Full wwPDB EM Validation Report

Mar 30, 2026 – 04:24 AM UTC

PDB ID	:	5XNL / pdb_00005xnl
EMDB ID	:	EMD-6741
Title	:	Structure of stacked C2S2M2-type PSII-LHCII supercomplex from Pisum sativum
Authors	:	Su, X.D.; Ma, J.; Wei, X.P.; Cao, P.; Zhu, D.J.; Chang, W.R.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on	:	2017-05-23
Resolution	:	2.70 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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

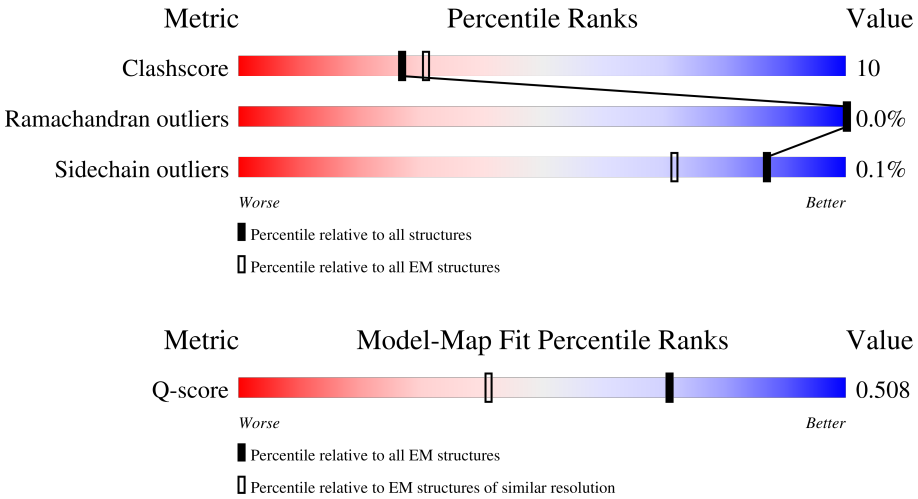
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.70 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.



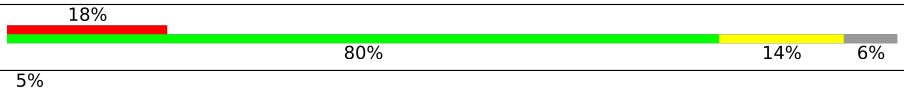
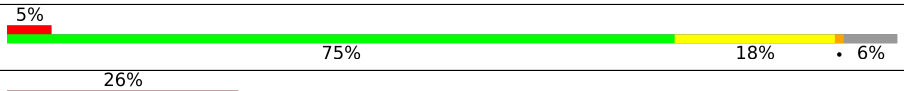
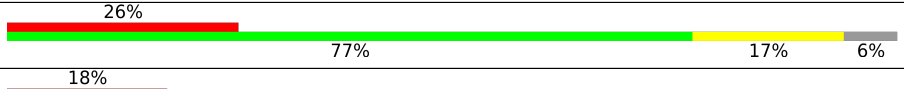
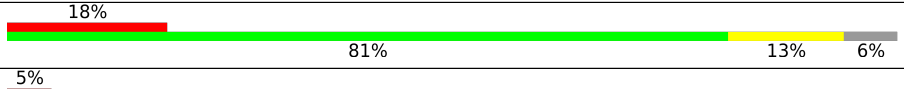
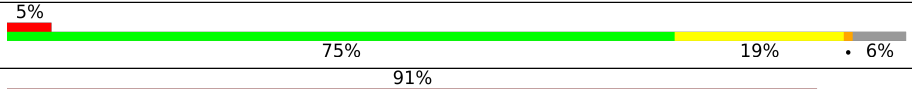
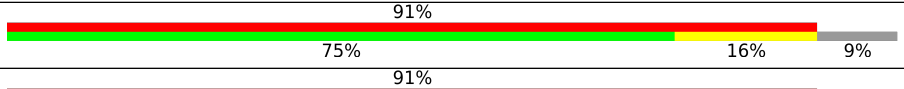
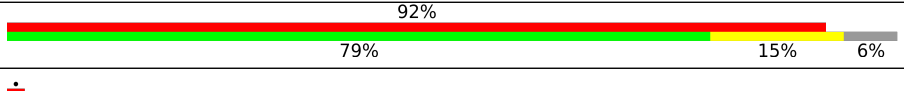
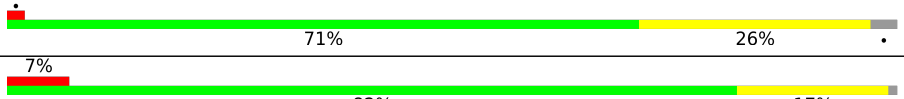
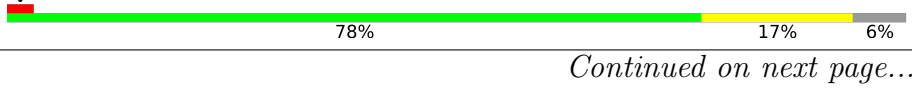
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	1	232	93% 80% 14% 6%
1	2	232	94% 80% 14% 6%
1	5	232	94% 81% 13% 6%
1	6	232	94% 80% 13% 6%

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Mol	Chain	Length	Quality of chain
1	G	232	
1	N	232	
1	Y	232	
1	g	232	
1	n	232	
1	y	232	
2	3	243	
2	7	243	
3	4	210	
3	8	210	
4	A	344	
4	a	344	
5	B	507	
5	b	507	
6	C	473	
6	c	473	
7	D	353	
7	d	353	
8	E	83	
8	e	83	
9	F	39	
9	f	39	
10	H	73	
10	h	73	
11	I	36	

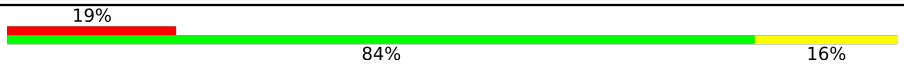
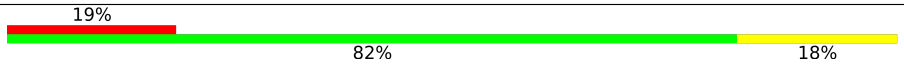
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Mol	Chain	Length	Quality of chain
11	i	36	78% 17% 6%
12	J	40	8% 78% 10% 12%
12	j	40	8% 78% 10% 12%
13	K	61	8% 49% 11% 39%
13	k	61	8% 51% 10% 39%
14	L	38	11% 68% 26%
14	l	38	11% 71% 24%
15	M	34	18% 79% 18%
15	m	34	18% 79% 18%
16	O	248	14% 79% 21%
16	o	248	13% 78% 22%
17	P	186	19% 83% 17%
17	p	186	19% 82% 18%
18	Q	148	85% 73% 14% 13%
18	q	148	84% 72% 15% 13%
19	R	246	21% 75% 20% 5%
19	r	246	21% 76% 20% 5%
20	S	244	32% 74% 15% 11%
20	s	244	32% 73% 16% 11%
21	T	35	6% 74% 17% 9%
21	t	35	6% 74% 17% 9%
22	W	54	11% 89% 11%
22	w	54	11% 89% 11%
23	X	86	10% 35% 10% 55%
23	x	86	10% 35% 10% 55%

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Mol	Chain	Length	Quality of chain
24	Z	62	
24	z	62	

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
25	CHL	1	601	X	-	-	-
25	CHL	1	605	X	-	-	-
25	CHL	1	606	X	-	-	-
25	CHL	1	607	X	-	-	-
25	CHL	1	608	X	-	-	-
25	CHL	1	609	X	-	-	-
25	CHL	2	601	X	-	-	-
25	CHL	2	605	X	-	-	-
25	CHL	2	606	X	-	-	-
25	CHL	2	607	X	-	-	-
25	CHL	2	608	X	-	-	-
25	CHL	2	609	X	-	-	-
25	CHL	3	601	X	-	-	-
25	CHL	3	605	X	-	-	-
25	CHL	3	606	X	-	-	-
25	CHL	3	607	X	-	-	-
25	CHL	3	608	X	-	-	-
25	CHL	3	609	X	-	-	-
25	CHL	4	601	X	-	-	-
25	CHL	4	606	X	-	-	-
25	CHL	4	607	X	-	-	-
25	CHL	4	608	X	-	-	-
25	CHL	4	609	X	-	-	-
25	CHL	5	601	X	-	-	-
25	CHL	5	605	X	-	-	-
25	CHL	5	606	X	-	-	-
25	CHL	5	607	X	-	-	-
25	CHL	5	608	X	-	-	-
25	CHL	5	609	X	-	-	-
25	CHL	6	601	X	-	-	-
25	CHL	6	605	X	-	-	-
25	CHL	6	606	X	-	-	-
25	CHL	6	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CHL	6	608	X	-	-	-
25	CHL	6	609	X	-	-	-
25	CHL	7	601	X	-	-	-
25	CHL	7	605	X	-	-	-
25	CHL	7	606	X	-	-	-
25	CHL	7	607	X	-	-	-
25	CHL	7	608	X	-	-	-
25	CHL	7	609	X	-	-	-
25	CHL	8	601	X	-	-	-
25	CHL	8	606	X	-	-	-
25	CHL	8	607	X	-	-	-
25	CHL	8	608	X	-	-	-
25	CHL	8	609	X	-	-	-
25	CHL	G	601	X	-	-	-
25	CHL	G	605	X	-	-	-
25	CHL	G	606	X	-	-	-
25	CHL	G	607	X	-	-	-
25	CHL	G	608	X	-	-	-
25	CHL	G	609	X	-	-	-
25	CHL	N	601	X	-	-	-
25	CHL	N	605	X	-	-	-
25	CHL	N	606	X	-	-	-
25	CHL	N	607	X	-	-	-
25	CHL	N	608	X	-	-	-
25	CHL	N	609	X	-	-	-
25	CHL	R	606	X	-	-	-
25	CHL	R	607	X	-	-	-
25	CHL	R	608	X	-	-	-
25	CHL	R	614	X	-	-	-
25	CHL	S	601	X	-	-	-
25	CHL	S	606	X	-	-	-
25	CHL	S	607	X	-	-	-
25	CHL	S	608	X	-	-	-
25	CHL	Y	601	X	-	-	-
25	CHL	Y	605	X	-	-	-
25	CHL	Y	606	X	-	-	-
25	CHL	Y	607	X	-	-	-
25	CHL	Y	608	X	-	-	-
25	CHL	Y	609	X	-	-	-
25	CHL	g	601	X	-	-	-
25	CHL	g	605	X	-	-	-
25	CHL	g	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CHL	g	607	X	-	-	-
25	CHL	g	608	X	-	-	-
25	CHL	g	609	X	-	-	-
25	CHL	n	601	X	-	-	-
25	CHL	n	605	X	-	-	-
25	CHL	n	606	X	-	-	-
25	CHL	n	607	X	-	-	-
25	CHL	n	608	X	-	-	-
25	CHL	n	609	X	-	-	-
25	CHL	r	606	X	-	-	-
25	CHL	r	607	X	-	-	-
25	CHL	r	608	X	-	-	-
25	CHL	r	614	X	-	-	-
25	CHL	s	601	X	-	-	-
25	CHL	s	606	X	-	-	-
25	CHL	s	607	X	-	-	-
25	CHL	s	608	X	-	-	-
25	CHL	y	601	X	-	-	-
25	CHL	y	605	X	-	-	-
25	CHL	y	606	X	-	-	-
25	CHL	y	607	X	-	-	-
25	CHL	y	608	X	-	-	-
25	CHL	y	609	X	-	-	-
26	CLA	1	602	X	-	-	-
26	CLA	1	603	X	-	-	-
26	CLA	1	610	X	-	-	-
26	CLA	1	611	X	-	-	-
26	CLA	1	612	X	-	-	-
26	CLA	1	614	X	-	-	-
26	CLA	2	602	X	-	-	-
26	CLA	2	603	X	-	-	-
26	CLA	2	604	X	-	-	-
26	CLA	2	610	X	-	-	-
26	CLA	2	612	X	-	-	-
26	CLA	2	614	X	-	-	-
26	CLA	3	602	X	-	-	-
26	CLA	3	603	X	-	-	-
26	CLA	3	604	X	-	-	-
26	CLA	3	610	X	-	-	-
26	CLA	3	611	X	-	-	-
26	CLA	3	612	X	-	-	-
26	CLA	3	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	3	614	X	-	-	-
26	CLA	4	602	X	-	-	-
26	CLA	4	603	X	-	-	-
26	CLA	4	610	X	-	-	-
26	CLA	4	611	X	-	-	-
26	CLA	4	612	X	-	-	-
26	CLA	5	602	X	-	-	-
26	CLA	5	603	X	-	-	-
26	CLA	5	610	X	-	-	-
26	CLA	5	611	X	-	-	-
26	CLA	5	612	X	-	-	-
26	CLA	5	614	X	-	-	-
26	CLA	6	602	X	-	-	-
26	CLA	6	603	X	-	-	-
26	CLA	6	604	X	-	-	-
26	CLA	6	610	X	-	-	-
26	CLA	6	612	X	-	-	-
26	CLA	6	614	X	-	-	-
26	CLA	7	602	X	-	-	-
26	CLA	7	603	X	-	-	-
26	CLA	7	604	X	-	-	-
26	CLA	7	610	X	-	-	-
26	CLA	7	611	X	-	-	-
26	CLA	7	612	X	-	-	-
26	CLA	7	613	X	-	-	-
26	CLA	7	614	X	-	-	-
26	CLA	8	602	X	-	-	-
26	CLA	8	603	X	-	-	-
26	CLA	8	610	X	-	-	-
26	CLA	8	611	X	-	-	-
26	CLA	8	612	X	-	-	-
26	CLA	A	405	X	-	-	-
26	CLA	A	406	X	-	-	-
26	CLA	A	410	X	-	-	-
26	CLA	B	602	X	-	-	-
26	CLA	B	603	X	-	-	-
26	CLA	B	604	X	-	-	-
26	CLA	B	605	X	-	-	-
26	CLA	B	606	X	-	-	-
26	CLA	B	607	X	-	-	-
26	CLA	B	608	X	-	-	-
26	CLA	B	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	B	612	X	-	-	-
26	CLA	B	613	X	-	-	-
26	CLA	B	614	X	-	-	-
26	CLA	B	615	X	-	-	-
26	CLA	B	616	X	-	-	-
26	CLA	B	617	X	-	-	-
26	CLA	C	501	X	-	-	-
26	CLA	C	502	X	-	-	-
26	CLA	C	503	X	-	-	-
26	CLA	C	504	X	-	-	-
26	CLA	C	505	X	-	-	-
26	CLA	C	506	X	-	-	-
26	CLA	C	507	X	-	-	-
26	CLA	C	508	X	-	-	-
26	CLA	C	509	X	-	-	-
26	CLA	C	510	X	-	-	-
26	CLA	C	511	X	-	-	-
26	CLA	C	512	X	-	-	-
26	CLA	D	402	X	-	-	-
26	CLA	G	602	X	-	-	-
26	CLA	G	603	X	-	-	-
26	CLA	G	604	X	-	-	-
26	CLA	G	610	X	-	-	-
26	CLA	G	611	X	-	-	-
26	CLA	G	612	X	-	-	-
26	CLA	G	613	X	-	-	-
26	CLA	G	614	X	-	-	-
26	CLA	N	602	X	-	-	-
26	CLA	N	603	X	-	-	-
26	CLA	N	604	X	-	-	-
26	CLA	N	610	X	-	-	-
26	CLA	N	611	X	-	-	-
26	CLA	N	612	X	-	-	-
26	CLA	N	613	X	-	-	-
26	CLA	N	614	X	-	-	-
26	CLA	R	601	X	-	-	-
26	CLA	R	602	X	-	-	-
26	CLA	R	603	X	-	-	-
26	CLA	R	604	X	-	-	-
26	CLA	R	609	X	-	-	-
26	CLA	R	610	X	-	-	-
26	CLA	R	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	R	612	X	-	-	-
26	CLA	R	613	X	-	-	-
26	CLA	S	602	X	-	-	-
26	CLA	S	603	X	-	-	-
26	CLA	S	604	X	-	-	-
26	CLA	S	609	X	-	-	-
26	CLA	S	610	X	-	-	-
26	CLA	S	611	X	-	-	-
26	CLA	S	612	X	-	-	-
26	CLA	S	613	X	-	-	-
26	CLA	S	614	X	-	-	-
26	CLA	Y	602	X	-	-	-
26	CLA	Y	603	X	-	-	-
26	CLA	Y	604	X	-	-	-
26	CLA	Y	610	X	-	-	-
26	CLA	Y	611	X	-	-	-
26	CLA	Y	612	X	-	-	-
26	CLA	Y	613	X	-	-	-
26	CLA	Y	614	X	-	-	-
26	CLA	a	405	X	-	-	-
26	CLA	a	406	X	-	-	-
26	CLA	a	410	X	-	-	-
26	CLA	b	602	X	-	-	-
26	CLA	b	603	X	-	-	-
26	CLA	b	604	X	-	-	-
26	CLA	b	605	X	-	-	-
26	CLA	b	606	X	-	-	-
26	CLA	b	607	X	-	-	-
26	CLA	b	608	X	-	-	-
26	CLA	b	611	X	-	-	-
26	CLA	b	612	X	-	-	-
26	CLA	b	613	X	-	-	-
26	CLA	b	614	X	-	-	-
26	CLA	b	615	X	-	-	-
26	CLA	b	616	X	-	-	-
26	CLA	b	617	X	-	-	-
26	CLA	c	501	X	-	-	-
26	CLA	c	502	X	-	-	-
26	CLA	c	503	X	-	-	-
26	CLA	c	504	X	-	-	-
26	CLA	c	505	X	-	-	-
26	CLA	c	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	c	507	X	-	-	-
26	CLA	c	508	X	-	-	-
26	CLA	c	509	X	-	-	-
26	CLA	c	510	X	-	-	-
26	CLA	c	511	X	-	-	-
26	CLA	c	512	X	-	-	-
26	CLA	d	402	X	-	-	-
26	CLA	g	602	X	-	-	-
26	CLA	g	603	X	-	-	-
26	CLA	g	604	X	-	-	-
26	CLA	g	610	X	-	-	-
26	CLA	g	611	X	-	-	-
26	CLA	g	612	X	-	-	-
26	CLA	g	613	X	-	-	-
26	CLA	g	614	X	-	-	-
26	CLA	n	602	X	-	-	-
26	CLA	n	603	X	-	-	-
26	CLA	n	604	X	-	-	-
26	CLA	n	610	X	-	-	-
26	CLA	n	611	X	-	-	-
26	CLA	n	612	X	-	-	-
26	CLA	n	613	X	-	-	-
26	CLA	n	614	X	-	-	-
26	CLA	r	601	X	-	-	-
26	CLA	r	602	X	-	-	-
26	CLA	r	603	X	-	-	-
26	CLA	r	604	X	-	-	-
26	CLA	r	609	X	-	-	-
26	CLA	r	610	X	-	-	-
26	CLA	r	611	X	-	-	-
26	CLA	r	612	X	-	-	-
26	CLA	r	613	X	-	-	-
26	CLA	s	602	X	-	-	-
26	CLA	s	603	X	-	-	-
26	CLA	s	604	X	-	-	-
26	CLA	s	609	X	-	-	-
26	CLA	s	610	X	-	-	-
26	CLA	s	611	X	-	-	-
26	CLA	s	612	X	-	-	-
26	CLA	s	613	X	-	-	-
26	CLA	s	614	X	-	-	-
26	CLA	y	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	y	603	X	-	-	-
26	CLA	y	604	X	-	-	-
26	CLA	y	610	X	-	-	-
26	CLA	y	611	X	-	-	-
26	CLA	y	612	X	-	-	-
26	CLA	y	613	X	-	-	-
26	CLA	y	614	X	-	-	-

2 Entry composition (i)

There are 42 unique types of molecules in this entry. The entry contains 98986 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 Chlorophyll a-b binding protein 8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	2	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		
1	G	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	N	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	Y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	5	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	6	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		
1	g	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	n	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		
2	7	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		

- Molecule 3 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	197	Total	C	N	O	S	0	0
			1534	1009	247	274	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	197	Total	C	N	O	S	0	0
			1534	1009	247	274	4		

- Molecule 4 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	334	Total	C	N	O	S	0	0
			2616	1708	431	464	13		
4	a	334	Total	C	N	O	S	0	0
			2616	1708	431	464	13		

- Molecule 5 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	503	Total	C	N	O	S	0	0
			3948	2581	669	686	12		
5	b	503	Total	C	N	O	S	0	0
			3948	2581	669	686	12		

- Molecule 6 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	450	Total	C	N	O	S	0	0
			3497	2300	583	604	10		
6	c	450	Total	C	N	O	S	0	0
			3497	2300	583	604	10		

- Molecule 7 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	341	Total	C	N	O	S	0	0
			2712	1790	444	466	12		
7	d	341	Total	C	N	O	S	0	0
			2712	1790	444	466	12		

- Molecule 8 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	E	75	Total	C	N	O	0	0
			612	400	100	112		
8	e	75	Total	C	N	O	0	0
			612	400	100	112		

- Molecule 9 is a protein called Cytochrome b559 subunit beta, PsbF.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	30	Total	C	N	O	S	0	0
			241	162	41	37	1		
9	f	30	Total	C	N	O	S	0	0
			241	162	41	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	60	Total	C	N	O	S	0	0
			452	296	72	81	3		
10	h	60	Total	C	N	O	S	0	0
			452	296	72	81	3		

- Molecule 11 is a protein called Photosystem II reaction center protein I, PsbI.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	34	Total	C	N	O	S	0	0
			278	191	43	43	1		
11	i	34	Total	C	N	O	S	0	0
			278	191	43	43	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	35	Total	C	N	O	0	0
			256	174	39	43		
12	j	35	Total	C	N	O	0	0
			256	174	39	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	37	Total	C	N	O	S	0	0
			306	215	44	46	1		
13	k	37	Total	C	N	O	S	0	0
			306	215	44	46	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	L	37	Total 311	C 205	N 49	O 57	0	0
14	l	37	Total 311	C 205	N 49	O 57	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	33	Total 256	C 176	N 36	O 43	S 1	0	0
15	m	33	Total 256	C 176	N 36	O 43	S 1	0	0

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	248	Total 1870	C 1179	N 306	O 382	S 3	0	0
16	o	248	Total 1870	C 1179	N 306	O 382	S 3	0	0

- Molecule 17 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	186	Total 1434	C 909	N 238	O 286	S 1	0	0
17	p	186	Total 1434	C 909	N 238	O 286	S 1	0	0

- Molecule 18 is a protein called Oxygen-evolving enhancer protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	Q	129	Total 1034	C 661	N 177	O 196	0	0
18	q	129	Total 1034	C 661	N 177	O 196	0	0

- Molecule 19 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	234	Total 1835	C 1194	N 297	O 341	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	r	234	Total	C	N	O	S	0	0
			1835	1194	297	341	3		

- Molecule 20 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	218	Total	C	N	O	S	0	0
			1689	1107	273	305	4		
20	s	218	Total	C	N	O	S	0	0
			1689	1107	273	305	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	32	Total	C	N	O	S	0	0
			261	182	37	41	1		
21	t	32	Total	C	N	O	S	0	0
			261	182	37	41	1		

- Molecule 22 is a protein called Photosystem II reaction center protein W.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	54	Total	C	N	O	S	0	0
			419	275	61	82	1		
22	w	54	Total	C	N	O	S	0	0
			419	275	61	82	1		

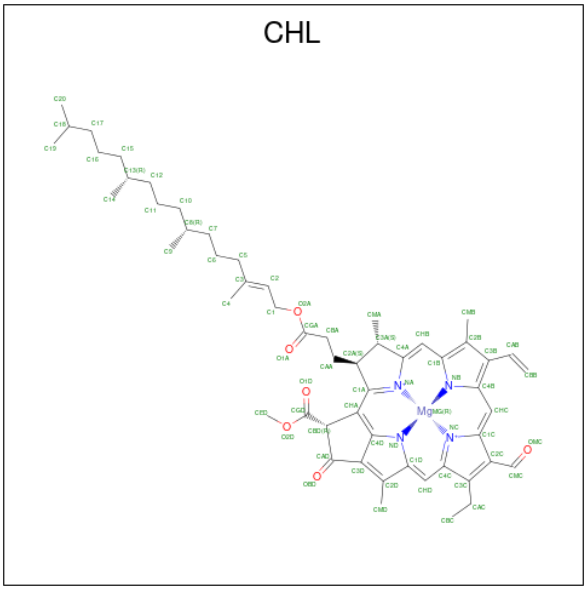
- Molecule 23 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	39	Total	C	N	O	0	0
			276	180	46	50		
23	x	39	Total	C	N	O	0	0
			276	180	46	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	62	Total	C	N	O	S	0	0
			464	312	69	82	1		
24	z	62	Total	C	N	O	S	0	0
			464	312	69	82	1		

- Molecule 25 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	3	1	Total	C	Mg	N	O	0
			64	53	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	3	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
25	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	3	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
25	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	G	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	N	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
25	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
25	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
25	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	R	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
25	R	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	R	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
25	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	S	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
25	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	Y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
25	Y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
25	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			62	51	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
25	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	7	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
25	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	7	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
25	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	g	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
25	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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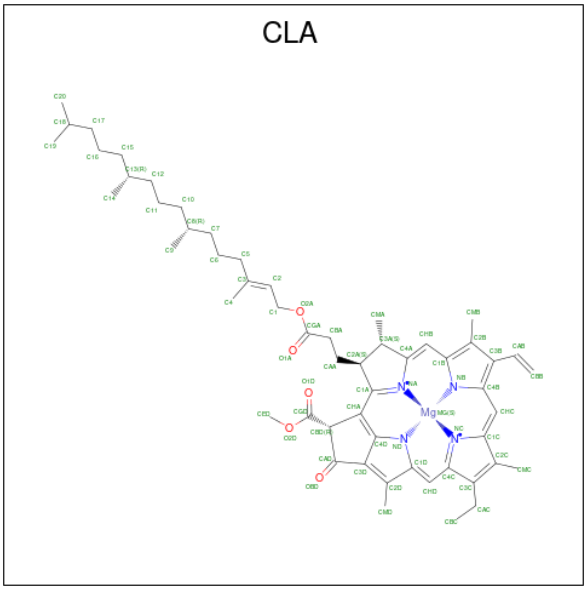
Mol	Chain	Residues	Atoms					AltConf
25	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	g	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	n	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
25	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
25	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	r	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
25	r	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	r	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
25	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	s	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
25	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
25	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
25	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
25	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
26	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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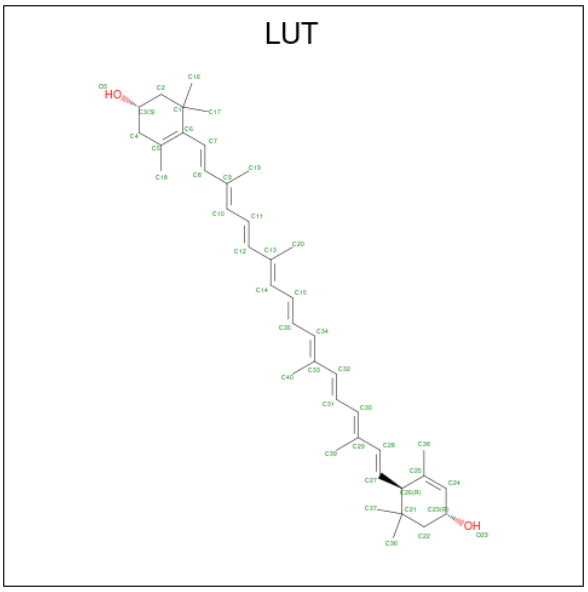
Mol	Chain	Residues	Atoms					AltConf
26	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	s	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

- Molecule 27 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



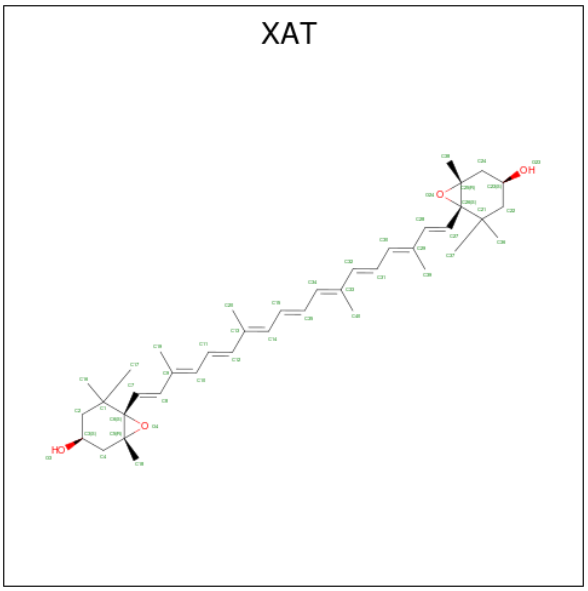
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			42	40	2	
27	1	1	Total	C	O	0
			42	40	2	
27	2	1	Total	C	O	0
			42	40	2	
27	2	1	Total	C	O	0
			42	40	2	
27	3	1	Total	C	O	0
			42	40	2	
27	3	1	Total	C	O	0
			42	40	2	
27	4	1	Total	C	O	0
			42	40	2	
27	G	1	Total	C	O	0
			42	40	2	
27	G	1	Total	C	O	0
			42	40	2	
27	N	1	Total	C	O	0
			42	40	2	
27	N	1	Total	C	O	0
			42	40	2	
27	R	1	Total	C	O	0
			42	40	2	
27	S	1	Total	C	O	0
			42	40	2	
27	S	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
27	Y	1	Total	C	O	0
			42	40	2	
27	Y	1	Total	C	O	0
			42	40	2	
27	5	1	Total	C	O	0
			42	40	2	
27	5	1	Total	C	O	0
			42	40	2	
27	6	1	Total	C	O	0
			42	40	2	
27	6	1	Total	C	O	0
			42	40	2	
27	7	1	Total	C	O	0
			42	40	2	
27	7	1	Total	C	O	0
			42	40	2	
27	8	1	Total	C	O	0
			42	40	2	
27	g	1	Total	C	O	0
			42	40	2	
27	g	1	Total	C	O	0
			42	40	2	
27	n	1	Total	C	O	0
			42	40	2	
27	n	1	Total	C	O	0
			42	40	2	
27	r	1	Total	C	O	0
			42	40	2	
27	s	1	Total	C	O	0
			42	40	2	
27	s	1	Total	C	O	0
			42	40	2	
27	y	1	Total	C	O	0
			42	40	2	
27	y	1	Total	C	O	0
			42	40	2	

- Molecule 28 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



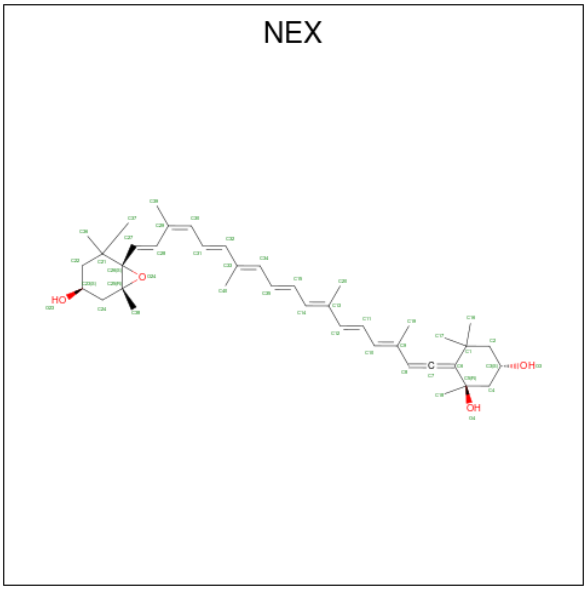
Mol	Chain	Residues	Atoms	AltConf
28	1	1	Total C O 44 40 4	0
28	2	1	Total C O 44 40 4	0
28	3	1	Total C O 44 40 4	0
28	4	1	Total C O 44 40 4	0
28	G	1	Total C O 44 40 4	0
28	N	1	Total C O 44 40 4	0
28	R	1	Total C O 44 40 4	0
28	Y	1	Total C O 44 40 4	0
28	5	1	Total C O 44 40 4	0
28	6	1	Total C O 44 40 4	0
28	7	1	Total C O 44 40 4	0
28	8	1	Total C O 44 40 4	0
28	g	1	Total C O 44 40 4	0
28	n	1	Total C O 44 40 4	0

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Mol	Chain	Residues	Atoms	AltConf
28	r	1	Total C O 44 40 4	0
28	y	1	Total C O 44 40 4	0

- Molecule 29 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



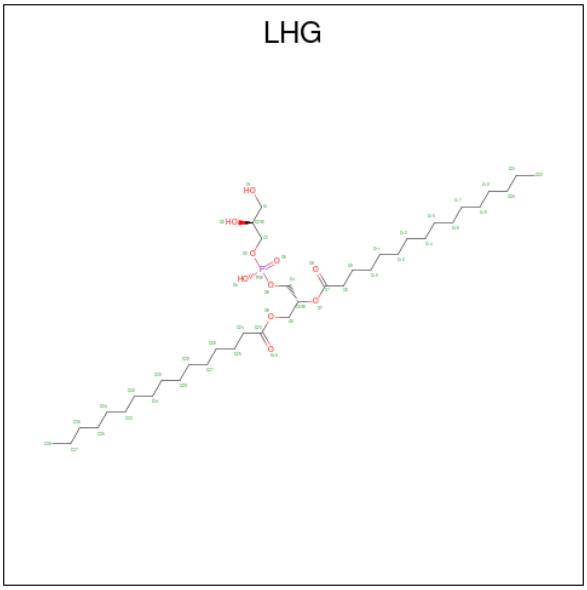
Mol	Chain	Residues	Atoms	AltConf
29	1	1	Total C O 44 40 4	0
29	2	1	Total C O 44 40 4	0
29	3	1	Total C O 44 40 4	0
29	G	1	Total C O 44 40 4	0
29	N	1	Total C O 44 40 4	0
29	R	1	Total C O 44 40 4	0
29	S	1	Total C O 44 40 4	0
29	Y	1	Total C O 44 40 4	0

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Mol	Chain	Residues	Atoms	AltConf
29	5	1	Total C O 44 40 4	0
29	6	1	Total C O 44 40 4	0
29	7	1	Total C O 44 40 4	0
29	g	1	Total C O 44 40 4	0
29	n	1	Total C O 44 40 4	0
29	r	1	Total C O 44 40 4	0
29	s	1	Total C O 44 40 4	0
29	y	1	Total C O 44 40 4	0

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
30	1	1	Total C O P 41 30 10 1	0
30	2	1	Total C O P 37 26 10 1	0
30	3	1	Total C O P 47 36 10 1	0

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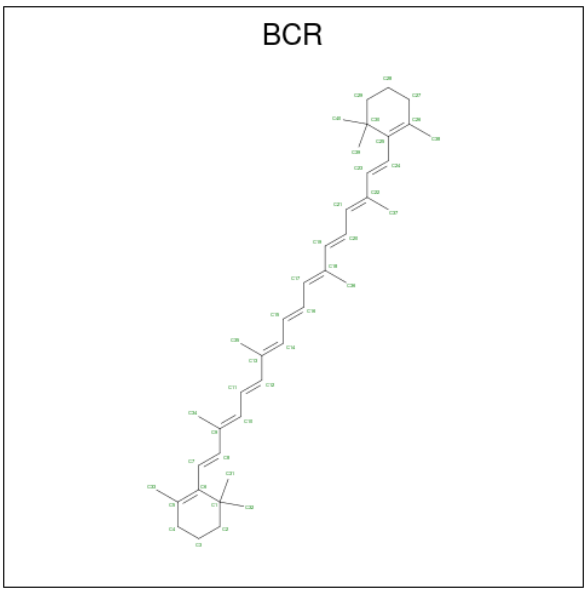
Mol	Chain	Residues	Atoms				AltConf
30	4	1	Total	C	O	P	0
			21	10	10	1	
30	B	1	Total	C	O	P	0
			47	36	10	1	
30	B	1	Total	C	O	P	0
			49	38	10	1	
30	C	1	Total	C	O	P	0
			49	38	10	1	
30	C	1	Total	C	O	P	0
			49	38	10	1	
30	C	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			46	35	10	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			43	32	10	1	
30	G	1	Total	C	O	P	0
			49	38	10	1	
30	L	1	Total	C	O	P	0
			49	38	10	1	
30	N	1	Total	C	O	P	0
			49	38	10	1	
30	R	1	Total	C	O	P	0
			42	31	10	1	
30	S	1	Total	C	O	P	0
			49	38	10	1	
30	Y	1	Total	C	O	P	0
			49	38	10	1	
30	5	1	Total	C	O	P	0
			41	30	10	1	
30	6	1	Total	C	O	P	0
			37	26	10	1	
30	7	1	Total	C	O	P	0
			47	36	10	1	
30	8	1	Total	C	O	P	0
			21	10	10	1	
30	b	1	Total	C	O	P	0
			47	36	10	1	
30	b	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
30	c	1	Total	C	O	P	0
			49	38	10	1	
30	c	1	Total	C	O	P	0
			49	38	10	1	
30	c	1	Total	C	O	P	0
			49	38	10	1	
30	d	1	Total	C	O	P	0
			46	35	10	1	
30	d	1	Total	C	O	P	0
			49	38	10	1	
30	d	1	Total	C	O	P	0
			43	32	10	1	
30	g	1	Total	C	O	P	0
			49	38	10	1	
30	l	1	Total	C	O	P	0
			49	38	10	1	
30	n	1	Total	C	O	P	0
			49	38	10	1	
30	r	1	Total	C	O	P	0
			42	31	10	1	
30	s	1	Total	C	O	P	0
			49	38	10	1	
30	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



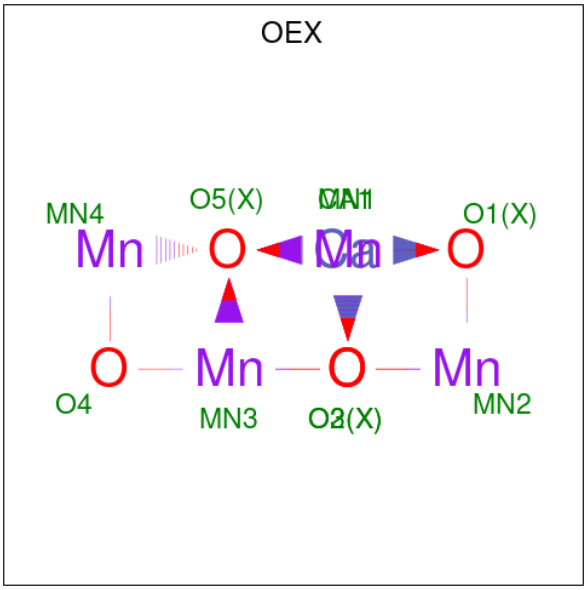
Mol	Chain	Residues	Atoms	AltConf
31	4	1	Total C 40 40	0
31	A	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	D	1	Total C 40 40	0
31	H	1	Total C 40 40	0
31	T	1	Total C 40 40	0
31	8	1	Total C 40 40	0
31	a	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
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	d	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
31	h	1	Total C 40 40	0
31	t	1	Total C 40 40	0

- Molecule 32 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 33 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 34 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

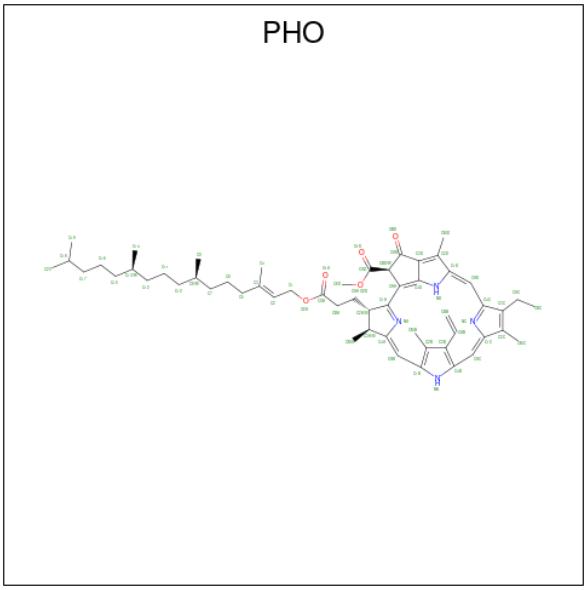
Mol	Chain	Residues	Atoms	AltConf
34	A	2	Total Cl 2 2	0

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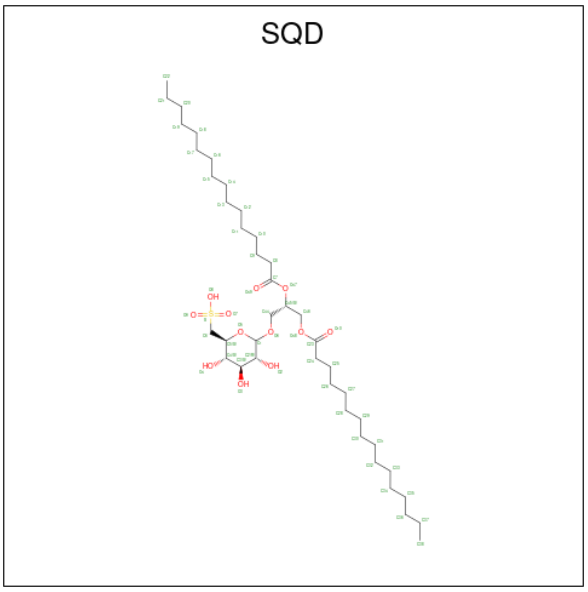
Mol	Chain	Residues	Atoms	AltConf
34	a	2	Total Cl 2 2	0

- Molecule 35 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



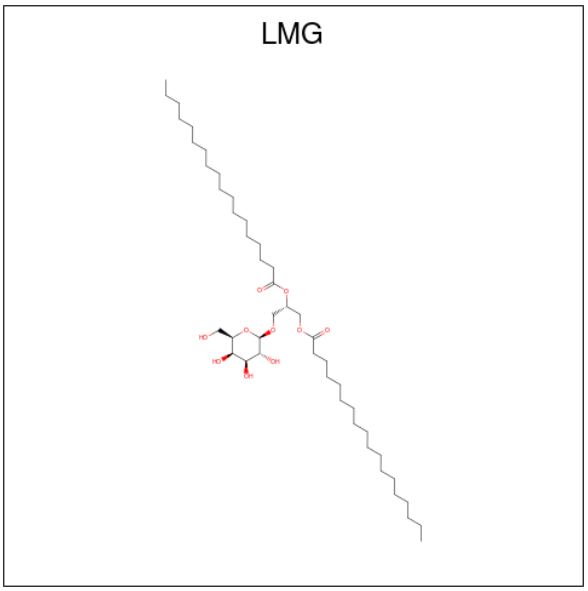
Mol	Chain	Residues	Atoms	AltConf
35	A	1	Total C N O 64 55 4 5	0
35	A	1	Total C N O 64 55 4 5	0
35	a	1	Total C N O 64 55 4 5	0
35	a	1	Total C N O 64 55 4 5	0

- Molecule 36 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



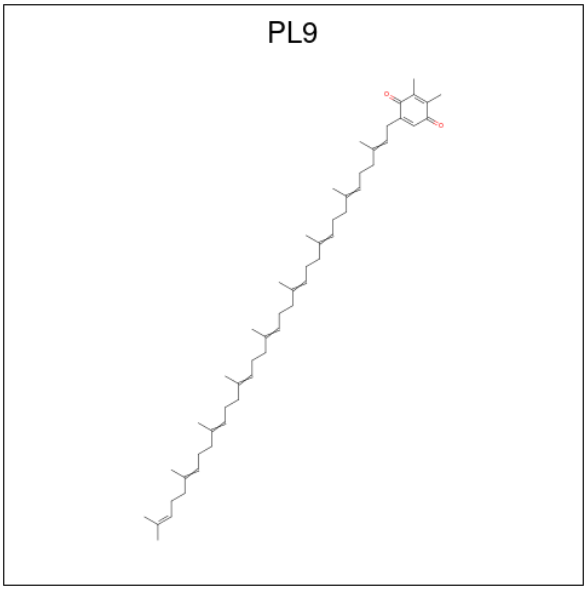
Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total 50	C 37	O 12	S 1	0
36	A	1	Total 54	C 41	O 12	S 1	0
36	B	1	Total 54	C 41	O 12	S 1	0
36	B	1	Total 42	C 29	O 12	S 1	0
36	a	1	Total 50	C 37	O 12	S 1	0
36	a	1	Total 54	C 41	O 12	S 1	0
36	b	1	Total 54	C 41	O 12	S 1	0
36	b	1	Total 42	C 29	O 12	S 1	0

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



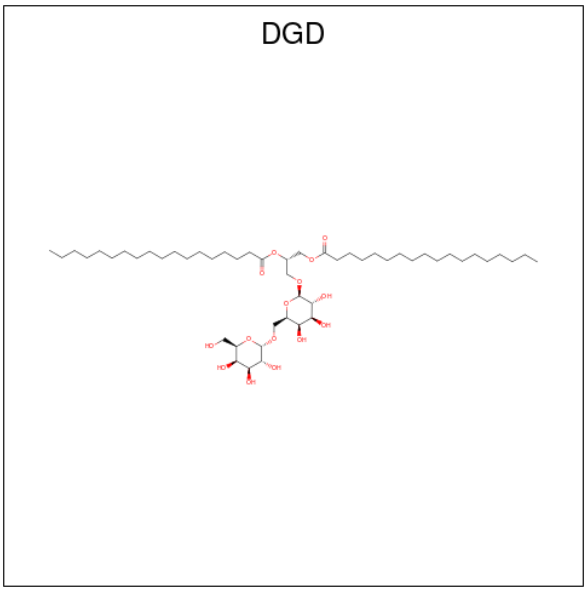
Mol	Chain	Residues	Atoms	AltConf
37	A	1	Total C O 48 38 10	0
37	A	1	Total C O 40 30 10	0
37	B	1	Total C O 51 41 10	0
37	B	1	Total C O 55 45 10	0
37	C	1	Total C O 51 41 10	0
37	D	1	Total C O 46 36 10	0
37	Z	1	Total C O 51 41 10	0
37	a	1	Total C O 48 38 10	0
37	a	1	Total C O 40 30 10	0
37	b	1	Total C O 51 41 10	0
37	b	1	Total C O 55 45 10	0
37	c	1	Total C O 51 41 10	0
37	d	1	Total C O 46 36 10	0
37	z	1	Total C O 51 41 10	0

- Molecule 38 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: $C_{53}H_{80}O_2$).



