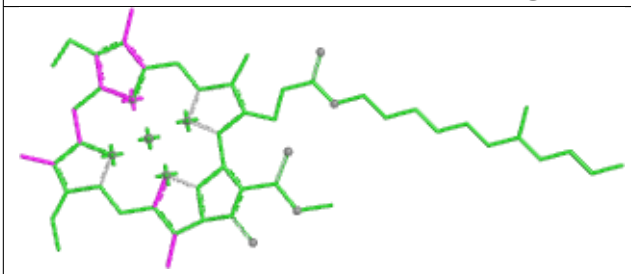


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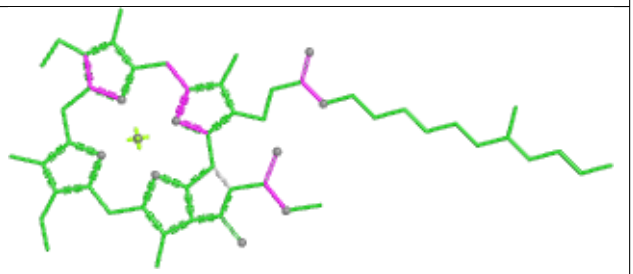


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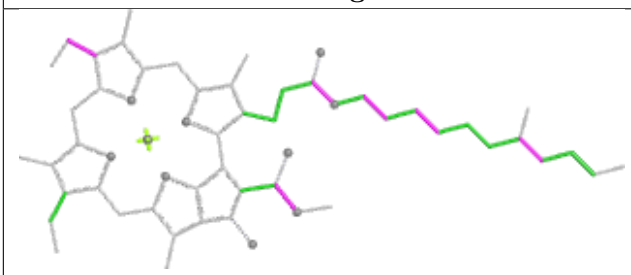
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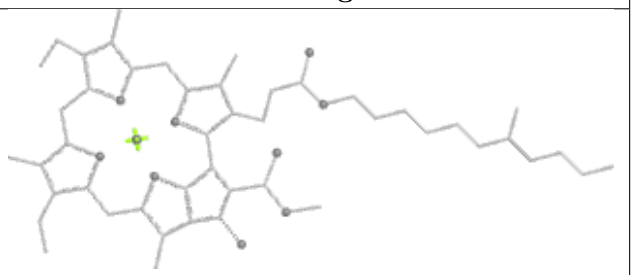
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Bond angles

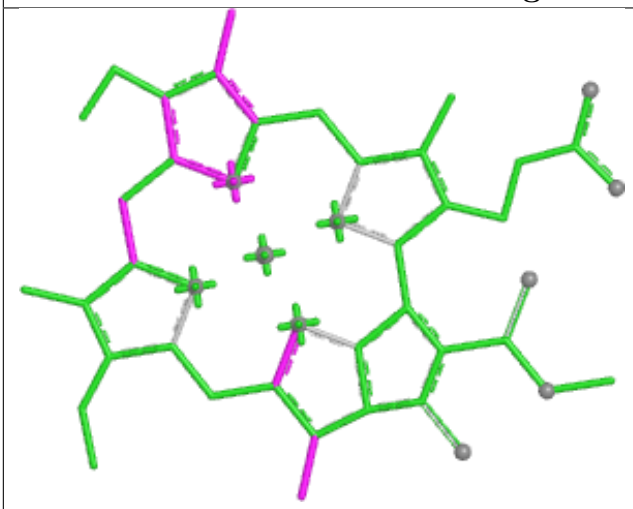


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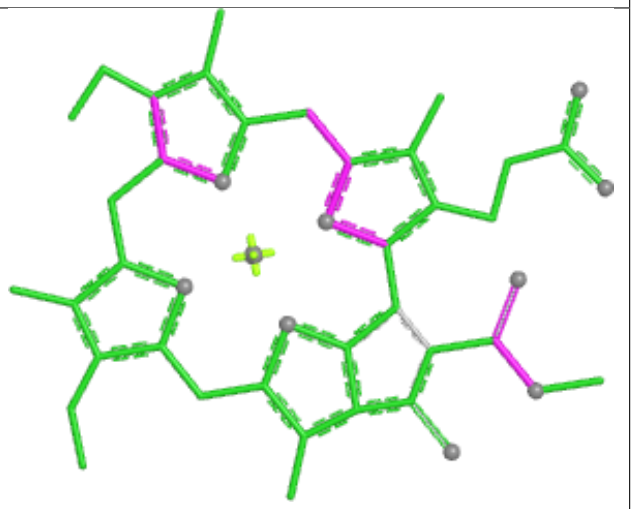


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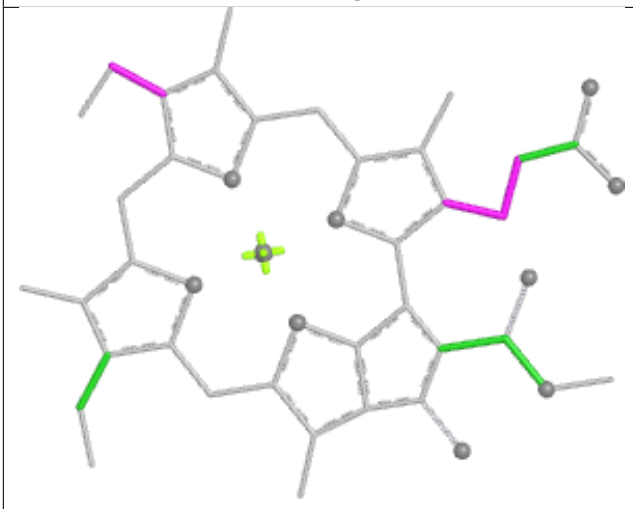
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Bond lengths



Bond angles

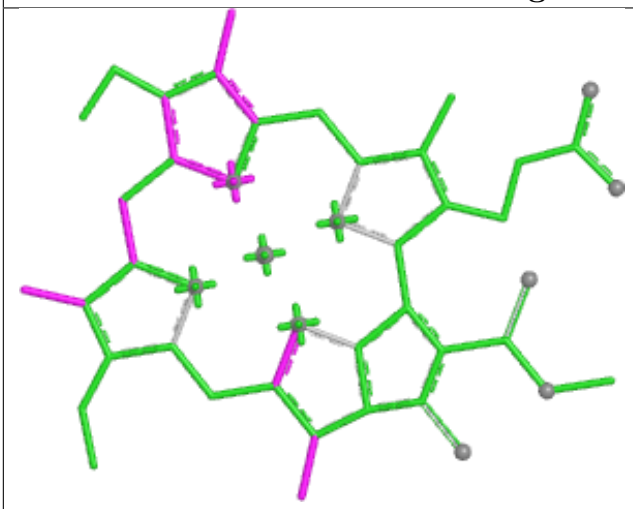


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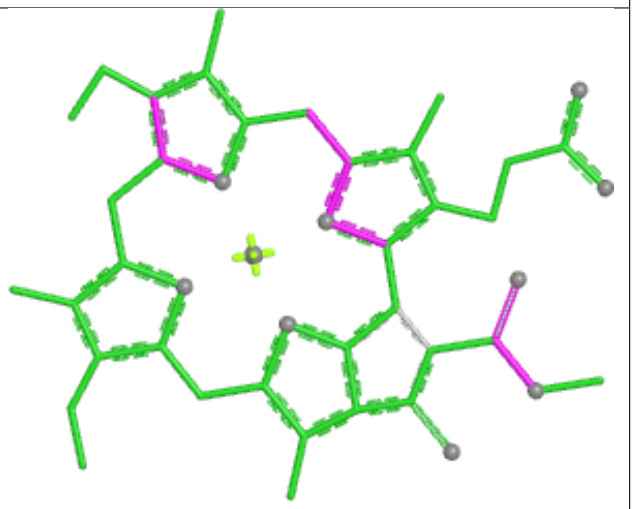


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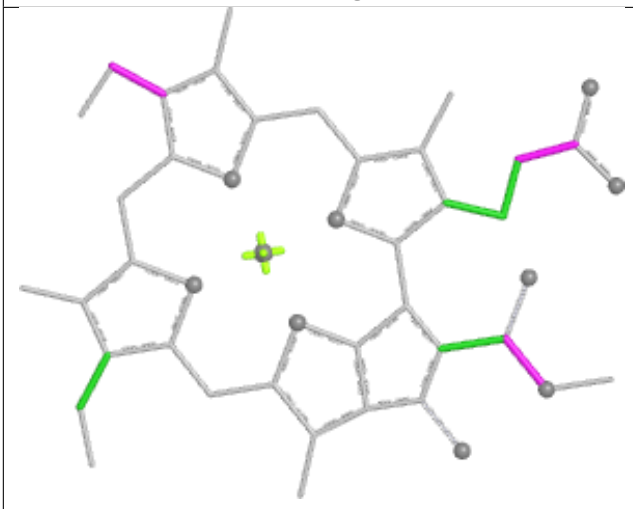
Ligand CLA 6 610



Bond lengths



Bond angles

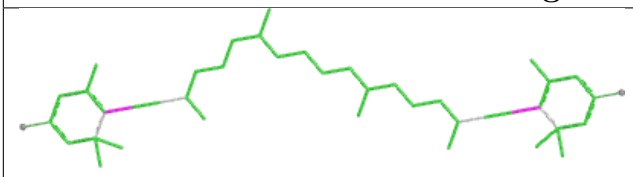


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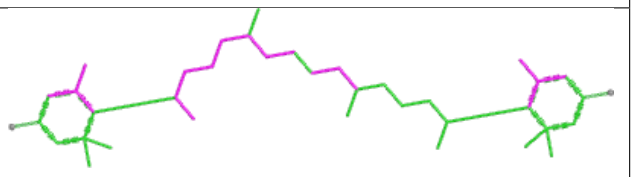


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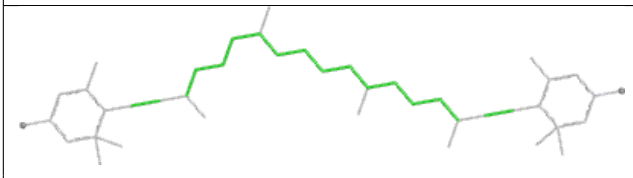
Ligand II0 8 613



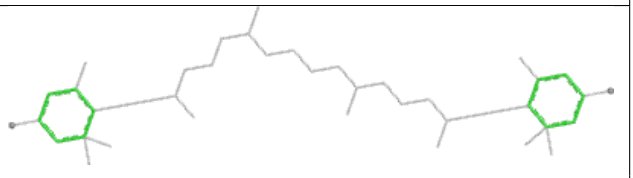
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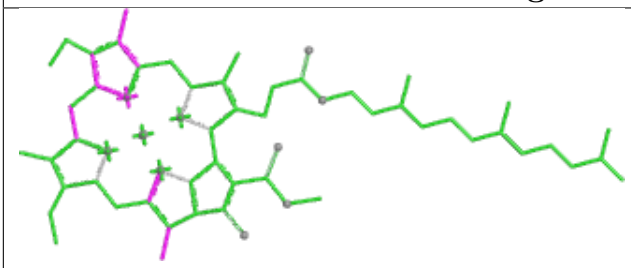


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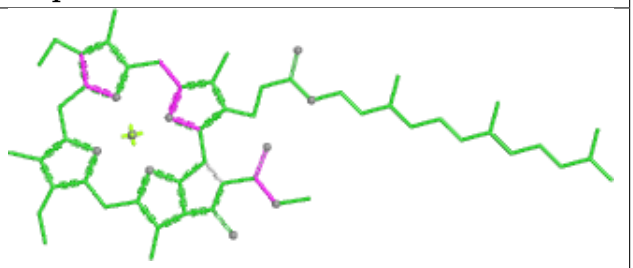


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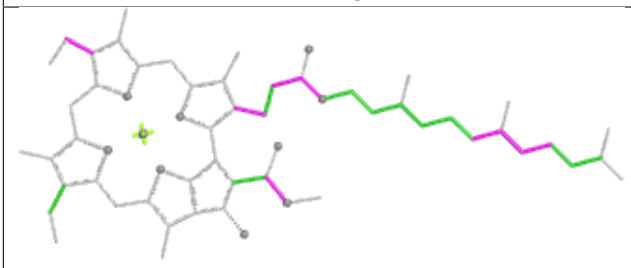
Ligand CLA p 306



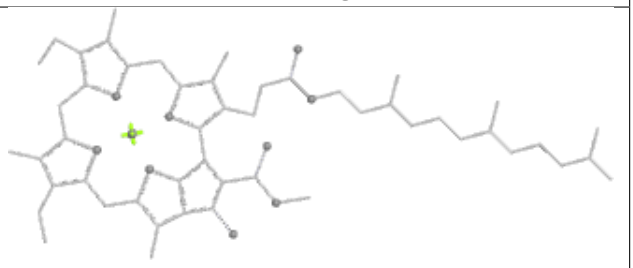
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Bond angles

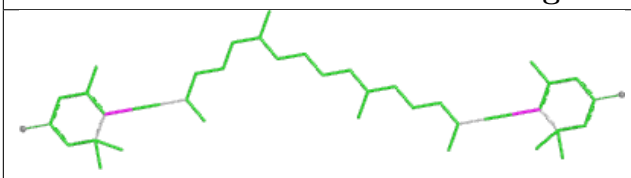


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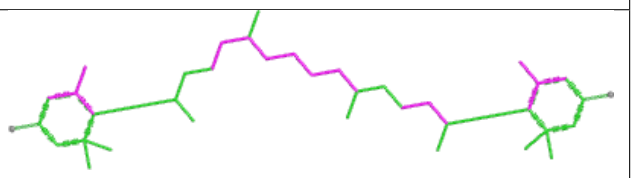


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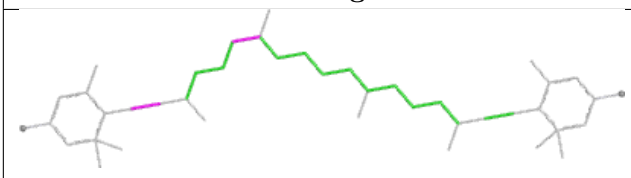
Ligand II0 1 617



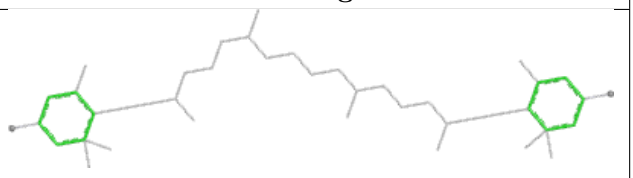
Bond lengths



Bond angles

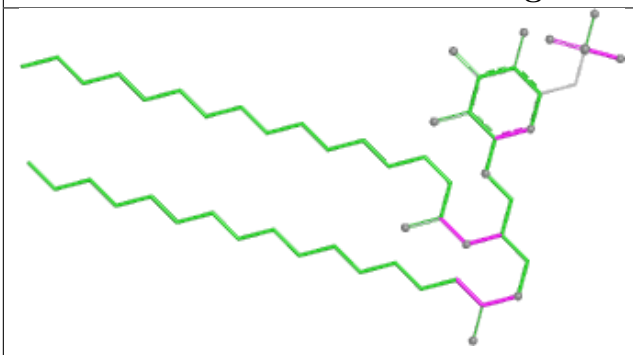


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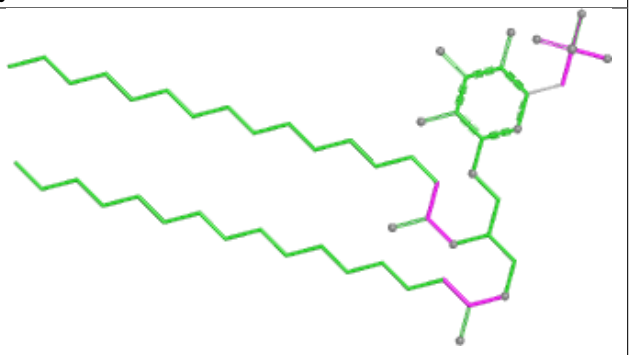


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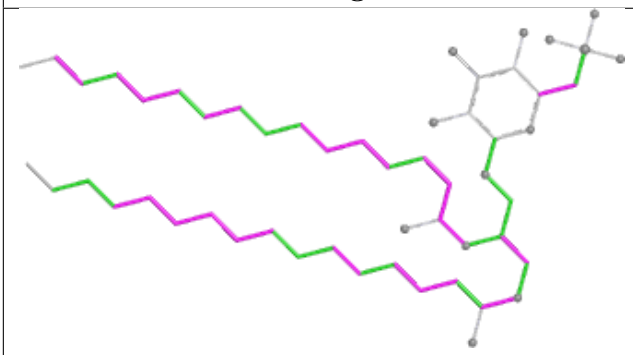
Ligand SQD B 620



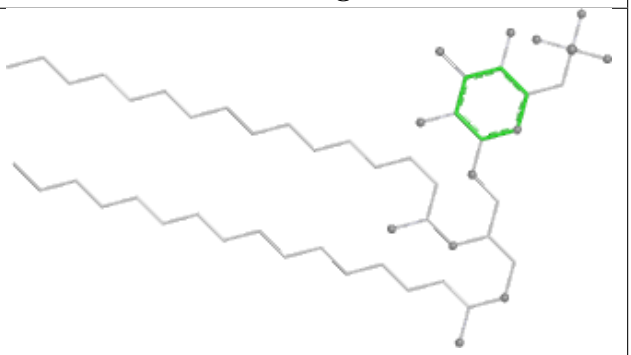
Bond lengths



Bond angles

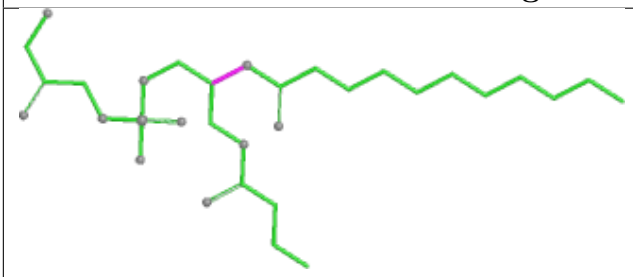


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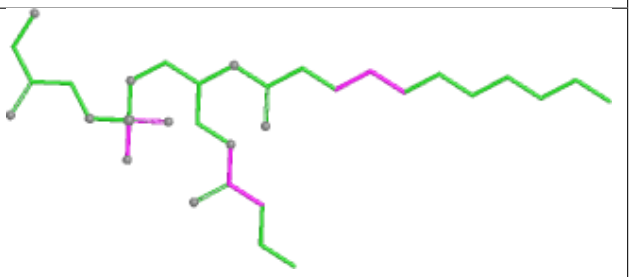


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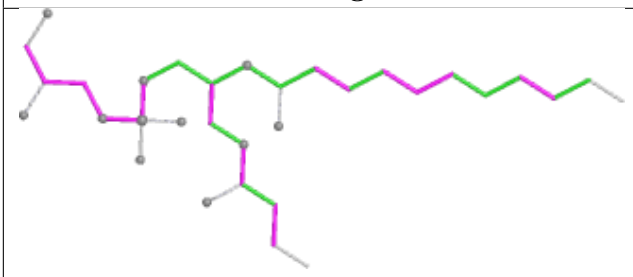
Ligand LHG D 410



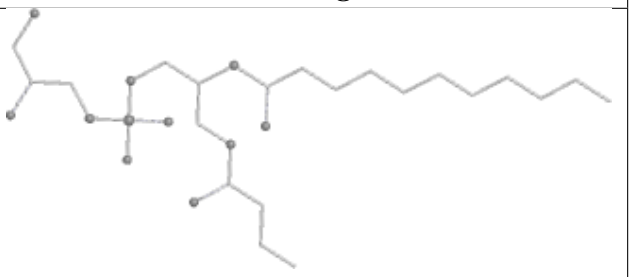
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Bond angles

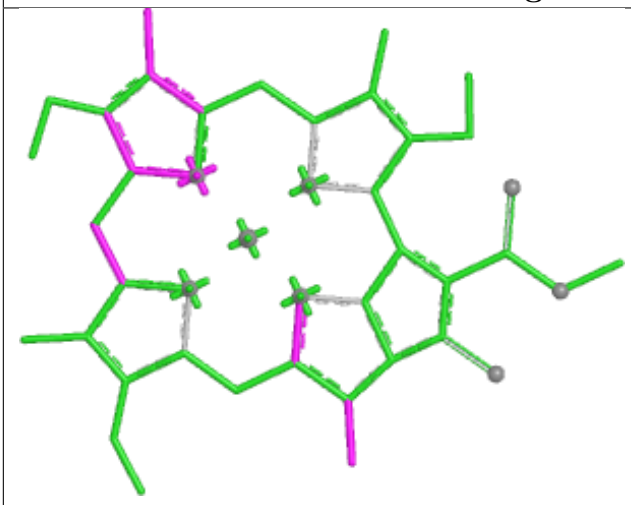


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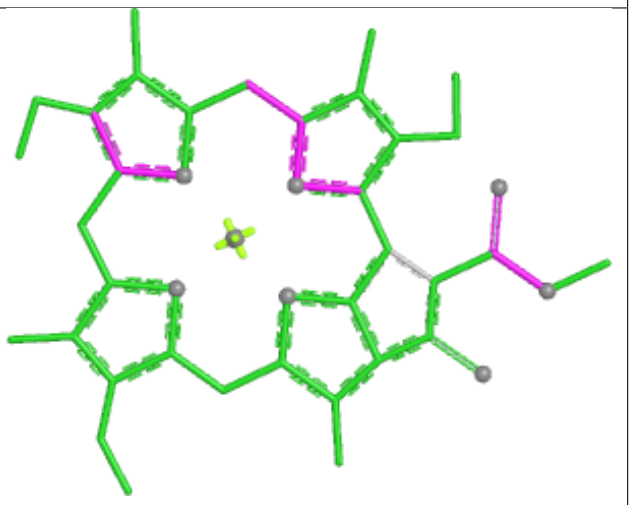


Rings

Ligand CLA P 601



Bond lengths



Bond angles

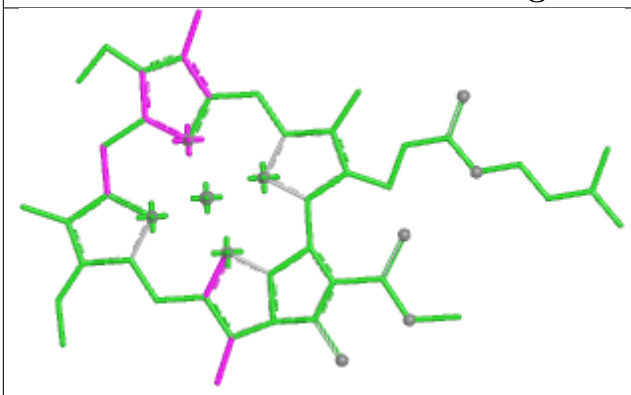


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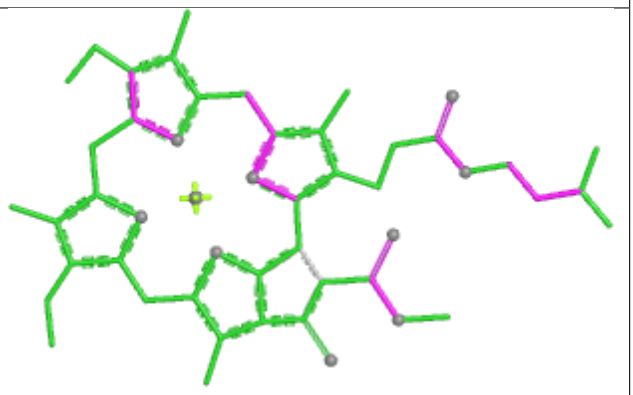


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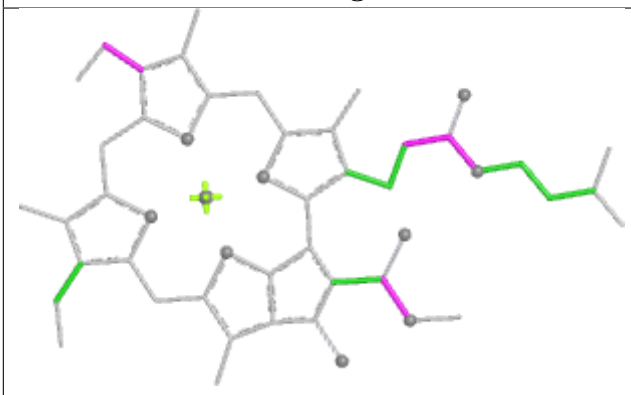
Ligand CLA 0 605



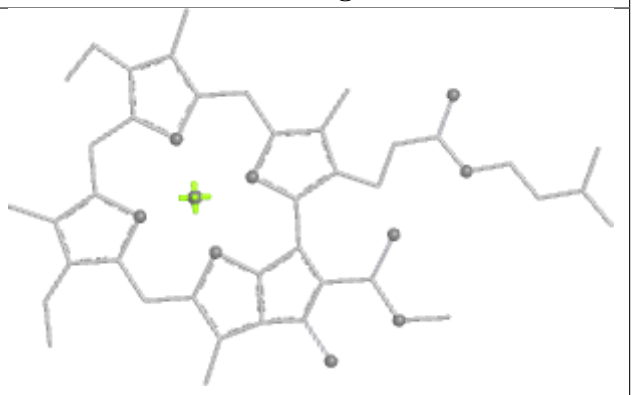
Bond lengths



Bond angles

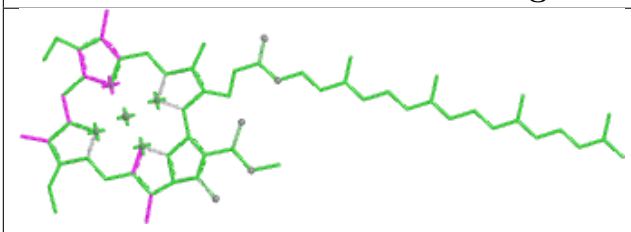


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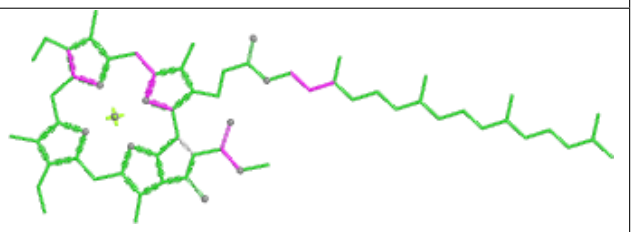


Rings

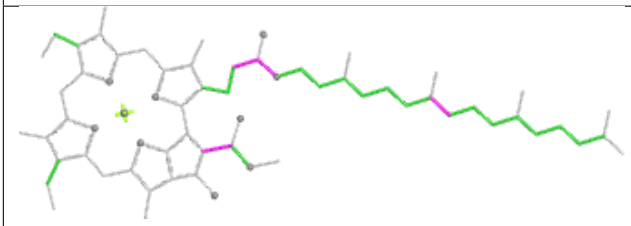
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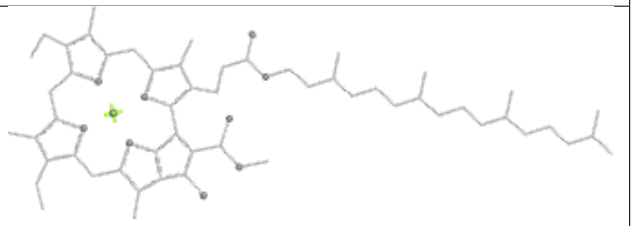
Bond lengths



Bond angles

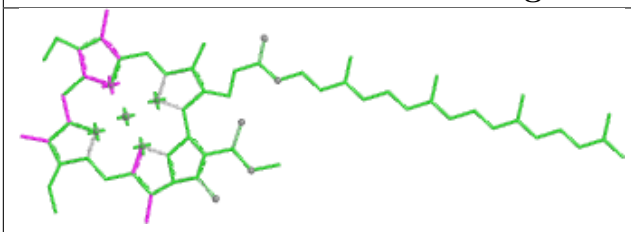


Torsions

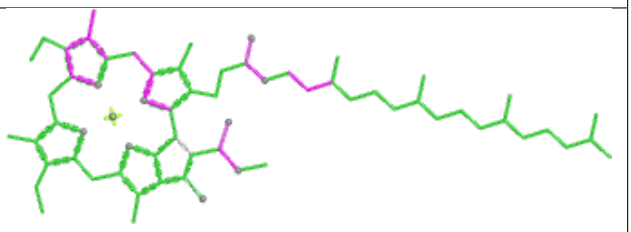


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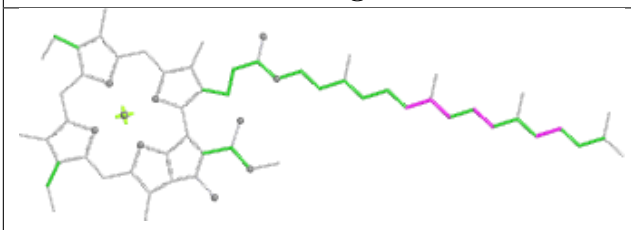
Ligand CLA C 509



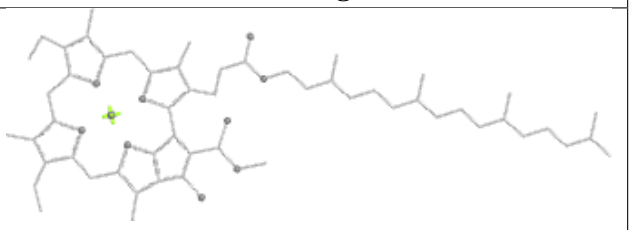
Bond lengths



Bond angles

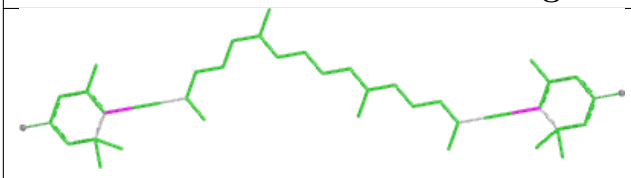


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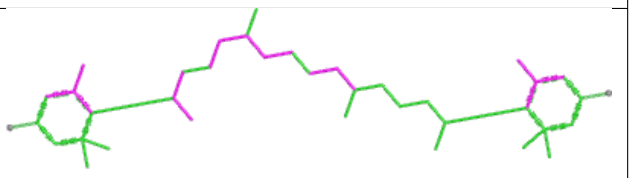


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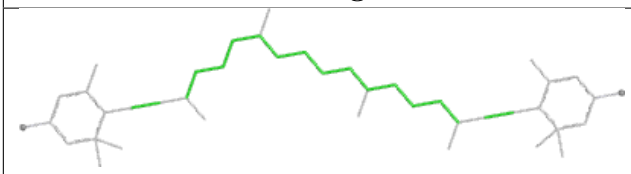
Ligand II0 1 614



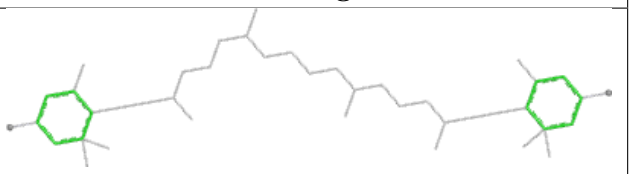
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Bond angles

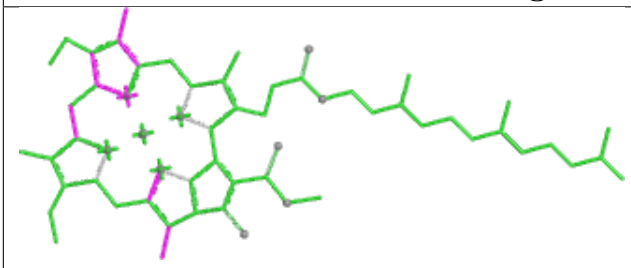


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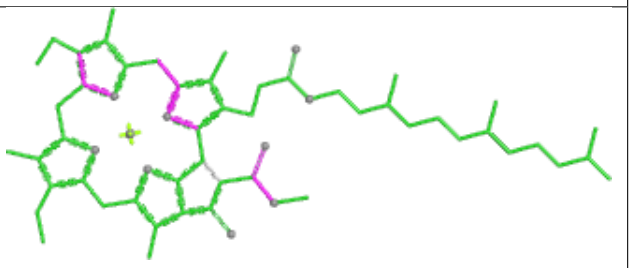


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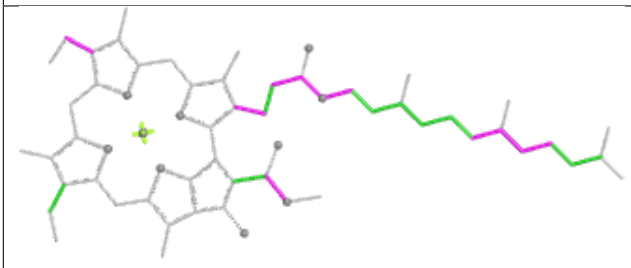
Ligand CLA 5 306



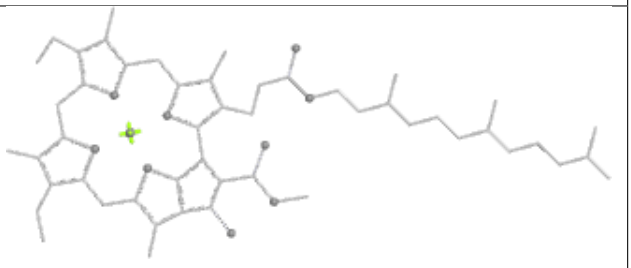
Bond lengths



Bond angles

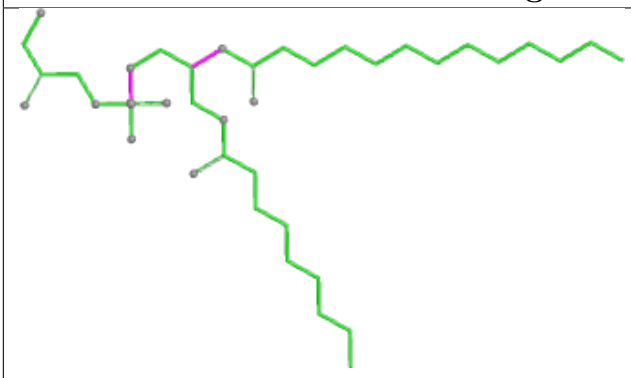


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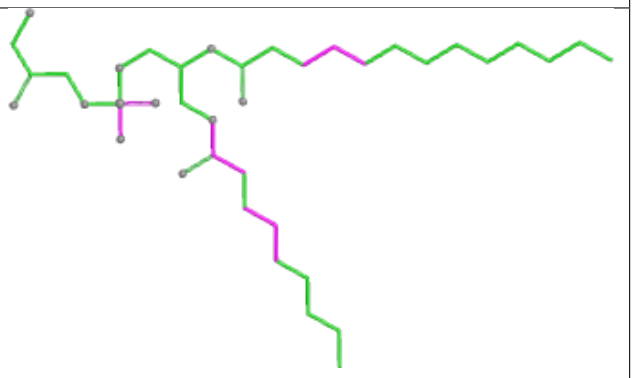


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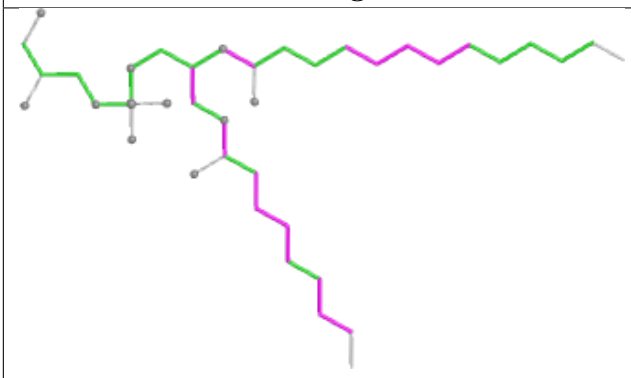
Ligand LHG b 621



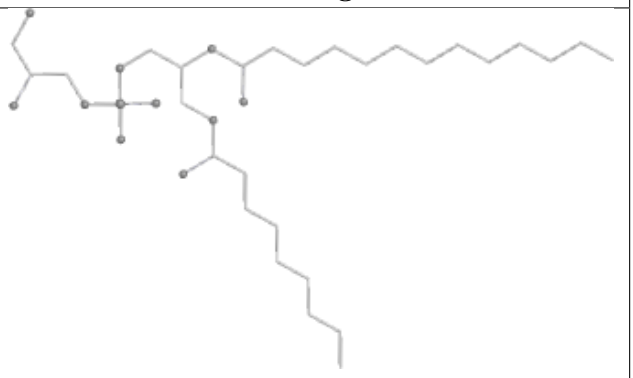
Bond lengths



Bond angles

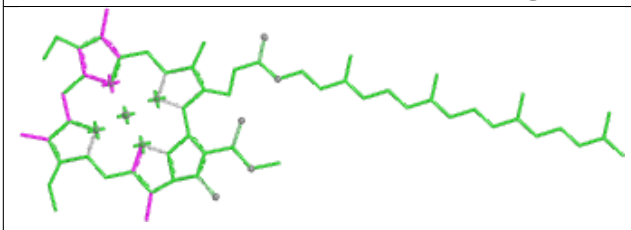


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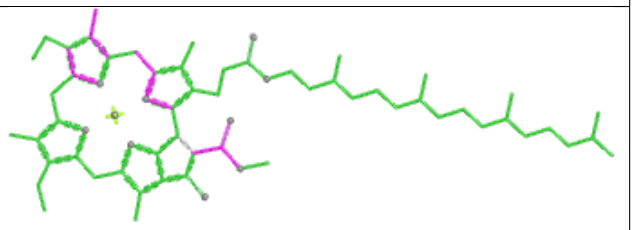


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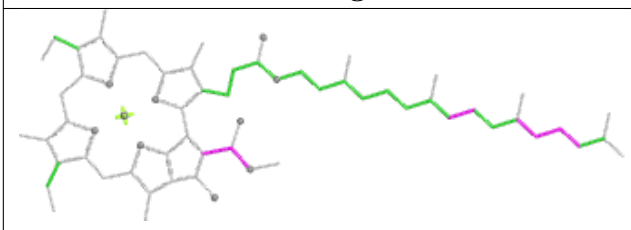
Ligand CLA C 508



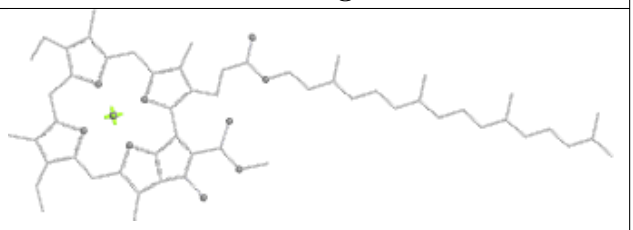
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Bond angles

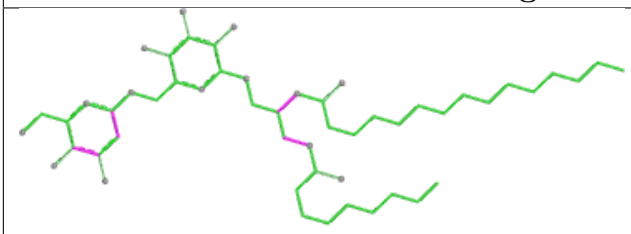


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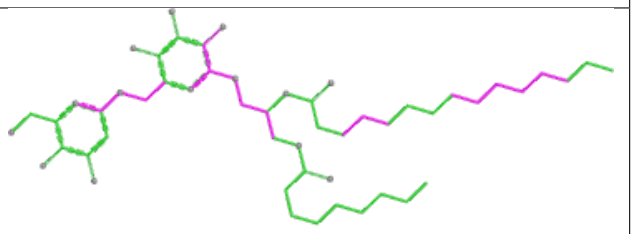


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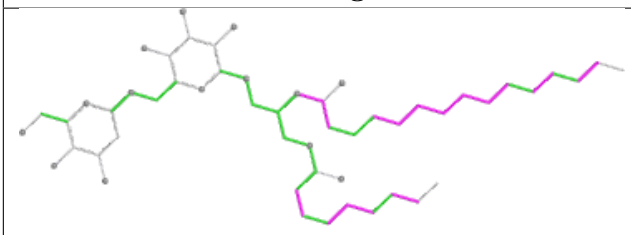
Ligand DGD A 614



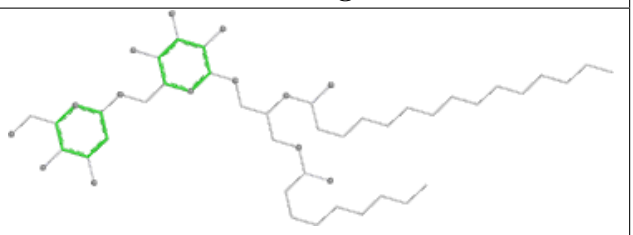
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Bond angles

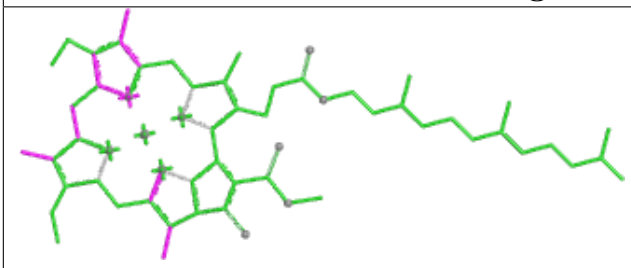


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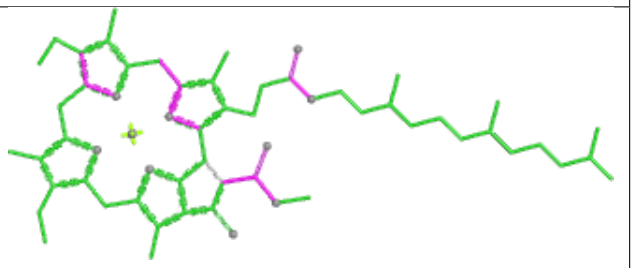


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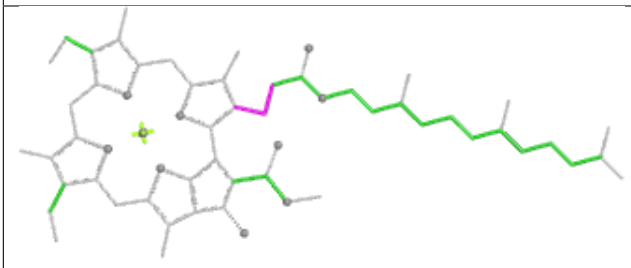
Ligand CLA a 408



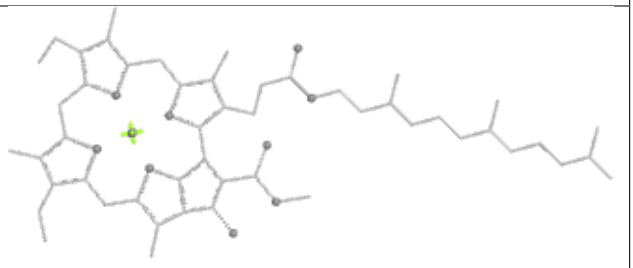
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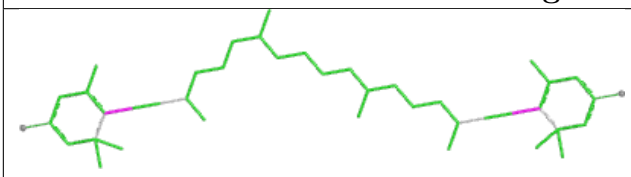


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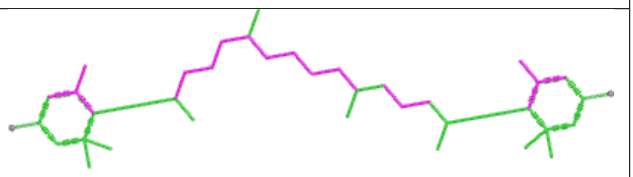


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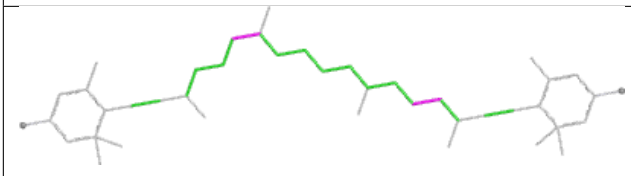
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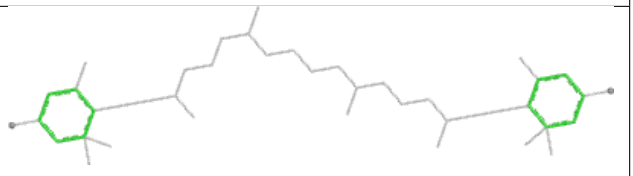
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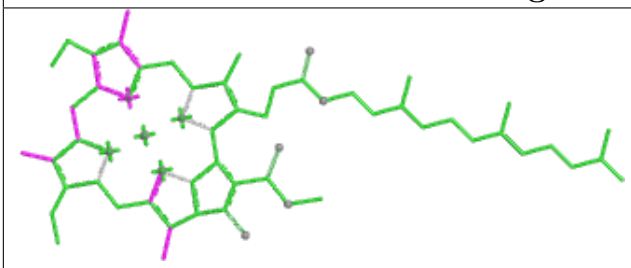


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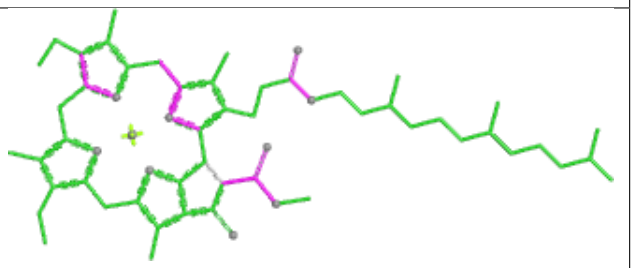


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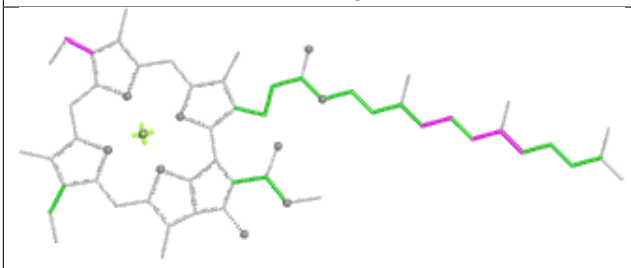
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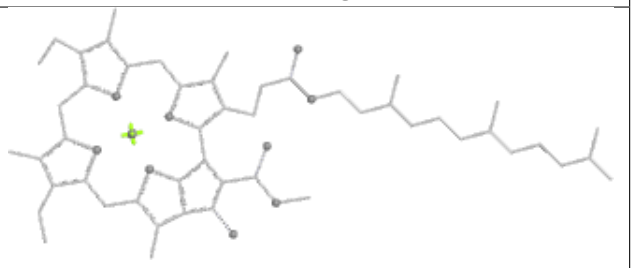
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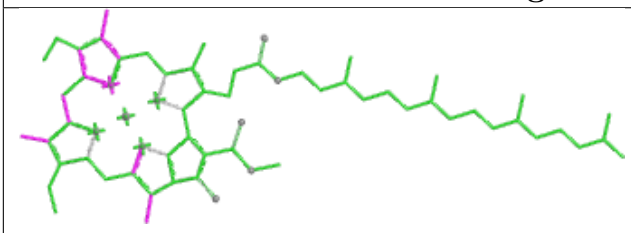


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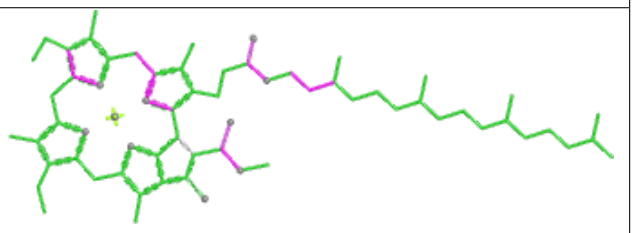


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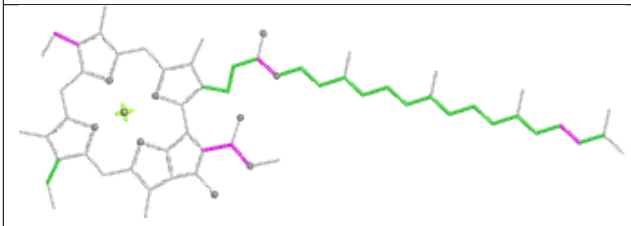
Ligand CLA b 610



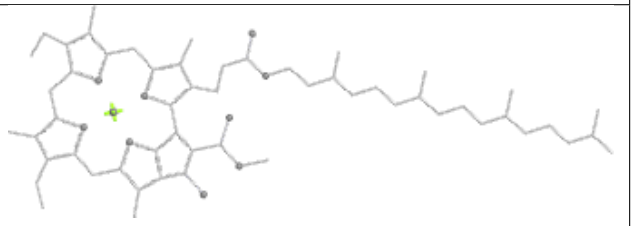
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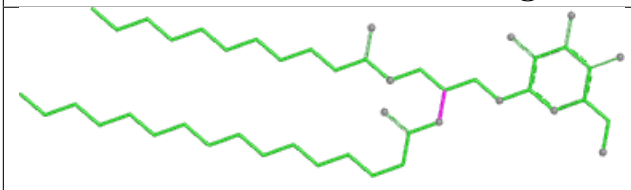


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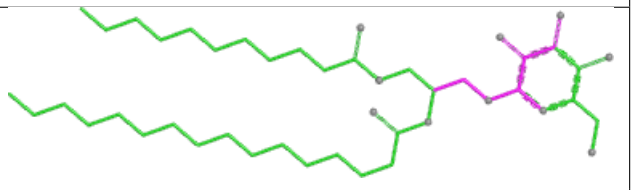


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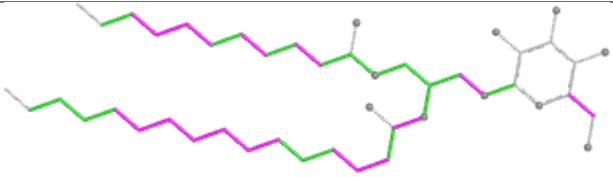
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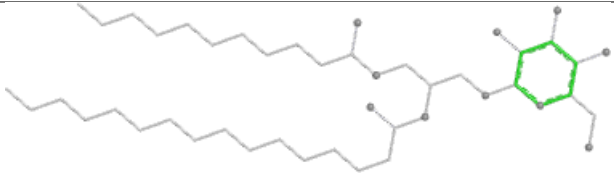
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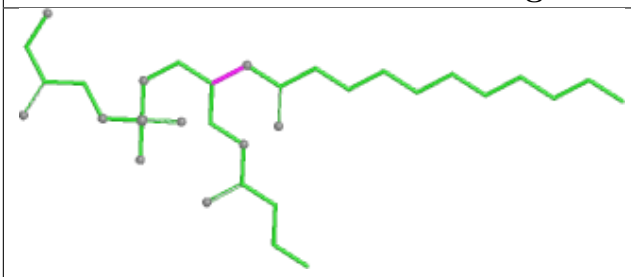


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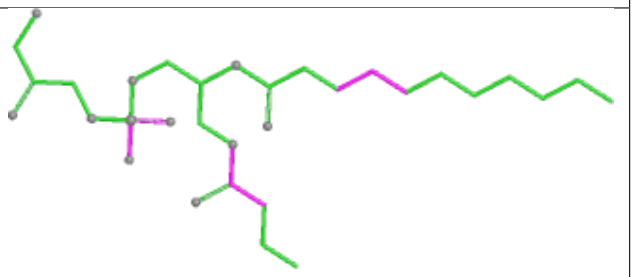


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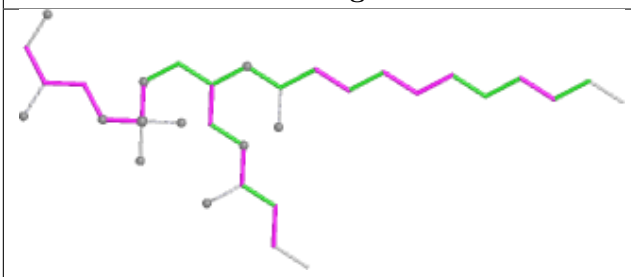
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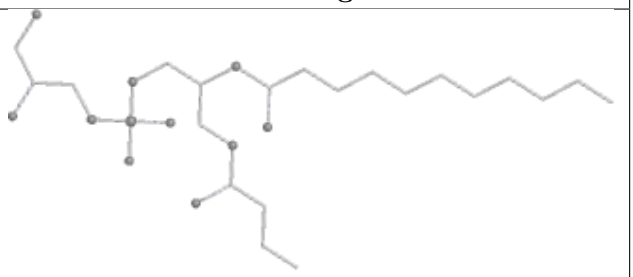
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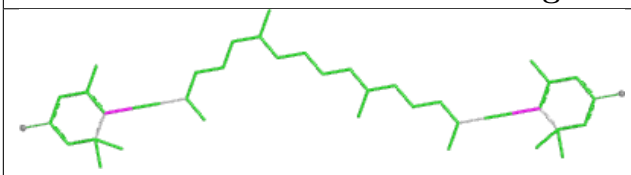


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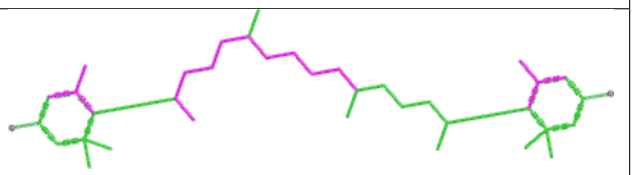


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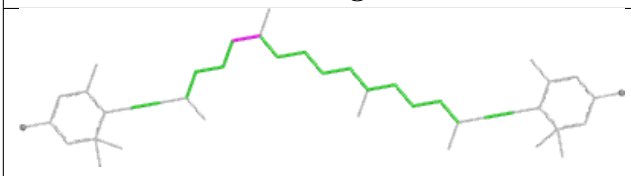
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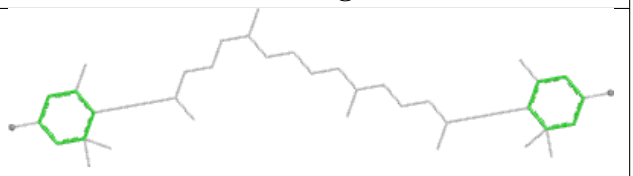
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Bond angles

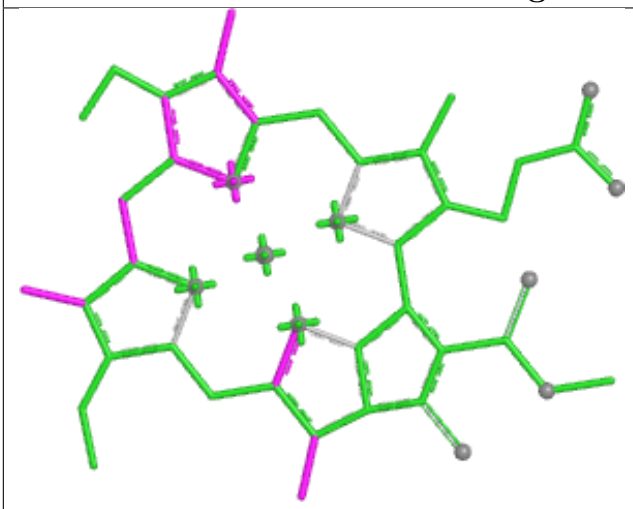


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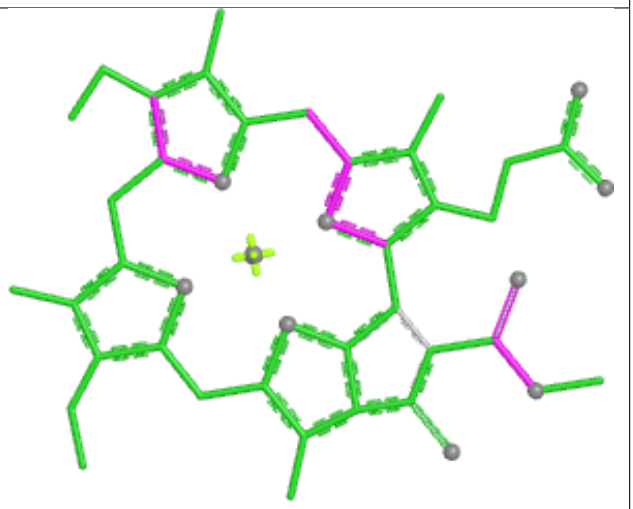


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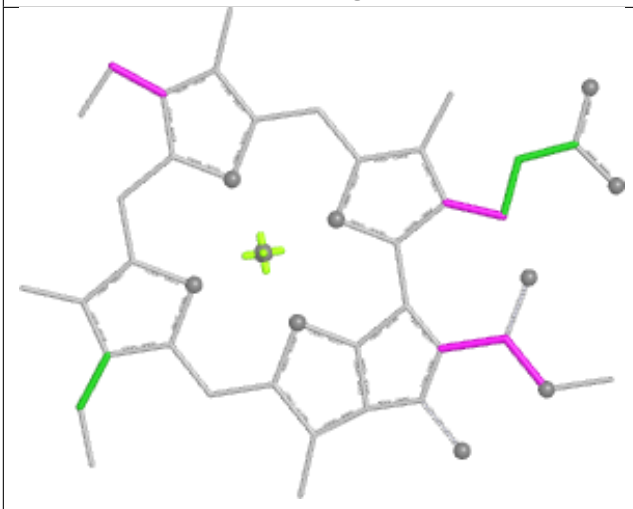
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Bond lengths



Bond angles

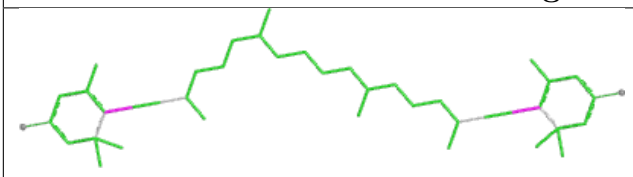


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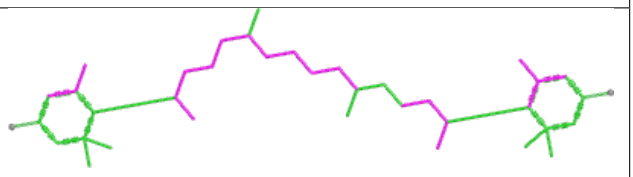


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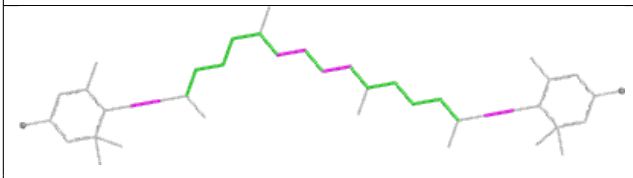
Ligand II0 4 616



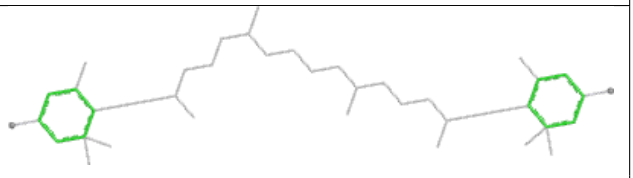
Bond lengths



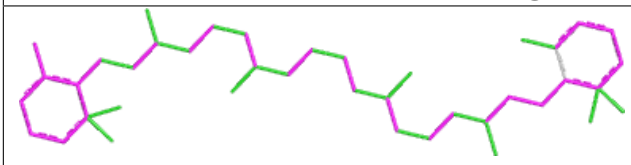
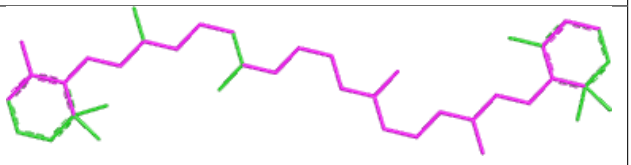
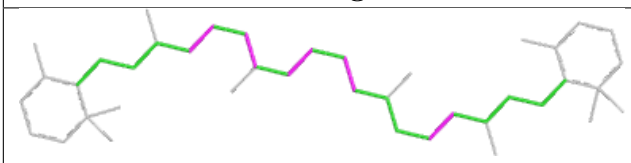
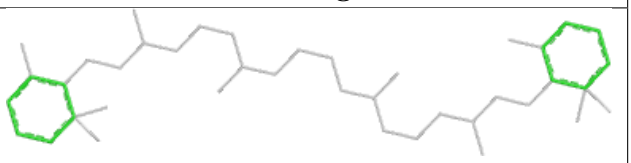
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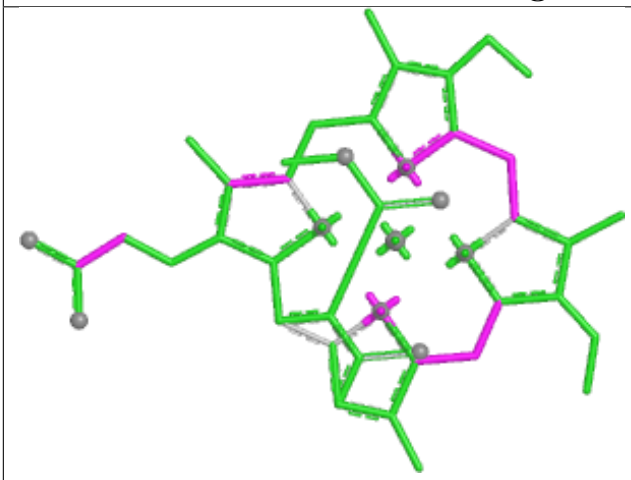
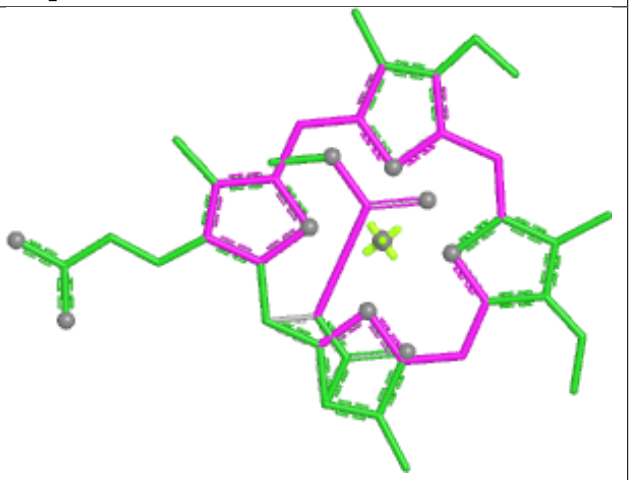
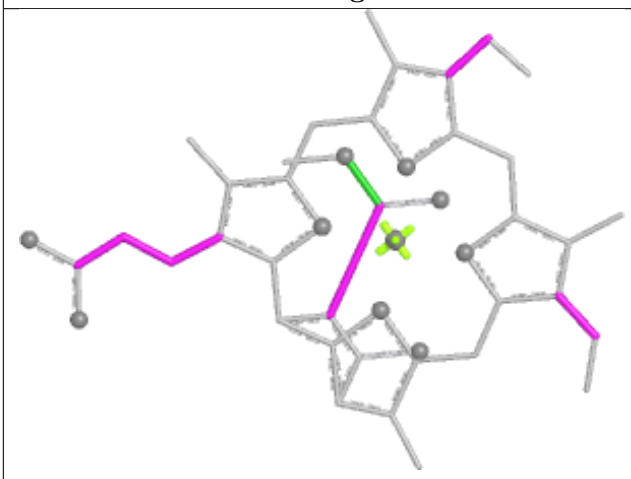
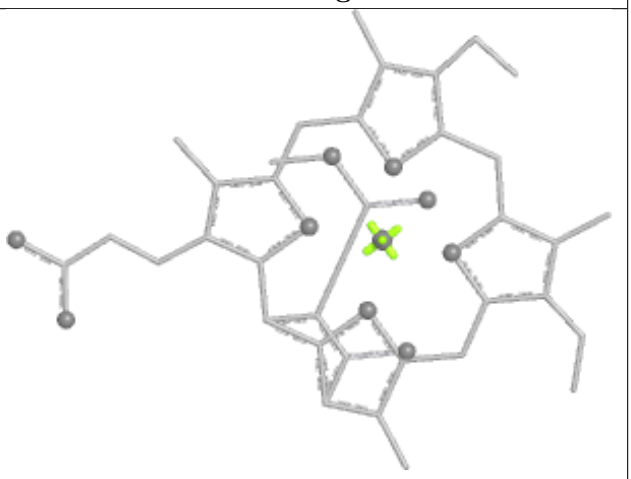


Torsions

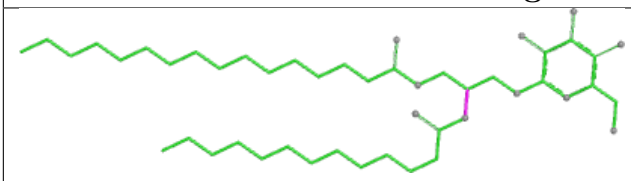


Rings

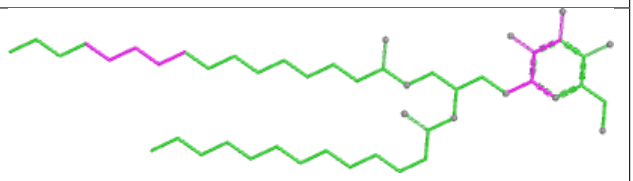
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 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC2 p 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

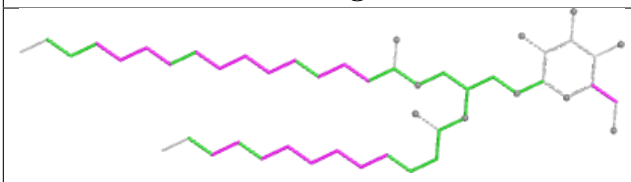
Ligand LMG a 410



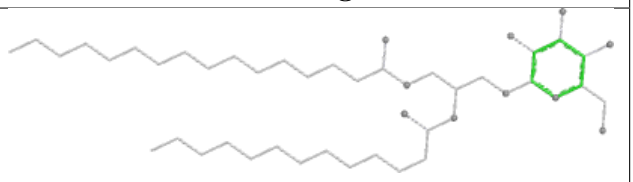
Bond lengths



Bond angles

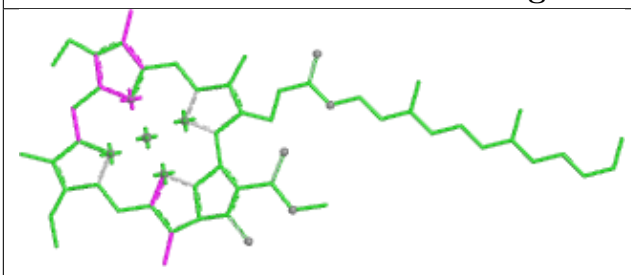


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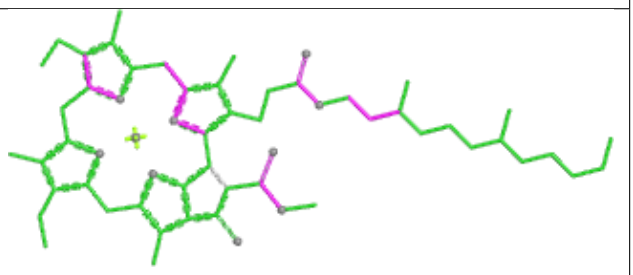


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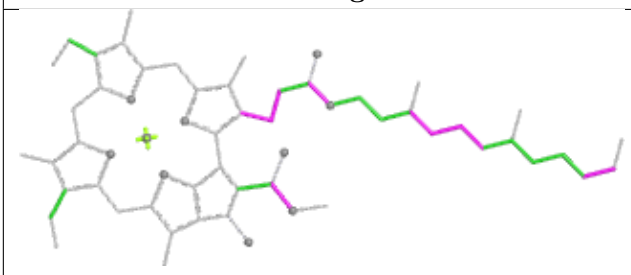
Ligand CLA 1 602



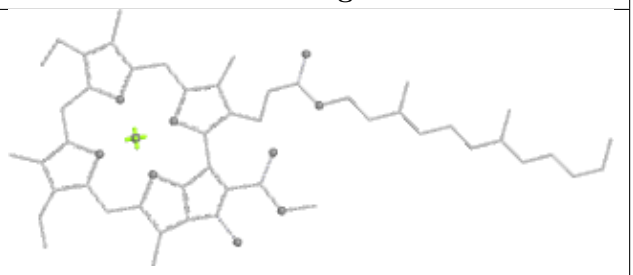
Bond lengths



Bond angles

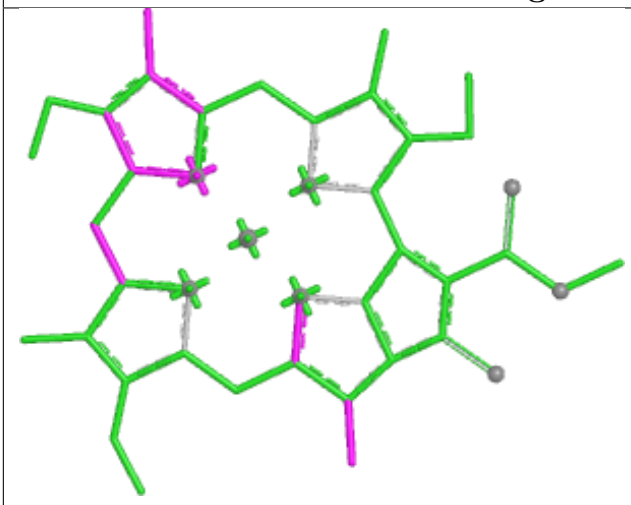


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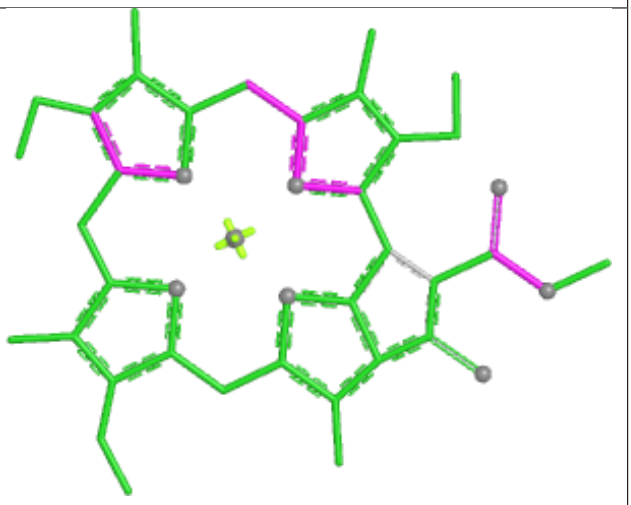


Rings

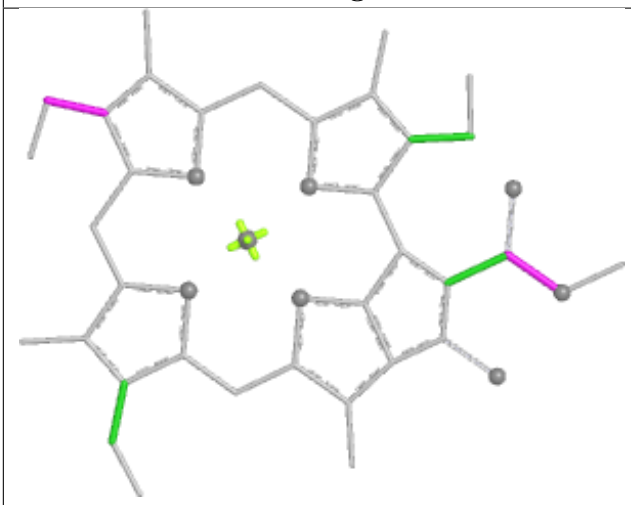
Ligand CLA 2 601



Bond lengths



Bond angles

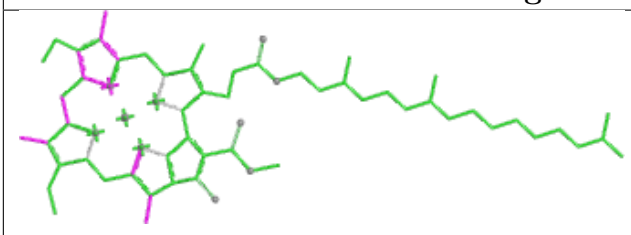


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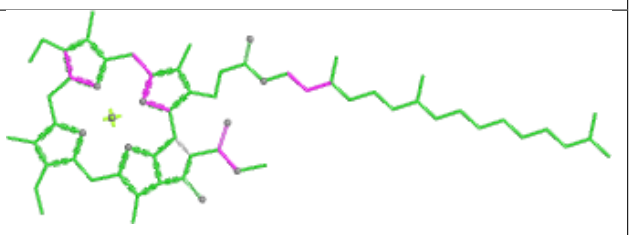


Rings

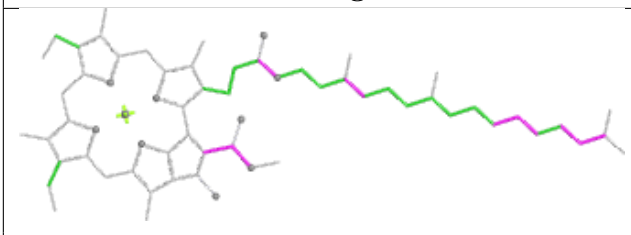
Ligand CLA B 615



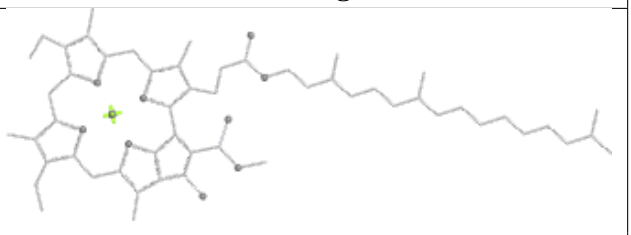
Bond lengths



Bond angles

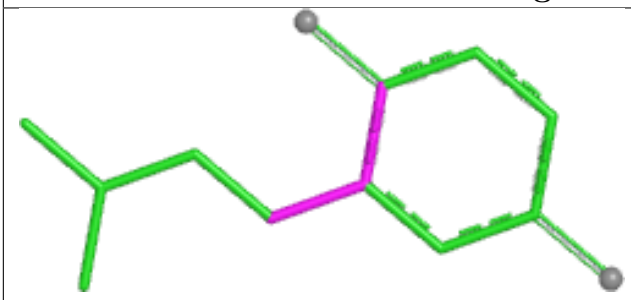


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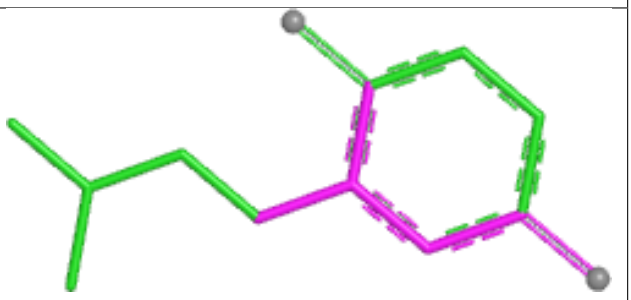


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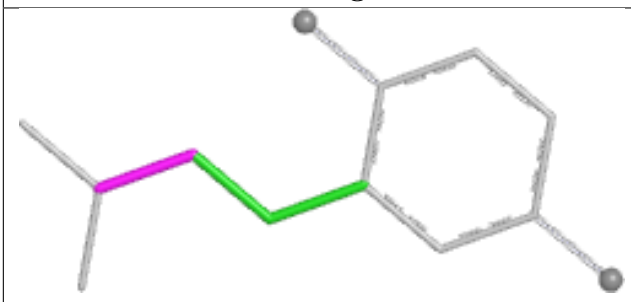
Ligand PL9 a 412



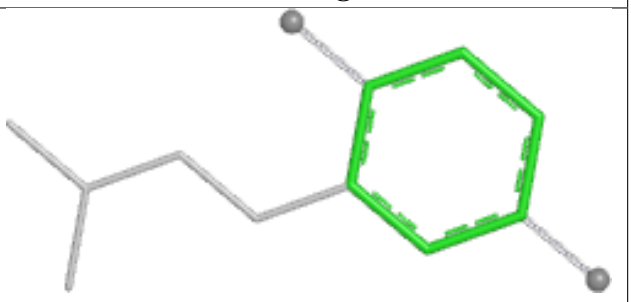
Bond lengths



Bond angles

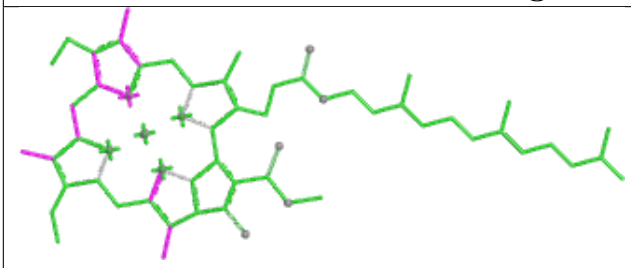


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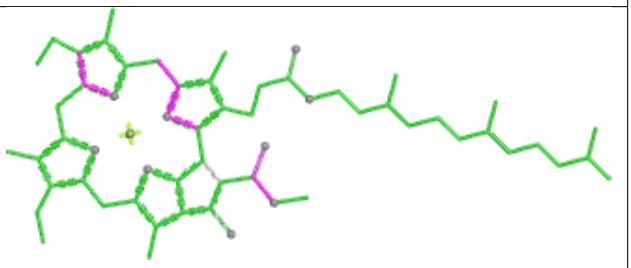


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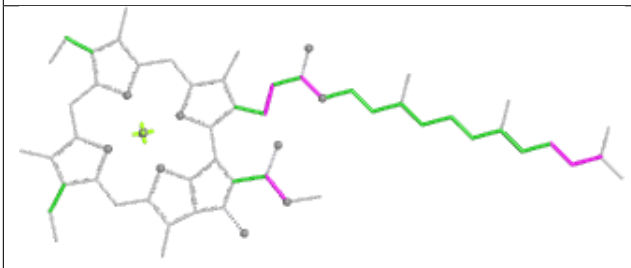
Ligand CLA 9 607



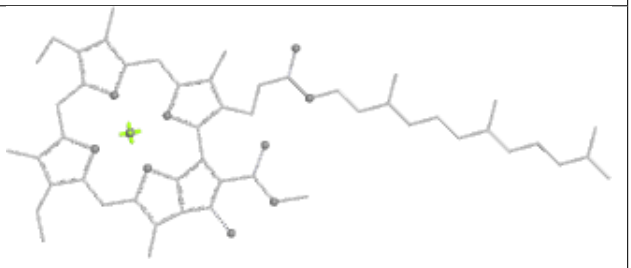
Bond lengths



Bond angles

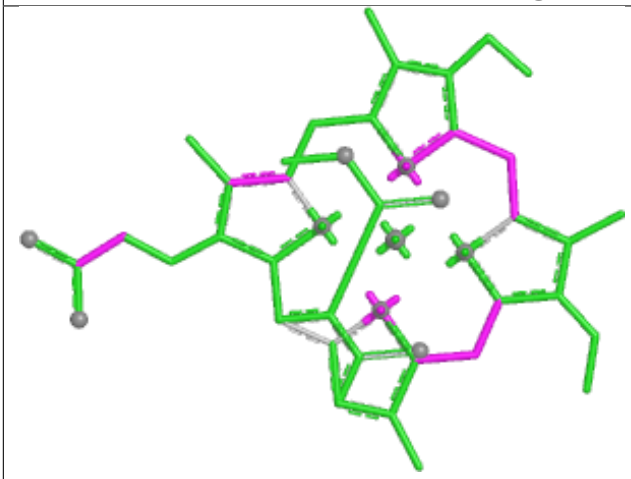


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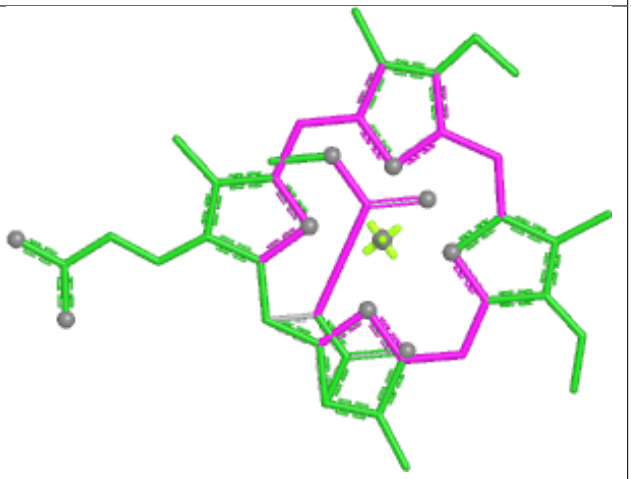


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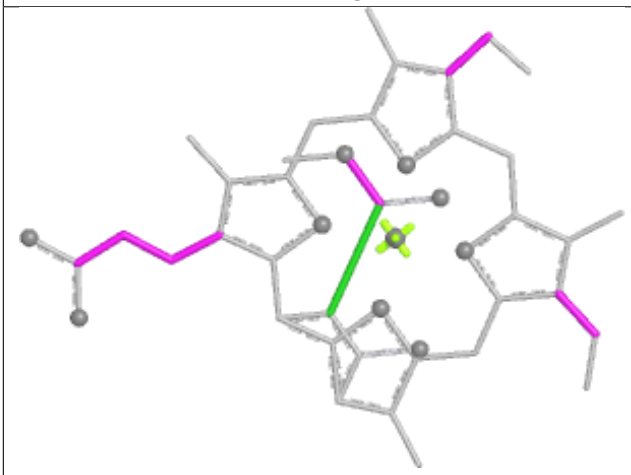
Ligand KC2 2 610



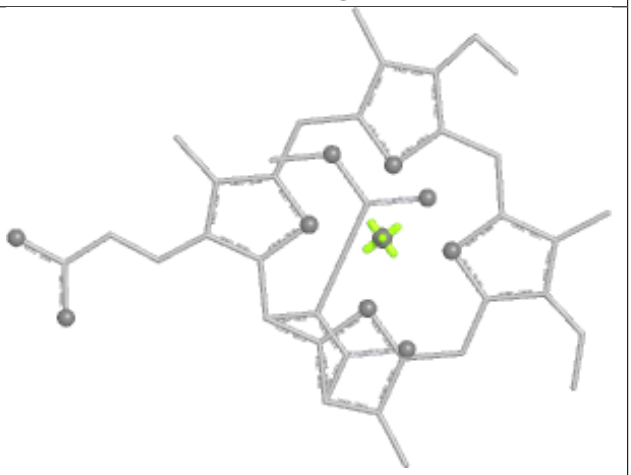
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Bond angles

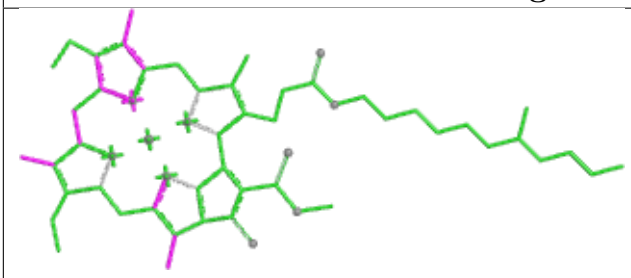


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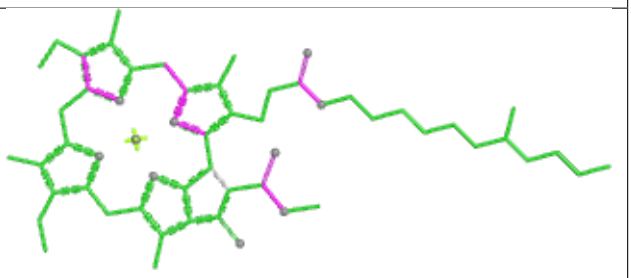


Rings

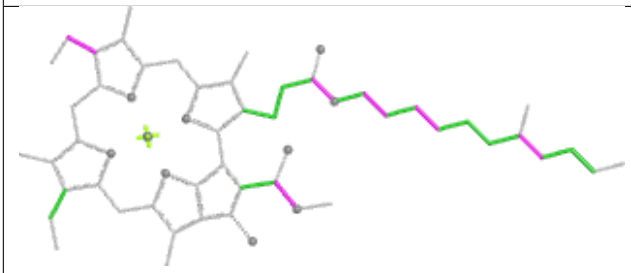
Ligand CLA c 512



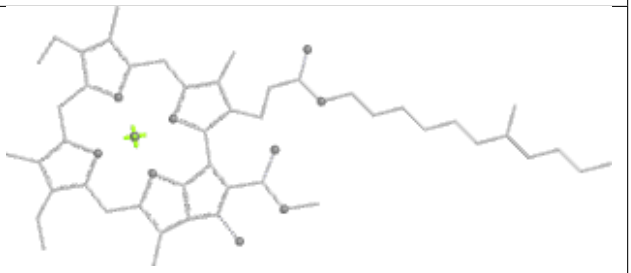
Bond lengths



Bond angles

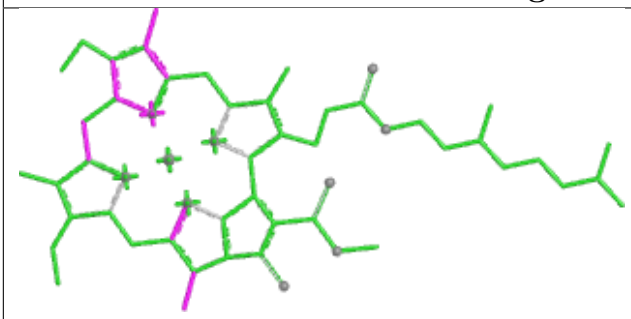


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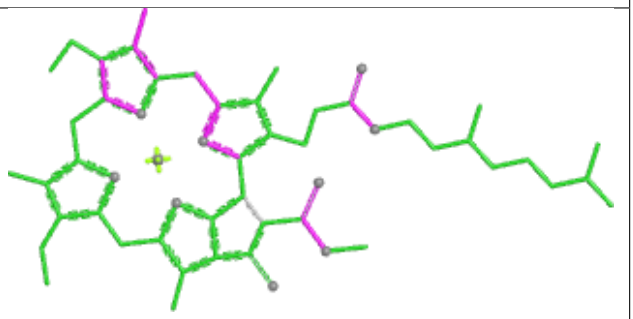


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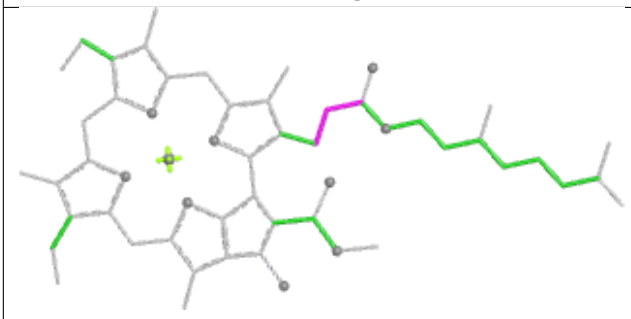
Ligand CLA 8 604



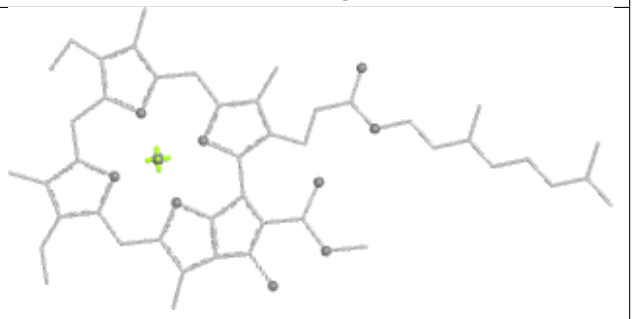
Bond lengths



Bond angles

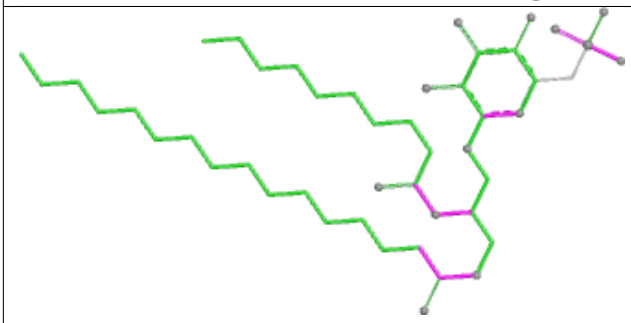


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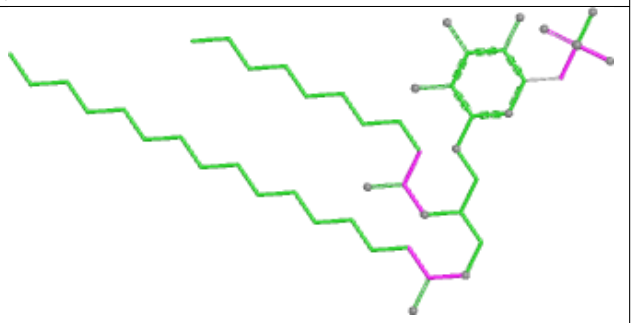


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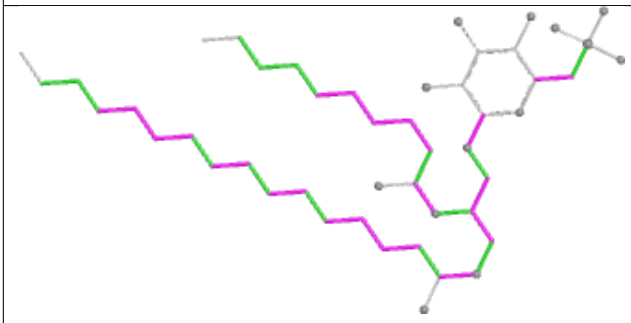
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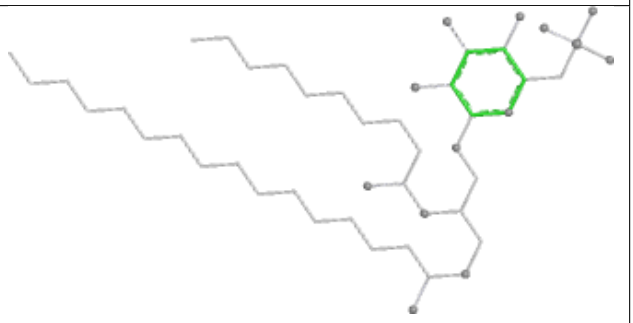
Bond lengths



Bond angles

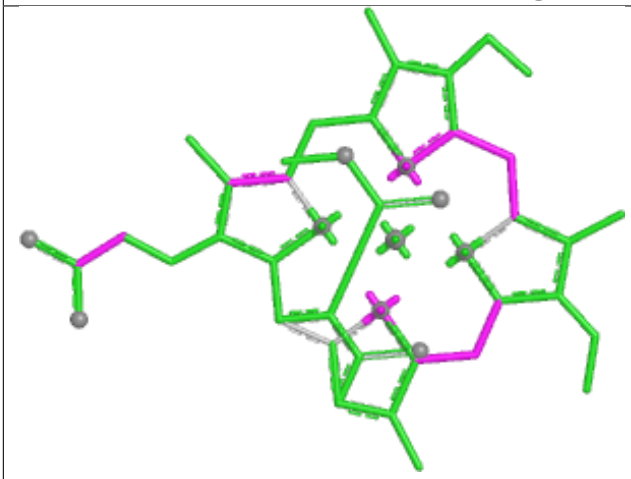


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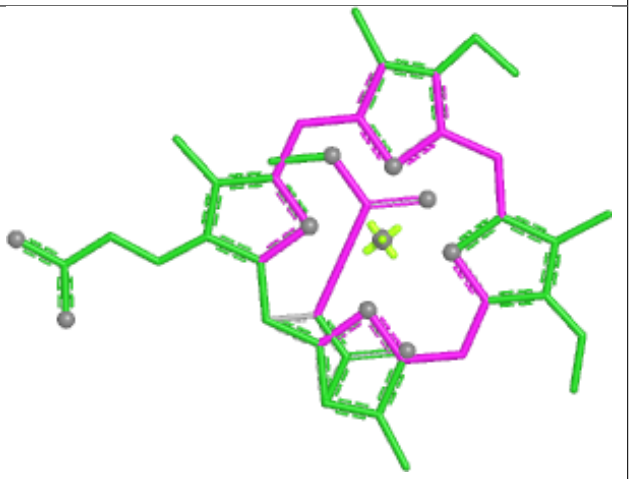


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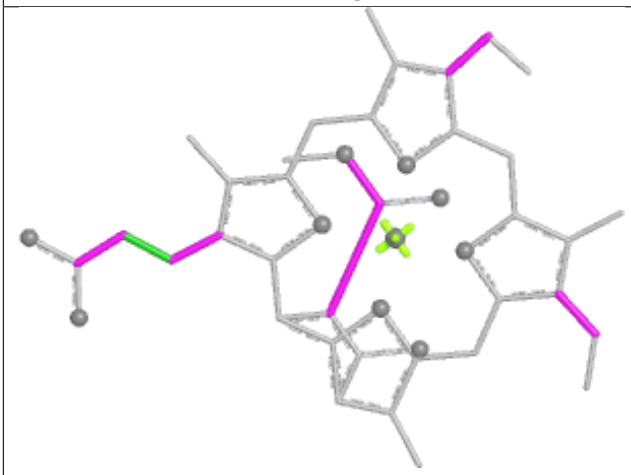
Ligand KC2 1 610



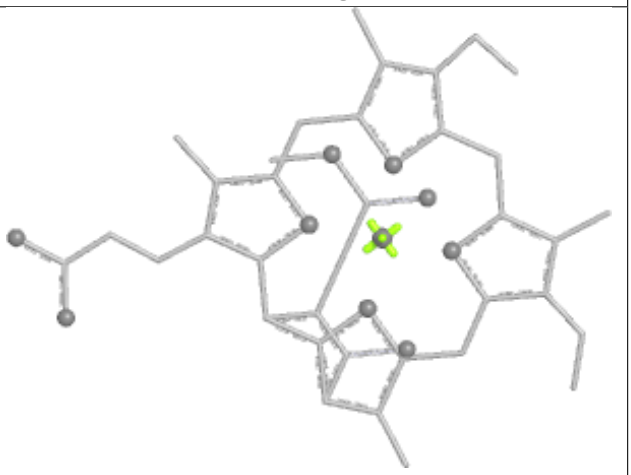
Bond lengths



Bond angles

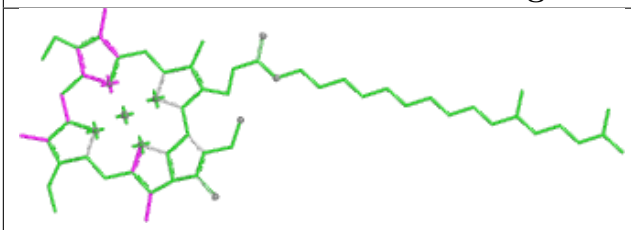


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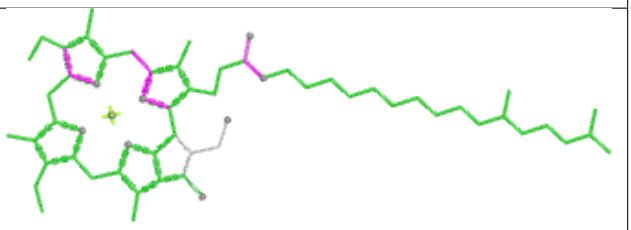


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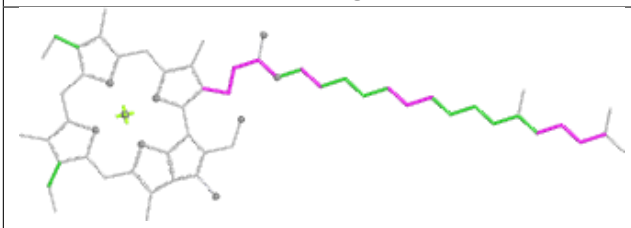
Ligand CLA b 603



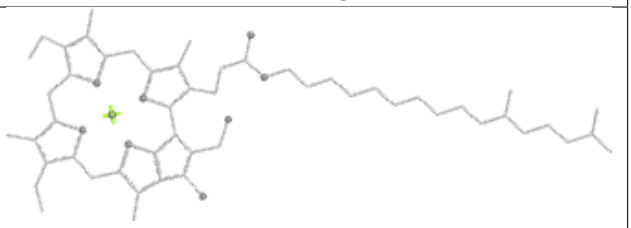
Bond lengths



Bond angles

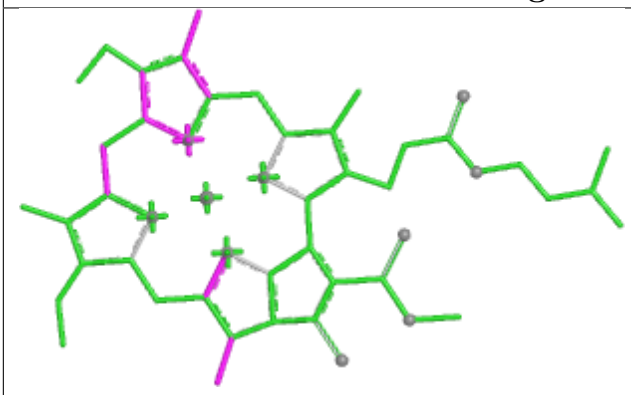


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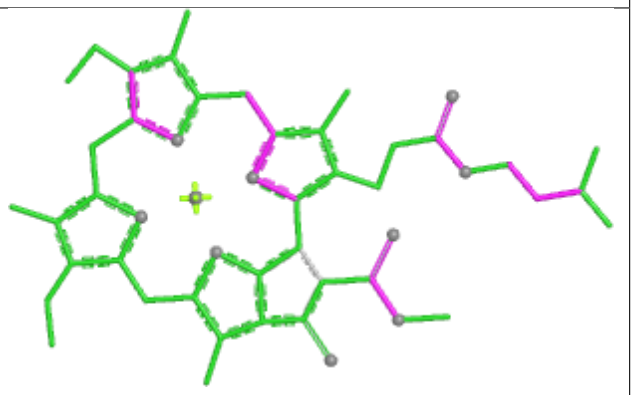


Rings

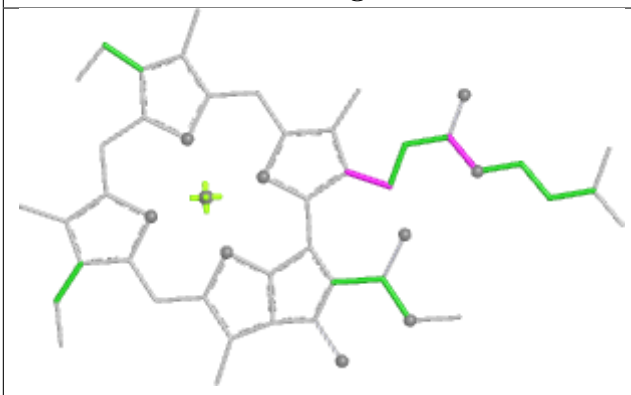
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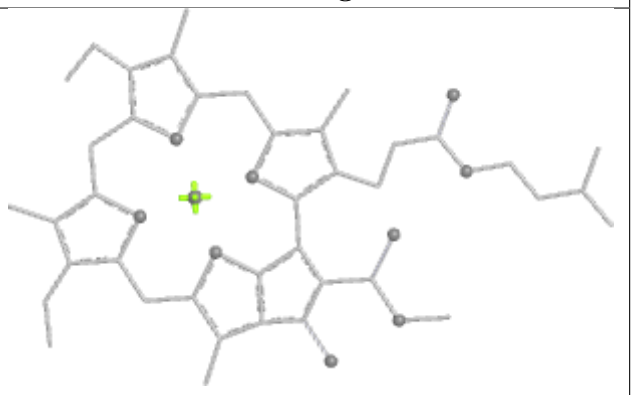
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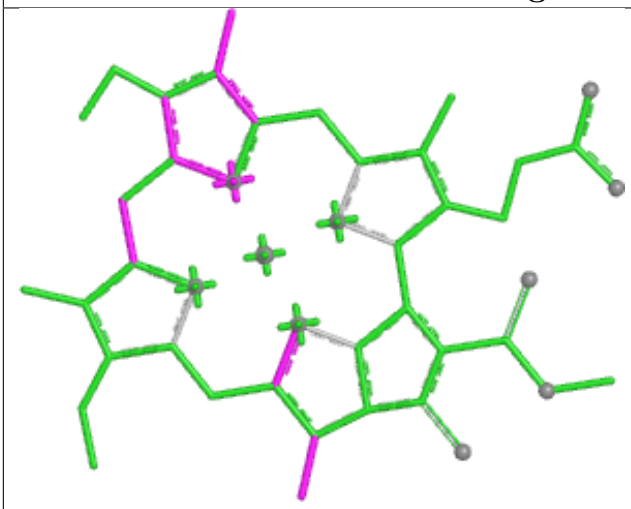


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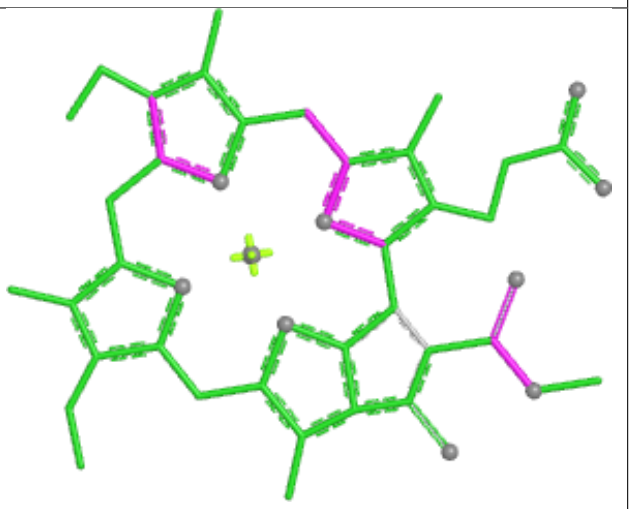


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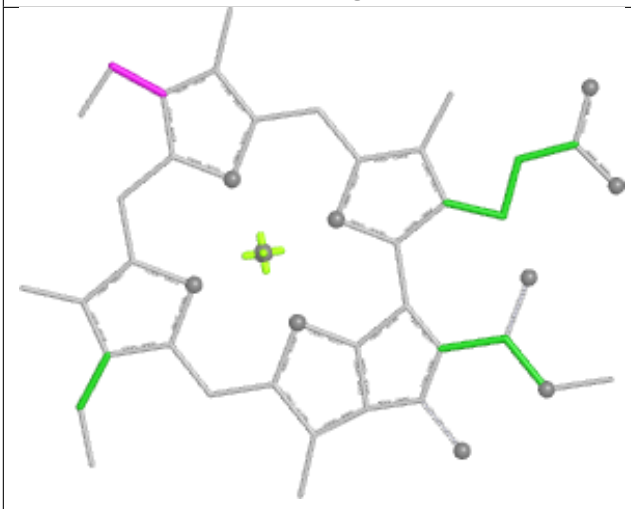
Ligand CLA 0 607



Bond lengths



Bond angles

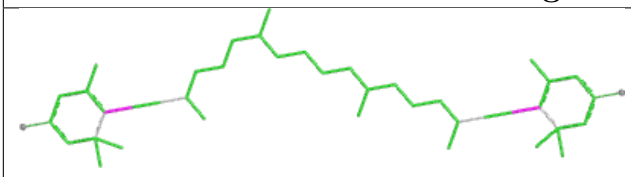


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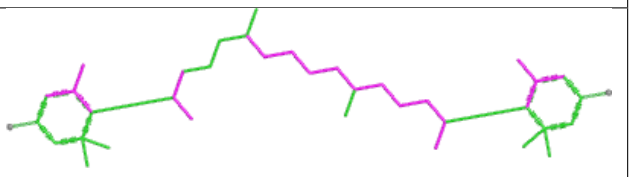


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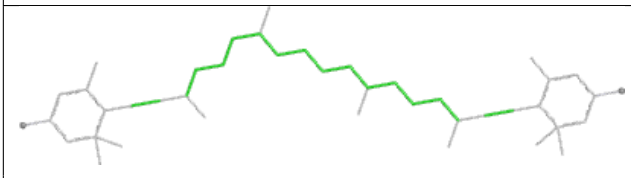
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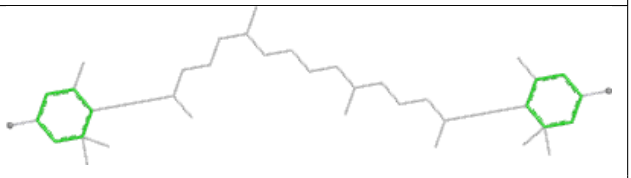
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Bond angles

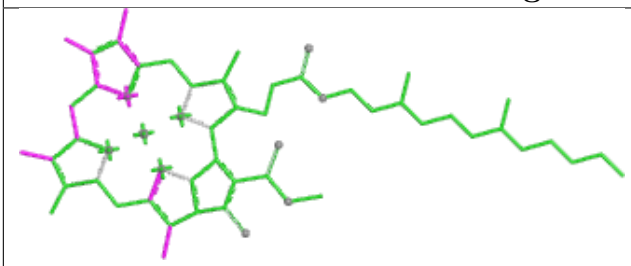


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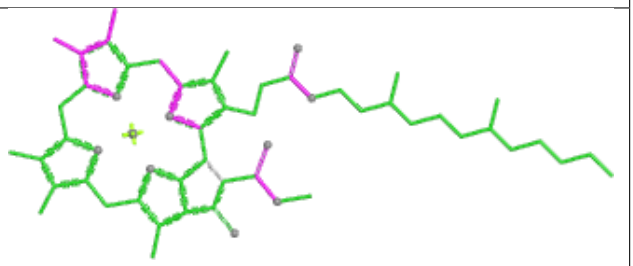


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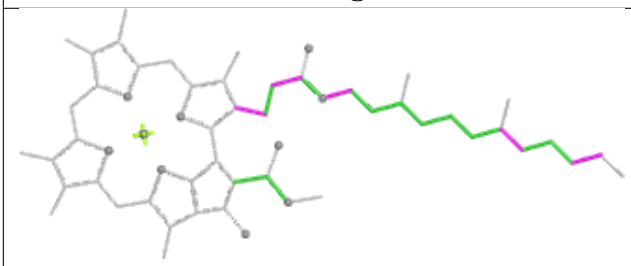
Ligand CLA D 403



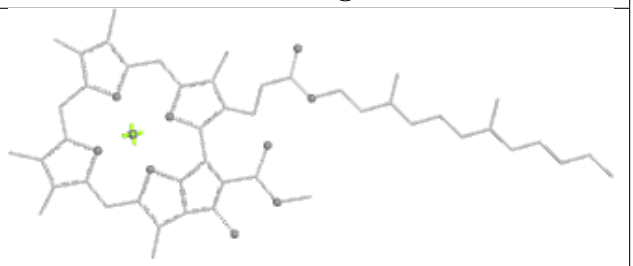
Bond lengths



Bond angles

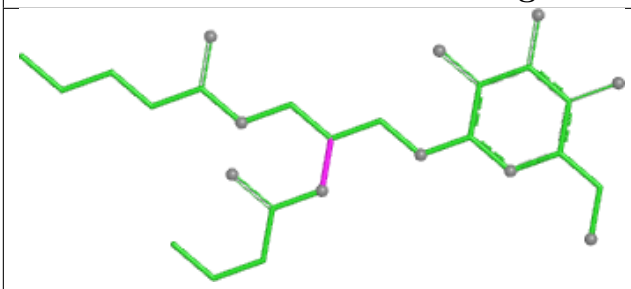


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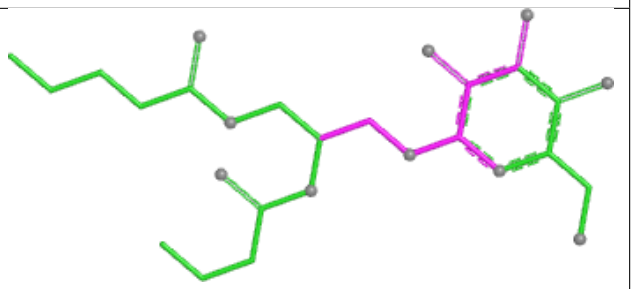


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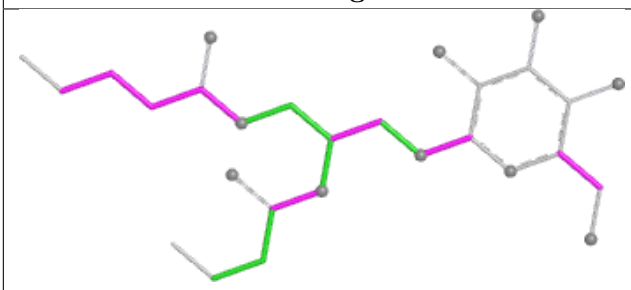
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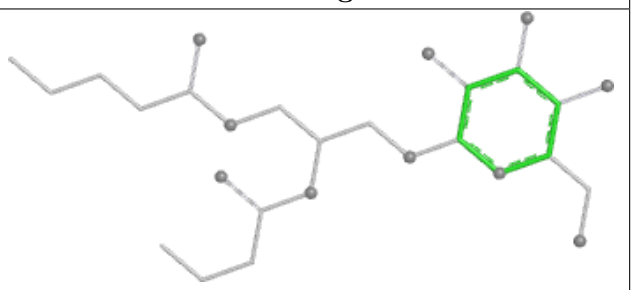
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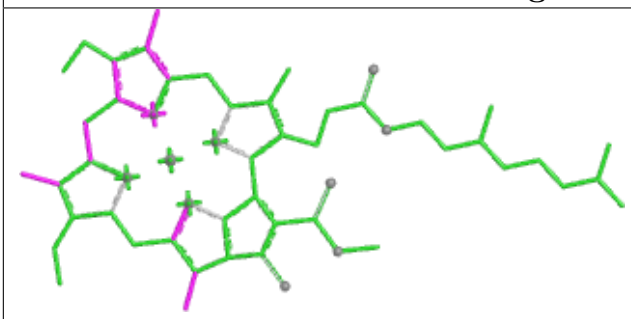
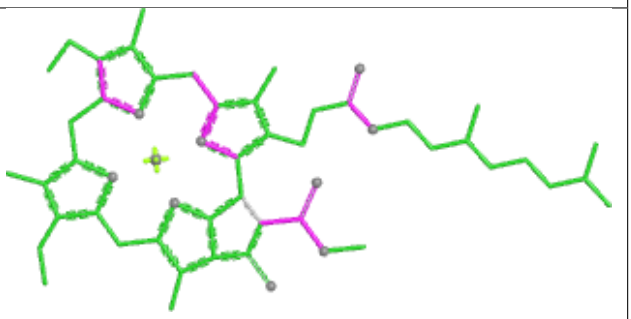
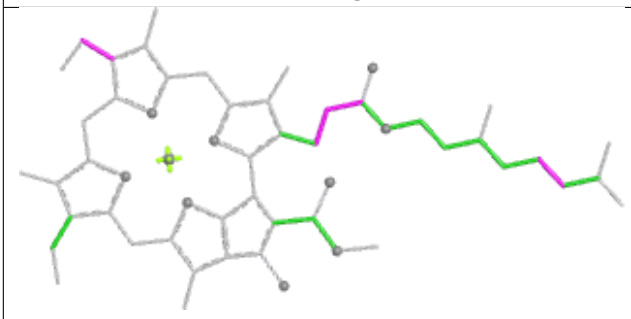
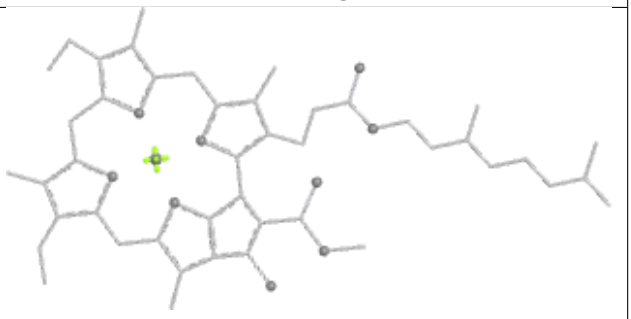
Bond angles

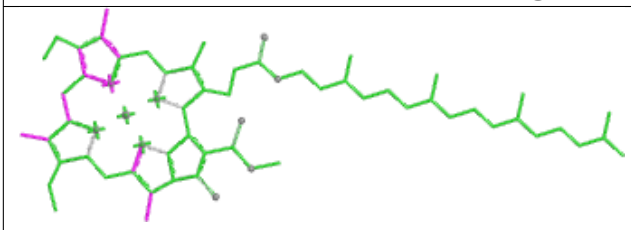
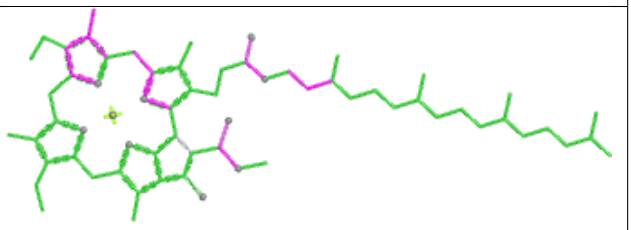
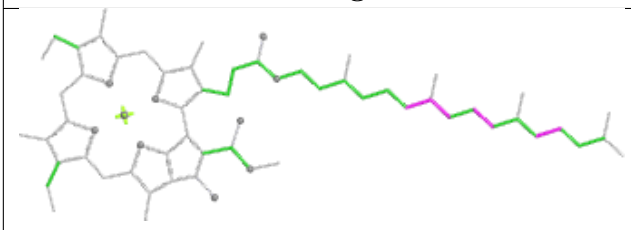
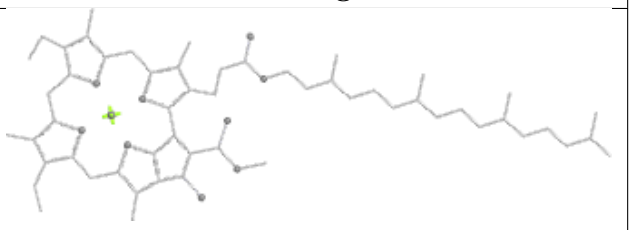


Torsions

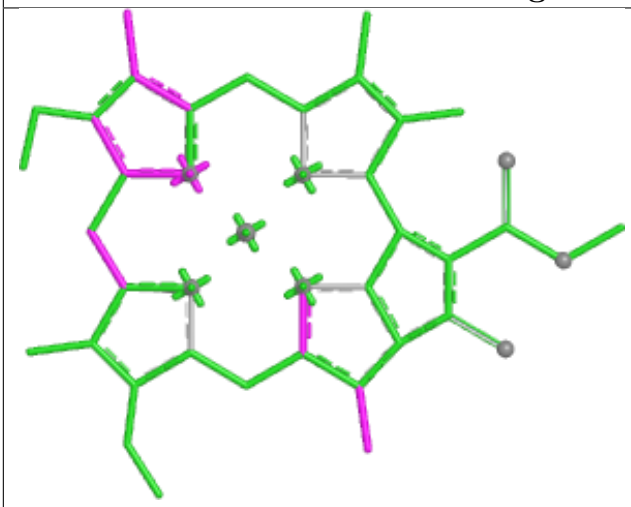


Rings

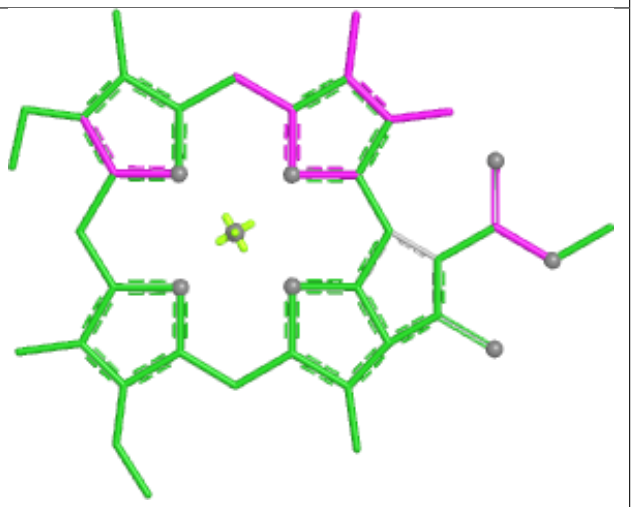
Ligand CLA 3 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