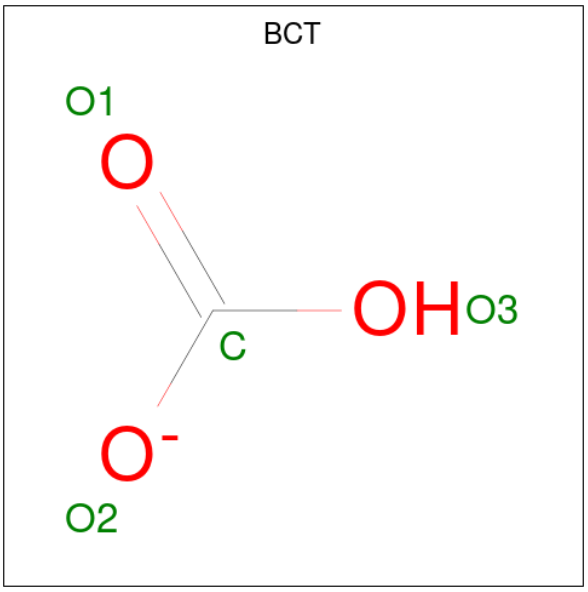
Mol	Chain	Residues	Atoms			AltConf
38	A	1	Total	C	O	0
			13	11	2	
38	D	1	Total	C	O	0
			55	53	2	
38	a	1	Total	C	O	0
			13	11	2	
38	d	1	Total	C	O	0
			55	53	2	

- Molecule 39 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



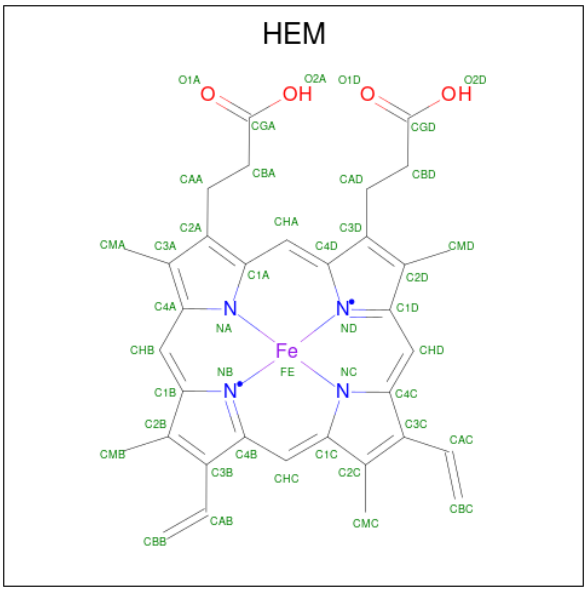
Mol	Chain	Residues	Atoms	AltConf
39	B	1	Total C O 59 44 15	0
39	C	1	Total C O 55 40 15	0
39	C	1	Total C O 62 47 15	0
39	C	1	Total C O 60 45 15	0
39	H	1	Total C O 62 47 15	0
39	b	1	Total C O 59 44 15	0
39	c	1	Total C O 55 40 15	0
39	c	1	Total C O 62 47 15	0
39	c	1	Total C O 60 45 15	0
39	h	1	Total C O 62 47 15	0

- Molecule 40 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
40	D	1	Total	C	O	0
			4	1	3	
40	d	1	Total	C	O	0
			4	1	3	

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		AltConf
42	A	96	Total	O	0
			96	96	
42	B	89	Total	O	0
			89	89	
42	C	68	Total	O	0
			68	68	
42	D	58	Total	O	0
			58	58	
42	E	10	Total	O	0
			10	10	
42	F	2	Total	O	0
			2	2	
42	G	15	Total	O	0
			15	15	
42	H	16	Total	O	0
			16	16	
42	J	3	Total	O	0
			3	3	
42	K	2	Total	O	0
			2	2	
42	L	10	Total	O	0
			10	10	
42	M	4	Total	O	0
			4	4	
42	N	20	Total	O	0
			20	20	
42	O	31	Total	O	0
			31	31	
42	P	16	Total	O	0
			16	16	
42	R	30	Total	O	0
			30	30	
42	S	14	Total	O	0
			14	14	
42	T	2	Total	O	0
			2	2	

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Mol	Chain	Residues	Atoms	AltConf
42	W	4	Total O 4 4	0
42	X	5	Total O 5 5	0
42	Y	39	Total O 39 39	0
42	Z	4	Total O 4 4	0
42	a	96	Total O 96 96	0
42	b	89	Total O 89 89	0
42	c	68	Total O 68 68	0
42	d	58	Total O 58 58	0
42	e	10	Total O 10 10	0
42	f	2	Total O 2 2	0
42	g	15	Total O 15 15	0
42	h	16	Total O 16 16	0
42	j	3	Total O 3 3	0
42	k	2	Total O 2 2	0
42	l	10	Total O 10 10	0
42	m	4	Total O 4 4	0
42	n	20	Total O 20 20	0
42	o	31	Total O 31 31	0
42	p	16	Total O 16 16	0
42	r	30	Total O 30 30	0
42	s	14	Total O 14 14	0

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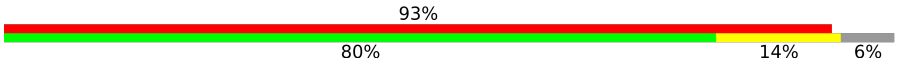
Mol	Chain	Residues	Atoms	AltConf
42	t	2	Total O 2 2	0
42	w	4	Total O 4 4	0
42	x	5	Total O 5 5	0
42	y	39	Total O 39 39	0
42	z	4	Total O 4 4	0

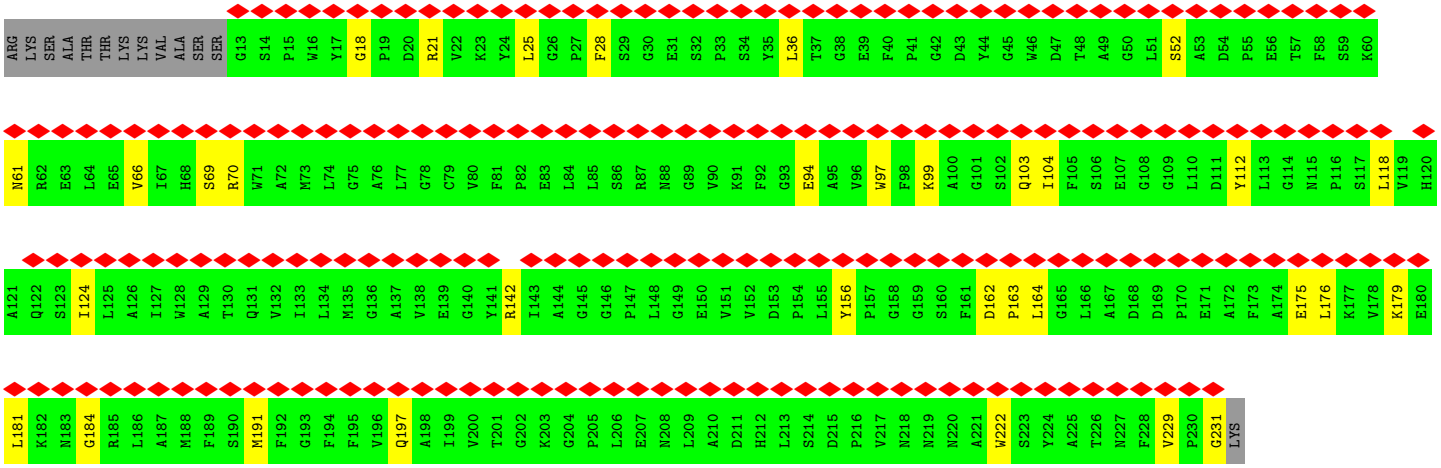
3 Residue-property plots (i)

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

• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

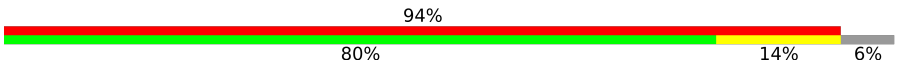
Chain 1:

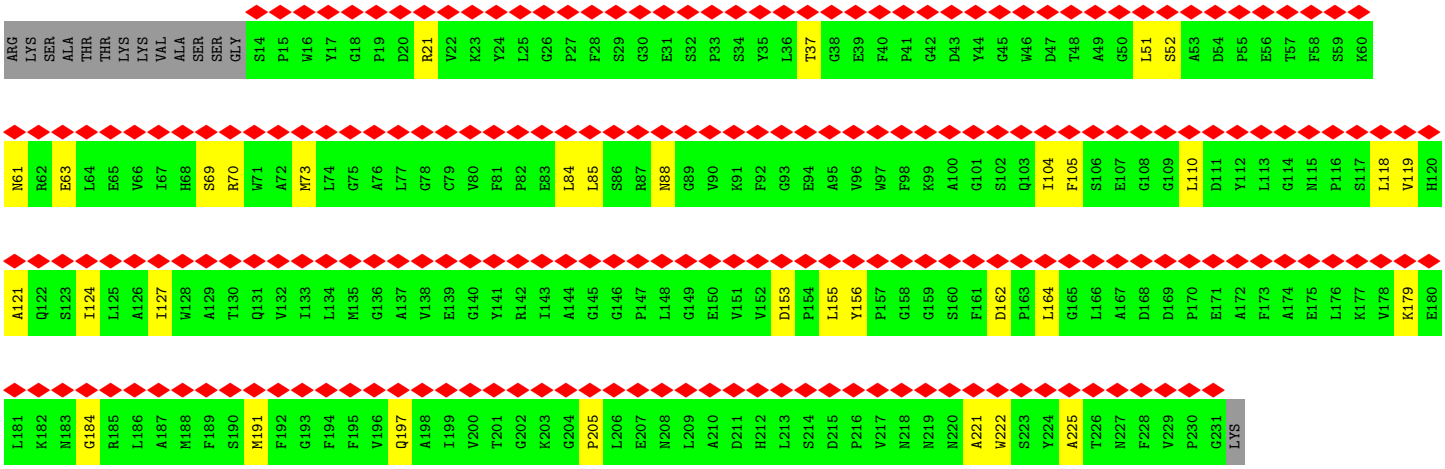




• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

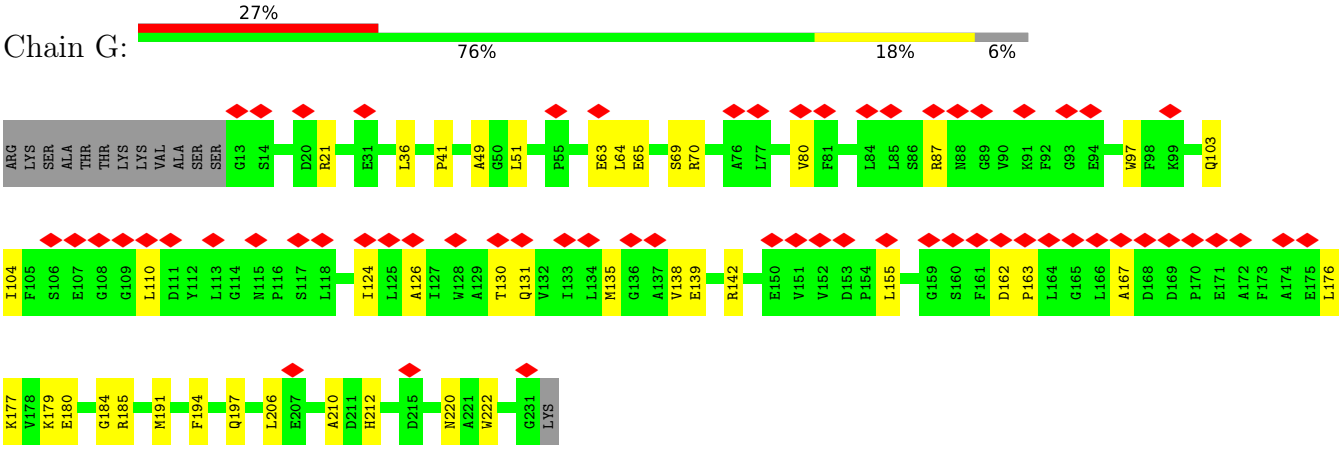
Chain 2:





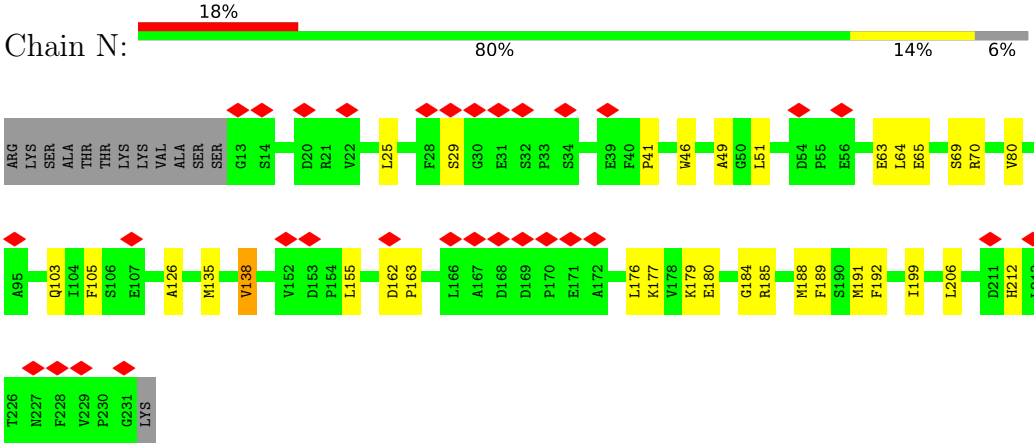
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain G:



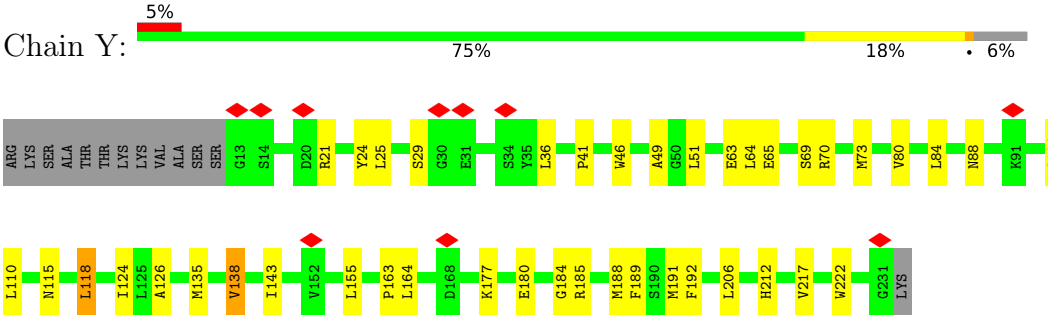
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain N:



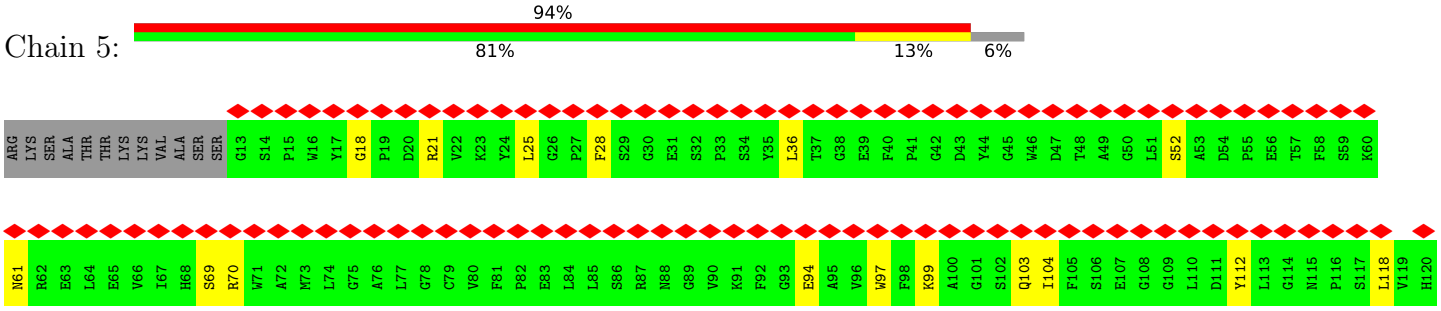
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

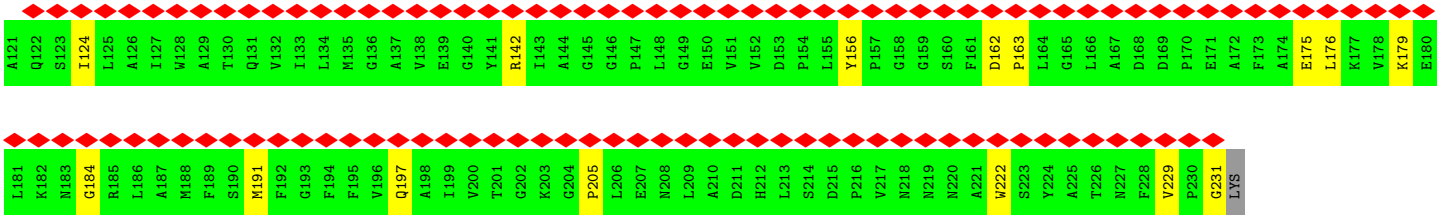
Chain Y:



• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

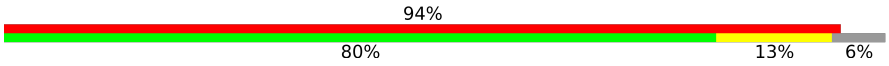
Chain 5:

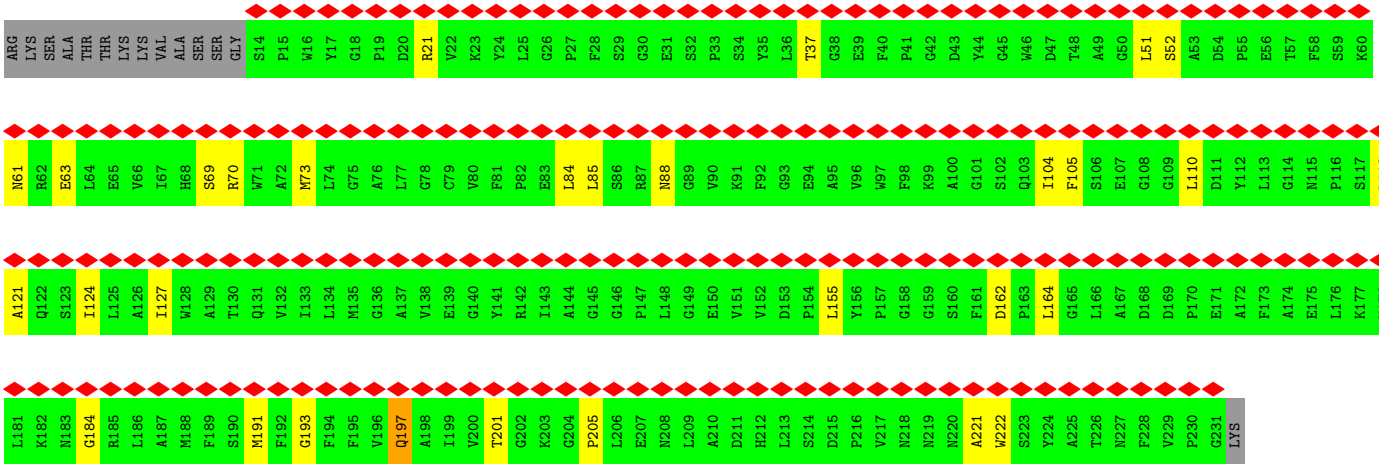




• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain 6:

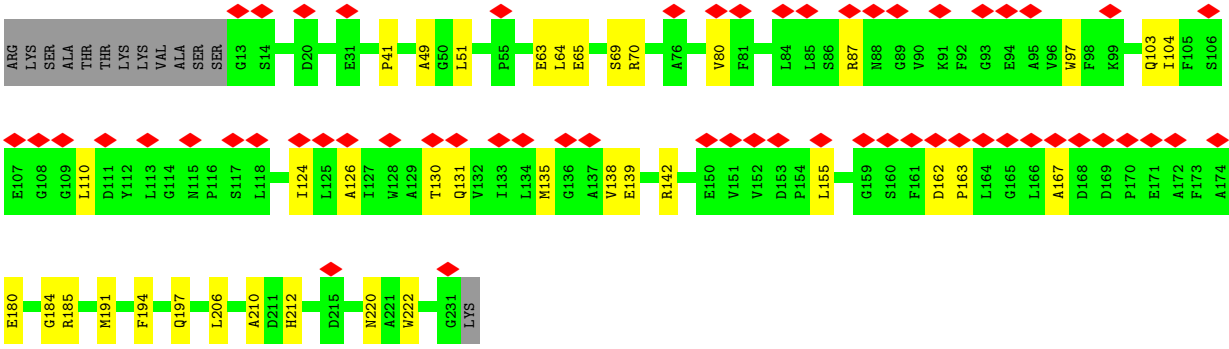




• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain g:

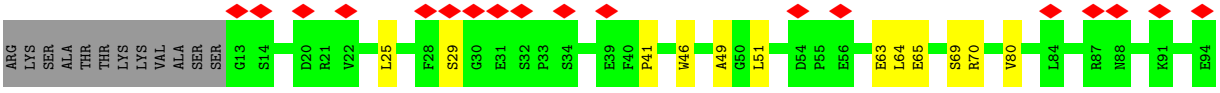


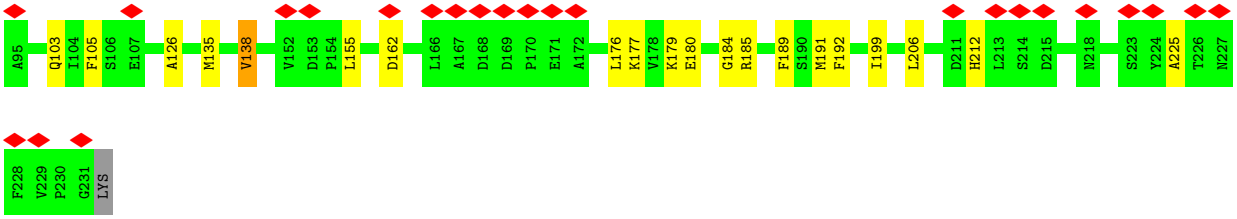


• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

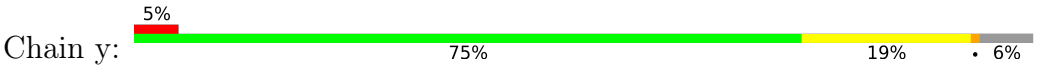
Chain n:

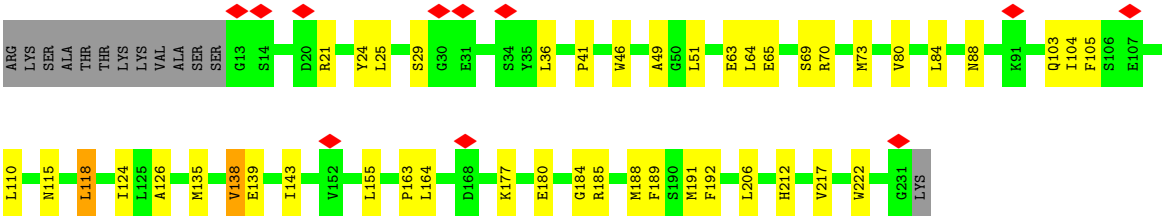




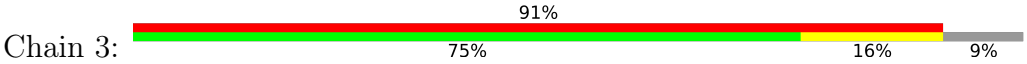


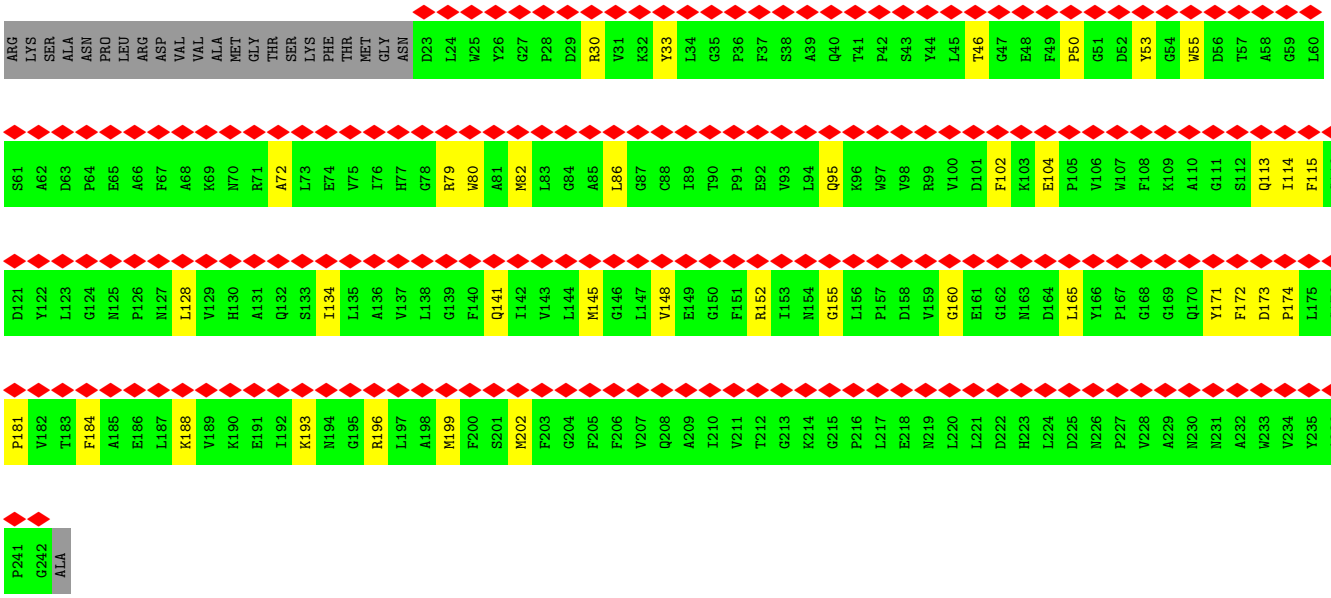
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



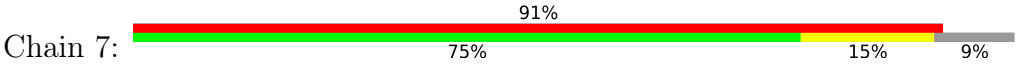


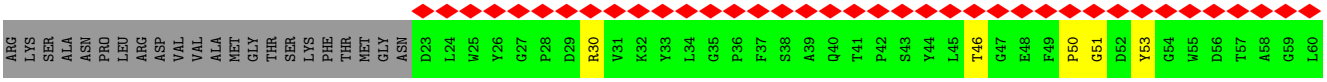
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic





• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

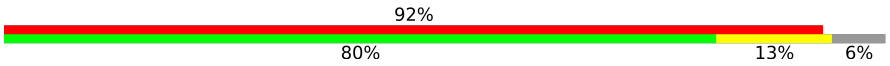


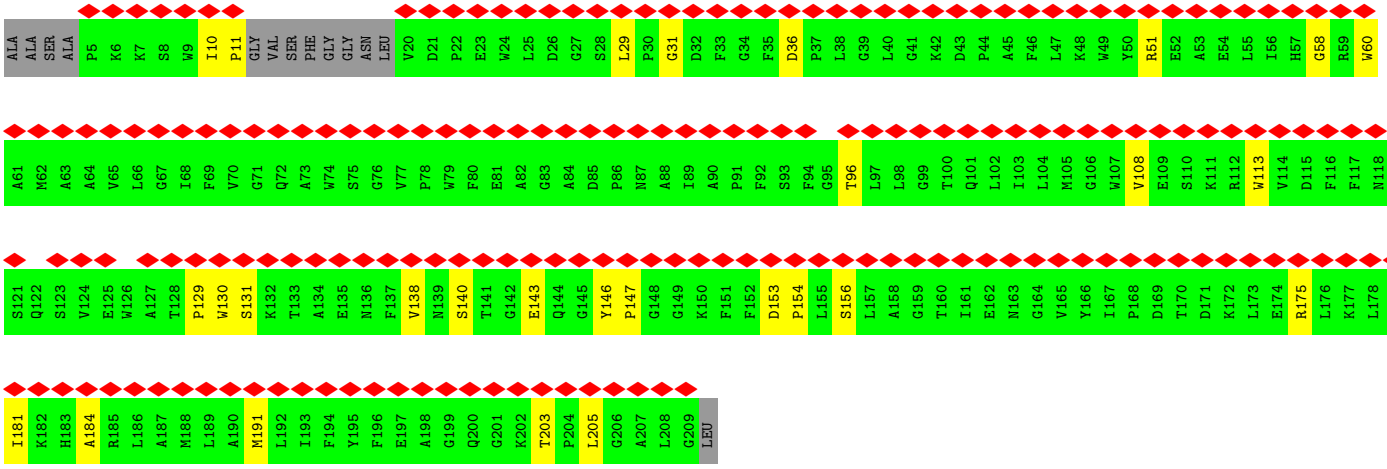




• Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24

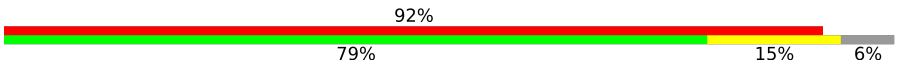
Chain 4:

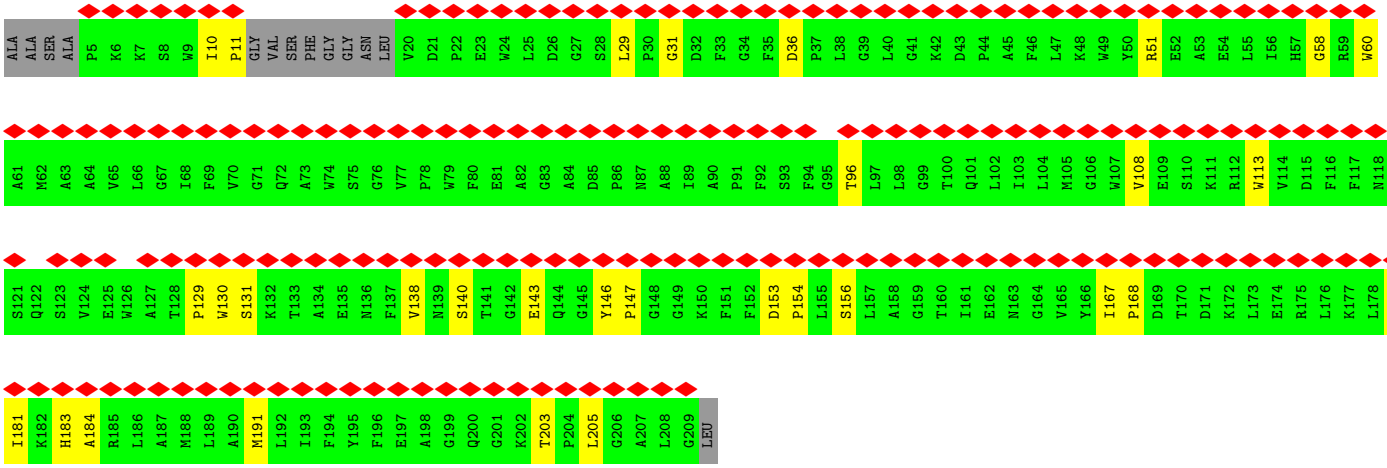




• Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24

Chain 8:





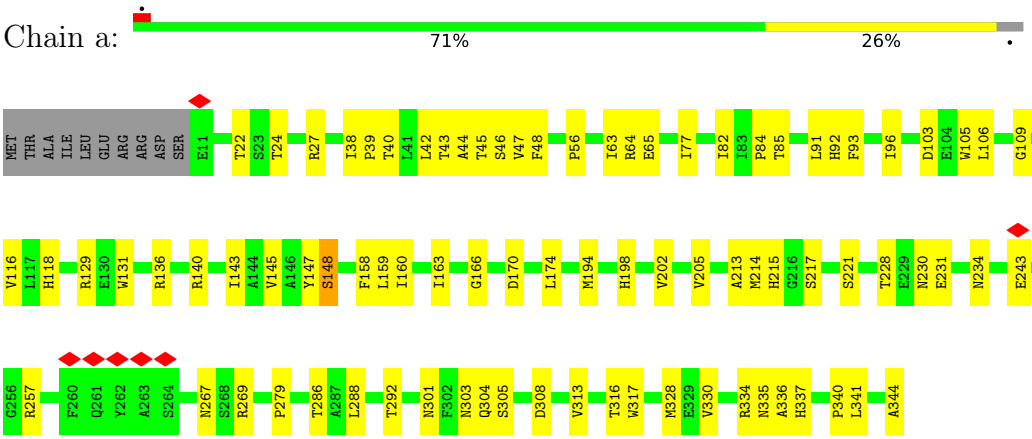
• Molecule 4: Photosystem II protein D1

Chain A:



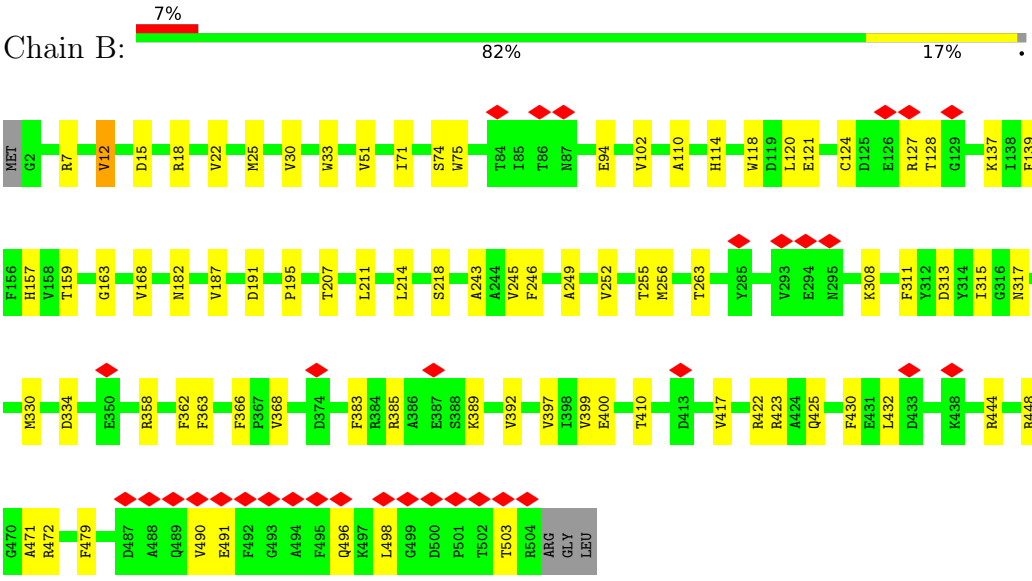
• Molecule 4: Photosystem II protein D1

Chain a:



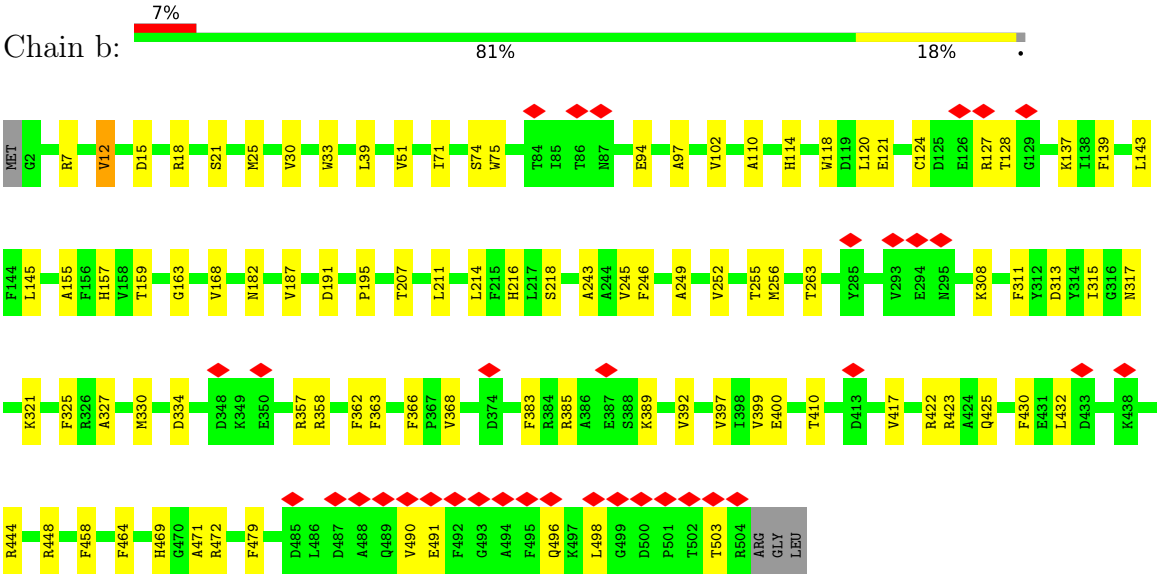
• Molecule 5: Photosystem II CP47 reaction center protein

Chain B:



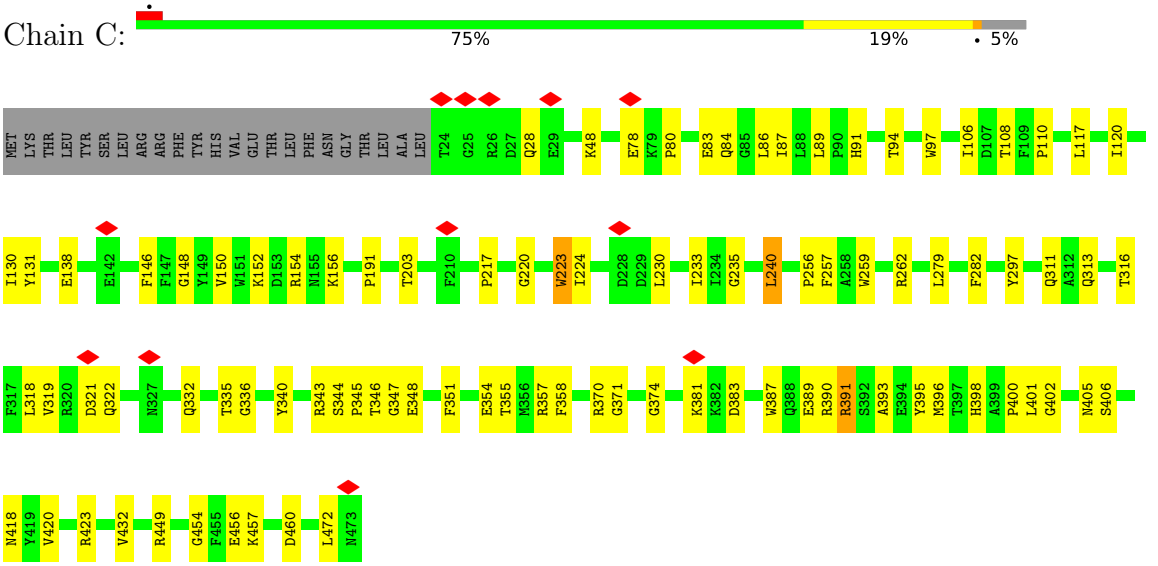
• Molecule 5: Photosystem II CP47 reaction center protein

Chain b:



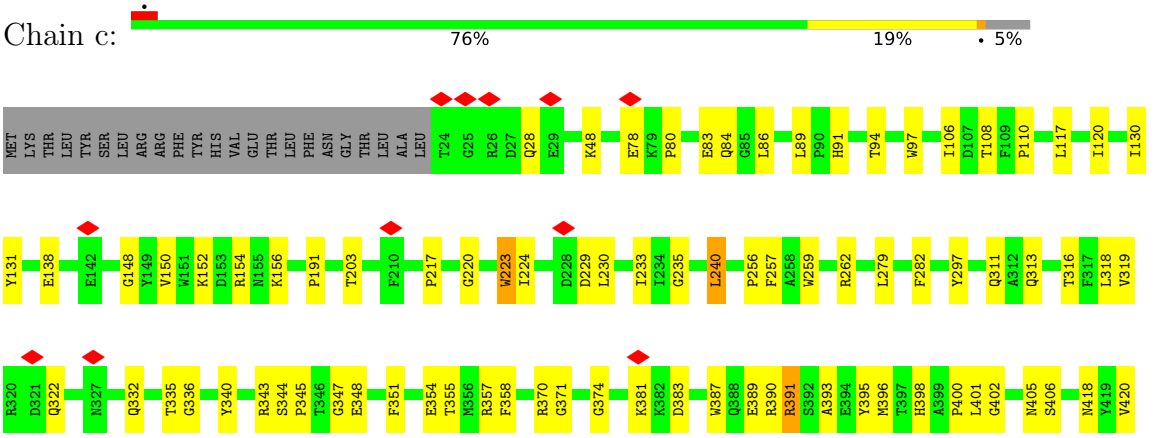
• Molecule 6: Photosystem II CP43 reaction center protein

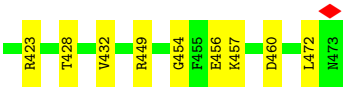
Chain C:



• Molecule 6: Photosystem II CP43 reaction center protein

Chain c:

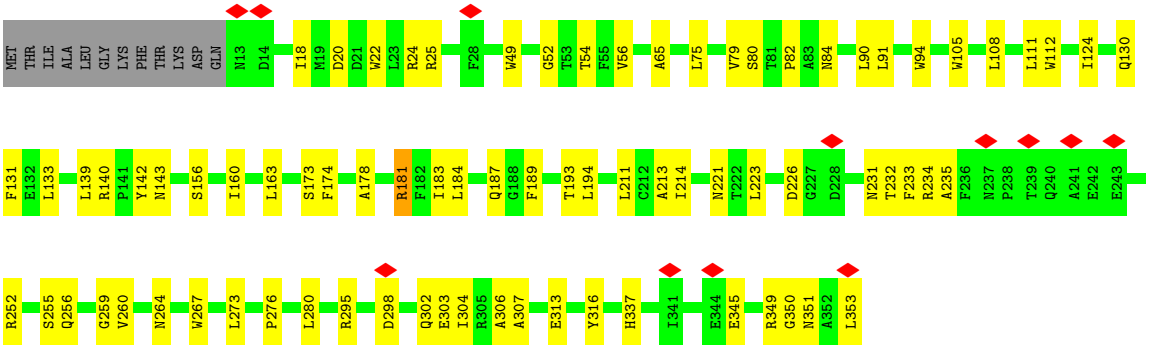




• Molecule 7: Photosystem II D2 protein

Chain D:

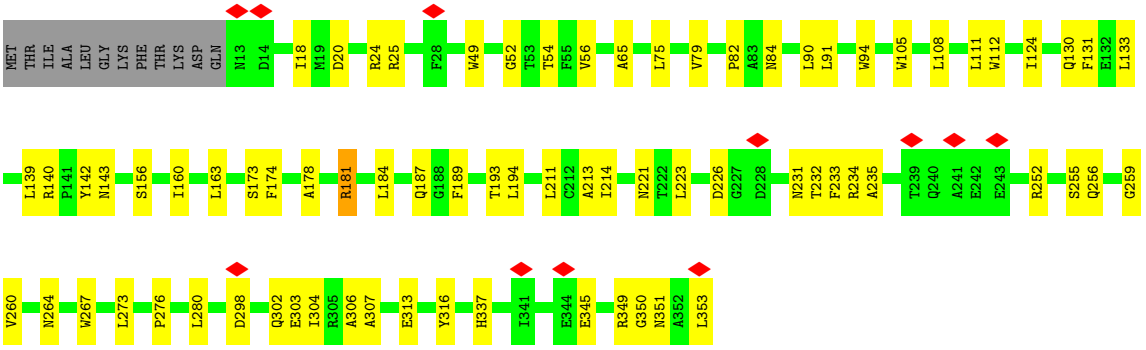




• Molecule 7: Photosystem II D2 protein

Chain d:

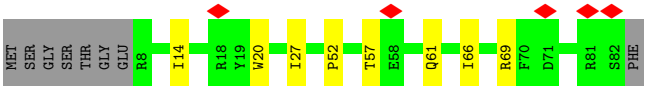




• Molecule 8: Cytochrome b559 subunit alpha

Chain E:

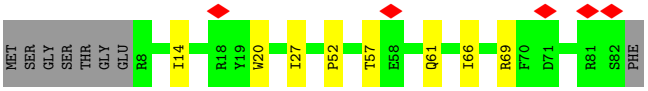




• Molecule 8: Cytochrome b559 subunit alpha

Chain e:

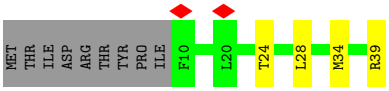




• Molecule 9: Cytochrome b559 subunit beta, PsbF

Chain F:

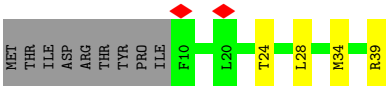




• Molecule 9: Cytochrome b559 subunit beta, PsbF

Chain f:

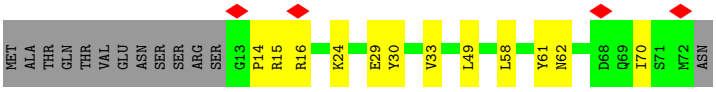




• Molecule 10: Photosystem II reaction center protein H

Chain H:

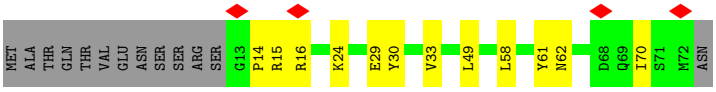




• Molecule 10: Photosystem II reaction center protein H

Chain h:

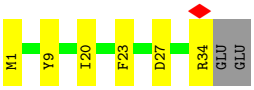




• Molecule 11: Photosystem II reaction center protein I, PsbI

Chain I:

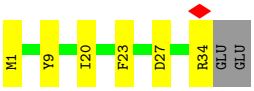




• Molecule 11: Photosystem II reaction center protein I, PsbI

Chain i:

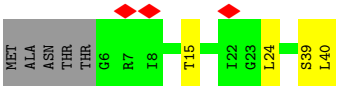




• Molecule 12: Photosystem II reaction center protein J

Chain J:

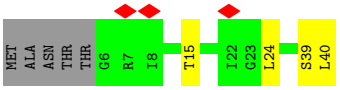




• Molecule 12: Photosystem II reaction center protein J

Chain j:

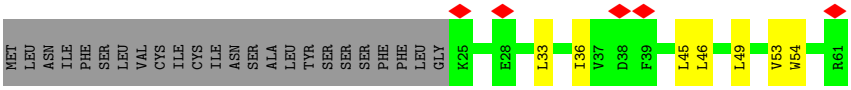




• Molecule 13: Photosystem II reaction center protein K

Chain K:

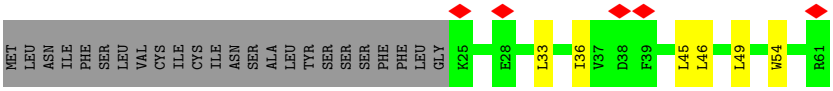




• Molecule 13: Photosystem II reaction center protein K

Chain k:

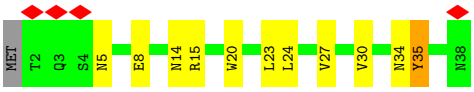




• Molecule 14: Photosystem II reaction center protein L

Chain L:

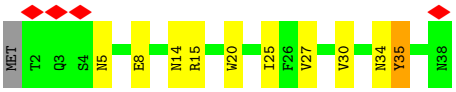




• Molecule 14: Photosystem II reaction center protein L

Chain l:





• Molecule 15: Photosystem II reaction center protein M

Chain M:

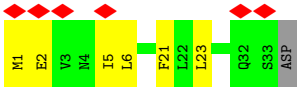




• Molecule 15: Photosystem II reaction center protein M

Chain m:

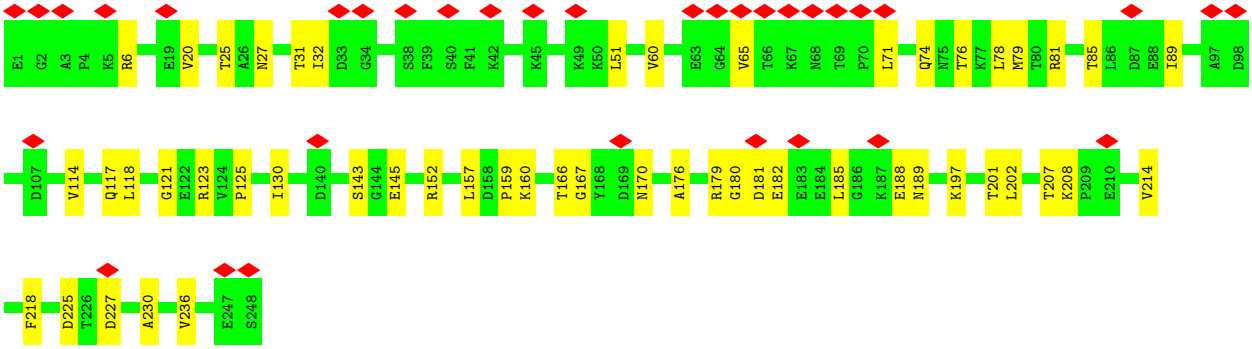




• Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic

Chain O:

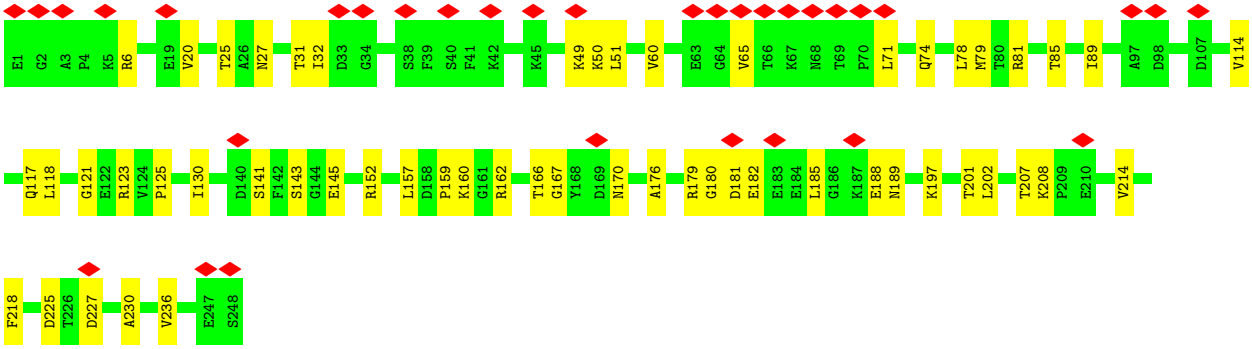




• Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic

Chain o:

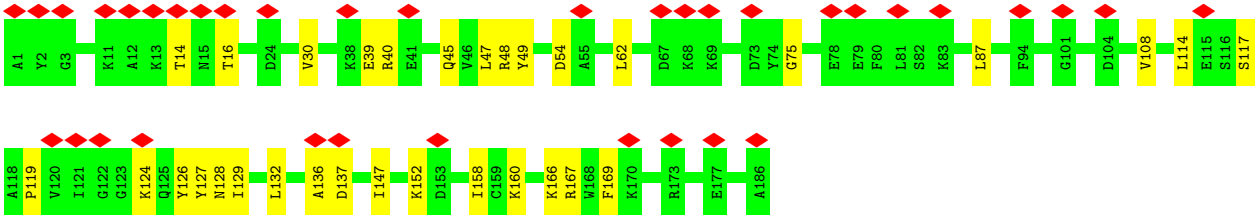




• Molecule 17: Oxygen-evolving enhancer protein 2, chloroplastic

Chain P:

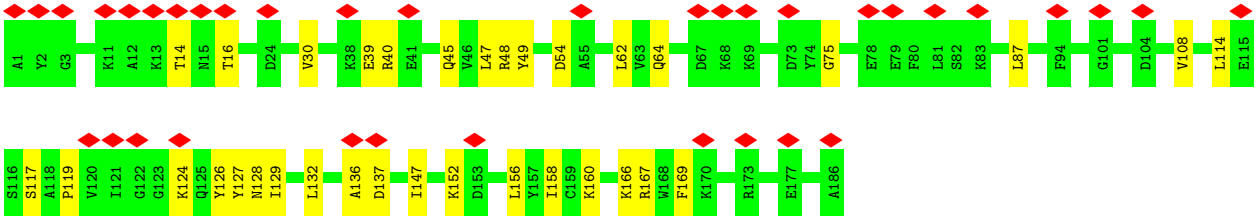




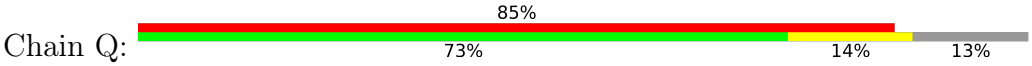
• Molecule 17: Oxygen-evolving enhancer protein 2, chloroplastic

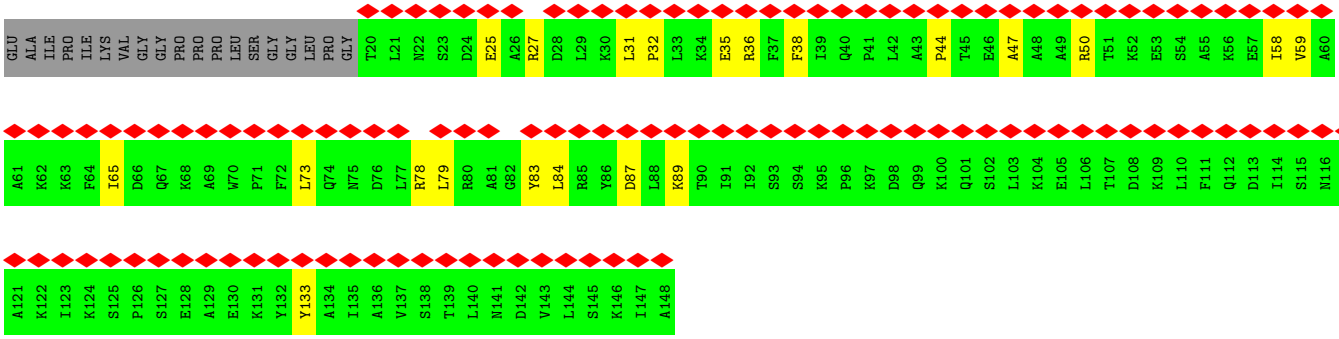
Chain p:



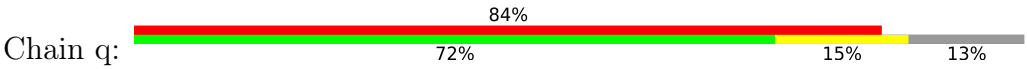


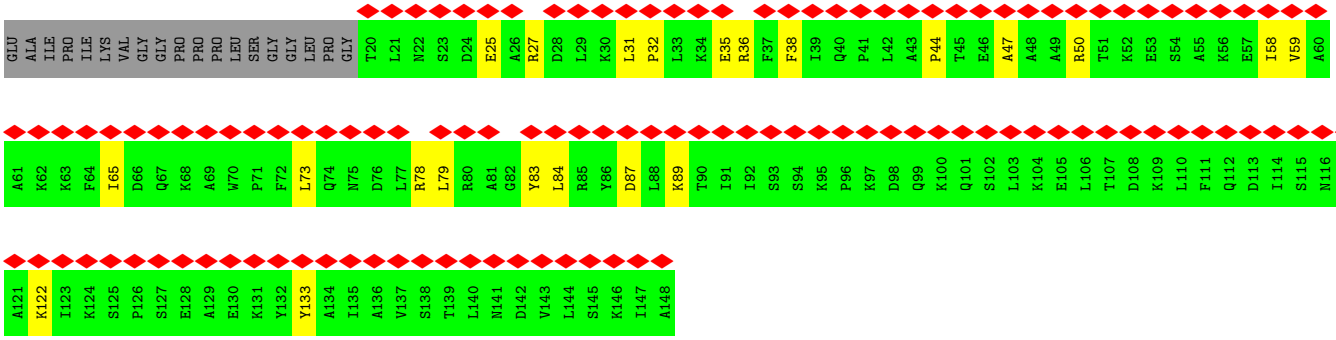
• Molecule 18: Oxygen-evolving enhancer protein 3



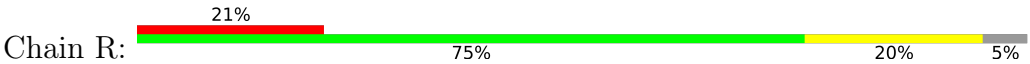


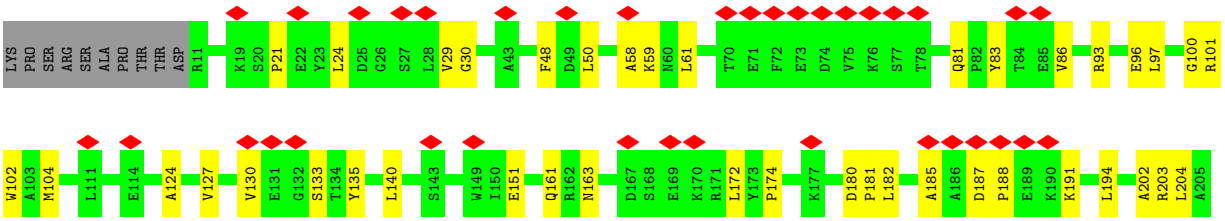
• Molecule 18: Oxygen-evolving enhancer protein 3

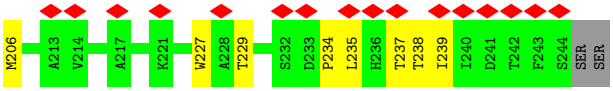




• Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29



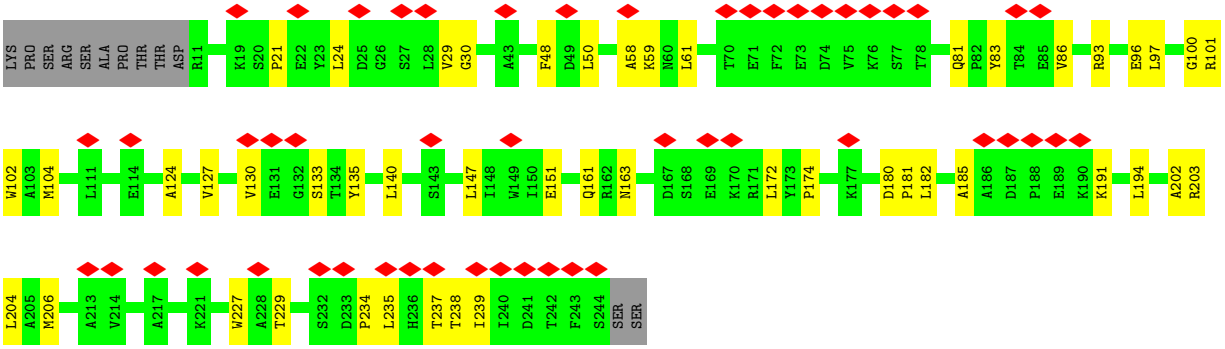




• Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29

Chain r:

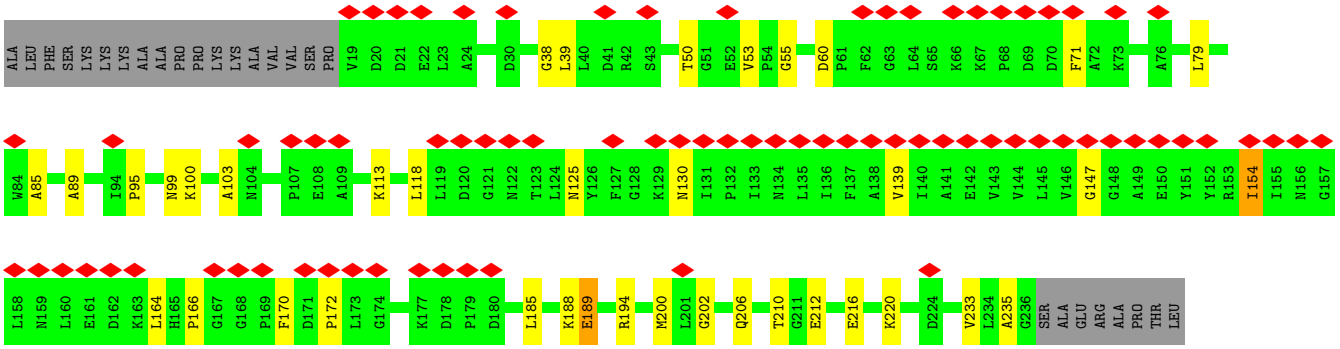




• Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

Chain S:

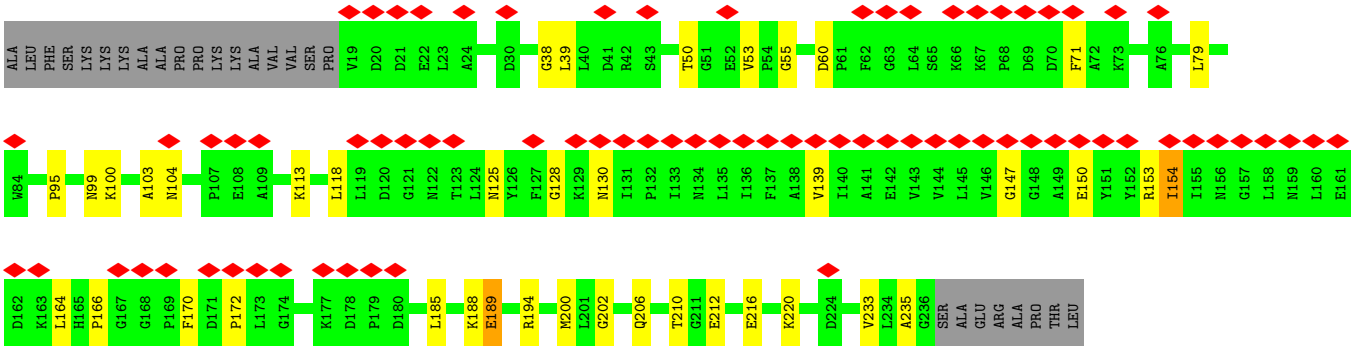




• Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

Chain s:

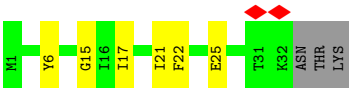




• Molecule 21: Photosystem II reaction center protein T

Chain T:

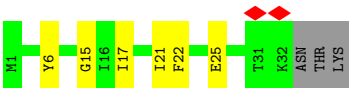




• Molecule 21: Photosystem II reaction center protein T

Chain t:

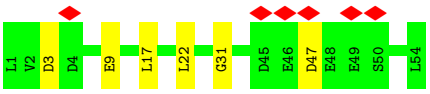




• Molecule 22: Photosystem II reaction center protein W

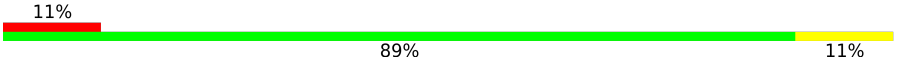
Chain W:

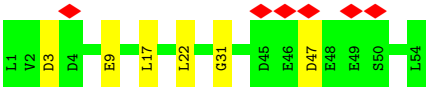




• Molecule 22: Photosystem II reaction center protein W

Chain w:

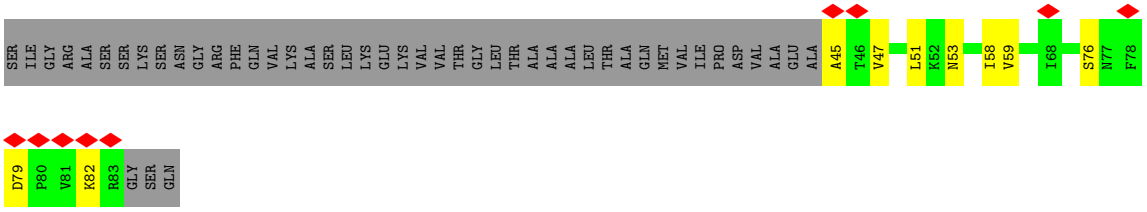




• Molecule 23: Photosystem II reaction center protein X

Chain X:

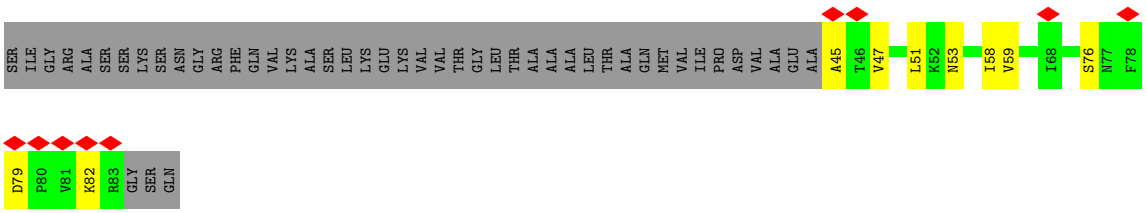




• Molecule 23: Photosystem II reaction center protein X

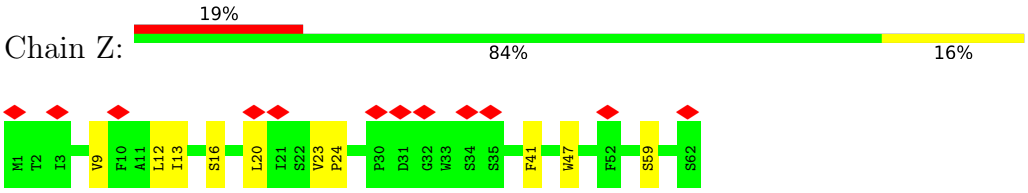
Chain x:





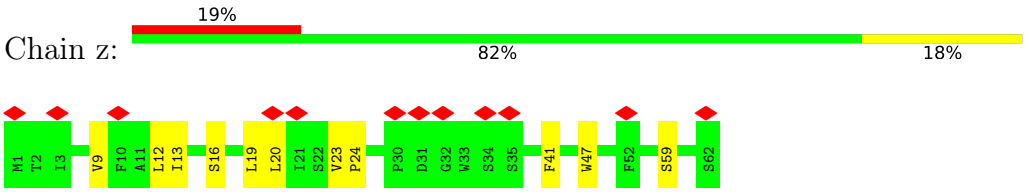
• Molecule 24: Photosystem II reaction center protein Z

Chain Z:



• Molecule 24: Photosystem II reaction center protein Z

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	136521	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	168.730	Depositor
Minimum map value	-94.103	Depositor
Average map value	0.061	Depositor
Map value standard deviation	6.582	Depositor
Recommended contour level	17.5	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	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: DGD, PL9, LMG, LHG, XAT, OEX, CL, CHL, HEM, CLA, BCR, FE2, NEX, LUT, BCT, PHO, SQD

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	1	0.27	0/1720	0.46	0/2342
1	2	0.25	0/1716	0.49	1/2337 (0.0%)
1	5	0.28	0/1720	0.46	0/2342
1	6	0.25	0/1716	0.49	1/2337 (0.0%)
1	G	0.39	0/1720	0.52	0/2342
1	N	0.50	0/1720	0.61	1/2342 (0.0%)
1	Y	0.44	0/1720	0.63	3/2342 (0.1%)
1	g	0.39	0/1720	0.52	0/2342
1	n	0.50	0/1720	0.61	1/2342 (0.0%)
1	y	0.44	0/1720	0.63	3/2342 (0.1%)
2	3	0.31	0/1759	0.50	0/2396
2	7	0.31	0/1759	0.50	0/2396
3	4	0.28	0/1586	0.59	0/2158
3	8	0.28	0/1586	0.59	0/2158
4	A	0.53	1/2697 (0.0%)	0.62	0/3677
4	a	0.53	1/2697 (0.0%)	0.62	0/3677
5	B	0.54	0/4081	0.61	0/5556
5	b	0.54	0/4081	0.61	0/5556
6	C	0.57	1/3614 (0.0%)	0.61	1/4922 (0.0%)
6	c	0.57	1/3614 (0.0%)	0.61	1/4922 (0.0%)
7	D	0.46	0/2804	0.62	0/3823
7	d	0.46	0/2804	0.62	0/3823
8	E	0.39	0/630	0.49	0/857
8	e	0.39	0/630	0.49	0/857
9	F	0.77	1/248 (0.4%)	0.78	0/335
9	f	0.78	1/248 (0.4%)	0.78	0/335
10	H	0.49	0/461	0.51	0/626
10	h	0.49	0/461	0.51	0/626
11	I	0.49	0/286	0.69	0/386
11	i	0.49	0/286	0.69	0/386
12	J	0.58	0/262	0.76	0/354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
12	j	0.58	0/262	0.76	0/354
13	K	0.45	0/318	0.71	0/434
13	k	0.45	0/318	0.71	0/434
14	L	0.59	0/319	0.68	1/434 (0.2%)
14	l	0.59	0/319	0.68	1/434 (0.2%)
15	M	0.44	0/260	0.68	0/355
15	m	0.45	0/260	0.68	0/355
16	O	0.45	1/1906 (0.1%)	0.61	0/2575
16	o	0.45	1/1906 (0.1%)	0.61	0/2575
17	P	0.55	0/1464	0.62	0/1978
17	p	0.55	0/1464	0.62	0/1978
18	Q	0.27	0/1051	0.56	0/1414
18	q	0.27	0/1051	0.56	0/1414
19	R	0.52	0/1886	0.64	1/2569 (0.0%)
19	r	0.52	0/1886	0.65	1/2569 (0.0%)
20	S	0.44	0/1736	0.70	3/2359 (0.1%)
20	s	0.44	0/1736	0.70	3/2359 (0.1%)
21	T	0.37	0/269	0.51	0/365
21	t	0.37	0/269	0.51	0/365
22	W	0.53	0/429	0.57	0/581
22	w	0.53	0/429	0.57	0/581
23	X	0.26	0/279	0.49	0/380
23	x	0.26	0/279	0.49	0/380
24	Z	0.39	0/474	0.61	0/648
24	z	0.40	0/474	0.61	0/648
All	All	0.46	8/74830 (0.0%)	0.60	22/101774 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	c	223	TRP	C-O	-5.55	1.19	1.24
6	C	223	TRP	C-O	-5.49	1.19	1.24
9	f	24	THR	C-O	-5.35	1.17	1.24
9	F	24	THR	C-O	-5.32	1.18	1.24
16	O	114	VAL	C-O	-5.31	1.18	1.24
16	o	114	VAL	C-O	-5.31	1.18	1.24
4	a	148	SER	C-O	-5.09	1.17	1.24
4	A	148	SER	C-O	-5.06	1.17	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	y	143	ILE	N-CA-C	8.60	120.38	111.00
1	Y	143	ILE	N-CA-C	8.59	120.36	111.00
1	N	138	VAL	N-CA-C	7.78	118.56	110.62
1	n	138	VAL	N-CA-C	7.78	118.56	110.62
1	Y	138	VAL	N-CA-C	7.77	118.55	110.62
1	y	138	VAL	N-CA-C	7.74	118.51	110.62
20	S	189	GLU	N-CA-C	6.86	118.55	111.14
20	s	189	GLU	N-CA-C	6.84	118.52	111.14
19	R	83	TYR	N-CA-C	6.71	118.67	111.36
19	r	83	TYR	N-CA-C	6.71	118.67	111.36
20	s	154	ILE	CA-C-N	-6.56	116.29	122.66
20	s	154	ILE	C-N-CA	-6.56	116.29	122.66
20	S	154	ILE	CA-C-N	-6.54	116.32	122.66
20	S	154	ILE	C-N-CA	-6.54	116.32	122.66
14	L	35	TYR	N-CA-C	6.33	118.26	111.36
14	l	35	TYR	N-CA-C	6.32	118.25	111.36
1	6	197	GLN	CA-CB-CG	5.92	125.94	114.10
1	2	197	GLN	CA-CB-CG	5.91	125.92	114.10
6	c	240	LEU	N-CA-C	5.74	117.61	111.36
6	C	240	LEU	N-CA-C	5.71	117.58	111.36
1	Y	118	LEU	N-CA-C	5.56	117.82	107.99
1	y	118	LEU	N-CA-C	5.56	117.82	107.99

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	1	1668	0	1596	25	0
1	2	1664	0	1593	24	0
1	5	1668	0	1596	23	0
1	6	1664	0	1593	24	0
1	G	1668	0	1596	33	0
1	N	1668	0	1596	28	0
1	Y	1668	0	1596	34	0
1	g	1668	0	1596	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	n	1668	0	1596	26	0
1	y	1668	0	1596	35	0
2	3	1707	0	1659	28	0
2	7	1707	0	1659	28	0
3	4	1534	0	1486	22	0
3	8	1534	0	1486	23	0
4	A	2616	0	2522	98	0
4	a	2616	0	2522	94	0
5	B	3948	0	3818	80	0
5	b	3948	0	3818	84	0
6	C	3497	0	3422	87	0
6	c	3497	0	3422	84	0
7	D	2712	0	2604	84	0
7	d	2712	0	2604	79	0
8	E	612	0	595	6	0
8	e	612	0	595	6	0
9	F	241	0	246	3	0
9	f	241	0	246	3	0
10	H	452	0	473	18	0
10	h	452	0	473	18	0
11	I	278	0	291	8	0
11	i	278	0	291	8	0
12	J	256	0	269	4	0
12	j	256	0	269	4	0
13	K	306	0	313	7	0
13	k	306	0	313	6	0
14	L	311	0	299	13	0
14	l	311	0	299	12	0
15	M	256	0	284	6	0
15	m	256	0	284	6	0
16	O	1870	0	1851	34	0
16	o	1870	0	1851	36	0
17	P	1434	0	1392	22	0
17	p	1434	0	1392	23	0
18	Q	1034	0	1075	22	0
18	q	1034	0	1075	23	0
19	R	1835	0	1801	43	0
19	r	1835	0	1801	42	0
20	S	1689	0	1670	33	0
20	s	1689	0	1670	35	0
21	T	261	0	280	9	0
21	t	261	0	280	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	W	419	0	402	5	0
22	w	419	0	402	5	0
23	X	276	0	301	8	0
23	x	276	0	301	8	0
24	Z	464	0	493	9	0
24	z	464	0	493	10	0
25	1	309	0	244	9	0
25	2	306	0	238	5	0
25	3	316	0	254	16	0
25	4	229	0	152	7	0
25	5	309	0	244	9	0
25	6	306	0	238	6	0
25	7	316	0	254	17	0
25	8	229	0	152	7	0
25	G	355	0	335	26	0
25	N	362	0	350	13	0
25	R	225	0	201	8	0
25	S	196	0	144	6	0
25	Y	362	0	350	11	0
25	g	355	0	335	26	0
25	n	362	0	350	12	0
25	r	225	0	201	9	0
25	s	196	0	144	5	0
25	y	362	0	350	13	0
26	1	412	0	348	8	0
26	2	391	0	314	7	0
26	3	426	0	373	12	0
26	4	270	0	198	3	0
26	5	412	0	348	8	0
26	6	391	0	314	8	0
26	7	426	0	373	10	0
26	8	270	0	198	2	0
26	A	240	0	242	16	0
26	B	1040	0	1152	53	0
26	C	845	0	936	37	0
26	D	130	0	144	7	0
26	G	477	0	477	19	0
26	N	473	0	468	25	0
26	R	543	0	490	29	0
26	S	465	0	393	14	0
26	Y	473	0	468	22	0
26	a	240	0	242	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	b	1040	0	1152	53	0
26	c	845	0	936	31	0
26	d	130	0	144	8	0
26	g	477	0	477	20	0
26	n	473	0	468	27	0
26	r	543	0	490	29	0
26	s	465	0	393	17	0
26	y	473	0	468	18	0
27	1	84	0	112	10	0
27	2	84	0	112	9	0
27	3	84	0	112	8	0
27	4	42	0	56	2	0
27	5	84	0	112	10	0
27	6	84	0	112	8	0
27	7	84	0	112	6	0
27	8	42	0	56	3	0
27	G	84	0	112	13	0
27	N	84	0	112	10	0
27	R	42	0	56	4	0
27	S	84	0	112	5	0
27	Y	84	0	112	10	0
27	g	84	0	112	15	0
27	n	84	0	112	9	0
27	r	42	0	56	5	0
27	s	84	0	112	6	0
27	y	84	0	112	9	0
28	1	44	0	56	4	0
28	2	44	0	56	6	0
28	3	44	0	56	3	0
28	4	44	0	56	3	0
28	5	44	0	56	3	0
28	6	44	0	56	4	0
28	7	44	0	56	3	0
28	8	44	0	56	4	0
28	G	44	0	56	5	0
28	N	44	0	56	6	0
28	R	44	0	56	4	0
28	Y	44	0	56	6	0
28	g	44	0	56	5	0
28	n	44	0	56	7	0
28	r	44	0	56	5	0
28	y	44	0	56	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	1	44	0	56	2	0
29	2	44	0	56	1	0
29	3	44	0	56	3	0
29	5	44	0	56	2	0
29	6	44	0	56	0	0
29	7	44	0	56	3	0
29	G	44	0	56	5	0
29	N	44	0	56	1	0
29	R	44	0	56	5	0
29	S	44	0	56	2	0
29	Y	44	0	56	2	0
29	g	44	0	56	2	0
29	n	44	0	56	1	0
29	r	44	0	56	4	0
29	s	44	0	56	3	0
29	y	44	0	56	1	0
30	1	41	0	55	2	0
30	2	37	0	44	1	0
30	3	47	0	67	3	0
30	4	21	0	12	1	0
30	5	41	0	55	2	0
30	6	37	0	44	1	0
30	7	47	0	67	2	0
30	8	21	0	12	1	0
30	B	96	0	141	5	0
30	C	147	0	222	12	0
30	D	138	0	195	17	0
30	G	49	0	74	4	0
30	L	49	0	74	3	0
30	N	49	0	74	4	0
30	R	42	0	57	4	0
30	S	49	0	74	4	0
30	Y	49	0	74	4	0
30	b	96	0	141	5	0
30	c	147	0	222	11	0
30	d	138	0	195	15	0
30	g	49	0	74	4	0
30	l	49	0	74	2	0
30	n	49	0	74	3	0
30	r	42	0	57	4	0
30	s	49	0	74	5	0
30	y	49	0	74	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	4	40	0	56	7	0
31	8	40	0	56	8	0
31	A	40	0	56	4	0
31	B	120	0	168	11	0
31	C	160	0	224	22	0
31	D	40	0	56	3	0
31	H	40	0	56	6	0
31	T	40	0	56	10	0
31	a	40	0	56	5	0
31	b	120	0	168	16	0
31	c	160	0	224	19	0
31	d	40	0	56	3	0
31	h	40	0	56	6	0
31	t	40	0	56	8	0
32	A	10	0	0	0	0
32	a	10	0	0	0	0
33	A	1	0	0	0	0
33	a	1	0	0	0	0
34	A	2	0	0	0	0
34	a	2	0	0	0	0
35	A	128	0	148	10	0
35	a	128	0	148	11	0
36	A	104	0	144	13	0
36	B	96	0	126	8	0
36	a	104	0	144	12	0
36	b	96	0	126	8	0
37	A	88	0	116	3	0
37	B	106	0	158	8	0
37	C	51	0	72	1	0
37	D	46	0	62	2	0
37	Z	51	0	72	5	0
37	a	88	0	116	3	0
37	b	106	0	158	8	0
37	c	51	0	72	1	0
37	d	46	0	62	2	0
37	z	51	0	72	5	0
38	A	13	0	7	1	0
38	D	55	0	80	2	0
38	a	13	0	7	1	0
38	d	55	0	80	1	0
39	B	59	0	76	5	0
39	C	177	0	227	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	H	62	0	82	3	0
39	b	59	0	76	5	0
39	c	177	0	227	5	0
39	h	62	0	82	4	0
40	D	4	0	0	0	0
40	d	4	0	0	0	0
41	F	43	0	30	1	0
41	f	43	0	30	1	0
42	A	96	0	0	0	0
42	B	89	0	0	0	0
42	C	68	0	0	0	0
42	D	58	0	0	0	0
42	E	10	0	0	0	0
42	F	2	0	0	0	0
42	G	15	0	0	1	0
42	H	16	0	0	0	0
42	J	3	0	0	0	0
42	K	2	0	0	0	0
42	L	10	0	0	0	0
42	M	4	0	0	0	0
42	N	20	0	0	0	0
42	O	31	0	0	0	0
42	P	16	0	0	0	0
42	R	30	0	0	0	0
42	S	14	0	0	1	0
42	T	2	0	0	0	0
42	W	4	0	0	0	0
42	X	5	0	0	0	0
42	Y	39	0	0	0	0
42	Z	4	0	0	0	0
42	a	96	0	0	0	0
42	b	89	0	0	0	0
42	c	68	0	0	0	0
42	d	58	0	0	0	0
42	e	10	0	0	0	0
42	f	2	0	0	0	0
42	g	15	0	0	1	0
42	h	16	0	0	0	0
42	j	3	0	0	0	0
42	k	2	0	0	0	0
42	l	10	0	0	0	0
42	m	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	n	20	0	0	0	0
42	o	31	0	0	0	0
42	p	16	0	0	0	0
42	r	30	0	0	0	0
42	s	14	0	0	1	0
42	t	2	0	0	0	0
42	w	4	0	0	0	0
42	x	5	0	0	0	0
42	y	39	0	0	0	0
42	z	4	0	0	0	0
All	All	98986	0	97642	1942	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 10.