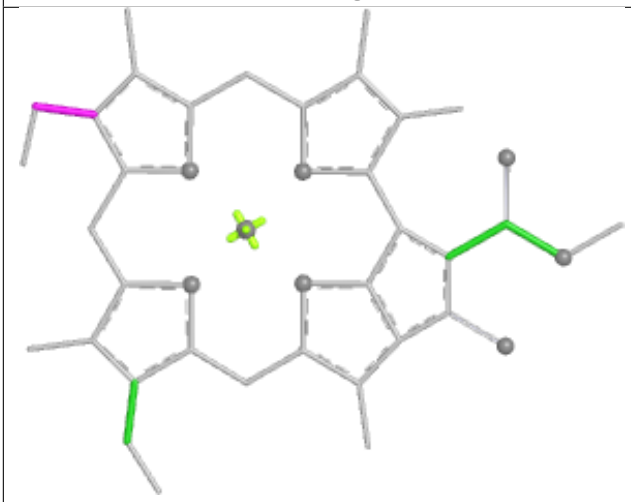
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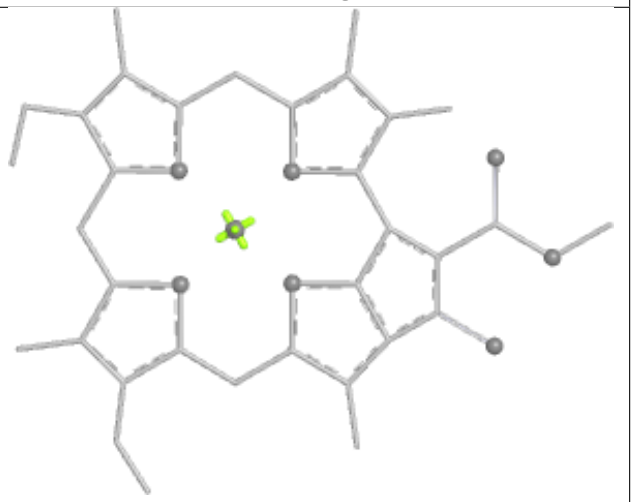
Bond lengths



Bond angles

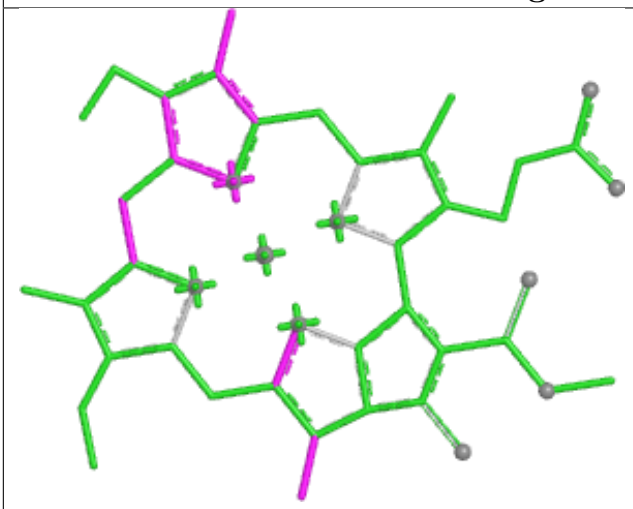


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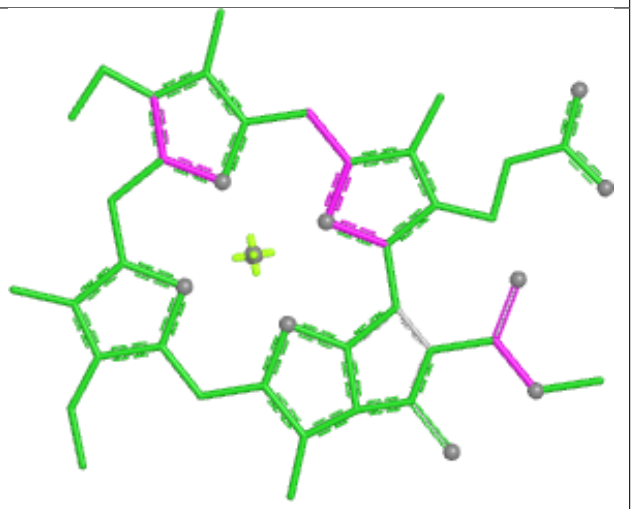


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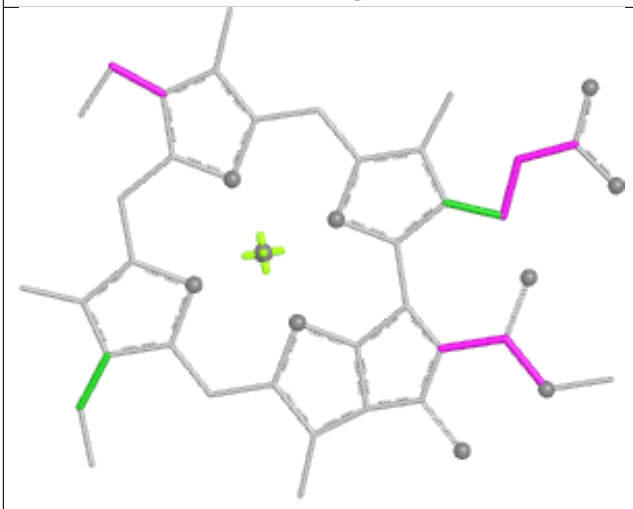
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Bond lengths



Bond angles

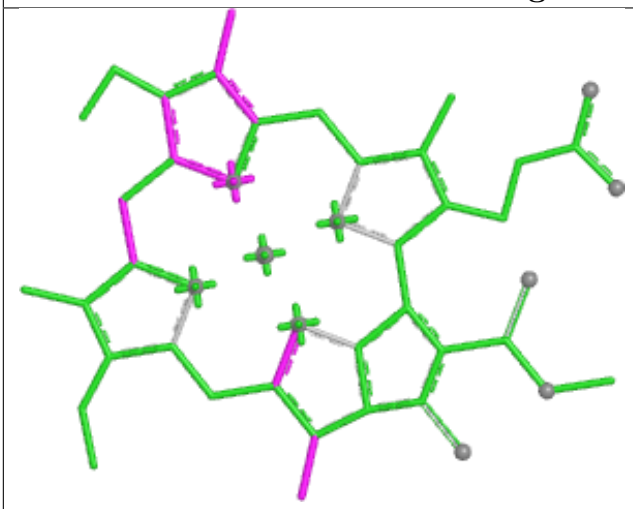


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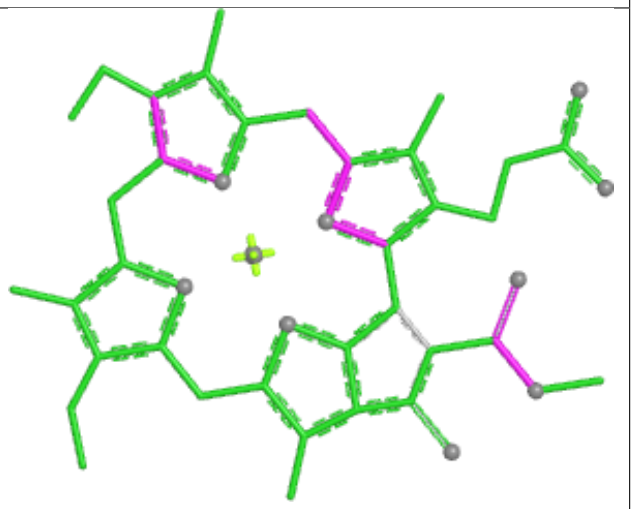


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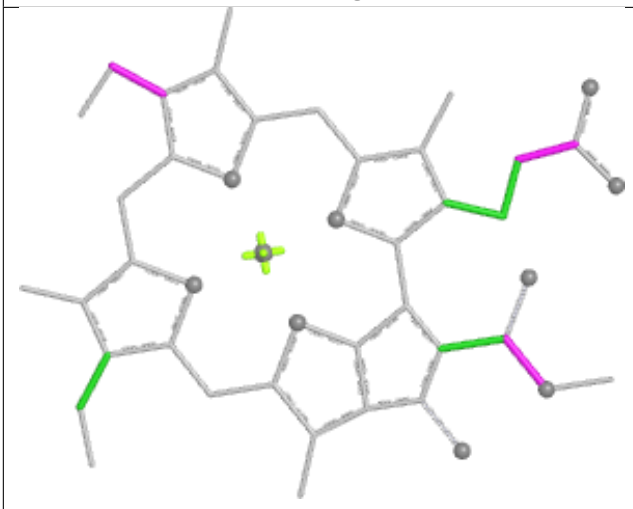
Ligand CLA 7 611



Bond lengths



Bond angles

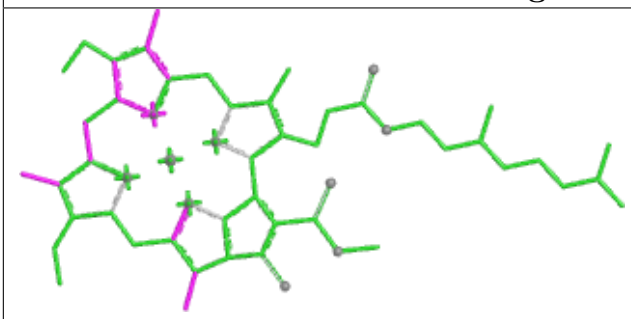


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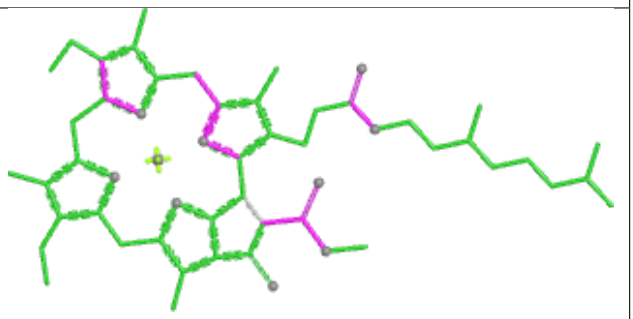


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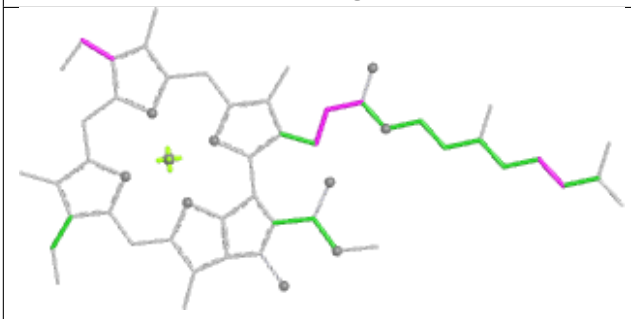
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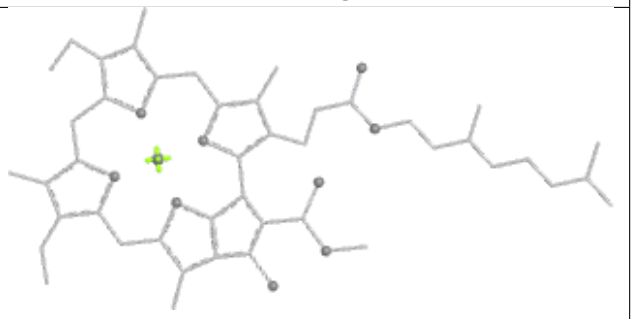
Bond lengths



Bond angles

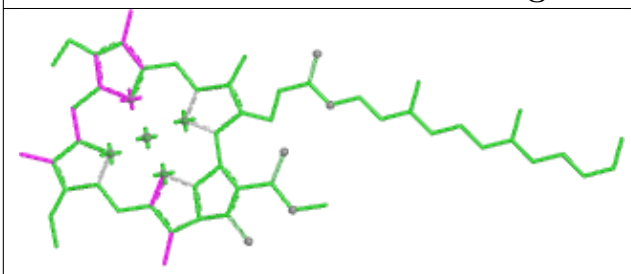


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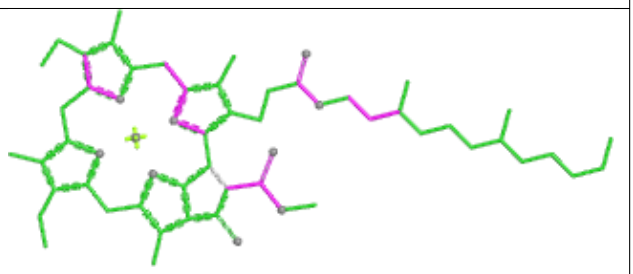


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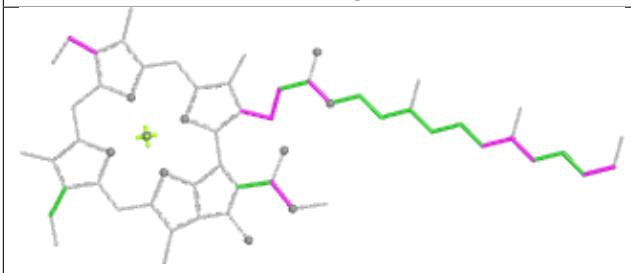
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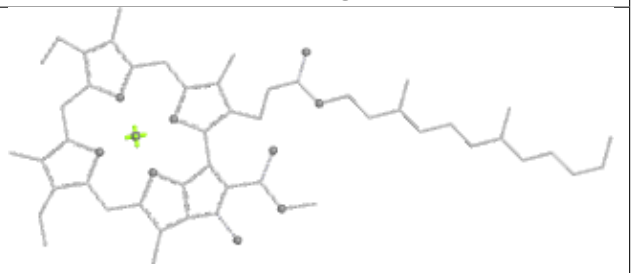
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Bond angles

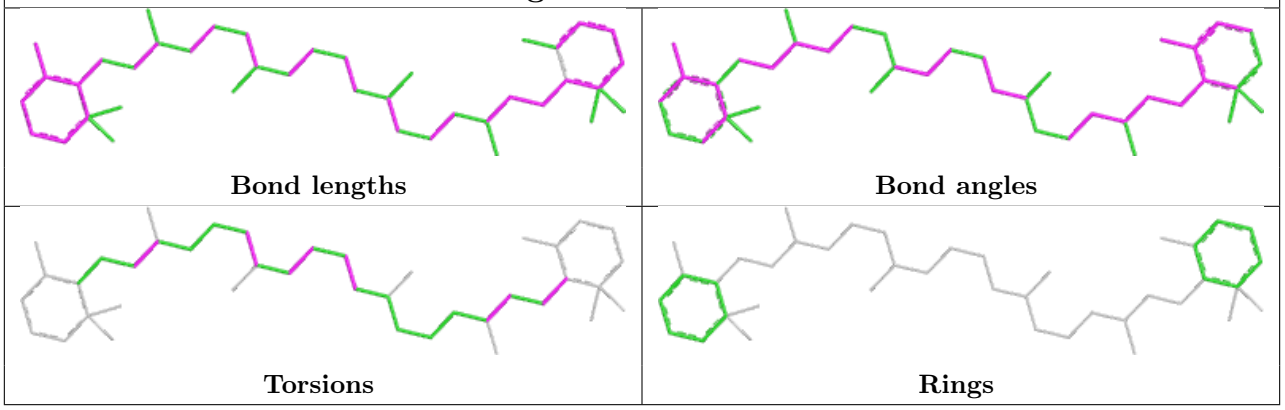


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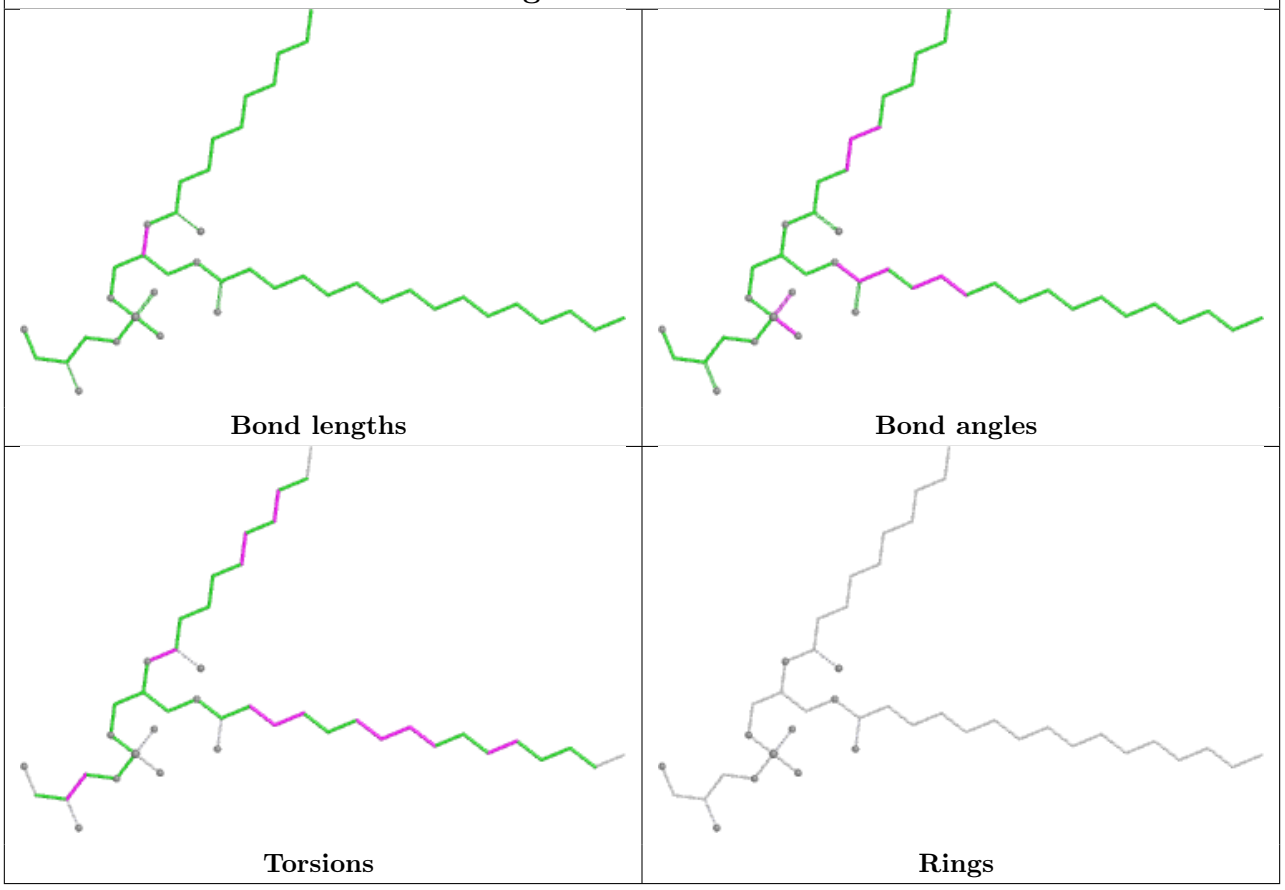


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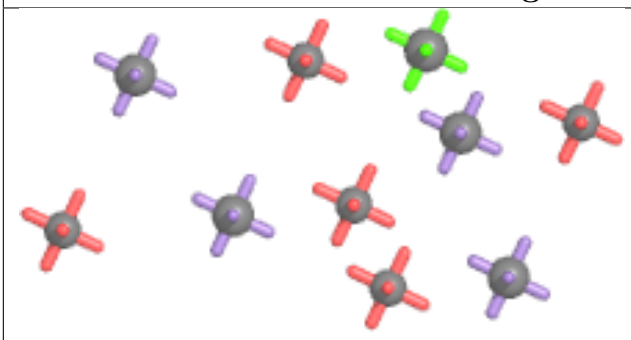
Ligand 8CT H 102



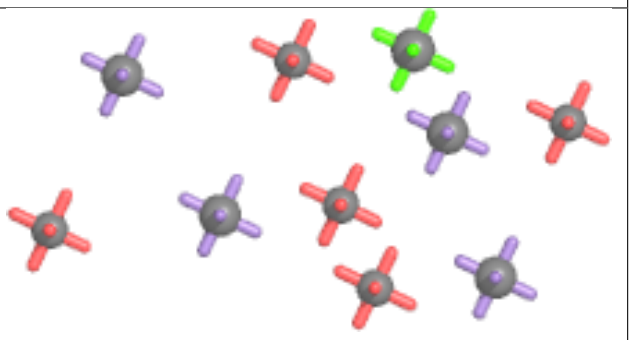
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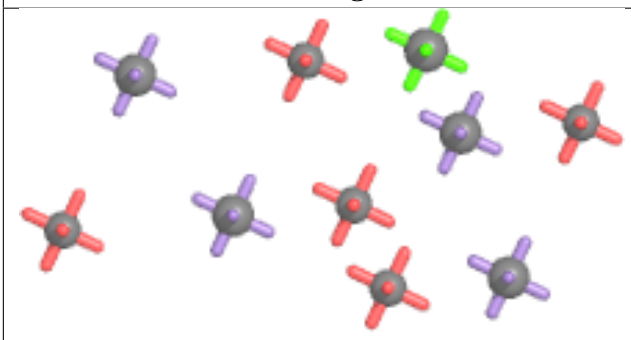
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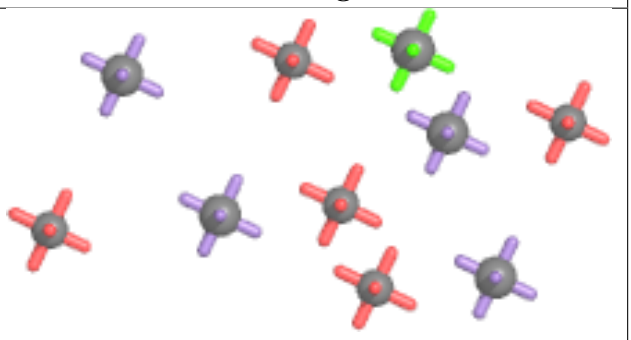
Bond lengths



Bond angles

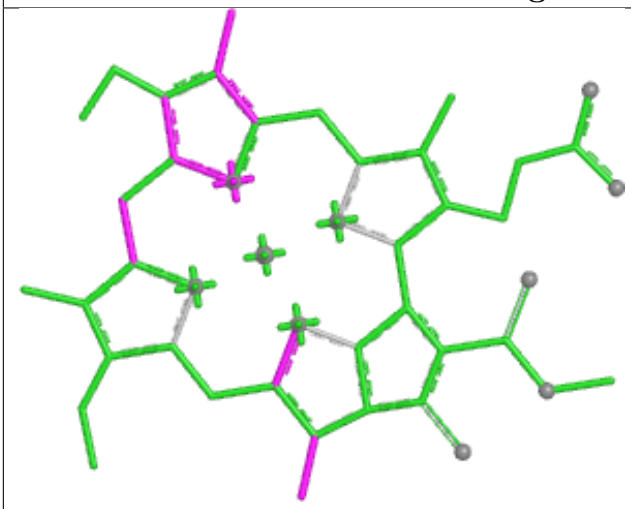


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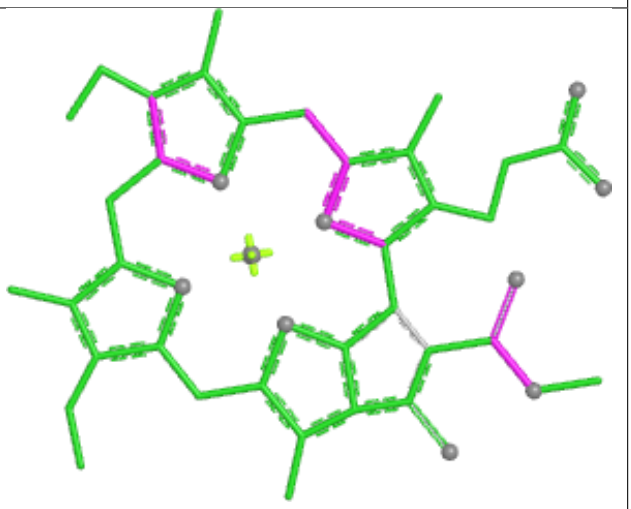


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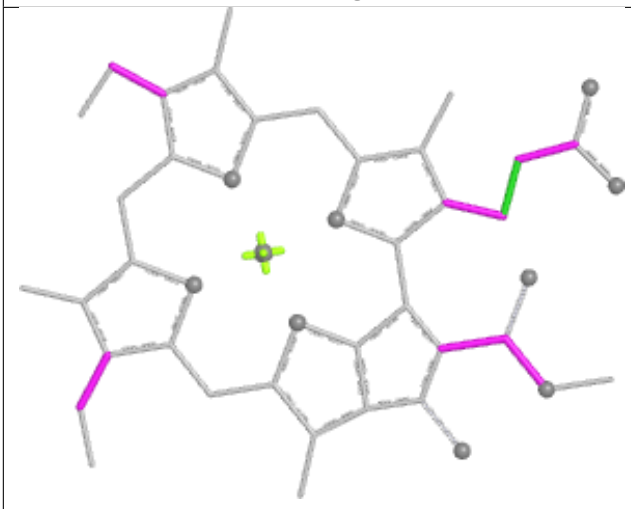
Ligand CLA 1 606



Bond lengths



Bond angles

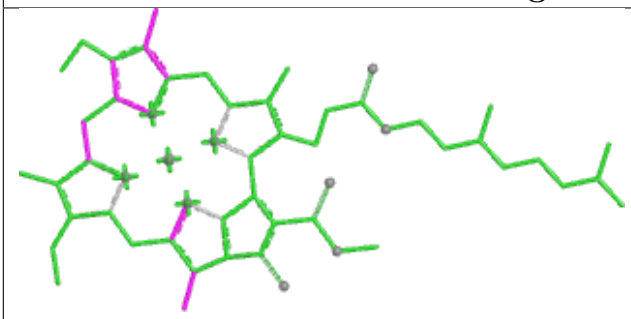


Torsions

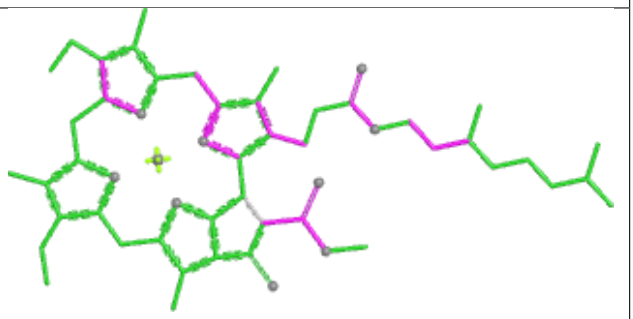


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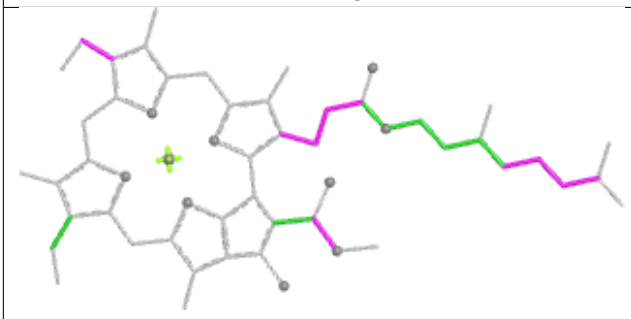
Ligand CLA 0 604



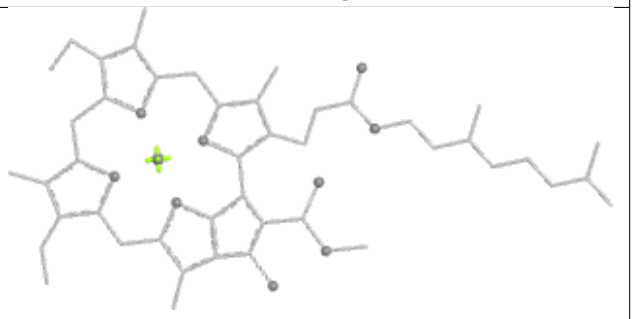
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Bond angles

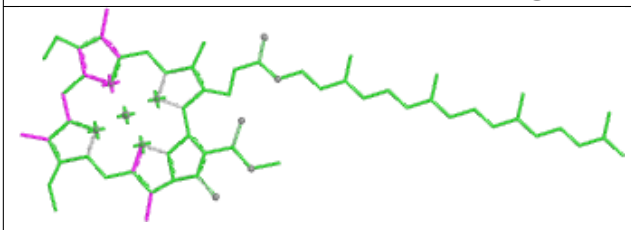


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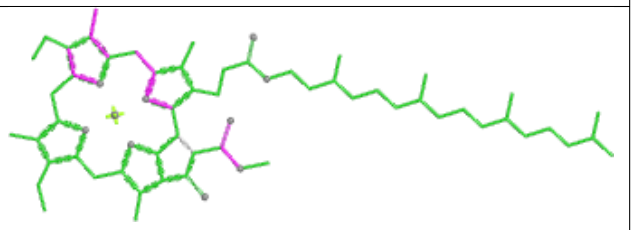


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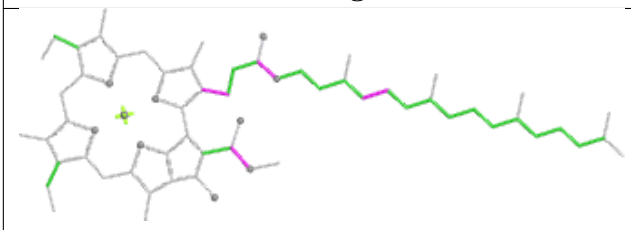
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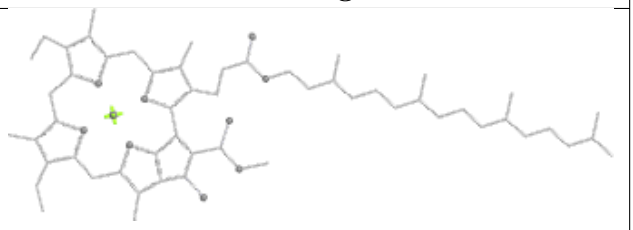
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Bond angles

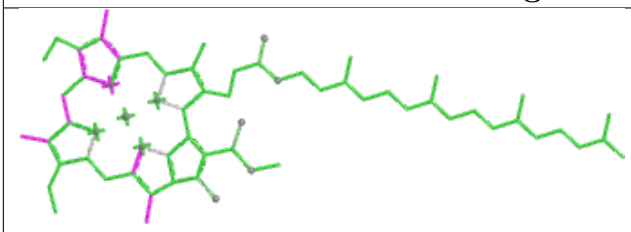


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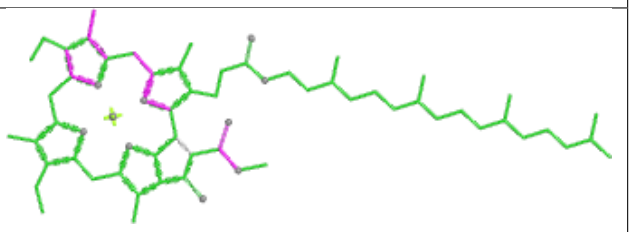


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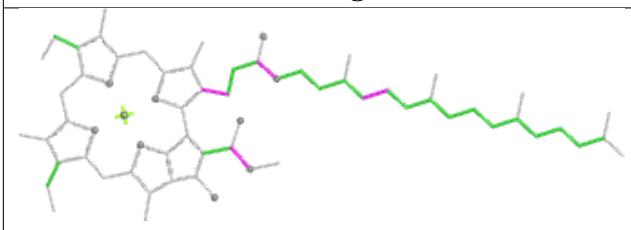
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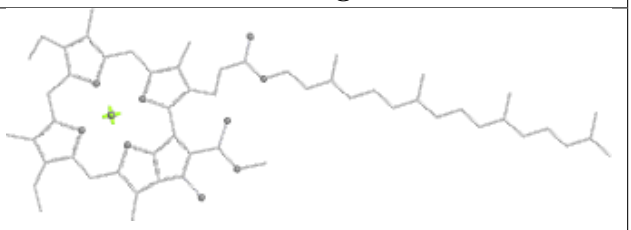
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Bond angles



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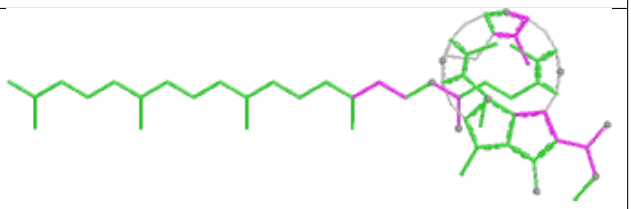


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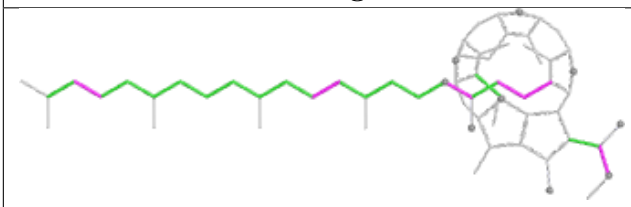
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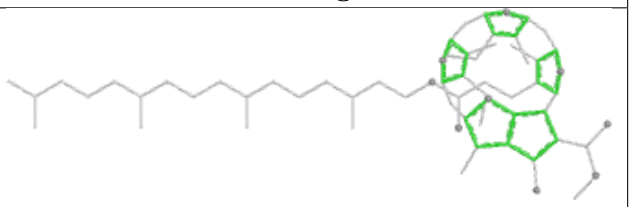
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Bond angles

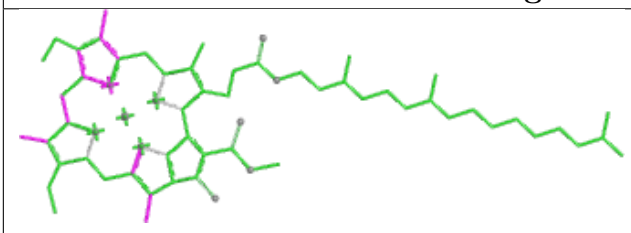


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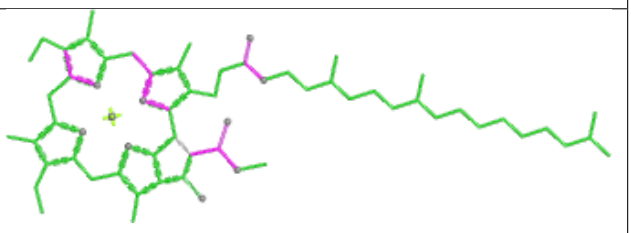


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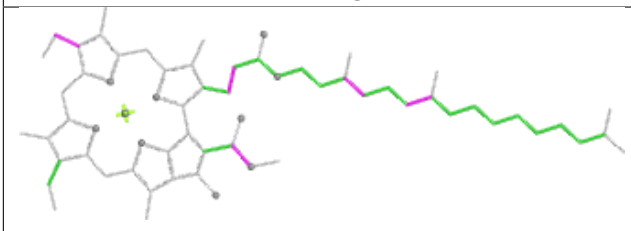
Ligand CLA B 604



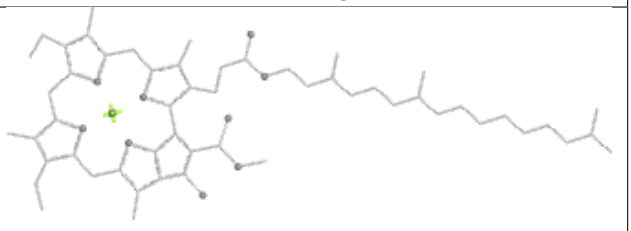
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Bond angles

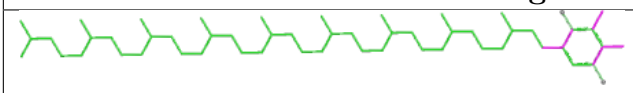


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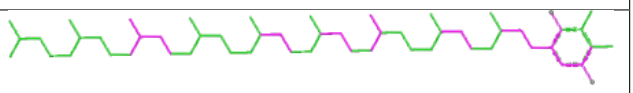


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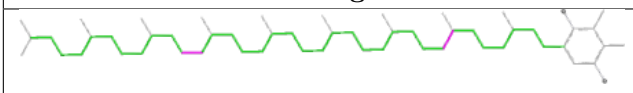
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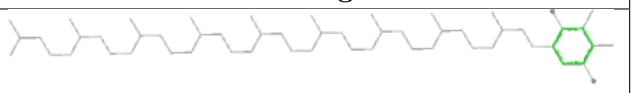
Bond lengths



Bond angles

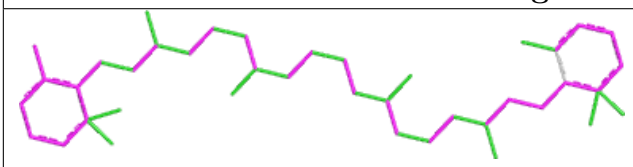


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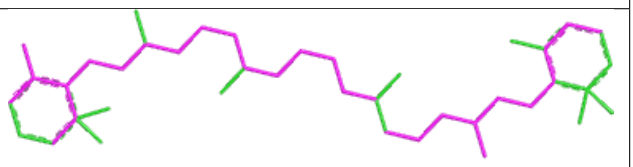


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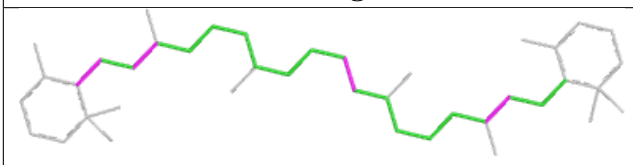
Ligand 8CT a 413



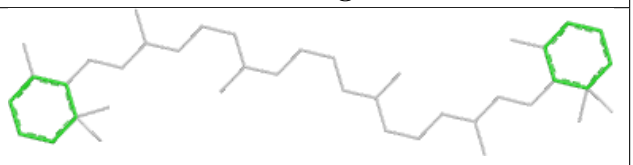
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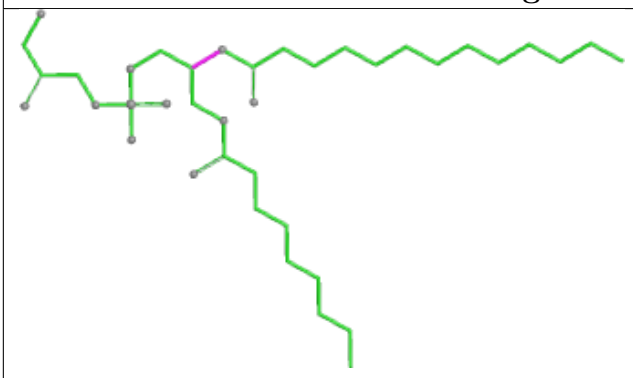


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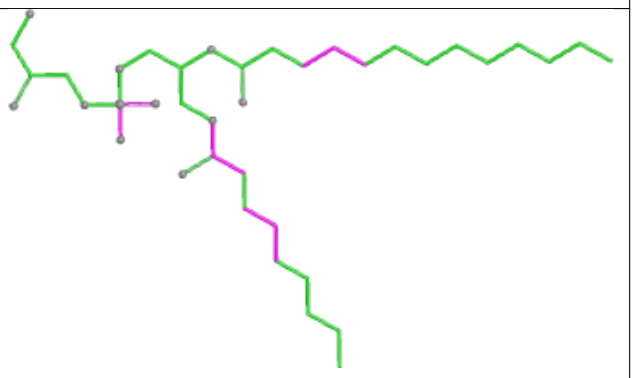


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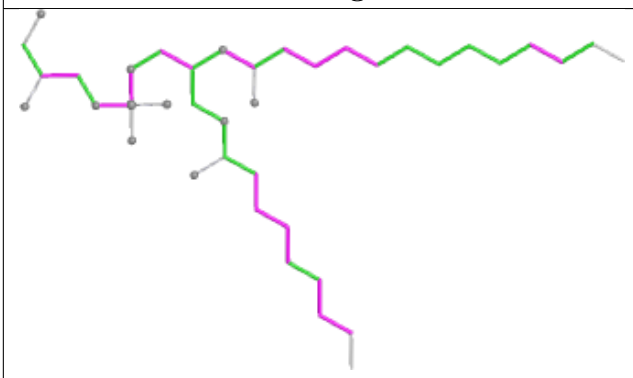
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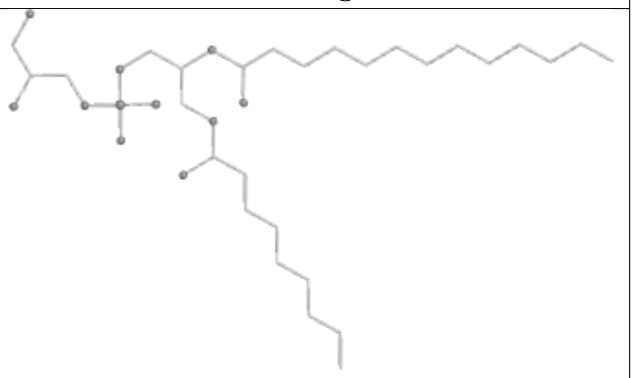
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Bond angles

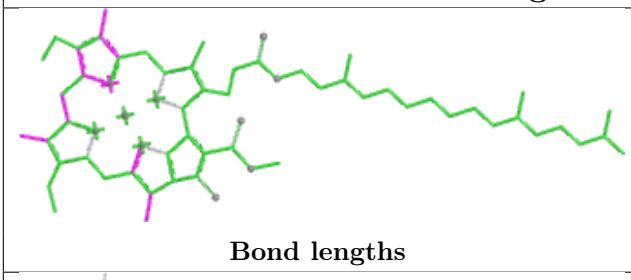


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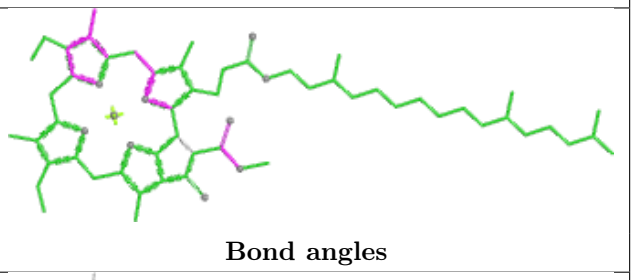


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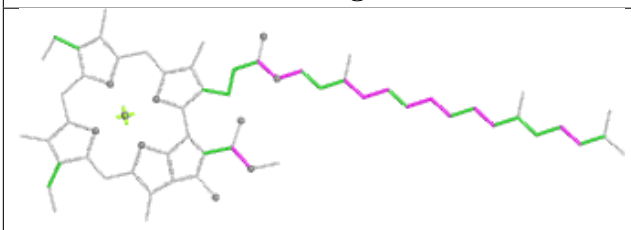
Ligand CLA c 504



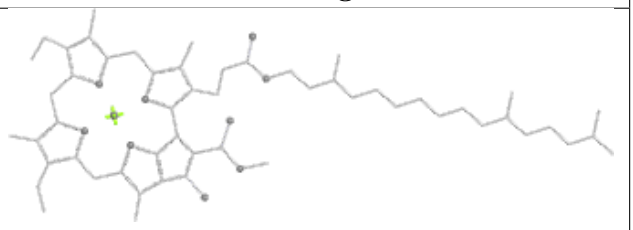
Bond lengths



Bond angles

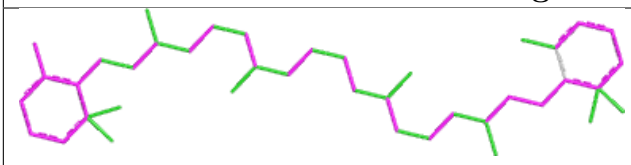


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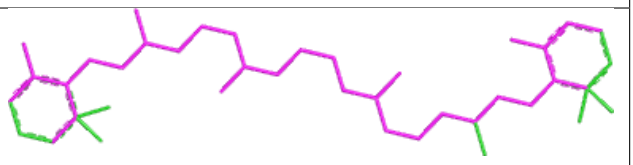


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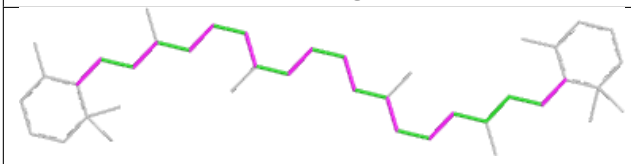
Ligand 8CT z 101



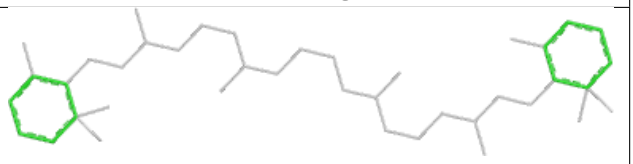
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Bond angles



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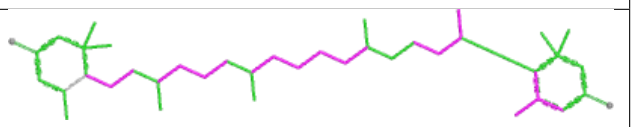


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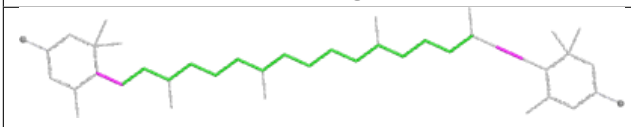
Ligand II3 7 615



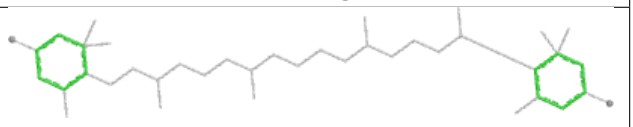
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Bond angles

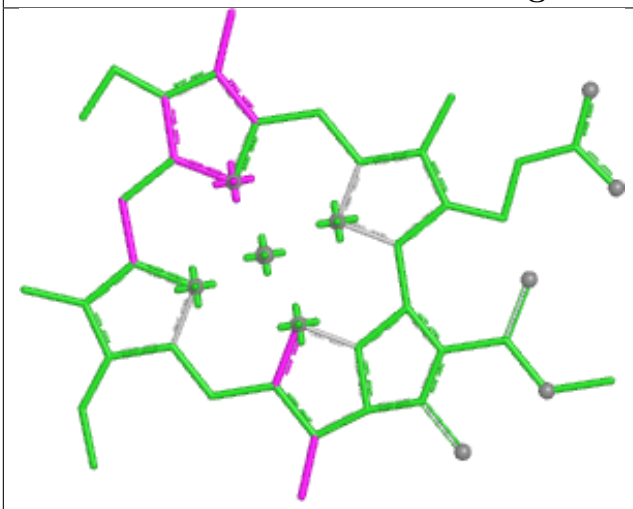


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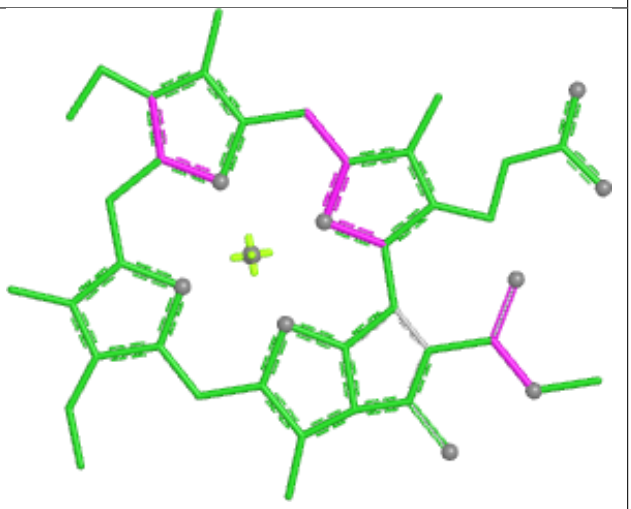


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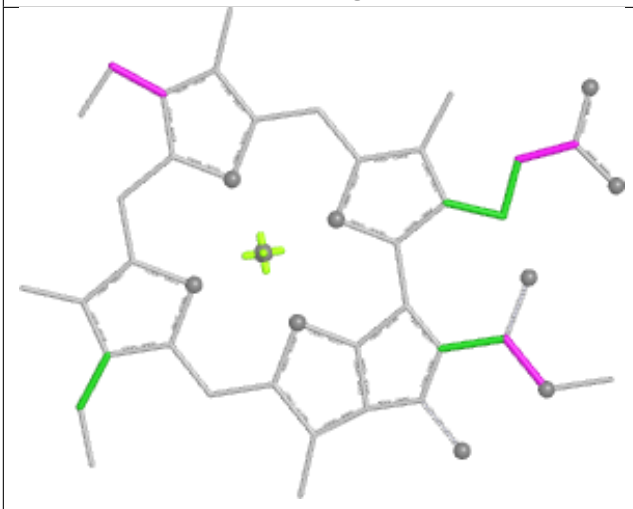
Ligand CLA 0 606



Bond lengths



Bond angles



Torsions

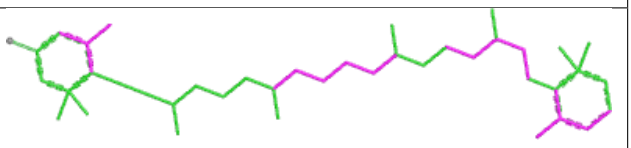


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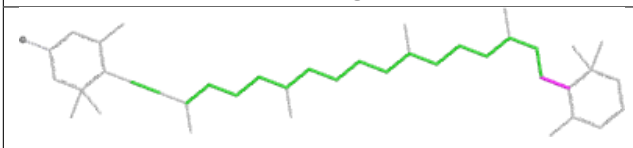
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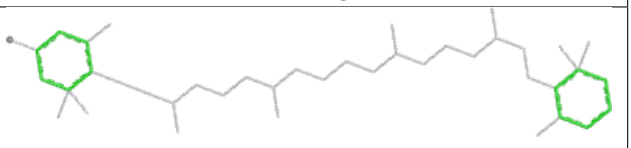
Bond lengths



Bond angles

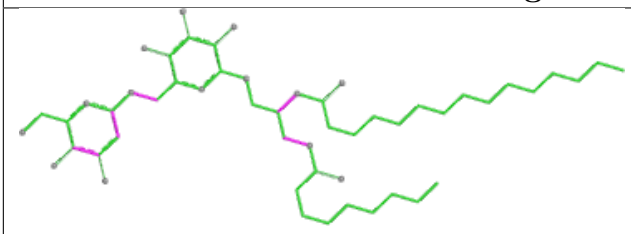


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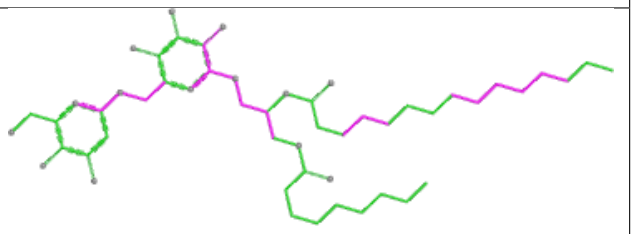


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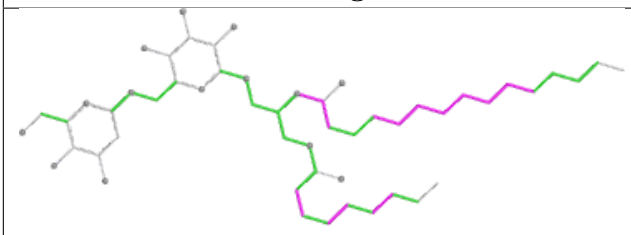
Ligand DGD a 414



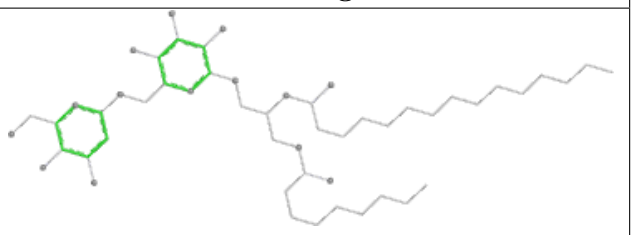
Bond lengths



Bond angles

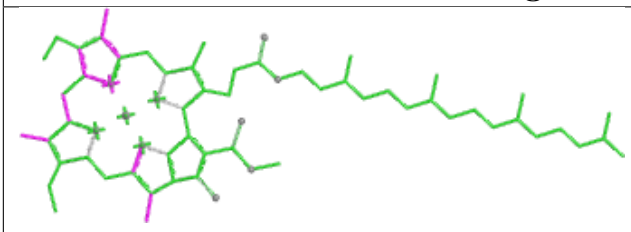


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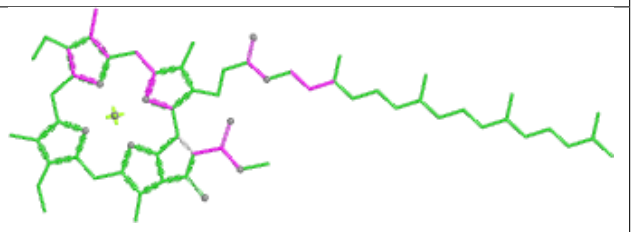


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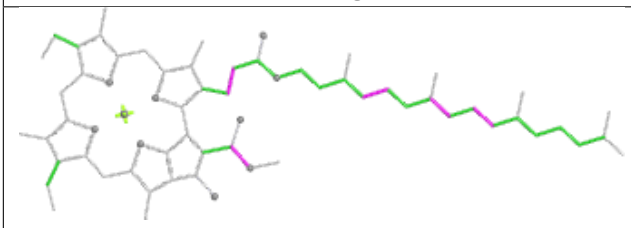
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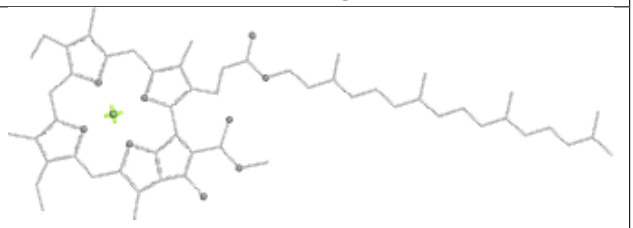
Bond lengths



Bond angles

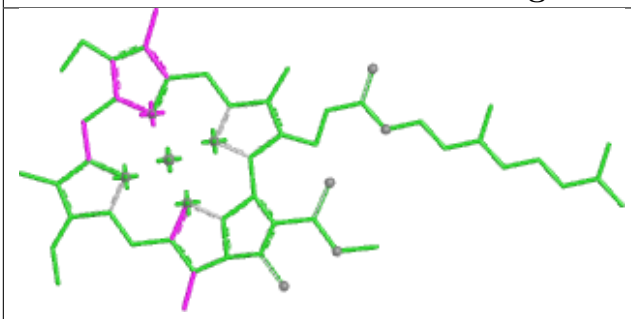


Torsions

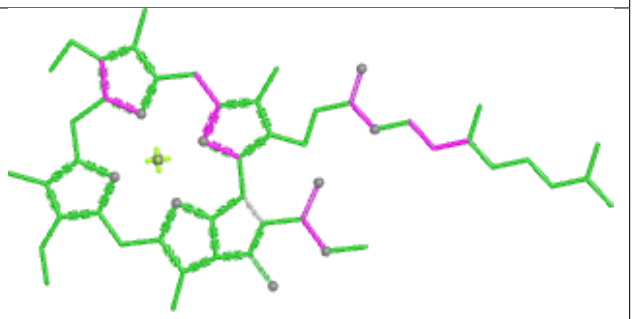


Rings

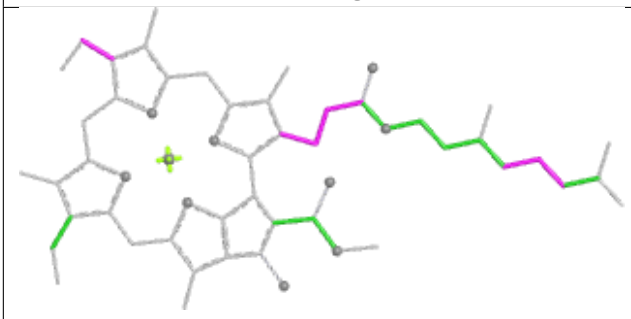
Ligand CLA 5 305



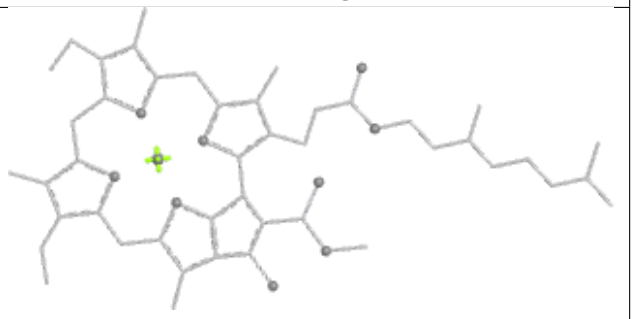
Bond lengths



Bond angles

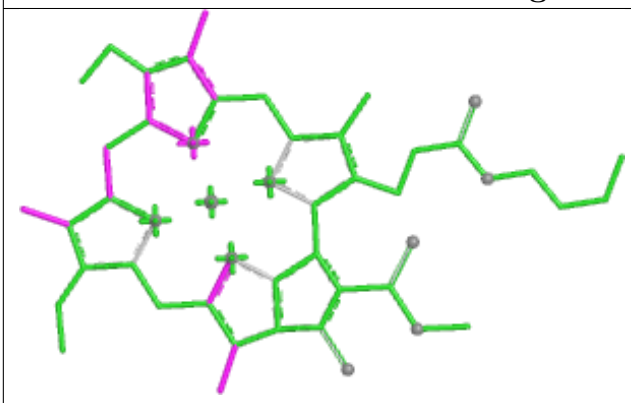


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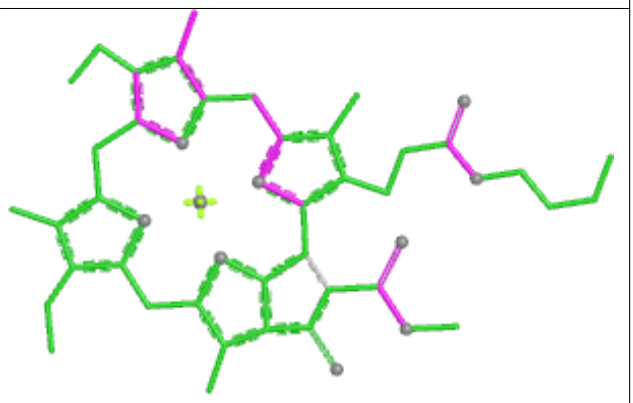


Rings

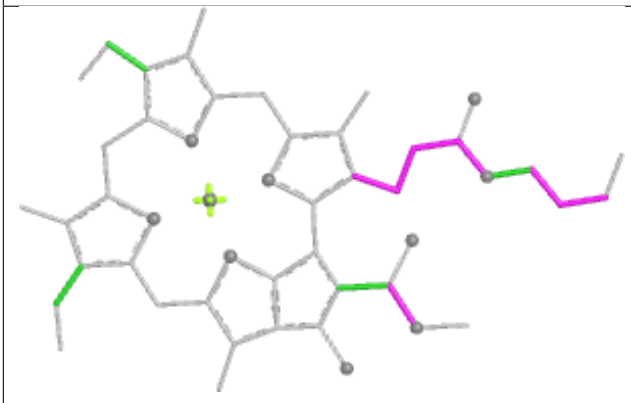
Ligand CLA c 513



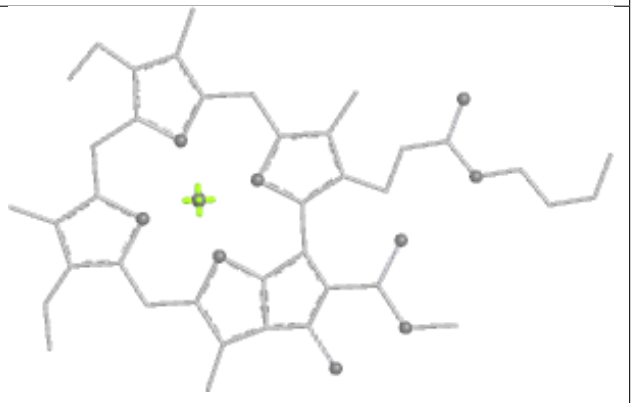
Bond lengths



Bond angles

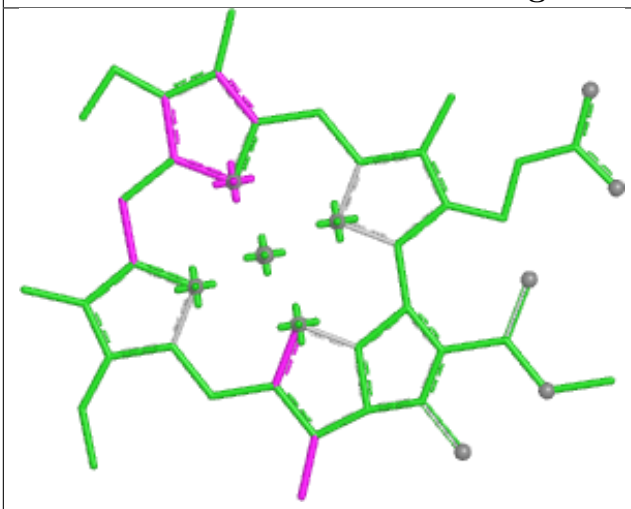


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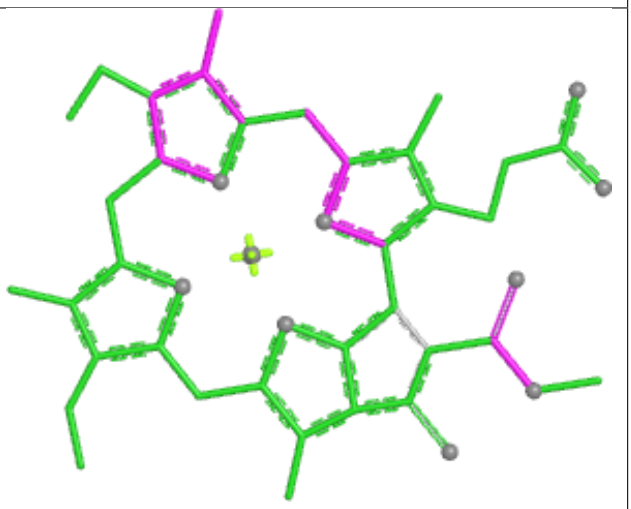


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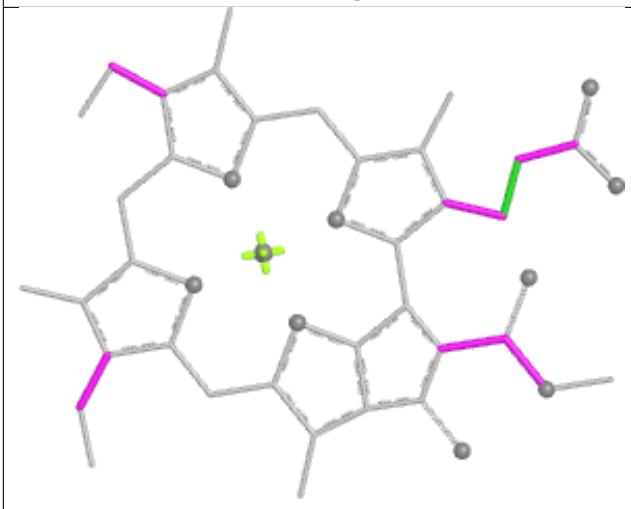
Ligand CLA 7 606



Bond lengths



Bond angles

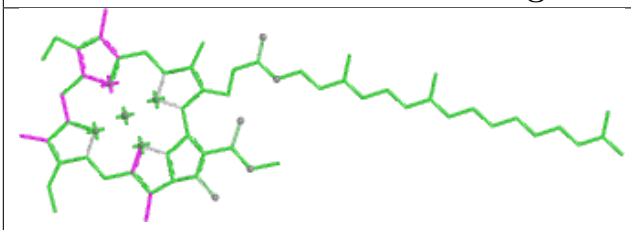


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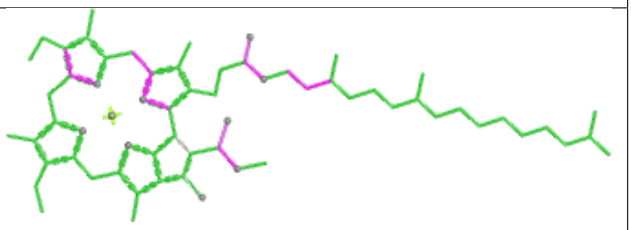


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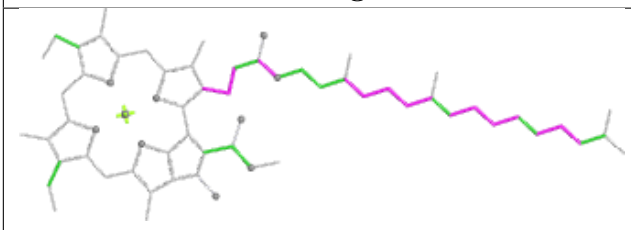
Ligand CLA b 612



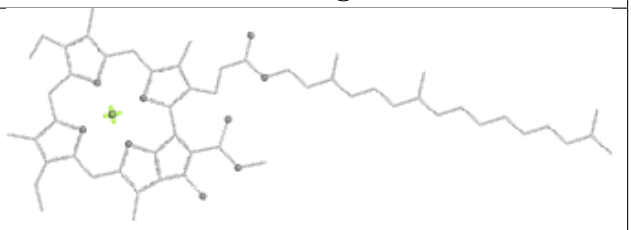
Bond lengths



Bond angles

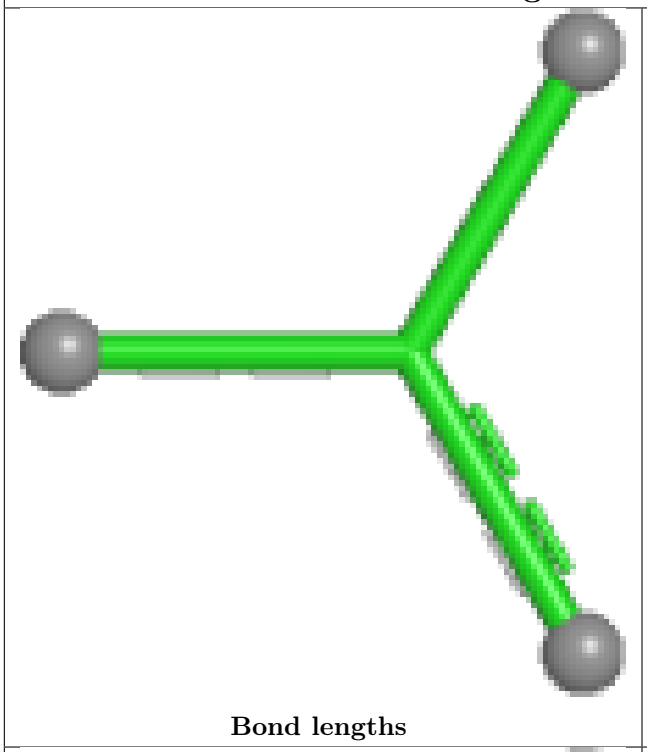


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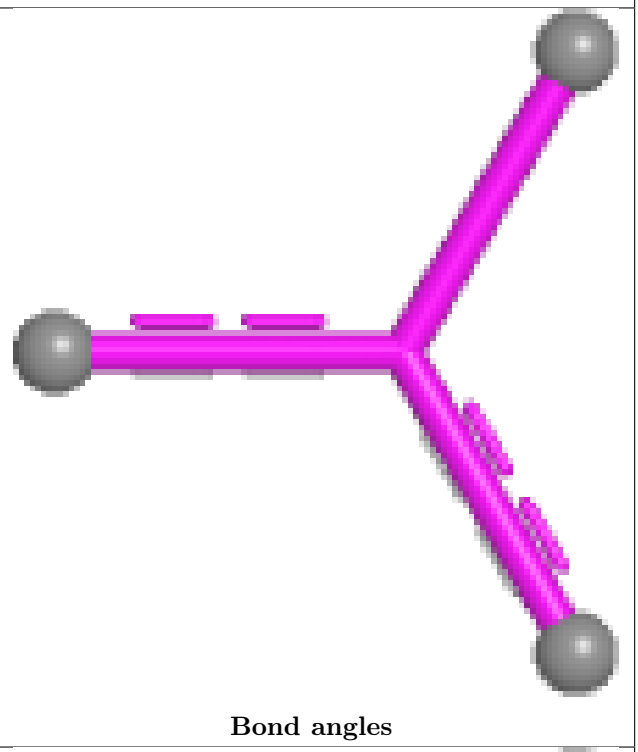


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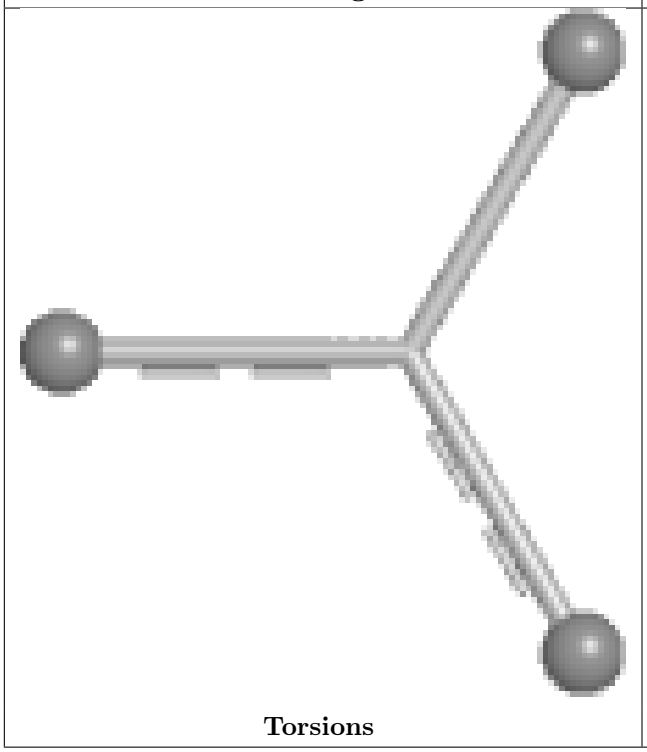
Ligand BCT A 611



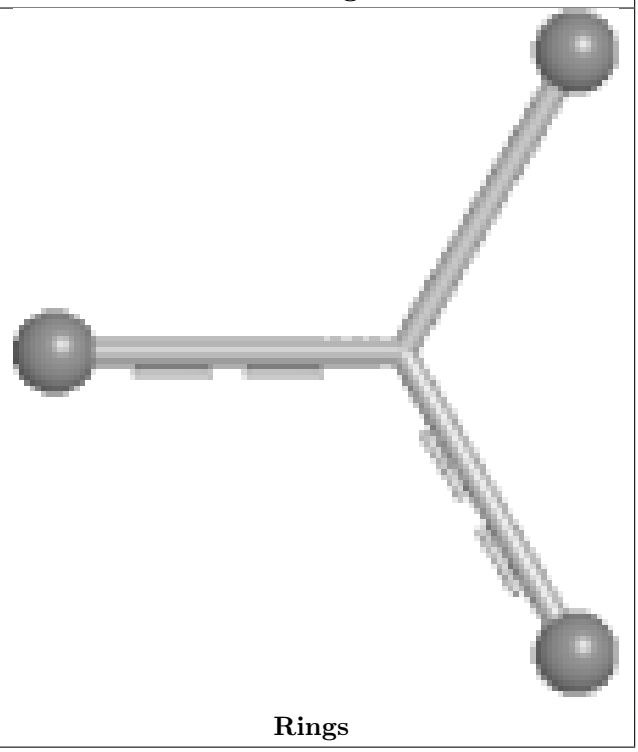
Bond lengths



Bond angles

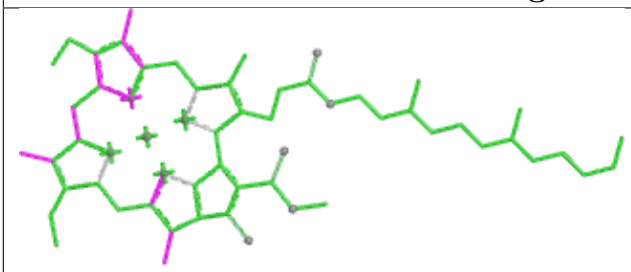


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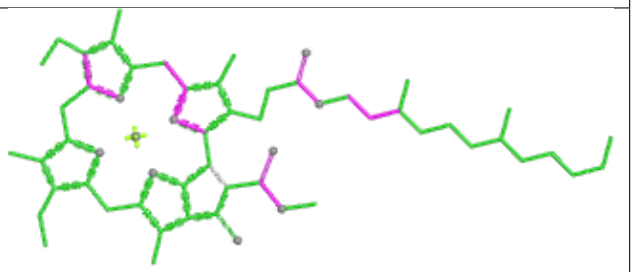


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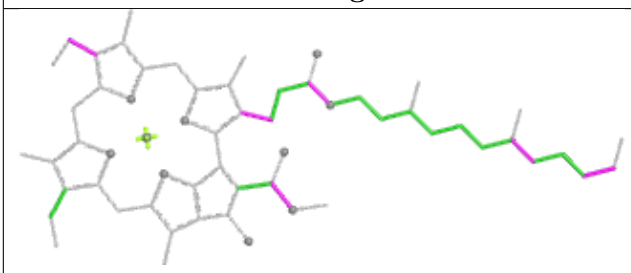
Ligand CLA 5 303



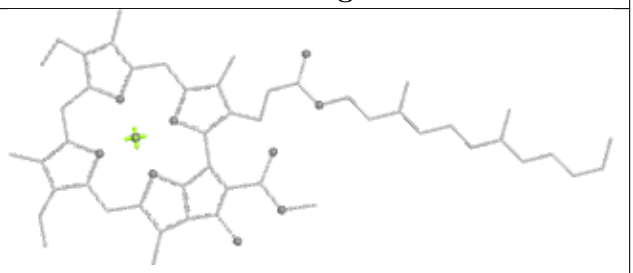
Bond lengths



Bond angles

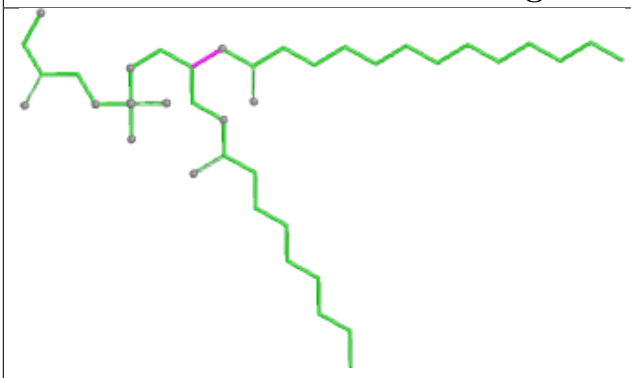


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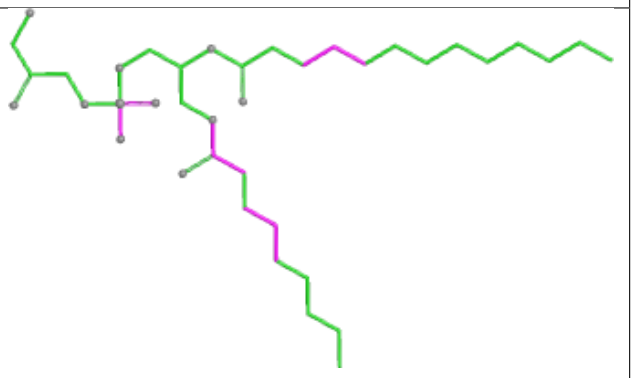


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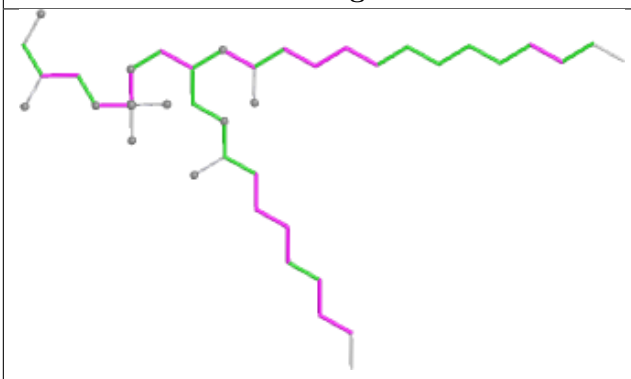
Ligand LHG b 619



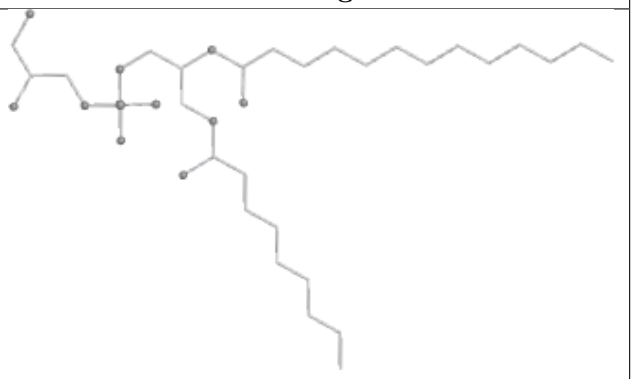
Bond lengths



Bond angles

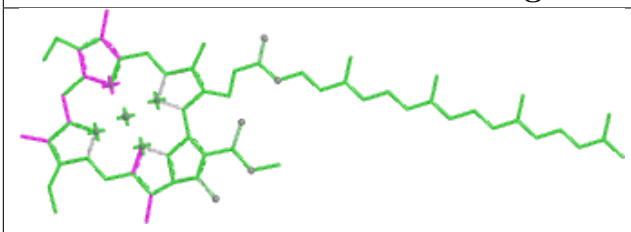


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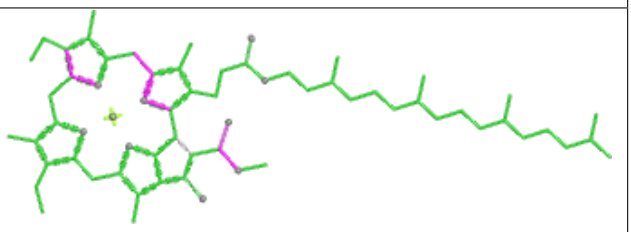


Rings

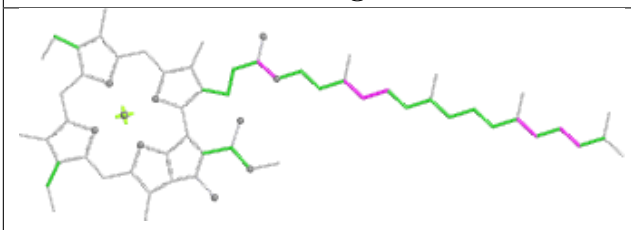
Ligand CLA C 511



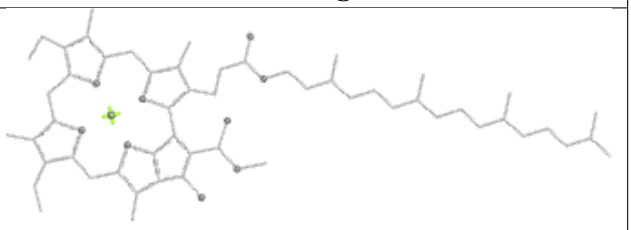
Bond lengths



Bond angles

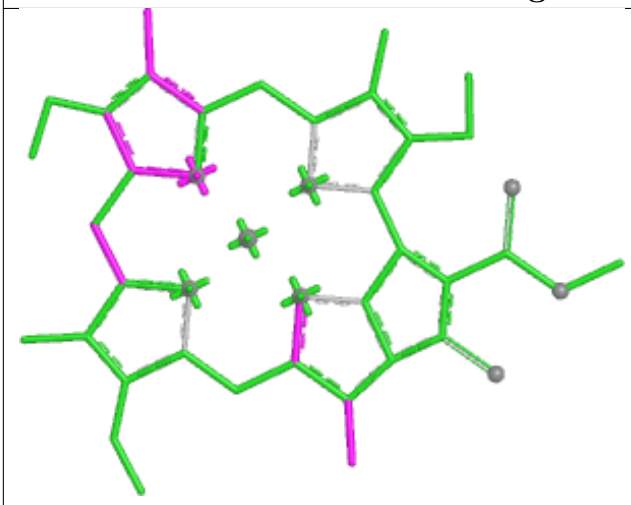


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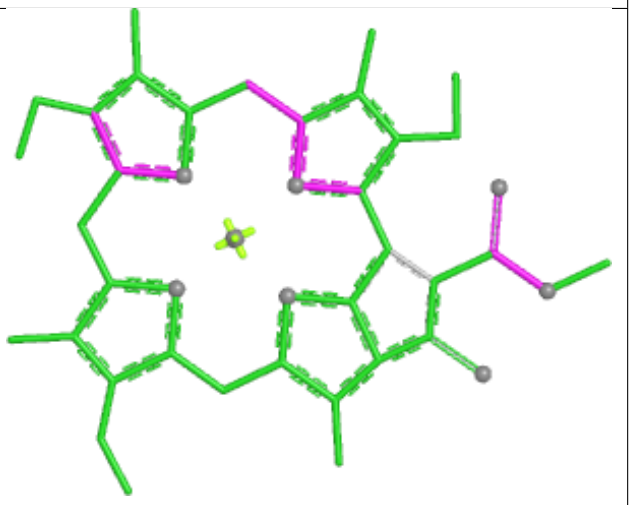


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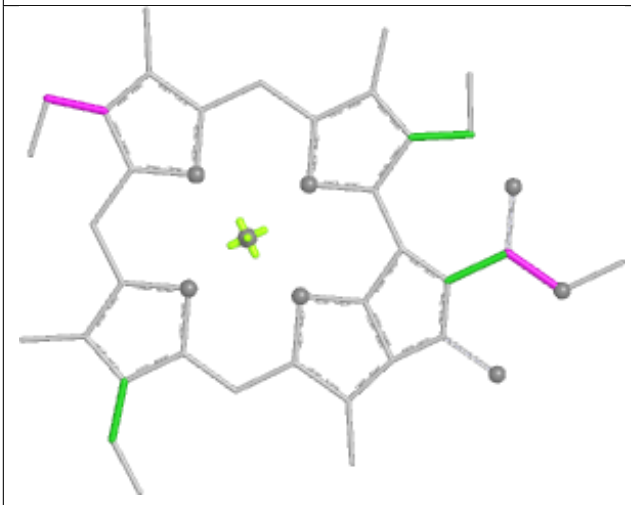
Ligand CLA 4 601



Bond lengths



Bond angles



Torsions

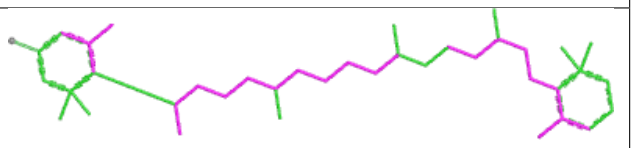


Rings

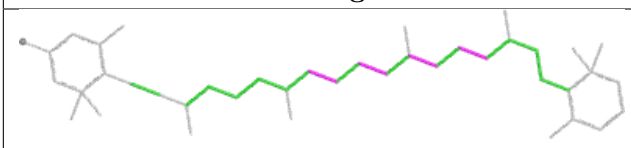
Ligand IHT 0 618



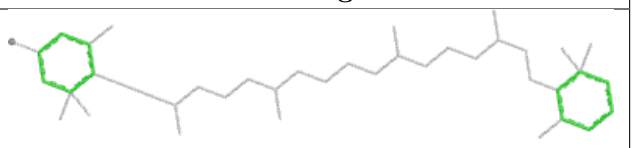
Bond lengths



Bond angles

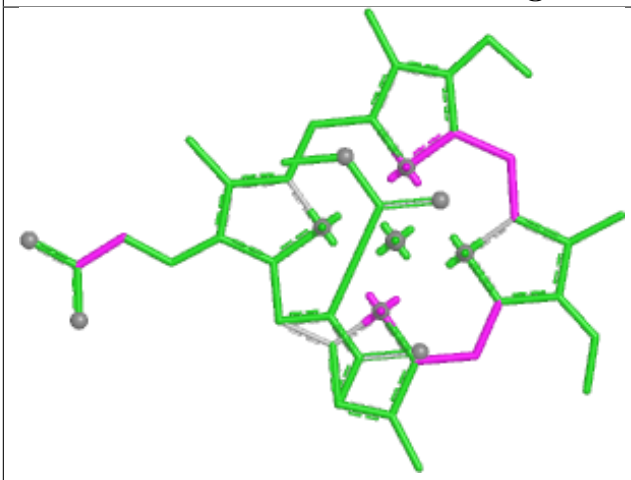


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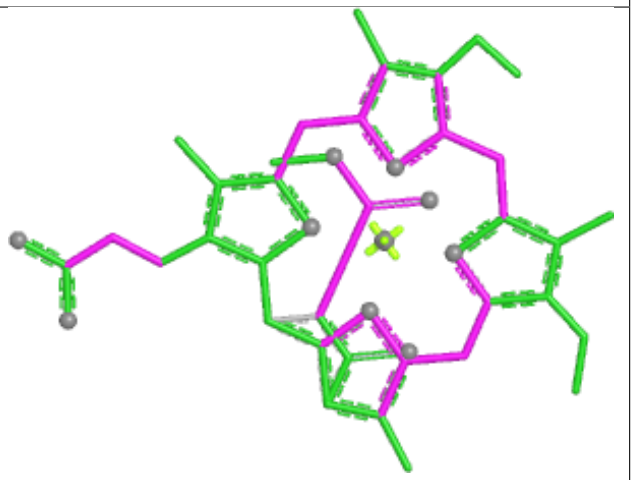


Rings

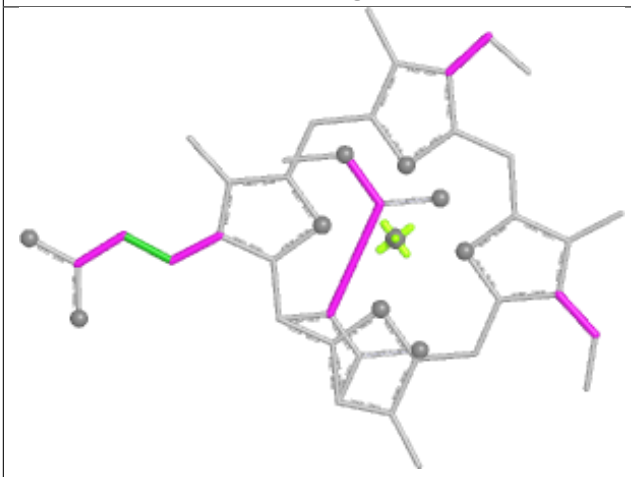
Ligand KC2 P 605



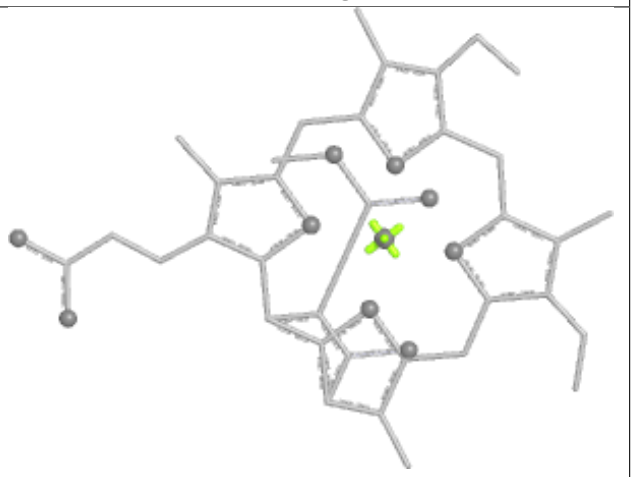
Bond lengths



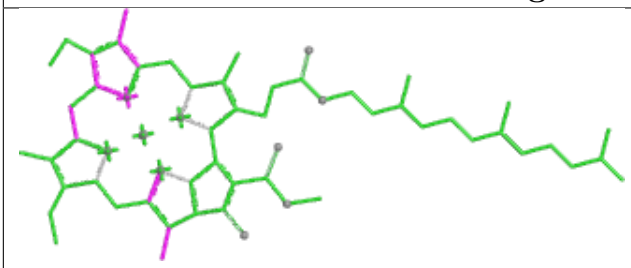
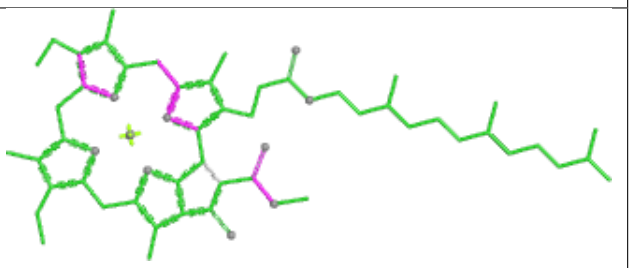
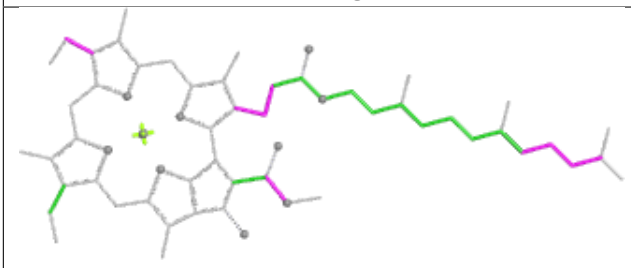
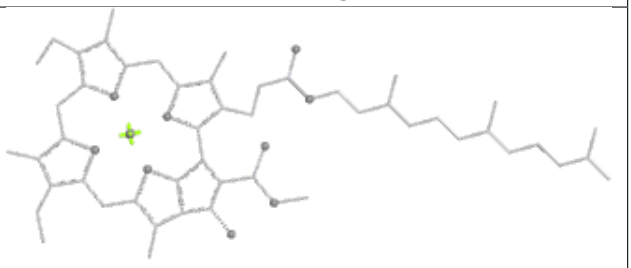
Bond angles

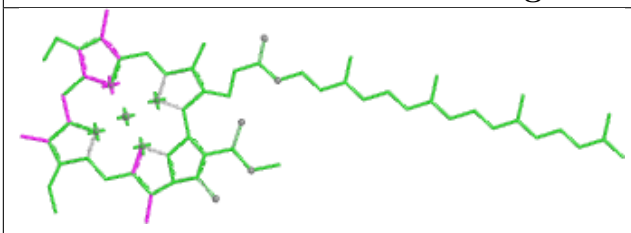
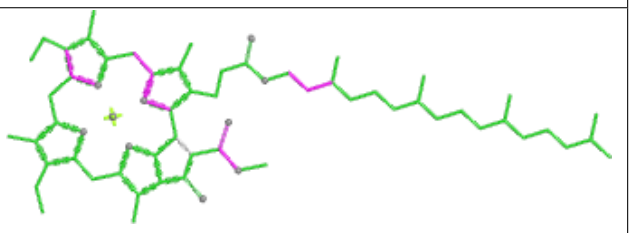
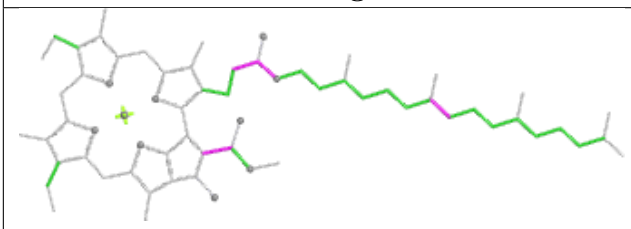
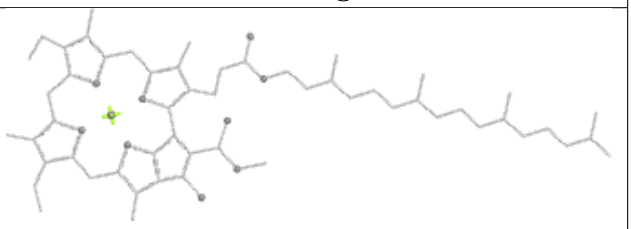


Torsions

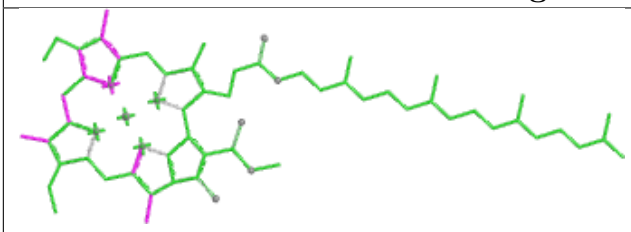


Rings

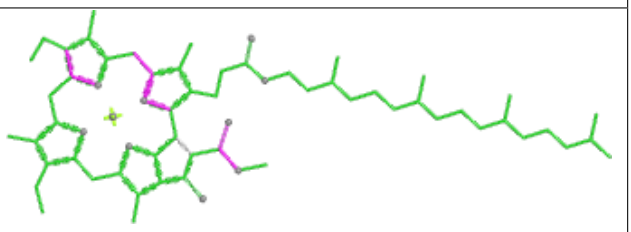
Ligand CLA 7 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

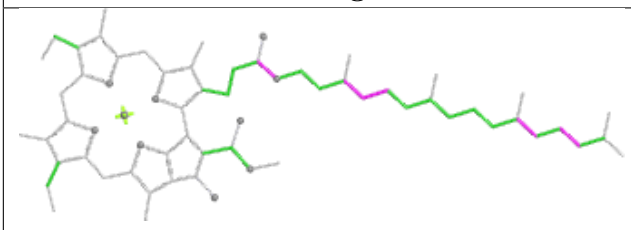
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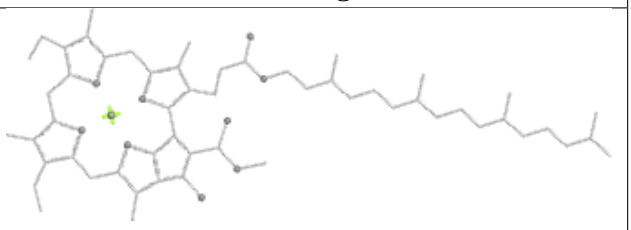
Bond lengths



Bond angles

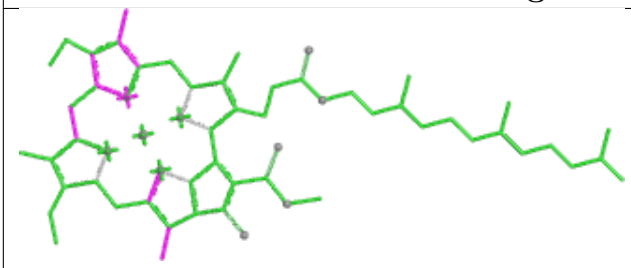


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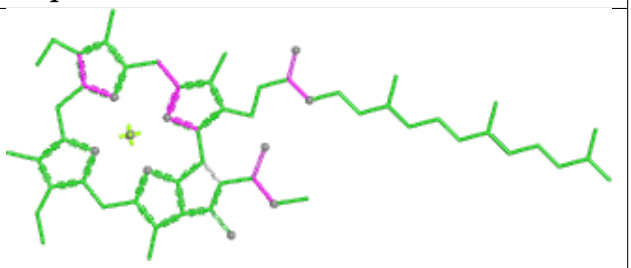


Rings

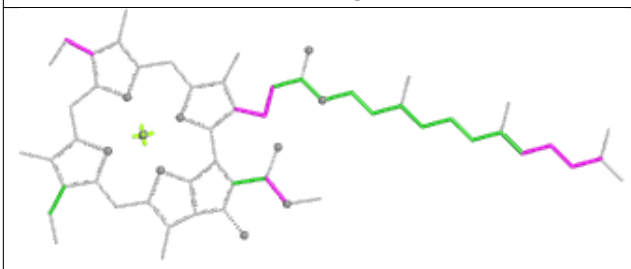
Ligand CLA p 309



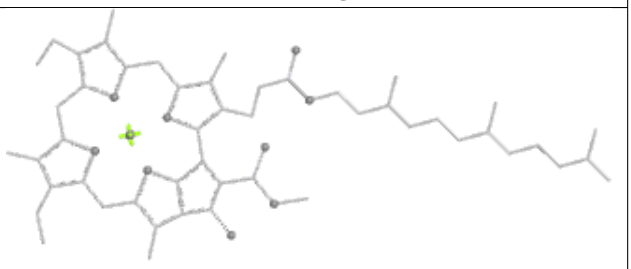
Bond lengths



Bond angles

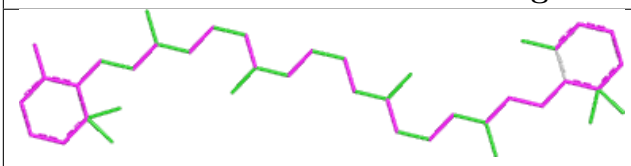


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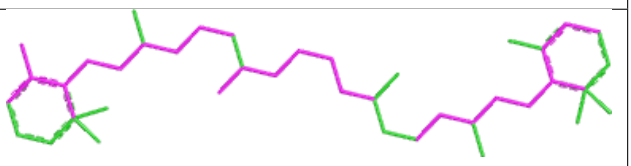


Rings

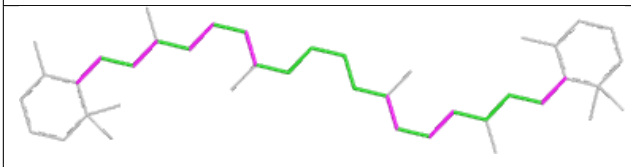
Ligand 8CT 9 615



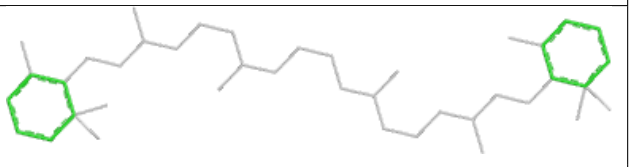
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Bond angles

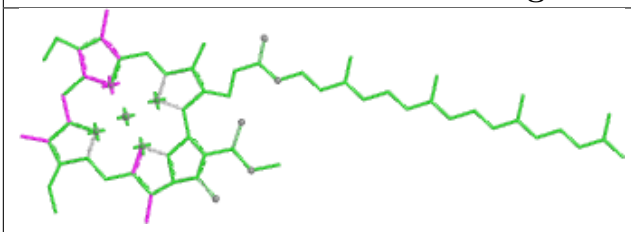


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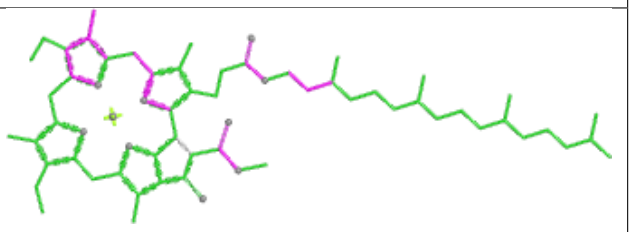


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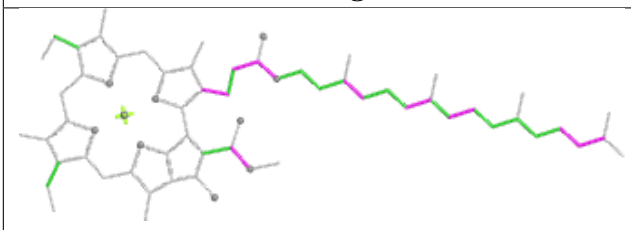
Ligand CLA b 613



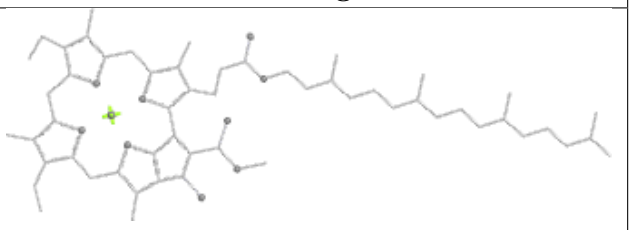
Bond lengths



Bond angles

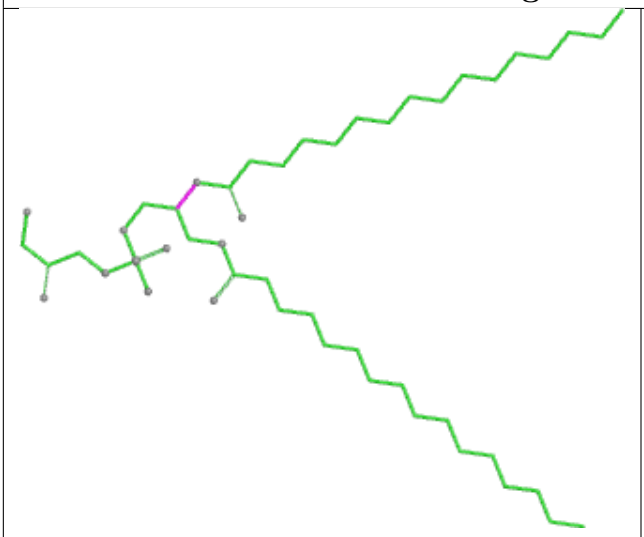


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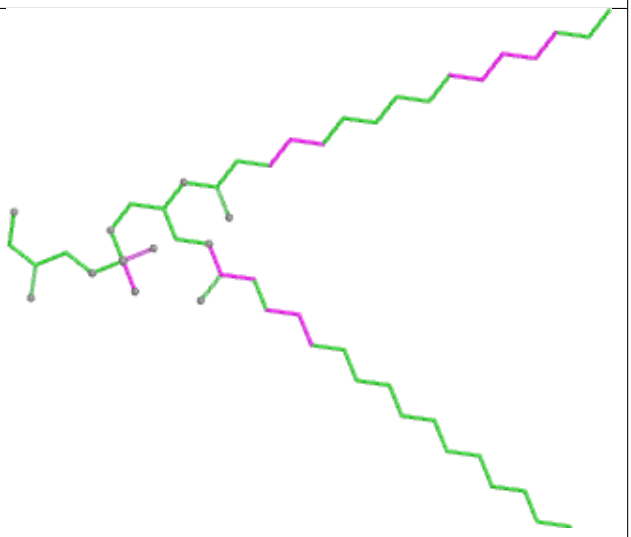


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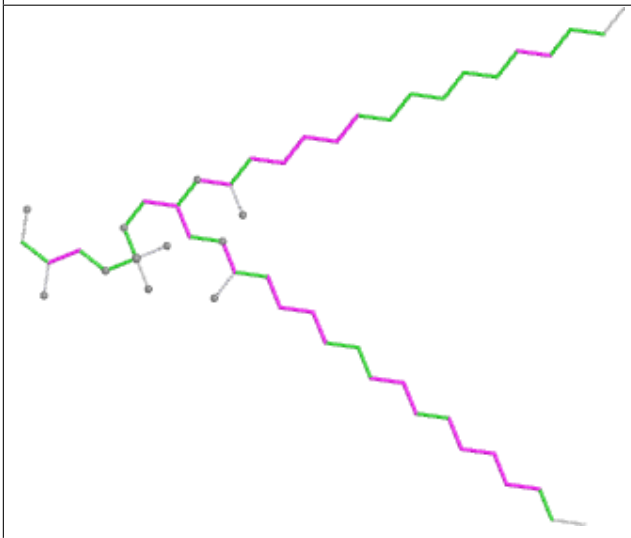
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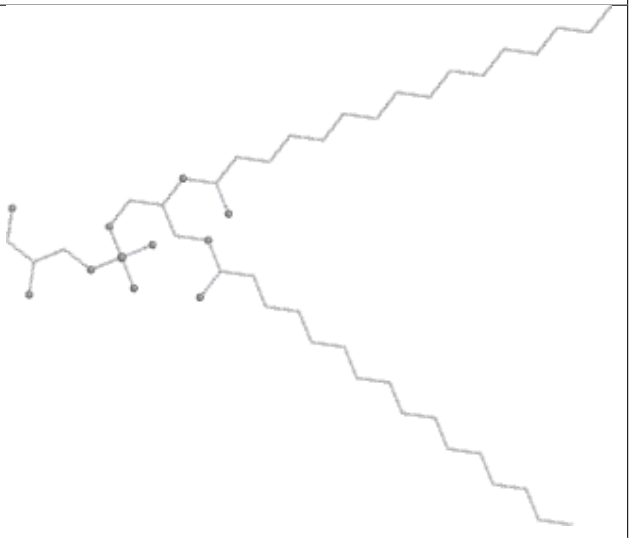
Bond lengths



Bond angles

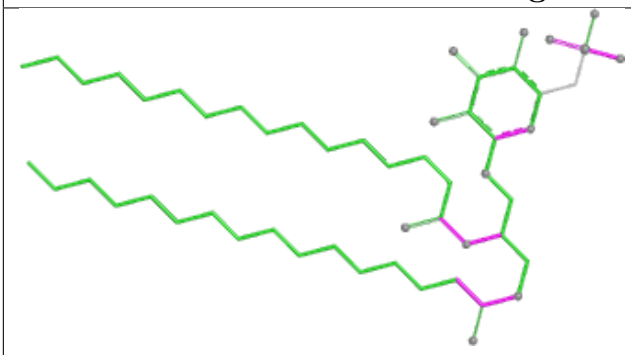


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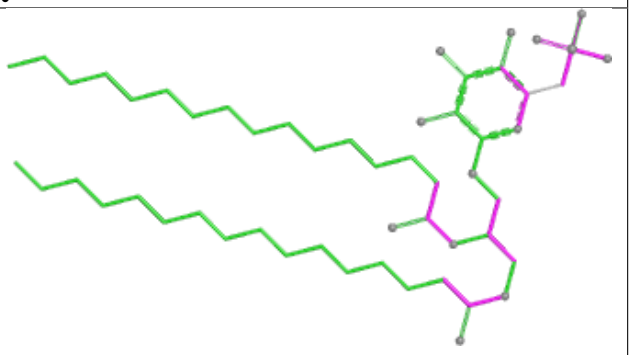


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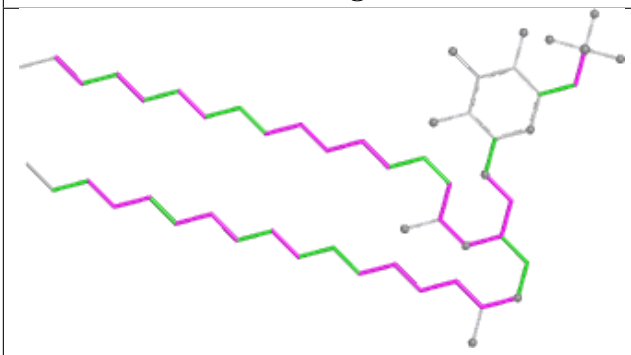
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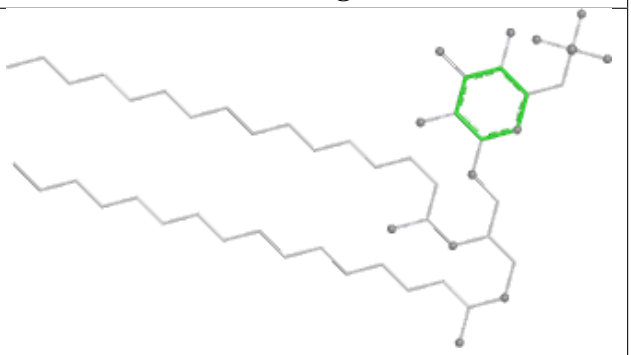
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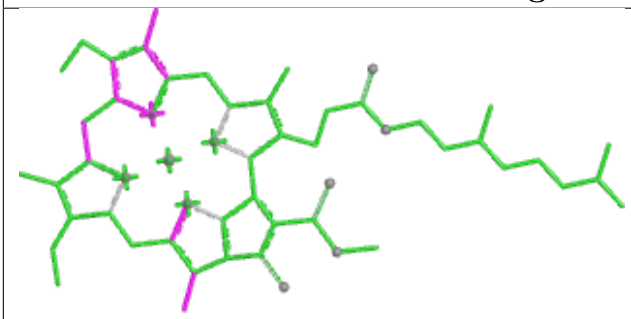


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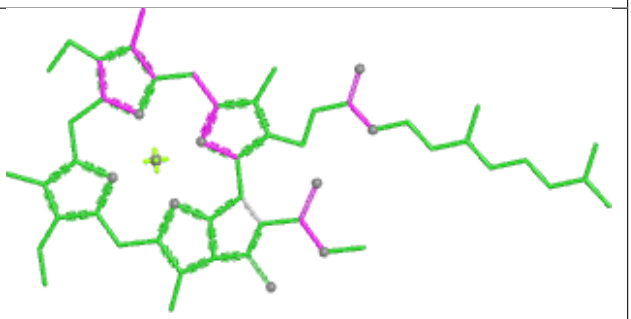


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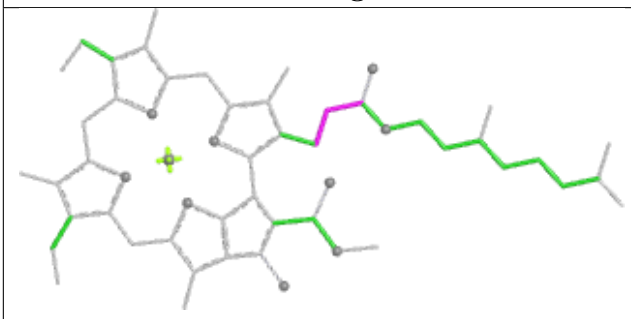
Ligand CLA 2 604



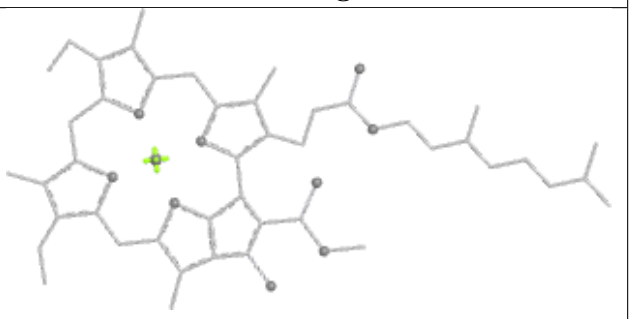
Bond lengths



Bond angles

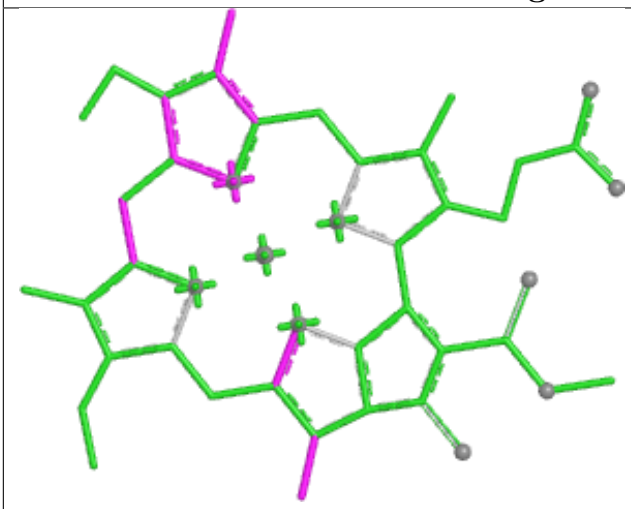


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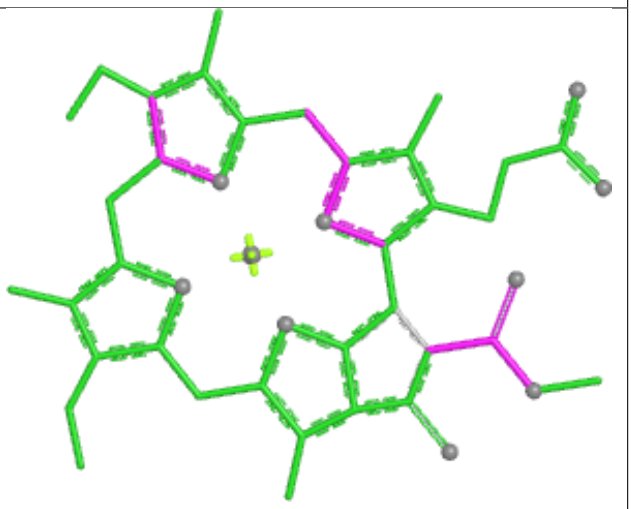


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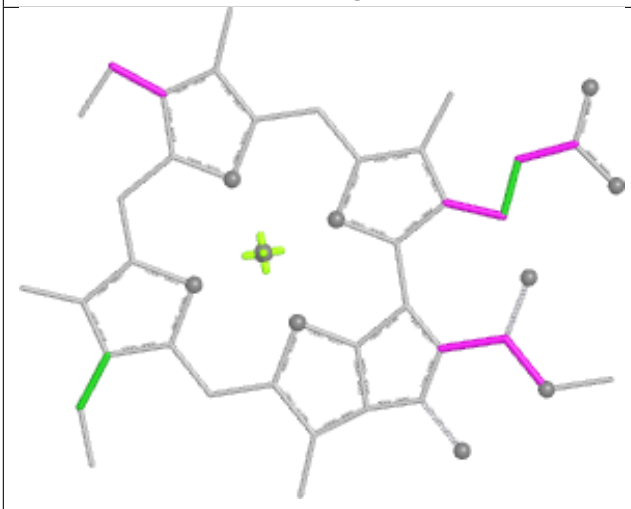
Ligand CLA 0 612



Bond lengths



Bond angles

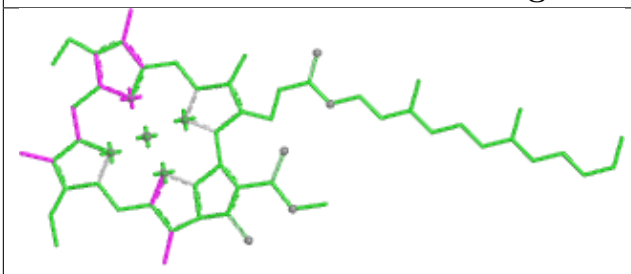


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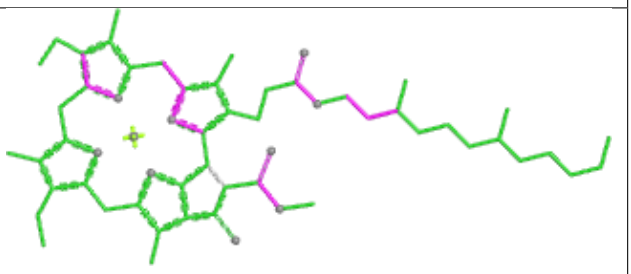


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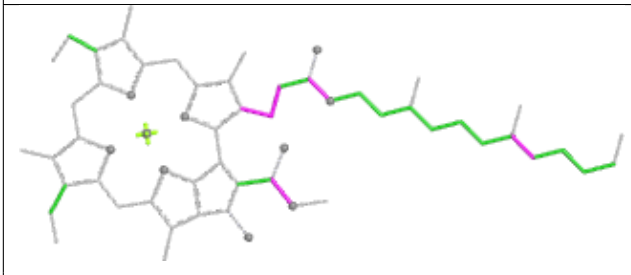
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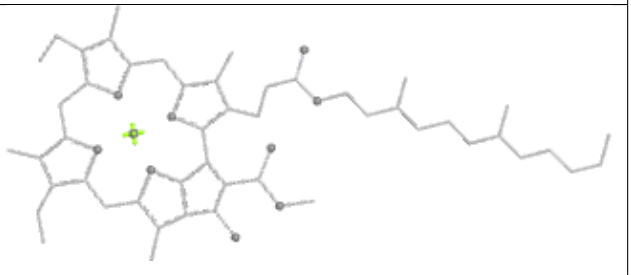
Bond lengths



Bond angles

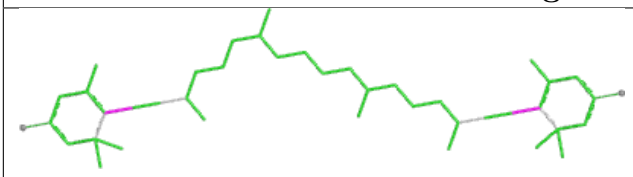


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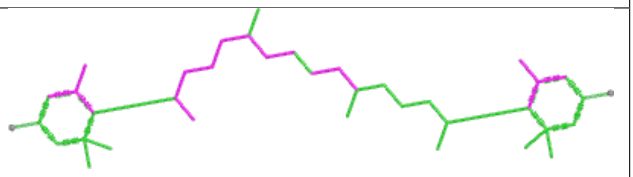


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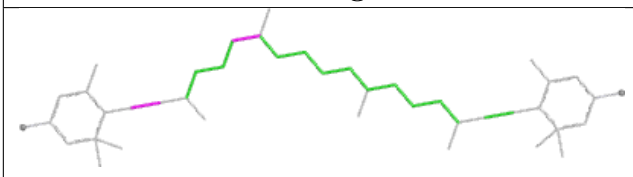
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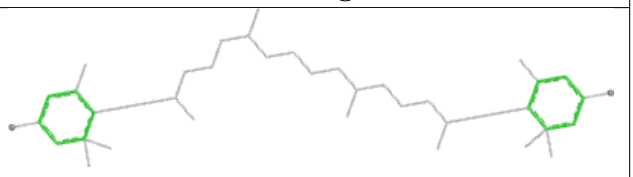
Bond lengths