All (1942) 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)
3:8:130:TRP:CD1	26:r:611:CLA:HAB	2.08	0.87
3:4:130:TRP:CD1	26:R:611:CLA:HAB	2.08	0.87
31:4:623:BCR:HC42	26:R:601:CLA:HBB1	1.62	0.82
31:8:623:BCR:HC42	26:r:601:CLA:HBB1	1.62	0.79
1:2:191:MET:HE2	27:2:1621:LUT:H10	1.65	0.78
1:6:191:MET:HE2	27:6:1621:LUT:H10	1.65	0.78
6:c:383:ASP:HB3	18:q:79:LEU:HD21	1.65	0.78
3:4:130:TRP:HD1	26:R:611:CLA:HAB	1.48	0.78
6:C:383:ASP:HB3	18:Q:79:LEU:HD21	1.65	0.77
3:8:130:TRP:HD1	26:r:611:CLA:HAB	1.48	0.76
26:7:602:CLA:HAB	27:7:1621:LUT:H32	1.67	0.75
20:s:139:VAL:HG22	25:s:607:CHL:HBC1	1.69	0.75
19:r:93:ARG:NH1	19:r:96:GLU:OE2	2.20	0.75
19:R:93:ARG:NH1	19:R:96:GLU:OE2	2.20	0.74
4:A:257:ARG:CD	5:B:498:LEU:HD21	2.18	0.74
26:3:602:CLA:HAB	27:3:1621:LUT:H32	1.67	0.74
20:S:139:VAL:HG22	25:S:607:CHL:HBC1	1.69	0.73
2:7:202:MET:HE2	27:7:1621:LUT:H10	1.71	0.73
4:a:257:ARG:CD	5:b:498:LEU:HD21	2.18	0.73
5:b:385:ARG:NH1	16:o:167:GLY:O	2.22	0.73
2:3:202:MET:HE2	27:3:1621:LUT:H10	1.71	0.73
31:c:517:BCR:H332	24:z:12:LEU:HD23	1.71	0.73
26:n:610:CLA:H71	26:n:612:CLA:H101	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:385:ARG:NH1	16:O:167:GLY:O	2.22	0.72
5:B:121:GLU:HG3	10:H:16:ARG:HD3	1.71	0.72
4:a:257:ARG:HD3	5:b:498:LEU:HD21	1.70	0.72
7:D:54:THR:HG22	9:F:34:MET:HE1	1.72	0.72
4:A:257:ARG:HD3	5:B:498:LEU:HD21	1.70	0.72
26:5:602:CLA:HAB	27:5:1621:LUT:H32	1.72	0.72
31:C:517:BCR:H332	24:Z:12:LEU:HD23	1.71	0.72
26:N:610:CLA:H71	26:N:612:CLA:H101	1.71	0.72
5:b:121:GLU:HG3	10:h:16:ARG:HD3	1.71	0.71
26:B:603:CLA:H12	10:H:61:TYR:CD2	2.26	0.71
26:b:603:CLA:H12	10:h:61:TYR:CD2	2.26	0.70
30:C:2630:LHG:H152	30:S:2630:LHG:H111	1.72	0.70
7:d:54:THR:HG22	9:f:34:MET:HE1	1.72	0.70
30:d:409:LHG:H291	21:t:17:ILE:HG23	1.72	0.70
4:A:243:GLU:N	4:A:243:GLU:OE2	2.24	0.70
26:1:602:CLA:HAB	27:1:1621:LUT:H32	1.72	0.70
30:c:2630:LHG:H152	30:s:2630:LHG:H111	1.72	0.70
26:g:610:CLA:H52	27:g:1620:LUT:H28	1.74	0.70
1:Y:191:MET:HE2	27:Y:1621:LUT:H10	1.74	0.69
36:a:418:SQD:C26	31:t:101:BCR:H333	2.21	0.69
1:y:191:MET:HE2	27:y:1621:LUT:H10	1.73	0.69
30:D:409:LHG:H291	21:T:17:ILE:HG23	1.72	0.69
35:A:409:PHO:HBC3	7:D:280:LEU:HD22	1.75	0.69
36:A:418:SQD:C26	31:T:101:BCR:H333	2.22	0.69
36:B:623:SQD:H281	15:M:21:PHE:HB2	1.75	0.69
26:G:610:CLA:H52	27:G:1620:LUT:H28	1.74	0.69
36:B:621:SQD:H352	31:t:101:BCR:H362	1.74	0.68
1:1:191:MET:HE2	27:1:1621:LUT:H10	1.75	0.68
1:5:191:MET:HE2	27:5:1621:LUT:H10	1.75	0.68
7:D:260:VAL:HG21	30:D:409:LHG:H281	1.76	0.68
30:d:409:LHG:H322	21:t:21:ILE:HD11	1.76	0.68
30:D:409:LHG:H322	21:T:21:ILE:HD11	1.76	0.68
4:a:243:GLU:N	4:a:243:GLU:OE2	2.24	0.68
1:g:191:MET:HE2	27:g:1621:LUT:H10	1.75	0.68
6:c:472:LEU:HD21	7:d:256:GLN:HE21	1.59	0.68
7:d:260:VAL:HG21	30:d:409:LHG:H281	1.76	0.68
35:a:409:PHO:HBC3	7:d:280:LEU:HD22	1.74	0.68
36:b:623:SQD:H281	15:m:21:PHE:HB2	1.75	0.67
4:A:221:SER:HA	7:D:140:ARG:HB2	1.75	0.67
20:S:202:GLY:O	20:S:206:GLN:HB3	1.93	0.67
20:s:202:GLY:O	20:s:206:GLN:HB3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:243:GLU:H	4:A:243:GLU:CD	2.03	0.67
1:G:191:MET:HE2	27:G:1621:LUT:H10	1.75	0.67
6:C:393:ALA:HB1	18:Q:27:ARG:HG3	1.77	0.67
4:a:221:SER:HA	7:d:140:ARG:HB2	1.75	0.67
5:B:75:TRP:HB3	39:B:626:DGD:HD5	1.76	0.67
26:7:611:CLA:H3A	3:8:131:SER:HA	1.77	0.67
19:r:30:GLY:H	19:r:93:ARG:NH2	1.93	0.66
6:C:472:LEU:HD21	7:D:256:GLN:HE21	1.58	0.66
20:S:100:LYS:NZ	20:S:216:GLU:OE1	2.28	0.66
5:b:15:ASP:OD2	14:l:5:ASN:ND2	2.28	0.66
5:B:311:PHE:O	5:B:317:ASN:ND2	2.29	0.66
7:D:193:THR:HG23	26:D:402:CLA:HBC2	1.78	0.66
26:b:604:CLA:HAB	26:b:606:CLA:H152	1.78	0.66
20:s:100:LYS:NZ	20:s:216:GLU:OE1	2.28	0.66
5:B:15:ASP:OD2	14:L:5:ASN:ND2	2.28	0.66
26:3:611:CLA:H3A	3:4:131:SER:HA	1.77	0.66
26:B:604:CLA:HAB	26:B:606:CLA:H152	1.78	0.66
31:T:101:BCR:H362	36:b:621:SQD:H352	1.78	0.66
4:a:40:THR:HG23	26:a:410:CLA:HBB1	1.78	0.66
5:b:75:TRP:HB3	39:b:626:DGD:HD5	1.76	0.66
7:d:193:THR:HG23	26:d:402:CLA:HBC2	1.78	0.66
28:N:1622:XAT:H363	30:N:2630:LHG:HC41	1.77	0.65
7:D:173:SER:HB2	7:D:178:ALA:HB1	1.79	0.65
19:r:163:ASN:HD22	26:r:616:CLA:HBC3	1.61	0.65
36:A:418:SQD:H181	30:D:409:LHG:H382	1.78	0.65
19:R:30:GLY:H	19:R:93:ARG:NH2	1.93	0.65
6:c:393:ALA:HB1	18:q:27:ARG:HG3	1.77	0.65
7:d:124:ILE:HD11	39:h:102:DGD:HAH2	1.79	0.65
19:R:163:ASN:HD22	26:R:616:CLA:HBC3	1.61	0.65
1:n:135:MET:HA	1:n:138:VAL:HG22	1.79	0.65
6:C:297:TYR:O	6:C:423:ARG:NH2	2.30	0.65
21:T:15:GLY:HA2	31:T:101:BCR:H12C	1.79	0.65
4:A:40:THR:HG23	26:A:410:CLA:HBB1	1.78	0.65
5:b:311:PHE:O	5:b:317:ASN:ND2	2.29	0.65
28:n:1622:XAT:H363	30:n:2630:LHG:HC41	1.77	0.65
7:D:124:ILE:HD11	39:H:102:DGD:HAH2	1.79	0.64
26:g:613:CLA:H162	26:g:614:CLA:H2	1.79	0.64
4:A:82:ILE:HB	4:A:174:LEU:HB2	1.79	0.64
4:A:217:SER:HA	7:D:273:LEU:HD12	1.79	0.64
26:G:613:CLA:H162	26:G:614:CLA:H2	1.79	0.64
1:g:139:GLU:HG3	25:g:609:CHL:C4B	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:135:MET:HA	1:N:138:VAL:HG22	1.79	0.64
31:C:517:BCR:H312	13:K:33:LEU:HD13	1.80	0.64
1:Y:135:MET:HA	1:Y:138:VAL:HG22	1.80	0.64
31:c:517:BCR:H312	13:k:33:LEU:HD13	1.80	0.64
8:e:57:THR:O	8:e:61:GLN:NE2	2.31	0.64
1:G:139:GLU:HG3	25:G:609:CHL:C4B	2.28	0.64
4:a:82:ILE:HB	4:a:174:LEU:HB2	1.79	0.64
4:a:217:SER:HA	7:d:273:LEU:HD12	1.79	0.64
36:a:418:SQD:H181	30:d:409:LHG:H382	1.78	0.64
8:E:57:THR:O	8:E:61:GLN:NE2	2.31	0.64
7:d:173:SER:HB2	7:d:178:ALA:HB1	1.79	0.64
6:c:86:LEU:HD13	6:c:89:LEU:HD12	1.80	0.63
6:c:297:TYR:O	6:c:423:ARG:NH2	2.30	0.63
17:p:117:SER:HB2	17:p:128:ASN:HB2	1.81	0.63
25:N:606:CHL:HMB1	25:N:609:CHL:HMC	1.81	0.63
4:A:143:ILE:HG13	7:D:221:ASN:HD22	1.63	0.63
6:C:86:LEU:HD13	6:C:89:LEU:HD12	1.80	0.63
1:N:191:MET:HE2	27:N:1621:LUT:H10	1.80	0.63
1:6:85:LEU:HD23	1:6:88:ASN:HD22	1.64	0.63
30:B:2631:LHG:H242	30:B:2631:LHG:HC91	1.81	0.63
30:c:2630:LHG:H101	26:s:611:CLA:HAB	1.81	0.63
1:n:191:MET:HE2	27:n:1621:LUT:H10	1.80	0.63
21:t:15:GLY:HA2	31:t:101:BCR:H12C	1.79	0.63
17:P:117:SER:HB2	17:P:128:ASN:HB2	1.80	0.63
4:a:143:ILE:HG13	7:d:221:ASN:HD22	1.63	0.62
12:J:40:LEU:HD11	17:P:14:THR:HG22	1.81	0.62
14:L:15:ARG:NH2	21:T:25:GLU:OE1	2.32	0.62
25:n:606:CHL:HMB1	25:n:609:CHL:HMC	1.80	0.62
14:l:15:ARG:NH2	21:t:25:GLU:OE1	2.32	0.62
19:R:21:PRO:HD2	19:R:24:LEU:HD13	1.80	0.62
1:G:70:ARG:NE	1:G:180:GLU:OE2	2.33	0.62
1:g:70:ARG:NE	1:g:180:GLU:OE2	2.33	0.62
12:j:40:LEU:HD11	17:p:14:THR:HG22	1.81	0.62
30:C:2630:LHG:H101	26:S:611:CLA:HAB	1.81	0.62
1:y:135:MET:HA	1:y:138:VAL:HG22	1.80	0.62
19:r:21:PRO:HD2	19:r:24:LEU:HD13	1.80	0.62
1:g:142:ARG:NH2	25:g:609:CHL:O1D	2.32	0.62
1:1:163:PRO:HD2	27:1:1620:LUT:H23	1.81	0.61
16:O:51:LEU:HB3	16:O:89:ILE:HB	1.82	0.61
16:O:117:GLN:HE21	16:O:121:GLY:HA2	1.65	0.61
25:7:606:CHL:HBB2	25:7:607:CHL:HBB1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:D:405:PL9:H111	30:D:409:LHG:HC92	1.81	0.61
1:Y:115:ASN:HB3	1:Y:118:LEU:HD12	1.82	0.61
26:A:407:CLA:HAB	26:D:402:CLA:H72	1.82	0.61
1:G:142:ARG:NH2	25:G:609:CHL:O1D	2.32	0.61
1:2:85:LEU:HD23	1:2:88:ASN:HD22	1.64	0.61
4:a:243:GLU:CD	4:a:243:GLU:H	2.03	0.61
30:b:2631:LHG:H242	30:b:2631:LHG:HC91	1.81	0.61
6:c:240:LEU:HD21	26:c:501:CLA:CHC	2.31	0.61
38:d:405:PL9:H111	30:d:409:LHG:HC92	1.82	0.61
20:s:147:GLY:HA2	26:s:609:CLA:HAB	1.83	0.61
2:3:171:TYR:O	2:3:172:PHE:HB2	2.00	0.61
25:3:606:CHL:HBB2	25:3:607:CHL:HBB1	1.82	0.61
4:A:159:LEU:HD22	26:C:505:CLA:H202	1.83	0.61
19:R:97:LEU:HB3	19:R:172:LEU:HD11	1.82	0.61
6:C:240:LEU:HD21	26:C:501:CLA:CHC	2.31	0.61
2:7:171:TYR:O	2:7:172:PHE:HB2	2.00	0.61
6:c:130:ILE:HD11	31:c:517:BCR:H21C	1.83	0.61
20:S:147:GLY:HA2	26:S:609:CLA:HAB	1.83	0.61
1:y:115:ASN:HB3	1:y:118:LEU:HD12	1.82	0.61
31:B:620:BCR:H271	21:t:22:PHE:HB3	1.83	0.60
1:5:163:PRO:HD2	27:5:1620:LUT:H23	1.81	0.60
25:R:606:CHL:HBA2	29:R:623:NEX:H403	1.83	0.60
4:a:159:LEU:HD22	26:c:505:CLA:H202	1.83	0.60
19:r:100:GLY:HA3	19:r:202:ALA:HB1	1.84	0.60
4:A:65:GLU:OE2	4:A:334:ARG:NH2	2.35	0.60
26:A:410:CLA:HAA2	37:A:413:LMG:H112	1.82	0.60
4:A:63:ILE:HB	6:C:335:THR:HG21	1.84	0.60
8:E:69:ARG:NH2	10:H:62:ASN:O	2.34	0.60
4:a:136:ARG:NH1	11:i:27:ASP:OD1	2.33	0.60
4:A:136:ARG:NH1	11:I:27:ASP:OD1	2.33	0.60
16:o:51:LEU:HB3	16:o:89:ILE:HB	1.82	0.60
19:r:97:LEU:HB3	19:r:172:LEU:HD11	1.82	0.60
1:y:164:LEU:HD12	27:y:1620:LUT:H222	1.84	0.60
26:a:407:CLA:HAB	26:d:402:CLA:H72	1.82	0.60
25:r:606:CHL:HBA2	29:r:623:NEX:H403	1.83	0.60
20:S:200:MET:HG2	27:S:1621:LUT:H14	1.83	0.60
26:8:610:CLA:HAB	27:8:620:LUT:H32	1.84	0.60
26:c:511:CLA:HBA1	31:c:517:BCR:H271	1.84	0.60
19:R:100:GLY:HA3	19:R:202:ALA:HB1	1.84	0.59
26:a:410:CLA:HAA2	37:a:413:LMG:H112	1.82	0.59
16:O:81:ARG:NH1	22:W:9:GLU:OE2	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:27:ARG:NH2	7:d:259:GLY:O	2.33	0.59
1:n:51:LEU:HD13	26:n:602:CLA:H42	1.84	0.59
6:C:130:ILE:HD11	31:C:517:BCR:H21C	1.83	0.59
1:Y:164:LEU:HD12	27:Y:1620:LUT:H222	1.84	0.59
1:N:51:LEU:HD13	26:N:602:CLA:H42	1.84	0.59
7:d:142:TYR:OH	30:d:408:LHG:O4	2.20	0.59
20:s:200:MET:HG2	27:s:1621:LUT:H14	1.83	0.59
26:C:511:CLA:HBA1	31:C:517:BCR:H271	1.84	0.59
4:a:63:ILE:HB	6:c:335:THR:HG21	1.84	0.59
5:b:191:ASP:HB2	10:h:70:ILE:HG12	1.84	0.59
1:g:103:GLN:NE2	26:g:604:CLA:O1D	2.36	0.59
26:c:503:CLA:H172	26:c:510:CLA:HBB2	1.85	0.59
31:c:516:BCR:H373	13:k:49:LEU:HD13	1.84	0.59
16:o:117:GLN:HE21	16:o:121:GLY:HA2	1.65	0.59
4:a:65:GLU:OE2	4:a:334:ARG:NH2	2.35	0.59
20:s:170:PHE:O	27:s:1620:LUT:H24	2.03	0.59
20:S:170:PHE:O	27:S:1620:LUT:H24	2.03	0.59
31:C:516:BCR:H373	13:K:49:LEU:HD13	1.84	0.59
1:G:103:GLN:NE2	26:G:604:CLA:O1D	2.36	0.58
25:1:607:CHL:HAA2	28:3:1622:XAT:H41	1.84	0.58
5:B:145:LEU:HB3	26:B:605:CLA:H162	1.84	0.58
18:q:50:ARG:NH1	18:q:87:ASP:OD1	2.36	0.58
35:A:409:PHO:H3A	26:D:402:CLA:H142	1.84	0.58
5:B:191:ASP:HB2	10:H:70:ILE:HG12	1.84	0.58
4:a:42:LEU:HD23	36:a:418:SQD:H212	1.85	0.58
5:b:145:LEU:HB3	26:b:605:CLA:H162	1.84	0.58
31:b:618:BCR:H322	37:b:622:LMG:H111	1.85	0.58
4:A:42:LEU:HD23	36:A:418:SQD:H212	1.85	0.58
4:a:335:ASN:HA	7:d:351:ASN:HD22	1.69	0.58
5:b:334:ASP:HB3	16:o:176:ALA:HB1	1.86	0.58
26:B:608:CLA:H2	37:B:622:LMG:H151	1.85	0.58
26:C:503:CLA:H172	26:C:510:CLA:HBB2	1.85	0.58
4:A:335:ASN:HA	7:D:351:ASN:HD22	1.69	0.58
6:C:391:ARG:NH1	6:C:395:TYR:OH	2.36	0.58
35:a:409:PHO:H3A	26:d:402:CLA:H142	1.84	0.58
6:c:78:GLU:HB2	18:q:32:PRO:HB3	1.86	0.58
18:Q:50:ARG:NH1	18:Q:87:ASP:OD1	2.36	0.58
25:g:606:CHL:CBA	29:g:1623:NEX:H403	2.34	0.58
26:4:610:CLA:HAB	27:4:620:LUT:H32	1.84	0.58
20:S:166:PRO:HB3	25:S:608:CHL:HBC2	1.85	0.58
3:4:191:MET:HE2	28:4:622:XAT:H10	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:27:ARG:NH2	7:D:259:GLY:O	2.33	0.58
7:D:142:TYR:OH	30:D:408:LHG:O4	2.20	0.58
7:D:187:GLN:HB2	26:D:402:CLA:HBC1	1.86	0.58
17:P:62:LEU:HD11	17:P:158:ILE:HD12	1.86	0.58
21:T:22:PHE:HB3	31:b:620:BCR:H271	1.85	0.58
4:A:131:TRP:CH2	6:C:449:ARG:HD2	2.39	0.57
1:n:70:ARG:NE	1:n:180:GLU:OE2	2.37	0.57
25:G:606:CHL:CBA	29:G:1623:NEX:H403	2.34	0.57
5:b:127:ARG:HG3	5:b:128:THR:HG23	1.86	0.57
26:b:608:CLA:H2	37:b:622:LMG:H151	1.85	0.57
5:B:334:ASP:HB3	16:O:176:ALA:HB1	1.86	0.57
6:C:148:GLY:O	6:C:156:LYS:NZ	2.37	0.57
1:N:70:ARG:NE	1:N:180:GLU:OE2	2.37	0.57
5:b:496:GLN:HB2	5:b:503:THR:HB	1.86	0.57
6:c:332:GLN:HE21	6:c:336:GLY:HA2	1.70	0.57
17:p:62:LEU:HD11	17:p:158:ILE:HD12	1.86	0.57
1:2:51:LEU:HD13	26:2:602:CLA:H42	1.86	0.57
6:C:78:GLU:HB2	18:Q:32:PRO:HB3	1.86	0.57
25:5:607:CHL:HAA2	28:7:1622:XAT:H41	1.84	0.57
4:a:341:LEU:H	6:c:313:GLN:HE22	1.53	0.57
20:s:166:PRO:HB3	25:s:608:CHL:HBC2	1.85	0.57
4:A:131:TRP:CZ2	6:C:449:ARG:HD2	2.40	0.57
4:A:341:LEU:H	6:C:313:GLN:HE22	1.53	0.57
31:B:618:BCR:H322	37:B:622:LMG:H111	1.85	0.57
6:C:343:ARG:NH1	6:C:347:GLY:O	2.38	0.57
8:E:14:ILE:O	8:E:20:TRP:NE1	2.38	0.57
26:R:613:CLA:H111	30:R:2630:LHG:H292	1.86	0.57
7:d:187:GLN:HB2	26:d:402:CLA:HBC1	1.86	0.57
1:6:51:LEU:HD13	26:6:602:CLA:H42	1.86	0.57
6:c:148:GLY:O	6:c:156:LYS:NZ	2.37	0.57
1:n:192:PHE:CD2	26:n:602:CLA:H171	2.40	0.57
4:a:140:ARG:NH1	7:d:232:THR:HG21	2.20	0.57
8:e:14:ILE:O	8:e:20:TRP:NE1	2.38	0.57
19:r:96:GLU:HB2	26:r:602:CLA:C1B	2.35	0.57
26:B:603:CLA:H12	10:H:61:TYR:HD2	1.69	0.57
26:8:612:CLA:HED2	26:8:612:CLA:H2A	1.87	0.57
5:b:30:VAL:HG11	26:b:613:CLA:H112	1.87	0.57
6:c:387:TRP:HB2	18:q:38:PHE:HD2	1.70	0.57
5:B:30:VAL:HG11	26:B:613:CLA:H112	1.87	0.56
5:B:127:ARG:HG3	5:B:128:THR:HG23	1.86	0.56
19:R:96:GLU:HB2	26:R:602:CLA:C1B	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:191:MET:HE2	28:8:622:XAT:H10	1.86	0.56
1:2:21:ARG:NH1	1:2:37:THR:O	2.38	0.56
4:A:340:PRO:HB2	17:P:166:LYS:HB3	1.86	0.56
26:B:615:CLA:H8	31:B:618:BCR:H362	1.88	0.56
26:N:610:CLA:H92	27:N:1620:LUT:H371	1.87	0.56
20:S:125:ASN:ND2	20:S:130:ASN:OD1	2.38	0.56
4:a:131:TRP:CZ2	6:c:449:ARG:HD2	2.40	0.56
4:a:140:ARG:HB2	7:d:221:ASN:HA	1.87	0.56
26:r:613:CLA:H111	30:r:2630:LHG:H292	1.86	0.56
26:4:612:CLA:HED2	26:4:612:CLA:H2A	1.87	0.56
4:A:103:ASP:HB3	16:O:79:MET:HE1	1.86	0.56
4:A:234:ASN:HB3	7:D:264:ASN:HD21	1.70	0.56
5:B:496:GLN:HB2	5:B:503:THR:HB	1.86	0.56
6:C:83:GLU:OE2	6:C:398:HIS:NE2	2.38	0.56
6:C:332:GLN:HE21	6:C:336:GLY:HA2	1.70	0.56
1:G:63:GLU:HA	1:G:155:LEU:HD21	1.86	0.56
4:a:131:TRP:CH2	6:c:449:ARG:HD2	2.39	0.56
4:a:340:PRO:HB2	17:p:166:LYS:HB3	1.86	0.56
1:g:63:GLU:HA	1:g:155:LEU:HD21	1.86	0.56
16:o:81:ARG:NH1	22:w:9:GLU:OE2	2.30	0.56
5:B:334:ASP:OD1	5:B:334:ASP:N	2.39	0.56
1:N:192:PHE:CD2	26:N:602:CLA:H171	2.40	0.56
4:a:147:TYR:OH	35:a:408:PHO:O1A	2.22	0.56
26:b:615:CLA:H8	31:b:618:BCR:H362	1.88	0.56
1:g:126:ALA:HB3	25:g:605:CHL:HMC	1.88	0.56
17:p:39:GLU:O	17:p:40:ARG:NH1	2.35	0.56
26:b:605:CLA:H203	30:b:2631:LHG:H342	1.87	0.56
6:c:83:GLU:OE2	6:c:398:HIS:NE2	2.38	0.56
26:n:610:CLA:H92	27:n:1620:LUT:H371	1.87	0.56
1:G:126:ALA:HB3	25:G:605:CHL:HMC	1.88	0.56
1:6:222:TRP:HB3	2:7:115:PHE:HZ	1.71	0.56
25:y:601:CHL:HMA3	30:y:2630:LHG:H121	1.88	0.56
4:a:103:ASP:HB3	16:o:79:MET:HE1	1.86	0.56
6:c:391:ARG:NH1	6:c:395:TYR:OH	2.36	0.56
4:A:140:ARG:NH1	7:D:232:THR:HG21	2.20	0.56
26:B:605:CLA:H203	30:B:2631:LHG:H342	1.87	0.56
1:6:21:ARG:NH1	1:6:37:THR:O	2.38	0.56
3:8:138:VAL:HG22	3:8:140:SER:H	1.71	0.56
4:a:234:ASN:HB3	7:d:264:ASN:HD21	1.70	0.56
6:c:343:ARG:NH1	6:c:347:GLY:O	2.38	0.56
8:e:69:ARG:NH2	10:h:62:ASN:O	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:64:ARG:O	16:O:152:ARG:NH1	2.33	0.56
4:A:140:ARG:HB2	7:D:221:ASN:HA	1.87	0.56
7:D:307:ALA:O	16:O:188:GLU:HG3	2.06	0.56
1:5:99:LYS:HA	25:5:607:CHL:HED3	1.87	0.56
26:c:501:CLA:HBB1	26:c:507:CLA:H41	1.88	0.56
26:g:603:CLA:H12	1:n:51:LEU:HD11	1.88	0.56
1:G:64:LEU:HD11	1:N:49:ALA:HA	1.88	0.55
17:P:39:GLU:O	17:P:40:ARG:NH1	2.35	0.55
4:a:64:ARG:O	16:o:152:ARG:NH1	2.33	0.55
1:1:99:LYS:HA	25:1:607:CHL:HED3	1.87	0.55
1:2:222:TRP:HB3	2:3:115:PHE:HZ	1.71	0.55
7:D:302:GLN:HG2	15:M:1:MET:HE1	1.89	0.55
26:G:603:CLA:H12	1:N:51:LEU:HD11	1.88	0.55
35:a:409:PHO:OBD	7:d:130:GLN:NE2	2.39	0.55
26:b:603:CLA:H12	10:h:61:TYR:HD2	1.69	0.55
16:o:74:GLN:HE21	16:o:118:LEU:HD22	1.70	0.55
4:A:147:TYR:OH	35:A:408:PHO:O1A	2.22	0.55
6:C:48:LYS:HE2	6:C:138:GLU:HG2	1.88	0.55
26:C:502:CLA:HBB2	26:C:510:CLA:H151	1.88	0.55
16:O:32:ILE:HG23	16:O:208:LYS:HE2	1.88	0.55
25:Y:601:CHL:HMA3	30:Y:2630:LHG:H121	1.88	0.55
26:c:502:CLA:HBB2	26:c:510:CLA:H151	1.88	0.55
31:c:516:BCR:H311	24:z:20:LEU:HD11	1.89	0.55
3:4:138:VAL:HG22	3:4:140:SER:H	1.71	0.55
35:A:409:PHO:OBD	7:D:130:GLN:NE2	2.39	0.55
6:C:387:TRP:HB2	18:Q:38:PHE:HD2	1.70	0.55
1:5:21:ARG:NH2	1:5:36:LEU:O	2.40	0.55
1:g:64:LEU:HD11	1:n:49:ALA:HA	1.88	0.55
16:O:74:GLN:HE21	16:O:118:LEU:HD22	1.70	0.55
1:6:110:LEU:HD21	26:6:604:CLA:HAA2	1.88	0.55
1:G:163:PRO:HD2	27:G:1620:LUT:H23	1.89	0.55
19:R:135:TYR:CD2	25:y:605:CHL:H11	2.41	0.55
4:A:305:SER:HA	12:J:39:SER:HB3	1.89	0.55
1:5:103:GLN:HE22	26:5:604:CLA:HED3	1.72	0.55
6:c:454:GLY:O	11:i:34:ARG:NH2	2.40	0.55
26:r:612:CLA:H2	26:r:612:CLA:H2A	1.89	0.55
1:2:110:LEU:HD21	26:2:604:CLA:HAA2	1.88	0.55
26:C:501:CLA:HBB1	26:C:507:CLA:H41	1.88	0.55
1:5:104:ILE:HG21	1:5:124:ILE:HD13	1.88	0.55
26:7:611:CLA:HBA1	26:7:612:CLA:HMD1	1.88	0.55
4:a:305:SER:HA	12:j:39:SER:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:302:GLN:HG2	15:m:1:MET:HE1	1.89	0.55
19:r:30:GLY:H	19:r:93:ARG:HH22	1.55	0.55
2:7:114:ILE:HG21	2:7:134:ILE:HD13	1.90	0.54
1:g:51:LEU:HD11	26:y:603:CLA:H12	1.89	0.54
1:1:103:GLN:HE22	26:1:604:CLA:HED3	1.72	0.54
1:G:51:LEU:HD11	26:Y:603:CLA:H12	1.90	0.54
1:N:64:LEU:HD11	1:Y:49:ALA:HA	1.89	0.54
1:5:197:GLN:HE22	27:5:1620:LUT:H42	1.71	0.54
2:7:79:ARG:NH1	25:7:608:CHL:OBD	2.40	0.54
5:B:124:CYS:O	10:H:24:LYS:NZ	2.40	0.54
19:R:30:GLY:H	19:R:93:ARG:HH22	1.55	0.54
26:R:612:CLA:H2	26:R:612:CLA:H2A	1.89	0.54
16:o:32:ILE:HG23	16:o:208:LYS:HE2	1.88	0.54
20:s:125:ASN:ND2	20:s:130:ASN:OD1	2.38	0.54
20:s:210:THR:HG22	20:s:233:VAL:HG11	1.89	0.54
1:1:104:ILE:HG21	1:1:124:ILE:HD13	1.88	0.54
1:N:63:GLU:HA	1:N:155:LEU:HD21	1.88	0.54
1:n:63:GLU:HA	1:n:155:LEU:HD21	1.88	0.54
1:n:64:LEU:HD11	1:y:49:ALA:HA	1.89	0.54
2:3:114:ILE:HG21	2:3:134:ILE:HD13	1.89	0.54
4:A:24:THR:O	7:D:252:ARG:NH2	2.39	0.54
6:C:318:LEU:HD12	6:C:340:TYR:HB3	1.90	0.54
20:S:60:ASP:OD1	27:S:1621:LUT:O23	2.26	0.54
1:Y:163:PRO:HD2	27:Y:1620:LUT:H23	1.90	0.54
5:b:124:CYS:O	10:h:24:LYS:NZ	2.40	0.54
6:c:48:LYS:HE2	6:c:138:GLU:HG2	1.88	0.54
7:d:307:ALA:O	16:o:188:GLU:HG3	2.06	0.54
3:4:129:PRO:HD3	26:R:601:CLA:HBB2	1.90	0.54
5:B:256:MET:HA	5:B:263:THR:HG21	1.90	0.54
20:S:50:THR:HG22	20:S:50:THR:O	2.08	0.54
30:b:2630:LHG:H341	37:b:2633:LMG:H202	1.89	0.54
1:1:197:GLN:HE22	27:1:1620:LUT:H42	1.71	0.54
2:7:173:ASP:OD1	27:7:1620:LUT:O23	2.26	0.54
4:A:267:ASN:ND2	7:D:233:PHE:O	2.40	0.54
31:C:516:BCR:HC21	24:Z:13:ILE:HG23	1.89	0.54
4:a:85:THR:HA	4:a:109:GLY:HA3	1.90	0.54
5:b:256:MET:HA	5:b:263:THR:HG21	1.90	0.54
20:s:50:THR:HG22	20:s:50:THR:O	2.08	0.54
1:y:163:PRO:HD2	27:y:1620:LUT:H23	1.90	0.54
1:1:21:ARG:NH2	1:1:36:LEU:O	2.40	0.54
19:R:135:TYR:HD2	25:y:605:CHL:H11	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:212:GLU:OE2	20:S:220:LYS:NZ	2.41	0.54
1:Y:80:VAL:HG13	1:Y:206:LEU:HD11	1.90	0.54
1:6:164:LEU:HD12	27:6:1620:LUT:H222	1.90	0.54
1:g:49:ALA:HA	1:y:64:LEU:HD11	1.90	0.54
25:Y:605:CHL:H11	19:r:135:TYR:CD2	2.43	0.53
2:7:53:TYR:OH	2:7:193:LYS:NZ	2.41	0.53
3:8:58:GLY:HA3	3:8:184:ALA:HB1	1.90	0.53
30:c:523:LHG:H112	30:c:523:LHG:H241	1.89	0.53
1:y:80:VAL:HG13	1:y:206:LEU:HD11	1.90	0.53
3:4:58:GLY:HA3	3:4:184:ALA:HB1	1.90	0.53
3:4:191:MET:HG2	28:4:622:XAT:H12	1.90	0.53
31:C:516:BCR:H311	24:Z:20:LEU:HD11	1.89	0.53
7:D:303:GLU:OE1	16:O:160:LYS:HE2	2.08	0.53
1:Y:217:VAL:O	1:Y:217:VAL:HG12	2.08	0.53
26:7:603:CLA:HED2	25:7:609:CHL:H93	1.91	0.53
4:A:85:THR:HA	4:A:109:GLY:HA3	1.90	0.53
1:G:49:ALA:HA	1:Y:64:LEU:HD11	1.90	0.53
25:Y:605:CHL:H11	19:r:135:TYR:HD2	1.74	0.53
25:6:606:CHL:HMB2	25:6:609:CHL:HMC	1.90	0.53
31:c:517:BCR:H333	24:z:9:VAL:HG13	1.91	0.53
1:n:212:HIS:CG	26:n:613:CLA:HAA2	2.44	0.53
20:s:60:ASP:OD1	27:s:1621:LUT:O23	2.26	0.53
20:s:172:PRO:HD2	27:s:1620:LUT:H23	1.90	0.53
31:C:517:BCR:H333	24:Z:9:VAL:HG13	1.91	0.53
3:8:191:MET:HG2	28:8:622:XAT:H12	1.90	0.53
7:d:303:GLU:OE1	16:o:160:LYS:HE2	2.08	0.53
20:s:212:GLU:OE2	20:s:220:LYS:NZ	2.41	0.53
5:B:121:GLU:HG3	10:H:16:ARG:CD	2.39	0.53
30:C:523:LHG:H112	30:C:523:LHG:H241	1.89	0.53
20:S:210:THR:HG22	20:S:233:VAL:HG11	1.89	0.53
6:c:318:LEU:HD12	6:c:340:TYR:HB3	1.90	0.53
7:d:313:GLU:HB2	16:o:159:PRO:HG3	1.90	0.53
16:o:207:THR:HG22	16:o:214:VAL:HG22	1.91	0.53
19:r:227:TRP:HB2	27:r:620:LUT:H21	1.90	0.53
4:A:45:THR:HG23	26:A:406:CLA:H201	1.91	0.53
30:B:2630:LHG:H341	37:B:2633:LMG:H202	1.89	0.53
31:c:516:BCR:HC21	24:z:13:ILE:HG23	1.89	0.53
1:n:65:GLU:OE2	1:n:185:ARG:NE	2.41	0.53
7:D:313:GLU:HB2	16:O:159:PRO:HG3	1.90	0.53
16:O:207:THR:HG22	16:O:214:VAL:HG22	1.91	0.53
1:Y:51:LEU:HD13	26:Y:602:CLA:H42	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:23:VAL:HB	24:Z:24:PRO:HD3	1.91	0.53
4:a:129:ARG:NH2	7:d:256:GLN:O	2.42	0.53
26:c:513:CLA:H71	30:c:2630:LHG:H122	1.91	0.53
25:g:606:CHL:HBA1	29:g:1623:NEX:H403	1.90	0.53
16:o:65:VAL:HA	16:o:71:LEU:HD21	1.91	0.53
2:3:173:ASP:OD1	27:3:1620:LUT:O23	2.26	0.53
1:g:163:PRO:HD2	27:g:1620:LUT:H23	1.89	0.53
5:B:472:ARG:HD3	5:B:479:PHE:CE1	2.44	0.53
16:O:143:SER:HA	16:O:201:THR:HA	1.91	0.53
20:S:172:PRO:HD2	27:S:1620:LUT:H23	1.89	0.53
1:y:104:ILE:HG21	1:y:124:ILE:HD13	1.91	0.53
25:2:606:CHL:HMB2	25:2:609:CHL:HMC	1.90	0.53
5:B:30:VAL:HG12	26:B:606:CLA:HHD	1.91	0.53
1:2:164:LEU:HD12	27:2:1620:LUT:H222	1.90	0.52
4:A:198:HIS:HA	4:A:286:THR:HG22	1.91	0.52
6:C:402:GLY:HA3	6:C:420:VAL:HG22	1.92	0.52
1:G:176:LEU:HD23	1:G:179:LYS:HD2	1.91	0.52
1:N:225:ALA:HA	28:N:1622:XAT:H42	1.91	0.52
2:7:141:GLN:HE22	25:7:607:CHL:HMC	1.74	0.52
3:8:129:PRO:HD3	26:r:601:CLA:HBB2	1.90	0.52
4:a:198:HIS:HA	4:a:286:THR:HG22	1.91	0.52
1:g:69:SER:HB3	1:g:184:GLY:HA3	1.91	0.52
17:p:87:LEU:O	17:p:160:LYS:NZ	2.41	0.52
26:r:602:CLA:H72	28:r:622:XAT:H28	1.90	0.52
4:A:129:ARG:NH2	7:D:256:GLN:O	2.42	0.52
14:L:20:TRP:HA	14:L:20:TRP:CE3	2.45	0.52
16:O:180:GLY:O	16:O:189:ASN:ND2	2.42	0.52
18:Q:50:ARG:HD2	18:Q:83:TYR:CD1	2.44	0.52
4:a:43:THR:HG23	31:a:411:BCR:H362	1.91	0.52
16:o:227:ASP:HB3	16:o:230:ALA:HB3	1.91	0.52
6:C:454:GLY:O	11:I:34:ARG:NH2	2.40	0.52
7:D:108:LEU:HD23	8:E:66:ILE:HD13	1.92	0.52
25:G:606:CHL:HBA1	29:G:1623:NEX:H403	1.90	0.52
1:N:212:HIS:CG	26:N:613:CLA:HAA2	2.44	0.52
16:O:65:VAL:HA	16:O:71:LEU:HD21	1.91	0.52
35:a:408:PHO:H51	36:a:418:SQD:H201	1.91	0.52
8:e:27:ILE:HG12	41:f:101:HEM:HMC3	1.91	0.52
6:C:282:PHE:HE1	26:C:501:CLA:H111	1.74	0.52
1:N:65:GLU:OE2	1:N:185:ARG:NE	2.41	0.52
17:P:87:LEU:O	17:P:160:LYS:NZ	2.41	0.52
19:R:227:TRP:HB2	27:R:620:LUT:H21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:472:ARG:HD3	5:b:479:PHE:CE1	2.44	0.52
6:c:282:PHE:HE1	26:c:501:CLA:H111	1.74	0.52
30:d:409:LHG:HC11	14:l:14:ASN:HD21	1.75	0.52
1:n:225:ALA:HA	28:n:1622:XAT:H42	1.91	0.52
26:y:602:CLA:H101	27:y:1621:LUT:H371	1.91	0.52
4:A:43:THR:HG23	31:A:411:BCR:H362	1.91	0.52
26:R:602:CLA:H72	28:R:622:XAT:H28	1.90	0.52
20:S:99:ASN:ND2	20:S:103:ALA:O	2.43	0.52
4:a:24:THR:O	7:d:252:ARG:NH2	2.39	0.52
4:a:288:LEU:HD22	6:c:432:VAL:HG22	1.91	0.52
5:b:255:THR:HG21	26:b:603:CLA:HED1	1.92	0.52
26:n:603:CLA:HMD3	25:n:609:CHL:HBA2	1.92	0.52
18:q:58:ILE:HD11	18:q:84:LEU:HD11	1.92	0.52
4:A:47:VAL:HG21	4:A:114:LEU:HD22	1.92	0.52
26:Y:602:CLA:H101	27:Y:1621:LUT:H371	1.91	0.52
1:y:51:LEU:HD13	26:y:602:CLA:H42	1.91	0.52
1:y:217:VAL:O	1:y:217:VAL:HG12	2.08	0.52
24:z:16:SER:HG	24:z:47:TRP:CD1	2.27	0.52
3:4:29:LEU:HD11	3:4:51:ARG:HD3	1.92	0.52
1:Y:63:GLU:HA	1:Y:155:LEU:HD21	1.92	0.52
1:Y:104:ILE:HG21	1:Y:124:ILE:HD13	1.91	0.52
5:b:30:VAL:HG12	26:b:606:CLA:HHD	1.91	0.52
1:g:176:LEU:HD23	1:g:179:LYS:HD2	1.91	0.52
19:r:59:LYS:HE2	19:r:61:LEU:HD21	1.92	0.52
26:3:603:CLA:HED2	25:3:609:CHL:H93	1.91	0.52
4:A:215:HIS:HB2	38:A:414:PL9:HC8	1.92	0.52
5:B:157:HIS:HE1	26:B:607:CLA:NA	2.07	0.52
7:D:79:VAL:HB	7:D:174:PHE:HB2	1.92	0.52
20:S:113:LYS:HA	25:S:607:CHL:HED3	1.91	0.52
4:a:215:HIS:HB2	38:a:414:PL9:HC8	1.92	0.52
16:o:180:GLY:O	16:o:189:ASN:ND2	2.42	0.52
8:E:27:ILE:HG12	41:F:101:HEM:HMC3	1.91	0.52
1:G:139:GLU:HG3	25:G:609:CHL:NB	2.25	0.52
25:8:606:CHL:HAA1	31:8:623:BCR:H19C	1.92	0.52
5:b:137:LYS:HZ1	10:h:29:GLU:CD	2.18	0.52
25:1:601:CHL:HMA3	30:1:2630:LHG:H121	1.92	0.52
2:3:104:GLU:O	2:3:113:GLN:NE2	2.43	0.52
25:4:606:CHL:HAA1	31:4:623:BCR:H19C	1.92	0.52
35:A:408:PHO:H51	36:A:418:SQD:H201	1.91	0.52
26:C:511:CLA:C4D	13:K:54:TRP:HH2	2.24	0.52
1:G:197:GLN:HG3	26:G:613:CLA:C1D	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:G:601:CHL:HHC	25:G:601:CHL:HBB1	1.92	0.52
16:O:227:ASP:HB3	16:O:230:ALA:HB3	1.91	0.52
18:Q:58:ILE:HD11	18:Q:84:LEU:HD11	1.92	0.52
6:C:131:TYR:OH	20:S:38:GLY:HA3	2.11	0.51
4:a:317:TRP:HZ3	7:d:181:ARG:HD2	1.75	0.51
26:c:511:CLA:C4D	13:k:54:TRP:HH2	2.24	0.51
1:g:197:GLN:HG3	26:g:613:CLA:C1D	2.39	0.51
1:n:80:VAL:HG13	1:n:206:LEU:HD11	1.91	0.51
2:3:141:GLN:HE22	25:3:607:CHL:HMC	1.74	0.51
2:7:30:ARG:NH1	2:7:46:THR:O	2.43	0.51
4:a:27:ARG:NH1	7:d:255:SER:O	2.37	0.51
4:a:45:THR:HG23	26:a:406:CLA:H201	1.91	0.51
6:c:131:TYR:OH	20:s:38:GLY:HA3	2.11	0.51
6:c:402:GLY:HA3	6:c:420:VAL:HG22	1.92	0.51
25:g:606:CHL:HBB2	25:g:607:CHL:HBB1	1.92	0.51
4:A:288:LEU:HD22	6:C:432:VAL:HG22	1.91	0.51
10:H:33:VAL:HG21	19:R:48:PHE:HE1	1.74	0.51
17:P:108:VAL:HB	17:P:136:ALA:HB2	1.92	0.51
25:5:607:CHL:HBB1	25:7:601:CHL:H141	1.92	0.51
28:6:1622:XAT:H41	25:7:607:CHL:HAA2	1.93	0.51
2:7:104:GLU:O	2:7:113:GLN:NE2	2.43	0.51
4:a:84:PRO:HA	4:a:112:TYR:CG	2.45	0.51
5:b:157:HIS:HE1	26:b:607:CLA:NA	2.07	0.51
6:c:28:GLN:NE2	7:d:234:ARG:NE	2.59	0.51
6:c:396:MET:SD	18:q:27:ARG:NH2	2.81	0.51
7:d:79:VAL:HB	7:d:174:PHE:HB2	1.92	0.51
1:g:139:GLU:HG3	25:g:609:CHL:NB	2.25	0.51
16:o:60:VAL:HG22	16:o:236:VAL:HG22	1.92	0.51
18:q:50:ARG:HD2	18:q:83:TYR:CD1	2.44	0.51
20:s:189:GLU:HG3	26:s:610:CLA:C4B	2.41	0.51
24:z:23:VAL:HB	24:z:24:PRO:HD3	1.91	0.51
2:3:30:ARG:NH1	2:3:46:THR:O	2.43	0.51
1:N:80:VAL:HG13	1:N:206:LEU:HD11	1.91	0.51
16:O:60:VAL:HG22	16:O:236:VAL:HG22	1.92	0.51
1:5:162:ASP:OD1	27:5:1620:LUT:O23	2.28	0.51
1:6:104:ILE:HG21	1:6:124:ILE:HD13	1.92	0.51
4:a:47:VAL:HG21	4:a:114:LEU:HD22	1.92	0.51
7:d:108:LEU:HD23	8:e:66:ILE:HD13	1.92	0.51
5:B:168:VAL:HG13	5:B:195:PRO:HG2	1.93	0.51
6:C:94:THR:HG22	26:C:501:CLA:HED1	1.93	0.51
26:C:513:CLA:H71	30:C:2630:LHG:H122	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:211:LEU:HA	7:D:214:ILE:HG22	1.92	0.51
20:S:189:GLU:HG3	26:S:610:CLA:C4B	2.41	0.51
24:Z:16:SER:HG	24:Z:47:TRP:CD1	2.27	0.51
3:8:29:LEU:HD11	3:8:51:ARG:HD3	1.92	0.51
25:g:601:CHL:HHC	25:g:601:CHL:HBB1	1.92	0.51
16:o:143:SER:HA	16:o:201:THR:HA	1.91	0.51
20:s:99:ASN:ND2	20:s:103:ALA:O	2.43	0.51
20:s:113:LYS:HA	25:s:607:CHL:HED3	1.91	0.51
21:t:17:ILE:HG22	31:t:101:BCR:H313	1.93	0.51
25:1:607:CHL:HBB1	25:3:601:CHL:H141	1.92	0.51
5:B:12:VAL:HG12	26:B:613:CLA:HMC2	1.93	0.51
5:B:71:ILE:HD13	26:B:607:CLA:HED3	1.92	0.51
5:B:423:ARG:NH1	5:B:430:PHE:O	2.44	0.51
6:C:108:THR:O	6:C:108:THR:HG22	2.11	0.51
7:D:306:ALA:HB3	16:O:160:LYS:HE3	1.93	0.51
1:G:69:SER:HB3	1:G:184:GLY:HA3	1.91	0.51
5:b:168:VAL:HG13	5:b:195:PRO:HG2	1.93	0.51
17:p:108:VAL:HB	17:p:136:ALA:HB2	1.92	0.51
1:2:162:ASP:OD1	27:2:1620:LUT:O23	2.29	0.51
28:2:1622:XAT:H41	25:3:607:CHL:HAA2	1.93	0.51
4:A:317:TRP:HZ3	7:D:181:ARG:HD2	1.75	0.51
5:B:255:THR:HG21	26:B:603:CLA:HED1	1.92	0.51
6:C:28:GLN:NE2	7:D:234:ARG:NE	2.59	0.51
7:D:25:ARG:NH1	23:X:79:ASP:O	2.43	0.51
4:a:170:ASP:OD2	6:c:357:ARG:NH1	2.40	0.51
5:b:12:VAL:HG12	26:b:613:CLA:HMC2	1.93	0.51
5:b:315:ILE:HG12	5:b:321:LYS:HG3	1.92	0.51
6:c:94:THR:HG22	26:c:501:CLA:HED1	1.93	0.51
10:h:33:VAL:HG21	19:r:48:PHE:HE1	1.74	0.51
1:2:104:ILE:HG21	1:2:124:ILE:HD13	1.92	0.51
30:C:2630:LHG:H223	26:S:614:CLA:H2	1.93	0.51
26:N:602:CLA:H203	27:N:1621:LUT:H391	1.93	0.51
25:5:601:CHL:HMA3	30:5:2630:LHG:H121	1.92	0.51
1:6:69:SER:HB3	1:6:184:GLY:HA3	1.93	0.51
25:7:606:CHL:HBA2	29:7:1623:NEX:H403	1.93	0.51
7:d:18:ILE:HG22	23:x:76:SER:HB3	1.93	0.51
1:2:69:SER:HB3	1:2:184:GLY:HA3	1.93	0.51
2:3:79:ARG:NH1	25:3:608:CHL:OBD	2.40	0.51
2:3:95:GLN:HE22	2:3:102:PHE:H	1.59	0.51
4:A:84:PRO:HA	4:A:112:TYR:CG	2.45	0.51
5:B:157:HIS:HA	5:B:163:GLY:HA3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:399:VAL:HG12	5:B:417:VAL:HG22	1.93	0.51
19:R:59:LYS:HE2	19:R:61:LEU:HD21	1.92	0.51
1:5:69:SER:HB3	1:5:184:GLY:HA3	1.93	0.51
2:7:95:GLN:HE22	2:7:102:PHE:H	1.59	0.51
4:a:267:ASN:ND2	7:d:233:PHE:O	2.40	0.51
5:b:71:ILE:HD13	26:b:607:CLA:HED3	1.92	0.51
7:d:211:LEU:HA	7:d:214:ILE:HG22	1.92	0.51
17:p:119:PRO:HG2	17:p:126:TYR:HB2	1.93	0.51
5:b:423:ARG:NH1	5:b:430:PHE:O	2.44	0.50
6:c:345:PRO:HB3	16:o:81:ARG:HD3	1.93	0.50
1:g:162:ASP:OD1	27:g:1620:LUT:O23	2.28	0.50
14:l:20:TRP:HA	14:l:20:TRP:CE3	2.45	0.50
5:b:399:VAL:HG12	5:b:417:VAL:HG22	1.93	0.50
6:c:370:ARG:HH11	6:c:370:ARG:HG3	1.77	0.50
1:y:63:GLU:HA	1:y:155:LEU:HD21	1.92	0.50
6:C:28:GLN:NE2	7:D:231:ASN:HD22	2.09	0.50
6:C:223:TRP:CG	6:C:224:ILE:H	2.28	0.50
1:G:162:ASP:OD1	27:G:1620:LUT:O23	2.28	0.50
1:Y:65:GLU:OE2	1:Y:185:ARG:NE	2.43	0.50
20:s:154:ILE:HD11	26:s:609:CLA:HMA1	1.93	0.50
1:1:69:SER:HB3	1:1:184:GLY:HA3	1.93	0.50
1:2:85:LEU:HA	1:2:88:ASN:HB2	1.94	0.50
4:A:116:VAL:HG13	4:A:158:PHE:HB3	1.93	0.50
26:B:615:CLA:H43	36:B:621:SQD:H122	1.94	0.50
6:C:117:LEU:HD22	37:Z:101:LMG:H391	1.94	0.50
6:C:345:PRO:HB3	16:O:81:ARG:HD3	1.94	0.50
26:C:507:CLA:H2	26:C:507:CLA:HMA1	1.94	0.50
1:G:135:MET:HA	1:G:138:VAL:HG22	1.93	0.50
25:Y:601:CHL:HHC	25:Y:601:CHL:HBB1	1.93	0.50
4:a:114:LEU:O	4:a:118:HIS:ND1	2.33	0.50
26:b:611:CLA:H141	26:b:613:CLA:HBD	1.94	0.50
26:b:614:CLA:H172	31:b:619:BCR:H312	1.94	0.50
6:c:223:TRP:CG	6:c:224:ILE:H	2.28	0.50
20:s:202:GLY:O	20:s:206:GLN:CB	2.59	0.50
1:1:162:ASP:OD1	27:1:1620:LUT:O23	2.28	0.50
25:3:606:CHL:HBA2	29:3:1623:NEX:H403	1.93	0.50
6:C:262:ARG:NH1	30:C:522:LHG:O5	2.34	0.50
6:C:370:ARG:HH11	6:C:370:ARG:HG3	1.77	0.50
26:N:603:CLA:HMD3	25:N:609:CHL:HBA2	1.92	0.50
1:Y:212:HIS:CG	26:Y:613:CLA:HAA2	2.47	0.50
26:6:603:CLA:HMD3	25:6:609:CHL:HBA2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:316:THR:HG22	7:D:65:ALA:HB3	1.93	0.50
5:B:330:MET:HA	5:B:444:ARG:HB2	1.94	0.50
6:C:460:ASP:HB2	11:I:34:ARG:NH1	2.26	0.50
5:b:121:GLU:HG3	10:h:16:ARG:CD	2.39	0.50
5:b:366:PHE:HD2	5:b:425:GLN:HE21	1.58	0.50
25:y:601:CHL:HBB1	25:y:601:CHL:HHC	1.93	0.50
1:1:176:LEU:HD23	1:1:179:LYS:HD2	1.93	0.50
4:A:96:ILE:HG12	4:A:105:TRP:CE2	2.47	0.50
5:B:315:ILE:HG12	5:B:321:LYS:HG3	1.92	0.50
5:B:366:PHE:HD2	5:B:425:GLN:HE21	1.58	0.50
1:5:176:LEU:HD23	1:5:179:LYS:HD2	1.93	0.50
5:b:256:MET:O	5:b:448:ARG:NH1	2.42	0.50
6:c:28:GLN:NE2	7:d:231:ASN:HD22	2.09	0.50
6:c:460:ASP:HB2	11:i:34:ARG:NH1	2.26	0.50
7:d:142:TYR:HB3	7:d:273:LEU:HD11	1.93	0.50
1:y:41:PRO:HG3	1:y:177:LYS:HB3	1.94	0.50
4:A:22:THR:HB	4:A:136:ARG:HE	1.77	0.50
30:D:409:LHG:HC11	14:L:14:ASN:HD21	1.75	0.50
25:G:606:CHL:HMB1	25:G:609:CHL:HMC	1.94	0.50
1:6:162:ASP:OD1	27:6:1620:LUT:O23	2.29	0.50
26:7:603:CLA:HMD3	25:7:609:CHL:HBA2	1.94	0.50
4:a:116:VAL:HG13	4:a:158:PHE:HB3	1.93	0.50
5:b:157:HIS:HA	5:b:163:GLY:HA3	1.93	0.50
26:b:604:CLA:H2	26:b:606:CLA:H91	1.94	0.50
30:c:2630:LHG:H223	26:s:614:CLA:H2	1.93	0.50
7:d:25:ARG:NH1	23:x:79:ASP:O	2.43	0.50
25:g:606:CHL:HMB1	25:g:609:CHL:HMC	1.94	0.50
26:B:604:CLA:H2	26:B:606:CLA:H91	1.94	0.50
26:B:611:CLA:H141	26:B:613:CLA:HBD	1.93	0.50
26:B:614:CLA:H172	31:B:619:BCR:H312	1.94	0.50
1:N:176:LEU:HD23	1:N:179:LYS:HD2	1.94	0.50
25:N:608:CHL:HHC	25:N:608:CHL:HBB1	1.93	0.50
1:5:18:GLY:O	1:5:21:ARG:NH1	2.41	0.50
6:c:150:VAL:HG12	6:c:152:LYS:H	1.77	0.50
20:s:39:LEU:HD22	24:z:41:PHE:HE1	1.77	0.50
26:D:403:CLA:H13	23:X:58:ILE:HG22	1.94	0.49
21:T:17:ILE:HG22	31:T:101:BCR:H313	1.93	0.49
4:a:254:TYR:CD1	7:d:133:LEU:HD22	2.47	0.49
26:b:615:CLA:H43	36:b:621:SQD:H122	1.94	0.49
7:d:306:ALA:HB3	16:o:160:LYS:HE3	1.93	0.49
17:p:45:GLN:HA	17:p:62:LEU:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:w:17:LEU:HA	22:w:22:LEU:HD23	1.94	0.49
28:2:1622:XAT:H393	30:2:2630:LHG:HC92	1.94	0.49
25:G:606:CHL:HBB2	25:G:607:CHL:HBB1	1.92	0.49
14:L:30:VAL:O	14:L:34:ASN:ND2	2.45	0.49
25:N:601:CHL:HBB1	25:N:601:CHL:HHC	1.94	0.49
17:P:45:GLN:HA	17:P:62:LEU:HA	1.94	0.49
4:a:22:THR:HB	4:a:136:ARG:HE	1.77	0.49
4:a:91:LEU:HD11	4:a:163:ILE:HA	1.95	0.49
26:a:405:CLA:H122	35:a:408:PHO:H3A	1.94	0.49
5:b:330:MET:HA	5:b:444:ARG:HB2	1.94	0.49
6:c:117:LEU:HD22	37:z:101:LMG:H391	1.94	0.49
26:n:602:CLA:H203	27:n:1621:LUT:H391	1.93	0.49
19:r:161:GLN:HG3	25:r:608:CHL:HBB1	1.93	0.49
6:C:150:VAL:HG12	6:C:152:LYS:H	1.77	0.49
17:P:119:PRO:HG2	17:P:126:TYR:HB2	1.93	0.49
20:S:154:ILE:HD11	26:S:609:CLA:HMA1	1.93	0.49
22:W:17:LEU:HA	22:W:22:LEU:HD23	1.94	0.49
1:6:85:LEU:HA	1:6:88:ASN:HB2	1.94	0.49
4:a:77:ILE:HD11	21:t:6:TYR:HB3	1.95	0.49
36:b:621:SQD:H262	36:b:623:SQD:H102	1.94	0.49
28:y:1622:XAT:H363	30:y:2630:LHG:HC41	1.94	0.49
4:A:77:ILE:HD11	21:T:6:TYR:HB3	1.95	0.49
5:B:249:ALA:HA	5:B:252:VAL:HG22	1.94	0.49
6:C:406:SER:HA	6:C:420:VAL:HG23	1.94	0.49
25:8:606:CHL:HAA1	31:8:623:BCR:H21C	1.94	0.49
4:a:96:ILE:HG12	4:a:105:TRP:CE2	2.47	0.49
20:S:39:LEU:HD22	24:Z:41:PHE:HE1	1.77	0.49
20:S:100:LYS:NZ	42:S:1101:HOH:O	2.45	0.49
6:c:262:ARG:NH1	30:c:522:LHG:O5	2.34	0.49
26:g:613:CLA:H91	30:g:2630:LHG:H321	1.95	0.49
26:n:610:CLA:H52	27:n:1620:LUT:H28	1.94	0.49
2:3:50:PRO:HG3	2:3:188:LYS:HD3	1.95	0.49
4:A:330:VAL:O	7:D:350:GLY:N	2.46	0.49
10:H:49:LEU:HB3	31:H:101:BCR:H14C	1.94	0.49
1:N:69:SER:HB3	1:N:184:GLY:HA3	1.93	0.49
4:a:316:THR:HG22	7:d:65:ALA:HB3	1.94	0.49
6:c:108:THR:O	6:c:108:THR:HG22	2.11	0.49
7:d:52:GLY:HA3	7:d:79:VAL:HG22	1.94	0.49
1:g:80:VAL:HG13	1:g:206:LEU:HD11	1.95	0.49
10:h:49:LEU:HB3	31:h:101:BCR:H14C	1.94	0.49
1:y:65:GLU:OE2	1:y:185:ARG:NE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:603:CLA:HMD3	25:2:609:CHL:HBA2	1.94	0.49
5:B:137:LYS:HZ1	10:H:29:GLU:CD	2.20	0.49
5:B:327:ALA:HB1	37:B:622:LMG:HC8	1.94	0.49
1:g:220:ASN:HB2	26:g:614:CLA:HED1	1.95	0.49
25:n:608:CHL:HHC	25:n:608:CHL:HBB1	1.94	0.49
26:3:603:CLA:HMD3	25:3:609:CHL:HBA2	1.94	0.49
25:4:606:CHL:HAA1	31:4:623:BCR:H21C	1.94	0.49
4:A:114:LEU:O	4:A:118:HIS:ND1	2.33	0.49
4:A:170:ASP:OD2	6:C:357:ARG:NH1	2.40	0.49
30:C:522:LHG:H181	22:W:31:GLY:HA3	1.94	0.49
26:N:610:CLA:H52	27:N:1620:LUT:H28	1.94	0.49
19:R:161:GLN:HG3	25:R:608:CHL:HBB1	1.93	0.49
5:b:327:ALA:HB1	37:b:622:LMG:HC8	1.94	0.49
7:d:267:TRP:HH2	30:l:101:LHG:H102	1.78	0.49
25:g:601:CHL:HMA3	30:g:2630:LHG:H121	1.95	0.49
25:n:601:CHL:HBB1	25:n:601:CHL:HHC	1.94	0.49
26:r:613:CLA:HHB	25:r:614:CHL:HHD	1.95	0.49
1:y:69:SER:HB3	1:y:184:GLY:HA3	1.94	0.49
25:y:608:CHL:H11	27:y:1620:LUT:H383	1.94	0.49
26:B:617:CLA:H91	31:B:620:BCR:H14C	1.95	0.49
7:D:18:ILE:HG22	23:X:76:SER:HB3	1.93	0.49
7:D:52:GLY:HA3	7:D:79:VAL:HG22	1.94	0.49
26:N:603:CLA:H12	1:Y:51:LEU:HD11	1.95	0.49
20:S:118:LEU:HD11	25:S:606:CHL:HMD3	1.94	0.49
25:Y:608:CHL:H11	27:Y:1620:LUT:H383	1.94	0.49
1:5:52:SER:OG	1:5:61:ASN:ND2	2.45	0.49
7:d:156:SER:HA	7:d:160:ILE:HB	1.95	0.49
1:y:212:HIS:CG	26:y:613:CLA:HAA2	2.47	0.49
1:1:52:SER:OG	1:1:61:ASN:ND2	2.45	0.49
2:3:53:TYR:OH	2:3:193:LYS:NZ	2.41	0.49
5:B:120:LEU:HD23	10:H:15:ARG:HB3	1.95	0.49
5:B:207:THR:HG21	37:B:2633:LMG:H351	1.94	0.49
6:C:80:PRO:O	6:C:84:GLN:HG3	2.13	0.49
6:C:217:PRO:HA	6:C:223:TRP:HB2	1.94	0.49
7:D:142:TYR:HB3	7:D:273:LEU:HD11	1.93	0.49
1:N:41:PRO:HG3	1:N:177:LYS:HB3	1.94	0.49
26:R:613:CLA:HHB	25:R:614:CHL:HHD	1.95	0.49
28:6:1622:XAT:H393	30:6:2630:LHG:HC92	1.94	0.49
1:g:135:MET:HA	1:g:138:VAL:HG22	1.93	0.49
1:g:194:PHE:HE1	27:g:1620:LUT:H41	1.78	0.49
25:g:609:CHL:H43	25:n:601:CHL:H12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:41:PRO:HG3	1:n:177:LYS:HB3	1.94	0.49
16:o:145:GLU:HB3	16:o:197:LYS:HE2	1.95	0.49
25:y:608:CHL:HHC	25:y:608:CHL:HBB1	1.95	0.49
4:A:254:TYR:CD1	7:D:133:LEU:HD22	2.47	0.48
6:C:370:ARG:HG3	6:C:370:ARG:NH1	2.28	0.48
20:S:235:ALA:HB2	24:Z:59:SER:HB3	1.95	0.48
3:8:154:PRO:HD2	27:8:620:LUT:H23	1.94	0.48
26:c:507:CLA:H2	26:c:507:CLA:HMA1	1.94	0.48
26:c:508:CLA:HBC2	30:d:410:LHG:H341	1.94	0.48
1:n:69:SER:HB3	1:n:184:GLY:HA3	1.93	0.48
36:B:621:SQD:H262	36:B:623:SQD:H102	1.94	0.48
7:D:20:ASP:OD2	7:D:24:ARG:NH1	2.39	0.48
31:D:404:BCR:H383	37:D:411:LMG:H182	1.94	0.48
26:G:613:CLA:H91	30:G:2630:LHG:H321	1.95	0.48
15:M:5:ILE:HG23	15:m:5:ILE:HG23	1.94	0.48
19:R:194:LEU:HB3	26:R:610:CLA:H3A	1.95	0.48
28:Y:1622:XAT:H363	30:Y:2630:LHG:HC41	1.94	0.48
2:7:50:PRO:HG3	2:7:188:LYS:HD3	1.95	0.48
5:b:207:THR:HG21	37:b:2633:LMG:H351	1.94	0.48
5:b:313:ASP:OD2	5:b:358:ARG:NH2	2.32	0.48
6:c:406:SER:HA	6:c:420:VAL:HG23	1.94	0.48
7:d:20:ASP:OD2	7:d:24:ARG:NH1	2.39	0.48
14:l:30:VAL:O	14:l:34:ASN:ND2	2.45	0.48
1:1:18:GLY:O	1:1:21:ARG:NH1	2.41	0.48
4:A:92:HIS:CE1	6:C:220:GLY:HA3	2.49	0.48
1:G:194:PHE:HE1	27:G:1620:LUT:H41	1.78	0.48
16:O:145:GLU:HB3	16:O:197:LYS:HE2	1.95	0.48
19:R:182:LEU:HD12	27:R:620:LUT:H222	1.95	0.48
6:c:80:PRO:O	6:c:84:GLN:HG3	2.13	0.48
6:c:217:PRO:HA	6:c:223:TRP:HB2	1.94	0.48
26:d:403:CLA:H13	23:x:58:ILE:HG22	1.94	0.48
25:g:606:CHL:HMB1	25:g:609:CHL:HAC1	1.95	0.48
26:1:603:CLA:HMD3	25:1:609:CHL:HBA2	1.95	0.48
31:4:623:BCR:HC22	30:R:2630:LHG:HC92	1.95	0.48
26:B:607:CLA:HBC1	30:B:2630:LHG:H101	1.96	0.48
1:G:87:ARG:HH12	1:G:210:ALA:CB	2.27	0.48
25:G:601:CHL:HMA3	30:G:2630:LHG:H121	1.95	0.48
1:Y:41:PRO:HG3	1:Y:177:LYS:HB3	1.94	0.48
1:5:156:TYR:HB3	26:5:610:CLA:HED2	1.94	0.48
26:5:603:CLA:HMD3	25:5:609:CHL:HBA2	1.95	0.48
1:n:176:LEU:HD23	1:n:179:LYS:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:r:194:LEU:HB3	26:r:610:CLA:H3A	1.95	0.48
20:s:118:LEU:HD11	25:s:606:CHL:HMD3	1.94	0.48
1:1:97:TRP:O	27:1:1621:LUT:O3	2.32	0.48
1:1:156:TYR:HB3	26:1:610:CLA:HED2	1.94	0.48
4:A:44:ALA:HB2	4:A:118:HIS:HB2	1.95	0.48
5:B:71:ILE:HD11	26:B:607:CLA:H2A	1.95	0.48
25:G:609:CHL:H43	25:N:601:CHL:H12	1.95	0.48
5:b:120:LEU:HD23	10:h:15:ARG:HB3	1.95	0.48
6:c:28:GLN:NE2	7:d:234:ARG:HE	2.12	0.48
26:c:504:CLA:H42	39:c:519:DGD:HB32	1.96	0.48
7:d:90:LEU:HG	10:h:62:ASN:HD22	1.78	0.48
7:d:90:LEU:HG	10:h:62:ASN:ND2	2.28	0.48
7:d:349:ARG:NH1	7:d:353:LEU:O	2.40	0.48
1:G:65:GLU:OE2	1:G:185:ARG:NE	2.47	0.48
20:S:202:GLY:O	20:S:206:GLN:CB	2.59	0.48
1:Y:110:LEU:HD23	1:Y:110:LEU:C	2.39	0.48
1:6:205:PRO:O	27:6:1620:LUT:O3	2.30	0.48
5:b:249:ALA:HA	5:b:252:VAL:HG22	1.94	0.48
1:g:65:GLU:OE2	1:g:185:ARG:NE	2.47	0.48
26:n:603:CLA:H12	1:y:51:LEU:HD11	1.95	0.48
20:s:100:LYS:NZ	42:s:1101:HOH:O	2.45	0.48
3:4:154:PRO:HD2	27:4:620:LUT:H23	1.94	0.48
3:4:203:THR:HG22	3:4:205:LEU:H	1.79	0.48
26:A:410:CLA:H11	11:I:9:TYR:CZ	2.48	0.48
5:B:392:VAL:HG13	5:B:397:VAL:HB	1.96	0.48
31:C:515:BCR:HC42	11:I:23:PHE:HB2	1.96	0.48
7:D:226:ASP:HB2	7:D:235:ALA:HB1	1.96	0.48
7:D:267:TRP:HH2	30:L:101:LHG:H102	1.78	0.48
16:O:6:ARG:HG2	16:O:31:THR:HB	1.96	0.48
25:Y:607:CHL:H142	25:Y:609:CHL:H101	1.96	0.48
26:5:613:CLA:H2	26:5:614:CLA:HMD1	1.95	0.48
4:a:330:VAL:O	7:d:350:GLY:N	2.46	0.48
4:a:341:LEU:H	6:c:313:GLN:NE2	2.12	0.48
1:2:179:LYS:HD3	26:2:612:CLA:HAA2	1.96	0.48
4:A:91:LEU:HD11	4:A:163:ILE:HA	1.94	0.48
26:A:405:CLA:H122	35:A:408:PHO:H3A	1.94	0.48
26:C:508:CLA:HBC2	30:D:410:LHG:H341	1.94	0.48
1:G:80:VAL:HG13	1:G:206:LEU:HD11	1.95	0.48
3:8:113:TRP:HB2	25:8:609:CHL:HMA1	1.96	0.48
26:a:410:CLA:H11	11:i:9:TYR:CZ	2.48	0.48
26:c:503:CLA:H151	26:c:510:CLA:HBB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:234:ASN:HB3	7:D:264:ASN:ND2	2.29	0.48
6:C:28:GLN:NE2	7:D:234:ARG:HE	2.12	0.48
7:D:90:LEU:HG	10:H:62:ASN:HD22	1.78	0.48
7:D:298:ASP:HA	7:D:316:TYR:OH	2.14	0.48
25:G:607:CHL:HAA2	28:N:1622:XAT:H41	1.96	0.48
26:S:603:CLA:HED2	26:S:603:CLA:H2A	1.96	0.48
1:Y:126:ALA:HB3	25:Y:605:CHL:HMC	1.96	0.48
1:6:121:ALA:HB1	1:6:127:ILE:HD11	1.95	0.48
30:c:522:LHG:H181	22:w:31:GLY:HA3	1.94	0.48
31:d:404:BCR:H383	37:d:411:LMG:H182	1.94	0.48
1:y:110:LEU:O	1:y:110:LEU:HD23	2.14	0.48
1:y:110:LEU:HD23	1:y:110:LEU:C	2.39	0.48
28:y:1622:XAT:H12	30:y:2630:LHG:H212	1.96	0.48
1:1:112:TYR:HD2	1:1:118:LEU:HD13	1.79	0.48
1:2:52:SER:OG	1:2:61:ASN:ND2	2.47	0.48
5:B:114:HIS:HE1	26:B:617:CLA:ND	2.11	0.48
5:B:321:LYS:NZ	5:B:363:PHE:O	2.47	0.48
26:C:506:CLA:H41	26:C:506:CLA:H62	1.68	0.48
7:D:90:LEU:HG	10:H:62:ASN:ND2	2.28	0.48
1:G:220:ASN:HB2	26:G:614:CLA:HED1	1.95	0.48
31:8:623:BCR:HC22	30:r:2630:LHG:HC92	1.95	0.48
4:A:228:THR:HA	19:R:58:ALA:HA	1.96	0.47
1:N:105:PHE:HZ	1:Y:222:TRP:HB3	1.79	0.47
25:Y:608:CHL:HHC	25:Y:608:CHL:HBB1	1.95	0.47
1:6:179:LYS:HD3	26:6:612:CLA:HAA2	1.96	0.47
2:7:72:ALA:HA	2:7:165:LEU:HD11	1.96	0.47
5:b:392:VAL:HG13	5:b:397:VAL:HB	1.96	0.47
16:o:6:ARG:HG2	16:o:31:THR:HB	1.96	0.47
20:s:53:VAL:HG21	20:s:71:PHE:HE2	1.79	0.47
1:1:94:GLU:N	1:1:103:GLN:OE1	2.45	0.47
26:1:613:CLA:H2	26:1:613:CLA:H61	1.67	0.47
4:A:231:GLU:O	5:B:7:ARG:NH1	2.47	0.47
6:C:91:HIS:NE2	26:C:502:CLA:O1D	2.44	0.47
1:Y:69:SER:HB3	1:Y:184:GLY:HA3	1.94	0.47
4:a:328:MET:HE1	7:d:184:LEU:HD22	1.96	0.47
26:b:607:CLA:HBC1	30:b:2630:LHG:H101	1.96	0.47
26:b:617:CLA:H91	31:b:620:BCR:H14C	1.95	0.47
6:c:230:LEU:HD23	6:c:233:ILE:HD12	1.96	0.47
1:g:87:ARG:HH12	1:g:210:ALA:CB	2.27	0.47
25:g:601:CHL:H152	25:y:607:CHL:HBB1	1.97	0.47
19:r:182:LEU:HD12	27:r:620:LUT:H222	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:603:CLA:HED2	26:s:603:CLA:H2A	1.96	0.47
17:P:169:PHE:HB2	18:Q:27:ARG:HB3	1.96	0.47
20:S:53:VAL:HG21	20:S:71:PHE:HE2	1.79	0.47
26:b:602:CLA:H12	26:b:602:CLA:H52	1.72	0.47
6:c:106:ILE:HG21	18:q:89:LYS:HE2	1.96	0.47
6:c:370:ARG:HG3	6:c:370:ARG:NH1	2.28	0.47
7:d:226:ASP:HB2	7:d:235:ALA:HB1	1.96	0.47
20:s:235:ALA:HB2	24:z:59:SER:HB3	1.95	0.47
5:B:490:VAL:HG23	5:B:491:GLU:HG3	1.96	0.47
7:D:156:SER:HA	7:D:160:ILE:HB	1.95	0.47
16:O:179:ARG:O	16:O:182:GLU:HG2	2.14	0.47
1:5:97:TRP:O	27:5:1621:LUT:O3	2.32	0.47
4:a:44:ALA:HB2	4:a:118:HIS:HB2	1.95	0.47
5:b:321:LYS:NZ	5:b:363:PHE:O	2.47	0.47
25:g:607:CHL:HAA2	28:n:1622:XAT:H41	1.96	0.47
20:s:154:ILE:CG1	26:s:609:CLA:HMA1	2.44	0.47
1:2:118:LEU:HD23	25:2:605:CHL:HED2	1.96	0.47
3:4:113:TRP:HB2	25:4:609:CHL:HMA1	1.96	0.47
4:A:39:PRO:HG3	31:A:411:BCR:HC8	1.97	0.47
4:A:279:PRO:HG2	7:D:213:ALA:HB2	1.97	0.47
4:A:341:LEU:H	6:C:313:GLN:NE2	2.12	0.47
6:C:311:GLN:OE1	6:C:355:THR:OG1	2.28	0.47
1:N:103:GLN:HE22	26:N:604:CLA:HED2	1.80	0.47
1:Y:110:LEU:HD23	1:Y:110:LEU:O	2.14	0.47
4:a:286:THR:HB	26:a:405:CLA:O1D	2.14	0.47
5:b:114:HIS:HE1	26:b:617:CLA:ND	2.11	0.47
5:b:334:ASP:OD1	5:b:334:ASP:N	2.39	0.47
7:d:298:ASP:HA	7:d:316:TYR:OH	2.14	0.47
1:n:105:PHE:HZ	1:y:222:TRP:HB3	1.79	0.47
28:n:1622:XAT:H15	28:n:1622:XAT:H201	1.64	0.47
17:p:169:PHE:HB2	18:q:27:ARG:HB3	1.96	0.47
25:y:607:CHL:H62	25:y:607:CHL:H2	1.57	0.47
1:2:121:ALA:HB1	1:2:127:ILE:HD11	1.95	0.47
5:B:33:TRP:CD1	31:t:101:BCR:H381	2.49	0.47
6:C:396:MET:SD	18:Q:27:ARG:NH2	2.81	0.47
30:C:2630:LHG:H222	30:S:2630:LHG:H331	1.96	0.47
19:R:204:LEU:HD13	26:R:611:CLA:HBC1	1.97	0.47
28:Y:1622:XAT:H12	30:Y:2630:LHG:H212	1.96	0.47
1:6:52:SER:OG	1:6:61:ASN:ND2	2.47	0.47
4:a:279:PRO:HG2	7:d:213:ALA:HB2	1.97	0.47
26:c:505:CLA:H43	31:c:515:BCR:H331	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:g:1622:XAT:H391	28:g:1622:XAT:H31	1.71	0.47
1:n:103:GLN:HE22	26:n:604:CLA:HED2	1.80	0.47
18:q:31:LEU:HB2	18:q:36:ARG:HD3	1.97	0.47
26:A:405:CLA:H162	26:A:406:CLA:H102	1.97	0.47
6:C:460:ASP:HB2	11:I:34:ARG:HH12	1.80	0.47
26:C:504:CLA:H42	39:C:519:DGD:HB32	1.96	0.47
1:G:41:PRO:HG3	1:G:177:LYS:HB3	1.97	0.47
1:G:110:LEU:HD21	26:G:604:CLA:HAA1	1.96	0.47
1:G:194:PHE:HE1	27:G:1620:LUT:C5	2.28	0.47
25:G:606:CHL:HMB1	25:G:609:CHL:HAC1	1.95	0.47
4:a:39:PRO:HG3	31:a:411:BCR:HC8	1.97	0.47
4:a:92:HIS:CE1	6:c:220:GLY:HA3	2.49	0.47
4:a:221:SER:HB2	7:d:140:ARG:O	2.15	0.47
4:a:231:GLU:O	5:b:7:ARG:NH1	2.47	0.47
26:a:405:CLA:H162	26:a:406:CLA:H102	1.97	0.47
5:b:471:ALA:HB2	7:d:131:PHE:HE1	1.80	0.47
5:b:490:VAL:HG23	5:b:491:GLU:HG3	1.96	0.47
30:b:2631:LHG:H161	30:b:2631:LHG:H341	1.97	0.47
26:c:503:CLA:HAB	26:c:512:CLA:H41	1.95	0.47
30:c:2630:LHG:H222	30:s:2630:LHG:H331	1.96	0.47
1:g:41:PRO:HG3	1:g:177:LYS:HB3	1.97	0.47
19:r:185:ALA:HB1	19:r:191:LYS:HG3	1.97	0.47
19:r:204:LEU:HD13	26:r:611:CLA:HBC1	1.97	0.47
29:s:1623:NEX:H15	29:s:1623:NEX:H201	1.79	0.47
28:y:1622:XAT:H15	28:y:1622:XAT:H201	1.76	0.47
4:A:328:MET:HE1	7:D:184:LEU:HD22	1.96	0.47
5:B:471:ALA:HB2	7:D:131:PHE:HE1	1.80	0.47
26:C:503:CLA:HAB	26:C:512:CLA:H41	1.95	0.47
20:S:154:ILE:CG1	26:S:609:CLA:HMA1	2.44	0.47
3:8:203:THR:HG22	3:8:205:LEU:H	1.79	0.47
31:8:623:BCR:H341	31:8:623:BCR:H11C	1.69	0.47
6:c:279:LEU:HD11	26:c:507:CLA:HBA1	1.97	0.47
1:g:194:PHE:HE1	27:g:1620:LUT:C5	2.28	0.47
25:y:607:CHL:H142	25:y:609:CHL:H101	1.96	0.47
6:C:387:TRP:HD1	18:Q:83:TYR:CZ	2.33	0.47
31:C:517:BCR:H24C	31:C:517:BCR:H371	1.72	0.47
26:G:613:CLA:H61	26:G:613:CLA:H2	1.64	0.47
18:Q:31:LEU:HB2	18:Q:36:ARG:HD3	1.97	0.47
4:a:228:THR:HA	19:r:58:ALA:HA	1.96	0.47
5:b:245:VAL:HG21	26:b:613:CLA:HED3	1.96	0.47
26:b:612:CLA:H8	26:b:614:CLA:H51	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:618:BCR:H15C	31:b:618:BCR:H351	1.75	0.47
6:c:456:GLU:OE2	6:c:457:LYS:NZ	2.48	0.47
31:c:515:BCR:HC42	11:i:23:PHE:HB2	1.96	0.47
1:g:110:LEU:HD21	26:g:604:CLA:HAA1	1.96	0.47
28:g:1622:XAT:O23	30:g:2630:LHG:O1	2.31	0.47
1:1:229:VAL:HG22	1:1:231:GLY:H	1.80	0.47
5:B:256:MET:O	5:B:448:ARG:NH1	2.42	0.47
7:D:260:VAL:HG12	30:D:409:LHG:HC82	1.97	0.47
27:G:1621:LUT:H15	27:G:1621:LUT:H201	1.79	0.47
1:Y:21:ARG:NH2	1:Y:36:LEU:O	2.48	0.47
28:6:1622:XAT:H15	28:6:1622:XAT:H201	1.79	0.47
4:a:214:MET:HE2	4:a:255:PHE:CE1	2.50	0.47
5:b:71:ILE:HD11	26:b:607:CLA:H2A	1.95	0.47
16:o:179:ARG:O	16:o:182:GLU:HG2	2.14	0.47
1:1:222:TRP:HB3	1:2:105:PHE:HZ	1.80	0.46
28:2:1622:XAT:H31	28:2:1622:XAT:H391	1.75	0.46
26:C:503:CLA:H151	26:C:510:CLA:HBB2	1.96	0.46
18:Q:50:ARG:HH11	18:Q:87:ASP:HB2	1.80	0.46
19:R:29:VAL:H	19:R:93:ARG:HH21	1.62	0.46
1:Y:41:PRO:HG3	1:Y:177:LYS:HD3	1.98	0.46
1:5:112:TYR:HD2	1:5:118:LEU:HD13	1.79	0.46
4:a:250:ALA:HB1	7:d:139:LEU:HD21	1.96	0.46
36:b:623:SQD:H62	14:l:8:GLU:HB3	1.97	0.46
19:r:180:ASP:OD1	27:r:620:LUT:O23	2.32	0.46
1:y:126:ALA:HB3	25:y:605:CHL:HMC	1.96	0.46
4:A:221:SER:HB2	7:D:140:ARG:O	2.15	0.46
4:A:286:THR:HB	26:A:405:CLA:O1D	2.14	0.46
5:B:102:VAL:HG11	36:a:418:SQD:H382	1.97	0.46
5:B:245:VAL:HG21	26:B:613:CLA:HED3	1.96	0.46
5:B:368:VAL:HG21	5:B:422:ARG:HG2	1.97	0.46
19:R:185:ALA:HB1	19:R:191:LYS:HG3	1.97	0.46
4:A:160:ILE:HD11	39:C:518:DGD:HBT2	1.97	0.46
4:A:250:ALA:HB1	7:D:139:LEU:HD21	1.97	0.46
31:B:619:BCR:H391	39:B:626:DGD:HBF1	1.97	0.46
6:C:456:GLU:OE2	6:C:457:LYS:NZ	2.48	0.46
28:G:1622:XAT:H15	28:G:1622:XAT:H201	1.71	0.46
25:N:607:CHL:H62	25:N:607:CHL:H2	1.56	0.46
19:R:133:SER:O	19:R:140:LEU:N	2.35	0.46
31:c:516:BCR:H363	13:k:46:LEU:HD22	1.98	0.46
19:r:151:GLU:OE1	25:r:607:CHL:HMC	2.16	0.46
28:1:1622:XAT:H31	28:1:1622:XAT:H391	1.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:84:LEU:O	1:2:88:ASN:N	2.48	0.46