Bond angles

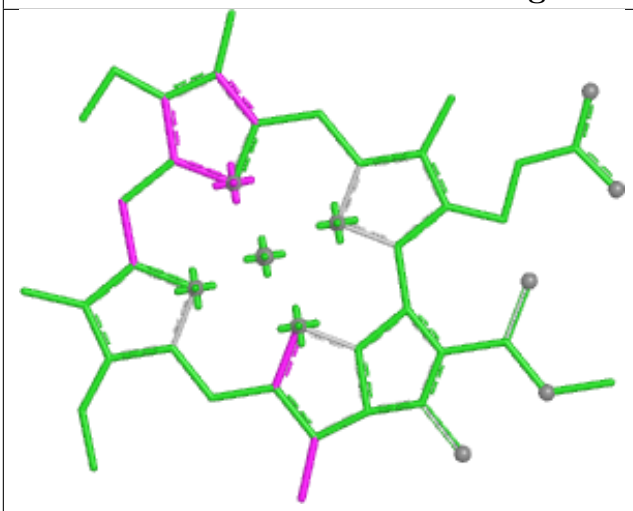


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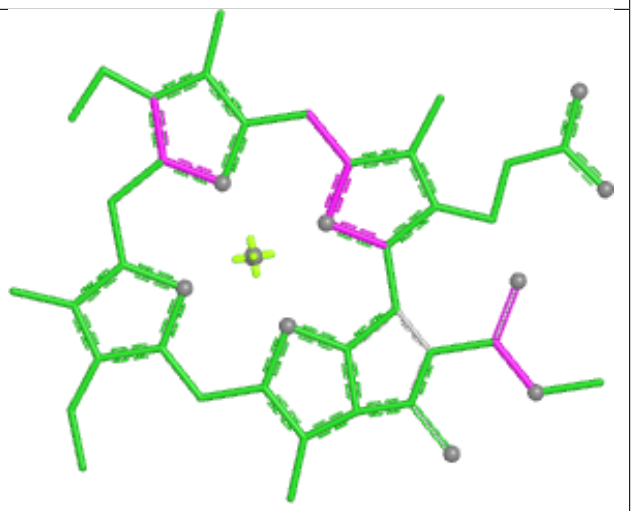


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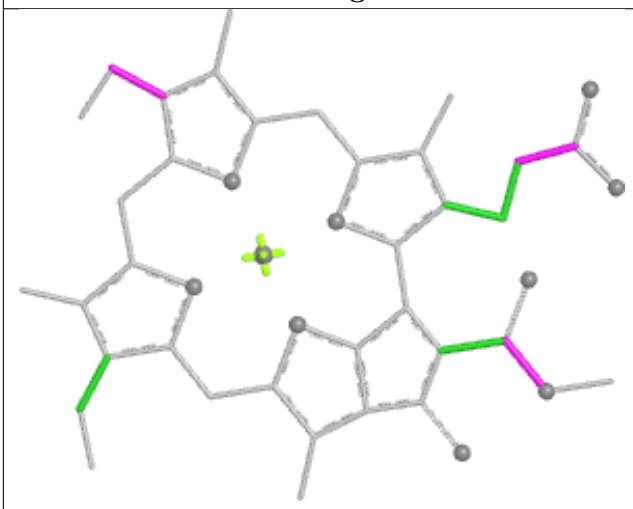
Ligand CLA 1 611



Bond lengths



Bond angles

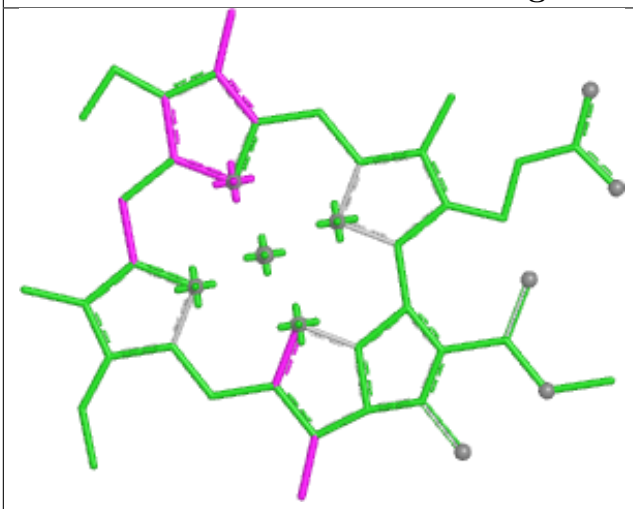


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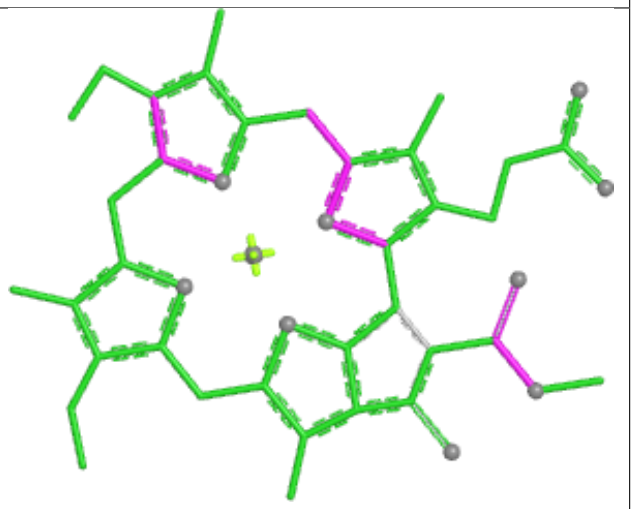


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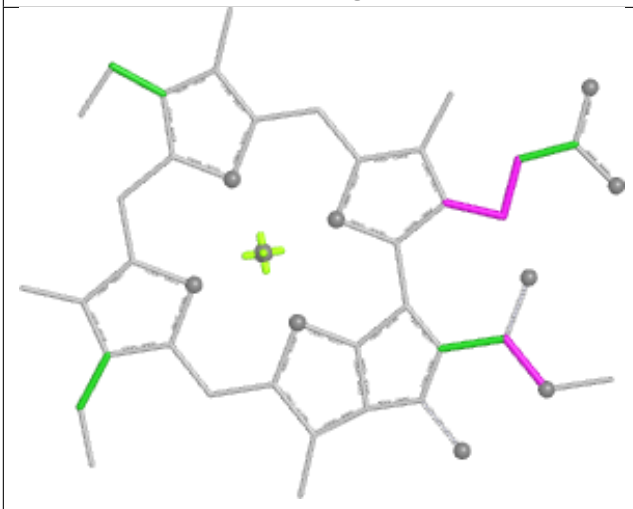
Ligand CLA 8 611



Bond lengths



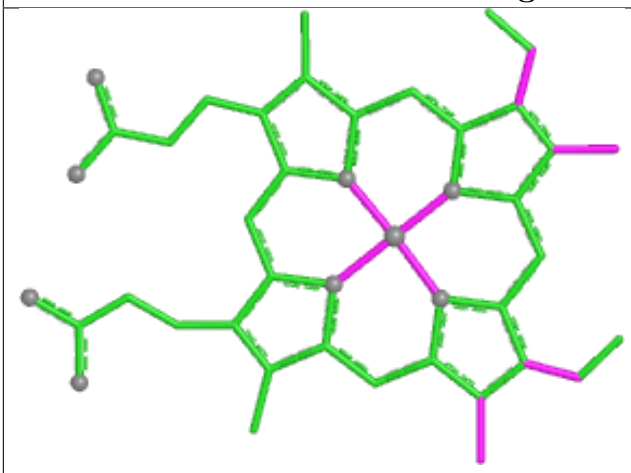
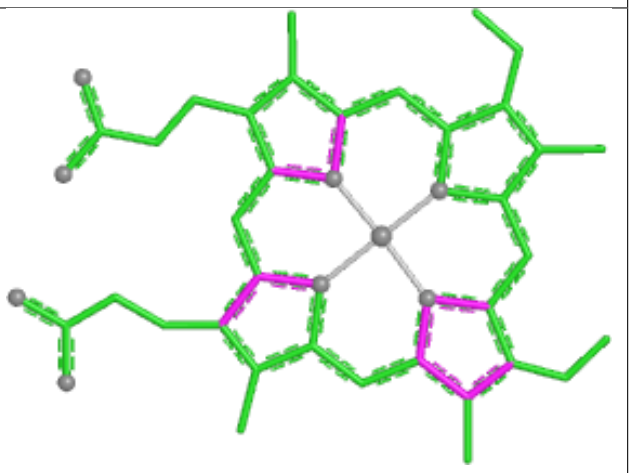
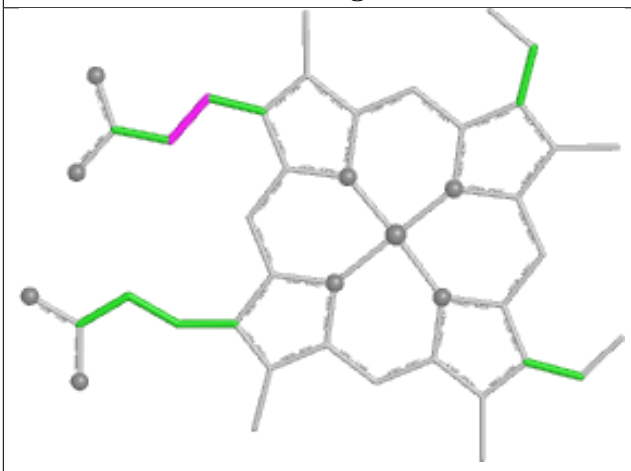
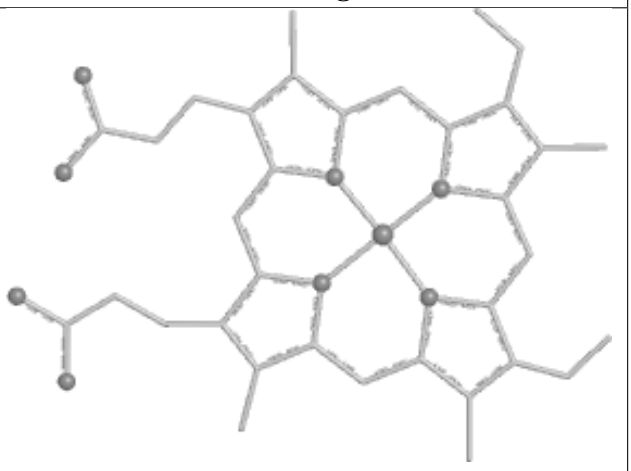
Bond angles

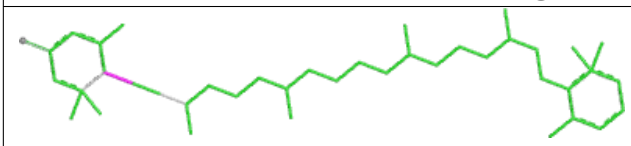
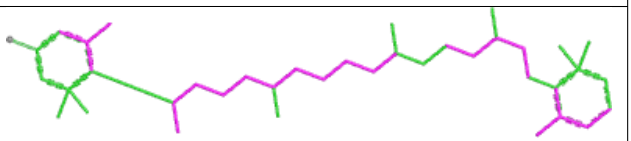
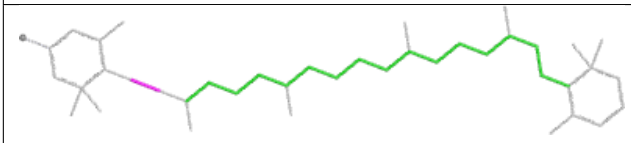
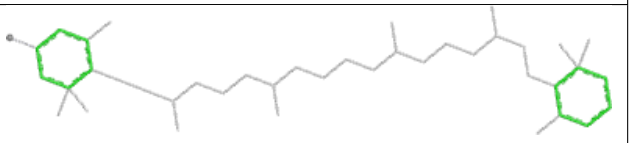


Torsions

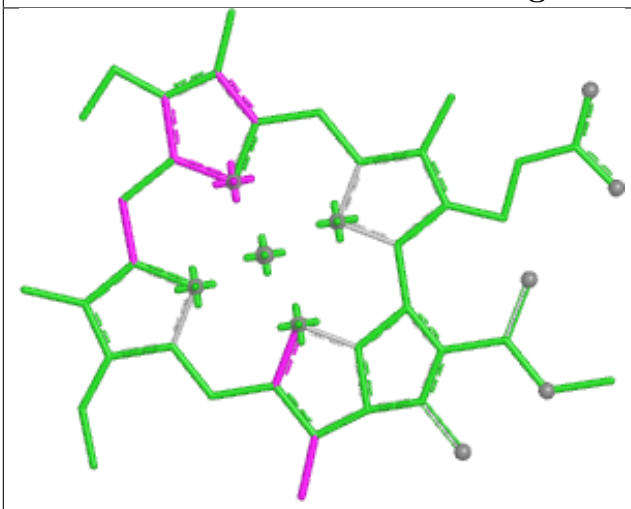


Rings

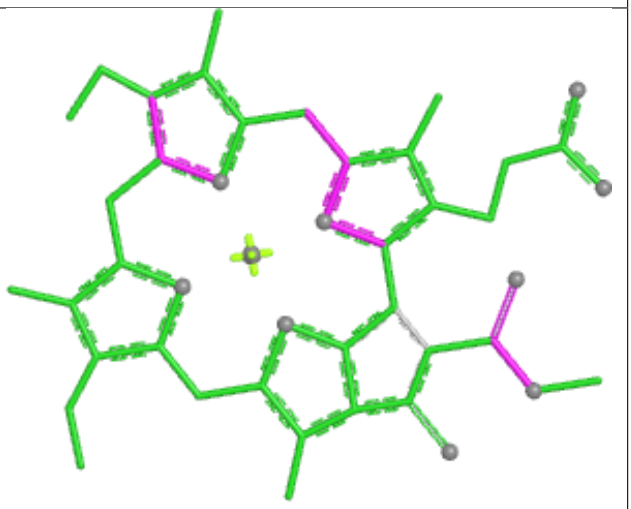
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 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand IHT 5 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

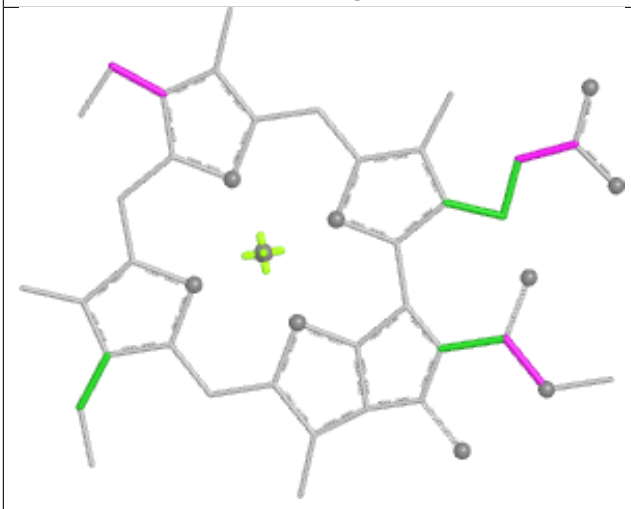
Ligand CLA 7 613



Bond lengths



Bond angles

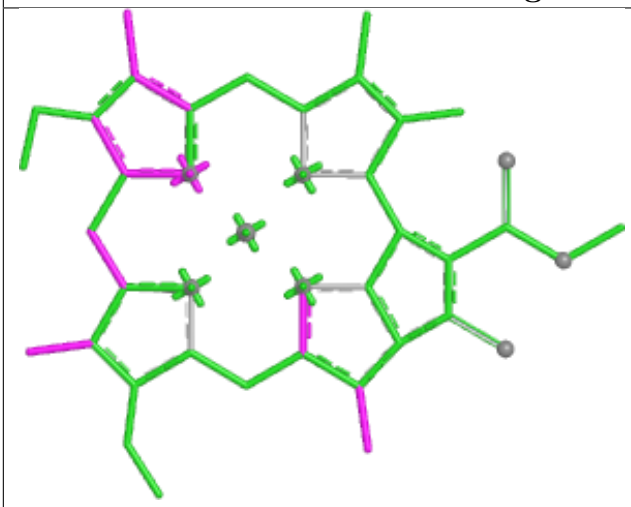


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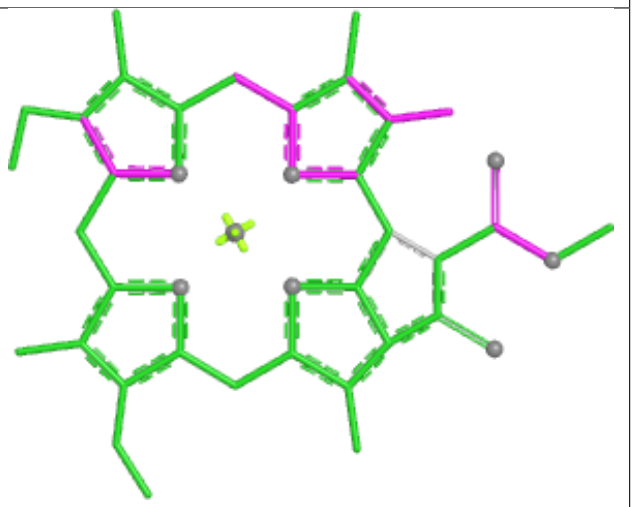


Rings

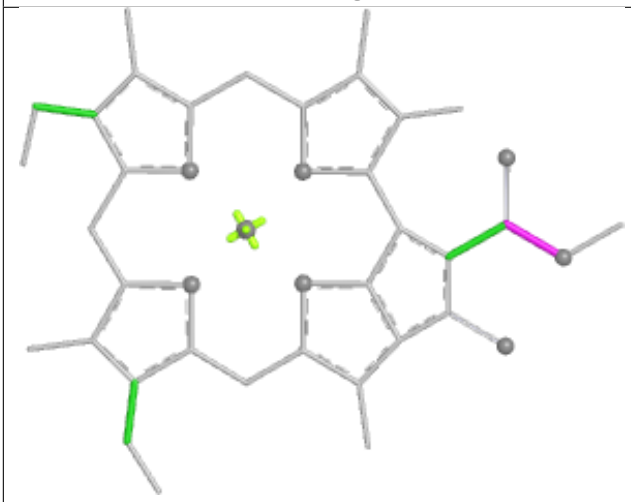
Ligand CLA B 608



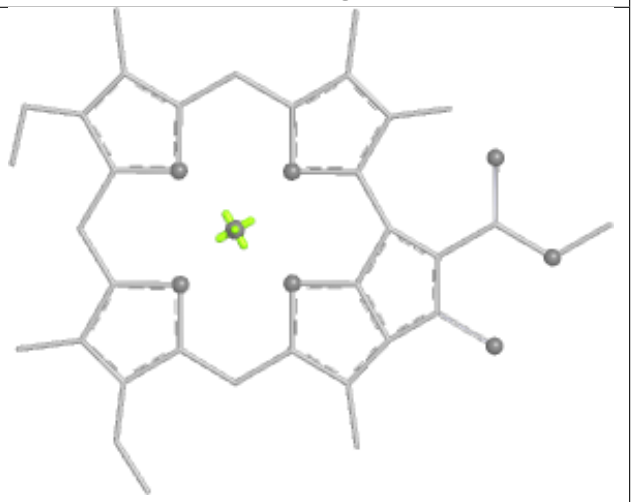
Bond lengths



Bond angles

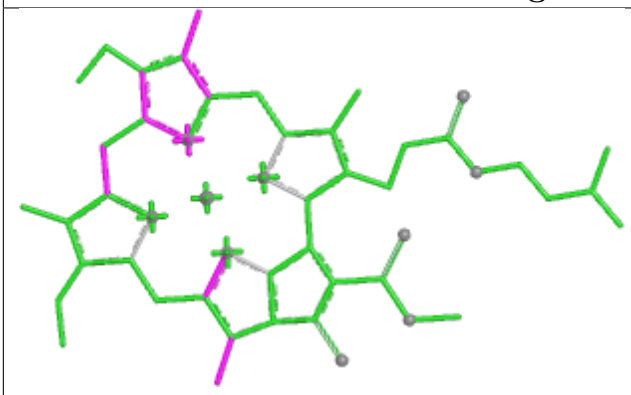


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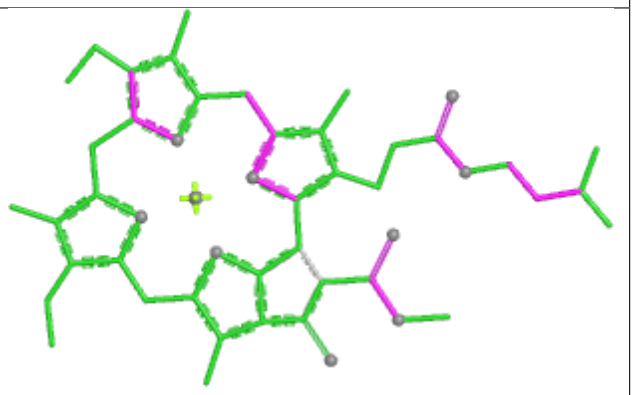


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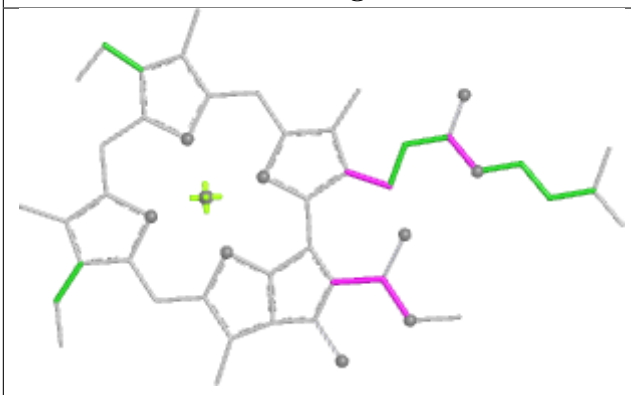
Ligand CLA 9 603



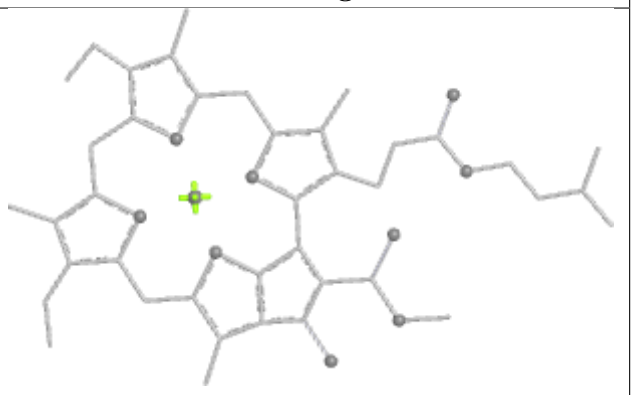
Bond lengths



Bond angles

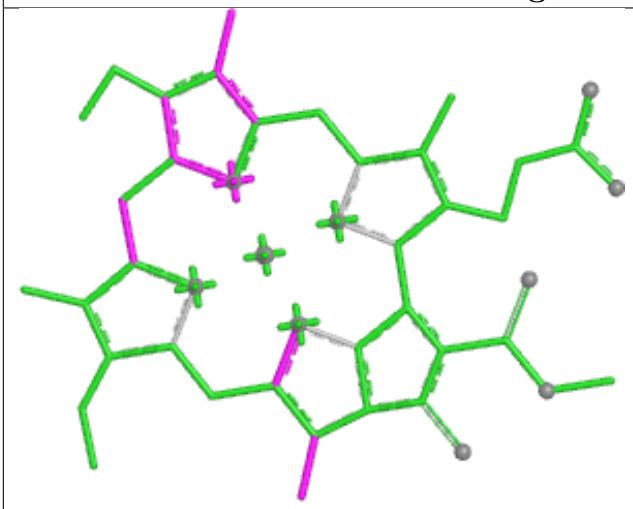


Torsions

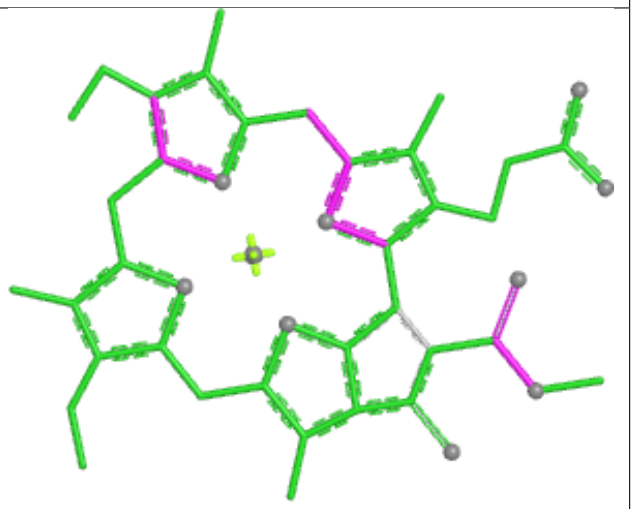


Rings

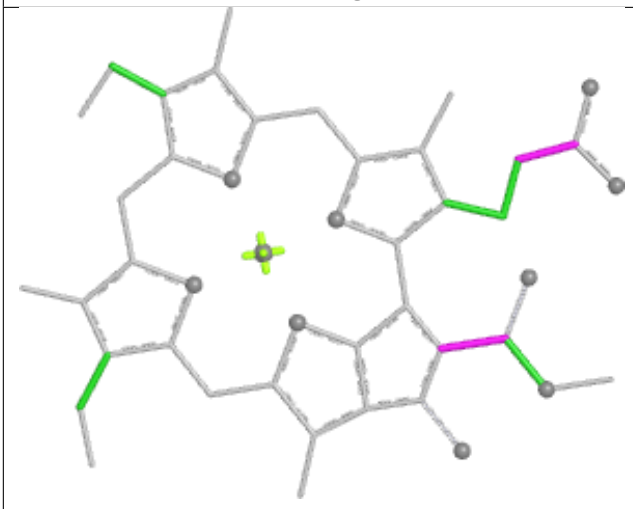
Ligand CLA 8 606



Bond lengths



Bond angles

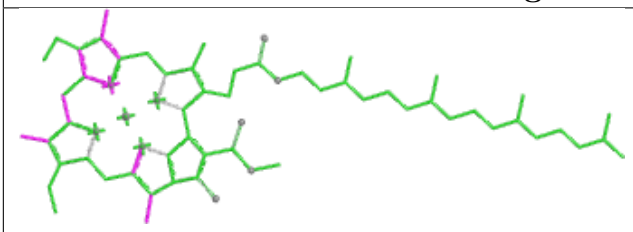


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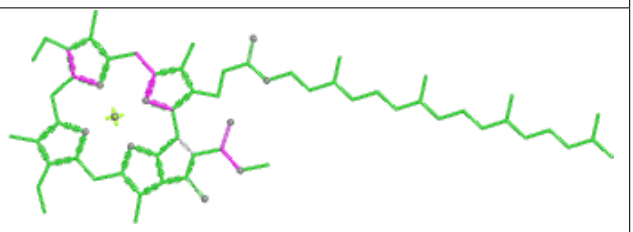


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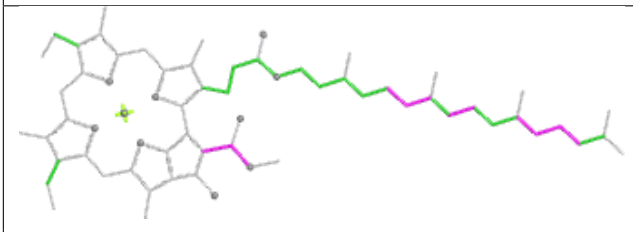
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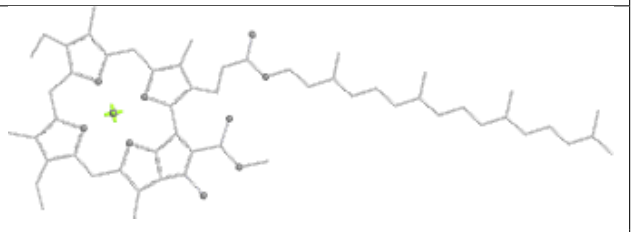
Bond lengths



Bond angles

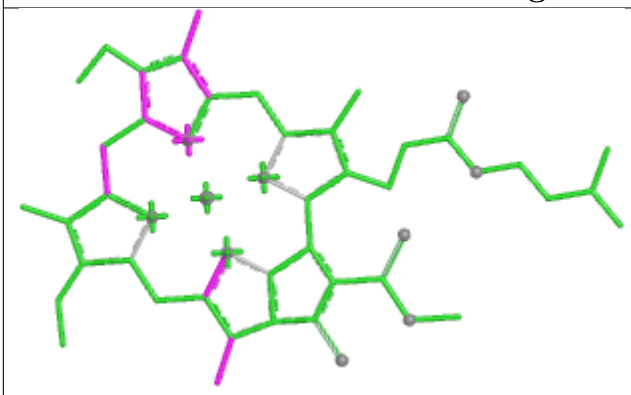


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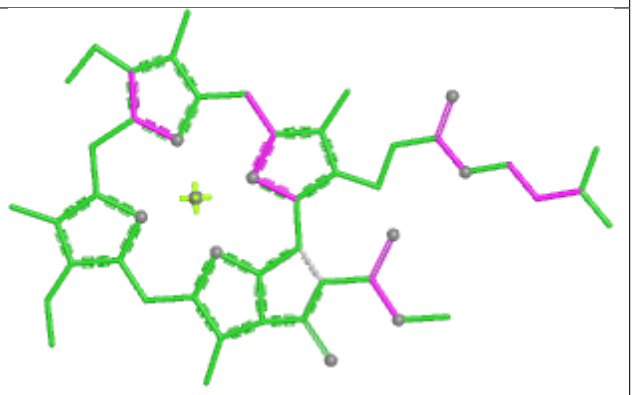


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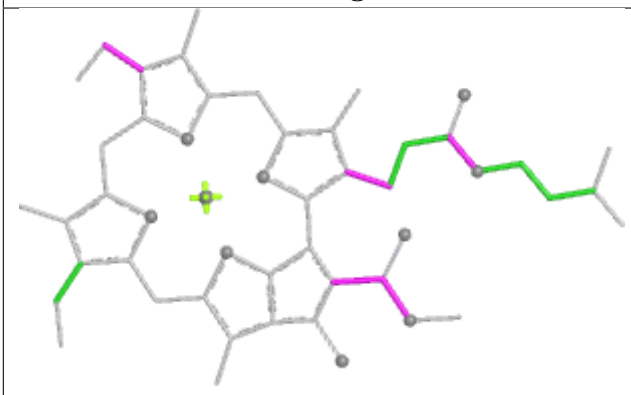
Ligand CLA 1 605



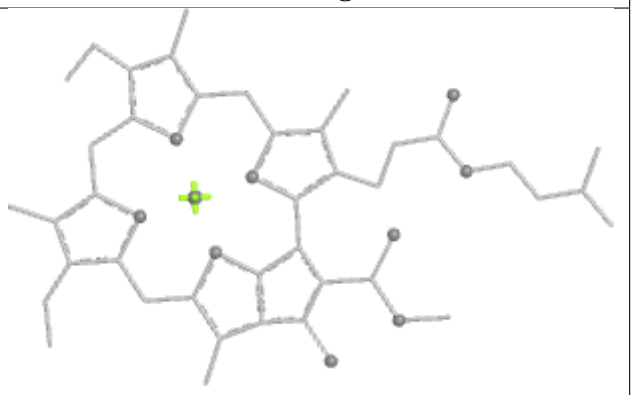
Bond lengths



Bond angles

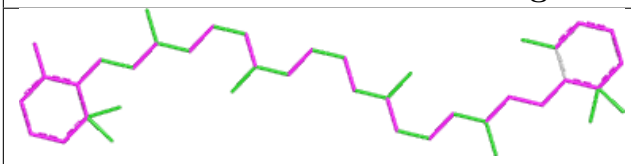


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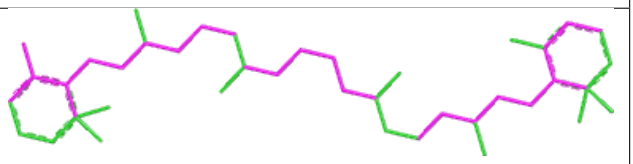


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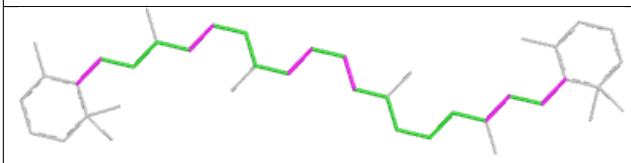
Ligand 8CT b 622



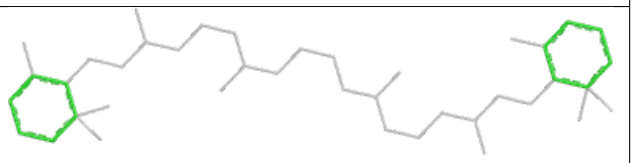
Bond lengths



Bond angles

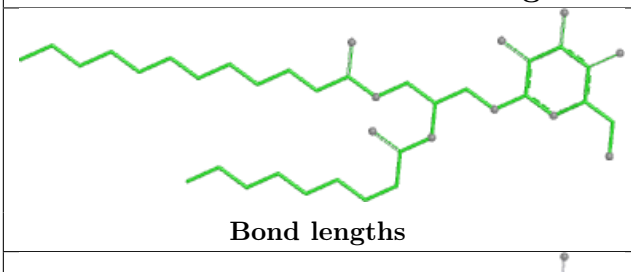


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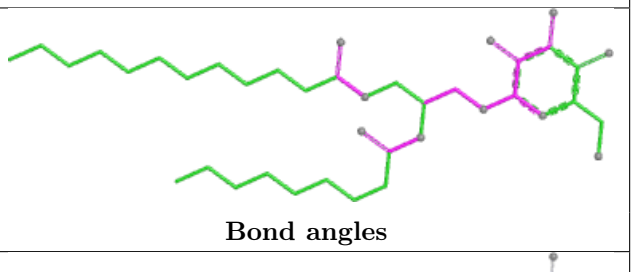


Rings

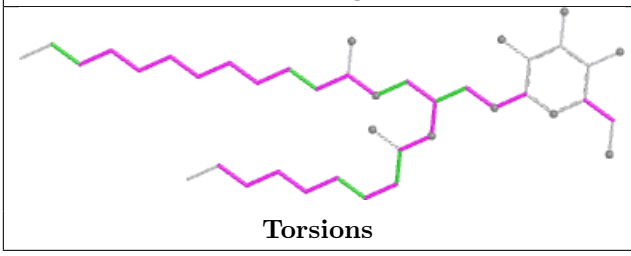
Ligand LMG d 401



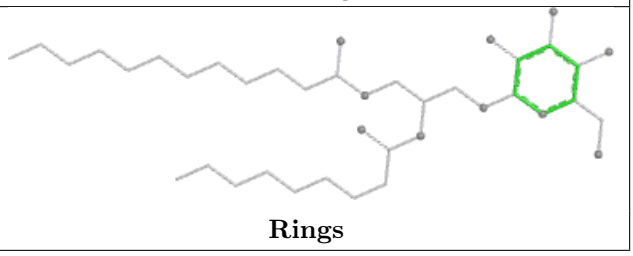
Bond lengths



Bond angles

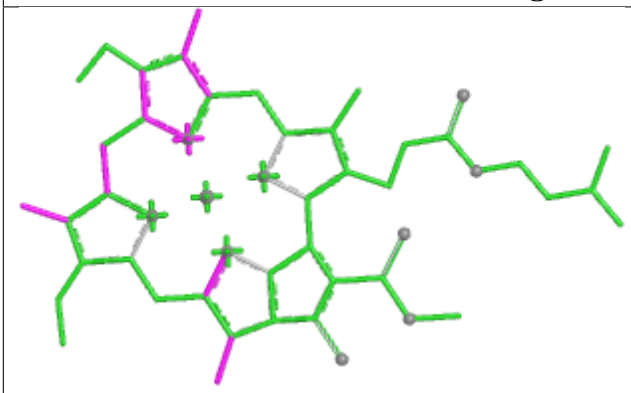


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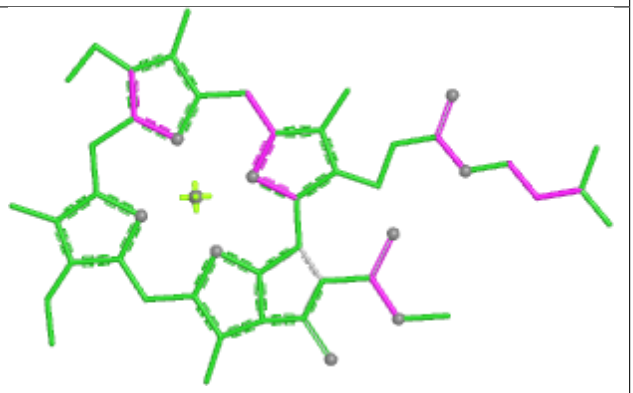


Rings

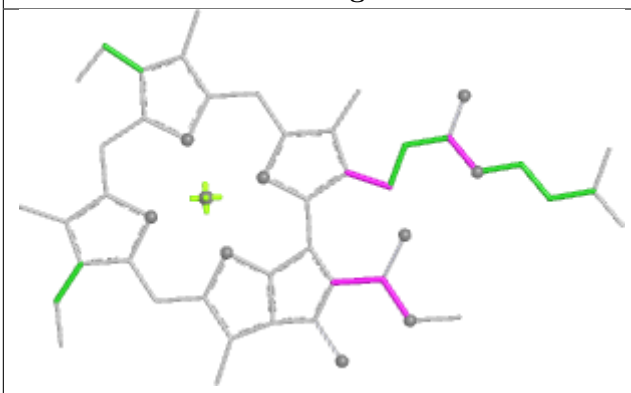
Ligand CLA 3 603



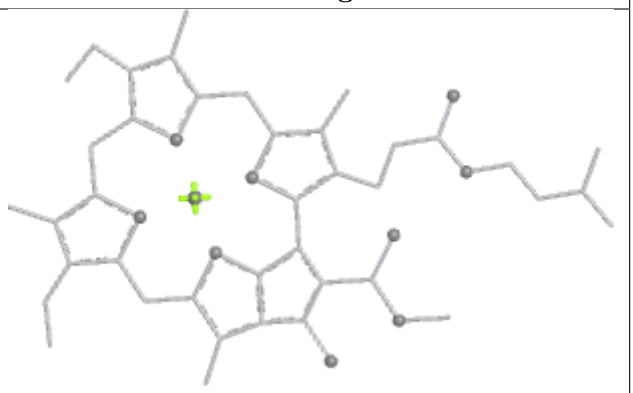
Bond lengths



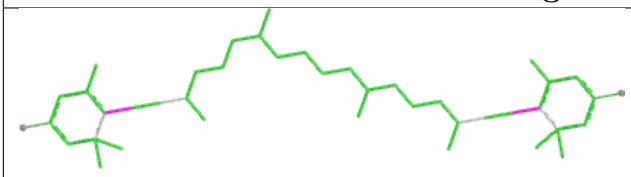
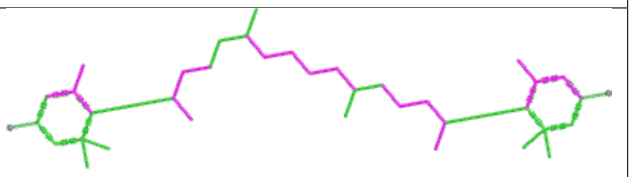
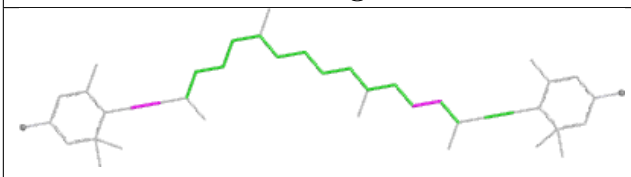
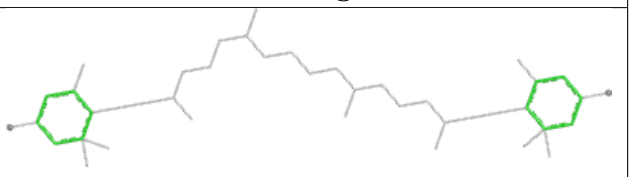
Bond angles

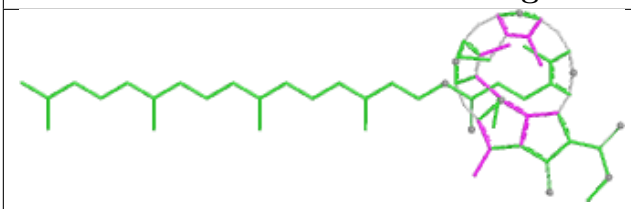
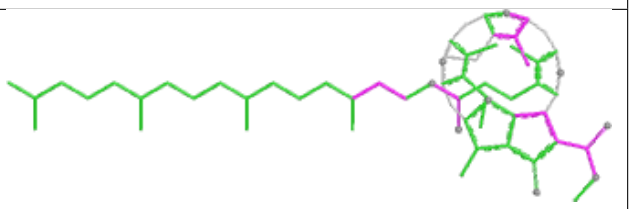
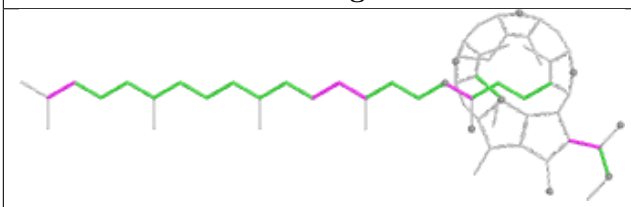
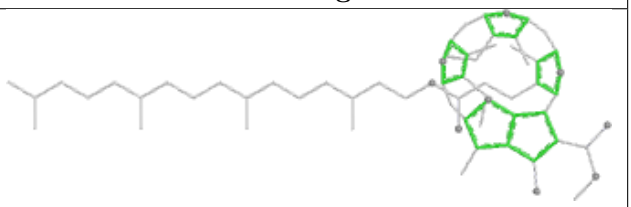


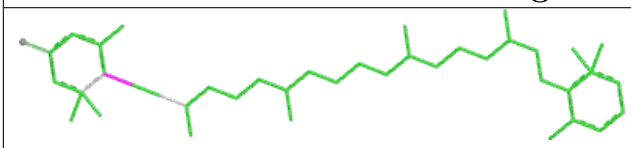
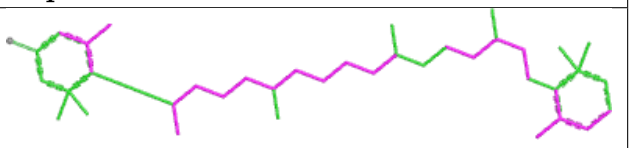
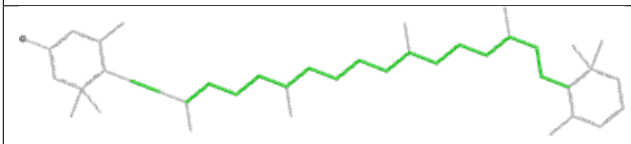
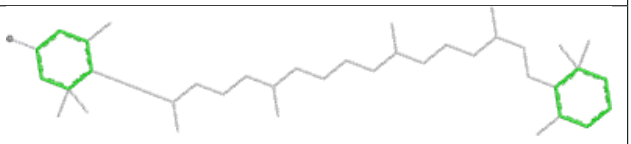
Torsions



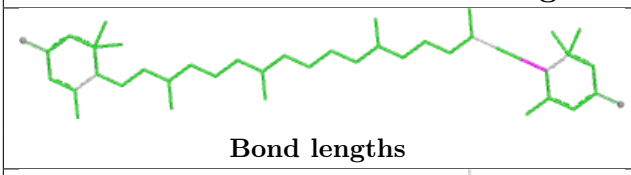
Rings

Ligand II0 4 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

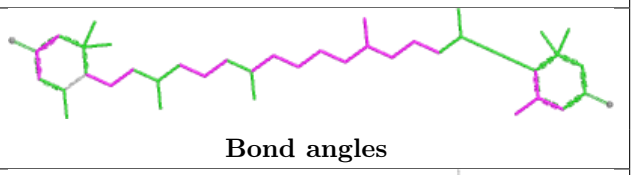
Ligand PHO A 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand IHT p 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

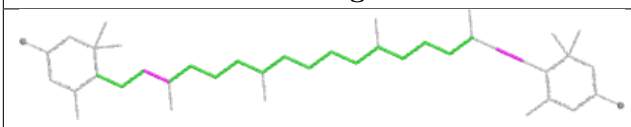
Ligand II3 P 613



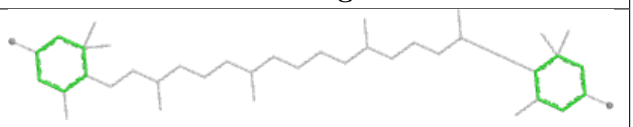
Bond lengths



Bond angles

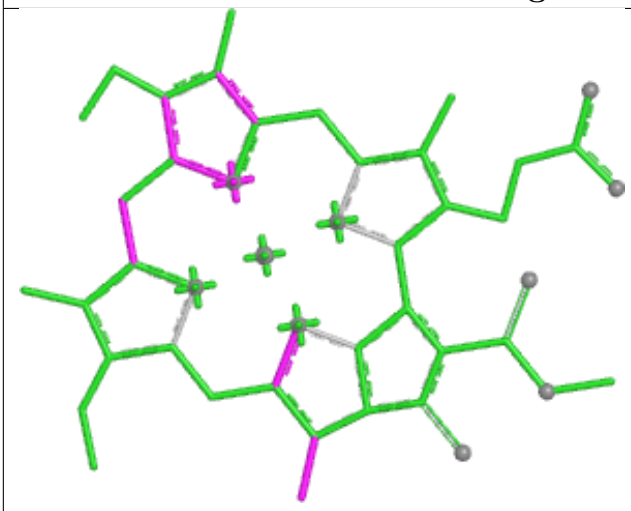


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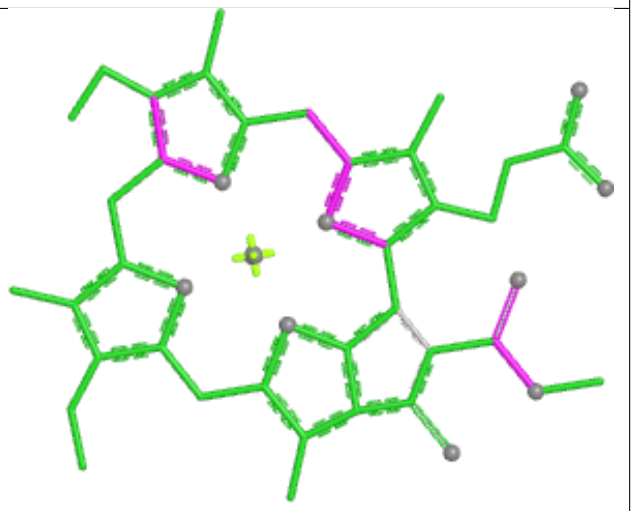


Rings

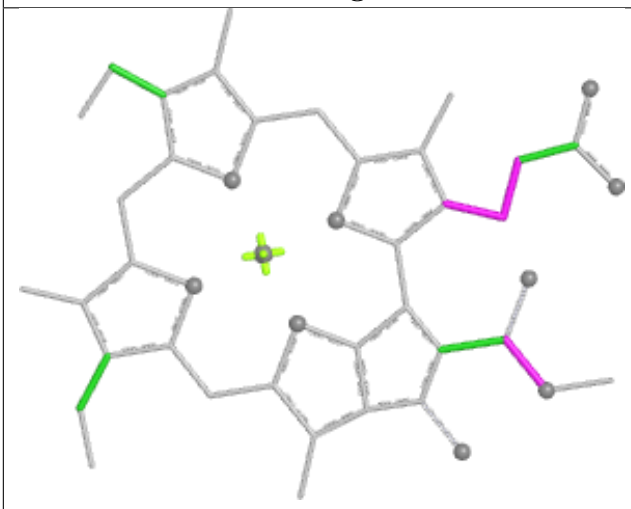
Ligand CLA 2 611



Bond lengths



Bond angles

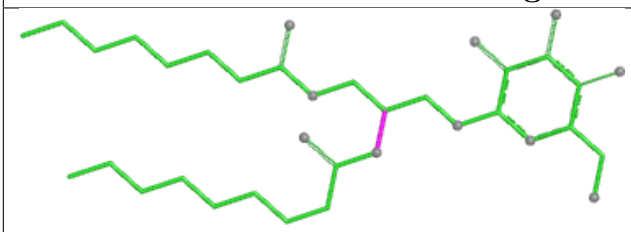


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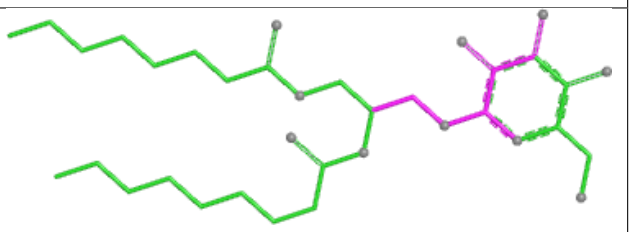


Rings

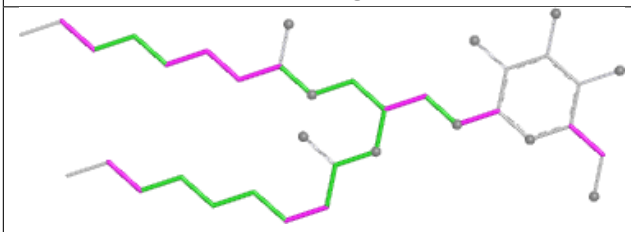
Ligand LMG 4 618



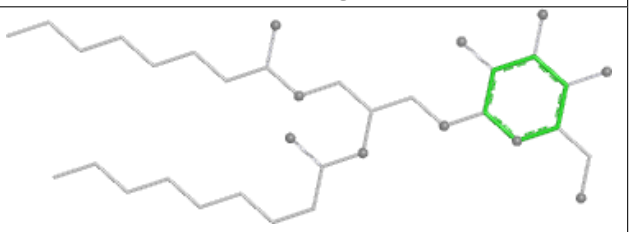
Bond lengths



Bond angles

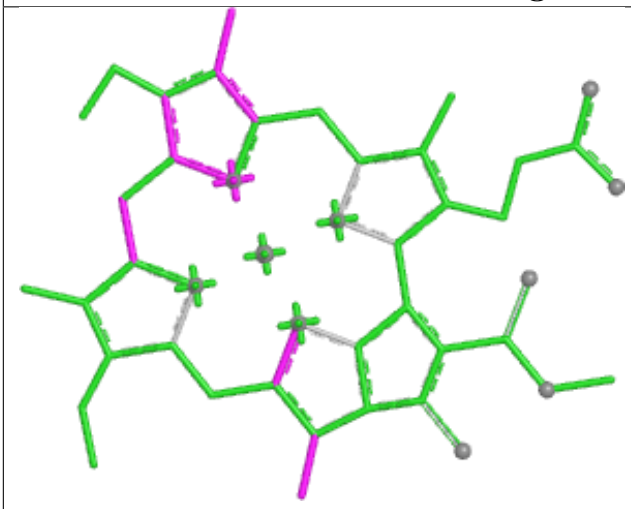


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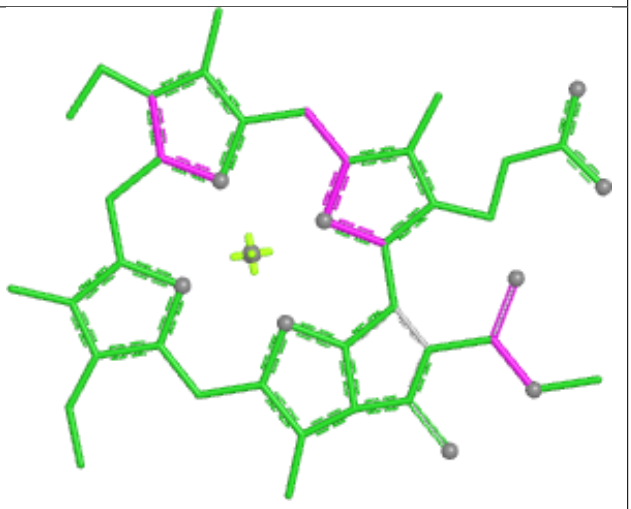


Rings

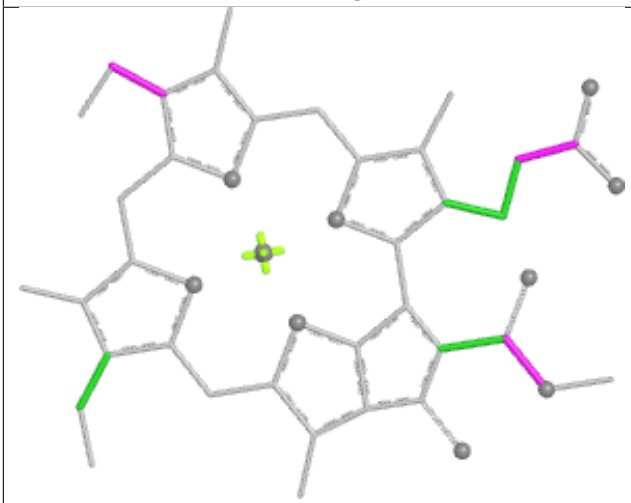
Ligand CLA 1 613



Bond lengths



Bond angles

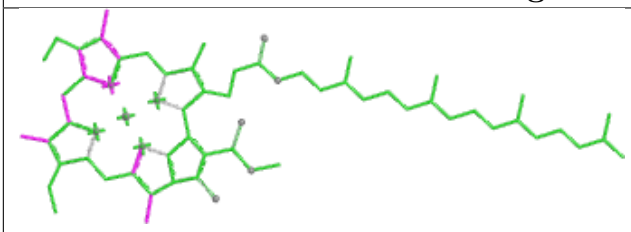


Torsions

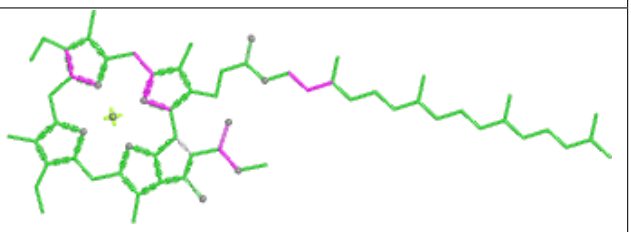


Rings

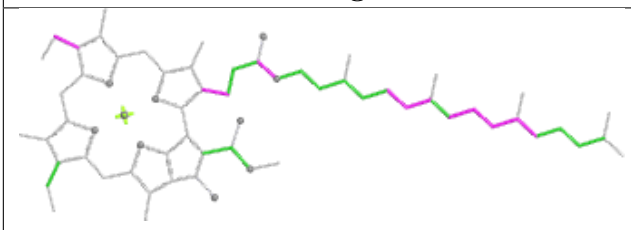
Ligand CLA b 617



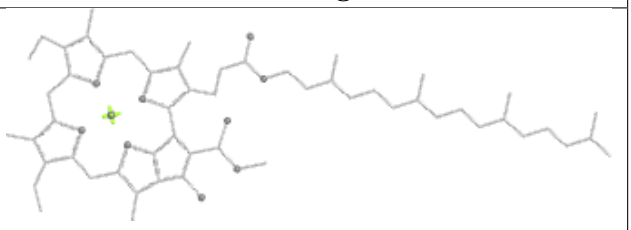
Bond lengths



Bond angles

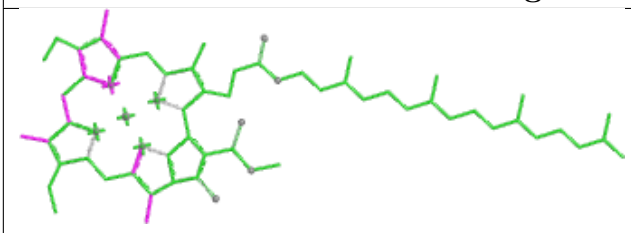


Torsions

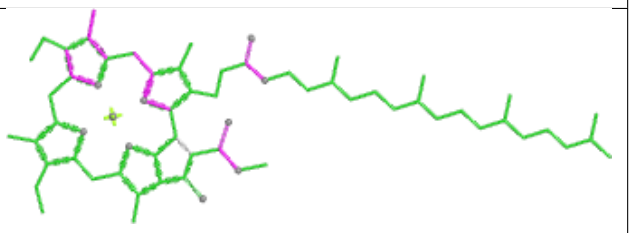


Rings

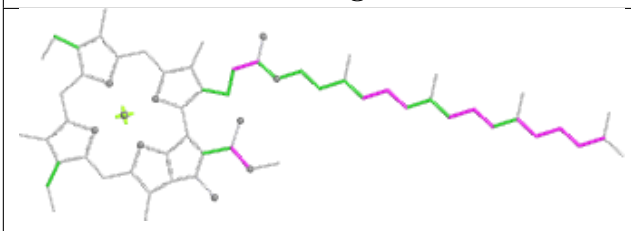
Ligand CLA B 614



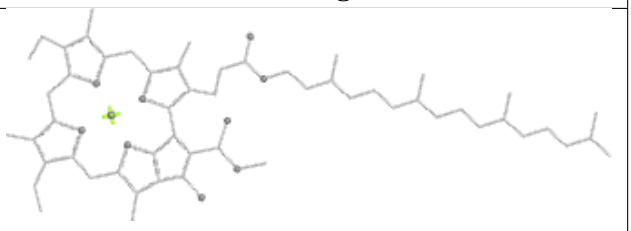
Bond lengths



Bond angles

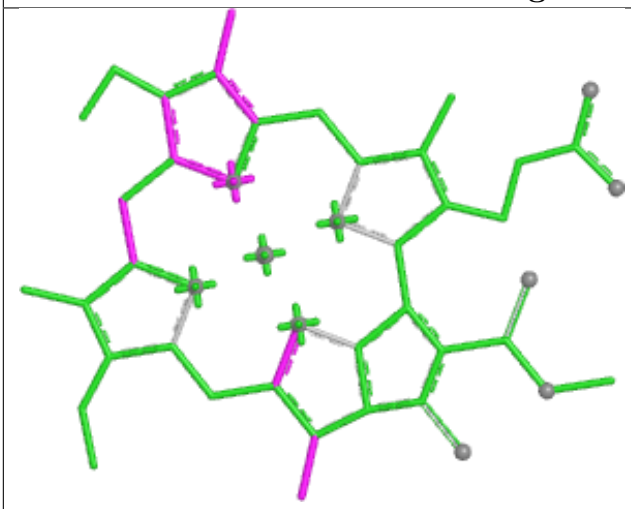


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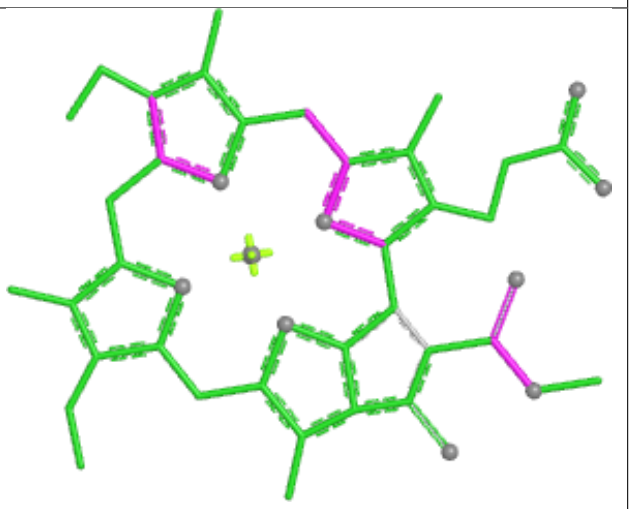


Rings

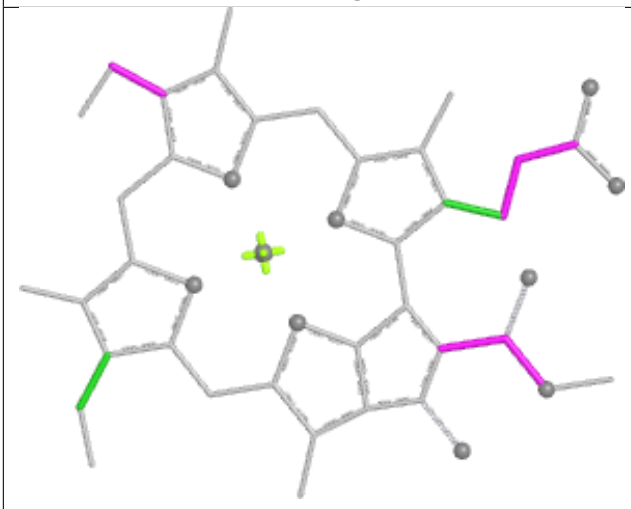
Ligand CLA 6 611



Bond lengths



Bond angles

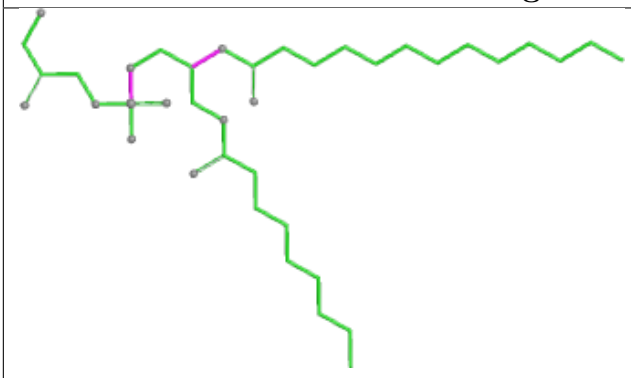


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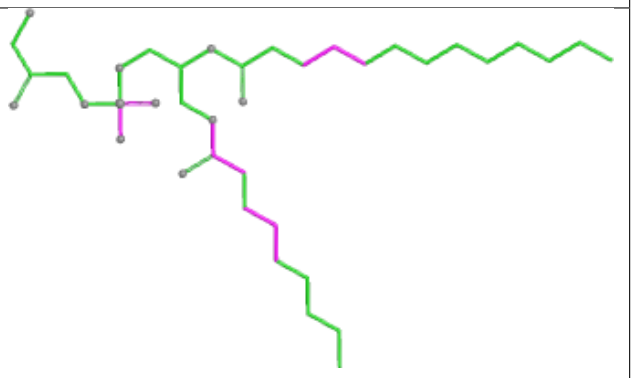


Rings

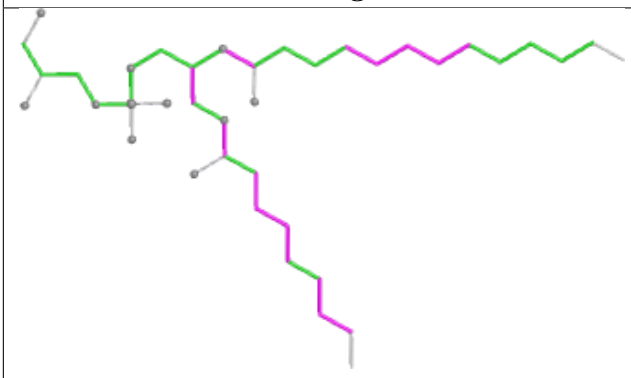
Ligand LHG B 621



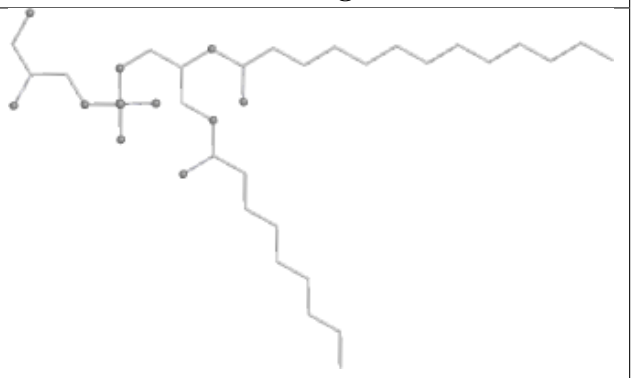
Bond lengths



Bond angles

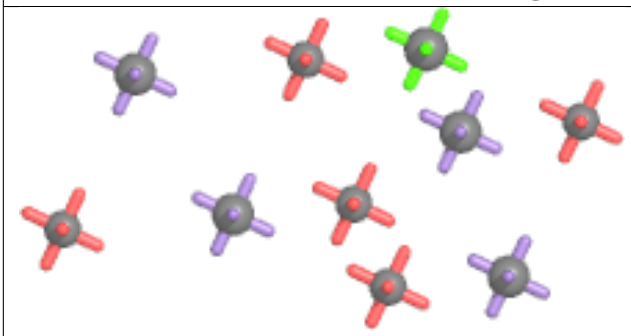


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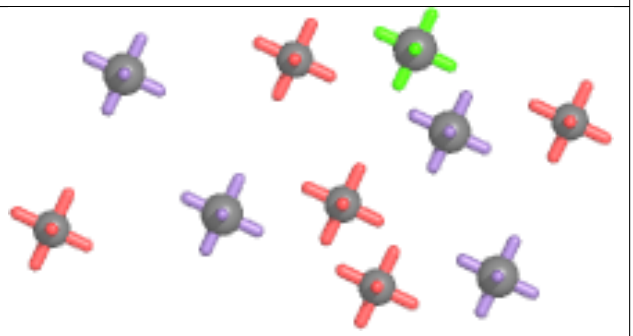


Rings

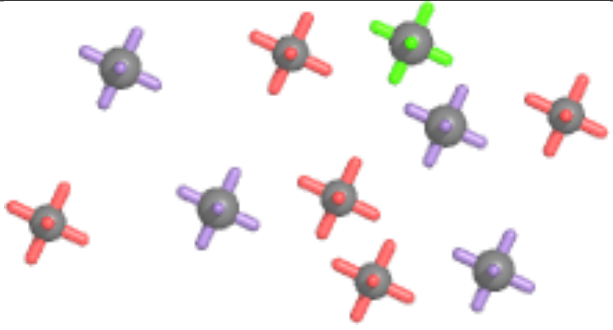
Ligand OEX a 404



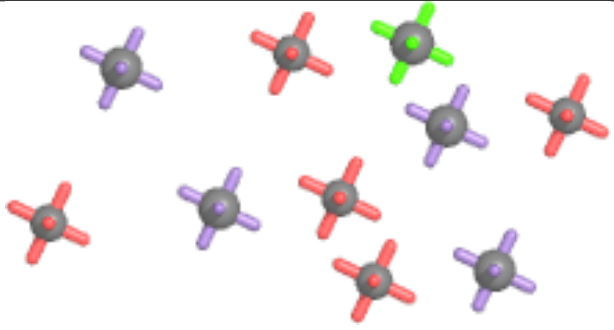
Bond lengths



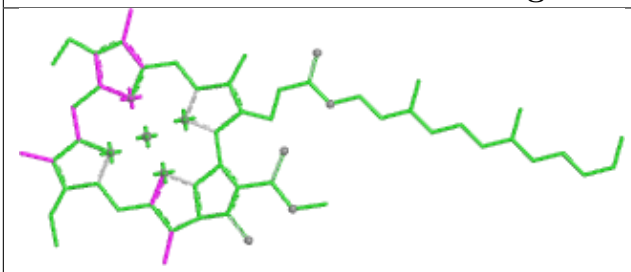
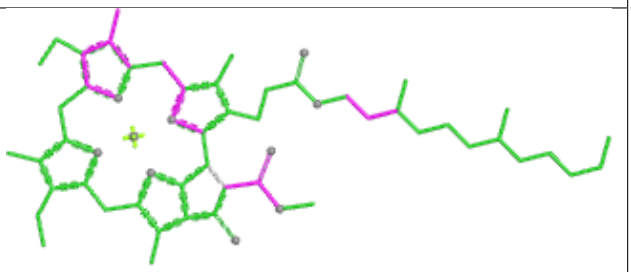
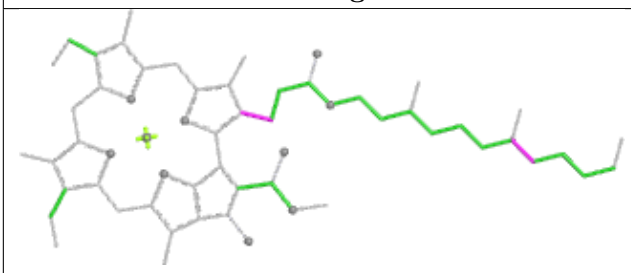
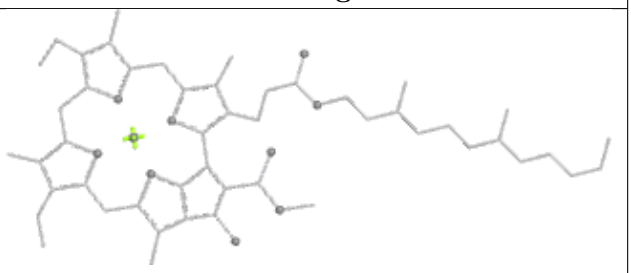
Bond angles

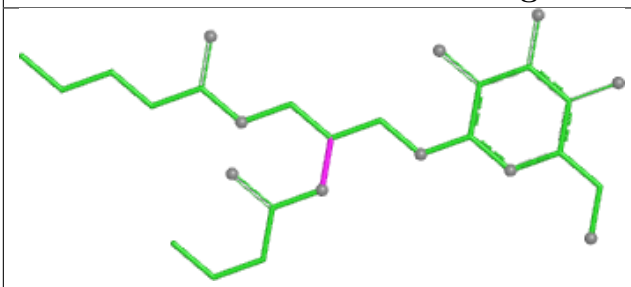
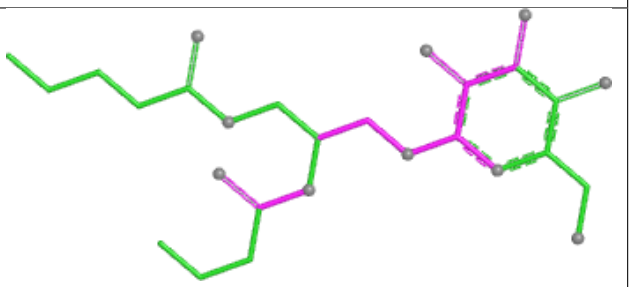
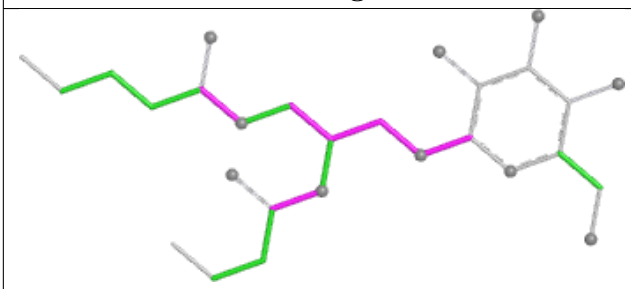
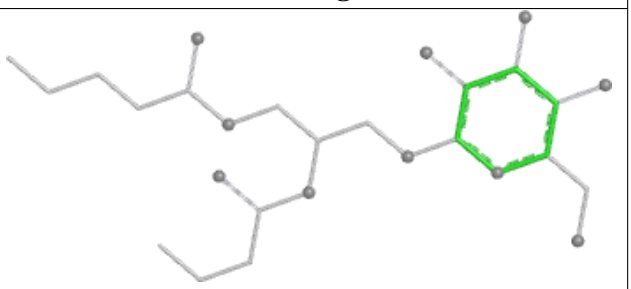


Torsions

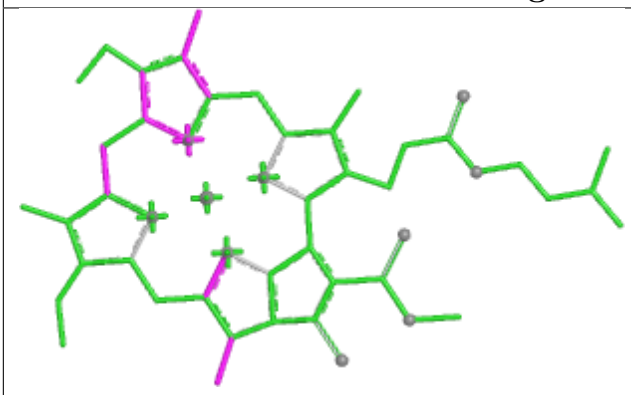


Rings

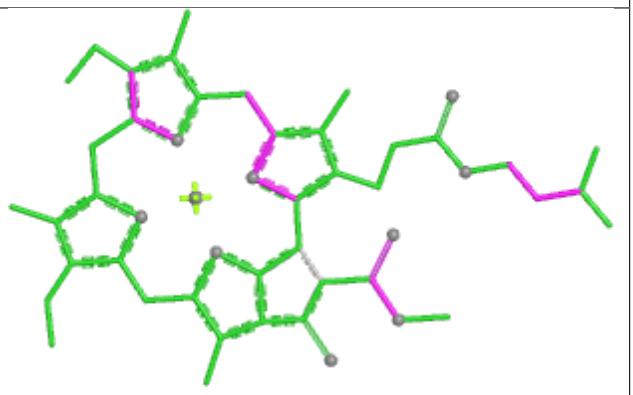
Ligand CLA d 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG P 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

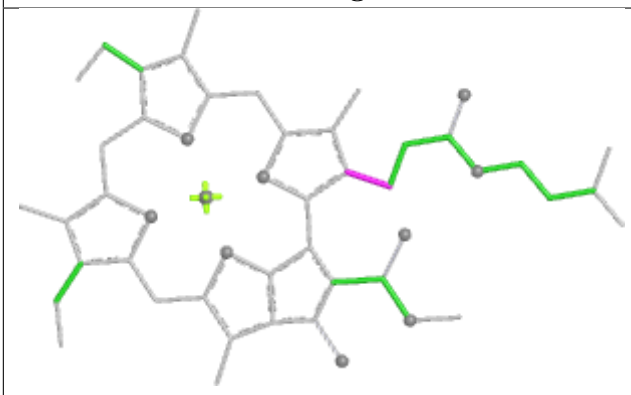
Ligand CLA 6 603



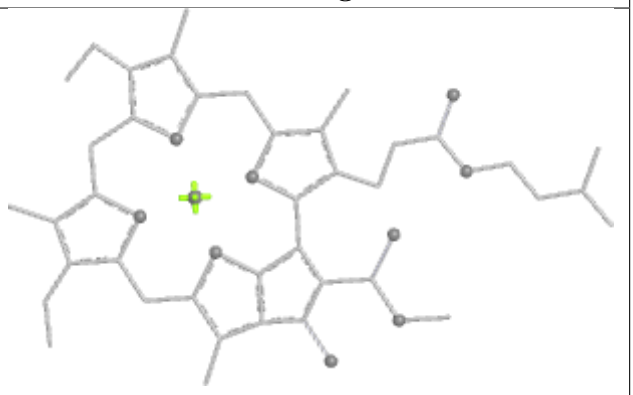
Bond lengths



Bond angles

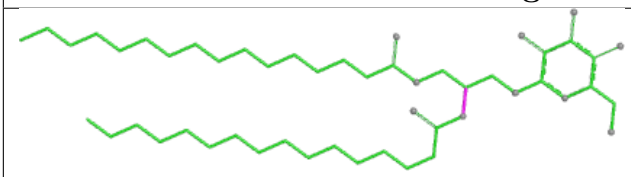


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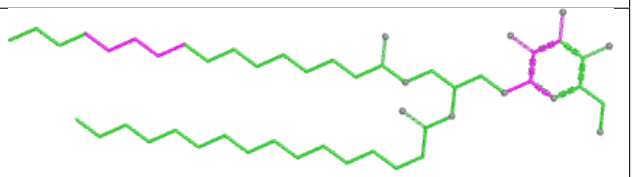


Rings

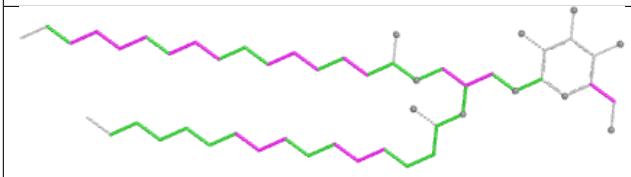
Ligand LMG b 618



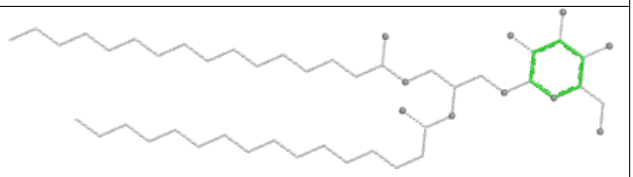
Bond lengths



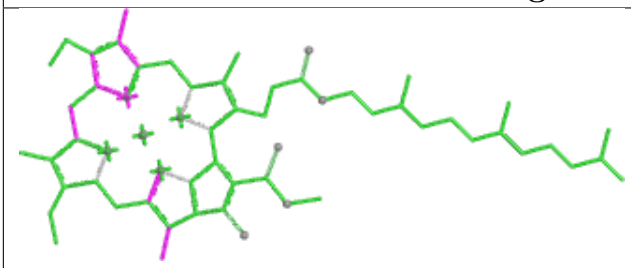
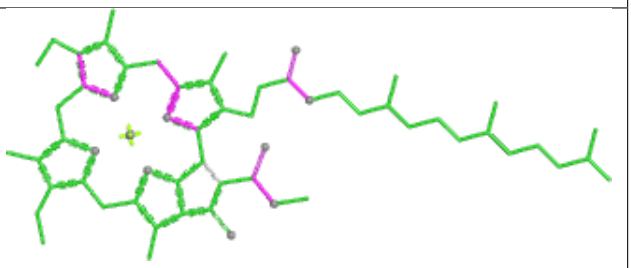
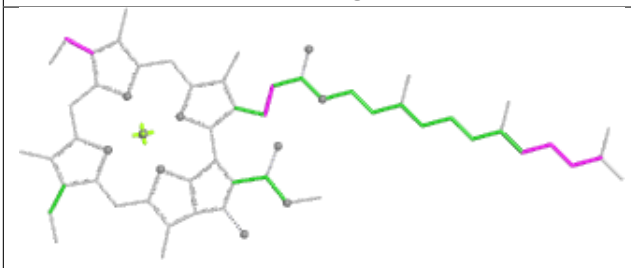
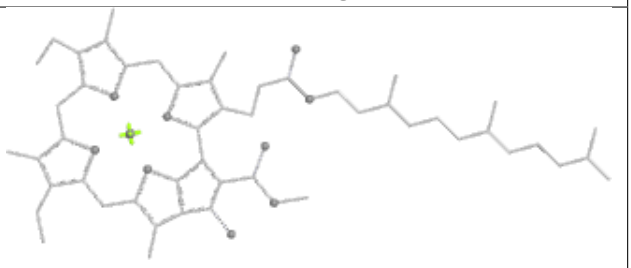
Bond angles

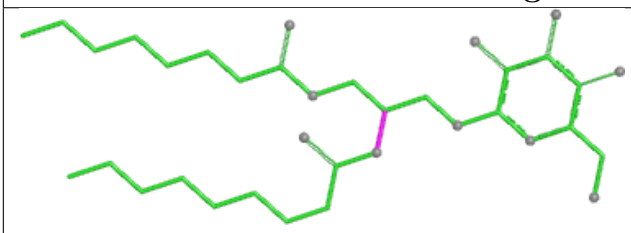
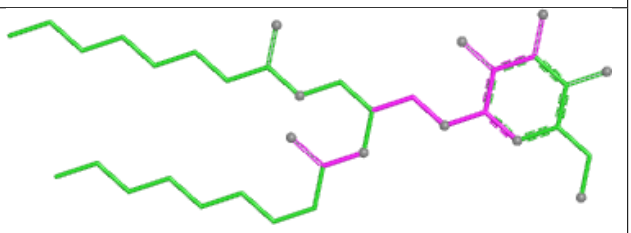
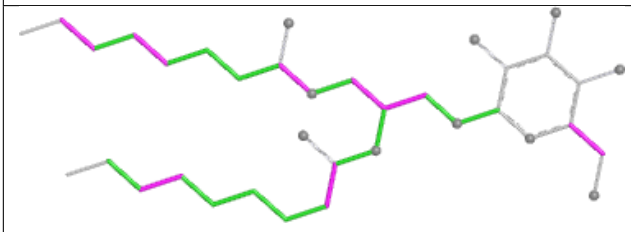
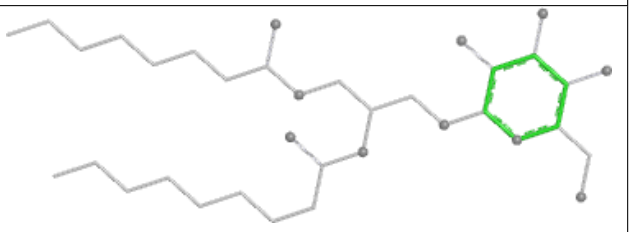


Torsions

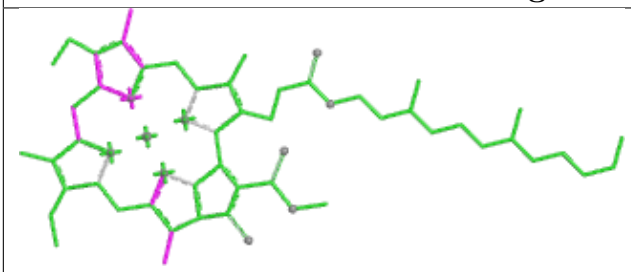


Rings

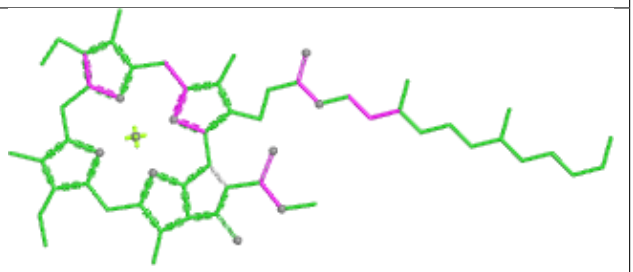
Ligand CLA 6 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG 8 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

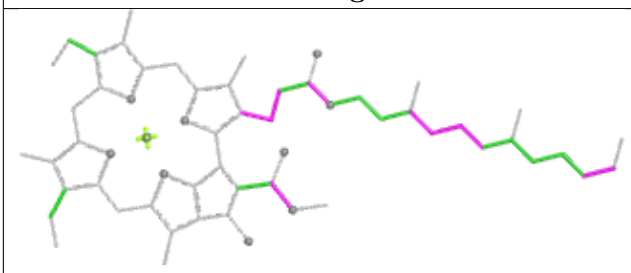
Ligand CLA 7 602



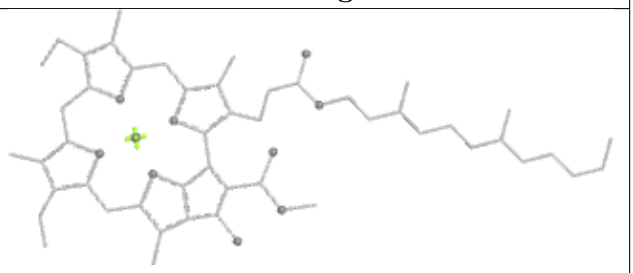
Bond lengths



Bond angles

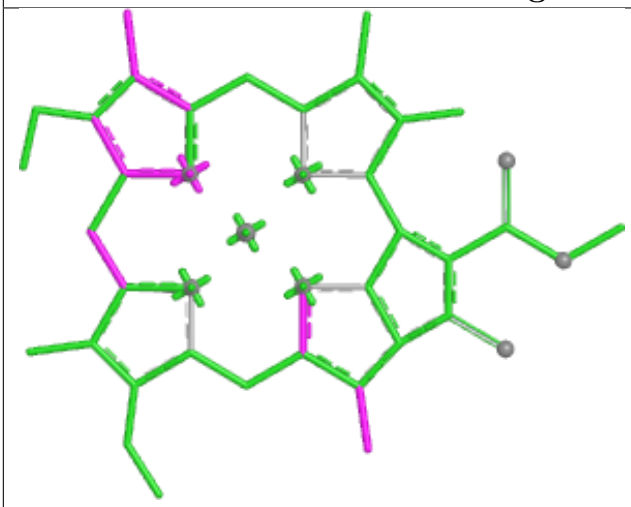


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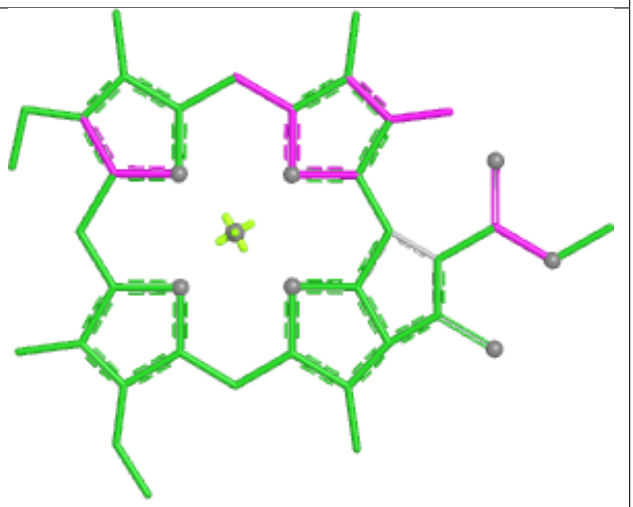


Rings

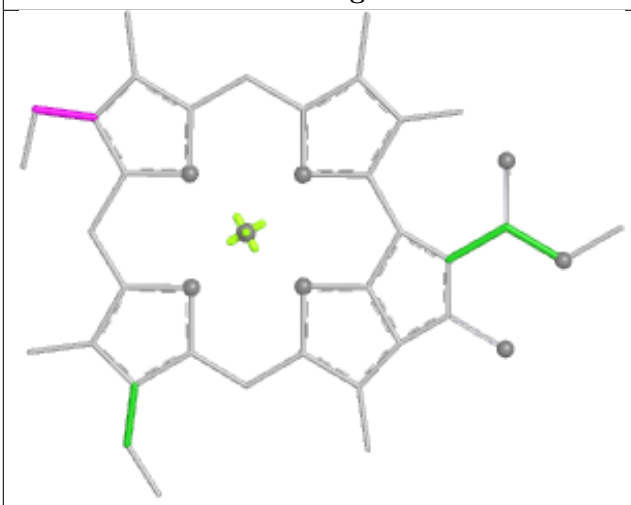
Ligand CLA 6 608



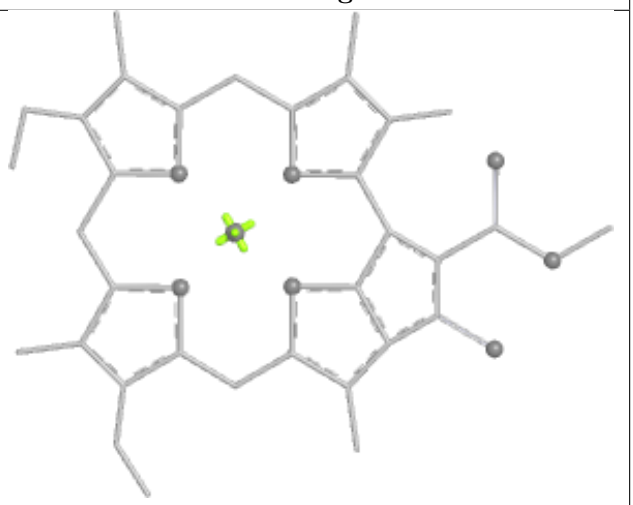
Bond lengths



Bond angles

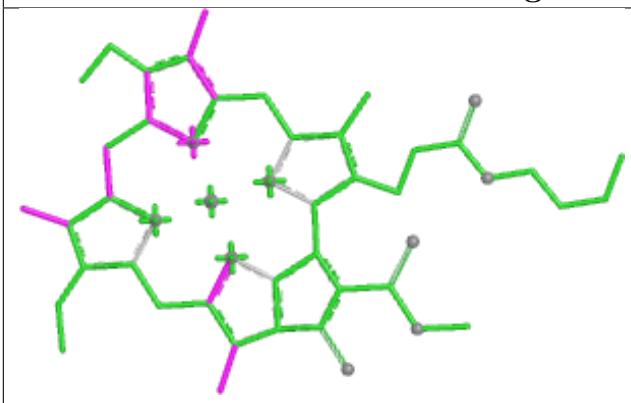


Torsions

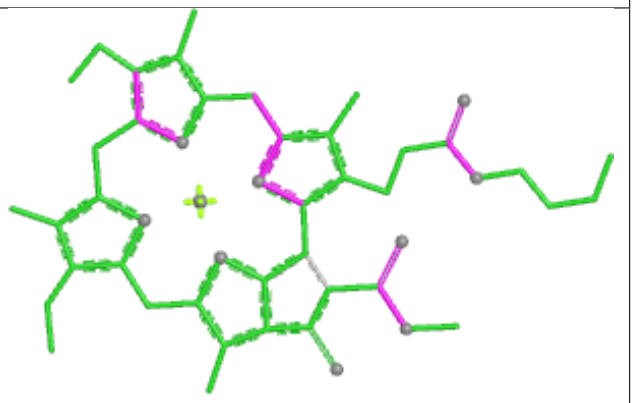


Rings

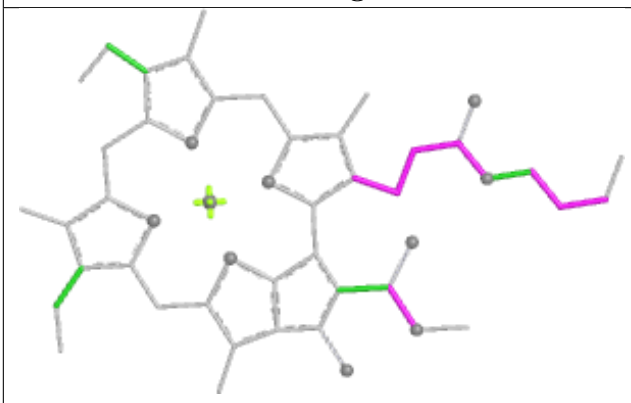
Ligand CLA C 513



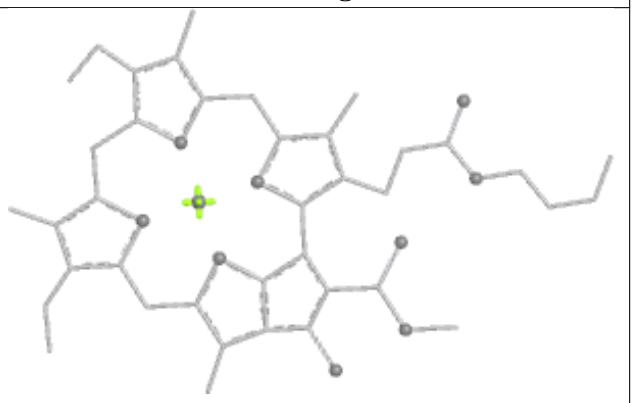
Bond lengths



Bond angles

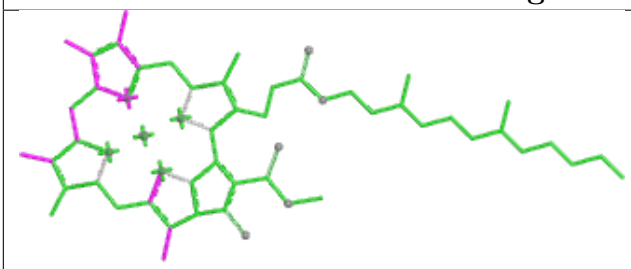


Torsions

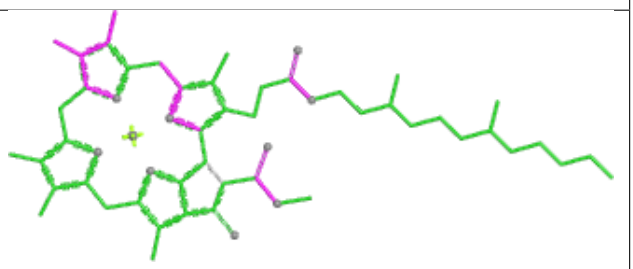


Rings

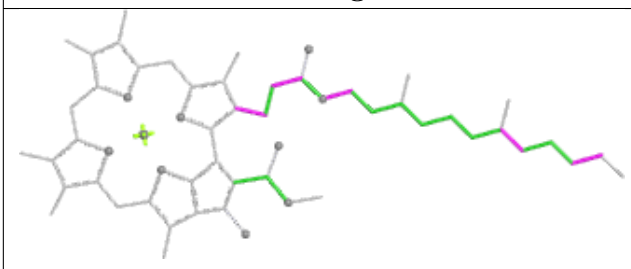
Ligand CLA d 402



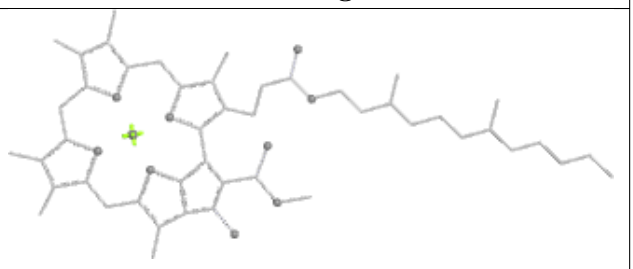
Bond lengths



Bond angles

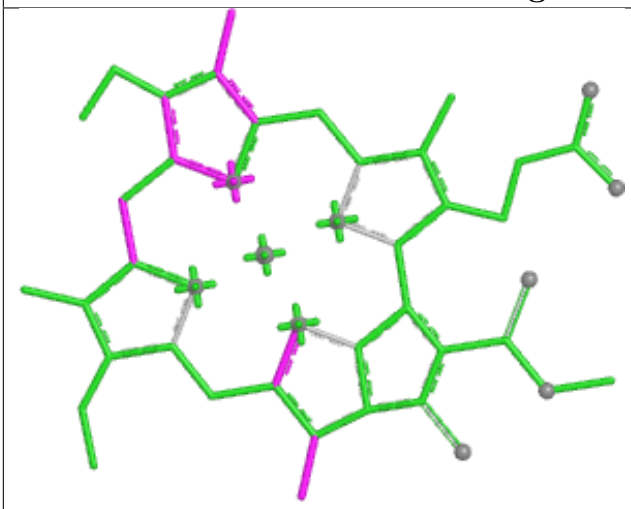


Torsions

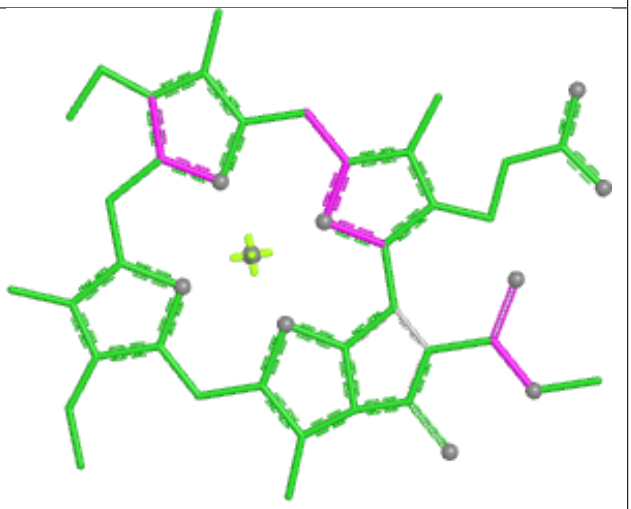


Rings

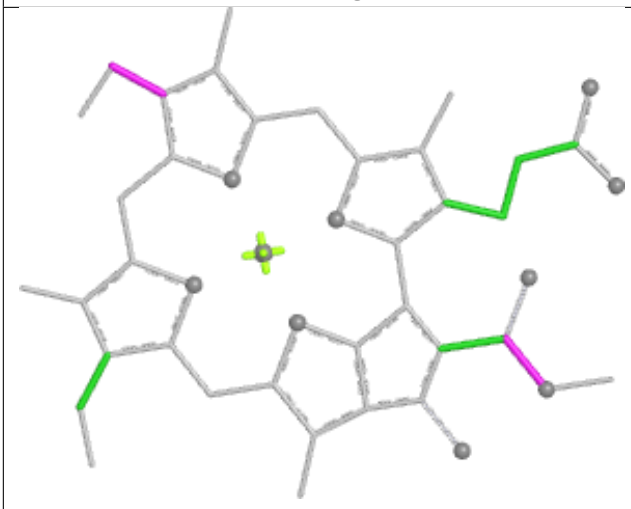
Ligand CLA 2 607



Bond lengths



Bond angles

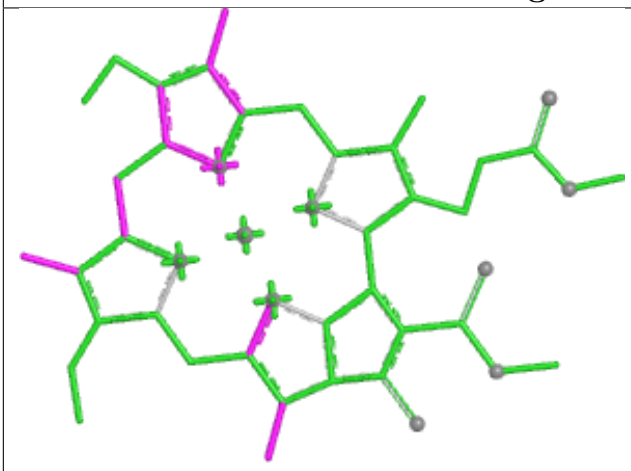


Torsions

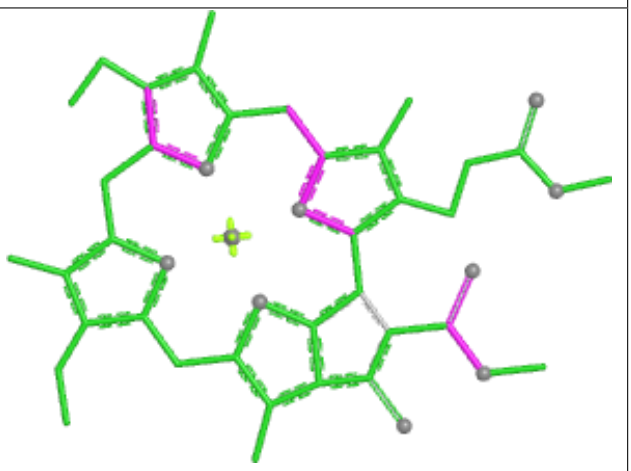


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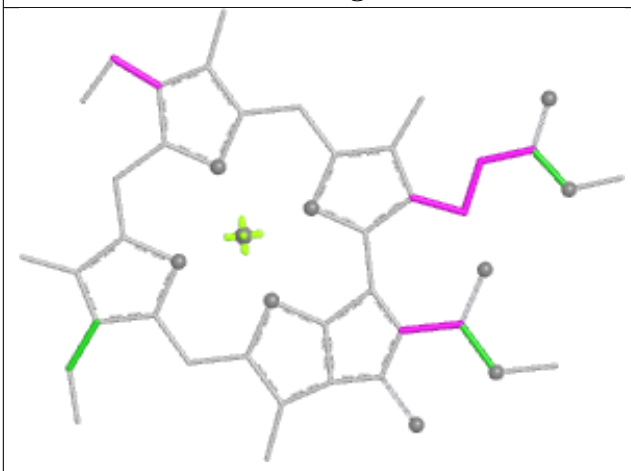
Ligand CLA 9 605



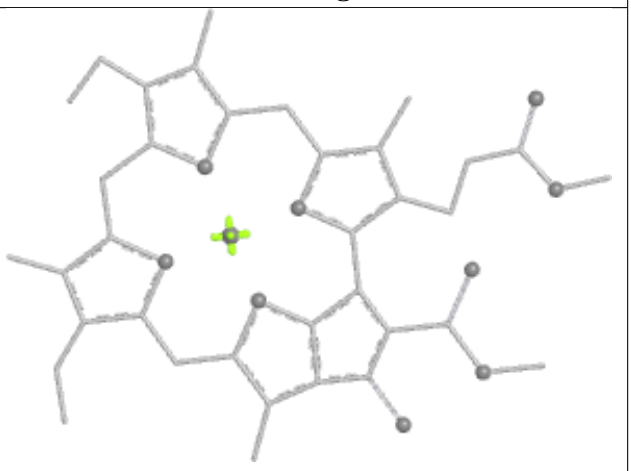
Bond lengths



Bond angles

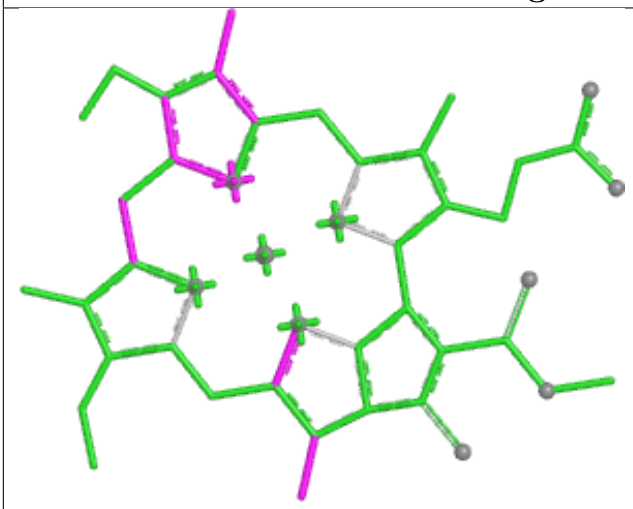


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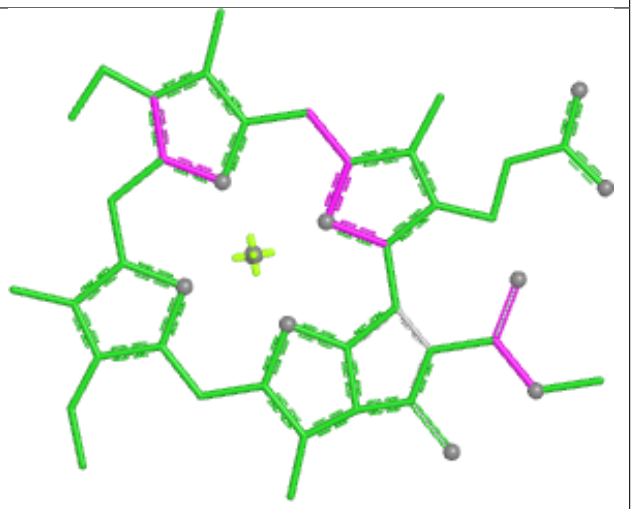


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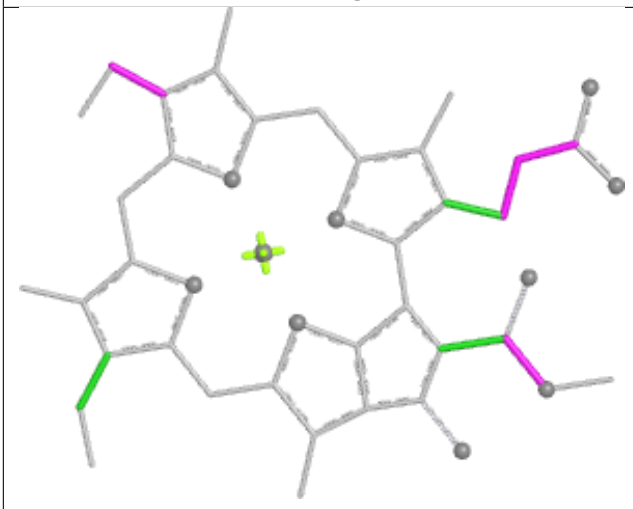
Ligand CLA 0 611



Bond lengths



Bond angles

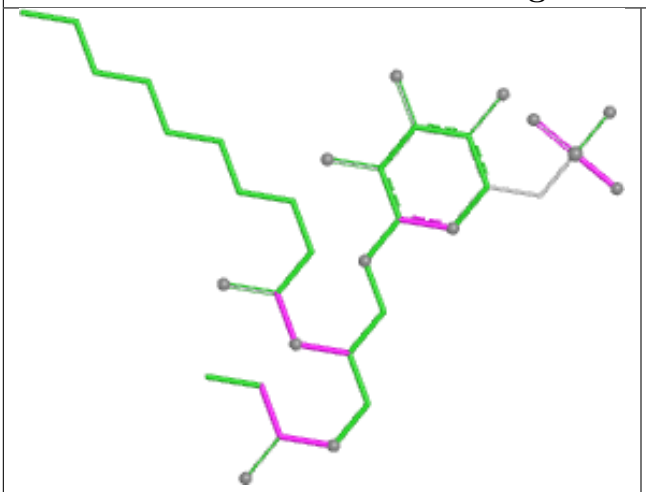


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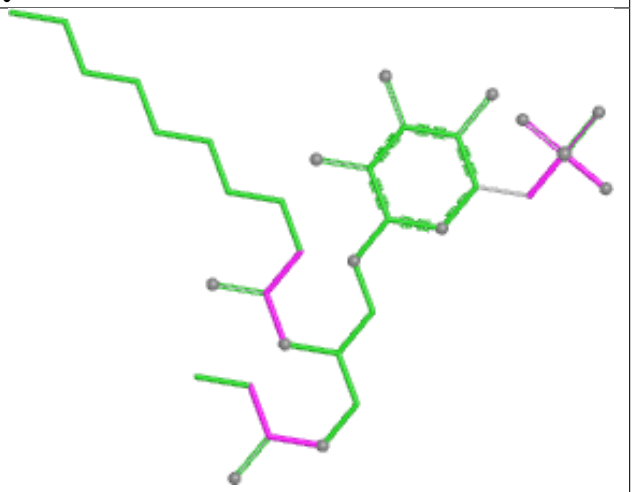


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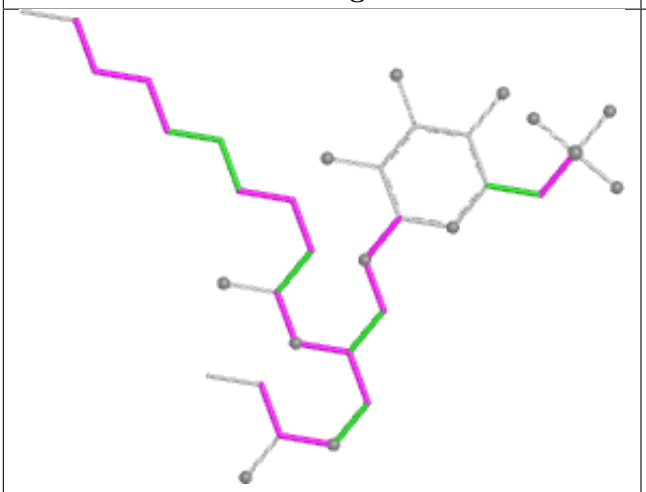
Ligand SQD 5 318



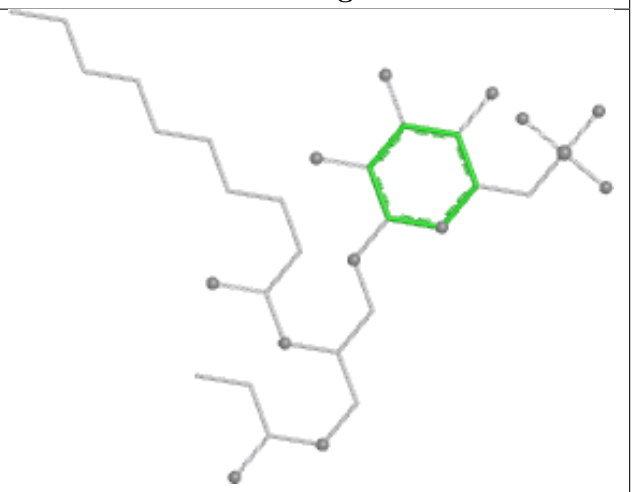
Bond lengths



Bond angles

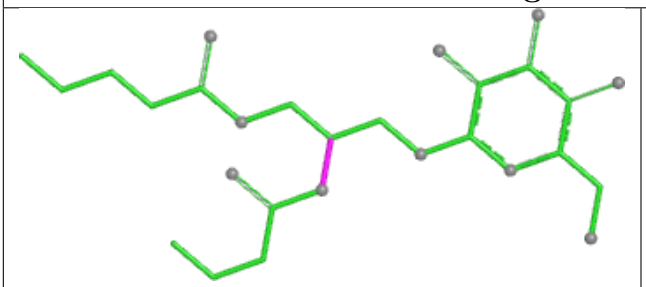


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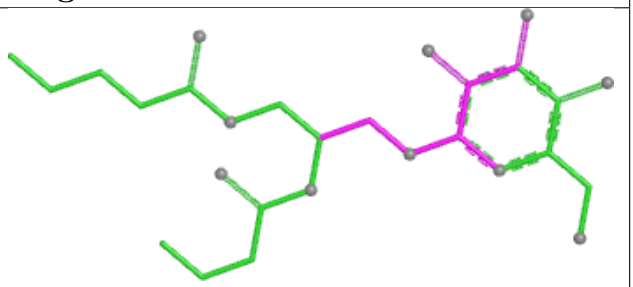


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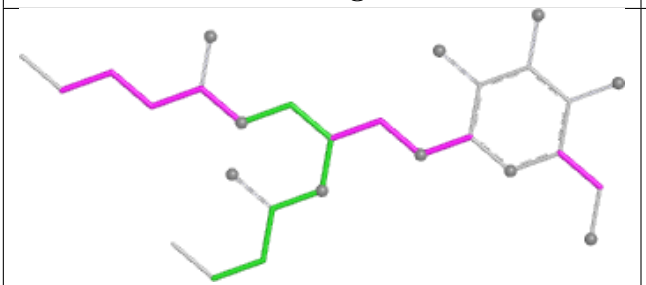
Ligand LMG g 101



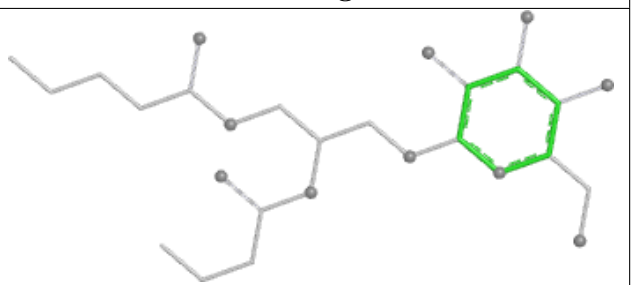
Bond lengths



Bond angles

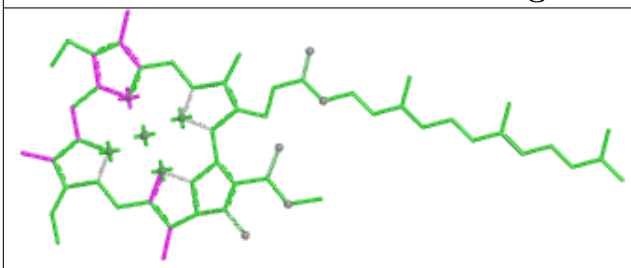


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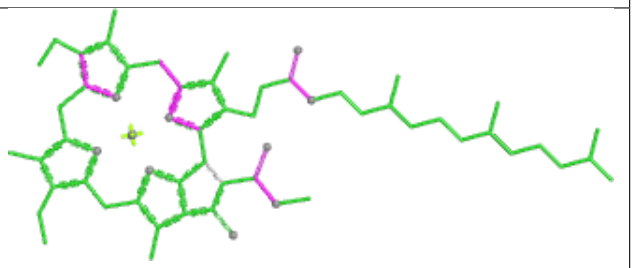


Rings

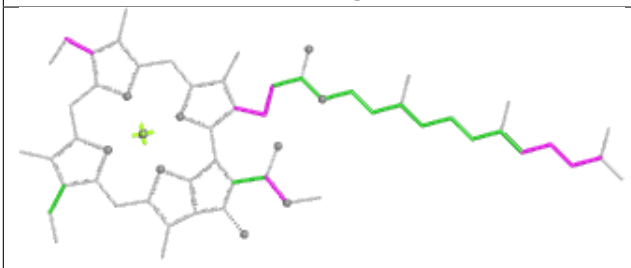
Ligand CLA 2 608



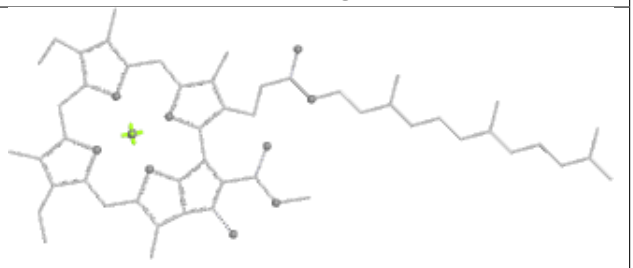
Bond lengths



Bond angles

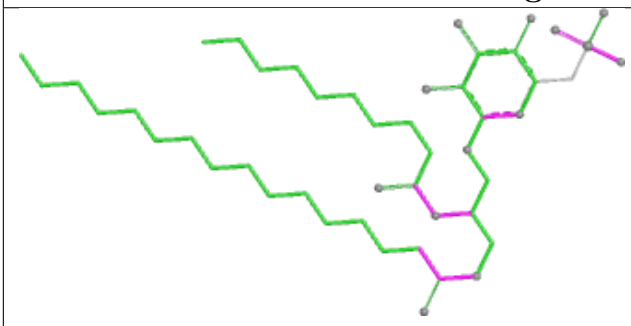


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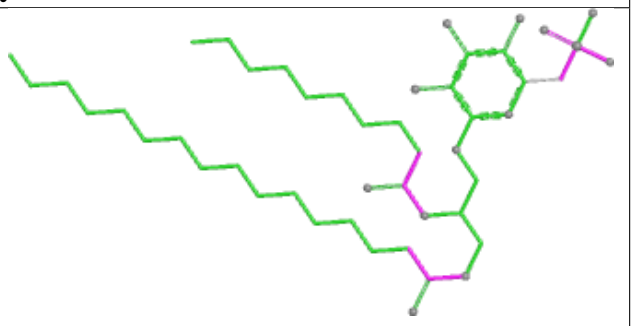


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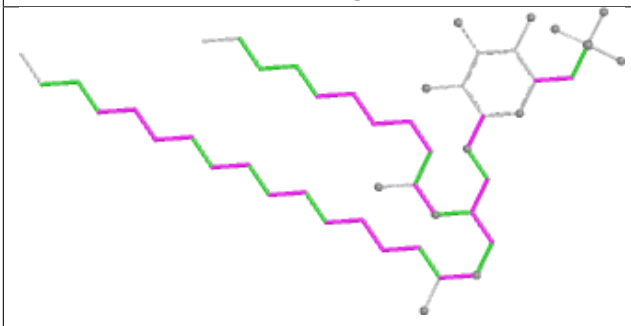
Ligand SQD B 601



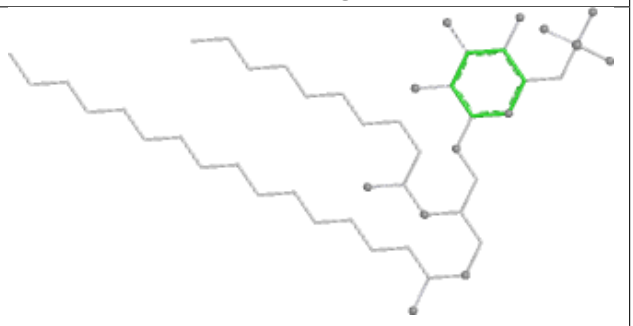
Bond lengths



Bond angles

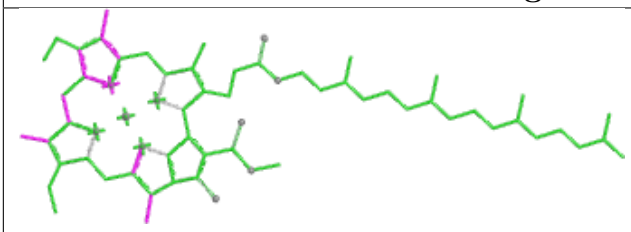


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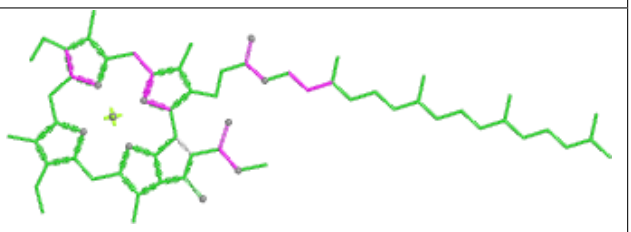


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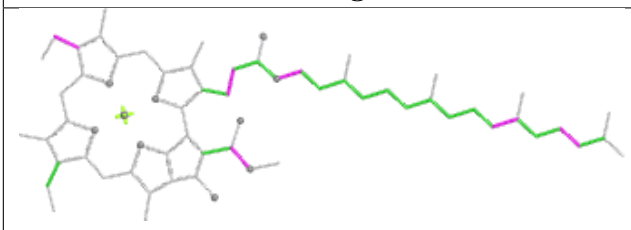
Ligand CLA B 611