4:A:214:MET:HE2	4:A:255:PHE:CE1	2.50	0.46
6:C:230:LEU:HD23	6:C:233:ILE:HD12	1.96	0.46
26:C:505:CLA:H43	31:C:515:BCR:H331	1.96	0.46
25:G:601:CHL:H152	25:Y:607:CHL:HBB1	1.97	0.46
19:R:101:ARG:NH2	25:R:608:CHL:OBD	2.37	0.46
4:a:234:ASN:HB3	7:d:264:ASN:ND2	2.29	0.46
35:a:408:PHO:H92	35:a:408:PHO:H62	1.77	0.46
37:a:415:LMG:HC1	11:i:1:MET:HE2	1.97	0.46
5:b:51:VAL:HG13	5:b:308:LYS:HB2	1.98	0.46
5:b:211:LEU:HD22	26:r:603:CLA:H111	1.98	0.46
31:b:618:BCR:H383	36:b:621:SQD:H101	1.97	0.46
7:d:260:VAL:HG12	30:d:409:LHG:HC82	1.97	0.46
17:p:54:ASP:HB2	17:p:167:ARG:HE	1.80	0.46
3:4:31:GLY:HA3	3:4:181:ILE:HG21	1.98	0.46
31:B:618:BCR:H383	36:B:621:SQD:H101	1.97	0.46
6:C:106:ILE:HG21	18:Q:89:LYS:HE2	1.96	0.46
6:C:257:PHE:HA	30:C:523:LHG:HC11	1.98	0.46
28:G:1622:XAT:H371	30:G:2630:LHG:H362	1.98	0.46
1:5:94:GLU:N	1:5:103:GLN:OE1	2.45	0.46
2:3:72:ALA:HA	2:3:165:LEU:HD11	1.96	0.46
4:A:77:ILE:HB	14:L:34:ASN:HD21	1.80	0.46
5:B:211:LEU:HD22	26:R:603:CLA:H111	1.98	0.46
30:B:2631:LHG:H161	30:B:2631:LHG:H341	1.97	0.46
1:N:199:ILE:HG13	25:N:607:CHL:H42	1.98	0.46
17:P:54:ASP:HB2	17:P:167:ARG:HE	1.80	0.46
26:S:614:CLA:HBC1	30:S:2630:LHG:H372	1.97	0.46
31:T:101:BCR:H381	5:b:33:TRP:CD1	2.51	0.46
28:Y:1622:XAT:H12	30:Y:2630:LHG:H191	1.98	0.46
1:5:222:TRP:HB3	1:6:105:PHE:HZ	1.80	0.46
26:5:613:CLA:H2	26:5:613:CLA:H61	1.67	0.46
2:7:181:PRO:HA	2:7:184:PHE:HB3	1.98	0.46
4:a:160:ILE:HD11	39:c:518:DGD:HBT2	1.97	0.46
26:d:403:CLA:H152	23:x:59:VAL:HA	1.97	0.46
1:n:199:ILE:HG13	25:n:607:CHL:H42	1.98	0.46
19:r:29:VAL:H	19:r:93:ARG:HH21	1.62	0.46
20:s:95:PRO:HG3	26:s:604:CLA:C1D	2.46	0.46
5:B:389:LYS:N	7:D:345:GLU:OE2	2.46	0.46
4:a:42:LEU:HD23	36:a:418:SQD:C21	2.46	0.46
4:a:63:ILE:HG21	4:a:336:ALA:HA	1.97	0.46
5:b:368:VAL:HG21	5:b:422:ARG:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:506:CLA:H71	11:i:20:ILE:HD13	1.98	0.46
31:d:404:BCR:H15C	31:d:404:BCR:H351	1.84	0.46
29:s:1623:NEX:H11	29:s:1623:NEX:H191	1.75	0.46
28:y:1622:XAT:H12	30:y:2630:LHG:H191	1.98	0.46
5:B:400:GLU:OE1	5:B:410:THR:OG1	2.25	0.46
31:C:517:BCR:H15C	31:C:517:BCR:H351	1.81	0.46
19:R:102:TRP:CD1	26:R:609:CLA:HMD3	2.51	0.46
20:S:95:PRO:HG3	26:S:604:CLA:C1D	2.46	0.46
1:6:118:LEU:HD23	25:6:605:CHL:HED2	1.96	0.46
5:b:114:HIS:HE1	26:b:617:CLA:C1D	2.29	0.46
6:c:257:PHE:HA	30:c:523:LHG:HC11	1.98	0.46
6:c:371:GLY:N	6:c:374:GLY:O	2.49	0.46
19:r:102:TRP:CD1	26:r:609:CLA:HMD3	2.51	0.46
37:A:415:LMG:HC1	11:I:1:MET:HE2	1.97	0.46
5:B:51:VAL:HG13	5:B:308:LYS:HB2	1.98	0.46
26:B:612:CLA:H8	26:B:614:CLA:H51	1.96	0.46
6:C:279:LEU:HD11	26:C:507:CLA:HBA1	1.97	0.46
31:C:516:BCR:H21C	12:J:15:THR:HG23	1.98	0.46
19:R:181:PRO:HD2	27:R:620:LUT:H23	1.98	0.46
31:b:619:BCR:H391	39:b:626:DGD:HBF1	1.97	0.46
6:c:91:HIS:NE2	26:c:502:CLA:O1D	2.44	0.46
6:c:316:THR:HG21	18:q:27:ARG:NH2	2.31	0.46
19:r:181:PRO:HD2	27:r:620:LUT:H23	1.98	0.46
1:y:21:ARG:NH2	1:y:36:LEU:O	2.48	0.46
1:y:41:PRO:HG3	1:y:177:LYS:HD3	1.97	0.46
2:3:155:GLY:HA2	25:3:608:CHL:HAC1	1.98	0.46
36:B:621:SQD:H351	36:B:621:SQD:H321	1.68	0.46
6:C:191:PRO:HA	18:Q:78:ARG:HG2	1.98	0.46
6:C:223:TRP:CG	6:C:224:ILE:N	2.83	0.46
30:C:522:LHG:H242	30:C:522:LHG:HC91	1.98	0.46
6:c:311:GLN:OE1	6:c:355:THR:OG1	2.28	0.46
37:c:521:LMG:H361	13:k:45:LEU:HD11	1.98	0.46
30:c:522:LHG:H242	30:c:522:LHG:HC91	1.98	0.46
26:n:610:CLA:H62	26:n:610:CLA:H41	1.71	0.46
18:q:50:ARG:HH11	18:q:87:ASP:HB2	1.80	0.46
27:1:1620:LUT:H35	27:1:1620:LUT:H401	1.84	0.45
28:1:1622:XAT:H15	28:1:1622:XAT:H201	1.73	0.45
25:4:601:CHL:HBA1	25:4:601:CHL:H3A	1.66	0.45
4:A:166:GLY:HA3	6:C:358:PHE:HE1	1.81	0.45
6:C:400:PRO:O	6:C:401:LEU:HD12	2.16	0.45
26:C:512:CLA:H202	26:C:513:CLA:H111	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:137:ASP:OD1	17:P:137:ASP:N	2.49	0.45
29:R:623:NEX:H11	29:R:623:NEX:H191	1.73	0.45
4:a:166:GLY:HA3	6:c:358:PHE:HE1	1.81	0.45
6:c:344:SER:OG	6:c:348:GLU:OE1	2.32	0.45
26:c:512:CLA:H202	26:c:513:CLA:H111	1.99	0.45
31:c:516:BCR:H21C	12:j:15:THR:HG23	1.98	0.45
9:f:39:ARG:NH2	17:p:16:THR:OG1	2.45	0.45
26:r:601:CLA:HBA1	26:r:601:CLA:H3A	1.44	0.45
3:4:36:ASP:OD1	28:4:622:XAT:O23	2.34	0.45
4:A:63:ILE:HG21	4:A:336:ALA:HA	1.97	0.45
6:C:316:THR:HG21	18:Q:27:ARG:NH2	2.30	0.45
1:N:41:PRO:HG3	1:N:177:LYS:HD3	1.98	0.45
36:a:418:SQD:H262	31:t:101:BCR:H333	1.96	0.45
36:b:621:SQD:H321	36:b:621:SQD:H351	1.68	0.45
6:c:400:PRO:O	6:c:401:LEU:HD12	2.16	0.45
26:c:510:CLA:H2	26:c:510:CLA:H61	1.77	0.45
7:d:56:VAL:HG21	7:d:111:LEU:HD12	1.99	0.45
26:g:602:CLA:H101	27:g:1621:LUT:H371	1.98	0.45
20:s:79:LEU:HD13	20:s:164:LEU:HD23	1.98	0.45
23:x:47:VAL:HA	23:x:51:LEU:HD23	1.98	0.45
1:y:103:GLN:HE22	26:y:604:CLA:HED2	1.81	0.45
26:y:603:CLA:HHC	26:y:603:CLA:HBB1	1.98	0.45
3:4:96:THR:HG21	19:R:235:LEU:HA	1.99	0.45
1:6:197:GLN:O	1:6:201:THR:OG1	2.31	0.45
6:c:387:TRP:HD1	18:q:83:TYR:CZ	2.33	0.45
26:r:616:CLA:HBA2	26:r:616:CLA:H3A	1.65	0.45
25:G:607:CHL:HBB2	25:G:609:CHL:HBC1	1.99	0.45
20:S:55:GLY:HA3	20:S:194:ARG:HH12	1.82	0.45
22:W:47:ASP:N	22:W:47:ASP:OD1	2.49	0.45
1:Y:24:TYR:CG	1:Y:46:TRP:HB2	2.51	0.45
1:Y:103:GLN:HE22	26:Y:604:CLA:HED2	1.81	0.45
26:Y:603:CLA:HHC	26:Y:603:CLA:HBB1	1.98	0.45
1:5:229:VAL:HG22	1:5:231:GLY:H	1.80	0.45
25:g:601:CHL:H102	28:g:1622:XAT:H14	1.98	0.45
1:y:70:ARG:NE	1:y:180:GLU:OE2	2.49	0.45
25:4:601:CHL:HBC1	30:4:2630:LHG:HC2	1.99	0.45
4:A:27:ARG:NH1	7:D:255:SER:O	2.37	0.45
6:C:110:PRO:HG3	37:Z:101:LMG:H121	1.97	0.45
14:L:5:ASN:HB3	14:L:8:GLU:HG3	1.98	0.45
25:N:601:CHL:HMA3	30:N:2630:LHG:H121	1.99	0.45
28:N:1622:XAT:H15	28:N:1622:XAT:H201	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:196:ARG:HA	2:7:199:MET:HE3	1.99	0.45
5:b:383:PHE:N	7:d:345:GLU:O	2.50	0.45
26:b:602:CLA:HBB2	31:h:101:BCR:H351	1.98	0.45
6:c:223:TRP:CG	6:c:224:ILE:N	2.83	0.45
7:d:194:LEU:O	14:l:35:TYR:OH	2.28	0.45
19:r:101:ARG:NH2	25:r:608:CHL:OBD	2.37	0.45
19:r:127:VAL:HA	19:r:130:VAL:HG22	1.98	0.45
27:3:1621:LUT:H15	27:3:1621:LUT:H201	1.80	0.45
6:C:371:GLY:N	6:C:374:GLY:O	2.49	0.45
31:C:516:BCR:H363	13:K:46:LEU:HD22	1.98	0.45
26:D:403:CLA:H152	23:X:59:VAL:HA	1.97	0.45
26:G:602:CLA:H101	27:G:1621:LUT:H371	1.98	0.45
28:G:1622:XAT:O23	30:G:2630:LHG:O1	2.31	0.45
29:N:1623:NEX:H35	29:N:1623:NEX:H401	1.86	0.45
16:O:202:LEU:HD23	16:O:218:PHE:HB3	1.98	0.45
19:R:187:ASP:HA	19:R:188:PRO:HD3	1.86	0.45
19:R:238:THR:HG22	19:R:239:ILE:H	1.81	0.45
1:Y:192:PHE:CD2	26:Y:602:CLA:H171	2.52	0.45
5:b:362:PHE:HB3	7:d:189:PHE:CD2	2.52	0.45
26:b:605:CLA:H141	26:b:605:CLA:H161	1.80	0.45
6:c:229:ASP:OD2	18:q:122:LYS:NZ	2.39	0.45
1:n:41:PRO:HG3	1:n:177:LYS:HD3	1.98	0.45
26:n:603:CLA:H91	25:n:609:CHL:H112	1.98	0.45
16:o:162:ARG:NH1	16:o:189:ASN:OD1	2.44	0.45
27:1:1621:LUT:H35	27:1:1621:LUT:H401	1.87	0.45
2:3:80:TRP:CE2	25:3:608:CHL:HED2	2.52	0.45
3:4:153:ASP:HB3	3:4:156:SER:HA	1.99	0.45
5:B:366:PHE:O	5:B:425:GLN:NE2	2.45	0.45
5:B:383:PHE:N	7:D:345:GLU:O	2.50	0.45
26:C:508:CLA:H142	26:C:510:CLA:H102	1.98	0.45
31:C:515:BCR:H15C	31:C:515:BCR:H351	1.81	0.45
1:G:97:TRP:O	27:G:1621:LUT:O3	2.35	0.45
26:Y:613:CLA:H2	26:Y:613:CLA:H61	1.66	0.45
3:8:31:GLY:HA3	3:8:181:ILE:HG21	1.98	0.45
25:8:601:CHL:HBC1	30:8:2630:LHG:HC2	1.99	0.45
4:a:77:ILE:HB	14:l:34:ASN:HD21	1.81	0.45
6:c:322:GLN:NE2	6:c:381:LYS:HA	2.32	0.45
26:g:611:CLA:H61	26:g:611:CLA:H41	1.84	0.45
1:n:162:ASP:OD1	27:n:1620:LUT:O23	2.35	0.45
17:p:129:ILE:HG23	17:p:147:ILE:HB	1.99	0.45
26:s:614:CLA:HBC1	30:s:2630:LHG:H372	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:24:TYR:CG	1:y:46:TRP:HB2	2.51	0.45
27:3:1620:LUT:H15	27:3:1620:LUT:H201	1.84	0.45
5:B:114:HIS:HE1	26:B:617:CLA:C1D	2.29	0.45
5:B:214:LEU:HB3	26:R:603:CLA:HED1	1.98	0.45
7:D:56:VAL:HG21	7:D:111:LEU:HD12	1.99	0.45
26:N:610:CLA:H92	26:N:610:CLA:H61	1.83	0.45
17:P:75:GLY:O	17:P:127:TYR:OH	2.31	0.45
20:S:79:LEU:HD13	20:S:164:LEU:HD23	1.98	0.45
25:Y:607:CHL:H62	25:Y:607:CHL:H2	1.57	0.45
5:b:187:VAL:HG23	26:b:602:CLA:HMD3	1.98	0.45
5:b:389:LYS:N	7:d:345:GLU:OE2	2.46	0.45
25:g:606:CHL:HBB2	25:g:607:CHL:CBB	2.47	0.45
28:g:1622:XAT:H371	30:g:2630:LHG:H362	1.98	0.45
31:h:101:BCR:H24C	31:h:101:BCR:H371	1.74	0.45
19:r:238:THR:HG22	19:r:239:ILE:H	1.81	0.45
1:y:185:ARG:HA	1:y:188:MET:HE3	1.99	0.45
5:B:30:VAL:HG13	26:B:614:CLA:HMC2	1.98	0.45
36:B:623:SQD:H62	14:L:8:GLU:HB3	1.97	0.45
28:R:622:XAT:H35	28:R:622:XAT:H401	1.77	0.45
3:8:36:ASP:OD1	28:8:622:XAT:O23	2.34	0.45
6:c:110:PRO:HG3	37:z:101:LMG:H121	1.97	0.45
26:c:512:CLA:C1B	31:c:514:BCR:H401	2.46	0.45
16:o:202:LEU:HD23	16:o:218:PHE:HB3	1.98	0.45
19:r:124:ALA:HB1	26:r:604:CLA:HED1	1.99	0.45
26:C:512:CLA:C1B	31:C:514:BCR:H401	2.46	0.45
7:D:163:LEU:HD13	39:H:102:DGD:HB92	1.99	0.45
1:N:162:ASP:OD1	27:N:1620:LUT:O23	2.35	0.45
27:Y:1621:LUT:H15	27:Y:1621:LUT:H201	1.81	0.45
28:7:1622:XAT:H15	28:7:1622:XAT:H201	1.77	0.45
6:c:191:PRO:HA	18:q:78:ARG:HG2	1.98	0.45
25:g:608:CHL:HHC	25:g:608:CHL:HBB1	1.99	0.45
2:3:181:PRO:HA	2:3:184:PHE:HB3	1.98	0.44
4:A:228:THR:OG1	4:A:230:ASN:OD1	2.28	0.44
7:D:52:GLY:HA2	7:D:56:VAL:HB	1.99	0.44
25:G:608:CHL:HBB1	25:G:608:CHL:HHC	1.99	0.44
1:N:192:PHE:CE2	26:N:602:CLA:H171	2.52	0.44
26:N:603:CLA:H91	25:N:609:CHL:H112	1.98	0.44
19:R:151:GLU:OE1	25:R:607:CHL:HMC	2.16	0.44
26:R:612:CLA:HHC	26:R:612:CLA:HBB1	1.99	0.44
31:T:101:BCR:H15C	31:T:101:BCR:H351	1.83	0.44
23:X:47:VAL:HA	23:X:51:LEU:HD23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:607:CHL:H61	25:6:607:CHL:HMB1	1.99	0.44
28:7:1622:XAT:H31	28:7:1622:XAT:H391	1.72	0.44
26:a:410:CLA:H112	26:a:410:CLA:H72	1.74	0.44
5:b:214:LEU:HB3	26:r:603:CLA:HED1	1.98	0.44
22:w:47:ASP:N	22:w:47:ASP:OD1	2.49	0.44
25:1:607:CHL:H142	25:1:609:CHL:H101	1.99	0.44
1:2:221:ALA:N	26:2:613:CLA:O1A	2.49	0.44
28:2:1622:XAT:H11	28:2:1622:XAT:H191	1.83	0.44
2:3:160:GLY:HA3	25:3:608:CHL:HBC3	1.99	0.44
26:3:603:CLA:H91	25:3:609:CHL:H121	1.99	0.44
4:A:267:ASN:HD22	36:A:412:SQD:H3	1.83	0.44
5:B:187:VAL:HG23	26:B:602:CLA:HMD3	1.98	0.44
5:B:458:PHE:HB3	26:B:605:CLA:HBC2	1.99	0.44
26:C:506:CLA:H71	11:I:20:ILE:HD13	1.98	0.44
37:C:521:LMG:H361	13:K:45:LEU:HD11	1.98	0.44
16:O:170:ASN:ND2	16:O:181:ASP:OD1	2.51	0.44
19:R:229:THR:HG22	19:R:237:THR:HG21	1.99	0.44
26:R:603:CLA:HED2	26:R:603:CLA:H2A	2.00	0.44
1:5:142:ARG:NH2	25:5:609:CHL:O1D	2.45	0.44
1:5:205:PRO:O	27:5:1620:LUT:O3	2.31	0.44
5:b:155:ALA:O	5:b:159:THR:OG1	2.36	0.44
6:c:97:TRP:HH2	26:c:502:CLA:H151	1.82	0.44
20:s:55:GLY:HA3	20:s:194:ARG:HH12	1.82	0.44
26:s:613:CLA:H2	26:s:613:CLA:H61	1.74	0.44
1:y:192:PHE:CD2	26:y:602:CLA:H171	2.52	0.44
1:2:205:PRO:O	27:2:1620:LUT:O3	2.30	0.44
26:B:605:CLA:H93	26:B:606:CLA:HAB	2.00	0.44
26:B:611:CLA:H102	26:B:616:CLA:HAA1	1.98	0.44
6:C:97:TRP:HH2	26:C:502:CLA:H151	1.82	0.44
6:C:319:VAL:HG11	6:C:389:GLU:HG2	1.99	0.44
19:R:124:ALA:HB1	26:R:604:CLA:HED1	1.99	0.44
1:Y:25:LEU:HB2	1:Y:29:SER:HA	1.99	0.44
1:6:51:LEU:HD12	27:6:1621:LUT:H221	2.00	0.44
1:6:84:LEU:O	1:6:88:ASN:N	2.48	0.44
2:7:155:GLY:HA2	25:7:608:CHL:HAC1	1.98	0.44
29:7:1623:NEX:H35	29:7:1623:NEX:H401	1.90	0.44
26:b:602:CLA:HAC1	31:h:101:BCR:H383	1.99	0.44
6:c:460:ASP:HB2	11:i:34:ARG:HH12	1.80	0.44
26:c:508:CLA:H142	26:c:510:CLA:H102	1.98	0.44
16:o:89:ILE:HD13	16:o:130:ILE:HD11	2.00	0.44
1:y:25:LEU:HB2	1:y:29:SER:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:602:CLA:HBA1	27:1:1621:LUT:H382	1.99	0.44
1:2:51:LEU:HD12	27:2:1621:LUT:H221	2.00	0.44
2:3:196:ARG:HA	2:3:199:MET:HE3	1.99	0.44
35:A:408:PHO:H42	30:D:409:LHG:H342	2.00	0.44
36:A:418:SQD:H262	31:T:101:BCR:H333	1.96	0.44
5:B:362:PHE:HB3	7:D:189:PHE:CD2	2.52	0.44
26:B:605:CLA:HAB	26:B:605:CLA:HHC	1.83	0.44
27:G:1621:LUT:H372	26:Y:603:CLA:HED3	2.00	0.44
19:R:180:ASP:OD1	27:R:620:LUT:O23	2.32	0.44
20:S:85:ALA:O	20:S:89:ALA:N	2.46	0.44
1:Y:70:ARG:NE	1:Y:180:GLU:OE2	2.49	0.44
1:Y:84:LEU:O	1:Y:88:ASN:ND2	2.51	0.44
2:7:80:TRP:CE2	25:7:608:CHL:HED2	2.52	0.44
4:a:304:GLN:HG2	4:a:313:VAL:HG11	2.00	0.44
6:c:154:ARG:HB3	6:c:256:PRO:HG2	1.98	0.44
19:r:21:PRO:CD	19:r:24:LEU:HD13	2.47	0.44
19:r:101:ARG:HA	19:r:104:MET:HE3	1.99	0.44
26:r:603:CLA:HED2	26:r:603:CLA:H2A	2.00	0.44
1:1:25:LEU:HB3	1:1:28:PHE:HB2	1.99	0.44
28:1:1622:XAT:H12	30:1:2630:LHG:H182	1.99	0.44
4:A:254:TYR:HE2	7:D:143:ASN:HD22	1.65	0.44
26:A:405:CLA:H161	26:A:405:CLA:H193	1.77	0.44
5:B:121:GLU:CD	10:H:14:PRO:HB2	2.43	0.44
25:G:601:CHL:H102	28:G:1622:XAT:H14	1.98	0.44
1:N:126:ALA:HB3	25:N:605:CHL:HMC	2.00	0.44
25:N:607:CHL:H143	25:N:607:CHL:H111	1.71	0.44
26:Y:602:CLA:H193	26:Y:602:CLA:H161	1.78	0.44
26:Y:612:CLA:H142	26:Y:612:CLA:H111	1.86	0.44
29:Y:1623:NEX:H11	29:Y:1623:NEX:H191	1.84	0.44
2:7:174:PRO:HD2	27:7:1620:LUT:H23	1.99	0.44
25:7:606:CHL:HMC	25:7:607:CHL:C4C	2.47	0.44
27:7:1620:LUT:H35	27:7:1620:LUT:H401	1.87	0.44
26:r:612:CLA:HHC	26:r:612:CLA:HBB1	1.99	0.44
29:r:623:NEX:H15	29:r:623:NEX:H201	1.80	0.44
2:3:174:PRO:HD2	27:3:1620:LUT:H23	1.99	0.44
27:3:1620:LUT:H35	27:3:1620:LUT:H401	1.87	0.44
5:B:334:ASP:HB2	5:B:432:LEU:HD13	1.99	0.44
26:B:602:CLA:HBB2	31:H:101:BCR:H351	1.98	0.44
26:B:614:CLA:H61	26:B:614:CLA:H41	1.68	0.44
6:C:154:ARG:HB3	6:C:256:PRO:HG2	1.98	0.44
26:C:502:CLA:H171	26:C:502:CLA:H13	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:1622:XAT:H12	30:5:2630:LHG:H182	1.99	0.44
5:b:30:VAL:HG13	26:b:614:CLA:HMC2	1.99	0.44
5:b:121:GLU:CD	10:h:14:PRO:HB2	2.43	0.44
5:b:464:PHE:HD2	26:b:612:CLA:HAC2	1.82	0.44
26:b:605:CLA:H93	26:b:606:CLA:HAB	2.00	0.44
26:b:611:CLA:H102	26:b:616:CLA:HAA1	1.98	0.44
14:l:5:ASN:HB3	14:l:8:GLU:HG3	1.98	0.44
25:n:601:CHL:HMA3	30:n:2630:LHG:H121	1.99	0.44
1:1:142:ARG:NH2	25:1:609:CHL:O1D	2.45	0.44
25:3:606:CHL:HMC	25:3:607:CHL:C4C	2.48	0.44
4:A:22:THR:HG22	4:A:136:ARG:HH11	1.83	0.44
6:C:322:GLN:NE2	6:C:381:LYS:HA	2.32	0.44
26:C:502:CLA:HHC	26:C:502:CLA:HAB	1.81	0.44
28:N:1622:XAT:H11	28:N:1622:XAT:H191	1.91	0.44
17:P:129:ILE:HG23	17:P:147:ILE:HB	1.99	0.44
18:Q:50:ARG:HH11	18:Q:87:ASP:CB	2.31	0.44
29:Y:1623:NEX:H35	29:Y:1623:NEX:H401	1.83	0.44
26:5:602:CLA:HBA1	27:5:1621:LUT:H382	1.99	0.44
2:7:79:ARG:HA	2:7:82:MET:HE3	1.99	0.44
5:b:334:ASP:HB2	5:b:432:LEU:HD13	1.99	0.44
31:b:620:BCR:H11C	31:b:620:BCR:H341	1.81	0.44
1:n:189:PHE:HD1	26:n:602:CLA:H201	1.82	0.44
19:r:229:THR:HG22	19:r:237:THR:HG21	1.99	0.44
26:r:611:CLA:H3A	26:r:611:CLA:HBA2	1.57	0.44
1:1:164:LEU:HG	26:g:611:CLA:HMB2	2.00	0.44
25:2:607:CHL:HMB1	25:2:607:CHL:H61	1.99	0.44
4:A:42:LEU:HD23	36:A:418:SQD:C21	2.46	0.44
26:B:613:CLA:H171	26:B:614:CLA:HBB2	2.00	0.44
39:B:626:DGD:HBN2	4:a:46:SER:HB3	1.98	0.44
7:D:84:ASN:HD22	7:D:337:HIS:CD2	2.36	0.44
26:D:403:CLA:H61	26:D:403:CLA:H102	1.78	0.44
1:N:189:PHE:HD1	26:N:602:CLA:H201	1.82	0.44
19:R:101:ARG:HA	19:R:104:MET:HE3	1.99	0.44
19:R:127:VAL:HA	19:R:130:VAL:HG22	1.98	0.44
2:7:160:GLY:HA3	25:7:608:CHL:HBC3	1.99	0.44
3:8:96:THR:HG21	19:r:235:LEU:HA	1.99	0.44
4:a:93:PHE:HZ	26:a:410:CLA:HAA1	1.83	0.44
4:a:267:ASN:HD22	36:a:412:SQD:H3	1.83	0.44
5:b:362:PHE:HB3	7:d:189:PHE:HD2	1.83	0.44
5:b:366:PHE:O	5:b:425:GLN:NE2	2.45	0.44
7:d:49:TRP:HA	7:d:79:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:163:LEU:HD13	39:h:102:DGD:HB92	1.99	0.44
1:g:97:TRP:O	27:g:1621:LUT:O3	2.35	0.44
25:g:607:CHL:HBB2	25:g:609:CHL:HBC1	1.99	0.44
26:g:613:CLA:H2	26:g:613:CLA:H61	1.64	0.44
1:n:192:PHE:CE2	26:n:602:CLA:H171	2.53	0.44
30:s:2630:LHG:H282	30:s:2630:LHG:HC91	1.99	0.44
1:y:73:MET:SD	26:y:610:CLA:HAB	2.58	0.44
26:y:602:CLA:H172	26:y:602:CLA:H13	1.64	0.44
28:3:1622:XAT:H31	28:3:1622:XAT:H391	1.72	0.44
35:A:408:PHO:H92	35:A:408:PHO:H62	1.77	0.44
26:A:410:CLA:H112	26:A:410:CLA:H72	1.74	0.44
26:B:603:CLA:H12	10:H:61:TYR:CE2	2.53	0.44
26:B:613:CLA:H61	26:B:613:CLA:H102	1.81	0.44
1:G:104:ILE:HG21	1:G:124:ILE:HD13	1.99	0.44
25:G:606:CHL:HBB2	25:G:607:CHL:CBB	2.47	0.44
26:R:613:CLA:H92	30:R:2630:LHG:H171	2.00	0.44
5:b:182:ASN:HA	37:b:2633:LMG:HC62	2.00	0.44
7:d:52:GLY:HA2	7:d:56:VAL:HB	1.98	0.44
27:g:1621:LUT:H35	27:g:1621:LUT:H401	1.83	0.44
25:y:601:CHL:H91	25:y:601:CHL:H112	1.80	0.44
35:A:409:PHO:HMC2	7:D:280:LEU:HD21	2.00	0.43
5:B:464:PHE:HD2	26:B:612:CLA:HAC2	1.82	0.43
18:Q:65:ILE:HG12	18:Q:73:LEU:HD22	1.99	0.43
30:S:2630:LHG:H282	30:S:2630:LHG:HC91	1.99	0.43
1:6:221:ALA:N	26:6:613:CLA:O1A	2.49	0.43
25:6:609:CHL:H93	25:6:609:CHL:H61	1.89	0.43
7:d:84:ASN:HD22	7:d:337:HIS:CD2	2.36	0.43
25:s:606:CHL:HMC	25:s:607:CHL:C1C	2.48	0.43
28:y:1622:XAT:H11	28:y:1622:XAT:H191	1.83	0.43
26:2:611:CLA:HBA2	26:2:612:CLA:HMD3	2.00	0.43
26:A:405:CLA:H102	35:A:408:PHO:HAA1	2.00	0.43
7:D:349:ARG:NH1	7:D:353:LEU:O	2.40	0.43
26:G:613:CLA:HBB1	27:G:1620:LUT:H192	2.00	0.43
19:R:81:GLN:HE21	26:R:616:CLA:HED3	1.83	0.43
1:5:70:ARG:NH1	25:5:608:CHL:OBD	2.42	0.43
25:6:607:CHL:H91	25:6:607:CHL:H112	1.80	0.43
26:b:603:CLA:H12	10:h:61:TYR:CE2	2.53	0.43
26:b:613:CLA:H171	26:b:614:CLA:HBB2	2.00	0.43
6:c:117:LEU:HD12	37:z:101:LMG:H202	2.00	0.43
6:c:319:VAL:HG11	6:c:389:GLU:HG2	2.00	0.43
27:g:1621:LUT:H372	26:y:603:CLA:HED3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:h:102:DGD:HB91	39:h:102:DGD:HB62	1.67	0.43
25:1:609:CHL:H91	25:1:609:CHL:H112	1.83	0.43
2:3:53:TYR:OH	30:3:2630:LHG:O5	2.33	0.43
2:3:79:ARG:HA	2:3:82:MET:HE3	1.99	0.43
37:B:622:LMG:HC91	15:M:6:LEU:HD22	2.01	0.43
16:O:89:ILE:HD13	16:O:130:ILE:HD11	2.00	0.43
1:Y:73:MET:SD	26:Y:610:CLA:HAB	2.58	0.43
1:6:63:GLU:HA	1:6:155:LEU:HD11	2.00	0.43
4:a:22:THR:HG22	4:a:136:ARG:HH11	1.83	0.43
26:a:405:CLA:H102	35:a:408:PHO:HAA1	2.00	0.43
6:c:120:ILE:HG23	24:z:47:TRP:CH2	2.53	0.43
26:c:506:CLA:H41	26:c:506:CLA:H62	1.68	0.43
30:d:409:LHG:H141	30:d:409:LHG:H292	2.00	0.43
2:3:152:ARG:NH2	25:3:609:CHL:O1D	2.52	0.43
26:B:602:CLA:HAC1	31:H:101:BCR:H383	1.99	0.43
26:C:501:CLA:H61	26:C:501:CLA:H41	1.90	0.43
30:D:409:LHG:H141	30:D:409:LHG:H292	2.00	0.43
17:P:30:VAL:HG11	17:P:49:TYR:CD2	2.53	0.43
1:5:25:LEU:HB3	1:5:28:PHE:HB2	1.99	0.43
26:6:611:CLA:HBA2	26:6:612:CLA:HMD3	2.00	0.43
27:7:1621:LUT:H15	27:7:1621:LUT:H201	1.80	0.43
3:8:153:ASP:HB3	3:8:156:SER:HA	1.99	0.43
28:8:622:XAT:H15	28:8:622:XAT:H201	1.87	0.43
35:a:409:PHO:HMC2	7:d:280:LEU:HD21	2.00	0.43
26:b:615:CLA:H92	26:b:615:CLA:H61	1.86	0.43
7:d:304:ILE:HD13	15:m:2:GLU:OE2	2.18	0.43
26:g:613:CLA:HBB1	27:g:1620:LUT:H192	2.00	0.43
1:n:126:ALA:HB3	25:n:605:CHL:HMC	2.00	0.43
26:n:603:CLA:C3D	25:n:609:CHL:H2	2.49	0.43
26:n:603:CLA:H92	26:n:603:CLA:H61	1.76	0.43
17:p:114:LEU:HD11	17:p:132:LEU:HB2	2.01	0.43
18:q:65:ILE:HG12	18:q:73:LEU:HD22	1.99	0.43
1:y:84:LEU:O	1:y:88:ASN:ND2	2.51	0.43
4:A:93:PHE:HZ	26:A:410:CLA:HAA1	1.83	0.43
4:A:145:VAL:O	4:A:148:SER:OG	2.29	0.43
36:A:418:SQD:H382	5:b:102:VAL:HG11	2.00	0.43
5:B:139:PHE:CZ	5:B:143:LEU:HD22	2.54	0.43
1:G:167:ALA:HB2	26:G:610:CLA:HAA1	2.01	0.43
26:G:603:CLA:HBB1	26:G:603:CLA:HHC	2.00	0.43
28:G:1622:XAT:H11	28:G:1622:XAT:H191	1.93	0.43
16:O:78:LEU:HB3	22:W:3:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:S:606:CHL:HMC	25:S:607:CHL:C1C	2.48	0.43
26:7:603:CLA:H91	25:7:609:CHL:H121	2.00	0.43
26:a:406:CLA:H202	26:a:406:CLA:H162	1.85	0.43
26:b:603:CLA:H93	26:b:603:CLA:H61	1.78	0.43
7:d:91:LEU:O	7:d:105:TRP:NE1	2.31	0.43
17:p:137:ASP:N	17:p:137:ASP:OD1	2.49	0.43
28:r:622:XAT:H15	28:r:622:XAT:H201	1.87	0.43
27:s:1621:LUT:H35	27:s:1621:LUT:H401	1.83	0.43
26:3:611:CLA:C4D	26:3:612:CLA:HMD2	2.49	0.43
5:B:469:HIS:CE1	26:B:612:CLA:NA	2.86	0.43
6:C:344:SER:OG	6:C:348:GLU:OE1	2.32	0.43
7:D:304:ILE:HD13	15:M:2:GLU:OE2	2.18	0.43
1:G:130:THR:HB	42:G:664:HOH:O	2.19	0.43
19:R:203:ARG:HA	19:R:206:MET:HE3	2.00	0.43
1:Y:185:ARG:HA	1:Y:188:MET:HE3	1.99	0.43
25:5:607:CHL:H142	25:5:609:CHL:H101	1.99	0.43
2:7:145:MET:HA	2:7:148:VAL:HG22	2.01	0.43
5:b:139:PHE:CZ	5:b:143:LEU:HD22	2.54	0.43
5:b:458:PHE:HB3	26:b:605:CLA:HBC2	1.99	0.43
5:b:469:HIS:CE1	26:b:612:CLA:NA	2.86	0.43
18:q:50:ARG:HH11	18:q:87:ASP:CB	2.31	0.43
26:r:613:CLA:H92	30:r:2630:LHG:H171	2.00	0.43
29:3:1623:NEX:H15	29:3:1623:NEX:H201	1.71	0.43
5:B:182:ASN:HA	37:B:2633:LMG:HC62	2.00	0.43
26:B:605:CLA:H141	26:B:605:CLA:H161	1.80	0.43
6:C:418:ASN:HD21	39:C:519:DGD:HD4	1.84	0.43
29:G:1623:NEX:H11	29:G:1623:NEX:H191	1.78	0.43
27:N:1621:LUT:H15	27:N:1621:LUT:H201	1.84	0.43
28:5:1622:XAT:H11	28:5:1622:XAT:H191	1.79	0.43
26:7:602:CLA:H93	26:7:602:CLA:H111	1.91	0.43
35:a:408:PHO:H42	30:d:409:LHG:H342	2.00	0.43
5:b:145:LEU:HD22	26:b:605:CLA:H18	2.00	0.43
6:c:28:GLN:HE22	7:d:231:ASN:HD22	1.65	0.43
1:g:131:GLN:OE1	25:g:607:CHL:HMC	2.19	0.43
16:o:125:PRO:HG2	16:o:225:ASP:HB3	2.00	0.43
19:r:81:GLN:HE21	26:r:616:CLA:HED3	1.83	0.43
19:r:203:ARG:HA	19:r:206:MET:HE3	2.00	0.43
4:A:304:GLN:HG2	4:A:313:VAL:HG11	2.00	0.43
6:C:117:LEU:HD12	37:Z:101:LMG:H202	2.00	0.43
6:C:120:ILE:HG23	24:Z:47:TRP:CH2	2.53	0.43
7:D:82:PRO:HD3	7:D:112:TRP:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:603:CLA:H2	26:Y:603:CLA:H61	1.75	0.43
4:a:337:HIS:CE1	7:d:353:LEU:HD11	2.54	0.43
26:b:614:CLA:H102	26:b:614:CLA:H62	1.81	0.43
6:c:217:PRO:HG3	39:c:518:DGD:HA71	2.01	0.43
26:n:602:CLA:H13	26:n:602:CLA:H172	1.83	0.43
17:p:30:VAL:HG11	17:p:49:TYR:CD2	2.53	0.43
26:3:613:CLA:H61	26:3:613:CLA:H2	1.77	0.43
4:A:337:HIS:CE1	7:D:353:LEU:HD11	2.54	0.43
31:A:411:BCR:H11C	31:A:411:BCR:H341	1.88	0.43
37:A:413:LMG:H352	6:C:217:PRO:HB3	2.01	0.43
36:A:418:SQD:H261	31:T:101:BCR:H333	2.00	0.43
5:B:313:ASP:OD2	5:B:358:ARG:NH2	2.32	0.43
26:N:613:CLA:H2	26:N:613:CLA:H61	1.61	0.43
28:N:1622:XAT:H31	28:N:1622:XAT:H391	1.81	0.43
16:O:185:LEU:HA	16:O:188:GLU:OE2	2.19	0.43
4:a:145:VAL:O	4:a:148:SER:OG	2.29	0.43
31:b:619:BCR:H361	31:b:619:BCR:H20C	1.87	0.43
37:b:622:LMG:HC91	15:m:6:LEU:HD22	2.01	0.43
26:c:502:CLA:HAB	26:c:502:CLA:HHC	1.81	0.43
26:g:603:CLA:HHC	26:g:603:CLA:HBB1	2.00	0.43
16:o:27:ASN:O	16:o:85:THR:OG1	2.33	0.43
17:p:75:GLY:O	17:p:127:TYR:OH	2.31	0.43
19:r:234:PRO:HB2	19:r:235:LEU:HD12	2.00	0.43
27:s:1620:LUT:H401	27:s:1620:LUT:H35	1.79	0.43
26:1:603:CLA:H8	26:3:602:CLA:H91	2.01	0.43
1:2:63:GLU:HA	1:2:155:LEU:HD11	2.00	0.43
4:A:308:ASP:HB2	8:E:52:PRO:O	2.19	0.43
5:B:362:PHE:HB3	7:D:189:PHE:HD2	1.83	0.43
1:G:131:GLN:OE1	25:G:607:CHL:HMC	2.19	0.43
2:7:152:ARG:NH2	25:7:609:CHL:O1D	2.52	0.43
4:a:228:THR:OG1	4:a:230:ASN:OD1	2.28	0.43
4:a:301:ASN:OD1	4:a:303:ASN:ND2	2.52	0.43
31:a:411:BCR:H15C	31:a:411:BCR:H351	1.86	0.43
6:c:28:GLN:HE21	7:d:234:ARG:HE	1.67	0.43
26:g:603:CLA:H42	26:y:603:CLA:H41	2.01	0.43
26:n:613:CLA:H2	26:n:613:CLA:H61	1.61	0.43
25:r:606:CHL:H92	25:r:606:CHL:H112	1.93	0.43
26:y:603:CLA:H61	26:y:603:CLA:H2	1.75	0.43
4:A:56:PRO:HB2	16:O:123:ARG:NH2	2.34	0.42
36:A:418:SQD:H461	36:A:418:SQD:H92	2.01	0.42
31:D:404:BCR:H15C	31:D:404:BCR:H351	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:157:LEU:HD21	16:O:166:THR:HG23	2.01	0.42
17:P:114:LEU:HD11	17:P:132:LEU:HB2	2.01	0.42
19:R:135:TYR:HD1	26:R:604:CLA:HBA1	1.84	0.42
26:Y:602:CLA:CAB	27:Y:1621:LUT:H32	2.49	0.42
25:7:609:CHL:H91	25:7:609:CHL:H112	1.83	0.42
3:8:143:GLU:H	3:8:146:TYR:HB2	1.84	0.42
26:b:612:CLA:H2	26:b:612:CLA:H61	1.69	0.42
26:b:613:CLA:H13	26:b:614:CLA:HBB2	2.01	0.42
31:b:619:BCR:HC42	37:b:622:LMG:H341	2.01	0.42
31:c:517:BCR:H15C	31:c:517:BCR:H351	1.81	0.42
7:d:82:PRO:HD3	7:d:112:TRP:HB3	2.01	0.42
4:A:131:TRP:CZ3	26:C:505:CLA:HAA2	2.54	0.42
5:B:110:ALA:HB2	31:B:620:BCR:H17C	2.01	0.42
5:B:145:LEU:HD22	26:B:605:CLA:H18	2.00	0.42
31:B:619:BCR:HC42	37:B:622:LMG:H341	2.01	0.42
7:D:49:TRP:HA	7:D:79:VAL:HG21	2.00	0.42
1:N:46:TRP:CE3	27:N:1621:LUT:H383	2.54	0.42
19:R:174:PRO:HB3	25:R:608:CHL:HBC2	2.00	0.42
20:S:185:LEU:HD23	20:S:188:LYS:HD2	2.01	0.42
31:T:101:BCR:H341	31:T:101:BCR:H11C	1.75	0.42
26:7:614:CLA:CBB	25:r:614:CHL:HAB	2.49	0.42
4:a:254:TYR:HE2	7:d:143:ASN:HD22	1.65	0.42
4:a:269:ARG:NH2	7:d:235:ALA:HB3	2.33	0.42
4:a:308:ASP:HB2	8:e:52:PRO:O	2.19	0.42
26:b:613:CLA:H61	26:b:613:CLA:H102	1.81	0.42
29:1:1623:NEX:H15	29:1:1623:NEX:H201	1.84	0.42
26:3:614:CLA:CBB	25:R:614:CHL:HAB	2.49	0.42
5:B:325:PHE:CG	14:L:35:TYR:HB3	2.55	0.42
6:C:28:GLN:HE22	7:D:231:ASN:HD22	1.65	0.42
6:C:28:GLN:HE21	7:D:234:ARG:HE	1.67	0.42
7:D:194:LEU:O	14:L:35:TYR:OH	2.28	0.42
26:R:602:CLA:H101	28:R:622:XAT:H371	2.02	0.42
28:Y:1622:XAT:H31	28:Y:1622:XAT:H391	1.73	0.42
27:5:1621:LUT:H35	27:5:1621:LUT:H401	1.87	0.42
5:b:18:ARG:HG3	5:b:118:TRP:HB3	2.02	0.42
5:b:325:PHE:CG	14:l:35:TYR:HB3	2.55	0.42
30:d:409:LHG:H181	21:t:17:ILE:HD11	2.00	0.42
25:g:607:CHL:HBB1	27:g:1621:LUT:H161	2.01	0.42
29:r:623:NEX:H35	29:r:623:NEX:H401	1.87	0.42
30:s:2630:LHG:H172	30:s:2630:LHG:H201	1.85	0.42
26:y:602:CLA:CAB	27:y:1621:LUT:H32	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:607:CHL:H91	25:2:607:CHL:H112	1.80	0.42
31:4:623:BCR:H11C	31:4:623:BCR:H341	1.69	0.42
4:A:166:GLY:HA3	6:C:358:PHE:CE1	2.54	0.42
4:A:194:MET:HE1	7:D:75:LEU:HB3	2.01	0.42
6:C:84:GLN:HB2	6:C:86:LEU:HG	2.02	0.42
31:C:514:BCR:H15C	31:C:514:BCR:H351	1.79	0.42
30:D:409:LHG:H181	21:T:17:ILE:HD11	2.00	0.42
25:G:607:CHL:HBB1	27:G:1621:LUT:H161	2.01	0.42
31:H:101:BCR:H11C	31:H:101:BCR:H341	1.82	0.42
31:H:101:BCR:H292	23:X:45:ALA:HB1	2.00	0.42
26:N:603:CLA:C3D	25:N:609:CHL:H2	2.49	0.42
26:R:609:CLA:HHC	26:R:609:CLA:HBB1	2.00	0.42
26:5:603:CLA:H8	26:7:602:CLA:H91	2.01	0.42
29:5:1623:NEX:H11	29:5:1623:NEX:H191	1.88	0.42
25:8:601:CHL:H3A	25:8:601:CHL:HBA1	1.66	0.42
4:a:38:ILE:HA	36:a:418:SQD:H171	2.02	0.42
36:a:418:SQD:H461	36:a:418:SQD:H92	2.01	0.42
5:b:110:ALA:HB2	31:b:620:BCR:H17C	2.01	0.42
26:b:603:CLA:H41	26:b:603:CLA:H62	1.84	0.42
31:b:619:BCR:H15C	31:b:619:BCR:H351	1.78	0.42
26:n:610:CLA:H92	26:n:610:CLA:H61	1.83	0.42
26:n:611:CLA:H92	26:n:611:CLA:H61	1.80	0.42
19:r:174:PRO:HB3	25:r:608:CHL:HBC2	1.99	0.42
26:r:609:CLA:HHC	26:r:609:CLA:HBB1	2.00	0.42
28:r:622:XAT:H35	28:r:622:XAT:H401	1.77	0.42
26:y:611:CLA:HHC	26:y:611:CLA:HBB1	2.01	0.42
27:1:1621:LUT:H15	27:1:1621:LUT:H201	1.79	0.42
28:3:1622:XAT:H11	28:3:1622:XAT:H191	1.88	0.42
4:A:269:ARG:NH2	7:D:235:ALA:HB3	2.33	0.42
31:A:411:BCR:H15C	31:A:411:BCR:H351	1.86	0.42
26:B:609:CLA:H192	10:H:58:LEU:CD2	2.50	0.42
26:B:616:CLA:H61	26:B:616:CLA:H2	1.78	0.42
26:a:405:CLA:H171	26:a:406:CLA:H111	2.01	0.42
6:c:418:ASN:HD21	39:c:519:DGD:HD4	1.84	0.42
1:g:104:ILE:HG21	1:g:124:ILE:HD13	1.99	0.42
25:g:601:CHL:HHB	25:y:609:CHL:HMB3	2.02	0.42
16:o:78:LEU:HB3	22:w:3:ASP:OD2	2.19	0.42
16:o:170:ASN:ND2	16:o:181:ASP:OD1	2.51	0.42
26:y:602:CLA:H193	26:y:602:CLA:H161	1.78	0.42
28:2:1622:XAT:H15	28:2:1622:XAT:H201	1.79	0.42
27:3:1621:LUT:H35	27:3:1621:LUT:H401	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:143:GLU:H	3:4:146:TYR:HB2	1.84	0.42
4:A:301:ASN:OD1	4:A:303:ASN:ND2	2.52	0.42
4:A:341:LEU:N	6:C:313:GLN:HE22	2.17	0.42
5:B:496:GLN:HE22	23:X:82:LYS:HG3	1.84	0.42
31:B:620:BCR:H15C	31:B:620:BCR:H351	1.82	0.42
6:C:217:PRO:HG3	39:C:518:DGD:HA71	2.01	0.42
13:K:33:LEU:HD22	13:K:36:ILE:HD11	2.01	0.42
26:N:613:CLA:H91	30:N:2630:LHG:H321	2.01	0.42
19:R:234:PRO:HB2	19:R:235:LEU:HD12	2.00	0.42
28:Y:1622:XAT:H15	28:Y:1622:XAT:H201	1.76	0.42
2:7:121:ASP:OD1	2:7:130:HIS:ND1	2.36	0.42
4:a:194:MET:HE1	7:d:75:LEU:HB3	2.01	0.42
26:b:614:CLA:H41	26:b:614:CLA:H61	1.68	0.42
1:n:46:TRP:CE3	27:n:1621:LUT:H383	2.54	0.42
26:r:602:CLA:H101	28:r:622:XAT:H371	2.02	0.42
3:4:60:TRP:CE2	25:4:608:CHL:HED2	2.55	0.42
31:4:623:BCR:H15C	31:4:623:BCR:H351	1.72	0.42
4:A:202:VAL:HA	4:A:205:VAL:HG22	2.01	0.42
5:B:155:ALA:O	5:B:159:THR:OG1	2.36	0.42
26:B:604:CLA:H62	26:B:604:CLA:H41	1.80	0.42
26:N:610:CLA:H41	26:N:610:CLA:H62	1.71	0.42
27:Y:1621:LUT:H35	27:Y:1621:LUT:H401	1.80	0.42
2:7:51:GLY:O	2:7:196:ARG:NH2	2.41	0.42
3:8:60:TRP:CE2	25:8:608:CHL:HED2	2.55	0.42
4:a:166:GLY:HA3	6:c:358:PHE:CE1	2.54	0.42
26:b:609:CLA:H192	10:h:58:LEU:CD2	2.50	0.42
31:h:101:BCR:H292	23:x:45:ALA:HB1	2.00	0.42
16:o:20:VAL:HG13	16:o:25:THR:HB	2.01	0.42
26:r:613:CLA:H91	26:r:613:CLA:H112	1.82	0.42
4:A:46:SER:HB3	39:b:626:DGD:HBN2	2.02	0.42
36:A:418:SQD:C22	31:T:101:BCR:H323	2.50	0.42
26:B:608:CLA:H93	26:B:608:CLA:H62	1.83	0.42
26:B:613:CLA:H13	26:B:614:CLA:HBB2	2.01	0.42
25:G:601:CHL:HHB	25:Y:609:CHL:HMB3	2.02	0.42
16:O:20:VAL:HG13	16:O:25:THR:HB	2.01	0.42
18:Q:44:PRO:HA	18:Q:47:ALA:HB3	2.01	0.42
19:R:21:PRO:CD	19:R:24:LEU:HD13	2.47	0.42
26:S:610:CLA:H43	26:S:612:CLA:HBA1	2.02	0.42
29:S:1623:NEX:H15	29:S:1623:NEX:H201	1.79	0.42
3:8:108:VAL:HG21	31:8:623:BCR:H16C	2.02	0.42
3:8:147:PRO:HB3	25:8:608:CHL:HBC2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:74:SER:OG	5:b:94:GLU:OE2	2.37	0.42
7:d:94:TRP:HB2	23:x:53:ASN:HB3	2.01	0.42
16:o:185:LEU:HA	16:o:188:GLU:OE2	2.19	0.42
20:s:150:GLU:OE1	20:s:153:ARG:NH2	2.42	0.42
26:C:513:CLA:H102	31:C:514:BCR:H23C	2.02	0.42
1:G:21:ARG:NH2	1:G:36:LEU:O	2.53	0.42
26:G:611:CLA:H112	26:G:611:CLA:H91	1.86	0.42
26:R:601:CLA:HBA1	26:R:601:CLA:H3A	1.44	0.42
26:S:604:CLA:C1C	29:S:1623:NEX:H222	2.50	0.42
29:5:1623:NEX:H15	29:5:1623:NEX:H201	1.85	0.42
31:8:623:BCR:H351	31:8:623:BCR:H15C	1.72	0.42
4:a:56:PRO:HB2	16:o:123:ARG:NH2	2.34	0.42
4:a:202:VAL:HA	4:a:205:VAL:HG22	2.01	0.42
5:b:400:GLU:OE1	5:b:410:THR:OG1	2.25	0.42
26:s:610:CLA:H43	26:s:612:CLA:HBA1	2.02	0.42
3:4:10:ILE:HG23	3:4:11:PRO:HD3	2.02	0.42
4:A:159:LEU:CD2	26:C:505:CLA:H202	2.49	0.42
5:B:218:SER:HA	19:R:86:VAL:HG21	2.02	0.42
6:C:321:ASP:OD2	6:C:340:TYR:OH	2.31	0.42
26:C:504:CLA:H143	26:C:504:CLA:H112	1.84	0.42
26:C:510:CLA:H162	26:C:510:CLA:H193	1.76	0.42
16:O:125:PRO:HG2	16:O:225:ASP:HB3	2.00	0.42
27:S:1620:LUT:H35	27:S:1620:LUT:H401	1.79	0.42
26:6:614:CLA:HBA1	26:6:614:CLA:H3A	1.86	0.42
5:b:496:GLN:HE22	23:x:82:LYS:HG3	1.84	0.42
31:b:620:BCR:H15C	31:b:620:BCR:H351	1.82	0.42
26:c:508:CLA:H161	26:c:508:CLA:H122	1.87	0.42
26:c:513:CLA:H11	31:c:514:BCR:H381	2.01	0.42
1:g:167:ALA:HB2	26:g:610:CLA:HAA1	2.01	0.42
29:n:1623:NEX:H15	29:n:1623:NEX:H201	1.75	0.42
16:o:157:LEU:HD21	16:o:166:THR:HG23	2.01	0.42
20:s:185:LEU:HD23	20:s:188:LYS:HD2	2.01	0.42
26:B:602:CLA:H12	26:B:602:CLA:H52	1.72	0.41
26:B:609:CLA:H192	10:H:58:LEU:HD23	2.02	0.41
27:G:1621:LUT:H35	27:G:1621:LUT:H401	1.82	0.41
16:O:27:ASN:O	16:O:85:THR:OG1	2.33	0.41
18:Q:32:PRO:HD2	18:Q:35:GLU:OE1	2.20	0.41
26:R:613:CLA:C1C	26:R:613:CLA:H51	2.50	0.41
3:8:167:ILE:HA	3:8:168:PRO:HD3	1.90	0.41
27:8:620:LUT:H15	27:8:620:LUT:H201	1.86	0.41
26:d:402:CLA:H142	26:d:402:CLA:H112	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:n:602:CLA:HBA1	27:n:1621:LUT:H382	2.02	0.41
19:r:21:PRO:HB2	19:r:24:LEU:CD1	2.50	0.41
20:s:154:ILE:HD11	26:s:609:CLA:CMA	2.50	0.41
1:1:175:GLU:HG2	1:1:179:LYS:HE3	2.01	0.41
27:2:1621:LUT:H15	27:2:1621:LUT:H201	1.80	0.41
29:2:1623:NEX:H15	29:2:1623:NEX:H201	1.83	0.41
5:B:18:ARG:HG3	5:B:118:TRP:HB3	2.02	0.41
26:C:513:CLA:H11	31:C:514:BCR:H381	2.01	0.41
30:D:409:LHG:H182	14:L:23:LEU:HD11	2.02	0.41
9:F:39:ARG:NH2	17:P:16:THR:OG1	2.45	0.41
17:P:45:GLN:NE2	17:P:48:ARG:HB2	2.36	0.41
26:Y:611:CLA:HBB1	26:Y:611:CLA:HHC	2.01	0.41
1:5:175:GLU:HG2	1:5:179:LYS:HE3	2.01	0.41
26:c:513:CLA:H102	31:c:514:BCR:H23C	2.02	0.41
31:c:515:BCR:H15C	31:c:515:BCR:H351	1.81	0.41
25:g:608:CHL:H202	26:g:610:CLA:H161	2.02	0.41
18:q:44:PRO:HA	18:q:47:ALA:HB3	2.01	0.41
19:r:133:SER:O	19:r:140:LEU:N	2.35	0.41
19:r:135:TYR:HD1	26:r:604:CLA:HBA1	1.84	0.41
2:3:145:MET:HA	2:3:148:VAL:HG22	2.01	0.41
5:B:74:SER:OG	5:B:94:GLU:OE2	2.37	0.41
26:B:603:CLA:H62	26:B:603:CLA:H41	1.84	0.41
6:C:390:ARG:HH12	18:Q:25:GLU:HB2	1.86	0.41
31:C:517:BCR:H20C	31:C:517:BCR:H361	1.89	0.41
1:G:212:HIS:CG	26:G:613:CLA:HAA2	2.55	0.41
26:G:603:CLA:H42	26:Y:603:CLA:H41	2.01	0.41
26:Y:602:CLA:H13	26:Y:602:CLA:H172	1.64	0.41
28:Y:1622:XAT:H35	28:Y:1622:XAT:H401	1.86	0.41
29:7:1623:NEX:H11	29:7:1623:NEX:H191	1.75	0.41
4:a:131:TRP:CZ3	26:c:505:CLA:HAA2	2.54	0.41
4:a:213:ALA:HB2	7:d:276:PRO:HG2	2.02	0.41
5:b:243:ALA:HA	5:b:246:PHE:CE2	2.56	0.41
25:g:607:CHL:H143	25:g:607:CHL:H111	1.72	0.41
1:n:25:LEU:HB2	1:n:29:SER:HA	2.02	0.41
26:n:613:CLA:H91	30:n:2630:LHG:H321	2.01	0.41
16:o:49:LYS:HE2	16:o:50:LYS:HZ3	1.86	0.41
2:3:193:LYS:HZ1	30:3:2630:LHG:P	2.43	0.41
4:A:143:ILE:HG13	7:D:221:ASN:ND2	2.34	0.41
4:A:213:ALA:HB2	7:D:276:PRO:HG2	2.02	0.41
4:A:286:THR:HG21	26:A:405:CLA:HMA3	2.03	0.41
7:D:94:TRP:HB2	23:X:53:ASN:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:D:409:LHG:C18	21:T:17:ILE:HD11	2.50	0.41
10:H:30:TYR:CE1	19:R:50:LEU:HG	2.55	0.41
30:R:2630:LHG:H102	30:R:2630:LHG:H281	2.02	0.41
26:S:613:CLA:H61	26:S:613:CLA:H2	1.74	0.41
36:a:418:SQD:C22	31:t:101:BCR:H323	2.50	0.41
26:b:603:CLA:H111	26:b:603:CLA:H91	1.82	0.41
6:c:259:TRP:HH2	26:c:507:CLA:H201	1.85	0.41
10:h:30:TYR:CE1	19:r:50:LEU:HG	2.55	0.41
26:n:602:CLA:H101	27:n:1621:LUT:H371	2.02	0.41
25:n:607:CHL:H62	25:n:607:CHL:H2	1.56	0.41
25:n:607:CHL:H143	25:n:607:CHL:H111	1.71	0.41
26:n:610:CLA:H101	26:n:612:CLA:H142	2.01	0.41
26:r:613:CLA:C1C	26:r:613:CLA:H51	2.50	0.41
26:2:602:CLA:HBA1	27:2:1621:LUT:H382	2.02	0.41
3:4:175:ARG:NH1	26:4:612:CLA:O1A	2.46	0.41
5:B:75:TRP:CE2	39:B:626:DGD:HG32	2.55	0.41
6:C:318:LEU:HD13	6:C:351:PHE:HE1	1.85	0.41
30:C:522:LHG:H192	26:Y:612:CLA:H101	2.03	0.41
26:G:602:CLA:H91	26:Y:603:CLA:H8	2.03	0.41
25:G:607:CHL:H203	25:G:607:CHL:H161	1.91	0.41
26:N:610:CLA:H101	26:N:612:CLA:H142	2.01	0.41
26:N:610:CLA:H141	26:N:610:CLA:H161	1.93	0.41
26:N:611:CLA:H61	26:N:611:CLA:H92	1.80	0.41
26:N:611:CLA:H43	26:N:612:CLA:HMD2	2.03	0.41
26:R:611:CLA:HBA2	26:R:611:CLA:H3A	1.57	0.41
4:a:257:ARG:HD2	5:b:498:LEU:HD21	2.01	0.41
6:c:97:TRP:NE1	37:z:101:LMG:H151	2.35	0.41
14:l:25:ILE:HD13	14:l:25:ILE:HA	1.91	0.41
26:n:610:CLA:HBB1	26:n:612:CLA:H3A	2.03	0.41
29:1:1623:NEX:H11	29:1:1623:NEX:H191	1.88	0.41
4:A:38:ILE:HA	36:A:418:SQD:H171	2.02	0.41
26:A:405:CLA:H171	26:A:406:CLA:H111	2.01	0.41
26:B:612:CLA:H92	26:B:612:CLA:H62	1.87	0.41
26:C:506:CLA:H143	26:C:506:CLA:H162	1.94	0.41
26:C:508:CLA:H161	26:C:508:CLA:H122	1.87	0.41
7:D:91:LEU:O	7:D:105:TRP:NE1	2.31	0.41
1:G:222:TRP:HB3	1:Y:105:PHE:HZ	1.85	0.41
25:G:608:CHL:H202	26:G:610:CLA:H161	2.02	0.41
31:H:101:BCR:H351	31:H:101:BCR:H15C	1.86	0.41
15:M:23:LEU:HD22	36:b:623:SQD:H101	2.03	0.41
20:S:55:GLY:O	20:S:194:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:154:ILE:HD11	26:S:609:CLA:CMA	2.50	0.41
26:b:603:CLA:H171	39:h:102:DGD:HAW1	2.02	0.41
6:c:390:ARG:HH12	18:q:25:GLU:HB2	1.86	0.41
30:d:409:LHG:C18	21:t:17:ILE:HD11	2.50	0.41
27:g:1621:LUT:H15	27:g:1621:LUT:H201	1.79	0.41
27:y:1621:LUT:H401	27:y:1621:LUT:H35	1.80	0.41
1:1:70:ARG:NH1	25:1:608:CHL:OBD	2.42	0.41
4:A:344:ALA:HB3	6:C:354:GLU:HB3	2.03	0.41
36:A:412:SQD:H131	30:D:410:LHG:H142	2.03	0.41
26:B:607:CLA:H142	26:B:607:CLA:H111	1.93	0.41
36:B:623:SQD:H101	15:m:23:LEU:HD22	2.01	0.41
26:G:610:CLA:H62	26:G:610:CLA:H41	1.91	0.41
26:N:602:CLA:H101	27:N:1621:LUT:H371	2.02	0.41
25:R:606:CHL:H8	29:R:623:NEX:H35	2.03	0.41
29:R:623:NEX:H15	29:R:623:NEX:H201	1.80	0.41
26:Y:613:CLA:H193	26:Y:613:CLA:H161	1.89	0.41
28:6:1622:XAT:H11	28:6:1622:XAT:H191	1.83	0.41
2:7:193:LYS:HZ1	30:7:2630:LHG:P	2.43	0.41
31:a:411:BCR:H371	31:a:411:BCR:H24C	1.88	0.41
37:a:413:LMG:H352	6:c:217:PRO:HB3	2.01	0.41
5:b:357:ARG:NH1	5:b:358:ARG:O	2.54	0.41
26:b:609:CLA:H192	10:h:58:LEU:HD23	2.02	0.41
6:c:318:LEU:HD13	6:c:351:PHE:HE1	1.85	0.41
26:d:402:CLA:H143	26:d:402:CLA:H161	1.90	0.41
31:d:404:BCR:H382	37:d:411:LMG:H341	2.02	0.41
13:k:33:LEU:HD22	13:k:36:ILE:HD11	2.01	0.41
18:q:32:PRO:HD2	18:q:35:GLU:OE1	2.20	0.41
19:r:147:LEU:HA	19:r:147:LEU:HD23	1.87	0.41
27:r:620:LUT:H15	27:r:620:LUT:H201	1.90	0.41
1:y:139:GLU:HG3	25:y:609:CHL:C4B	2.51	0.41
1:y:217:VAL:O	1:y:217:VAL:CG1	2.68	0.41
29:y:1623:NEX:H15	29:y:1623:NEX:H201	1.78	0.41
27:2:1620:LUT:H35	27:2:1620:LUT:H401	1.82	0.41
3:4:147:PRO:HB3	25:4:608:CHL:HBC2	2.01	0.41
26:A:405:CLA:HMC3	7:D:183:ILE:HG21	2.03	0.41
9:F:28:LEU:HD22	12:J:24:LEU:HD21	2.03	0.41
14:L:27:VAL:HG11	30:L:101:LHG:H201	2.02	0.41
17:P:124:LYS:HE3	17:P:152:LYS:HD2	2.03	0.41
3:8:10:ILE:HG23	3:8:11:PRO:HD3	2.02	0.41
5:b:75:TRP:CE2	39:b:626:DGD:HG32	2.55	0.41
26:b:611:CLA:H143	26:b:611:CLA:H162	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:194:PHE:CE1	27:g:1620:LUT:H41	2.55	0.41
17:p:124:LYS:HE3	17:p:152:LYS:HD2	2.03	0.41
18:q:59:VAL:O	18:q:133:TYR:OH	2.38	0.41
4:A:48:PHE:CD1	4:A:82:ILE:HD12	2.56	0.41
5:B:25:MET:HG2	31:B:618:BCR:H23C	2.03	0.41
26:B:603:CLA:H171	39:H:102:DGD:HAW1	2.02	0.41
6:C:97:TRP:NE1	37:Z:101:LMG:H151	2.36	0.41
29:G:1623:NEX:H15	29:G:1623:NEX:H201	1.80	0.41
27:N:1621:LUT:H35	27:N:1621:LUT:H401	1.88	0.41
30:N:2630:LHG:H341	30:N:2630:LHG:H312	1.81	0.41
17:P:47:LEU:HD13	17:P:49:TYR:HD1	1.86	0.41
17:P:87:LEU:HD11	17:P:158:ILE:HG21	2.02	0.41
25:5:607:CHL:H2	25:5:607:CHL:H62	1.88	0.41
4:a:269:ARG:NE	7:d:223:LEU:HD22	2.36	0.41
35:a:408:PHO:HBA2	35:a:408:PHO:H12	1.92	0.41
5:b:75:TRP:CZ2	39:b:626:DGD:HG11	2.56	0.41
31:b:619:BCR:H24C	31:b:619:BCR:H371	1.86	0.41
6:c:84:GLN:HB2	6:c:86:LEU:HG	2.02	0.41
30:d:410:LHG:O3	30:d:410:LHG:O1	2.34	0.41
1:g:130:THR:HB	42:g:664:HOH:O	2.19	0.41
25:g:607:CHL:H62	25:g:607:CHL:H2	1.70	0.41
25:g:607:CHL:H203	25:g:607:CHL:H161	1.91	0.41
31:h:101:BCR:H351	31:h:101:BCR:H15C	1.87	0.41
26:n:611:CLA:H43	26:n:612:CLA:HMD2	2.03	0.41
17:p:64:GLN:O	17:p:156:LEU:N	2.41	0.41
30:r:2630:LHG:H102	30:r:2630:LHG:H281	2.02	0.41
20:s:55:GLY:O	20:s:194:ARG:NH2	2.54	0.41
26:s:604:CLA:C1C	29:s:1623:NEX:H222	2.50	0.41
27:y:1620:LUT:H35	27:y:1620:LUT:H401	1.94	0.41
24:z:19:LEU:HD23	24:z:19:LEU:HA	1.94	0.41
37:z:101:LMG:H291	37:z:101:LMG:HC91	1.64	0.41
1:2:225:ALA:HB1	28:2:1622:XAT:H183	2.02	0.41
2:3:180:ASP:HA	2:3:181:PRO:HD3	1.93	0.41
6:C:203:THR:O	6:C:235:GLY:HA3	2.21	0.41
6:C:259:TRP:HH2	26:C:507:CLA:H201	1.85	0.41
31:D:404:BCR:H382	37:D:411:LMG:H341	2.02	0.41
25:G:601:CHL:H62	25:G:601:CHL:H41	1.88	0.41
25:G:607:CHL:H143	25:G:607:CHL:H111	1.72	0.41
1:N:25:LEU:HB2	1:N:29:SER:HA	2.02	0.41
16:O:76:THR:HG22	16:O:118:LEU:HD23	2.03	0.41
19:R:21:PRO:HB2	19:R:24:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:616:CLA:H3A	26:R:616:CLA:HBA2	1.65	0.41
1:Y:189:PHE:CE2	26:Y:613:CLA:HAB	2.57	0.41
1:Y:217:VAL:O	1:Y:217:VAL:CG1	2.68	0.41
26:Y:603:CLA:HBA1	26:Y:603:CLA:H3A	1.80	0.41
4:a:106:LEU:HD11	31:a:411:BCR:H292	2.03	0.41
36:a:418:SQD:H261	31:t:101:BCR:H333	2.00	0.41
5:b:218:SER:HA	19:r:86:VAL:HG21	2.02	0.41
6:c:405:ASN:HB3	39:c:520:DGD:HG2	2.02	0.41
17:p:47:LEU:HD13	17:p:49:TYR:HD1	1.86	0.41
26:r:602:CLA:CAB	28:r:622:XAT:H32	2.51	0.41
20:s:154:ILE:HG13	26:s:609:CLA:HMA1	2.03	0.41
1:1:181:LEU:HD23	1:1:181:LEU:HA	1.95	0.40
1:2:70:ARG:HA	1:2:73:MET:HE3	2.03	0.40
26:B:602:CLA:H142	26:B:602:CLA:H112	1.90	0.40
26:B:613:CLA:H122	26:B:613:CLA:H162	1.93	0.40
26:C:507:CLA:H142	31:C:515:BCR:H362	2.02	0.40
7:D:80:SER:HA	7:D:173:SER:HB3	2.03	0.40
20:S:154:ILE:HG13	26:S:609:CLA:HMA1	2.03	0.40
27:Y:1620:LUT:H15	27:Y:1620:LUT:H201	1.92	0.40
37:Z:101:LMG:HC91	37:Z:101:LMG:H291	1.64	0.40
28:5:1622:XAT:H201	28:5:1622:XAT:H15	1.73	0.40
26:6:602:CLA:HBA1	27:6:1621:LUT:H382	2.02	0.40
2:7:152:ARG:HH21	25:7:609:CHL:HMA3	1.86	0.40
2:7:193:LYS:NZ	30:7:2630:LHG:O5	2.52	0.40
31:8:623:BCR:H20C	31:8:623:BCR:H361	1.86	0.40
4:a:140:ARG:HH11	4:a:140:ARG:HD2	1.68	0.40
5:b:25:MET:HG2	31:b:618:BCR:H23C	2.03	0.40
26:b:610:CLA:HAB	26:b:610:CLA:HHC	1.85	0.40
31:c:514:BCR:H15C	31:c:514:BCR:H351	1.79	0.40
27:g:1620:LUT:H35	27:g:1620:LUT:H401	1.87	0.40
14:l:27:VAL:HG11	30:l:101:LHG:H201	2.02	0.40
17:p:45:GLN:NE2	17:p:48:ARG:HB2	2.35	0.40
17:p:87:LEU:HD11	17:p:158:ILE:HG21	2.02	0.40
25:r:606:CHL:H8	29:r:623:NEX:H35	2.03	0.40
1:1:66:VAL:HG22	1:1:181:LEU:HD21	2.04	0.40
28:1:1622:XAT:H35	28:1:1622:XAT:H401	1.89	0.40
2:3:33:TYR:CG	2:3:55:TRP:HB2	2.56	0.40
26:3:603:CLA:HBC1	25:3:609:CHL:HBC2	2.04	0.40
29:3:1623:NEX:H191	29:3:1623:NEX:H11	1.75	0.40
3:4:108:VAL:HG21	31:4:623:BCR:H16C	2.02	0.40
4:A:140:ARG:HH22	30:D:410:LHG:HC41	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:C:519:DGD:HBN1	39:C:519:DGD:HBW1	1.85	0.40
7:D:22:TRP:CD1	7:D:25:ARG:HE	2.39	0.40
29:G:1623:NEX:H35	29:G:1623:NEX:H401	1.88	0.40
26:R:602:CLA:CAB	28:R:622:XAT:H32	2.51	0.40
1:6:70:ARG:HA	1:6:73:MET:HE3	2.03	0.40
5:b:216:HIS:HE1	26:b:610:CLA:C1A	2.35	0.40
6:c:203:THR:O	6:c:235:GLY:HA3	2.21	0.40
30:c:522:LHG:H192	26:y:612:CLA:H101	2.03	0.40
1:g:222:TRP:HB3	1:y:105:PHE:HZ	1.85	0.40
27:n:1620:LUT:H15	27:n:1620:LUT:H201	1.93	0.40
28:n:1622:XAT:H11	28:n:1622:XAT:H191	1.91	0.40
17:p:169:PHE:CB	18:q:27:ARG:HD3	2.52	0.40
26:s:604:CLA:HBA2	26:s:604:CLA:H3A	1.95	0.40
26:A:405:CLA:C19	30:D:409:LHG:H332	2.52	0.40
31:C:516:BCR:H19C	13:K:53:VAL:HG21	2.04	0.40
7:D:189:PHE:O	7:D:295:ARG:NE	2.55	0.40
25:G:605:CHL:H3A	25:G:605:CHL:HBA2	1.86	0.40
14:L:24:LEU:HB2	30:L:101:LHG:H162	2.03	0.40
1:N:185:ARG:HA	1:N:188:MET:HE3	2.03	0.40
17:P:169:PHE:CB	18:Q:27:ARG:HD3	2.52	0.40
26:R:604:CLA:C1C	29:R:623:NEX:H222	2.52	0.40
27:Y:1620:LUT:H31	27:Y:1620:LUT:H391	1.96	0.40
25:7:601:CHL:H92	25:7:601:CHL:H62	1.86	0.40
3:8:179:ALA:O	3:8:183:HIS:ND1	2.38	0.40
4:a:292:THR:HG22	6:c:428:THR:HB	2.03	0.40
26:a:405:CLA:C19	30:d:409:LHG:H332	2.52	0.40
1:g:51:LEU:HD13	26:g:602:CLA:H42	2.04	0.40
1:g:212:HIS:CG	26:g:613:CLA:HAA2	2.55	0.40
26:g:610:CLA:H13	26:g:610:CLA:H172	1.85	0.40
20:s:154:ILE:HD11	26:s:609:CLA:H3A	2.04	0.40
1:y:189:PHE:CE2	26:y:613:CLA:HAB	2.56	0.40
27:2:1620:LUT:H11	27:2:1620:LUT:H191	1.94	0.40
2:3:86:LEU:HB3	26:3:604:CLA:HMC2	2.03	0.40
4:A:104:GLU:OE2	4:A:108:ASN:ND2	2.55	0.40
4:A:269:ARG:NE	7:D:223:LEU:HD22	2.36	0.40
5:B:12:VAL:HG11	5:B:22:VAL:HG21	2.04	0.40
5:B:243:ALA:HA	5:B:246:PHE:CE2	2.56	0.40
6:C:346:THR:OG1	6:C:348:GLU:OE1	2.37	0.40
6:C:405:ASN:HB3	39:C:520:DGD:HG2	2.02	0.40
1:N:163:PRO:HD2	27:N:1620:LUT:H23	2.03	0.40
26:N:610:CLA:HBB1	26:N:612:CLA:H3A	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:93:ARG:HA	19:R:93:ARG:HD3	1.97	0.40
27:5:1621:LUT:H201	27:5:1621:LUT:H15	1.79	0.40
1:6:193:GLY:O	1:6:197:GLN:HG2	2.22	0.40
2:7:86:LEU:HB3	26:7:604:CLA:HMC2	2.03	0.40
4:a:48:PHE:CD1	4:a:82:ILE:HD12	2.56	0.40
5:b:39:LEU:HG	5:b:97:ALA:HB1	2.04	0.40
9:f:28:LEU:HD22	12:j:24:LEU:HD21	2.03	0.40
28:g:1622:XAT:H201	28:g:1622:XAT:H15	1.71	0.40
26:n:613:CLA:H121	28:n:1622:XAT:H34	2.03	0.40
28:n:1622:XAT:H31	28:n:1622:XAT:H391	1.81	0.40
16:o:141:SER:OG	16:o:201:THR:OG1	2.39	0.40
26:s:610:CLA:H62	26:s:610:CLA:H41	1.98	0.40
27:y:1621:LUT:H201	27:y:1621:LUT:H15	1.81	0.40
26:1:602:CLA:H93	26:1:602:CLA:H111	1.91	0.40
1:2:153:ASP:OD2	1:2:156:TYR:N	2.53	0.40
2:3:128:LEU:HD23	25:3:605:CHL:HED2	2.03	0.40
26:3:611:CLA:C1B	30:3:2630:LHG:HC31	2.52	0.40
4:A:49:ILE:HG23	38:D:405:PL9:H501	2.04	0.40
4:A:214:MET:HE2	4:A:255:PHE:HE1	1.87	0.40
5:B:75:TRP:CZ2	39:B:626:DGD:HG11	2.56	0.40
6:C:87:ILE:O	6:C:91:HIS:ND1	2.55	0.40
6:C:146:PHE:HB3	30:C:2630:LHG:HC12	2.03	0.40
26:N:603:CLA:HAC2	25:N:607:CHL:H18	2.04	0.40
18:Q:59:VAL:O	18:Q:133:TYR:OH	2.38	0.40
25:S:607:CHL:H91	25:S:607:CHL:H112	1.92	0.40
27:6:1620:LUT:H401	27:6:1620:LUT:H35	1.82	0.40
27:6:1621:LUT:H35	27:6:1621:LUT:H401	1.85	0.40
4:a:344:ALA:HB3	6:c:354:GLU:HB3	2.03	0.40
5:b:18:ARG:O	5:b:21:SER:HB3	2.22	0.40
31:c:517:BCR:H24C	31:c:517:BCR:H371	1.72	0.40
25:g:601:CHL:H112	25:g:601:CHL:H91	1.74	0.40
20:s:104:ASN:HB3	20:s:128:GLY:HA2	2.03	0.40
26:y:613:CLA:H2	26:y:613:CLA:H61	1.66	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	1	217/232 (94%)	209 (96%)	8 (4%)	0	100	100
1	2	216/232 (93%)	210 (97%)	5 (2%)	1 (0%)	24	48
1	5	217/232 (94%)	209 (96%)	8 (4%)	0	100	100
1	6	216/232 (93%)	210 (97%)	5 (2%)	1 (0%)	24	48
1	G	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
1	N	217/232 (94%)	214 (99%)	3 (1%)	0	100	100
1	Y	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
1	g	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
1	n	217/232 (94%)	214 (99%)	3 (1%)	0	100	100
1	y	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
2	3	218/243 (90%)	209 (96%)	9 (4%)	0	100	100
2	7	218/243 (90%)	209 (96%)	9 (4%)	0	100	100
3	4	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
3	8	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
4	A	332/344 (96%)	326 (98%)	6 (2%)	0	100	100
4	a	332/344 (96%)	326 (98%)	6 (2%)	0	100	100
5	B	501/507 (99%)	493 (98%)	8 (2%)	0	100	100
5	b	501/507 (99%)	493 (98%)	8 (2%)	0	100	100
6	C	448/473 (95%)	441 (98%)	7 (2%)	0	100	100
6	c	448/473 (95%)	442 (99%)	6 (1%)	0	100	100
7	D	339/353 (96%)	335 (99%)	4 (1%)	0	100	100
7	d	339/353 (96%)	335 (99%)	4 (1%)	0	100	100
8	E	73/83 (88%)	73 (100%)	0	0	100	100
8	e	73/83 (88%)	73 (100%)	0	0	100	100
9	F	28/39 (72%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	f	28/39 (72%)	28 (100%)	0	0	100	100
10	H	58/73 (80%)	58 (100%)	0	0	100	100
10	h	58/73 (80%)	58 (100%)	0	0	100	100
11	I	32/36 (89%)	32 (100%)	0	0	100	100
11	i	32/36 (89%)	32 (100%)	0	0	100	100
12	J	33/40 (82%)	33 (100%)	0	0	100	100
12	j	33/40 (82%)	33 (100%)	0	0	100	100
13	K	35/61 (57%)	35 (100%)	0	0	100	100
13	k	35/61 (57%)	35 (100%)	0	0	100	100
14	L	35/38 (92%)	35 (100%)	0	0	100	100
14	l	35/38 (92%)	35 (100%)	0	0	100	100
15	M	31/34 (91%)	29 (94%)	2 (6%)	0	100	100
15	m	31/34 (91%)	29 (94%)	2 (6%)	0	100	100
16	O	246/248 (99%)	240 (98%)	6 (2%)	0	100	100
16	o	246/248 (99%)	240 (98%)	6 (2%)	0	100	100
17	P	184/186 (99%)	183 (100%)	1 (0%)	0	100	100
17	p	184/186 (99%)	183 (100%)	1 (0%)	0	100	100
18	Q	127/148 (86%)	125 (98%)	2 (2%)	0	100	100
18	q	127/148 (86%)	125 (98%)	2 (2%)	0	100	100
19	R	232/246 (94%)	228 (98%)	4 (2%)	0	100	100
19	r	232/246 (94%)	228 (98%)	4 (2%)	0	100	100
20	S	216/244 (88%)	209 (97%)	7 (3%)	0	100	100
20	s	216/244 (88%)	208 (96%)	8 (4%)	0	100	100
21	T	30/35 (86%)	30 (100%)	0	0	100	100
21	t	30/35 (86%)	30 (100%)	0	0	100	100
22	W	52/54 (96%)	52 (100%)	0	0	100	100
22	w	52/54 (96%)	52 (100%)	0	0	100	100
23	X	37/86 (43%)	36 (97%)	1 (3%)	0	100	100
23	x	37/86 (43%)	36 (97%)	1 (3%)	0	100	100
24	Z	60/62 (97%)	60 (100%)	0	0	100	100
24	z	60/62 (97%)	60 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	9248/10006 (92%)	9056 (98%)	190 (2%)	2 (0%)	100 100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	119	VAL
1	6	119	VAL