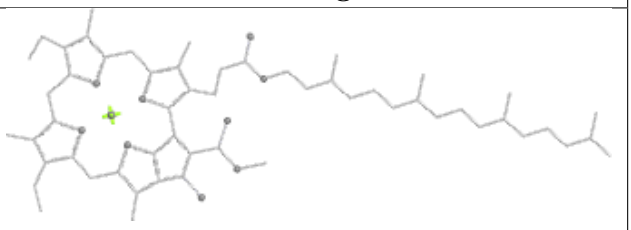
Bond lengths



Bond angles

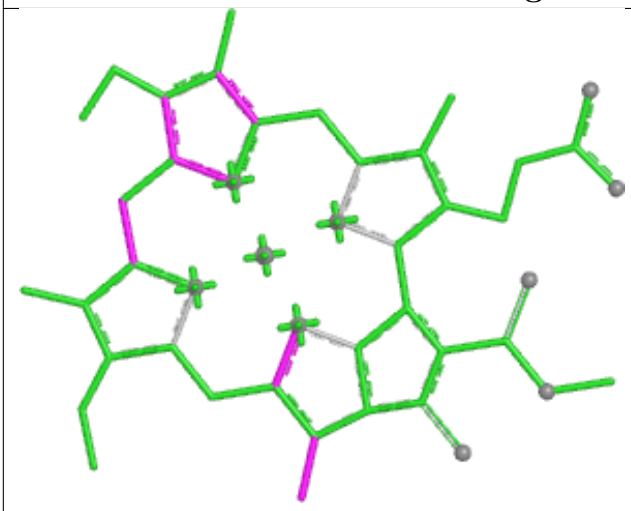


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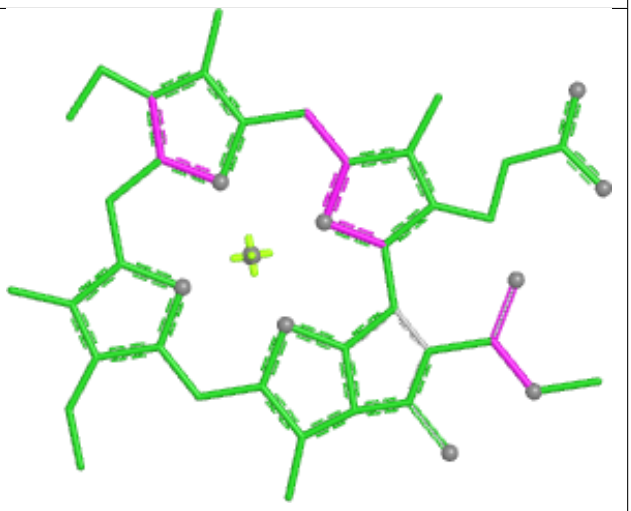


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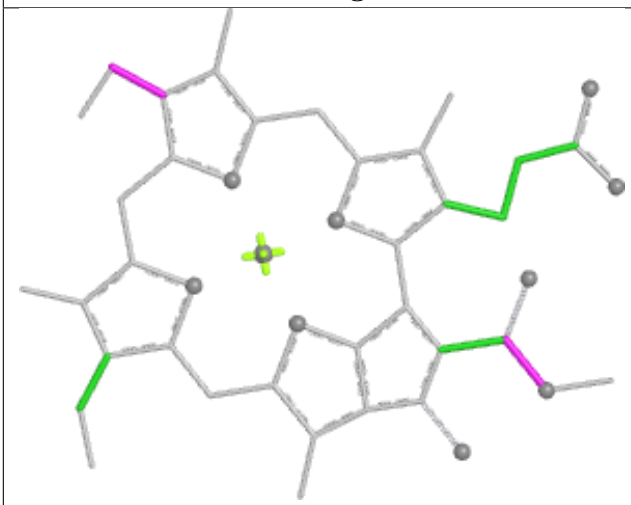
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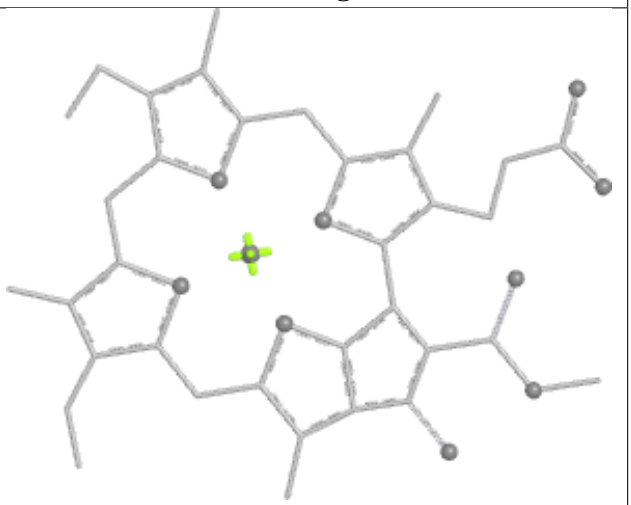
Bond lengths



Bond angles

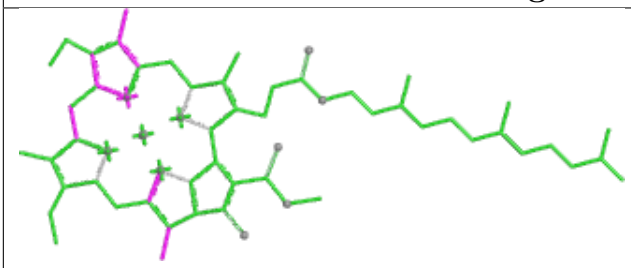


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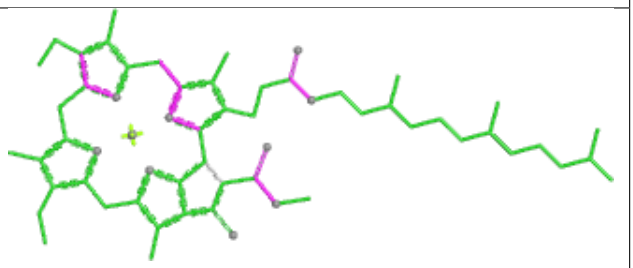


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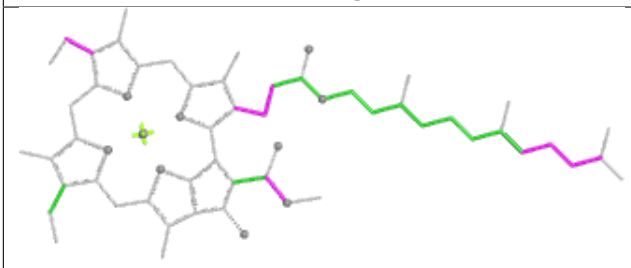
Ligand CLA 5 309



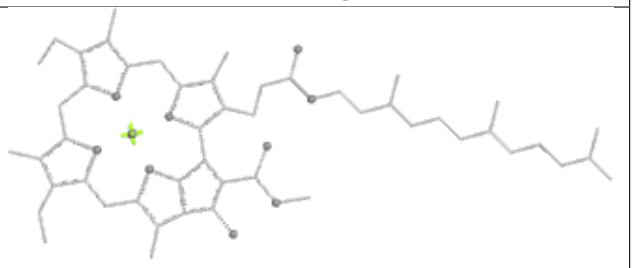
Bond lengths



Bond angles

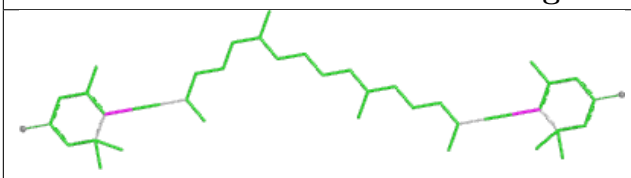


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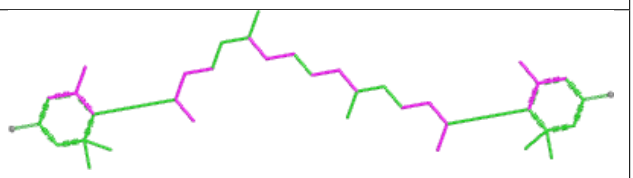


Rings

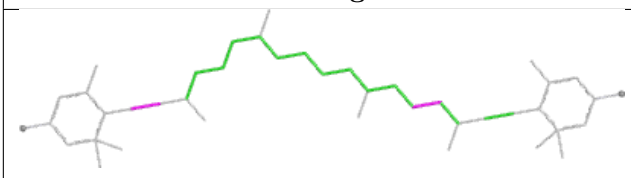
Ligand II0 2 619



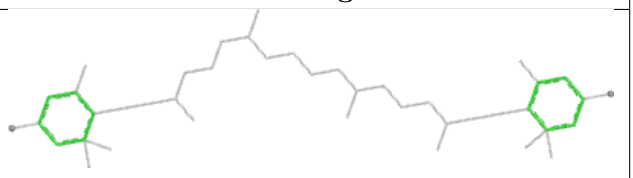
Bond lengths



Bond angles

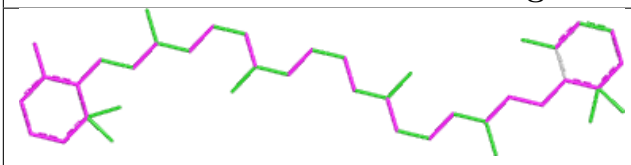


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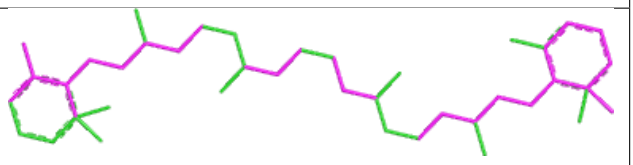


Rings

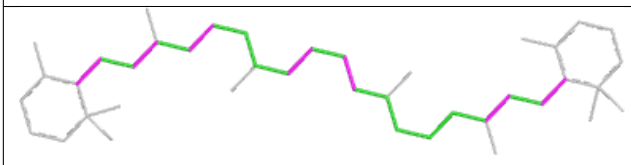
Ligand 8CT C 518



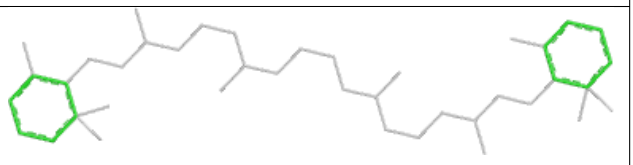
Bond lengths



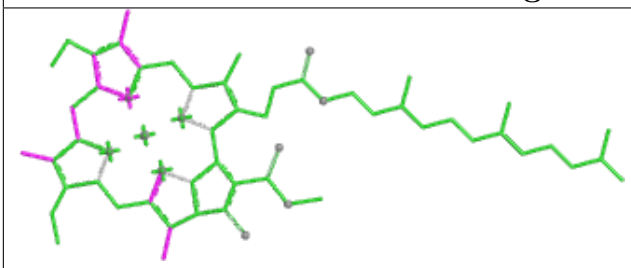
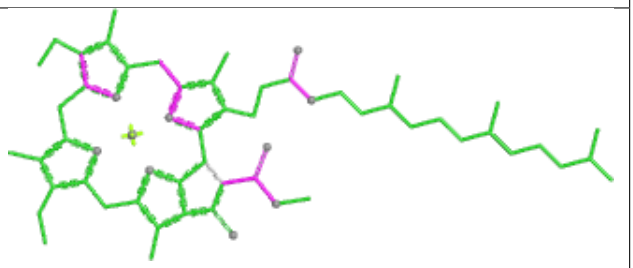
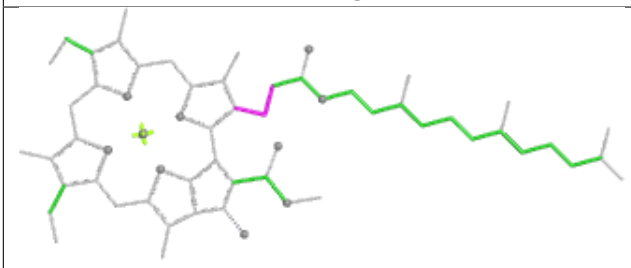
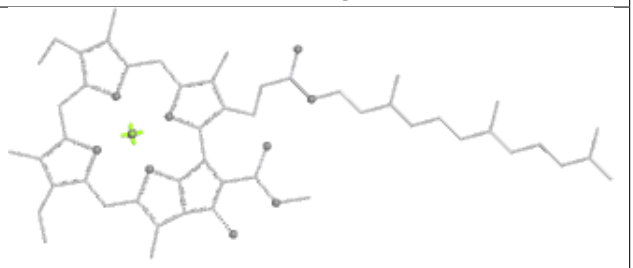
Bond angles

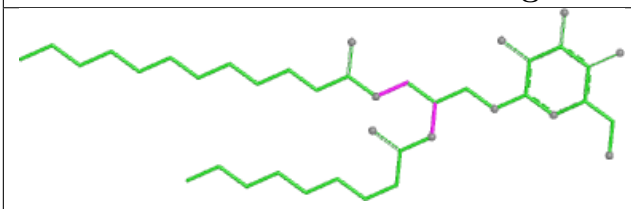
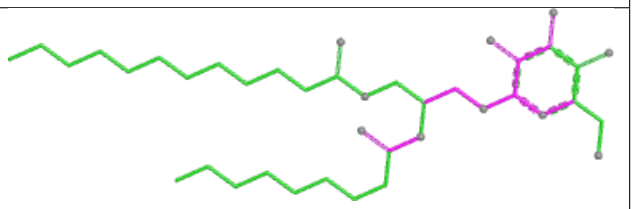
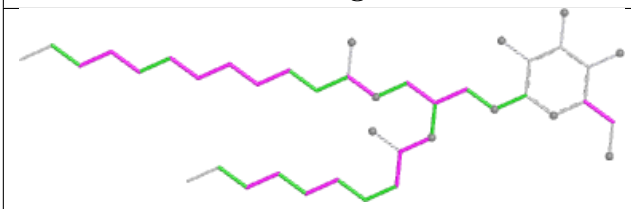
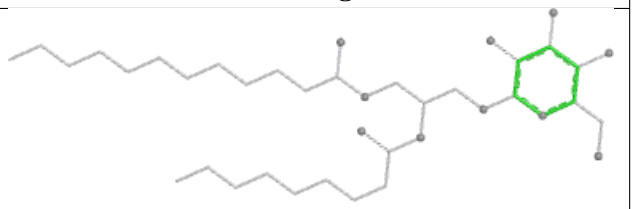


Torsions

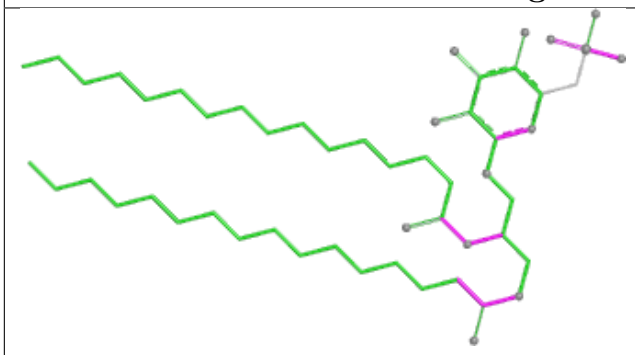


Rings

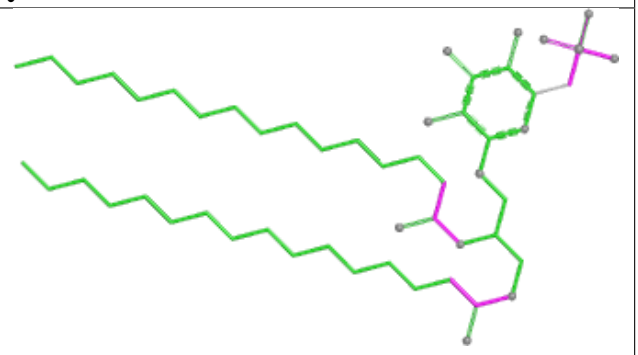
Ligand CLA A 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG L 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

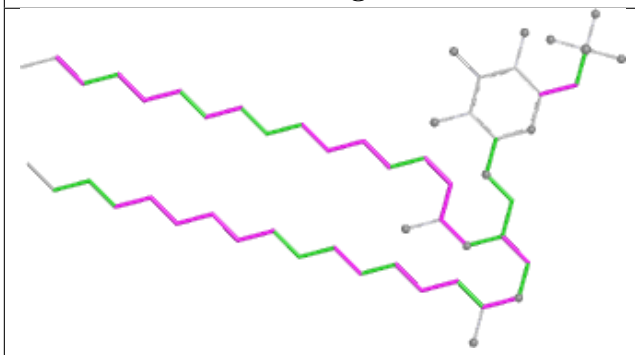
Ligand SQD b 620



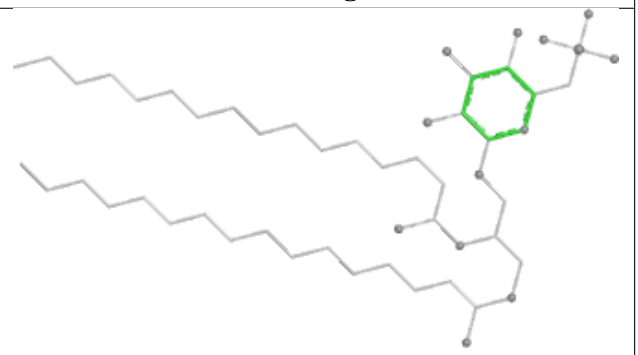
Bond lengths



Bond angles

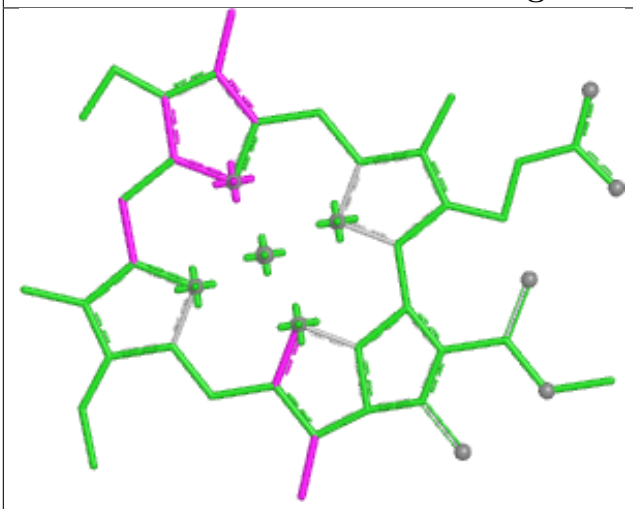


Torsions

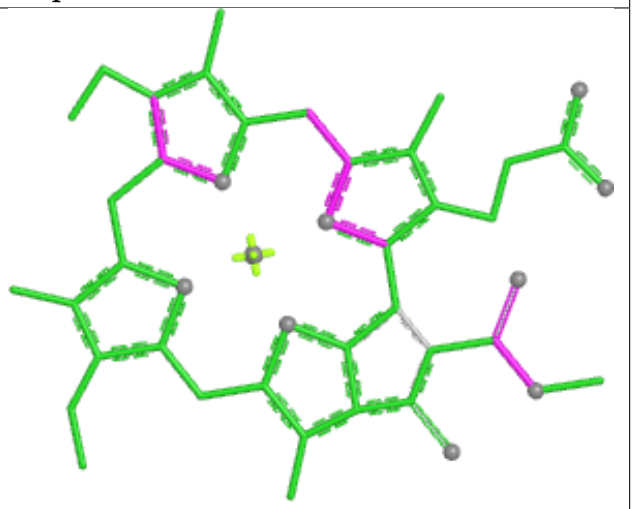


Rings

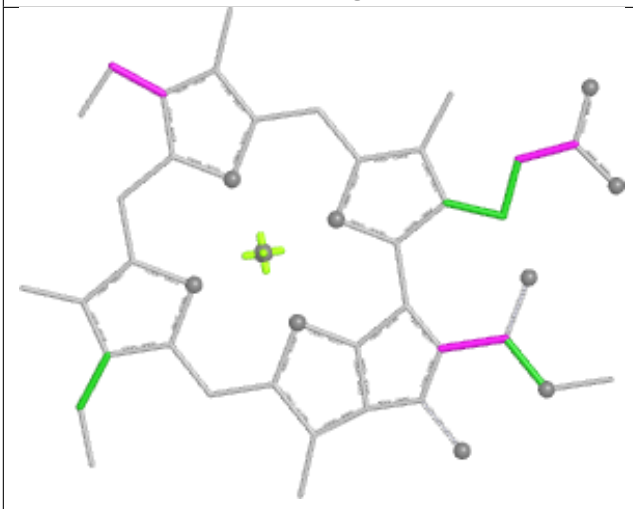
Ligand CLA p 307



Bond lengths



Bond angles

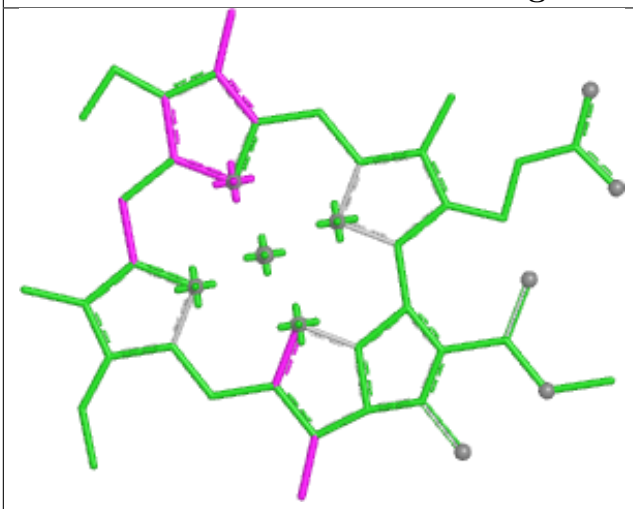


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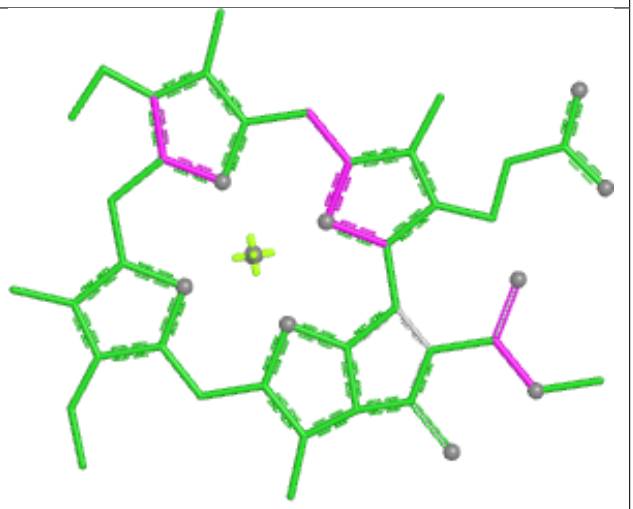


Rings

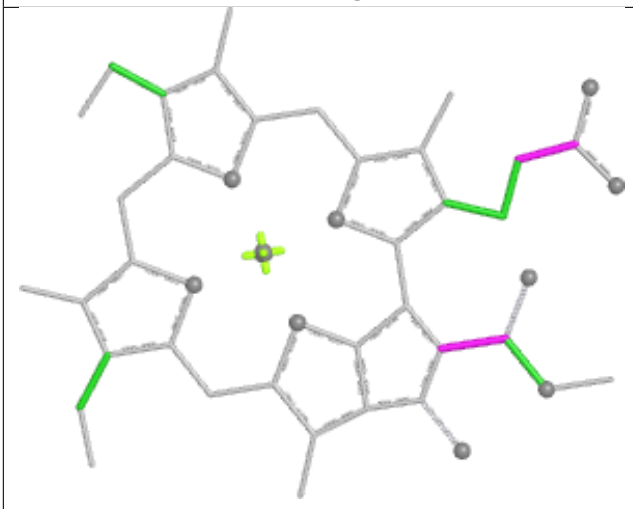
Ligand CLA 2 606



Bond lengths



Bond angles

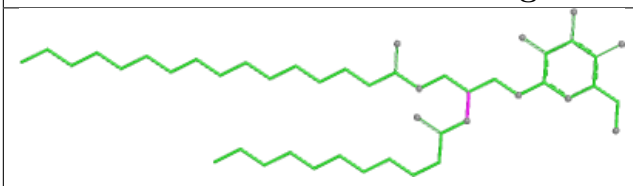


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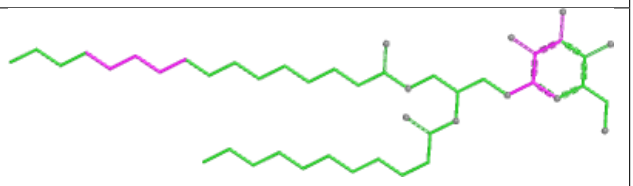


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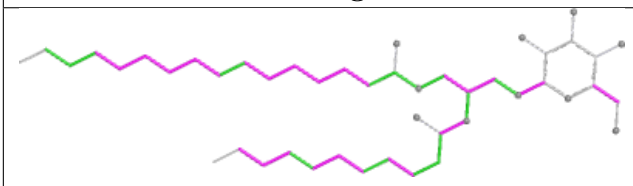
Ligand LMG C 517



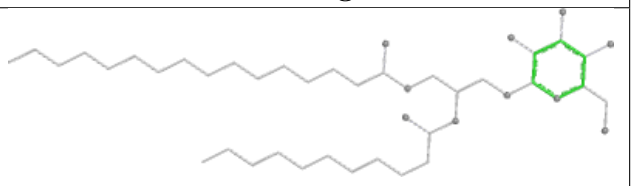
Bond lengths



Bond angles

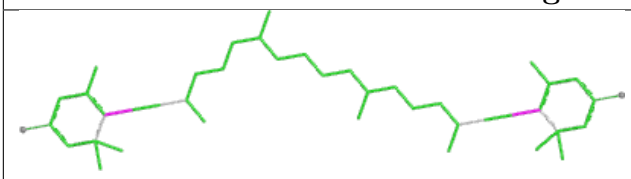


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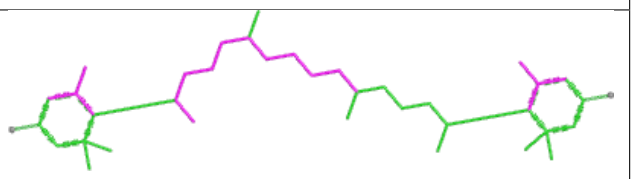


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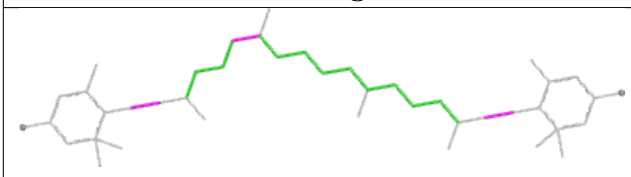
Ligand II0 3 614



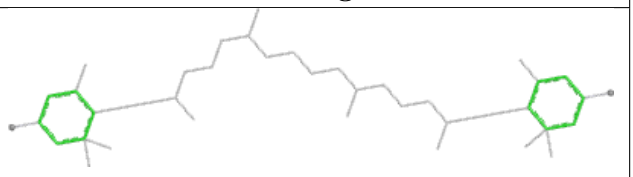
Bond lengths



Bond angles

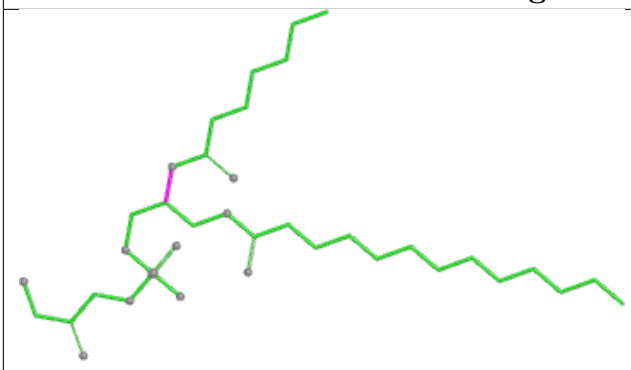


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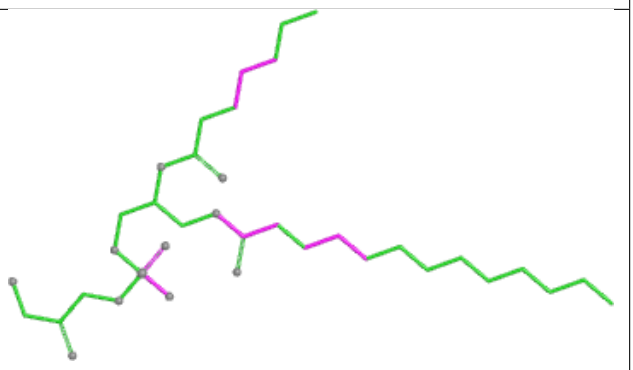


Rings

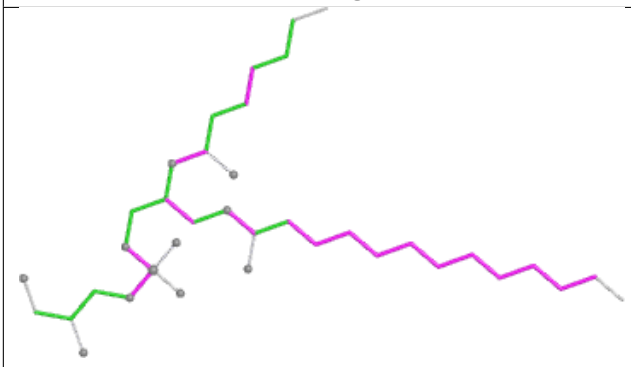
Ligand LHG s 301



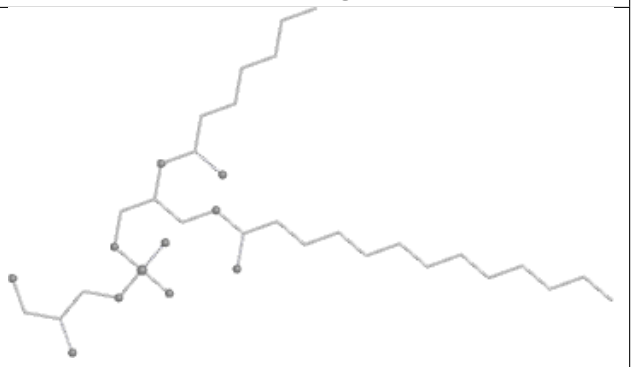
Bond lengths



Bond angles

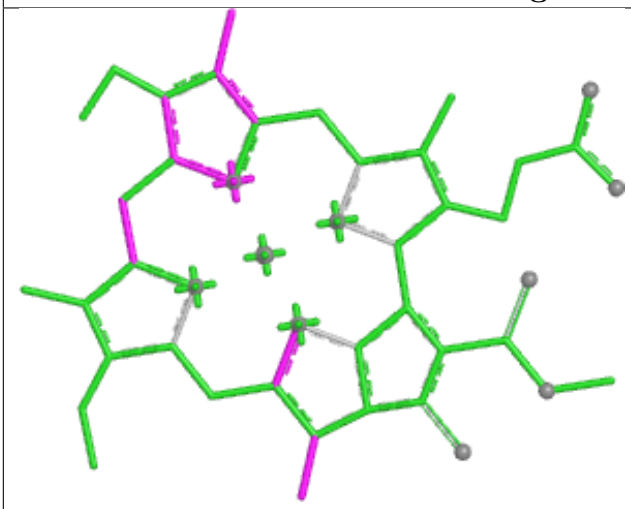


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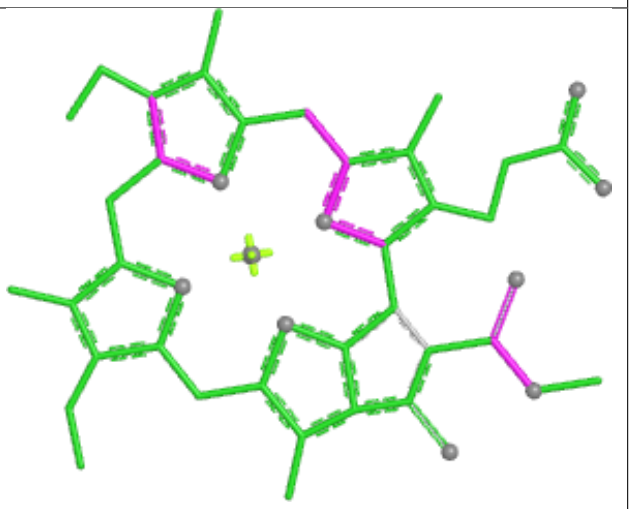


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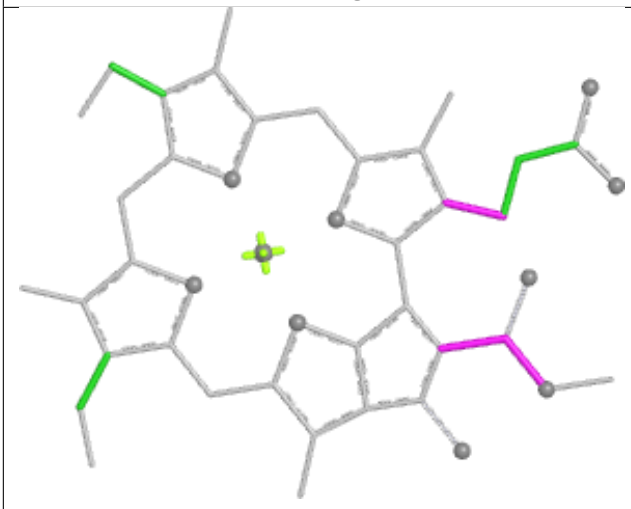
Ligand CLA s 302



Bond lengths



Bond angles

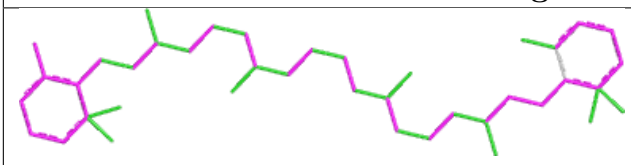


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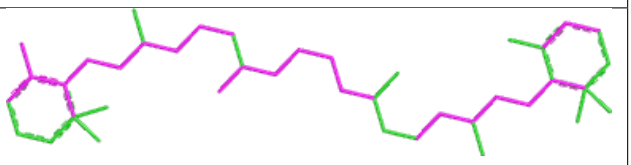


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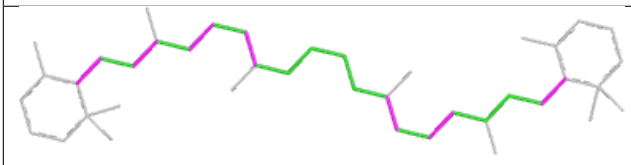
Ligand 8CT 3 615



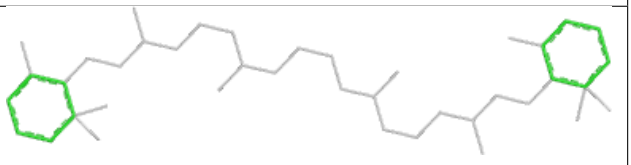
Bond lengths



Bond angles

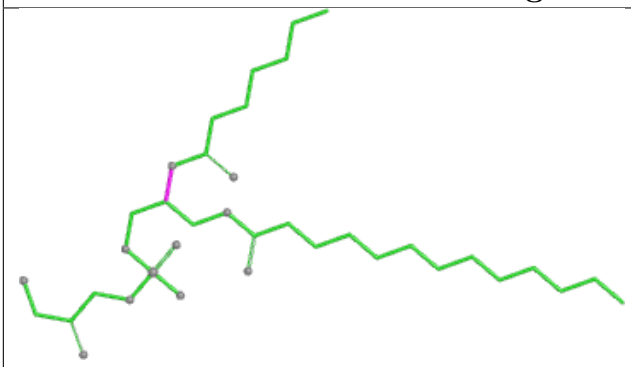


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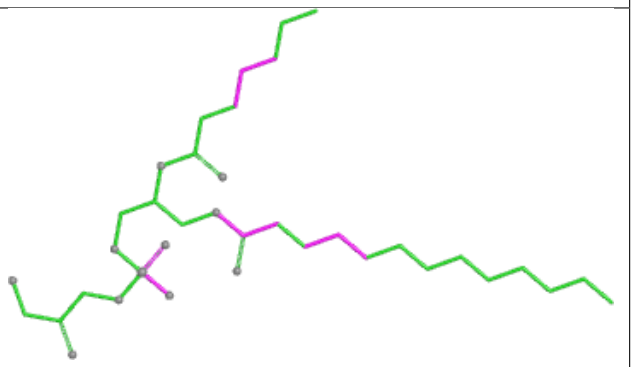


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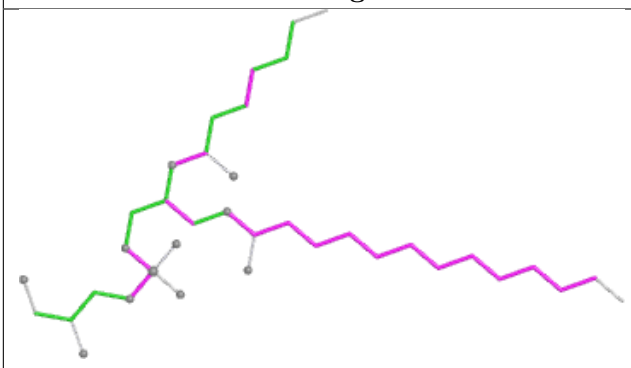
Ligand LHG S 301



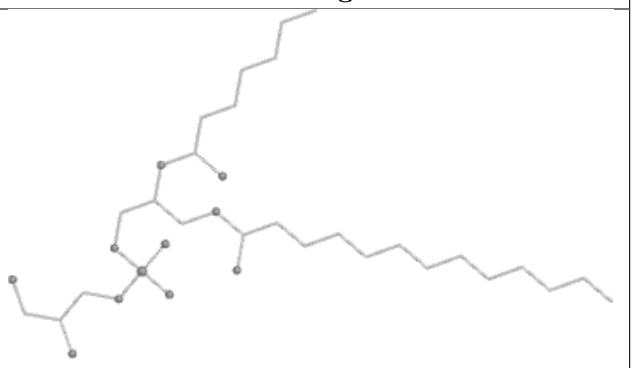
Bond lengths



Bond angles



Torsions

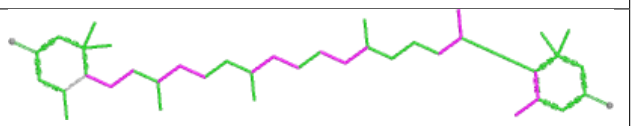


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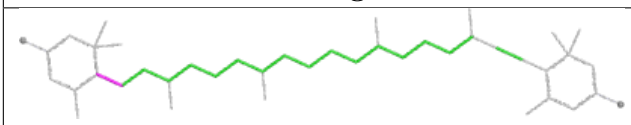
Ligand II3 1 615



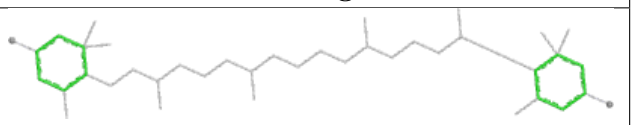
Bond lengths



Bond angles

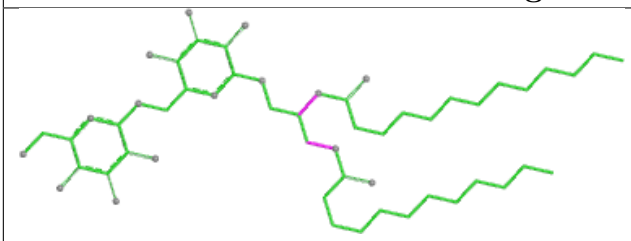


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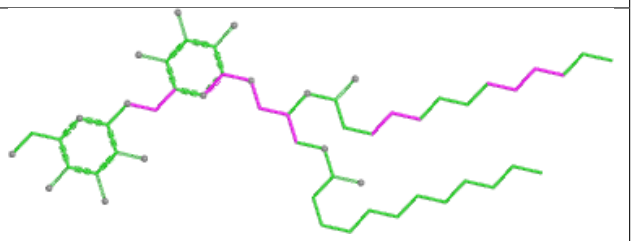


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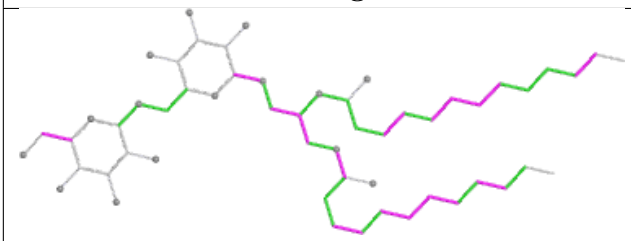
Ligand DGD c 516



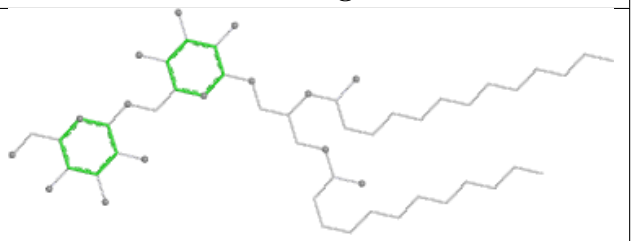
Bond lengths



Bond angles

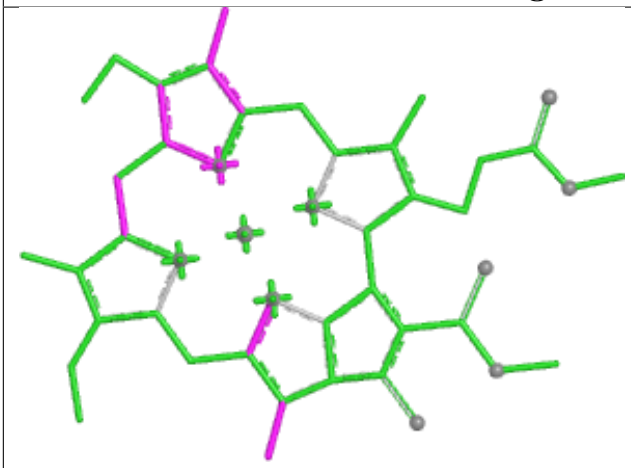


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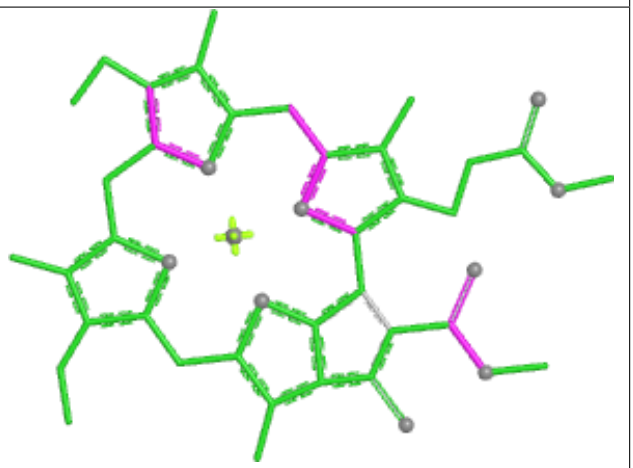


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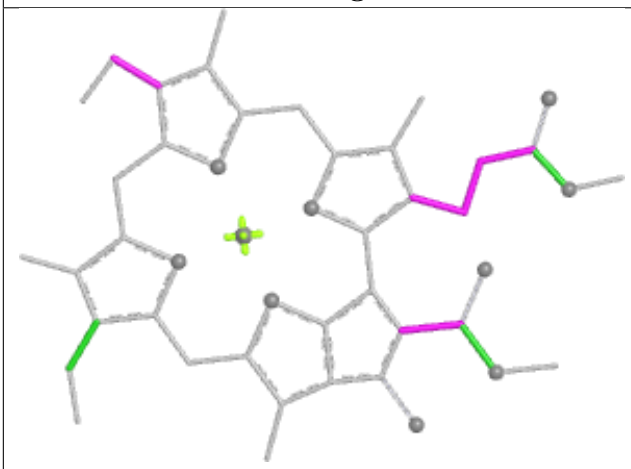
Ligand CLA 3 605



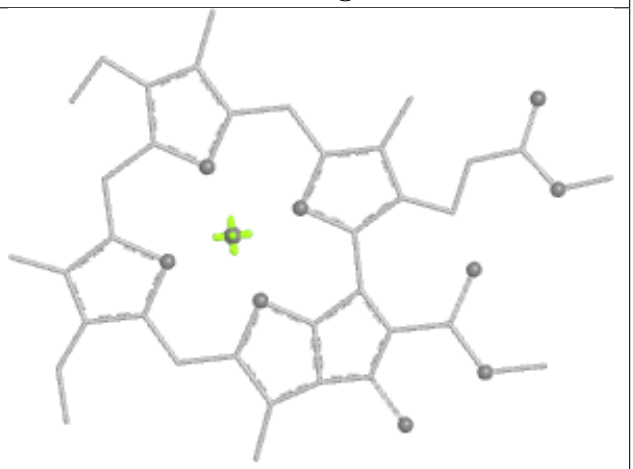
Bond lengths



Bond angles

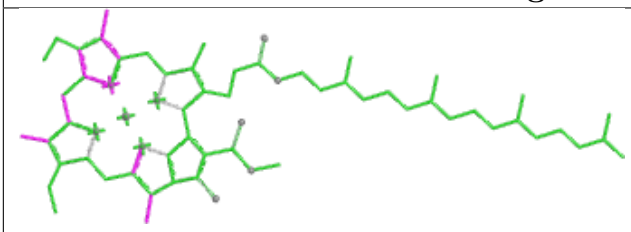


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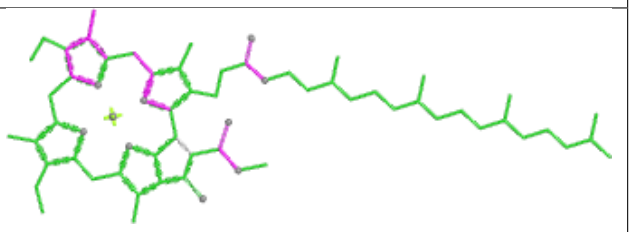


Rings

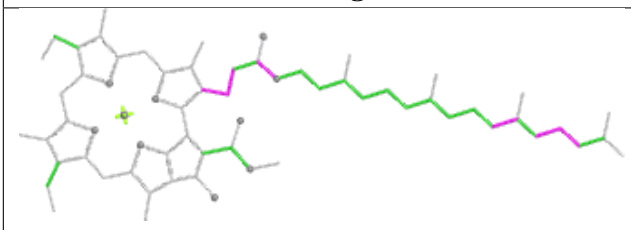
Ligand CLA b 609



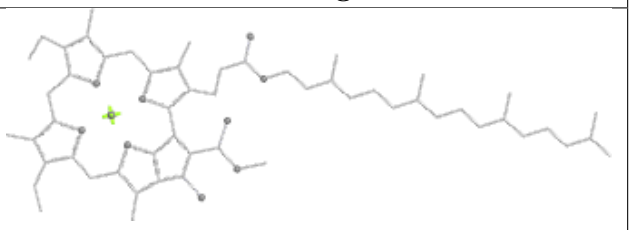
Bond lengths



Bond angles

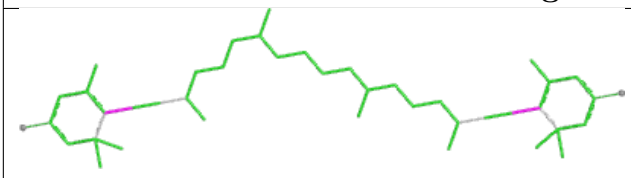


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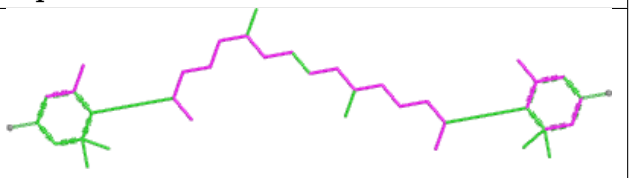


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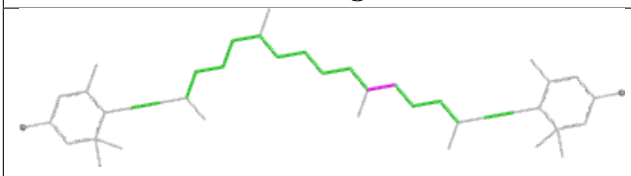
Ligand II0 p 301



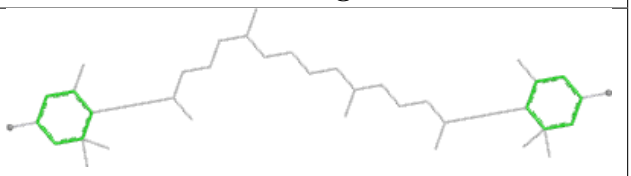
Bond lengths



Bond angles

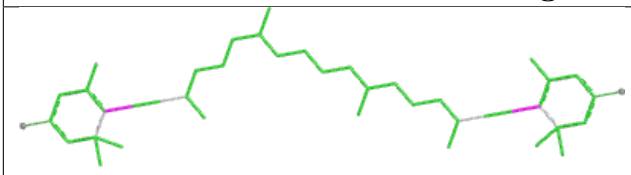


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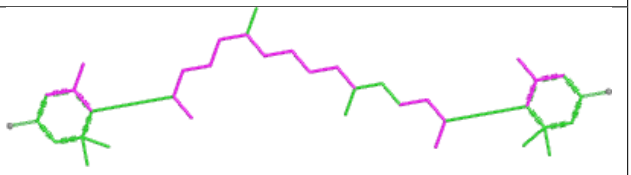


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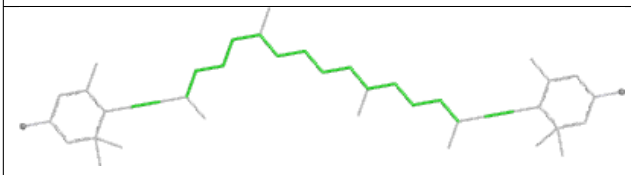
Ligand II0 P 612



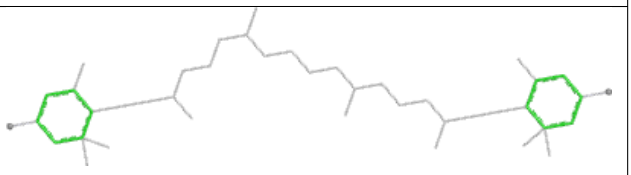
Bond lengths



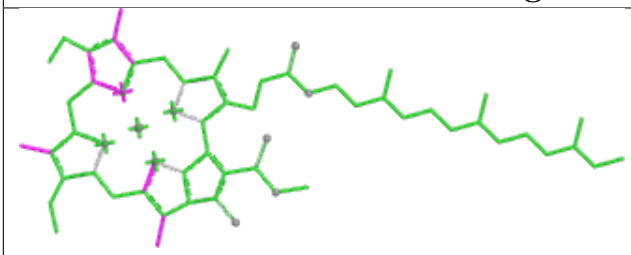
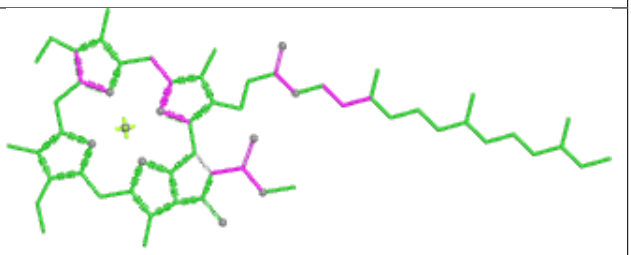
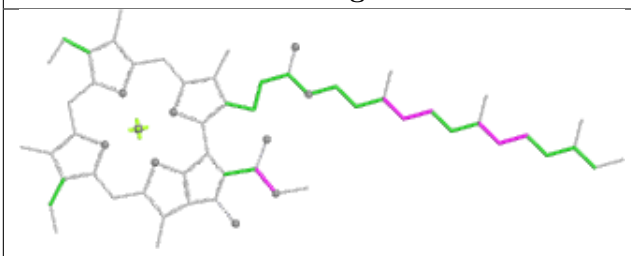
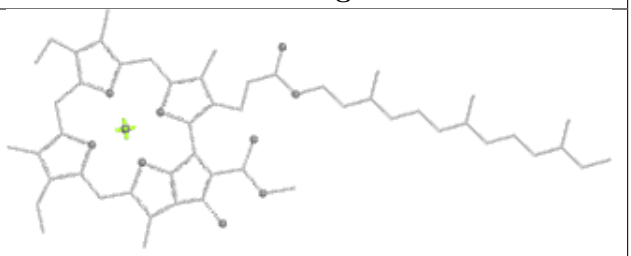
Bond angles

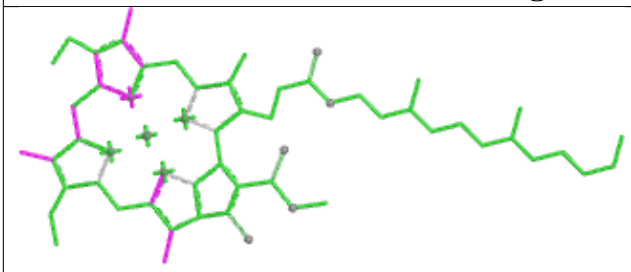
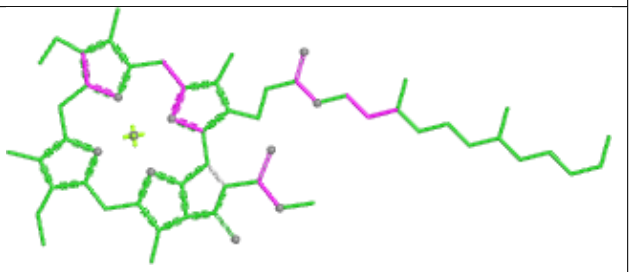
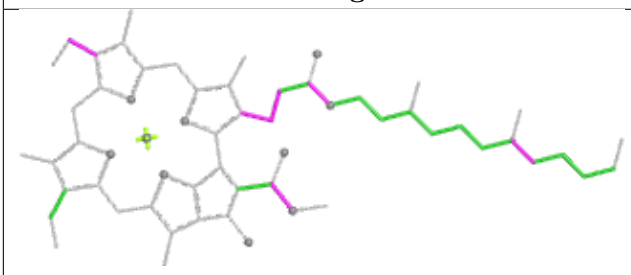
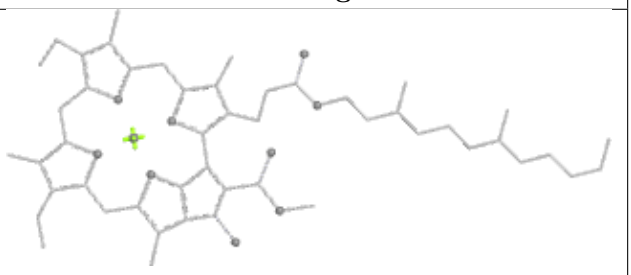


Torsions

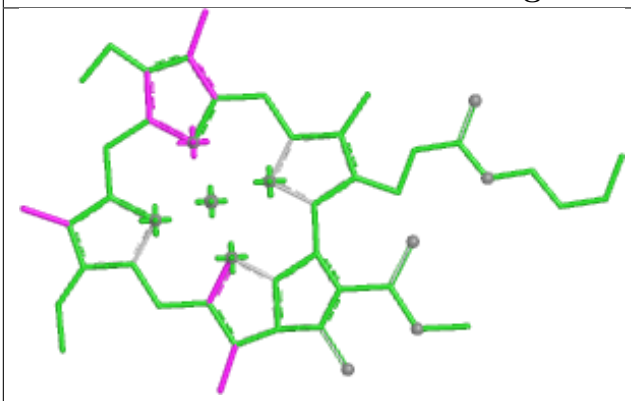


Rings

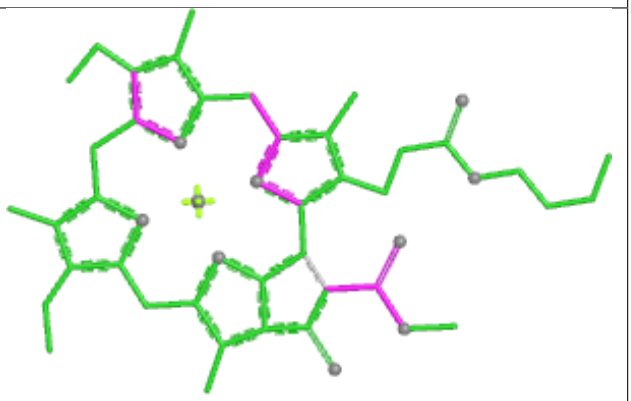
Ligand CLA B 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 8 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