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	1	171/182 (94%)	171 (100%)	0	100 100
1	2	171/182 (94%)	171 (100%)	0	100 100
1	5	171/182 (94%)	171 (100%)	0	100 100
1	6	171/182 (94%)	171 (100%)	0	100 100
1	G	171/182 (94%)	171 (100%)	0	100 100
1	N	171/182 (94%)	171 (100%)	0	100 100
1	Y	171/182 (94%)	171 (100%)	0	100 100
1	g	171/182 (94%)	171 (100%)	0	100 100
1	n	171/182 (94%)	171 (100%)	0	100 100
1	y	171/182 (94%)	171 (100%)	0	100 100
2	3	175/193 (91%)	175 (100%)	0	100 100
2	7	175/193 (91%)	175 (100%)	0	100 100
3	4	154/162 (95%)	154 (100%)	0	100 100
3	8	154/162 (95%)	154 (100%)	0	100 100
4	A	270/279 (97%)	270 (100%)	0	100 100
4	a	270/279 (97%)	270 (100%)	0	100 100
5	B	400/403 (99%)	399 (100%)	1 (0%)	86 94
5	b	400/403 (99%)	399 (100%)	1 (0%)	86 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	C	352/373 (94%)	351 (100%)	1 (0%)	86	94
6	c	352/373 (94%)	351 (100%)	1 (0%)	86	94
7	D	275/285 (96%)	274 (100%)	1 (0%)	84	93
7	d	275/285 (96%)	274 (100%)	1 (0%)	84	93
8	E	67/73 (92%)	67 (100%)	0	100	100
8	e	67/73 (92%)	67 (100%)	0	100	100
9	F	25/34 (74%)	25 (100%)	0	100	100
9	f	25/34 (74%)	25 (100%)	0	100	100
10	H	49/61 (80%)	49 (100%)	0	100	100
10	h	49/61 (80%)	49 (100%)	0	100	100
11	I	31/33 (94%)	31 (100%)	0	100	100
11	i	31/33 (94%)	31 (100%)	0	100	100
12	J	26/30 (87%)	26 (100%)	0	100	100
12	j	26/30 (87%)	26 (100%)	0	100	100
13	K	32/54 (59%)	32 (100%)	0	100	100
13	k	32/54 (59%)	32 (100%)	0	100	100
14	L	35/36 (97%)	35 (100%)	0	100	100
14	l	35/36 (97%)	35 (100%)	0	100	100
15	M	29/30 (97%)	29 (100%)	0	100	100
15	m	29/30 (97%)	29 (100%)	0	100	100
16	O	204/204 (100%)	204 (100%)	0	100	100
16	o	204/204 (100%)	204 (100%)	0	100	100
17	P	150/150 (100%)	150 (100%)	0	100	100
17	p	150/150 (100%)	150 (100%)	0	100	100
18	Q	112/125 (90%)	112 (100%)	0	100	100
18	q	112/125 (90%)	112 (100%)	0	100	100
19	R	191/202 (95%)	191 (100%)	0	100	100
19	r	191/202 (95%)	191 (100%)	0	100	100
20	S	170/190 (90%)	170 (100%)	0	100	100
20	s	170/190 (90%)	170 (100%)	0	100	100
21	T	29/32 (91%)	29 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	t	29/32 (91%)	29 (100%)	0	100 100
22	W	44/44 (100%)	44 (100%)	0	100 100
22	w	44/44 (100%)	44 (100%)	0	100 100
23	X	32/67 (48%)	32 (100%)	0	100 100
23	x	32/67 (48%)	32 (100%)	0	100 100
24	Z	54/54 (100%)	54 (100%)	0	100 100
24	z	54/54 (100%)	54 (100%)	0	100 100
All	All	7522/8048 (94%)	7516 (100%)	6 (0%)	87 96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	12	VAL
6	C	391	ARG
7	D	181	ARG
5	b	12	VAL
6	c	391	ARG
7	d	181	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	ASN
1	2	61	ASN
1	2	88	ASN
2	3	95	GLN
2	3	113	GLN
2	3	219	ASN
4	A	234	ASN
4	A	266	ASN
4	A	303	ASN
5	B	216	HIS
5	B	296	GLN
5	B	496	GLN
6	C	28	GLN
6	C	313	GLN
6	C	332	GLN
6	C	418	ASN