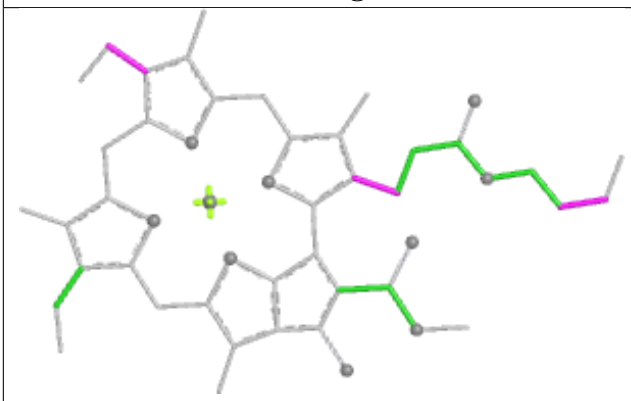
Ligand CLA A 603



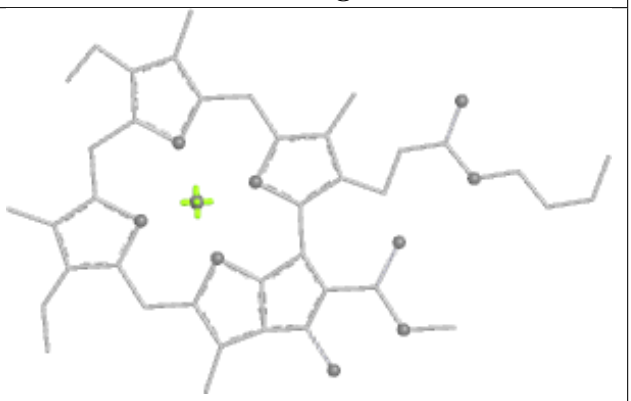
Bond lengths



Bond angles

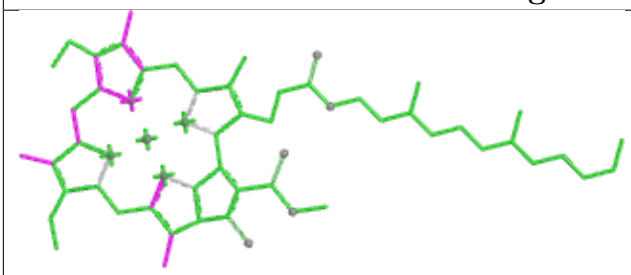


Torsions

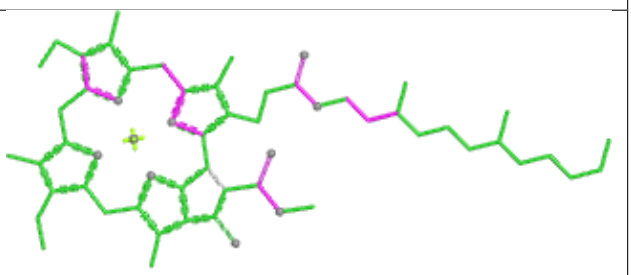


Rings

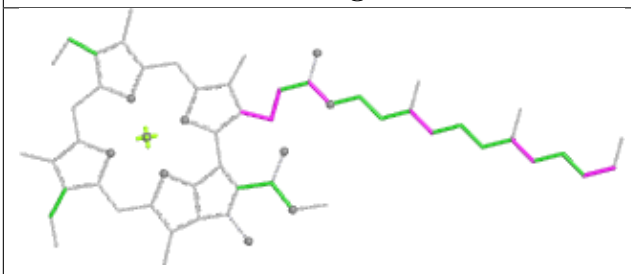
Ligand CLA 3 602



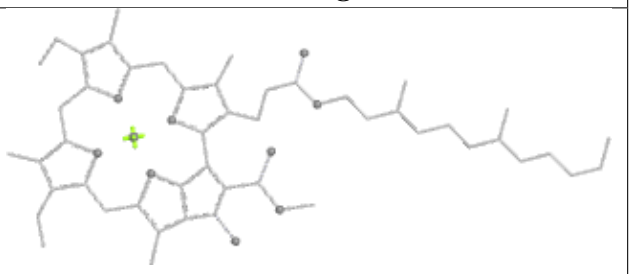
Bond lengths



Bond angles

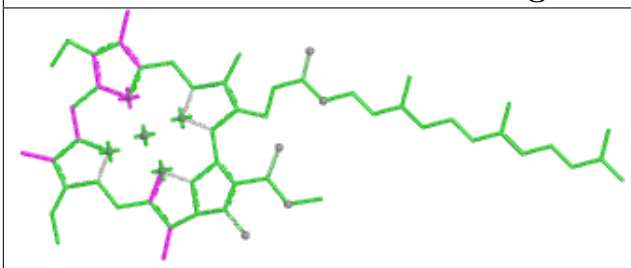


Torsions

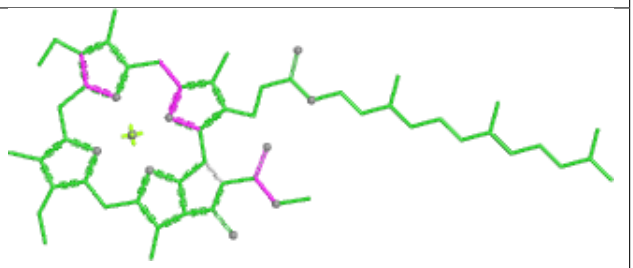


Rings

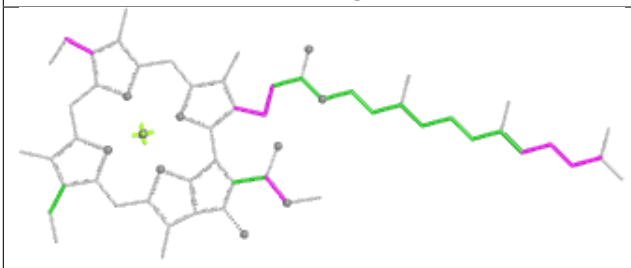
Ligand CLA 1 608



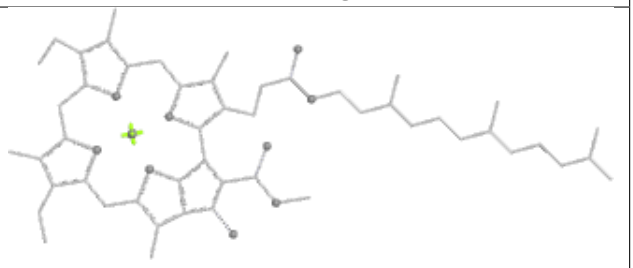
Bond lengths



Bond angles

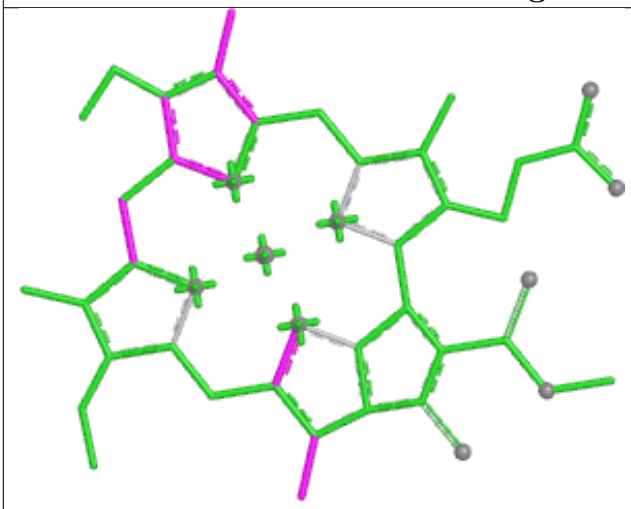


Torsions

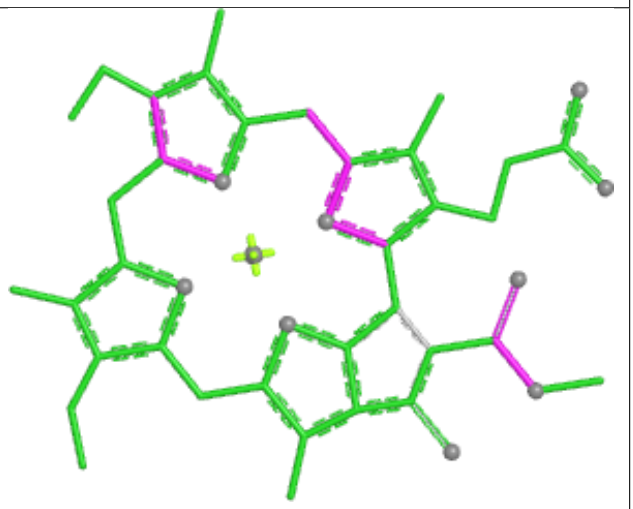


Rings

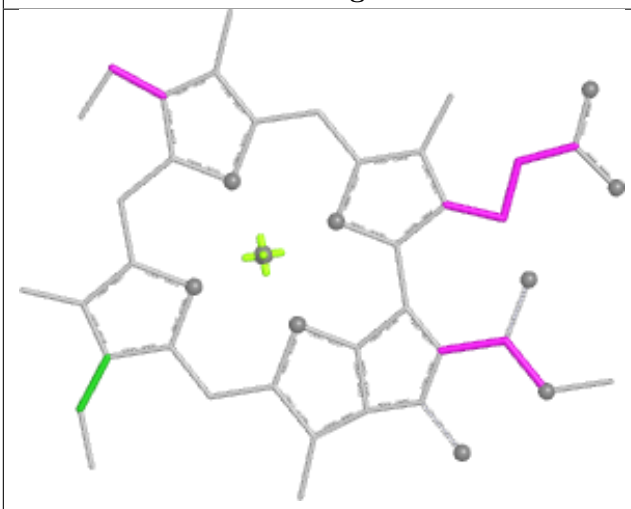
Ligand CLA 5 313



Bond lengths



Bond angles

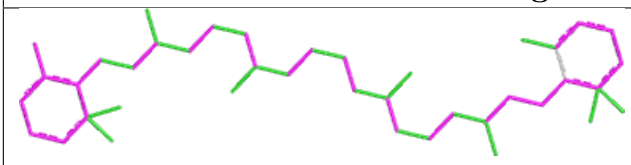


Torsions

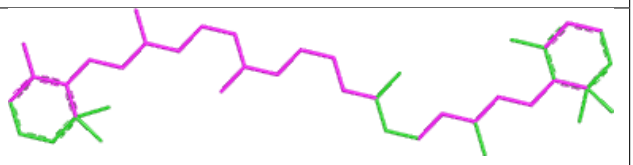


Rings

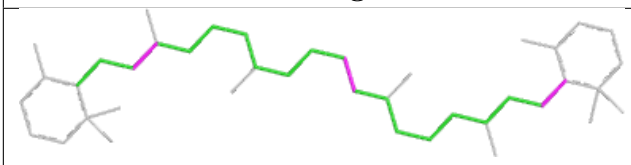
Ligand 8CT 6 615



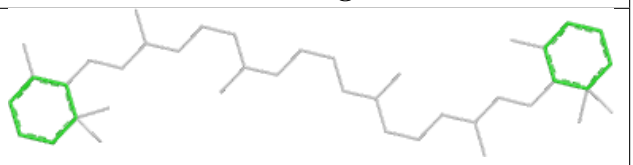
Bond lengths



Bond angles

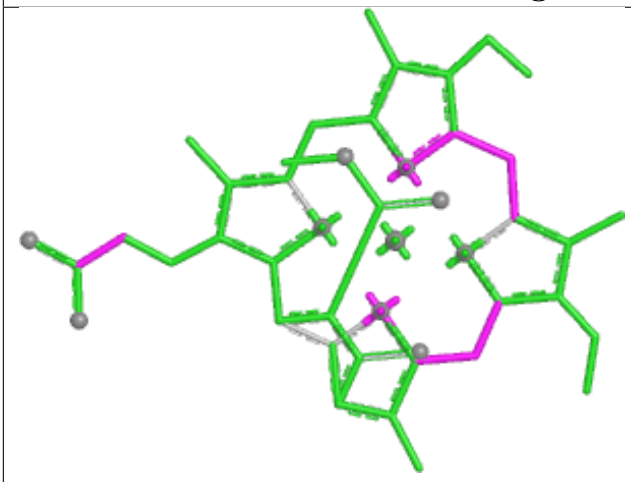


Torsions

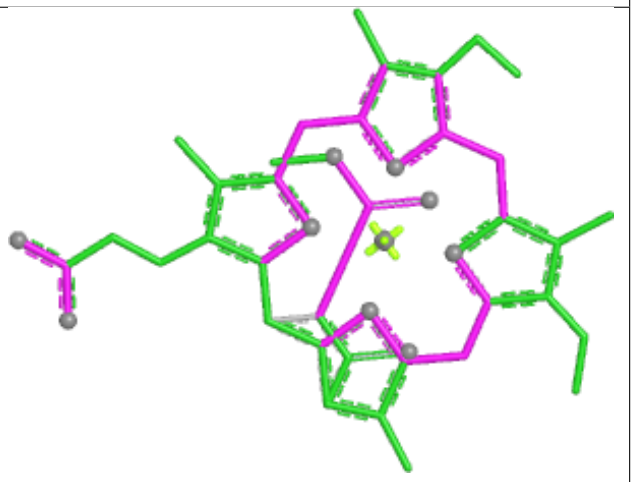


Rings

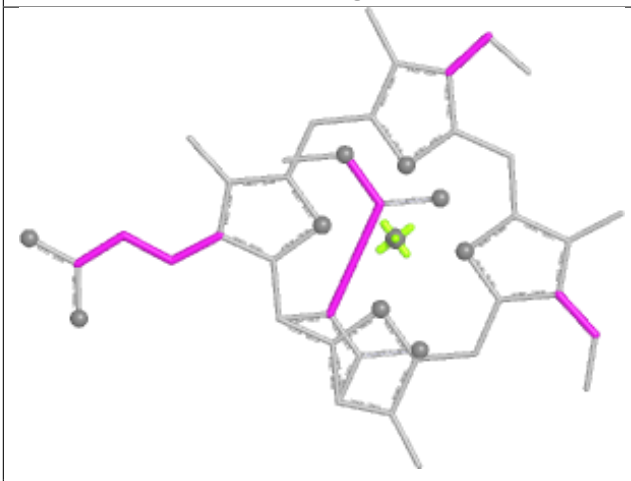
Ligand KC2 4 610



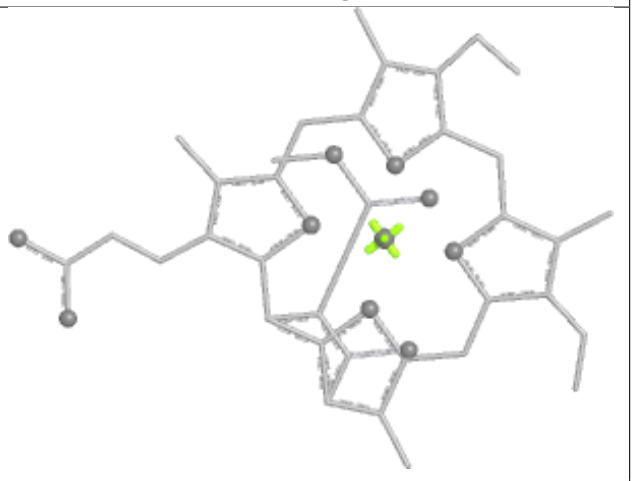
Bond lengths



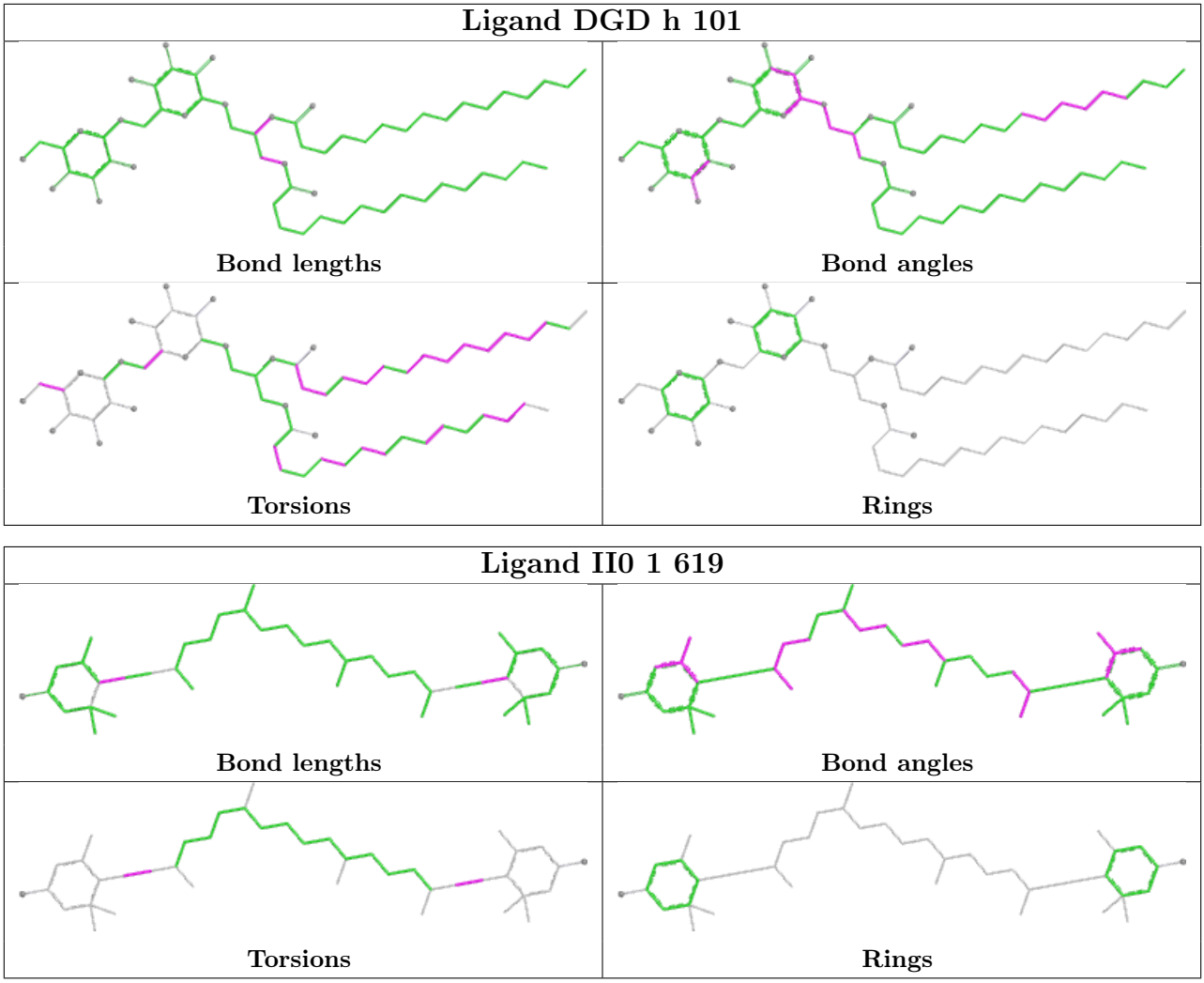
Bond angles



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.

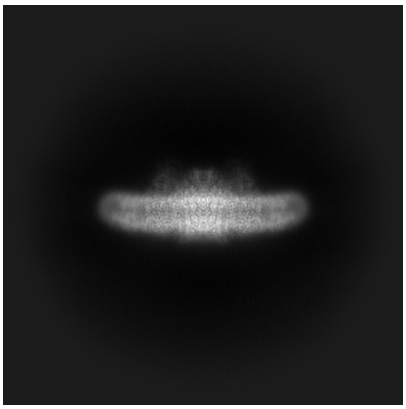
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37414. These allow visual inspection of the internal detail of the map and identification of artifacts.

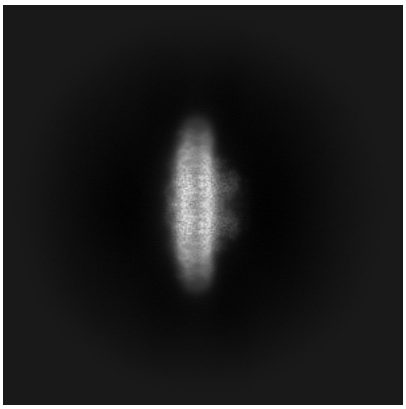
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

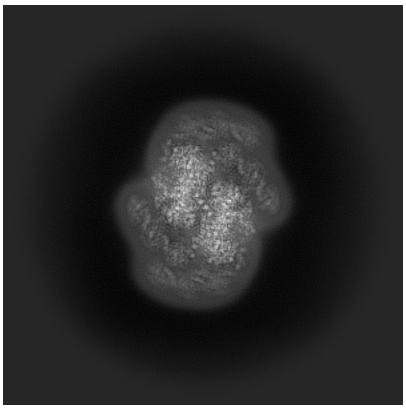
6.1.1 Primary map



X

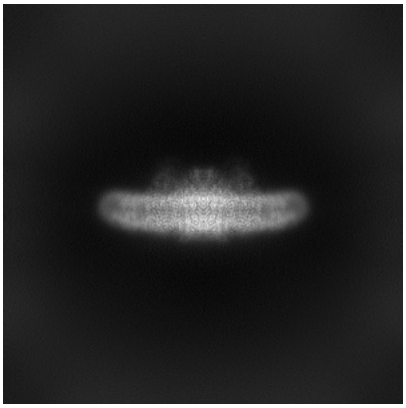


Y

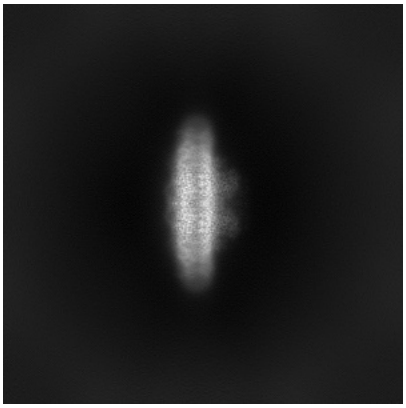


Z

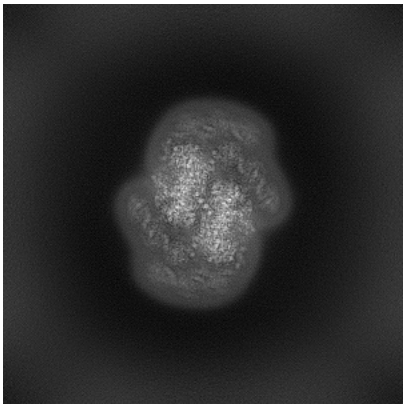
6.1.2 Raw map



X



Y

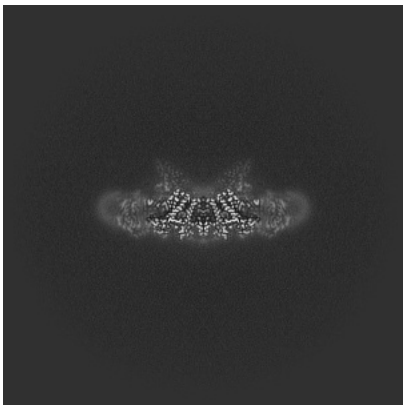


Z

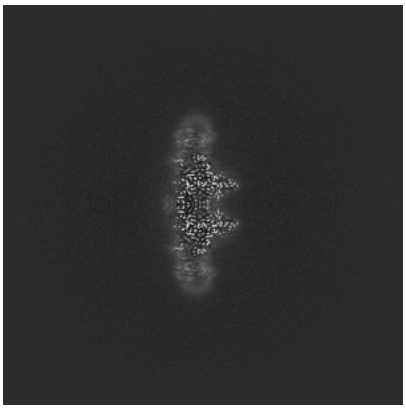
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

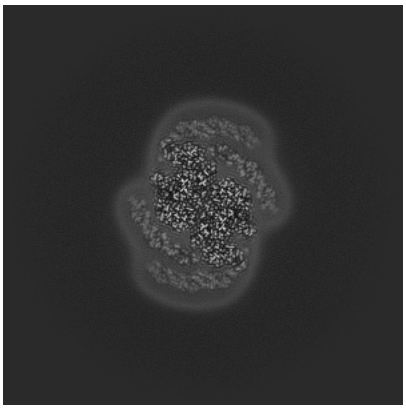
6.2.1 Primary map



X Index: 256

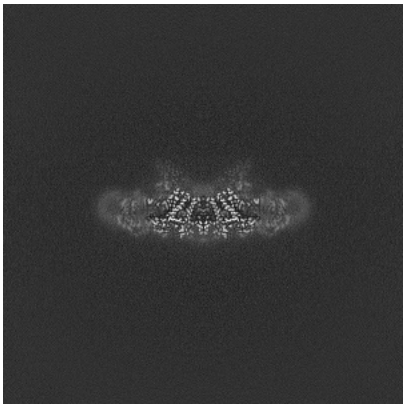


Y Index: 256

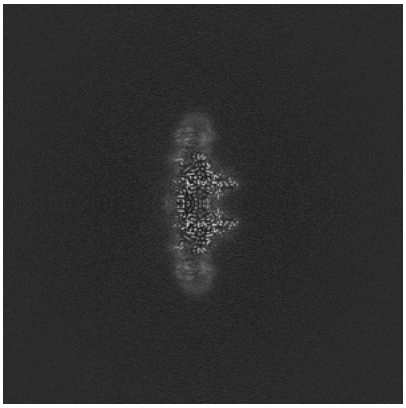


Z Index: 256

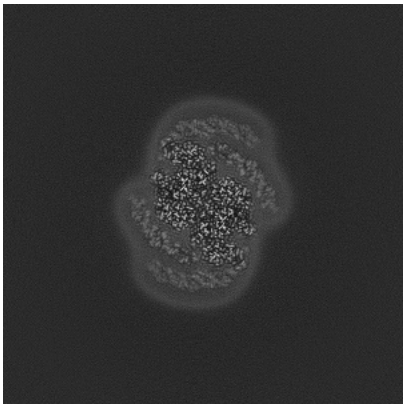
6.2.2 Raw map



X Index: 256



Y Index: 256

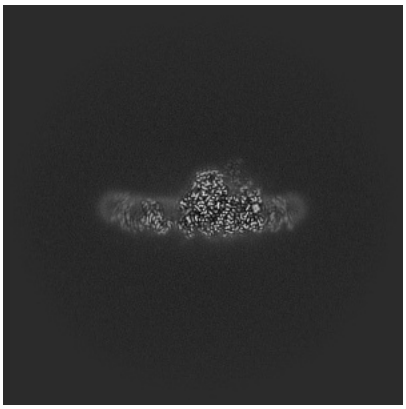


Z Index: 256

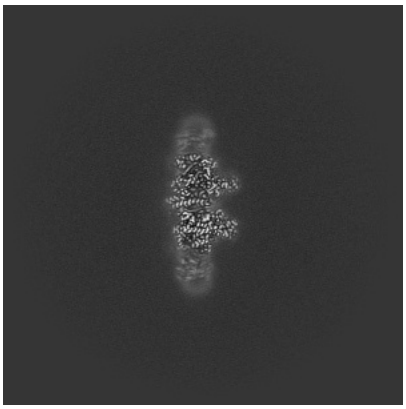
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

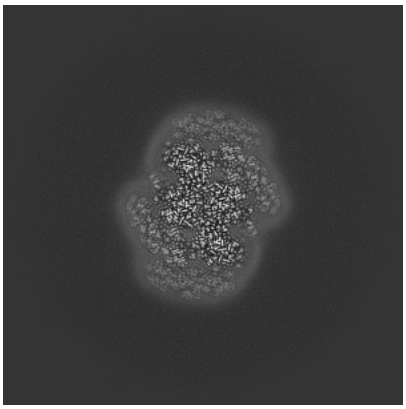
6.3.1 Primary map



X Index: 229

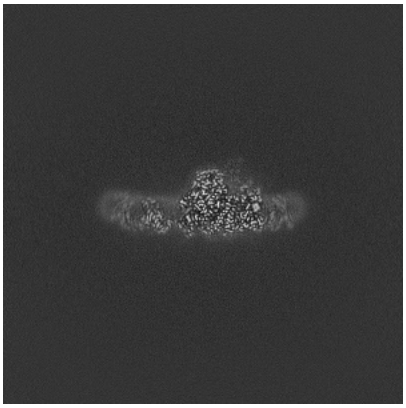


Y Index: 251

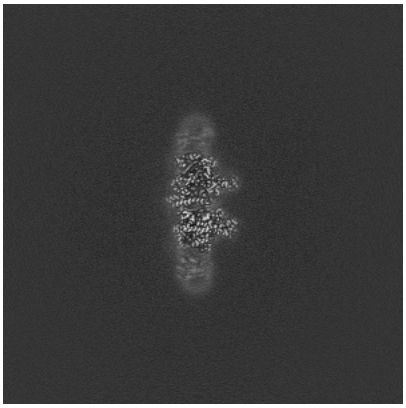


Z Index: 235

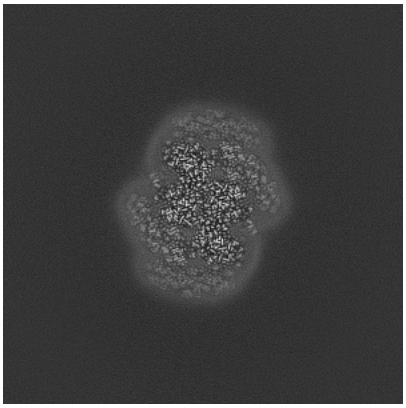
6.3.2 Raw map



X Index: 229



Y Index: 251

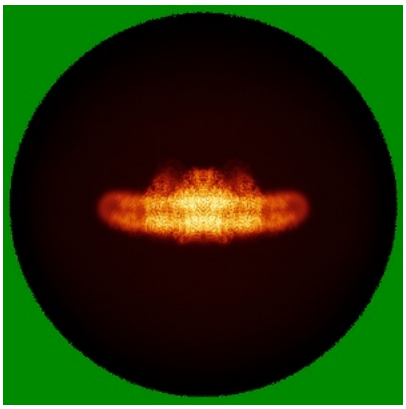


Z Index: 235

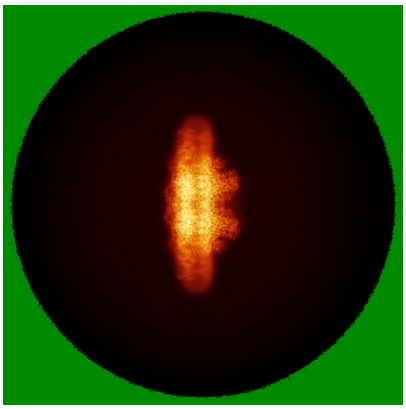
The images above show the largest variance slices of the map in three orthogonal directions.

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

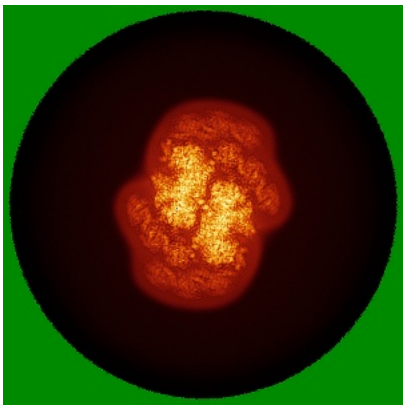
6.4.1 Primary map



X

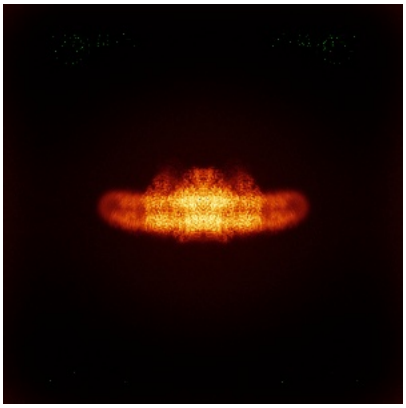


Y

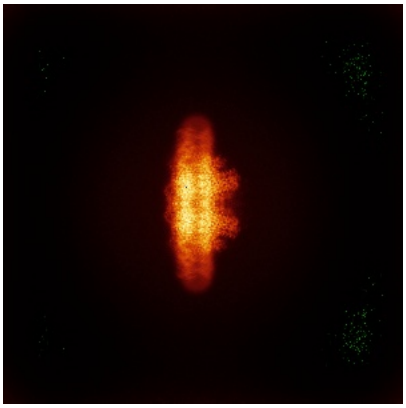


Z

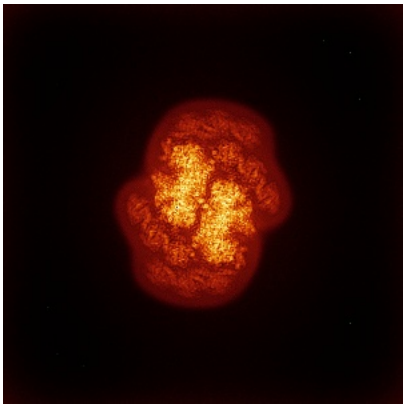
6.4.2 Raw map



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)

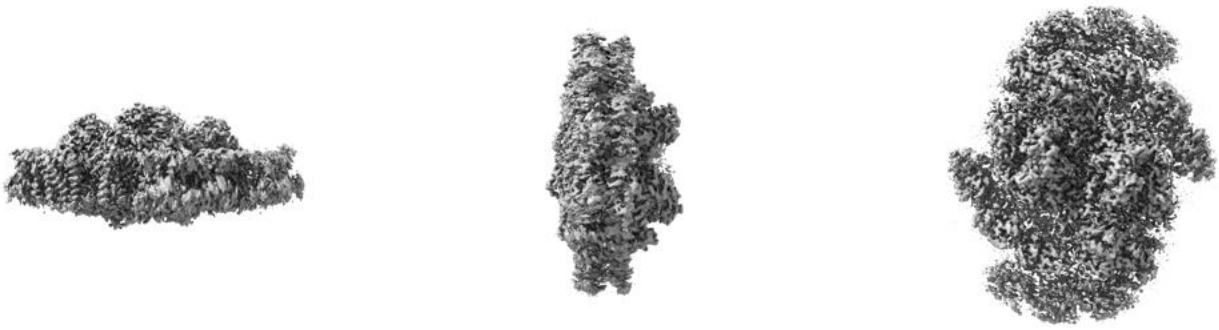
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.253. 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.

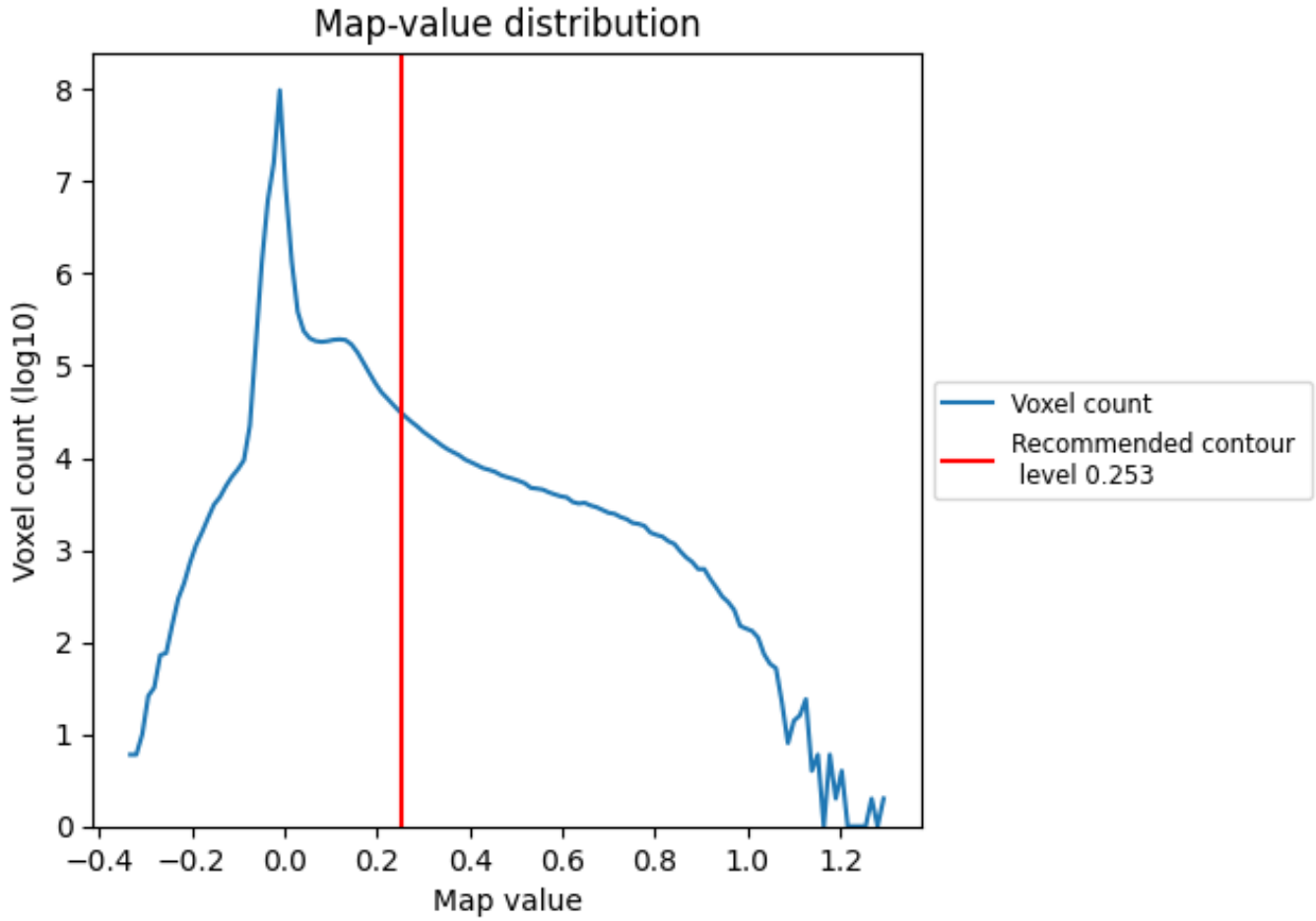
6.6 Mask visualisation (i)

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

7 Map analysis

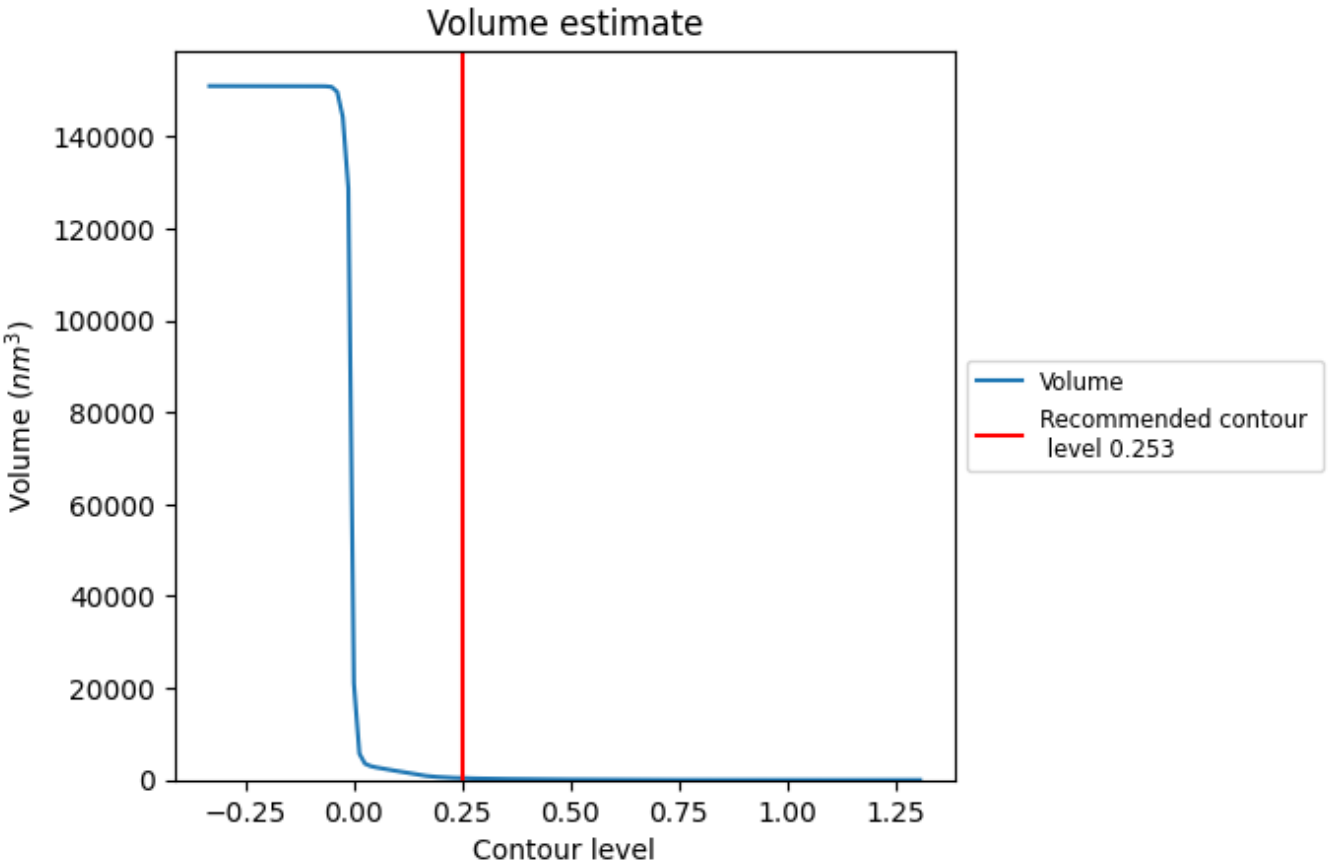
This section contains the results of statistical analysis of the map.

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.

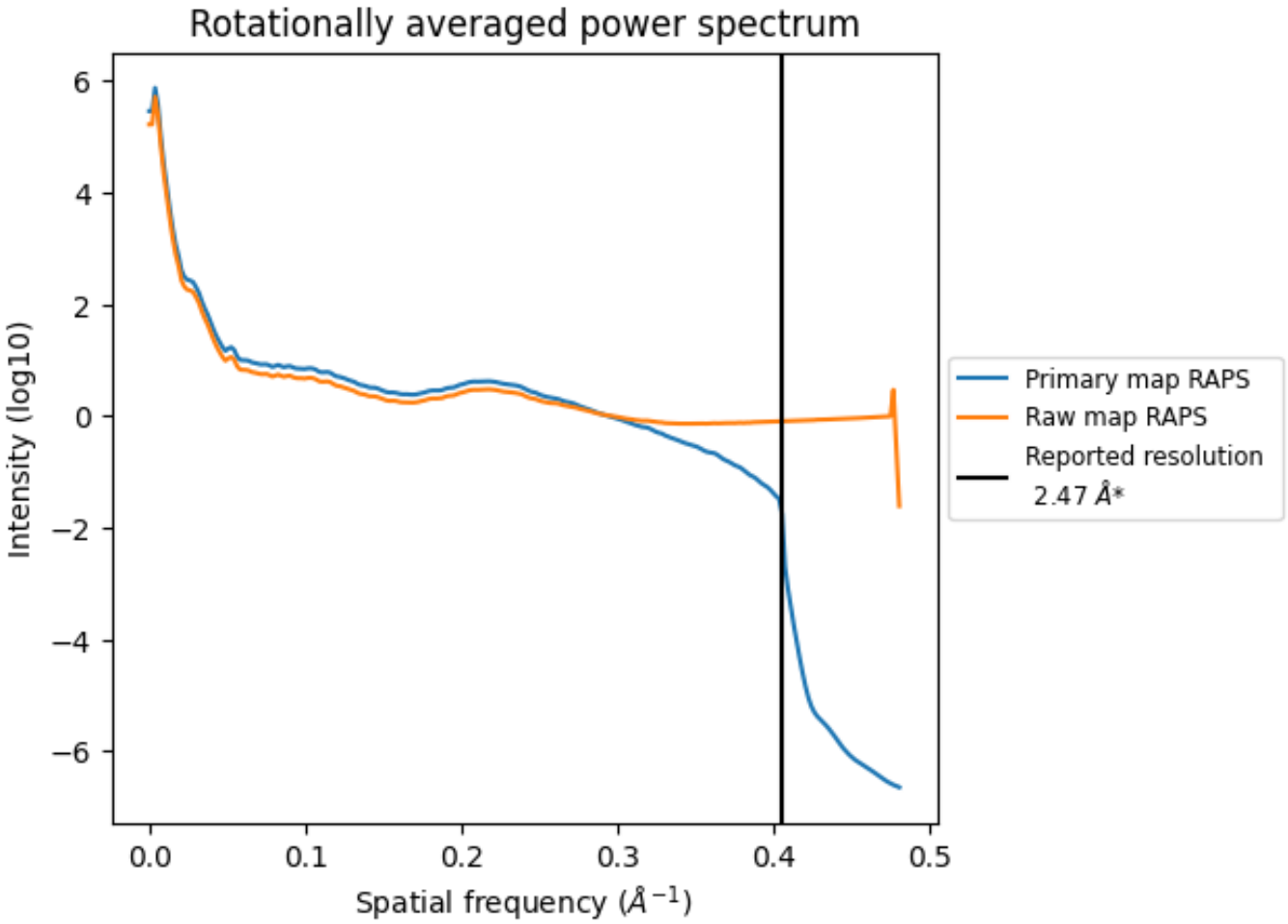
7.2 Volume estimate



The volume at the recommended contour level is 394 nm^3; this corresponds to an approximate mass of 356 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)

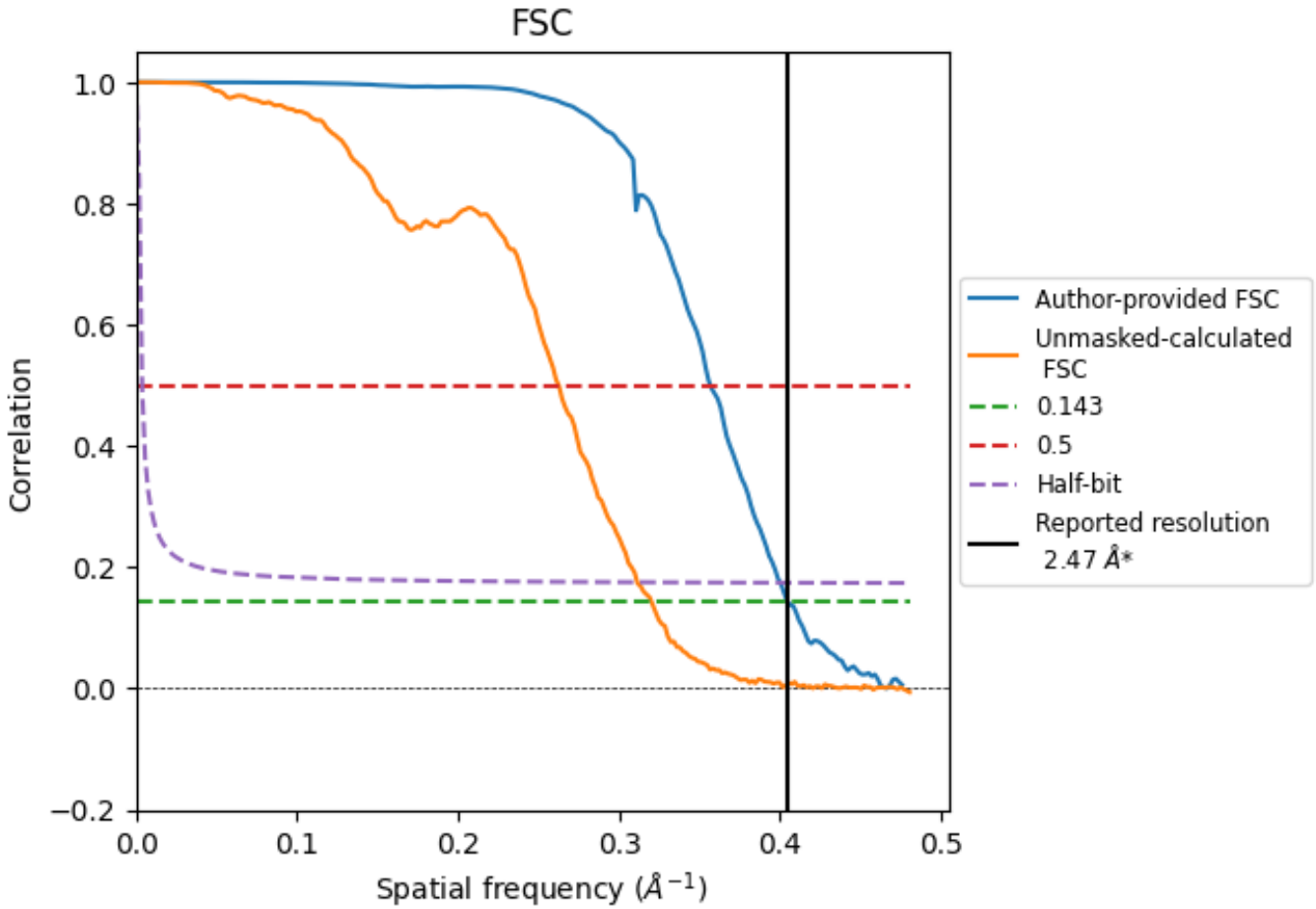


*Reported resolution corresponds to spatial frequency of 0.405 Å^{-1}

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 0.405 Å^{-1}

8.2 Resolution estimates (i)

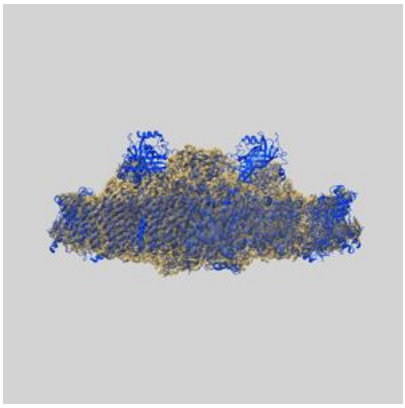
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.47	-	-
Author-provided FSC curve	2.47	2.80	2.50
Unmasked-calculated*	3.12	3.81	3.21

*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 3.12 differs from the reported value 2.47 by more than 10 %

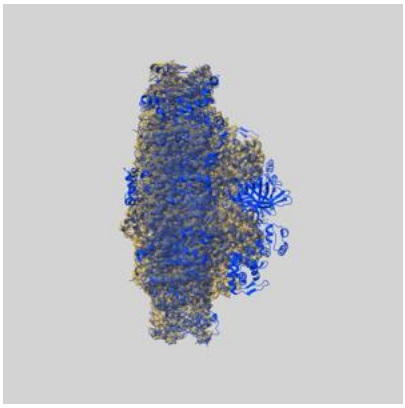
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37414 and PDB model 8WB4. Per-residue inclusion information can be found in section 3 on page 43.

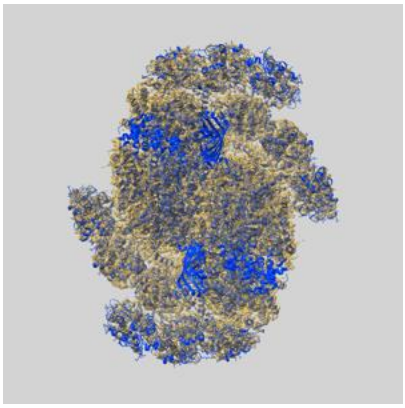
9.1 Map-model overlay



X



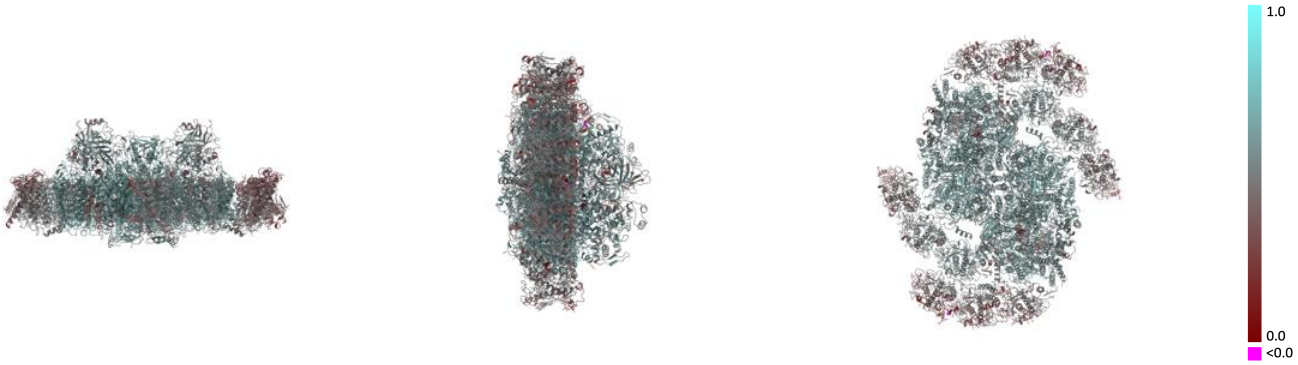
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.253 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.

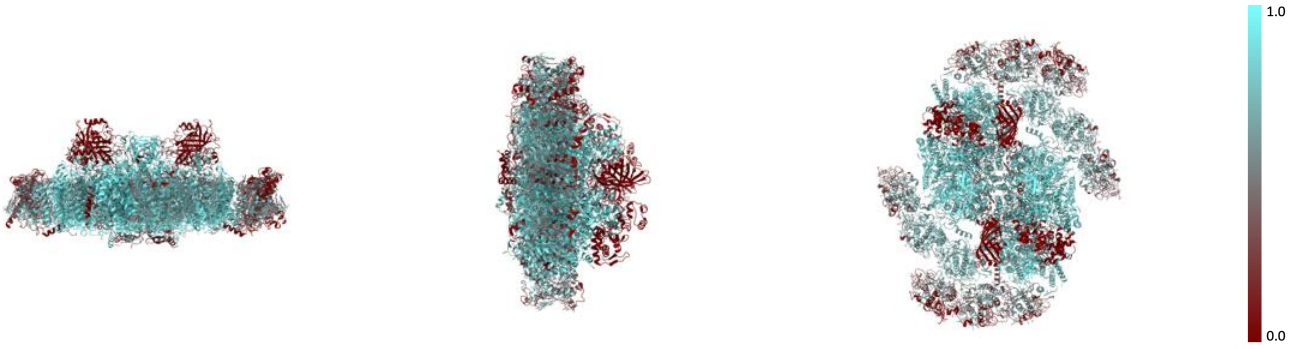
9.2 Q-score mapped to coordinate model (i)



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.

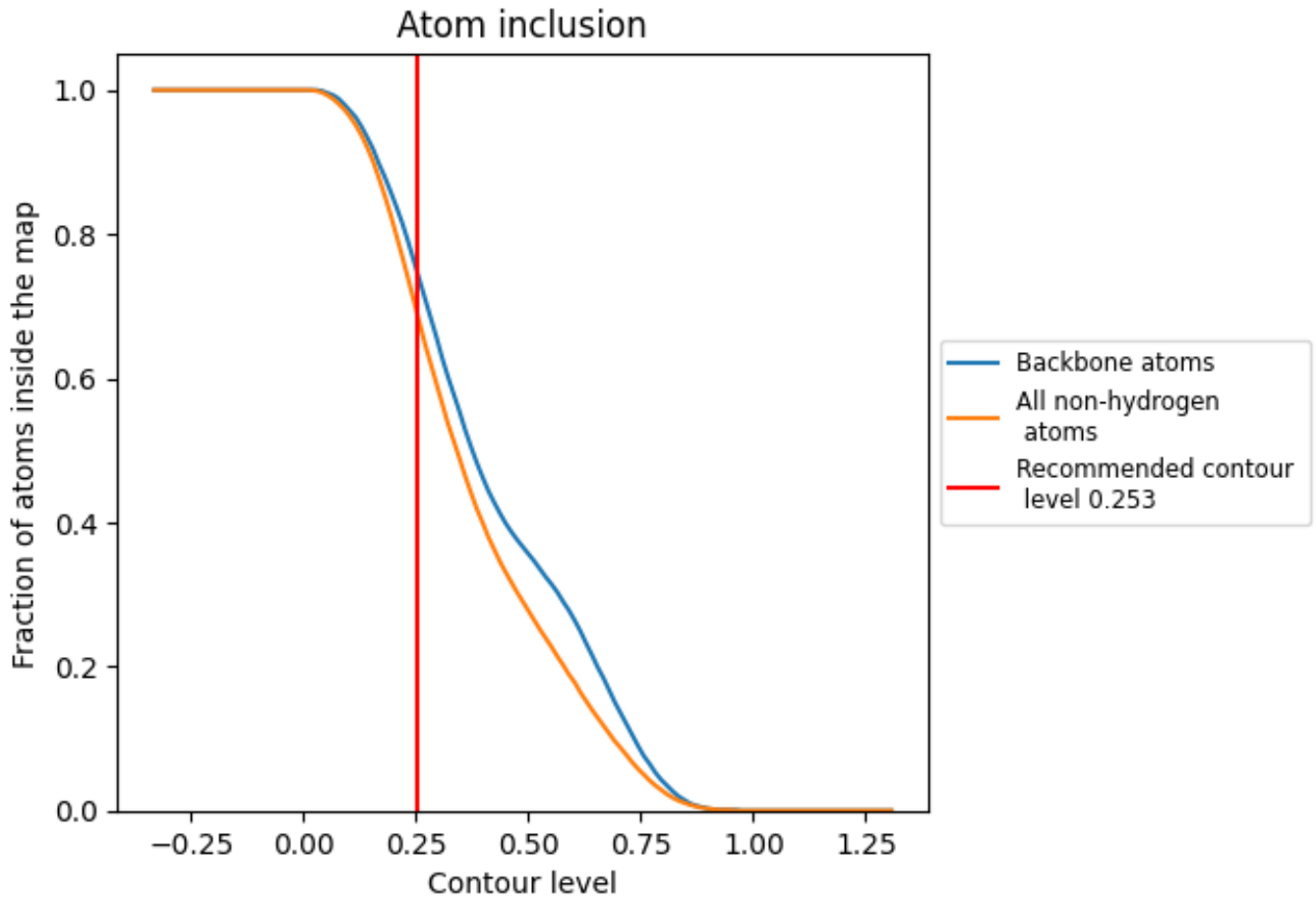
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.253).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 69% 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 (0.253) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6870	0.5390
0	0.3220	0.3940
1	0.5160	0.4300
2	0.7030	0.5030
3	0.8210	0.5590
4	0.3280	0.3940
5	0.3860	0.4010
6	0.4790	0.4320
7	0.5140	0.4320
8	0.7060	0.5030
9	0.8200	0.5590
A	0.9490	0.6200
B	0.9280	0.6140
C	0.9050	0.6000
D	0.9620	0.6290
E	0.7590	0.5330
F	0.8680	0.5520
G	0.4320	0.5120
H	0.9650	0.6130
I	0.9890	0.6320
J	0.2870	0.4670
K	0.9140	0.5930
L	0.9340	0.6010
M	0.9440	0.6050
O	0.0060	0.4920
P	0.4830	0.4330
Q	0.0570	0.5560
R	0.4620	0.4100
S	0.6270	0.5060
T	0.9250	0.6230
U	0.0110	0.4830
V	0.0170	0.5160
W	0.8750	0.5900
X	0.8780	0.5930
Y	0.6150	0.4860



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Chain	Atom inclusion	Q-score
Z	0.7650	0.5140
a	0.9470	0.6180
b	0.9290	0.6150
c	0.9040	0.6010
d	0.9620	0.6310
e	0.7600	0.5390
f	0.8430	0.5560
g	0.4160	0.4930
h	0.9650	0.6160
i	0.9890	0.6260
j	0.2870	0.4630
k	0.9110	0.5940
l	0.9340	0.5980
m	0.9350	0.6030
o	0.0070	0.4880
p	0.3940	0.4020
q	0.0570	0.5540
r	0.4620	0.4120
s	0.6270	0.5080
t	0.9250	0.6230
u	0.0110	0.4850
v	0.0160	0.5190
w	0.8750	0.5860
x	0.8780	0.5880
y	0.6110	0.4880
z	0.7570	0.5180