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Mol	Chain	Res	Type
7	D	84	ASN
7	D	143	ASN
7	D	221	ASN
7	D	256	GLN
7	D	264	ASN
7	D	351	ASN
1	G	122	GLN
16	O	74	GLN
16	O	190	ASN
17	P	112	ASN
18	Q	40	GLN
18	Q	75	ASN
18	Q	99	GLN
19	R	47	GLN
19	R	56	ASN
19	R	226	ASN
19	R	236	HIS
20	S	206	GLN
1	Y	88	ASN
1	5	61	ASN
1	6	61	ASN
1	6	88	ASN
2	7	95	GLN
2	7	113	GLN
2	7	219	ASN
4	a	234	ASN
4	a	266	ASN
4	a	303	ASN
5	b	216	HIS
5	b	296	GLN
5	b	496	GLN
6	c	28	GLN
6	c	313	GLN
6	c	332	GLN
6	c	418	ASN
7	d	84	ASN
7	d	143	ASN
7	d	221	ASN
7	d	256	GLN
7	d	264	ASN
7	d	351	ASN
1	g	122	GLN

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Mol	Chain	Res	Type
16	o	47	ASN
16	o	74	GLN
16	o	190	ASN
17	p	144	HIS
18	q	40	GLN
18	q	75	ASN
18	q	99	GLN
19	r	47	GLN
19	r	56	ASN
19	r	60	ASN
19	r	226	ASN
19	r	236	HIS
20	s	206	GLN
1	y	88	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 490 ligands modelled in this entry, 6 are monoatomic - leaving 484 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	$\#\|Z\|>2$
26	CLA	g	602	1	69,73,73	1.16	10 (14%)	82,113,113	1.42	10 (12%)
25	CHL	4	606	-	40,54,74	4.14	19 (47%)	34,90,114	2.90	16 (47%)
32	OEX	A	401	6,4	0,15,15	-	-	-		
26	CLA	C	511	6	69,73,73	1.15	10 (14%)	82,113,113	1.41	8 (9%)
38	PL9	d	405	-	55,55,55	1.76	13 (23%)	68,69,69	1.52	12 (17%)
30	LHG	N	2630	26	48,48,48	0.68	1 (2%)	51,54,54	1.32	6 (11%)
31	BCR	c	514	-	41,41,41	0.77	0	56,56,56	1.78	14 (25%)
26	CLA	6	614	1	49,53,73	1.38	7 (14%)	58,89,113	1.23	3 (5%)
28	XAT	Y	1622	-	41,47,47	0.96	2 (4%)	54,74,74	2.94	22 (40%)
30	LHG	D	410	-	42,42,48	0.70	1 (2%)	45,48,54	1.24	4 (8%)
26	CLA	R	612	19	53,57,73	1.32	7 (13%)	61,93,113	1.50	6 (9%)
26	CLA	G	612	1	64,68,73	1.19	7 (10%)	76,107,113	1.22	5 (6%)
25	CHL	1	608	-	40,54,74	4.04	19 (47%)	34,90,114	2.83	11 (32%)
25	CHL	8	607	-	40,54,74	4.12	19 (47%)	34,90,114	2.61	13 (38%)
26	CLA	b	612	5	69,73,73	1.22	8 (11%)	82,113,113	1.48	8 (9%)
25	CHL	5	607	-	57,71,74	3.43	19 (33%)	54,110,114	2.54	15 (27%)
25	CHL	7	609	2	55,69,74	3.47	20 (36%)	52,108,114	2.35	15 (28%)
25	CHL	6	601	1	40,54,74	4.09	18 (45%)	34,90,114	3.24	16 (47%)
31	BCR	A	411	-	41,41,41	0.67	0	56,56,56	1.81	14 (25%)
31	BCR	h	101	-	41,41,41	0.71	0	56,56,56	1.91	11 (19%)
25	CHL	N	608	42	60,74,74	3.27	19 (31%)	58,114,114	2.46	18 (31%)
26	CLA	1	610	1	60,64,73	1.21	8 (13%)	71,102,113	1.13	5 (7%)
28	XAT	G	1622	-	41,47,47	0.93	2 (4%)	54,74,74	2.80	22 (40%)
32	OEX	a	401	6,4	0,15,15	-	-	-		
26	CLA	s	613	20	59,63,73	1.23	8 (13%)	70,101,113	1.33	5 (7%)
31	BCR	D	404	-	41,41,41	0.71	0	56,56,56	1.86	12 (21%)
30	LHG	b	2631	-	48,48,48	0.69	2 (4%)	51,54,54	1.24	6 (11%)
29	NEX	r	623	-	40,46,46	1.10	3 (7%)	50,70,70	2.42	20 (40%)
25	CHL	1	606	-	40,54,74	3.98	19 (47%)	34,90,114	3.03	14 (41%)
25	CHL	4	609	3	40,54,74	4.11	19 (47%)	34,90,114	2.63	11 (32%)
26	CLA	A	407	42	54,58,73	1.25	7 (12%)	64,95,113	1.46	7 (10%)
26	CLA	B	611	42	69,73,73	1.16	9 (13%)	82,113,113	1.57	13 (15%)
26	CLA	Y	613	1	69,73,73	1.13	8 (11%)	82,113,113	1.31	7 (8%)
25	CHL	1	605	1	40,54,74	4.06	19 (47%)	34,90,114	3.05	15 (44%)
36	SQD	B	623	-	40,42,54	1.10	4 (10%)	50,53,65	1.72	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	XAT	5	1622	-	41,47,47	0.90	1 (2%)	54,74,74	2.62	21 (38%)
25	CHL	7	607	-	47,61,74	3.93	19 (40%)	41,98,114	2.22	14 (34%)
26	CLA	S	611	30	60,64,73	1.21	8 (13%)	71,102,113	1.36	6 (8%)
25	CHL	g	605	1	40,54,74	4.18	18 (45%)	34,90,114	3.04	11 (32%)
26	CLA	g	603	1	69,73,73	1.19	10 (14%)	82,113,113	1.47	10 (12%)
25	CHL	1	601	1	40,54,74	4.15	19 (47%)	34,90,114	2.78	15 (44%)
31	BCR	8	623	-	41,41,41	0.70	0	56,56,56	2.33	15 (26%)
30	LHG	L	101	-	48,48,48	0.94	1 (2%)	51,54,54	1.33	6 (11%)
26	CLA	s	602	20	65,69,73	1.18	10 (15%)	77,108,113	1.34	11 (14%)
25	CHL	s	607	42	52,66,74	3.49	18 (34%)	48,104,114	2.67	14 (29%)
26	CLA	r	612	19	53,57,73	1.32	8 (15%)	61,93,113	1.50	6 (9%)
31	BCR	T	101	-	41,41,41	0.69	0	56,56,56	2.58	19 (33%)
26	CLA	c	509	6	69,73,73	1.18	9 (13%)	82,113,113	1.55	11 (13%)
25	CHL	8	608	-	40,54,74	3.93	19 (47%)	34,90,114	2.90	13 (38%)
27	LUT	N	1621	-	42,43,43	0.80	1 (2%)	51,60,60	1.93	15 (29%)
38	PL9	D	405	-	55,55,55	1.77	13 (23%)	68,69,69	1.52	11 (16%)
31	BCR	C	514	-	41,41,41	0.77	0	56,56,56	1.78	14 (25%)
41	HEM	f	101	9,8	50,50,50	1.36	7 (14%)	67,82,82	1.10	4 (5%)
35	PHO	a	409	-	58,69,69	2.01	10 (17%)	55,99,99	1.70	11 (20%)
25	CHL	Y	606	42	44,58,74	3.53	18 (40%)	37,94,114	3.04	13 (35%)
26	CLA	C	506	6	69,73,73	1.16	8 (11%)	82,113,113	1.43	11 (13%)
25	CHL	5	608	-	40,54,74	4.04	19 (47%)	34,90,114	2.83	11 (32%)
26	CLA	R	602	19	64,68,73	1.15	9 (14%)	76,107,113	1.47	8 (10%)
26	CLA	S	604	42	54,58,73	1.30	10 (18%)	64,95,113	1.74	8 (12%)
26	CLA	B	605	5	69,73,73	1.35	9 (13%)	82,113,113	1.90	21 (25%)
26	CLA	2	614	1	49,53,73	1.38	6 (12%)	58,89,113	1.23	3 (5%)
30	LHG	g	2630	26	48,48,48	0.68	1 (2%)	51,54,54	1.30	6 (11%)
39	DGD	C	519	-	63,63,67	1.11	6 (9%)	77,77,81	1.46	12 (15%)
31	BCR	b	618	-	41,41,41	0.71	0	56,56,56	1.88	14 (25%)
26	CLA	4	611	30	49,53,73	1.38	7 (14%)	58,89,113	1.29	4 (6%)
31	BCR	b	619	-	41,41,41	0.69	0	56,56,56	1.83	17 (30%)
26	CLA	R	610	19	69,73,73	1.12	8 (11%)	82,113,113	1.24	9 (10%)
25	CHL	Y	608	42	60,74,74	3.18	19 (31%)	58,114,114	2.42	16 (27%)
30	LHG	4	2630	26	20,20,48	0.93	2 (10%)	23,26,54	1.34	2 (8%)
39	DGD	H	102	-	63,63,67	1.09	7 (11%)	77,77,81	1.40	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	b	606	5	69,73,73	1.25	10 (14%)	82,113,113	1.54	10 (12%)
30	LHG	C	523	-	48,48,48	0.66	2 (4%)	51,54,54	1.22	5 (9%)
26	CLA	G	611	30	64,68,73	1.25	9 (14%)	76,107,113	1.47	6 (7%)
25	CHL	y	601	1	60,74,74	3.24	20 (33%)	58,114,114	2.64	16 (27%)
25	CHL	7	606	-	40,54,74	3.93	19 (47%)	34,90,114	3.06	13 (38%)
25	CHL	G	607	42	60,74,74	3.34	19 (31%)	58,114,114	2.17	17 (29%)
25	CHL	2	605	1	40,54,74	4.16	18 (45%)	34,90,114	2.64	13 (38%)
39	DGD	c	518	-	56,56,67	1.18	6 (10%)	70,70,81	1.56	12 (17%)
26	CLA	3	610	2	64,68,73	1.20	8 (12%)	76,107,113	1.13	6 (7%)
26	CLA	B	615	5	69,73,73	1.13	8 (11%)	82,113,113	1.36	8 (9%)
26	CLA	s	611	30	60,64,73	1.21	8 (13%)	71,102,113	1.37	6 (8%)
26	CLA	4	603	3	49,53,73	1.39	9 (18%)	58,89,113	1.42	5 (8%)
26	CLA	G	602	1	69,73,73	1.16	10 (14%)	82,113,113	1.42	10 (12%)
31	BCR	t	101	-	41,41,41	0.69	0	56,56,56	2.58	19 (33%)
30	LHG	Y	2630	26	48,48,48	0.81	2 (4%)	51,54,54	1.25	6 (11%)
26	CLA	5	610	1	60,64,73	1.21	6 (10%)	71,102,113	1.13	5 (7%)
26	CLA	a	410	4	64,68,73	1.16	6 (9%)	76,107,113	1.53	8 (10%)
26	CLA	Y	602	1	69,73,73	1.16	8 (11%)	82,113,113	1.38	10 (12%)
26	CLA	g	612	1	64,68,73	1.20	7 (10%)	76,107,113	1.22	5 (6%)
26	CLA	C	503	6	69,73,73	1.18	10 (14%)	82,113,113	1.32	7 (8%)
26	CLA	a	405	4	69,73,73	1.26	9 (13%)	82,113,113	1.46	11 (13%)
26	CLA	g	611	30	64,68,73	1.26	9 (14%)	76,107,113	1.47	6 (7%)
26	CLA	n	603	1	69,73,73	1.21	9 (13%)	82,113,113	1.49	13 (15%)
26	CLA	B	612	5	69,73,73	1.22	8 (11%)	82,113,113	1.49	8 (9%)
25	CHL	s	601	20	40,54,74	4.10	19 (47%)	34,90,114	2.85	13 (38%)
27	LUT	5	1621	-	42,43,43	0.83	2 (4%)	51,60,60	1.76	15 (29%)
38	PL9	A	414	-	13,13,55	0.85	0	17,17,69	1.83	4 (23%)
26	CLA	R	611	30	53,57,73	1.30	9 (16%)	61,93,113	1.59	10 (16%)
26	CLA	c	504	42	69,73,73	1.12	12 (17%)	82,113,113	1.46	6 (7%)
37	LMG	Z	101	-	51,51,55	0.84	1 (1%)	59,59,63	1.32	5 (8%)
29	NEX	7	1623	-	40,46,46	0.95	2 (5%)	50,70,70	2.32	16 (32%)
29	NEX	Y	1623	-	40,46,46	1.04	3 (7%)	50,70,70	2.46	19 (38%)
27	LUT	2	1620	-	42,43,43	0.70	0	51,60,60	1.98	16 (31%)
30	LHG	G	2630	26	48,48,48	0.68	1 (2%)	51,54,54	1.30	6 (11%)
25	CHL	y	608	42	60,74,74	3.18	19 (31%)	58,114,114	2.42	16 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CHL	8	601	3	39,53,74	4.34	19 (48%)	33,89,114	2.02	10 (30%)
31	BCR	H	101	-	41,41,41	0.70	0	56,56,56	1.92	11 (19%)
27	LUT	S	1621	-	42,43,43	0.72	0	51,60,60	1.95	19 (37%)
26	CLA	r	604	42	52,56,73	1.28	9 (17%)	61,92,113	1.55	8 (13%)
30	LHG	B	2631	-	48,48,48	0.69	2 (4%)	51,54,54	1.24	6 (11%)
26	CLA	Y	614	1	52,56,73	1.29	9 (17%)	61,92,113	1.43	6 (9%)
26	CLA	B	614	5	69,73,73	1.19	8 (11%)	82,113,113	1.31	5 (6%)
30	LHG	7	2630	26	46,46,48	0.72	1 (2%)	49,52,54	1.27	5 (10%)
26	CLA	1	603	1	59,63,73	1.22	9 (15%)	70,101,113	1.41	5 (7%)
26	CLA	6	610	1	54,58,73	1.27	7 (12%)	64,95,113	1.19	6 (9%)
25	CHL	5	609	1	56,70,74	3.41	19 (33%)	53,109,114	2.26	14 (26%)
26	CLA	b	611	42	69,73,73	1.15	9 (13%)	82,113,113	1.57	13 (15%)
31	BCR	c	517	-	41,41,41	0.79	1 (2%)	56,56,56	2.12	11 (19%)
31	BCR	b	620	-	41,41,41	0.72	1 (2%)	56,56,56	2.00	18 (32%)
27	LUT	1	1620	-	42,43,43	0.70	0	51,60,60	1.88	15 (29%)
28	XAT	6	1622	-	41,47,47	0.91	1 (2%)	54,74,74	2.58	21 (38%)
29	NEX	N	1623	-	40,46,46	1.02	3 (7%)	50,70,70	2.28	16 (32%)
25	CHL	y	607	42	60,74,74	3.14	20 (33%)	58,114,114	2.21	14 (24%)
26	CLA	1	604	-	54,58,73	1.32	9 (16%)	64,95,113	1.33	9 (14%)
27	LUT	7	1621	-	42,43,43	0.81	1 (2%)	51,60,60	1.71	14 (27%)
25	CHL	Y	605	1	42,56,74	3.92	19 (45%)	36,92,114	2.77	11 (30%)
25	CHL	8	606	-	40,54,74	4.14	19 (47%)	34,90,114	2.90	16 (47%)
25	CHL	G	608	42	60,74,74	3.33	18 (30%)	58,114,114	2.37	17 (29%)
25	CHL	s	608	-	40,54,74	4.05	19 (47%)	34,90,114	2.27	9 (26%)
39	DGD	B	626	-	60,60,67	1.05	3 (5%)	74,74,81	1.40	12 (16%)
26	CLA	3	614	2	52,56,73	1.30	7 (13%)	61,92,113	1.15	5 (8%)
26	CLA	Y	611	30	64,68,73	1.21	7 (10%)	76,107,113	1.45	8 (10%)
25	CHL	S	606	42	40,54,74	4.21	18 (45%)	34,90,114	3.28	12 (35%)
36	SQD	b	623	-	40,42,54	1.10	4 (10%)	50,53,65	1.72	10 (20%)
25	CHL	5	606	-	40,54,74	3.97	19 (47%)	34,90,114	3.04	13 (38%)
26	CLA	c	511	6	69,73,73	1.15	10 (14%)	82,113,113	1.41	8 (9%)
31	BCR	B	620	-	41,41,41	0.72	1 (2%)	56,56,56	2.01	19 (33%)
25	CHL	N	607	42	60,74,74	3.16	19 (31%)	58,114,114	2.29	16 (27%)
25	CHL	6	609	1	55,69,74	3.50	20 (36%)	52,108,114	2.28	14 (26%)
26	CLA	N	604	42	54,58,73	1.38	9 (16%)	64,95,113	1.58	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	XAT	g	1622	-	41,47,47	0.93	2 (4%)	54,74,74	2.81	22 (40%)
26	CLA	c	510	6	69,73,73	1.16	6 (8%)	82,113,113	1.41	9 (10%)
25	CHL	7	601	2	58,72,74	3.37	19 (32%)	55,111,114	2.69	18 (32%)
26	CLA	2	612	1	49,53,73	1.40	7 (14%)	58,89,113	1.36	6 (10%)
26	CLA	3	612	2	49,53,73	1.36	8 (16%)	58,89,113	1.36	7 (12%)
25	CHL	5	601	1	40,54,74	4.15	19 (47%)	34,90,114	2.78	15 (44%)
30	LHG	C	522	-	48,48,48	0.71	1 (2%)	51,54,54	1.28	7 (13%)
30	LHG	s	2630	26	48,48,48	0.76	1 (2%)	51,54,54	1.28	7 (13%)
26	CLA	c	502	6	69,73,73	1.15	10 (14%)	82,113,113	1.56	9 (10%)
39	DGD	h	102	-	63,63,67	1.09	7 (11%)	77,77,81	1.41	10 (12%)
41	HEM	F	101	9,8	50,50,50	1.36	7 (14%)	67,82,82	1.10	4 (5%)
25	CHL	n	605	1	42,56,74	3.95	18 (42%)	36,92,114	3.13	14 (38%)
30	LHG	c	2630	-	48,48,48	0.68	1 (2%)	51,54,54	1.33	7 (13%)
28	XAT	r	622	-	41,47,47	0.93	2 (4%)	54,74,74	2.67	21 (38%)
26	CLA	2	610	1	54,58,73	1.26	7 (12%)	64,95,113	1.19	6 (9%)
25	CHL	r	607	42	50,64,74	3.56	19 (38%)	46,102,114	2.71	16 (34%)
26	CLA	c	512	6	69,73,73	1.15	9 (13%)	82,113,113	1.37	9 (10%)
26	CLA	G	610	1	68,72,73	1.16	7 (10%)	80,111,113	1.22	6 (7%)
26	CLA	d	403	7	69,73,73	1.11	7 (10%)	82,113,113	1.50	9 (10%)
26	CLA	a	407	42	54,58,73	1.25	7 (12%)	64,95,113	1.45	6 (9%)
26	CLA	C	504	42	69,73,73	1.12	12 (17%)	82,113,113	1.46	6 (7%)
30	LHG	d	408	-	45,45,48	0.81	1 (2%)	48,51,54	1.30	5 (10%)
38	PL9	a	414	-	13,13,55	0.85	0	17,17,69	1.84	4 (23%)
26	CLA	b	605	5	69,73,73	1.35	10 (14%)	82,113,113	1.90	21 (25%)
26	CLA	r	616	19	49,53,73	1.42	7 (14%)	58,89,113	1.31	3 (5%)
26	CLA	N	613	1	64,68,73	1.15	7 (10%)	76,107,113	1.42	5 (6%)
37	LMG	b	622	-	51,51,55	0.84	1 (1%)	59,59,63	1.30	4 (6%)
29	NEX	5	1623	-	40,46,46	1.02	3 (7%)	50,70,70	2.26	15 (30%)
27	LUT	G	1621	-	42,43,43	0.80	1 (2%)	51,60,60	2.00	16 (31%)
26	CLA	6	612	1	49,53,73	1.40	7 (14%)	58,89,113	1.36	6 (10%)
26	CLA	8	610	3	49,53,73	1.36	9 (18%)	58,89,113	1.15	4 (6%)
25	CHL	2	609	1	55,69,74	3.50	20 (36%)	52,108,114	2.28	14 (26%)
26	CLA	s	603	20	49,53,73	1.37	6 (12%)	58,89,113	1.72	9 (15%)
26	CLA	n	604	42	54,58,73	1.38	9 (16%)	64,95,113	1.58	11 (17%)
27	LUT	1	1621	-	42,43,43	0.84	2 (4%)	51,60,60	1.76	16 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	6	611	30	49,53,73	1.34	7 (14%)	58,89,113	1.35	5 (8%)
26	CLA	6	602	1	65,69,73	1.20	9 (13%)	77,108,113	1.18	6 (7%)
29	NEX	S	1623	-	40,46,46	1.02	3 (7%)	50,70,70	2.18	16 (32%)
37	LMG	c	521	-	51,51,55	0.80	3 (5%)	59,59,63	1.38	6 (10%)
25	CHL	g	608	42	60,74,74	3.32	18 (30%)	58,114,114	2.36	17 (29%)
26	CLA	N	610	1	69,73,73	1.12	7 (10%)	82,113,113	1.27	10 (12%)
26	CLA	A	405	4	69,73,73	1.26	9 (13%)	82,113,113	1.47	11 (13%)
25	CHL	Y	607	42	60,74,74	3.14	20 (33%)	58,114,114	2.22	14 (24%)
28	XAT	3	1622	-	41,47,47	0.92	1 (2%)	54,74,74	2.77	24 (44%)
25	CHL	8	609	3	40,54,74	4.11	19 (47%)	34,90,114	2.64	11 (32%)
25	CHL	N	606	42	44,58,74	3.84	18 (40%)	37,94,114	2.98	13 (35%)
26	CLA	R	603	19	64,68,73	1.16	7 (10%)	76,107,113	1.48	10 (13%)
26	CLA	c	501	6	69,73,73	1.13	7 (10%)	82,113,113	1.27	8 (9%)
27	LUT	S	1620	-	42,43,43	0.69	0	51,60,60	1.90	14 (27%)
26	CLA	c	513	6	69,73,73	1.10	7 (10%)	82,113,113	1.45	14 (17%)
26	CLA	8	612	3	49,53,73	1.37	6 (12%)	58,89,113	1.33	6 (10%)
40	BCT	D	401	33	3,3,3	1.18	0	2,3,3	4.24	2 (100%)
26	CLA	Y	610	1	64,68,73	1.20	9 (14%)	76,107,113	1.16	9 (11%)
26	CLA	C	502	6	69,73,73	1.16	10 (14%)	82,113,113	1.56	9 (10%)
25	CHL	r	608	42	55,69,74	3.33	19 (34%)	52,108,114	2.60	15 (28%)
26	CLA	S	612	20	53,57,73	1.28	7 (13%)	61,93,113	1.45	7 (11%)
26	CLA	b	613	5	69,73,73	1.24	7 (10%)	82,113,113	1.68	11 (13%)
25	CHL	S	607	42	52,66,74	3.49	18 (34%)	48,104,114	2.66	14 (29%)
26	CLA	2	603	1	59,63,73	1.25	9 (15%)	70,101,113	1.38	6 (8%)
27	LUT	6	1620	-	42,43,43	0.70	0	51,60,60	1.98	16 (31%)
37	LMG	A	415	-	40,40,55	0.86	0	48,48,63	1.29	6 (12%)
26	CLA	2	611	30	49,53,73	1.34	7 (14%)	58,89,113	1.36	5 (8%)
26	CLA	C	512	6	69,73,73	1.15	9 (13%)	82,113,113	1.38	9 (10%)
26	CLA	3	602	2	64,68,73	1.19	7 (10%)	76,107,113	1.18	9 (11%)
26	CLA	b	614	5	69,73,73	1.19	8 (11%)	82,113,113	1.31	5 (6%)
37	LMG	A	413	-	48,48,55	0.79	0	56,56,63	1.31	6 (10%)
26	CLA	D	403	7	69,73,73	1.11	7 (10%)	82,113,113	1.50	10 (12%)
26	CLA	5	613	1	59,63,73	1.26	8 (13%)	70,101,113	1.20	3 (4%)
27	LUT	y	1621	-	42,43,43	0.80	1 (2%)	51,60,60	1.82	13 (25%)
31	BCR	C	517	-	41,41,41	0.79	1 (2%)	56,56,56	2.11	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	C	507	42	69,73,73	1.19	11 (15%)	82,113,113	1.60	10 (12%)
26	CLA	7	614	2	52,56,73	1.30	7 (13%)	61,92,113	1.15	5 (8%)
30	LHG	r	2630	26	41,41,48	0.72	1 (2%)	44,47,54	1.29	6 (13%)
26	CLA	C	505	6	69,73,73	1.21	9 (13%)	82,113,113	1.60	9 (10%)
25	CHL	R	608	42	55,69,74	3.33	19 (34%)	52,108,114	2.60	15 (28%)
39	DGD	b	626	-	60,60,67	1.05	3 (5%)	74,74,81	1.40	12 (16%)
25	CHL	1	609	1	56,70,74	3.41	19 (33%)	53,109,114	2.26	14 (26%)
26	CLA	S	613	20	59,63,73	1.23	8 (13%)	70,101,113	1.33	5 (7%)
26	CLA	B	613	5	69,73,73	1.25	7 (10%)	82,113,113	1.67	11 (13%)
27	LUT	Y	1620	-	42,43,43	0.73	0	51,60,60	1.89	15 (29%)
26	CLA	7	610	2	64,68,73	1.20	8 (12%)	76,107,113	1.14	6 (7%)
26	CLA	5	604	-	54,58,73	1.32	9 (16%)	64,95,113	1.33	9 (14%)
26	CLA	7	612	2	49,53,73	1.35	8 (16%)	58,89,113	1.36	7 (12%)
30	LHG	B	2630	-	46,46,48	0.67	1 (2%)	49,52,54	1.30	6 (12%)
26	CLA	b	609	5	69,73,73	1.10	8 (11%)	82,113,113	1.49	8 (9%)
25	CHL	N	601	1	60,74,74	3.28	18 (30%)	58,114,114	2.67	17 (29%)
27	LUT	N	1620	-	42,43,43	0.70	0	51,60,60	1.84	13 (25%)
26	CLA	7	602	2	64,68,73	1.20	7 (10%)	76,107,113	1.18	9 (11%)
26	CLA	N	603	1	69,73,73	1.21	9 (13%)	82,113,113	1.49	13 (15%)
26	CLA	y	610	1	64,68,73	1.20	8 (12%)	76,107,113	1.16	10 (13%)
29	NEX	1	1623	-	40,46,46	1.03	3 (7%)	50,70,70	2.27	16 (32%)
26	CLA	n	612	1	64,68,73	1.21	7 (10%)	76,107,113	1.30	7 (9%)
26	CLA	c	508	6	69,73,73	1.19	8 (11%)	82,113,113	1.63	11 (13%)
26	CLA	4	612	3	49,53,73	1.36	6 (12%)	58,89,113	1.33	7 (12%)
26	CLA	D	402	7	69,73,73	1.28	8 (11%)	82,113,113	1.58	9 (10%)
26	CLA	G	604	42	54,58,73	1.38	8 (14%)	64,95,113	1.53	8 (12%)
25	CHL	R	607	42	50,64,74	3.57	19 (38%)	46,102,114	2.71	16 (34%)
26	CLA	3	611	30	59,63,73	1.28	9 (15%)	70,101,113	1.42	9 (12%)
39	DGD	c	519	-	63,63,67	1.11	6 (9%)	77,77,81	1.47	12 (15%)
31	BCR	c	516	-	41,41,41	0.70	0	56,56,56	2.01	16 (28%)
26	CLA	B	616	5	69,73,73	1.13	8 (11%)	82,113,113	1.35	9 (10%)
26	CLA	7	604	-	49,53,73	1.37	7 (14%)	58,89,113	1.29	6 (10%)
26	CLA	b	602	42	69,73,73	1.16	8 (11%)	82,113,113	1.30	6 (7%)
26	CLA	s	604	42	54,58,73	1.30	10 (18%)	64,95,113	1.75	9 (14%)
31	BCR	B	619	-	41,41,41	0.69	0	56,56,56	1.84	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	Y	603	1	69,73,73	1.21	9 (13%)	82,113,113	1.47	14 (17%)
27	LUT	6	1621	-	42,43,43	0.78	1 (2%)	51,60,60	1.79	15 (29%)
35	PHO	A	408	-	58,69,69	2.01	12 (20%)	55,99,99	1.66	11 (20%)
26	CLA	b	608	42	69,73,73	1.22	10 (14%)	82,113,113	1.52	9 (10%)
26	CLA	5	602	1	65,69,73	1.19	9 (13%)	77,108,113	1.17	7 (9%)
26	CLA	1	611	30	49,53,73	1.36	9 (18%)	58,89,113	1.24	4 (6%)
26	CLA	B	610	5	69,73,73	1.13	10 (14%)	82,113,113	1.46	9 (10%)
28	XAT	2	1622	-	41,47,47	0.92	2 (4%)	54,74,74	2.59	21 (38%)
30	LHG	1	2630	26	40,40,48	0.74	1 (2%)	43,46,54	1.36	6 (13%)
31	BCR	C	515	-	41,41,41	0.77	0	56,56,56	2.05	17 (30%)
30	LHG	l	101	-	48,48,48	0.94	1 (2%)	51,54,54	1.33	6 (11%)
25	CHL	y	606	42	44,58,74	3.53	18 (40%)	37,94,114	3.03	13 (35%)
26	CLA	R	604	42	52,56,73	1.28	9 (17%)	61,92,113	1.55	8 (13%)
31	BCR	a	411	-	41,41,41	0.67	0	56,56,56	1.81	14 (25%)
28	XAT	7	1622	-	41,47,47	0.92	1 (2%)	54,74,74	2.77	24 (44%)
28	XAT	4	622	-	41,47,47	0.90	2 (4%)	54,74,74	2.51	21 (38%)
26	CLA	r	609	19	62,66,73	1.20	7 (11%)	73,104,113	1.42	5 (6%)
26	CLA	7	613	2	62,66,73	1.21	8 (12%)	73,104,113	1.23	3 (4%)
26	CLA	N	614	1	52,56,73	1.29	5 (9%)	61,92,113	1.44	6 (9%)
26	CLA	8	603	3	49,53,73	1.39	9 (18%)	58,89,113	1.41	5 (8%)
29	NEX	y	1623	-	40,46,46	1.04	3 (7%)	50,70,70	2.46	19 (38%)
26	CLA	G	613	1	69,73,73	1.15	9 (13%)	82,113,113	1.24	5 (6%)
26	CLA	5	603	1	59,63,73	1.22	10 (16%)	70,101,113	1.41	5 (7%)
37	LMG	z	101	-	51,51,55	0.83	1 (1%)	59,59,63	1.33	6 (10%)
28	XAT	n	1622	-	41,47,47	0.89	1 (2%)	54,74,74	2.88	23 (42%)
25	CHL	n	608	42	60,74,74	3.27	19 (31%)	58,114,114	2.46	18 (31%)
25	CHL	n	601	1	60,74,74	3.28	18 (30%)	58,114,114	2.67	17 (29%)
30	LHG	d	409	-	48,48,48	0.79	1 (2%)	51,54,54	1.33	7 (13%)
26	CLA	A	410	4	64,68,73	1.15	6 (9%)	76,107,113	1.52	8 (10%)
35	PHO	A	409	-	58,69,69	2.01	9 (15%)	55,99,99	1.69	11 (20%)
25	CHL	g	607	42	60,74,74	3.34	19 (31%)	58,114,114	2.17	17 (29%)
30	LHG	C	2630	-	48,48,48	0.68	1 (2%)	51,54,54	1.33	7 (13%)
27	LUT	r	620	-	42,43,43	0.74	1 (2%)	51,60,60	1.98	15 (29%)
26	CLA	b	610	5	69,73,73	1.13	10 (14%)	82,113,113	1.46	9 (10%)
27	LUT	g	1620	-	42,43,43	0.69	0	51,60,60	1.82	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	SQD	B	621	-	52,54,54	0.94	2 (3%)	62,65,65	1.60	12 (19%)
25	CHL	s	606	42	40,54,74	4.21	18 (45%)	34,90,114	3.28	12 (35%)
28	XAT	8	622	-	41,47,47	0.91	2 (4%)	54,74,74	2.51	21 (38%)
26	CLA	B	607	5	69,73,73	1.20	10 (14%)	82,113,113	1.45	13 (15%)
29	NEX	3	1623	-	40,46,46	0.95	2 (5%)	50,70,70	2.32	16 (32%)
26	CLA	n	614	1	52,56,73	1.29	5 (9%)	61,92,113	1.45	6 (9%)
39	DGD	c	520	-	61,61,67	1.18	7 (11%)	75,75,81	1.46	12 (16%)
26	CLA	Y	604	42	54,58,73	1.35	8 (14%)	64,95,113	1.60	9 (14%)
26	CLA	S	614	20	53,57,73	1.25	6 (11%)	61,93,113	1.51	6 (9%)
26	CLA	A	406	42	69,73,73	1.13	8 (11%)	82,113,113	1.56	15 (18%)
29	NEX	G	1623	-	40,46,46	1.09	4 (10%)	50,70,70	2.27	14 (28%)
26	CLA	1	602	1	65,69,73	1.19	9 (13%)	77,108,113	1.17	7 (9%)
26	CLA	n	611	30	64,68,73	1.20	8 (12%)	76,107,113	1.35	5 (6%)
25	CHL	5	605	1	40,54,74	4.06	19 (47%)	34,90,114	3.05	15 (44%)
26	CLA	C	501	6	69,73,73	1.14	7 (10%)	82,113,113	1.27	8 (9%)
36	SQD	a	412	-	48,50,54	0.97	5 (10%)	58,61,65	1.70	10 (17%)
26	CLA	4	602	3	49,53,73	1.34	9 (18%)	58,89,113	1.40	5 (8%)
25	CHL	7	608	-	40,54,74	3.99	20 (50%)	34,90,114	2.98	15 (44%)
27	LUT	R	620	-	42,43,43	0.73	1 (2%)	51,60,60	1.98	15 (29%)
26	CLA	y	612	1	64,68,73	1.22	9 (14%)	76,107,113	1.32	5 (6%)
26	CLA	n	602	1	69,73,73	1.16	9 (13%)	82,113,113	1.40	11 (13%)
27	LUT	3	1621	-	42,43,43	0.80	1 (2%)	51,60,60	1.70	14 (27%)
26	CLA	R	616	19	49,53,73	1.42	8 (16%)	58,89,113	1.30	3 (5%)
26	CLA	B	603	5	69,73,73	1.14	9 (13%)	82,113,113	1.33	7 (8%)
28	XAT	1	1622	-	41,47,47	0.89	1 (2%)	54,74,74	2.62	21 (38%)
29	NEX	6	1623	-	40,46,46	1.02	3 (7%)	50,70,70	2.26	16 (32%)
30	LHG	b	2630	-	46,46,48	0.67	1 (2%)	49,52,54	1.30	6 (12%)
25	CHL	G	606	42	44,58,74	3.90	18 (40%)	37,94,114	2.86	15 (40%)
30	LHG	8	2630	26	20,20,48	0.93	2 (10%)	23,26,54	1.34	2 (8%)
27	LUT	2	1621	-	42,43,43	0.78	1 (2%)	51,60,60	1.79	15 (29%)
37	LMG	b	2633	-	55,55,55	0.78	2 (3%)	63,63,63	1.32	7 (11%)
26	CLA	y	614	1	52,56,73	1.29	9 (17%)	61,92,113	1.43	6 (9%)
30	LHG	5	2630	26	40,40,48	0.74	1 (2%)	43,46,54	1.36	6 (13%)
26	CLA	y	611	30	64,68,73	1.21	7 (10%)	76,107,113	1.45	8 (10%)
25	CHL	n	609	1	60,74,74	3.27	20 (33%)	58,114,114	2.42	17 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	LUT	y	1620	-	42,43,43	0.74	1 (2%)	51,60,60	1.89	15 (29%)
30	LHG	c	522	-	48,48,48	0.71	1 (2%)	51,54,54	1.28	6 (11%)
26	CLA	y	604	42	54,58,73	1.35	8 (14%)	64,95,113	1.60	7 (10%)
26	CLA	g	610	1	68,72,73	1.16	7 (10%)	80,111,113	1.21	6 (7%)
30	LHG	R	2630	26	41,41,48	0.72	1 (2%)	44,47,54	1.29	6 (13%)
25	CHL	7	605	2	40,54,74	4.18	19 (47%)	34,90,114	2.70	15 (44%)
26	CLA	7	603	2	59,63,73	1.22	9 (15%)	70,101,113	1.44	8 (11%)
26	CLA	8	602	3	49,53,73	1.34	8 (16%)	58,89,113	1.41	5 (8%)
26	CLA	C	509	6	69,73,73	1.18	9 (13%)	82,113,113	1.55	11 (13%)
36	SQD	b	621	-	52,54,54	0.93	2 (3%)	62,65,65	1.60	12 (19%)
26	CLA	b	607	5	69,73,73	1.20	10 (14%)	82,113,113	1.45	13 (15%)
26	CLA	b	616	5	69,73,73	1.13	8 (11%)	82,113,113	1.35	9 (10%)
26	CLA	G	603	1	69,73,73	1.18	10 (14%)	82,113,113	1.47	11 (13%)
25	CHL	G	609	1	55,69,74	3.43	20 (36%)	52,108,114	2.49	17 (32%)
26	CLA	S	602	20	65,69,73	1.18	10 (15%)	77,108,113	1.34	11 (14%)
26	CLA	6	604	-	49,53,73	1.37	8 (16%)	58,89,113	1.32	4 (6%)
26	CLA	B	608	42	69,73,73	1.22	9 (13%)	82,113,113	1.52	9 (10%)
25	CHL	2	606	-	40,54,74	4.09	19 (47%)	34,90,114	2.88	11 (32%)
37	LMG	a	415	-	40,40,55	0.86	0	48,48,63	1.29	6 (12%)
27	LUT	Y	1621	-	42,43,43	0.80	1 (2%)	51,60,60	1.82	13 (25%)
25	CHL	S	608	-	40,54,74	4.06	19 (47%)	34,90,114	2.28	8 (23%)
25	CHL	Y	601	1	60,74,74	3.24	19 (31%)	58,114,114	2.63	16 (27%)
26	CLA	5	614	1	49,53,73	1.36	7 (14%)	58,89,113	1.27	4 (6%)
39	DGD	C	520	-	61,61,67	1.18	7 (11%)	75,75,81	1.47	12 (16%)
26	CLA	n	613	1	64,68,73	1.16	7 (10%)	76,107,113	1.42	5 (6%)
26	CLA	c	506	6	69,73,73	1.17	8 (11%)	82,113,113	1.43	10 (12%)
37	LMG	B	622	-	51,51,55	0.84	1 (1%)	59,59,63	1.30	4 (6%)
26	CLA	8	604	-	49,53,73	1.36	8 (16%)	58,89,113	1.24	4 (6%)
28	XAT	y	1622	-	41,47,47	0.96	2 (4%)	54,74,74	2.95	22 (40%)
25	CHL	n	607	42	60,74,74	3.16	19 (31%)	58,114,114	2.29	16 (27%)
26	CLA	5	611	30	49,53,73	1.36	9 (18%)	58,89,113	1.25	4 (6%)
25	CHL	4	601	3	39,53,74	4.34	19 (48%)	33,89,114	2.01	10 (30%)
26	CLA	B	604	5	69,73,73	1.21	8 (11%)	82,113,113	1.33	11 (13%)
26	CLA	6	613	1	49,53,73	1.35	8 (16%)	58,89,113	1.23	3 (5%)
30	LHG	S	2630	26	48,48,48	0.76	1 (2%)	51,54,54	1.28	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	R	609	19	62,66,73	1.20	7 (11%)	73,104,113	1.41	5 (6%)
25	CHL	G	601	1	60,74,74	3.24	18 (30%)	58,114,114	2.71	18 (31%)
25	CHL	G	605	1	40,54,74	4.18	18 (45%)	34,90,114	3.04	12 (35%)
25	CHL	R	606	42	60,74,74	3.38	19 (31%)	58,114,114	2.55	16 (27%)
26	CLA	s	609	20	49,53,73	1.38	6 (12%)	58,89,113	1.23	6 (10%)
28	XAT	R	622	-	41,47,47	0.92	2 (4%)	54,74,74	2.66	21 (38%)
27	LUT	g	1621	-	42,43,43	0.81	1 (2%)	51,60,60	1.99	16 (31%)
27	LUT	s	1620	-	42,43,43	0.68	0	51,60,60	1.91	14 (27%)
30	LHG	D	409	-	48,48,48	0.78	1 (2%)	51,54,54	1.33	7 (13%)
29	NEX	n	1623	-	40,46,46	1.02	3 (7%)	50,70,70	2.28	16 (32%)
25	CHL	S	601	20	40,54,74	4.09	19 (47%)	34,90,114	2.84	13 (38%)
26	CLA	C	508	6	69,73,73	1.18	9 (13%)	82,113,113	1.64	11 (13%)
26	CLA	N	612	1	64,68,73	1.21	7 (10%)	76,107,113	1.30	7 (9%)
26	CLA	y	613	1	69,73,73	1.14	8 (11%)	82,113,113	1.30	7 (8%)
26	CLA	s	610	20	59,63,73	1.25	9 (15%)	70,101,113	1.38	9 (12%)
25	CHL	2	608	-	40,54,74	4.08	20 (50%)	34,90,114	3.01	11 (32%)
25	CHL	g	601	1	60,74,74	3.24	18 (30%)	58,114,114	2.71	19 (32%)
29	NEX	2	1623	-	40,46,46	1.02	3 (7%)	50,70,70	2.27	16 (32%)
27	LUT	5	1620	-	42,43,43	0.70	0	51,60,60	1.88	15 (29%)
25	CHL	g	609	1	55,69,74	3.43	20 (36%)	52,108,114	2.48	17 (32%)
37	LMG	C	521	-	51,51,55	0.80	3 (5%)	59,59,63	1.38	6 (10%)
27	LUT	n	1621	-	42,43,43	0.80	1 (2%)	51,60,60	1.93	15 (29%)
31	BCR	B	618	-	41,41,41	0.70	0	56,56,56	1.88	14 (25%)
25	CHL	Y	609	1	60,74,74	3.25	20 (33%)	58,114,114	2.52	16 (27%)
39	DGD	C	518	-	56,56,67	1.17	6 (10%)	70,70,81	1.56	12 (17%)
25	CHL	N	605	1	42,56,74	3.95	18 (42%)	36,92,114	3.13	14 (38%)
26	CLA	B	606	5	69,73,73	1.25	9 (13%)	82,113,113	1.54	10 (12%)
25	CHL	R	614	19	36,50,74	4.29	18 (50%)	29,85,114	2.68	11 (37%)
31	BCR	c	515	-	41,41,41	0.78	0	56,56,56	2.06	17 (30%)
26	CLA	2	604	-	49,53,73	1.37	7 (14%)	58,89,113	1.32	4 (6%)
26	CLA	3	604	-	49,53,73	1.37	8 (16%)	58,89,113	1.29	6 (10%)
26	CLA	r	603	19	64,68,73	1.16	7 (10%)	76,107,113	1.48	10 (13%)
37	LMG	d	411	-	46,46,55	0.93	3 (6%)	54,54,63	1.46	4 (7%)
26	CLA	n	610	1	69,73,73	1.12	7 (10%)	82,113,113	1.27	9 (10%)
25	CHL	g	606	42	44,58,74	3.89	18 (40%)	37,94,114	2.86	15 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	y	602	1	69,73,73	1.16	8 (11%)	82,113,113	1.38	10 (12%)
25	CHL	3	606	-	40,54,74	3.92	19 (47%)	34,90,114	3.05	13 (38%)
26	CLA	b	603	5	69,73,73	1.13	9 (13%)	82,113,113	1.33	7 (8%)
25	CHL	n	606	42	44,58,74	3.85	18 (40%)	37,94,114	2.99	13 (35%)
29	NEX	g	1623	-	40,46,46	1.09	4 (10%)	50,70,70	2.27	14 (28%)
37	LMG	B	2633	-	55,55,55	0.78	2 (3%)	63,63,63	1.32	7 (11%)
26	CLA	G	614	1	52,56,73	1.34	6 (11%)	61,92,113	1.28	7 (11%)
25	CHL	3	607	-	47,61,74	3.93	19 (40%)	41,98,114	2.22	14 (34%)
26	CLA	r	602	19	64,68,73	1.15	9 (14%)	76,107,113	1.48	8 (10%)
27	LUT	G	1620	-	42,43,43	0.69	0	51,60,60	1.82	13 (25%)
26	CLA	2	602	1	65,69,73	1.20	9 (13%)	77,108,113	1.17	6 (7%)
26	CLA	1	614	1	49,53,73	1.36	7 (14%)	58,89,113	1.27	4 (6%)
37	LMG	a	413	-	48,48,55	0.79	0	56,56,63	1.31	6 (10%)
25	CHL	1	607	-	57,71,74	3.43	19 (33%)	54,110,114	2.54	15 (27%)
27	LUT	7	1620	-	42,43,43	0.73	0	51,60,60	1.87	13 (25%)
26	CLA	3	613	2	62,66,73	1.21	8 (12%)	73,104,113	1.23	3 (4%)
28	XAT	N	1622	-	41,47,47	0.89	1 (2%)	54,74,74	2.88	24 (44%)
26	CLA	r	601	19	53,57,73	1.28	6 (11%)	61,93,113	1.73	10 (16%)
26	CLA	B	617	5	69,73,73	1.20	10 (14%)	82,113,113	1.46	10 (12%)
26	CLA	r	613	19	64,68,73	1.21	7 (10%)	76,107,113	1.14	4 (5%)
26	CLA	1	612	1	49,53,73	1.40	9 (18%)	58,89,113	1.39	9 (15%)
25	CHL	y	609	1	60,74,74	3.25	20 (33%)	58,114,114	2.51	16 (27%)
27	LUT	8	620	-	42,43,43	0.74	1 (2%)	51,60,60	2.05	19 (37%)
25	CHL	4	607	-	40,54,74	4.12	19 (47%)	34,90,114	2.61	14 (41%)
25	CHL	3	609	2	55,69,74	3.48	20 (36%)	52,108,114	2.35	15 (28%)
25	CHL	6	607	-	55,69,74	3.48	19 (34%)	52,108,114	2.31	15 (28%)
25	CHL	6	606	-	40,54,74	4.09	19 (47%)	34,90,114	2.88	11 (32%)
26	CLA	N	602	1	69,73,73	1.17	9 (13%)	82,113,113	1.40	11 (13%)
26	CLA	S	610	20	59,63,73	1.25	9 (15%)	70,101,113	1.38	9 (12%)
36	SQD	A	418	-	52,54,54	0.92	4 (7%)	62,65,65	1.61	13 (20%)
26	CLA	C	513	6	69,73,73	1.10	7 (10%)	82,113,113	1.45	14 (17%)
26	CLA	N	611	30	64,68,73	1.20	7 (10%)	76,107,113	1.35	5 (6%)
26	CLA	R	613	19	64,68,73	1.21	7 (10%)	76,107,113	1.13	4 (5%)
25	CHL	y	605	1	42,56,74	3.92	19 (45%)	36,92,114	2.76	11 (30%)
26	CLA	y	603	1	69,73,73	1.21	9 (13%)	82,113,113	1.47	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	NEX	s	1623	-	40,46,46	1.02	3 (7%)	50,70,70	2.18	16 (32%)
40	BCT	d	401	33	3,3,3	1.18	0	2,3,3	4.23	2 (100%)
26	CLA	r	611	30	53,57,73	1.30	8 (15%)	61,93,113	1.59	10 (16%)
26	CLA	b	604	5	69,73,73	1.21	8 (11%)	82,113,113	1.32	11 (13%)
36	SQD	A	412	-	48,50,54	0.97	5 (10%)	58,61,65	1.70	10 (17%)
26	CLA	b	617	5	69,73,73	1.20	10 (14%)	82,113,113	1.46	10 (12%)
25	CHL	6	605	1	40,54,74	4.16	19 (47%)	34,90,114	2.64	13 (38%)
26	CLA	6	603	1	59,63,73	1.26	9 (15%)	70,101,113	1.38	6 (8%)
30	LHG	d	410	-	42,42,48	0.70	1 (2%)	45,48,54	1.25	4 (8%)
37	LMG	D	411	-	46,46,55	0.94	3 (6%)	54,54,63	1.46	4 (7%)
25	CHL	3	608	-	40,54,74	3.99	20 (50%)	34,90,114	2.98	15 (44%)
26	CLA	g	614	1	52,56,73	1.34	6 (11%)	61,92,113	1.28	7 (11%)
26	CLA	8	611	30	49,53,73	1.38	7 (14%)	58,89,113	1.30	4 (6%)
35	PHO	a	408	-	58,69,69	2.01	13 (22%)	55,99,99	1.66	12 (21%)
26	CLA	c	507	42	69,73,73	1.19	11 (15%)	82,113,113	1.59	10 (12%)
25	CHL	N	609	1	60,74,74	3.27	20 (33%)	58,114,114	2.42	17 (29%)
26	CLA	C	510	6	69,73,73	1.16	7 (10%)	82,113,113	1.41	9 (10%)
30	LHG	c	523	-	48,48,48	0.66	2 (4%)	51,54,54	1.22	5 (9%)
30	LHG	n	2630	26	48,48,48	0.68	1 (2%)	51,54,54	1.32	6 (11%)
29	NEX	R	623	-	40,46,46	1.11	3 (7%)	50,70,70	2.42	20 (40%)
26	CLA	g	604	42	54,58,73	1.38	9 (16%)	64,95,113	1.53	8 (12%)
26	CLA	c	505	6	69,73,73	1.21	9 (13%)	82,113,113	1.60	9 (10%)
26	CLA	4	610	3	49,53,73	1.36	9 (18%)	58,89,113	1.14	4 (6%)
30	LHG	y	2630	26	48,48,48	0.81	2 (4%)	51,54,54	1.25	6 (11%)
26	CLA	R	601	19	53,57,73	1.28	6 (11%)	61,93,113	1.74	10 (16%)
26	CLA	s	614	20	53,57,73	1.26	6 (11%)	61,93,113	1.51	6 (9%)
26	CLA	4	604	-	49,53,73	1.36	7 (14%)	58,89,113	1.25	4 (6%)
31	BCR	d	404	-	41,41,41	0.71	0	56,56,56	1.86	12 (21%)
26	CLA	b	615	5	69,73,73	1.12	8 (11%)	82,113,113	1.36	8 (9%)
26	CLA	1	613	1	59,63,73	1.25	8 (13%)	70,101,113	1.20	3 (4%)
27	LUT	4	620	-	42,43,43	0.74	1 (2%)	51,60,60	2.06	19 (37%)
25	CHL	r	614	19	36,50,74	4.29	18 (50%)	29,85,114	2.69	11 (37%)
30	LHG	2	2630	26	36,36,48	0.75	1 (2%)	39,42,54	1.30	4 (10%)
30	LHG	3	2630	26	46,46,48	0.72	1 (2%)	49,52,54	1.27	5 (10%)
26	CLA	g	613	1	69,73,73	1.15	9 (13%)	82,113,113	1.23	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	r	610	19	69,73,73	1.13	7 (10%)	82,113,113	1.24	9 (10%)
25	CHL	4	608	-	40,54,74	3.93	19 (47%)	34,90,114	2.89	13 (38%)
30	LHG	D	408	-	45,45,48	0.80	1 (2%)	48,51,54	1.30	5 (10%)
26	CLA	a	406	42	69,73,73	1.13	8 (11%)	82,113,113	1.56	15 (18%)
25	CHL	6	608	-	40,54,74	4.08	20 (50%)	34,90,114	3.01	11 (32%)
26	CLA	s	612	20	53,57,73	1.28	7 (13%)	61,93,113	1.45	7 (11%)
25	CHL	r	606	42	60,74,74	3.39	19 (31%)	58,114,114	2.55	16 (27%)
25	CHL	3	605	2	40,54,74	4.18	19 (47%)	34,90,114	2.71	14 (41%)
26	CLA	3	603	2	59,63,73	1.22	9 (15%)	70,101,113	1.43	8 (11%)
26	CLA	S	609	20	49,53,73	1.38	6 (12%)	58,89,113	1.24	6 (10%)
26	CLA	B	609	5	69,73,73	1.10	8 (11%)	82,113,113	1.48	8 (9%)
26	CLA	7	611	30	59,63,73	1.28	9 (15%)	70,101,113	1.42	8 (11%)
26	CLA	2	613	1	49,53,73	1.36	8 (16%)	58,89,113	1.24	3 (5%)
26	CLA	c	503	6	69,73,73	1.18	10 (14%)	82,113,113	1.32	7 (8%)
26	CLA	Y	612	1	64,68,73	1.22	9 (14%)	76,107,113	1.32	5 (6%)
31	BCR	4	623	-	41,41,41	0.70	0	56,56,56	2.33	15 (26%)
36	SQD	a	418	-	52,54,54	0.92	4 (7%)	62,65,65	1.61	13 (20%)
26	CLA	d	402	7	69,73,73	1.28	9 (13%)	82,113,113	1.58	9 (10%)
31	BCR	C	516	-	41,41,41	0.70	0	56,56,56	2.01	16 (28%)
25	CHL	2	601	1	40,54,74	4.10	18 (45%)	34,90,114	3.24	16 (47%)
25	CHL	3	601	2	58,72,74	3.38	19 (32%)	55,111,114	2.69	18 (32%)
27	LUT	3	1620	-	42,43,43	0.73	0	51,60,60	1.88	14 (27%)
26	CLA	S	603	20	49,53,73	1.37	6 (12%)	58,89,113	1.72	9 (15%)
25	CHL	2	607	-	55,69,74	3.49	19 (34%)	52,108,114	2.31	15 (28%)
27	LUT	s	1621	-	42,43,43	0.72	0	51,60,60	1.95	19 (37%)
26	CLA	5	612	1	49,53,73	1.40	9 (18%)	58,89,113	1.39	9 (15%)
27	LUT	n	1620	-	42,43,43	0.69	0	51,60,60	1.83	13 (25%)
26	CLA	B	602	42	69,73,73	1.16	8 (11%)	82,113,113	1.30	6 (7%)
30	LHG	6	2630	26	36,36,48	0.75	1 (2%)	39,42,54	1.30	4 (10%)

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
26	CLA	g	602	1	1/1/15/20	12/39/115/115	-
25	CHL	4	606	-	3/3/16/26	8/15/113/137	-
26	CLA	C	511	6	1/1/15/20	12/39/115/115	-
38	PL9	d	405	-	-	10/53/73/73	0/1/1/1
30	LHG	N	2630	26	-	24/53/53/53	-
31	BCR	c	514	-	-	2/29/63/63	0/2/2/2
26	CLA	6	614	1	1/1/11/20	6/15/91/115	-
28	XAT	Y	1622	-	-	2/31/93/93	0/4/4/4
30	LHG	D	410	-	-	28/47/47/53	-
26	CLA	R	612	19	1/1/11/20	6/20/96/115	-
26	CLA	G	612	1	1/1/14/20	14/33/109/115	-
25	CHL	1	608	-	3/3/16/26	8/15/113/137	-
25	CHL	8	607	-	3/3/16/26	8/15/113/137	-
26	CLA	b	612	5	1/1/15/20	12/39/115/115	-
25	CHL	5	607	-	4/4/19/26	22/36/134/137	-
25	CHL	7	609	2	4/4/19/26	13/33/131/137	-
25	CHL	6	601	1	3/3/16/26	4/15/113/137	-
31	BCR	A	411	-	-	6/29/63/63	0/2/2/2
31	BCR	h	101	-	-	2/29/63/63	0/2/2/2
25	CHL	N	608	42	4/4/20/26	13/39/137/137	-
26	CLA	1	610	1	1/1/13/20	7/29/105/115	-
28	XAT	G	1622	-	-	2/31/93/93	0/4/4/4
26	CLA	s	613	20	1/1/13/20	2/27/103/115	-
31	BCR	D	404	-	-	7/29/63/63	0/2/2/2
30	LHG	b	2631	-	-	21/53/53/53	-
29	NEX	r	623	-	-	4/27/83/83	0/3/3/3
25	CHL	1	606	-	3/3/16/26	8/15/113/137	-
25	CHL	4	609	3	3/3/16/26	5/15/113/137	-
26	CLA	A	407	42	-	3/21/97/115	-
26	CLA	B	611	42	1/1/15/20	10/39/115/115	-
26	CLA	Y	613	1	1/1/15/20	10/39/115/115	-
25	CHL	1	605	1	3/3/16/26	7/15/113/137	-
36	SQD	B	623	-	-	18/37/57/69	0/1/1/1
28	XAT	5	1622	-	-	2/31/93/93	0/4/4/4
25	CHL	7	607	-	3/3/17/26	5/24/122/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	S	611	30	1/1/13/20	9/29/105/115	-
25	CHL	g	605	1	3/3/16/26	7/15/113/137	-
26	CLA	g	603	1	1/1/15/20	11/39/115/115	-
25	CHL	1	601	1	3/3/16/26	4/15/113/137	-
31	BCR	8	623	-	-	8/29/63/63	0/2/2/2
30	LHG	L	101	-	-	19/53/53/53	-
26	CLA	s	602	20	1/1/14/20	12/35/111/115	-
25	CHL	s	607	42	4/4/18/26	16/30/128/137	-
26	CLA	r	612	19	1/1/11/20	6/20/96/115	-
31	BCR	T	101	-	-	13/29/63/63	0/2/2/2
26	CLA	c	509	6	1/1/15/20	8/39/115/115	-
25	CHL	8	608	-	3/3/16/26	5/15/113/137	-
27	LUT	N	1621	-	-	3/29/67/67	0/2/2/2
38	PL9	D	405	-	-	10/53/73/73	0/1/1/1
31	BCR	C	514	-	-	2/29/63/63	0/2/2/2
41	HEM	f	101	9,8	-	1/14/54/54	-
35	PHO	a	409	-	-	7/37/103/103	0/5/6/6
25	CHL	Y	606	42	3/3/16/26	6/20/118/137	-
26	CLA	C	506	6	1/1/15/20	19/39/115/115	-
25	CHL	5	608	-	3/3/16/26	8/15/113/137	-
26	CLA	R	602	19	1/1/14/20	8/33/109/115	-
26	CLA	S	604	42	1/1/12/20	6/21/97/115	-
26	CLA	B	605	5	1/1/15/20	12/39/115/115	-
26	CLA	2	614	1	1/1/11/20	6/15/91/115	-
30	LHG	g	2630	26	-	26/53/53/53	-
39	DGD	C	519	-	-	24/51/91/95	0/2/2/2
31	BCR	b	618	-	-	2/29/63/63	0/2/2/2
26	CLA	4	611	30	1/1/11/20	6/15/91/115	-
31	BCR	b	619	-	-	2/29/63/63	0/2/2/2
26	CLA	R	610	19	1/1/15/20	13/39/115/115	-
25	CHL	Y	608	42	4/4/20/26	15/39/137/137	-
30	LHG	4	2630	26	-	8/23/23/53	-
39	DGD	H	102	-	-	21/51/91/95	0/2/2/2
26	CLA	b	606	5	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LHG	C	523	-	-	20/53/53/53	-
26	CLA	G	611	30	1/1/14/20	13/33/109/115	-
25	CHL	y	601	1	4/4/20/26	16/39/137/137	-
25	CHL	7	606	-	3/3/16/26	9/15/113/137	-
25	CHL	G	607	42	4/4/20/26	16/39/137/137	-
25	CHL	2	605	1	3/3/16/26	9/15/113/137	-
39	DGD	c	518	-	-	15/44/84/95	0/2/2/2
26	CLA	3	610	2	1/1/14/20	9/33/109/115	-
26	CLA	B	615	5	1/1/15/20	12/39/115/115	-
26	CLA	s	611	30	1/1/13/20	9/29/105/115	-
26	CLA	4	603	3	1/1/11/20	6/15/91/115	-
26	CLA	G	602	1	1/1/15/20	12/39/115/115	-
31	BCR	t	101	-	-	13/29/63/63	0/2/2/2
30	LHG	Y	2630	26	-	25/53/53/53	-
26	CLA	5	610	1	1/1/13/20	7/29/105/115	-
26	CLA	a	410	4	1/1/14/20	8/33/109/115	-
26	CLA	Y	602	1	1/1/15/20	10/39/115/115	-
26	CLA	g	612	1	1/1/14/20	14/33/109/115	-
26	CLA	C	503	6	1/1/15/20	11/39/115/115	-
26	CLA	a	405	4	1/1/15/20	6/39/115/115	-
26	CLA	g	611	30	1/1/14/20	13/33/109/115	-
26	CLA	n	603	1	1/1/15/20	12/39/115/115	-
26	CLA	B	612	5	1/1/15/20	12/39/115/115	-
25	CHL	s	601	20	3/3/16/26	5/15/113/137	-
27	LUT	5	1621	-	-	3/29/67/67	0/2/2/2
38	PL9	A	414	-	-	1/5/18/73	0/1/1/1
26	CLA	R	611	30	1/1/11/20	8/20/96/115	-
26	CLA	c	504	42	1/1/15/20	17/39/115/115	-
37	LMG	Z	101	-	-	23/46/66/70	0/1/1/1
29	NEX	7	1623	-	-	4/27/83/83	0/3/3/3
29	NEX	Y	1623	-	-	6/27/83/83	0/3/3/3
27	LUT	2	1620	-	-	2/29/67/67	0/2/2/2
30	LHG	G	2630	26	-	26/53/53/53	-
25	CHL	y	608	42	4/4/20/26	15/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	8	601	3	3/3/16/26	8/13/111/137	-
31	BCR	H	101	-	-	2/29/63/63	0/2/2/2
27	LUT	S	1621	-	-	2/29/67/67	0/2/2/2
26	CLA	r	604	42	1/1/11/20	6/19/95/115	-
30	LHG	B	2631	-	-	21/53/53/53	-
26	CLA	Y	614	1	1/1/11/20	5/19/95/115	-
26	CLA	B	614	5	1/1/15/20	13/39/115/115	-
30	LHG	7	2630	26	-	24/51/51/53	-
26	CLA	1	603	1	1/1/13/20	13/27/103/115	-
26	CLA	6	610	1	1/1/12/20	6/21/97/115	-
25	CHL	5	609	1	4/4/19/26	16/35/133/137	-
26	CLA	b	611	42	1/1/15/20	10/39/115/115	-
31	BCR	c	517	-	-	4/29/63/63	0/2/2/2
31	BCR	b	620	-	-	6/29/63/63	0/2/2/2
27	LUT	1	1620	-	-	2/29/67/67	0/2/2/2
28	XAT	6	1622	-	-	3/31/93/93	0/4/4/4
29	NEX	N	1623	-	-	4/27/83/83	0/3/3/3
25	CHL	y	607	42	4/4/20/26	17/39/137/137	-
26	CLA	1	604	-	-	10/21/97/115	-
27	LUT	7	1621	-	-	3/29/67/67	0/2/2/2
25	CHL	Y	605	1	3/3/16/26	8/18/116/137	-
25	CHL	8	606	-	3/3/16/26	8/15/113/137	-
25	CHL	G	608	42	4/4/20/26	15/39/137/137	-
25	CHL	s	608	-	3/3/16/26	6/15/113/137	-
39	DGD	B	626	-	-	24/48/88/95	0/2/2/2
26	CLA	3	614	2	1/1/11/20	10/19/95/115	-
26	CLA	Y	611	30	1/1/14/20	8/33/109/115	-
25	CHL	S	606	42	3/3/16/26	8/15/113/137	-
36	SQD	b	623	-	-	18/37/57/69	0/1/1/1
25	CHL	5	606	-	3/3/16/26	8/15/113/137	-
26	CLA	c	511	6	1/1/15/20	12/39/115/115	-
31	BCR	B	620	-	-	6/29/63/63	0/2/2/2
25	CHL	N	607	42	4/4/20/26	16/39/137/137	-
25	CHL	6	609	1	4/4/19/26	13/33/131/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	N	604	42	1/1/12/20	4/21/97/115	-
28	XAT	g	1622	-	-	2/31/93/93	0/4/4/4
26	CLA	c	510	6	1/1/15/20	15/39/115/115	-
25	CHL	7	601	2	4/4/19/26	17/37/135/137	-
26	CLA	2	612	1	1/1/11/20	6/15/91/115	-
26	CLA	3	612	2	1/1/11/20	8/15/91/115	-
25	CHL	5	601	1	3/3/16/26	4/15/113/137	-
30	LHG	C	522	-	-	19/53/53/53	-
30	LHG	s	2630	26	-	27/53/53/53	-
26	CLA	c	502	6	1/1/15/20	18/39/115/115	-
39	DGD	h	102	-	-	21/51/91/95	0/2/2/2
41	HEM	F	101	9,8	-	1/14/54/54	-
25	CHL	n	605	1	3/3/16/26	9/18/116/137	-
30	LHG	c	2630	-	-	27/53/53/53	-
28	XAT	r	622	-	-	3/31/93/93	0/4/4/4
26	CLA	2	610	1	1/1/12/20	6/21/97/115	-
25	CHL	r	607	42	4/4/18/26	9/27/125/137	-
26	CLA	c	512	6	1/1/15/20	11/39/115/115	-
26	CLA	G	610	1	1/1/14/20	15/38/114/115	-
26	CLA	d	403	7	-	10/39/115/115	-
26	CLA	a	407	42	-	3/21/97/115	-
26	CLA	C	504	42	1/1/15/20	17/39/115/115	-
30	LHG	d	408	-	-	19/50/50/53	-
38	PL9	a	414	-	-	1/5/18/73	0/1/1/1
26	CLA	b	605	5	1/1/15/20	12/39/115/115	-
26	CLA	r	616	19	-	6/15/91/115	-
26	CLA	N	613	1	1/1/14/20	7/33/109/115	-
37	LMG	b	622	-	-	24/46/66/70	0/1/1/1
29	NEX	5	1623	-	-	6/27/83/83	0/3/3/3
27	LUT	G	1621	-	-	1/29/67/67	0/2/2/2
26	CLA	6	612	1	1/1/11/20	6/15/91/115	-
26	CLA	8	610	3	1/1/11/20	6/15/91/115	-
25	CHL	2	609	1	4/4/19/26	13/33/131/137	-
26	CLA	s	603	20	1/1/11/20	7/15/91/115	-
26	CLA	n	604	42	1/1/12/20	4/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LUT	1	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	6	611	30	-	4/15/91/115	-
26	CLA	6	602	1	1/1/14/20	12/35/111/115	-
29	NEX	S	1623	-	-	5/27/83/83	0/3/3/3
37	LMG	c	521	-	-	22/46/66/70	0/1/1/1
25	CHL	g	608	42	4/4/20/26	15/39/137/137	-
26	CLA	N	610	1	1/1/15/20	10/39/115/115	-
26	CLA	A	405	4	1/1/15/20	6/39/115/115	-
25	CHL	Y	607	42	4/4/20/26	17/39/137/137	-
28	XAT	3	1622	-	-	2/31/93/93	0/4/4/4
25	CHL	8	609	3	3/3/16/26	5/15/113/137	-
25	CHL	N	606	42	3/3/16/26	8/20/118/137	-
26	CLA	R	603	19	1/1/14/20	14/33/109/115	-
26	CLA	c	501	6	1/1/15/20	16/39/115/115	-
27	LUT	S	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	c	513	6	-	10/39/115/115	-
26	CLA	8	612	3	1/1/11/20	7/15/91/115	-
26	CLA	Y	610	1	1/1/14/20	9/33/109/115	-
26	CLA	C	502	6	1/1/15/20	18/39/115/115	-
25	CHL	r	608	42	4/4/19/26	15/33/131/137	-
26	CLA	S	612	20	1/1/11/20	4/20/96/115	-
26	CLA	b	613	5	1/1/15/20	12/39/115/115	-
25	CHL	S	607	42	4/4/18/26	16/30/128/137	-
26	CLA	2	603	1	1/1/13/20	11/27/103/115	-
27	LUT	6	1620	-	-	2/29/67/67	0/2/2/2
37	LMG	A	415	-	-	14/35/55/70	0/1/1/1
26	CLA	b	614	5	1/1/15/20	13/39/115/115	-
26	CLA	C	512	6	1/1/15/20	11/39/115/115	-
26	CLA	3	602	2	1/1/14/20	15/33/109/115	-
26	CLA	2	611	30	-	4/15/91/115	-
37	LMG	A	413	-	-	28/43/63/70	0/1/1/1
26	CLA	D	403	7	-	10/39/115/115	-
26	CLA	5	613	1	-	8/27/103/115	-
27	LUT	y	1621	-	-	1/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	C	517	-	-	4/29/63/63	0/2/2/2
26	CLA	C	507	42	1/1/15/20	23/39/115/115	-
26	CLA	7	614	2	1/1/11/20	10/19/95/115	-
30	LHG	r	2630	26	-	18/46/46/53	-
26	CLA	C	505	6	1/1/15/20	13/39/115/115	-
25	CHL	R	608	42	4/4/19/26	15/33/131/137	-
39	DGD	b	626	-	-	24/48/88/95	0/2/2/2
25	CHL	1	609	1	4/4/19/26	16/35/133/137	-
26	CLA	S	613	20	1/1/13/20	2/27/103/115	-
26	CLA	B	613	5	1/1/15/20	12/39/115/115	-
27	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	7	610	2	1/1/14/20	9/33/109/115	-
26	CLA	5	604	-	-	10/21/97/115	-
26	CLA	7	612	2	1/1/11/20	8/15/91/115	-
30	LHG	B	2630	-	-	31/51/51/53	-
26	CLA	b	609	5	-	8/39/115/115	-
25	CHL	N	601	1	4/4/20/26	17/39/137/137	-
27	LUT	N	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	7	602	2	1/1/14/20	15/33/109/115	-
26	CLA	N	603	1	1/1/15/20	12/39/115/115	-
26	CLA	y	610	1	1/1/14/20	9/33/109/115	-
29	NEX	1	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	n	612	1	1/1/14/20	10/33/109/115	-
26	CLA	c	508	6	1/1/15/20	10/39/115/115	-
26	CLA	4	612	3	1/1/11/20	7/15/91/115	-
26	CLA	D	402	7	1/1/15/20	4/39/115/115	-
26	CLA	G	604	42	1/1/12/20	5/21/97/115	-
25	CHL	R	607	42	4/4/18/26	9/27/125/137	-
26	CLA	3	611	30	1/1/13/20	9/27/103/115	-
39	DGD	c	519	-	-	24/51/91/95	0/2/2/2
31	BCR	c	516	-	-	7/29/63/63	0/2/2/2
26	CLA	B	616	5	1/1/15/20	13/39/115/115	-
26	CLA	7	604	-	1/1/11/20	10/15/91/115	-
26	CLA	b	602	42	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	s	604	42	1/1/12/20	6/21/97/115	-
31	BCR	B	619	-	-	2/29/63/63	0/2/2/2
26	CLA	Y	603	1	1/1/15/20	12/39/115/115	-
27	LUT	6	1621	-	-	2/29/67/67	0/2/2/2
35	PHO	A	408	-	-	10/37/103/103	0/5/6/6
26	CLA	b	608	42	1/1/15/20	10/39/115/115	-
26	CLA	5	602	1	1/1/14/20	14/35/111/115	-
26	CLA	1	611	30	1/1/11/20	8/15/91/115	-
26	CLA	B	610	5	-	10/39/115/115	-
28	XAT	2	1622	-	-	3/31/93/93	0/4/4/4
30	LHG	1	2630	26	-	15/45/45/53	-
31	BCR	C	515	-	-	6/29/63/63	0/2/2/2
30	LHG	l	101	-	-	19/53/53/53	-
25	CHL	y	606	42	3/3/16/26	6/20/118/137	-
26	CLA	R	604	42	1/1/11/20	6/19/95/115	-
31	BCR	a	411	-	-	6/29/63/63	0/2/2/2
28	XAT	7	1622	-	-	2/31/93/93	0/4/4/4
28	XAT	4	622	-	-	2/31/93/93	0/4/4/4
26	CLA	r	609	19	1/1/13/20	3/31/107/115	-
26	CLA	7	613	2	1/1/13/20	9/31/107/115	-
26	CLA	N	614	1	1/1/11/20	5/19/95/115	-
26	CLA	8	603	3	1/1/11/20	6/15/91/115	-
29	NEX	y	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	G	613	1	1/1/15/20	14/39/115/115	-
26	CLA	5	603	1	1/1/13/20	13/27/103/115	-
37	LMG	z	101	-	-	23/46/66/70	0/1/1/1
28	XAT	n	1622	-	-	3/31/93/93	0/4/4/4
25	CHL	n	608	42	4/4/20/26	13/39/137/137	-
25	CHL	n	601	1	4/4/20/26	16/39/137/137	-
30	LHG	d	409	-	-	26/53/53/53	-
26	CLA	A	410	4	1/1/14/20	8/33/109/115	-
35	PHO	A	409	-	-	7/37/103/103	0/5/6/6
25	CHL	g	607	42	4/4/20/26	16/39/137/137	-
30	LHG	C	2630	-	-	27/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LUT	r	620	-	-	3/29/67/67	0/2/2/2
26	CLA	b	610	5	-	10/39/115/115	-
27	LUT	g	1620	-	-	2/29/67/67	0/2/2/2
36	SQD	B	621	-	-	31/49/69/69	0/1/1/1
25	CHL	s	606	42	3/3/16/26	8/15/113/137	-
28	XAT	8	622	-	-	2/31/93/93	0/4/4/4
26	CLA	B	607	5	1/1/15/20	8/39/115/115	-
29	NEX	3	1623	-	-	4/27/83/83	0/3/3/3
26	CLA	n	614	1	1/1/11/20	5/19/95/115	-
39	DGD	c	520	-	-	21/49/89/95	0/2/2/2
26	CLA	Y	604	42	1/1/12/20	2/21/97/115	-
26	CLA	S	614	20	1/1/11/20	4/20/96/115	-
26	CLA	A	406	42	1/1/15/20	10/39/115/115	-
29	NEX	G	1623	-	-	5/27/83/83	0/3/3/3
26	CLA	1	602	1	1/1/14/20	14/35/111/115	-
26	CLA	n	611	30	1/1/14/20	6/33/109/115	-
25	CHL	5	605	1	3/3/16/26	7/15/113/137	-
26	CLA	C	501	6	1/1/15/20	16/39/115/115	-
36	SQD	a	412	-	-	13/45/65/69	0/1/1/1
26	CLA	4	602	3	1/1/11/20	9/15/91/115	-
25	CHL	7	608	-	3/3/16/26	3/15/113/137	-
27	LUT	R	620	-	-	4/29/67/67	0/2/2/2
26	CLA	y	612	1	1/1/14/20	14/33/109/115	-
26	CLA	n	602	1	1/1/15/20	11/39/115/115	-
27	LUT	3	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	R	616	19	-	6/15/91/115	-
26	CLA	B	603	5	1/1/15/20	7/39/115/115	-
28	XAT	1	1622	-	-	2/31/93/93	0/4/4/4
29	NEX	6	1623	-	-	7/27/83/83	0/3/3/3
30	LHG	b	2630	-	-	31/51/51/53	-
25	CHL	G	606	42	3/3/16/26	8/20/118/137	-
30	LHG	8	2630	26	-	8/23/23/53	-
27	LUT	2	1621	-	-	2/29/67/67	0/2/2/2
37	LMG	b	2633	-	-	24/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	y	614	1	1/1/11/20	5/19/95/115	-
30	LHG	5	2630	26	-	15/45/45/53	-
26	CLA	y	611	30	1/1/14/20	8/33/109/115	-
25	CHL	n	609	1	4/4/20/26	15/39/137/137	-
27	LUT	y	1620	-	-	2/29/67/67	0/2/2/2
30	LHG	c	522	-	-	19/53/53/53	-
26	CLA	y	604	42	1/1/12/20	2/21/97/115	-
26	CLA	g	610	1	1/1/14/20	15/38/114/115	-
30	LHG	R	2630	26	-	18/46/46/53	-
25	CHL	7	605	2	3/3/16/26	9/15/113/137	-
26	CLA	7	603	2	1/1/13/20	14/27/103/115	-
26	CLA	8	602	3	1/1/11/20	9/15/91/115	-
26	CLA	C	509	6	1/1/15/20	8/39/115/115	-
36	SQD	b	621	-	-	31/49/69/69	0/1/1/1
26	CLA	b	607	5	1/1/15/20	8/39/115/115	-
26	CLA	b	616	5	1/1/15/20	13/39/115/115	-
26	CLA	G	603	1	1/1/15/20	11/39/115/115	-
25	CHL	G	609	1	4/4/19/26	10/33/131/137	-
26	CLA	S	602	20	1/1/14/20	12/35/111/115	-
26	CLA	6	604	-	1/1/11/20	9/15/91/115	-
26	CLA	B	608	42	1/1/15/20	10/39/115/115	-
25	CHL	2	606	-	3/3/16/26	6/15/113/137	-
37	LMG	a	415	-	-	14/35/55/70	0/1/1/1
27	LUT	Y	1621	-	-	1/29/67/67	0/2/2/2
25	CHL	S	608	-	3/3/16/26	6/15/113/137	-
25	CHL	Y	601	1	4/4/20/26	16/39/137/137	-
26	CLA	5	614	1	1/1/11/20	4/15/91/115	-
39	DGD	C	520	-	-	21/49/89/95	0/2/2/2
26	CLA	n	613	1	1/1/14/20	7/33/109/115	-
26	CLA	c	506	6	1/1/15/20	19/39/115/115	-
37	LMG	B	622	-	-	24/46/66/70	0/1/1/1
26	CLA	8	604	-	-	8/15/91/115	-
28	XAT	y	1622	-	-	2/31/93/93	0/4/4/4
25	CHL	n	607	42	4/4/20/26	16/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	5	611	30	1/1/11/20	8/15/91/115	-
25	CHL	4	601	3	3/3/16/26	8/13/111/137	-
26	CLA	B	604	5	1/1/15/20	12/39/115/115	-
26	CLA	6	613	1	-	5/15/91/115	-
30	LHG	S	2630	26	-	27/53/53/53	-
26	CLA	R	609	19	1/1/13/20	3/31/107/115	-
25	CHL	G	601	1	4/4/20/26	16/39/137/137	-
25	CHL	G	605	1	3/3/16/26	7/15/113/137	-
25	CHL	R	606	42	4/4/20/26	18/39/137/137	-
26	CLA	s	609	20	1/1/11/20	7/15/91/115	-
28	XAT	R	622	-	-	3/31/93/93	0/4/4/4
27	LUT	g	1621	-	-	1/29/67/67	0/2/2/2
27	LUT	s	1620	-	-	2/29/67/67	0/2/2/2
30	LHG	D	409	-	-	26/53/53/53	-
29	NEX	n	1623	-	-	4/27/83/83	0/3/3/3
25	CHL	S	601	20	3/3/16/26	5/15/113/137	-
26	CLA	C	508	6	1/1/15/20	10/39/115/115	-
26	CLA	N	612	1	1/1/14/20	10/33/109/115	-
26	CLA	y	613	1	1/1/15/20	10/39/115/115	-
26	CLA	s	610	20	1/1/13/20	6/27/103/115	-
25	CHL	2	608	-	3/3/16/26	7/15/113/137	-
25	CHL	g	601	1	4/4/20/26	16/39/137/137	-
29	NEX	2	1623	-	-	7/27/83/83	0/3/3/3
27	LUT	5	1620	-	-	2/29/67/67	0/2/2/2
25	CHL	g	609	1	4/4/19/26	10/33/131/137	-
37	LMG	C	521	-	-	22/46/66/70	0/1/1/1
27	LUT	n	1621	-	-	3/29/67/67	0/2/2/2
31	BCR	B	618	-	-	2/29/63/63	0/2/2/2
25	CHL	Y	609	1	4/4/20/26	13/39/137/137	-
39	DGD	C	518	-	-	15/44/84/95	0/2/2/2
25	CHL	N	605	1	3/3/16/26	9/18/116/137	-
26	CLA	B	606	5	1/1/15/20	15/39/115/115	-
25	CHL	R	614	19	3/3/15/26	4/10/108/137	-
31	BCR	c	515	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	2	604	-	1/1/11/20	9/15/91/115	-
26	CLA	3	604	-	1/1/11/20	10/15/91/115	-
26	CLA	r	603	19	1/1/14/20	14/33/109/115	-
37	LMG	d	411	-	-	14/41/61/70	0/1/1/1
26	CLA	n	610	1	1/1/15/20	10/39/115/115	-
25	CHL	g	606	42	3/3/16/26	8/20/118/137	-
26	CLA	y	602	1	1/1/15/20	10/39/115/115	-
25	CHL	3	606	-	3/3/16/26	9/15/113/137	-
26	CLA	b	603	5	1/1/15/20	7/39/115/115	-
25	CHL	n	606	42	3/3/16/26	8/20/118/137	-
29	NEX	g	1623	-	-	5/27/83/83	0/3/3/3
37	LMG	B	2633	-	-	24/50/70/70	0/1/1/1
26	CLA	G	614	1	1/1/11/20	3/19/95/115	-
25	CHL	3	607	-	3/3/17/26	5/24/122/137	-
26	CLA	r	602	19	1/1/14/20	8/33/109/115	-
27	LUT	G	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	2	602	1	1/1/14/20	12/35/111/115	-
26	CLA	1	614	1	1/1/11/20	4/15/91/115	-
37	LMG	a	413	-	-	28/43/63/70	0/1/1/1
25	CHL	1	607	-	4/4/19/26	22/36/134/137	-
27	LUT	7	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	3	613	2	1/1/13/20	9/31/107/115	-
28	XAT	N	1622	-	-	3/31/93/93	0/4/4/4
26	CLA	r	601	19	1/1/11/20	12/20/96/115	-
26	CLA	B	617	5	1/1/15/20	16/39/115/115	-
26	CLA	r	613	19	1/1/14/20	10/33/109/115	-
26	CLA	1	612	1	1/1/11/20	5/15/91/115	-
25	CHL	y	609	1	4/4/20/26	13/39/137/137	-
27	LUT	8	620	-	-	4/29/67/67	0/2/2/2
25	CHL	4	607	-	3/3/16/26	8/15/113/137	-
25	CHL	3	609	2	4/4/19/26	13/33/131/137	-
25	CHL	6	607	-	4/4/19/26	14/33/131/137	-
25	CHL	6	606	-	3/3/16/26	6/15/113/137	-
26	CLA	N	602	1	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	S	610	20	1/1/13/20	6/27/103/115	-
36	SQD	A	418	-	-	22/49/69/69	0/1/1/1
26	CLA	C	513	6	-	10/39/115/115	-
26	CLA	N	611	30	1/1/14/20	6/33/109/115	-
26	CLA	R	613	19	1/1/14/20	10/33/109/115	-
25	CHL	y	605	1	3/3/16/26	8/18/116/137	-
26	CLA	y	603	1	1/1/15/20	12/39/115/115	-
29	NEX	s	1623	-	-	5/27/83/83	0/3/3/3
26	CLA	r	611	30	1/1/11/20	8/20/96/115	-
26	CLA	b	604	5	1/1/15/20	12/39/115/115	-
36	SQD	A	412	-	-	13/45/65/69	0/1/1/1
26	CLA	b	617	5	1/1/15/20	16/39/115/115	-
25	CHL	6	605	1	3/3/16/26	9/15/113/137	-
26	CLA	6	603	1	1/1/13/20	12/27/103/115	-
30	LHG	d	410	-	-	29/47/47/53	-
37	LMG	D	411	-	-	14/41/61/70	0/1/1/1
25	CHL	3	608	-	3/3/16/26	3/15/113/137	-
26	CLA	g	614	1	1/1/11/20	3/19/95/115	-
26	CLA	8	611	30	1/1/11/20	6/15/91/115	-
35	PHO	a	408	-	-	10/37/103/103	0/5/6/6
26	CLA	c	507	42	1/1/15/20	23/39/115/115	-
25	CHL	N	609	1	4/4/20/26	15/39/137/137	-
26	CLA	C	510	6	1/1/15/20	15/39/115/115	-
30	LHG	c	523	-	-	20/53/53/53	-
30	LHG	n	2630	26	-	24/53/53/53	-
29	NEX	R	623	-	-	4/27/83/83	0/3/3/3
26	CLA	g	604	42	1/1/12/20	5/21/97/115	-
26	CLA	c	505	6	1/1/15/20	13/39/115/115	-
26	CLA	4	610	3	1/1/11/20	6/15/91/115	-
30	LHG	y	2630	26	-	25/53/53/53	-
26	CLA	R	601	19	1/1/11/20	12/20/96/115	-
26	CLA	s	614	20	1/1/11/20	4/20/96/115	-
26	CLA	4	604	-	-	8/15/91/115	-
31	BCR	d	404	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	b	615	5	1/1/15/20	12/39/115/115	-
26	CLA	1	613	1	-	8/27/103/115	-
27	LUT	4	620	-	-	4/29/67/67	0/2/2/2
25	CHL	r	614	19	3/3/15/26	4/10/108/137	-
30	LHG	2	2630	26	-	14/41/41/53	-
30	LHG	3	2630	26	-	24/51/51/53	-
26	CLA	g	613	1	1/1/15/20	14/39/115/115	-
26	CLA	r	610	19	1/1/15/20	13/39/115/115	-
25	CHL	4	608	-	3/3/16/26	5/15/113/137	-
30	LHG	D	408	-	-	19/50/50/53	-
26	CLA	a	406	42	1/1/15/20	10/39/115/115	-
25	CHL	6	608	-	3/3/16/26	7/15/113/137	-
26	CLA	s	612	20	1/1/11/20	4/20/96/115	-
25	CHL	r	606	42	4/4/20/26	18/39/137/137	-
25	CHL	3	605	2	3/3/16/26	9/15/113/137	-
26	CLA	3	603	2	1/1/13/20	14/27/103/115	-
26	CLA	S	609	20	1/1/11/20	7/15/91/115	-
26	CLA	B	609	5	-	8/39/115/115	-
26	CLA	7	611	30	1/1/13/20	9/27/103/115	-
26	CLA	2	613	1	-	5/15/91/115	-
26	CLA	c	503	6	1/1/15/20	11/39/115/115	-
26	CLA	Y	612	1	1/1/14/20	14/33/109/115	-
31	BCR	4	623	-	-	8/29/63/63	0/2/2/2
36	SQD	a	418	-	-	22/49/69/69	0/1/1/1
26	CLA	d	402	7	1/1/15/20	4/39/115/115	-
31	BCR	C	516	-	-	7/29/63/63	0/2/2/2
25	CHL	2	601	1	3/3/16/26	4/15/113/137	-
25	CHL	3	601	2	4/4/19/26	17/37/135/137	-
27	LUT	3	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	S	603	20	1/1/11/20	7/15/91/115	-
25	CHL	2	607	-	4/4/19/26	14/33/131/137	-
27	LUT	s	1621	-	-	2/29/67/67	0/2/2/2
26	CLA	5	612	1	1/1/11/20	5/15/91/115	-
27	LUT	n	1620	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	602	42	1/1/15/20	16/39/115/115	-
30	LHG	6	2630	26	-	14/41/41/53	-

All (3947) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	601	CHL	C2C-C3C	11.12	1.47	1.36
25	S	601	CHL	C2C-C3C	11.10	1.47	1.36
25	s	601	CHL	C2C-C3C	11.10	1.47	1.36
25	8	601	CHL	C2C-C3C	11.07	1.47	1.36
25	3	607	CHL	C2C-C3C	10.91	1.46	1.36
25	7	607	CHL	C2C-C3C	10.85	1.46	1.36
25	r	614	CHL	C2C-C3C	10.64	1.46	1.36
25	r	606	CHL	C2C-C3C	10.63	1.46	1.36
25	7	609	CHL	C2C-C3C	10.63	1.46	1.36
25	6	606	CHL	C2C-C3C	10.62	1.46	1.36
25	R	614	CHL	C2C-C3C	10.61	1.46	1.36
25	3	609	CHL	C2C-C3C	10.60	1.46	1.36
25	2	605	CHL	C2C-C3C	10.56	1.46	1.36
25	6	605	CHL	C2C-C3C	10.56	1.46	1.36
25	2	606	CHL	C2C-C3C	10.56	1.46	1.36
25	6	609	CHL	C2C-C3C	10.54	1.46	1.36
25	R	606	CHL	C2C-C3C	10.53	1.46	1.36
25	2	609	CHL	C2C-C3C	10.51	1.46	1.36
25	4	606	CHL	C2C-C3C	10.51	1.46	1.36
25	g	609	CHL	C2C-C3C	10.50	1.46	1.36
25	S	608	CHL	C2C-C3C	10.50	1.46	1.36
25	s	608	CHL	C2C-C3C	10.50	1.46	1.36
25	G	609	CHL	C2C-C3C	10.49	1.46	1.36
25	N	606	CHL	C2C-C3C	10.45	1.46	1.36
25	n	606	CHL	C2C-C3C	10.45	1.46	1.36
25	8	606	CHL	C2C-C3C	10.44	1.46	1.36
25	4	607	CHL	C2C-C3C	10.33	1.46	1.36
25	G	607	CHL	C2C-C3C	10.33	1.46	1.36
25	g	607	CHL	C2C-C3C	10.33	1.46	1.36
25	7	605	CHL	C2C-C3C	10.31	1.46	1.36
25	3	605	CHL	C2C-C3C	10.30	1.46	1.36
25	8	607	CHL	C2C-C3C	10.28	1.46	1.36
25	1	601	CHL	C2C-C3C	10.26	1.46	1.36
25	1	607	CHL	C2C-C3C	10.24	1.46	1.36
25	5	601	CHL	C2C-C3C	10.23	1.46	1.36
25	1	609	CHL	C2C-C3C	10.23	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	609	CHL	C2C-C3C	10.23	1.46	1.36
25	5	607	CHL	C2C-C3C	10.20	1.46	1.36
25	G	606	CHL	C2C-C3C	10.20	1.46	1.36
25	g	606	CHL	C2C-C3C	10.20	1.46	1.36
25	g	608	CHL	C2C-C3C	10.19	1.46	1.36
25	R	614	CHL	C1D-C2D	10.18	1.51	1.39
25	r	614	CHL	C1D-C2D	10.18	1.51	1.39
25	S	606	CHL	C2C-C3C	10.17	1.46	1.36
25	8	609	CHL	C2C-C3C	10.16	1.46	1.36
25	Y	609	CHL	C2C-C3C	10.15	1.46	1.36
25	G	608	CHL	C2C-C3C	10.15	1.46	1.36
25	N	605	CHL	C2C-C3C	10.15	1.46	1.36
25	n	605	CHL	C2C-C3C	10.15	1.46	1.36
25	4	609	CHL	C2C-C3C	10.15	1.46	1.36
25	y	609	CHL	C2C-C3C	10.15	1.46	1.36
25	s	606	CHL	C2C-C3C	10.14	1.46	1.36
25	4	609	CHL	C1D-C2D	10.13	1.51	1.39
25	8	607	CHL	C1D-C2D	10.13	1.51	1.39
25	n	609	CHL	C2C-C3C	10.12	1.46	1.36
25	2	601	CHL	C1D-C2D	10.11	1.51	1.39
25	7	608	CHL	C2C-C3C	10.11	1.46	1.36
25	4	607	CHL	C1D-C2D	10.10	1.51	1.39
25	8	609	CHL	C1D-C2D	10.10	1.51	1.39
25	6	601	CHL	C1D-C2D	10.09	1.51	1.39
25	2	608	CHL	C2C-C3C	10.09	1.46	1.36
25	N	609	CHL	C2C-C3C	10.09	1.46	1.36
25	3	608	CHL	C2C-C3C	10.07	1.46	1.36
25	2	607	CHL	C2C-C3C	10.07	1.46	1.36
25	1	601	CHL	C1D-C2D	10.06	1.51	1.39
25	5	601	CHL	C1D-C2D	10.06	1.51	1.39
25	y	605	CHL	C2C-C3C	10.05	1.46	1.36
25	6	608	CHL	C2C-C3C	10.04	1.46	1.36
25	Y	601	CHL	C1D-C2D	10.03	1.51	1.39
25	4	601	CHL	C1D-C2D	10.02	1.51	1.39
25	y	601	CHL	C1D-C2D	10.02	1.51	1.39
25	8	601	CHL	C1D-C2D	10.01	1.51	1.39
25	R	608	CHL	C2C-C3C	10.01	1.46	1.36
25	Y	605	CHL	C2C-C3C	10.01	1.46	1.36
25	N	601	CHL	C1D-C2D	10.01	1.51	1.39
25	n	601	CHL	C1D-C2D	10.01	1.51	1.39
25	6	607	CHL	C2C-C3C	9.98	1.46	1.36
25	g	605	CHL	C1D-C2D	9.97	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	608	CHL	C2C-C3C	9.97	1.46	1.36
25	1	606	CHL	C2C-C3C	9.95	1.46	1.36
25	5	606	CHL	C2C-C3C	9.95	1.46	1.36
25	G	605	CHL	C2C-C3C	9.93	1.46	1.36
25	3	607	CHL	C1D-C2D	9.93	1.50	1.39
25	R	606	CHL	C1D-C2D	9.93	1.50	1.39
25	1	607	CHL	C1D-C2D	9.93	1.50	1.39
25	7	607	CHL	C1D-C2D	9.92	1.50	1.39
25	G	605	CHL	C1D-C2D	9.90	1.50	1.39
25	3	601	CHL	C1D-C2D	9.90	1.50	1.39
25	5	607	CHL	C1D-C2D	9.89	1.50	1.39
25	r	606	CHL	C1D-C2D	9.89	1.50	1.39
25	s	606	CHL	C1D-C2D	9.88	1.50	1.39
25	S	606	CHL	C1D-C2D	9.88	1.50	1.39
25	g	605	CHL	C2C-C3C	9.86	1.45	1.36
25	R	607	CHL	C2C-C3C	9.85	1.45	1.36
25	3	609	CHL	C1D-C2D	9.85	1.50	1.39
25	7	609	CHL	C1D-C2D	9.85	1.50	1.39
25	7	601	CHL	C1D-C2D	9.85	1.50	1.39
25	7	605	CHL	C1D-C2D	9.83	1.50	1.39
25	r	607	CHL	C2C-C3C	9.81	1.45	1.36
25	3	605	CHL	C1D-C2D	9.78	1.50	1.39
25	5	608	CHL	C2C-C3C	9.77	1.45	1.36
25	8	608	CHL	C2C-C3C	9.77	1.45	1.36
25	N	607	CHL	C2C-C3C	9.75	1.45	1.36
25	n	607	CHL	C2C-C3C	9.75	1.45	1.36
25	g	601	CHL	C1D-C2D	9.74	1.50	1.39
25	2	605	CHL	C1D-C2D	9.73	1.50	1.39
25	6	605	CHL	C1D-C2D	9.73	1.50	1.39
25	G	601	CHL	C1D-C2D	9.73	1.50	1.39
25	1	608	CHL	C2C-C3C	9.72	1.45	1.36
25	2	601	CHL	C2C-C3C	9.71	1.45	1.36
25	6	601	CHL	C2C-C3C	9.70	1.45	1.36
25	5	605	CHL	C2C-C3C	9.69	1.45	1.36
25	4	608	CHL	C2C-C3C	9.69	1.45	1.36
25	1	605	CHL	C2C-C3C	9.69	1.45	1.36
25	4	606	CHL	C1D-C2D	9.69	1.50	1.39
25	8	606	CHL	C1D-C2D	9.69	1.50	1.39
25	G	606	CHL	C1D-C2D	9.66	1.50	1.39
25	g	606	CHL	C1D-C2D	9.66	1.50	1.39
25	5	609	CHL	C1D-C2D	9.65	1.50	1.39
25	y	607	CHL	C2C-C3C	9.63	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	601	CHL	C1D-C2D	9.62	1.50	1.39
25	1	609	CHL	C1D-C2D	9.62	1.50	1.39
25	Y	607	CHL	C2C-C3C	9.61	1.45	1.36
25	S	601	CHL	C1D-C2D	9.61	1.50	1.39
25	g	609	CHL	C1D-C2D	9.57	1.50	1.39
25	5	605	CHL	C1D-C2D	9.56	1.50	1.39
25	G	609	CHL	C1D-C2D	9.54	1.50	1.39
25	Y	609	CHL	C1D-C2D	9.51	1.50	1.39
25	6	607	CHL	C1D-C2D	9.51	1.50	1.39
25	1	605	CHL	C1D-C2D	9.50	1.50	1.39
25	y	609	CHL	C1D-C2D	9.50	1.50	1.39
25	2	608	CHL	C1D-C2D	9.50	1.50	1.39
25	6	608	CHL	C1D-C2D	9.50	1.50	1.39
25	2	607	CHL	C1D-C2D	9.48	1.50	1.39
25	N	607	CHL	C1A-CHA	9.47	1.50	1.40
25	n	607	CHL	C1A-CHA	9.47	1.50	1.40
25	N	608	CHL	C2C-C3C	9.46	1.45	1.36
25	S	607	CHL	C1D-C2D	9.44	1.50	1.39
25	2	606	CHL	C1D-C2D	9.43	1.50	1.39
25	6	606	CHL	C1D-C2D	9.43	1.50	1.39
25	s	607	CHL	C1D-C2D	9.43	1.50	1.39
25	G	608	CHL	C1D-C2D	9.42	1.50	1.39
25	3	601	CHL	C2C-C3C	9.41	1.45	1.36
25	7	601	CHL	C2C-C3C	9.40	1.45	1.36
25	N	609	CHL	C1D-C2D	9.40	1.50	1.39
25	n	609	CHL	C1D-C2D	9.40	1.50	1.39
25	g	608	CHL	C1D-C2D	9.39	1.50	1.39
25	n	608	CHL	C2C-C3C	9.39	1.45	1.36
25	G	601	CHL	C2C-C3C	9.38	1.45	1.36
25	g	601	CHL	C2C-C3C	9.38	1.45	1.36
25	G	607	CHL	C1D-C2D	9.24	1.50	1.39
25	g	607	CHL	C1D-C2D	9.23	1.50	1.39
25	2	609	CHL	C1D-C2D	9.21	1.50	1.39
25	Y	606	CHL	C2C-C3C	9.19	1.45	1.36
25	y	606	CHL	C2C-C3C	9.18	1.45	1.36
25	6	609	CHL	C1D-C2D	9.17	1.50	1.39
25	S	607	CHL	C1A-CHA	9.17	1.50	1.40
25	s	607	CHL	C1A-CHA	9.17	1.50	1.40
25	n	606	CHL	C1D-C2D	9.16	1.50	1.39
25	Y	608	CHL	C2C-C3C	9.15	1.45	1.36
25	7	608	CHL	C1D-C2D	9.15	1.50	1.39
25	4	608	CHL	C1D-C2D	9.14	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	608	CHL	C1D-C2D	9.14	1.50	1.39
25	N	606	CHL	C1D-C2D	9.13	1.50	1.39
25	y	608	CHL	C2C-C3C	9.11	1.45	1.36
25	S	607	CHL	C2C-C3C	9.09	1.45	1.36
25	y	601	CHL	C2C-C3C	9.09	1.45	1.36
25	Y	601	CHL	C2C-C3C	9.08	1.45	1.36
25	N	601	CHL	C2C-C3C	9.08	1.45	1.36
25	8	608	CHL	C1D-C2D	9.08	1.49	1.39
25	n	601	CHL	C2C-C3C	9.08	1.45	1.36
25	5	608	CHL	C1D-C2D	9.08	1.49	1.39
25	R	607	CHL	C1D-C2D	9.05	1.49	1.39
25	r	607	CHL	C1D-C2D	9.05	1.49	1.39
25	7	606	CHL	C1D-C2D	9.04	1.49	1.39
25	s	607	CHL	C2C-C3C	9.03	1.45	1.36
25	1	606	CHL	C1D-C2D	9.03	1.49	1.39
25	1	608	CHL	C1D-C2D	9.03	1.49	1.39
25	Y	605	CHL	C1D-C2D	9.02	1.49	1.39
25	3	606	CHL	C1D-C2D	9.02	1.49	1.39
25	y	607	CHL	C1A-CHA	9.00	1.50	1.40
25	y	605	CHL	C1D-C2D	9.00	1.49	1.39
25	5	606	CHL	C1D-C2D	8.99	1.49	1.39
25	Y	607	CHL	C1A-CHA	8.97	1.50	1.40
25	4	601	CHL	C1A-CHA	8.97	1.50	1.40
25	N	608	CHL	C1D-C2D	8.96	1.49	1.39
25	n	608	CHL	C1D-C2D	8.96	1.49	1.39
25	S	606	CHL	C3B-C4B	8.94	1.50	1.41
25	s	606	CHL	C3B-C4B	8.93	1.50	1.41
25	8	601	CHL	C1A-CHA	8.92	1.50	1.40
25	2	607	CHL	C1A-CHA	8.89	1.50	1.40
25	6	607	CHL	C1A-CHA	8.87	1.50	1.40
25	7	606	CHL	C2C-C3C	8.86	1.45	1.36
25	3	606	CHL	C2C-C3C	8.79	1.44	1.36
25	S	608	CHL	C1D-C2D	8.79	1.49	1.39
25	s	608	CHL	C1D-C2D	8.79	1.49	1.39
25	N	605	CHL	C1D-C2D	8.78	1.49	1.39
25	n	605	CHL	C1D-C2D	8.78	1.49	1.39
25	y	608	CHL	C1D-C2D	8.77	1.49	1.39
25	Y	608	CHL	C1D-C2D	8.75	1.49	1.39
35	a	409	PHO	C3B-C4B	8.73	1.50	1.41
25	R	608	CHL	C1A-CHA	8.72	1.49	1.40
25	r	608	CHL	C1A-CHA	8.70	1.49	1.40
25	G	605	CHL	C3B-C4B	8.69	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	605	CHL	C3B-C4B	8.66	1.49	1.41
35	A	409	PHO	C3B-C4B	8.66	1.50	1.41
25	n	608	CHL	C3B-C4B	8.64	1.49	1.41
25	3	605	CHL	C1A-CHA	8.60	1.49	1.40
25	G	609	CHL	C1A-CHA	8.60	1.49	1.40
25	g	609	CHL	C1A-CHA	8.60	1.49	1.40
25	7	605	CHL	C1B-C2B	8.59	1.49	1.39
25	N	608	CHL	C3B-C4B	8.58	1.49	1.41
25	3	607	CHL	C1A-CHA	8.58	1.49	1.40
25	7	607	CHL	C1A-CHA	8.58	1.49	1.40
25	7	605	CHL	C1A-CHA	8.57	1.49	1.40
35	a	408	PHO	C1B-C2B	8.55	1.48	1.39
25	3	605	CHL	C1B-C2B	8.54	1.49	1.39
25	N	605	CHL	C1A-CHA	8.53	1.49	1.40
25	n	605	CHL	C1A-CHA	8.53	1.49	1.40
35	A	408	PHO	C1B-C2B	8.52	1.48	1.39
25	8	601	CHL	C1B-C2B	8.51	1.49	1.39
25	G	608	CHL	C3B-C4B	8.47	1.49	1.41
25	4	601	CHL	C1B-C2B	8.45	1.49	1.39
25	N	601	CHL	C3B-C4B	8.42	1.49	1.41
25	R	614	CHL	C1B-C2B	8.40	1.49	1.39
25	r	614	CHL	C1B-C2B	8.40	1.49	1.39
25	n	601	CHL	C3B-C4B	8.39	1.49	1.41
25	g	608	CHL	C3B-C4B	8.39	1.49	1.41
25	3	601	CHL	C3B-C4B	8.36	1.49	1.41
25	7	601	CHL	C3B-C4B	8.34	1.49	1.41
25	s	608	CHL	C1B-C2B	8.33	1.49	1.39
25	S	608	CHL	C1B-C2B	8.31	1.49	1.39
25	2	609	CHL	C1B-C2B	8.30	1.49	1.39
25	6	609	CHL	C1B-C2B	8.27	1.49	1.39
25	2	605	CHL	C1A-CHA	8.27	1.49	1.40
25	r	608	CHL	C1D-C2D	8.26	1.48	1.39
25	R	608	CHL	C1D-C2D	8.24	1.48	1.39
25	6	605	CHL	C1A-CHA	8.24	1.49	1.40
25	6	609	CHL	C1A-CHA	8.24	1.49	1.40
25	Y	605	CHL	C1A-CHA	8.23	1.49	1.40
25	2	605	CHL	C1B-C2B	8.23	1.48	1.39
25	6	605	CHL	C1B-C2B	8.23	1.48	1.39
25	1	607	CHL	C1A-CHA	8.23	1.49	1.40
25	5	607	CHL	C1A-CHA	8.23	1.49	1.40
25	2	609	CHL	C1A-CHA	8.22	1.49	1.40
25	r	606	CHL	C3B-C4B	8.22	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	608	CHL	C1A-CHA	8.21	1.49	1.40
25	R	614	CHL	C1A-CHA	8.18	1.49	1.40
25	r	614	CHL	C1A-CHA	8.18	1.49	1.40
25	1	605	CHL	C1B-C2B	8.16	1.48	1.39
25	8	607	CHL	C1B-C2B	8.15	1.48	1.39
25	5	608	CHL	C1A-CHA	8.15	1.49	1.40
25	y	605	CHL	C1A-CHA	8.15	1.49	1.40
25	R	606	CHL	C3B-C4B	8.14	1.49	1.41
25	5	605	CHL	C1B-C2B	8.13	1.48	1.39
25	2	601	CHL	C3B-C4B	8.13	1.49	1.41
25	G	601	CHL	C3B-C4B	8.13	1.49	1.41
25	4	607	CHL	C1B-C2B	8.13	1.48	1.39
25	g	601	CHL	C3B-C4B	8.13	1.49	1.41
25	6	607	CHL	C1B-C2B	8.12	1.48	1.39
25	6	601	CHL	C3B-C4B	8.12	1.49	1.41
25	7	608	CHL	C1B-C2B	8.10	1.48	1.39
25	1	601	CHL	C1B-C2B	8.09	1.48	1.39
25	5	601	CHL	C1B-C2B	8.09	1.48	1.39
25	3	608	CHL	C1B-C2B	8.09	1.48	1.39
25	5	608	CHL	C3B-C4B	8.09	1.49	1.41
25	r	607	CHL	C1A-CHA	8.09	1.49	1.40
25	N	605	CHL	C1B-C2B	8.09	1.48	1.39
25	n	605	CHL	C1B-C2B	8.09	1.48	1.39
25	R	607	CHL	C1A-CHA	8.08	1.49	1.40
25	2	607	CHL	C1B-C2B	8.08	1.48	1.39
25	n	606	CHL	C1A-CHA	8.07	1.49	1.40
25	y	608	CHL	C3B-C4B	8.07	1.49	1.41
25	5	607	CHL	C1B-C2B	8.06	1.48	1.39
25	N	606	CHL	C1A-CHA	8.06	1.49	1.40
25	1	607	CHL	C1B-C2B	8.06	1.48	1.39
25	g	608	CHL	C1A-CHA	8.05	1.49	1.40
25	G	606	CHL	C1A-CHA	8.03	1.49	1.40
25	1	608	CHL	C3B-C4B	8.03	1.49	1.41
25	Y	608	CHL	C3B-C4B	8.02	1.49	1.41
25	G	608	CHL	C1A-CHA	8.00	1.49	1.40
25	2	606	CHL	C1A-CHA	8.00	1.49	1.40
25	g	606	CHL	C1A-CHA	7.99	1.49	1.40
25	4	608	CHL	C1B-C2B	7.98	1.48	1.39
25	y	605	CHL	C3B-C4B	7.98	1.49	1.41
25	y	606	CHL	C1A-CHA	7.98	1.49	1.40
25	s	608	CHL	C1A-CHA	7.97	1.49	1.40
25	N	607	CHL	C1D-C2D	7.97	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	608	CHL	C1B-C2B	7.97	1.48	1.39
25	y	601	CHL	C3B-C4B	7.97	1.49	1.41
25	n	607	CHL	C1D-C2D	7.97	1.48	1.39
25	G	605	CHL	C1A-CHA	7.96	1.49	1.40
25	3	607	CHL	C1B-C2B	7.95	1.48	1.39
25	S	608	CHL	C1A-CHA	7.94	1.49	1.40
25	Y	606	CHL	C1A-CHA	7.94	1.49	1.40
25	Y	601	CHL	C3B-C4B	7.94	1.49	1.41
25	S	607	CHL	C1B-C2B	7.94	1.48	1.39
25	g	605	CHL	C1A-CHA	7.93	1.49	1.40
25	Y	605	CHL	C3B-C4B	7.93	1.49	1.41
25	s	607	CHL	C1B-C2B	7.93	1.48	1.39
25	6	606	CHL	C1A-CHA	7.92	1.49	1.40
25	7	607	CHL	C1B-C2B	7.92	1.48	1.39
25	8	607	CHL	C1A-CHA	7.91	1.49	1.40
25	N	608	CHL	C1A-CHA	7.91	1.49	1.40
25	n	608	CHL	C1A-CHA	7.91	1.49	1.40
25	4	606	CHL	C1B-C2B	7.90	1.48	1.39
25	G	607	CHL	C1A-CHA	7.89	1.49	1.40
25	g	607	CHL	C1A-CHA	7.89	1.49	1.40
25	4	607	CHL	C1A-CHA	7.88	1.49	1.40
25	2	601	CHL	C1B-C2B	7.88	1.48	1.39
25	6	601	CHL	C1B-C2B	7.88	1.48	1.39
25	6	608	CHL	C1A-CHA	7.87	1.48	1.40
25	N	606	CHL	C1B-C2B	7.87	1.48	1.39
25	n	606	CHL	C1B-C2B	7.87	1.48	1.39
25	8	606	CHL	C3B-C4B	7.87	1.49	1.41
25	6	608	CHL	C1B-C2B	7.86	1.48	1.39
25	8	606	CHL	C1B-C2B	7.86	1.48	1.39
25	S	606	CHL	C1B-C2B	7.85	1.48	1.39
25	2	608	CHL	C1B-C2B	7.85	1.48	1.39
25	1	609	CHL	C1A-CHA	7.84	1.48	1.40
25	5	609	CHL	C1A-CHA	7.84	1.48	1.40
25	s	606	CHL	C1B-C2B	7.84	1.48	1.39
25	1	608	CHL	C1B-C2B	7.82	1.48	1.39
25	5	608	CHL	C1B-C2B	7.82	1.48	1.39
25	g	607	CHL	C3B-C4B	7.81	1.49	1.41
25	5	606	CHL	C1A-CHA	7.81	1.48	1.40
25	4	606	CHL	C3B-C4B	7.81	1.49	1.41
25	2	608	CHL	C1A-CHA	7.81	1.48	1.40
25	1	609	CHL	C1B-C2B	7.80	1.48	1.39
25	5	609	CHL	C1B-C2B	7.80	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	608	CHL	C3B-C4B	7.79	1.49	1.41
25	R	607	CHL	C3B-C4B	7.79	1.49	1.41
25	r	607	CHL	C3B-C4B	7.79	1.49	1.41
25	G	607	CHL	C3B-C4B	7.77	1.49	1.41
25	1	606	CHL	C1A-CHA	7.77	1.48	1.40
25	S	601	CHL	C3B-C4B	7.77	1.49	1.41
25	s	601	CHL	C3B-C4B	7.77	1.49	1.41
25	3	608	CHL	C1A-CHA	7.76	1.48	1.40
25	7	608	CHL	C1A-CHA	7.76	1.48	1.40
25	Y	607	CHL	C1D-C2D	7.75	1.48	1.39
25	s	606	CHL	C1A-CHA	7.74	1.48	1.40
25	N	609	CHL	C1A-CHA	7.73	1.48	1.40
25	n	609	CHL	C1A-CHA	7.73	1.48	1.40
25	Y	609	CHL	C1A-CHA	7.73	1.48	1.40
25	y	609	CHL	C1A-CHA	7.73	1.48	1.40
25	S	606	CHL	C1A-CHA	7.72	1.48	1.40
25	s	608	CHL	C3B-C4B	7.71	1.48	1.41
25	2	608	CHL	C3B-C4B	7.71	1.48	1.41
25	6	608	CHL	C3B-C4B	7.71	1.48	1.41
25	G	605	CHL	C1B-C2B	7.70	1.48	1.39
25	g	605	CHL	C1B-C2B	7.70	1.48	1.39
35	A	409	PHO	C1B-C2B	7.70	1.48	1.39
25	3	607	CHL	C3B-C4B	7.69	1.48	1.41
25	7	607	CHL	C3B-C4B	7.69	1.48	1.41
35	a	409	PHO	C1B-C2B	7.67	1.47	1.39
25	y	607	CHL	C1D-C2D	7.66	1.48	1.39
25	1	601	CHL	C3B-C4B	7.65	1.48	1.41
25	5	601	CHL	C3B-C4B	7.65	1.48	1.41
25	G	608	CHL	C1B-C2B	7.65	1.48	1.39
25	n	605	CHL	C3B-C4B	7.65	1.48	1.41
25	8	609	CHL	C1B-C2B	7.64	1.48	1.39
25	g	608	CHL	C1B-C2B	7.64	1.48	1.39
25	4	609	CHL	C1B-C2B	7.61	1.48	1.39
25	N	605	CHL	C3B-C4B	7.60	1.48	1.41
25	r	606	CHL	C1A-CHA	7.60	1.48	1.40
25	Y	605	CHL	C1B-C2B	7.58	1.48	1.39
25	y	605	CHL	C1B-C2B	7.58	1.48	1.39
25	N	601	CHL	C1B-C2B	7.57	1.48	1.39
25	n	601	CHL	C1B-C2B	7.57	1.48	1.39
25	R	606	CHL	C1A-CHA	7.56	1.48	1.40
25	2	606	CHL	C1B-C2B	7.55	1.48	1.39
25	4	601	CHL	C3B-C4B	7.53	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	601	CHL	C3B-C4B	7.53	1.48	1.41
25	1	605	CHL	C1A-CHA	7.52	1.48	1.40
25	5	605	CHL	C1A-CHA	7.52	1.48	1.40
25	6	606	CHL	C1B-C2B	7.50	1.48	1.39
25	4	606	CHL	C1A-CHA	7.48	1.48	1.40
35	a	408	PHO	C3B-C4B	7.48	1.49	1.41
25	3	606	CHL	C3B-C4B	7.47	1.48	1.41
25	y	601	CHL	C1B-C2B	7.46	1.48	1.39
25	Y	606	CHL	C1D-C2D	7.45	1.48	1.39
25	y	606	CHL	C1D-C2D	7.45	1.48	1.39
25	Y	601	CHL	C1B-C2B	7.44	1.48	1.39
25	4	608	CHL	C1A-CHA	7.44	1.48	1.40
25	8	608	CHL	C1A-CHA	7.44	1.48	1.40
35	A	408	PHO	C3B-C4B	7.43	1.49	1.41
25	7	606	CHL	C3B-C4B	7.42	1.48	1.41
25	N	608	CHL	C1B-C2B	7.42	1.48	1.39
25	n	608	CHL	C1B-C2B	7.42	1.48	1.39
25	6	605	CHL	C3B-C4B	7.42	1.48	1.41
25	8	606	CHL	C1A-CHA	7.42	1.48	1.40
25	2	606	CHL	C3B-C4B	7.41	1.48	1.41
25	6	606	CHL	C3B-C4B	7.41	1.48	1.41
25	G	601	CHL	C1B-C2B	7.41	1.48	1.39
25	g	601	CHL	C1B-C2B	7.41	1.48	1.39
25	3	606	CHL	C1A-CHA	7.41	1.48	1.40
25	y	608	CHL	C1A-CHA	7.41	1.48	1.40
25	8	609	CHL	C1A-CHA	7.39	1.48	1.40
25	R	606	CHL	C1B-C2B	7.38	1.47	1.39
25	4	609	CHL	C1A-CHA	7.38	1.48	1.40
25	Y	608	CHL	C1A-CHA	7.37	1.48	1.40
25	7	606	CHL	C1A-CHA	7.37	1.48	1.40
25	2	605	CHL	C3B-C4B	7.36	1.48	1.41
25	r	606	CHL	C1B-C2B	7.33	1.47	1.39
25	3	601	CHL	C1B-C2B	7.33	1.47	1.39
25	7	601	CHL	C1B-C2B	7.33	1.47	1.39
25	N	601	CHL	C1A-CHA	7.30	1.48	1.40
25	n	601	CHL	C1A-CHA	7.30	1.48	1.40
25	7	605	CHL	C3B-C4B	7.30	1.48	1.41
25	g	606	CHL	C1B-C2B	7.29	1.47	1.39
25	G	606	CHL	C1B-C2B	7.27	1.47	1.39
25	3	605	CHL	C3B-C4B	7.26	1.48	1.41
25	7	606	CHL	C1B-C2B	7.25	1.47	1.39
25	n	609	CHL	C3B-C4B	7.25	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	607	CHL	C1B-C2B	7.24	1.47	1.39
25	N	609	CHL	C3B-C4B	7.22	1.48	1.41
25	Y	601	CHL	C1A-CHA	7.19	1.48	1.40
25	s	607	CHL	C3B-C4B	7.19	1.48	1.41
25	r	607	CHL	C1B-C2B	7.18	1.47	1.39
25	3	606	CHL	C1B-C2B	7.17	1.47	1.39
25	3	609	CHL	C1B-C2B	7.17	1.47	1.39
25	G	609	CHL	C3B-C4B	7.15	1.48	1.41
25	5	605	CHL	C3B-C4B	7.14	1.48	1.41
25	5	606	CHL	C1B-C2B	7.14	1.47	1.39
25	7	609	CHL	C1B-C2B	7.14	1.47	1.39
25	1	605	CHL	C3B-C4B	7.13	1.48	1.41
25	y	601	CHL	C1A-CHA	7.13	1.48	1.40
25	2	607	CHL	C3B-C4B	7.13	1.48	1.41
25	1	606	CHL	C1B-C2B	7.12	1.47	1.39
25	g	606	CHL	C3B-C4B	7.12	1.48	1.41
25	S	607	CHL	C3B-C4B	7.11	1.48	1.41
25	G	606	CHL	C3B-C4B	7.10	1.48	1.41
25	G	601	CHL	C1A-CHA	7.10	1.48	1.40
25	g	601	CHL	C1A-CHA	7.10	1.48	1.40
25	6	607	CHL	C3B-C4B	7.10	1.48	1.41
25	3	609	CHL	C1A-CHA	7.09	1.48	1.40
25	7	609	CHL	C1A-CHA	7.09	1.48	1.40
25	g	609	CHL	C3B-C4B	7.08	1.48	1.41
25	N	607	CHL	C1B-C2B	7.07	1.47	1.39
25	n	607	CHL	C1B-C2B	7.05	1.47	1.39
25	3	609	CHL	C3B-C4B	7.03	1.48	1.41
25	7	609	CHL	C3B-C4B	7.03	1.48	1.41
25	4	607	CHL	C3B-C4B	6.98	1.48	1.41
25	5	607	CHL	C3B-C4B	6.97	1.48	1.41
25	y	607	CHL	C1B-C2B	6.97	1.47	1.39
25	1	607	CHL	C3B-C4B	6.94	1.48	1.41
25	Y	607	CHL	C1B-C2B	6.93	1.47	1.39
25	8	607	CHL	C3B-C4B	6.91	1.48	1.41
25	y	609	CHL	C3B-C4B	6.91	1.48	1.41
25	y	608	CHL	C1B-C2B	6.90	1.47	1.39
25	Y	609	CHL	C3B-C4B	6.90	1.48	1.41
25	4	609	CHL	C3B-C4B	6.89	1.48	1.41
25	8	609	CHL	C3B-C4B	6.89	1.48	1.41
25	6	601	CHL	C1A-CHA	6.89	1.47	1.40
25	2	601	CHL	C1A-CHA	6.89	1.47	1.40
25	n	606	CHL	C3B-C4B	6.89	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	608	CHL	C1B-C2B	6.88	1.47	1.39
25	2	609	CHL	C3B-C4B	6.86	1.48	1.41
25	6	609	CHL	C3B-C4B	6.84	1.48	1.41
25	G	607	CHL	C1B-C2B	6.83	1.47	1.39
25	g	607	CHL	C1B-C2B	6.82	1.47	1.39
25	N	606	CHL	C3B-C4B	6.80	1.48	1.41
25	1	601	CHL	C1A-CHA	6.80	1.47	1.40
25	5	601	CHL	C1A-CHA	6.80	1.47	1.40
25	r	608	CHL	C1B-C2B	6.76	1.47	1.39
25	S	601	CHL	C1A-CHA	6.76	1.47	1.40
25	s	601	CHL	C1A-CHA	6.76	1.47	1.40
25	3	608	CHL	C3B-C4B	6.76	1.48	1.41
25	R	608	CHL	C1B-C2B	6.75	1.47	1.39
25	1	606	CHL	C3B-C4B	6.74	1.48	1.41
25	R	608	CHL	C3D-C4D	-6.74	1.31	1.41
25	7	608	CHL	C3B-C4B	6.73	1.47	1.41
25	r	608	CHL	C3B-C4B	6.72	1.47	1.41
25	r	608	CHL	C3D-C4D	-6.72	1.31	1.41
25	Y	601	CHL	C3D-C4D	-6.71	1.31	1.41
25	y	601	CHL	C3D-C4D	-6.71	1.31	1.41
25	5	606	CHL	C3B-C4B	6.71	1.47	1.41
25	S	601	CHL	C1B-C2B	6.69	1.47	1.39
25	G	609	CHL	C1B-C2B	6.69	1.47	1.39
25	g	609	CHL	C1B-C2B	6.69	1.47	1.39
25	s	601	CHL	C1B-C2B	6.68	1.47	1.39
25	y	608	CHL	C3D-C4D	-6.67	1.31	1.41
25	Y	608	CHL	C3D-C4D	-6.67	1.31	1.41
25	Y	606	CHL	C1B-C2B	6.65	1.47	1.39
25	y	606	CHL	C1B-C2B	6.65	1.47	1.39
25	R	608	CHL	C3B-C4B	6.65	1.47	1.41
25	S	606	CHL	C3A-C2A	-6.63	1.49	1.54
25	s	606	CHL	C3A-C2A	-6.59	1.49	1.54
25	3	601	CHL	C1A-CHA	6.59	1.47	1.40
25	7	601	CHL	C1A-CHA	6.59	1.47	1.40
25	4	608	CHL	C3B-C4B	6.57	1.47	1.41
25	8	608	CHL	C3B-C4B	6.57	1.47	1.41
25	Y	606	CHL	C3B-C4B	6.52	1.47	1.41
25	r	614	CHL	C3B-C4B	6.50	1.47	1.41
25	y	606	CHL	C3B-C4B	6.49	1.47	1.41
25	R	614	CHL	C3B-C4B	6.46	1.47	1.41
25	3	601	CHL	C3D-C4D	-6.37	1.31	1.41
25	7	601	CHL	C3D-C4D	-6.37	1.31	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	609	CHL	C3A-C2A	-6.36	1.49	1.54
25	n	609	CHL	C3A-C2A	-6.36	1.49	1.54
25	Y	609	CHL	C1B-C2B	6.35	1.46	1.39
25	S	601	CHL	C3D-C4D	-6.35	1.31	1.41
25	s	601	CHL	C3D-C4D	-6.35	1.31	1.41
25	y	609	CHL	C1B-C2B	6.33	1.46	1.39
25	G	601	CHL	C3D-C4D	-6.31	1.31	1.41
25	g	601	CHL	C3D-C4D	-6.31	1.31	1.41
25	y	606	CHL	C3D-C4D	-6.29	1.31	1.41
25	g	608	CHL	C3D-C4D	-6.27	1.32	1.41
25	n	601	CHL	C3D-C4D	-6.26	1.32	1.41
25	G	608	CHL	C3D-C4D	-6.25	1.32	1.41
25	Y	606	CHL	C3D-C4D	-6.24	1.32	1.41
25	Y	607	CHL	C3B-C4B	6.23	1.47	1.41
25	N	601	CHL	C3D-C4D	-6.22	1.32	1.41
25	1	601	CHL	C3D-C4D	-6.19	1.32	1.41
25	1	609	CHL	C3B-C4B	6.18	1.47	1.41
25	5	609	CHL	C3B-C4B	6.18	1.47	1.41
25	N	608	CHL	C3D-C4D	-6.17	1.32	1.41
25	n	608	CHL	C3D-C4D	-6.17	1.32	1.41
25	y	607	CHL	C3B-C4B	6.16	1.47	1.41
25	5	601	CHL	C3D-C4D	-6.16	1.32	1.41
25	6	601	CHL	C3D-C4D	-6.15	1.32	1.41
25	n	609	CHL	C1B-C2B	6.13	1.46	1.39
25	N	607	CHL	C3B-C4B	6.13	1.47	1.41
25	n	607	CHL	C3B-C4B	6.13	1.47	1.41
25	2	601	CHL	C3D-C4D	-6.12	1.32	1.41
25	N	609	CHL	C1B-C2B	6.09	1.46	1.39
25	R	606	CHL	C3D-C4D	-6.00	1.32	1.41
25	r	606	CHL	C3D-C4D	-6.00	1.32	1.41
25	7	606	CHL	C3D-C4D	-5.99	1.32	1.41
25	Y	609	CHL	C3D-C4D	-5.98	1.32	1.41
25	y	609	CHL	C3D-C4D	-5.98	1.32	1.41
25	Y	607	CHL	C3D-C4D	-5.96	1.32	1.41
25	S	608	CHL	C3D-C4D	-5.95	1.32	1.41
25	3	608	CHL	C3D-C4D	-5.94	1.32	1.41
25	3	606	CHL	C3D-C4D	-5.92	1.32	1.41
25	8	609	CHL	C3D-C4D	-5.92	1.32	1.41
25	1	608	CHL	C3D-C4D	-5.92	1.32	1.41
25	5	608	CHL	C3D-C4D	-5.92	1.32	1.41
25	y	607	CHL	C3D-C4D	-5.92	1.32	1.41
25	s	601	CHL	CHB-C4A	-5.92	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	608	CHL	C3D-C4D	-5.91	1.32	1.41
25	S	601	CHL	CHB-C4A	-5.91	1.31	1.38
25	s	608	CHL	C3D-C4D	-5.90	1.32	1.41
25	N	609	CHL	C3D-C4D	-5.89	1.32	1.41
25	n	609	CHL	C3D-C4D	-5.89	1.32	1.41
25	R	607	CHL	C3D-C4D	-5.87	1.32	1.41
25	r	607	CHL	C3D-C4D	-5.87	1.32	1.41
25	1	606	CHL	C3D-C4D	-5.86	1.32	1.41
25	4	609	CHL	C3D-C4D	-5.86	1.32	1.41
25	5	606	CHL	C3D-C4D	-5.85	1.32	1.41
25	G	607	CHL	C3A-C2A	-5.85	1.49	1.54
25	g	607	CHL	C3A-C2A	-5.85	1.49	1.54
25	Y	605	CHL	C3D-C4D	-5.85	1.32	1.41
25	1	609	CHL	C3D-C4D	-5.84	1.32	1.41
25	5	609	CHL	C3D-C4D	-5.84	1.32	1.41
25	4	608	CHL	C3D-C4D	-5.84	1.32	1.41
25	y	605	CHL	C3D-C4D	-5.83	1.32	1.41
25	G	607	CHL	C3D-C4D	-5.82	1.32	1.41
25	8	608	CHL	C3D-C4D	-5.81	1.32	1.41
25	3	609	CHL	C3D-C4D	-5.80	1.32	1.41
25	7	609	CHL	C3D-C4D	-5.80	1.32	1.41
25	4	606	CHL	C3D-C4D	-5.80	1.32	1.41
25	8	606	CHL	C3D-C4D	-5.79	1.32	1.41
25	g	607	CHL	C3D-C4D	-5.79	1.32	1.41
25	7	607	CHL	C3D-C4D	-5.78	1.32	1.41
25	y	607	CHL	C3A-C2A	-5.78	1.49	1.54
25	y	609	CHL	C3A-C2A	-5.77	1.49	1.54
25	Y	609	CHL	C3A-C2A	-5.77	1.49	1.54
25	2	608	CHL	C3D-C4D	-5.76	1.32	1.41
25	1	608	CHL	C3A-C2A	-5.75	1.49	1.54
25	5	608	CHL	C3A-C2A	-5.75	1.49	1.54
25	1	607	CHL	C3A-C2A	-5.74	1.49	1.54
25	6	608	CHL	C3D-C4D	-5.74	1.32	1.41
25	3	607	CHL	C3D-C4D	-5.74	1.32	1.41
25	Y	607	CHL	C3A-C2A	-5.74	1.49	1.54
25	1	605	CHL	C3D-C4D	-5.74	1.32	1.41
25	5	605	CHL	C3D-C4D	-5.74	1.32	1.41
25	5	607	CHL	C3A-C2A	-5.74	1.49	1.54
25	R	606	CHL	C3A-C2A	-5.74	1.49	1.54
25	r	606	CHL	C3A-C2A	-5.74	1.49	1.54
25	6	609	CHL	C3D-C4D	-5.72	1.32	1.41
25	6	606	CHL	C3D-C4D	-5.71	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	605	CHL	C3D-C4D	-5.71	1.32	1.41
25	N	605	CHL	C3D-C4D	-5.70	1.32	1.41
25	N	606	CHL	C3D-C4D	-5.70	1.32	1.41
25	n	606	CHL	C3D-C4D	-5.70	1.32	1.41
25	2	609	CHL	C3D-C4D	-5.67	1.32	1.41
25	2	606	CHL	C3D-C4D	-5.66	1.32	1.41
25	G	606	CHL	C3D-C4D	-5.65	1.32	1.41
25	N	609	CHL	CHB-C4A	-5.65	1.31	1.38
25	n	609	CHL	CHB-C4A	-5.65	1.31	1.38
25	1	606	CHL	C3A-C2A	-5.64	1.49	1.54
25	g	606	CHL	C3D-C4D	-5.64	1.32	1.41
25	7	606	CHL	C3A-C2A	-5.63	1.49	1.54
25	2	601	CHL	C3A-C2A	-5.62	1.49	1.54
25	8	607	CHL	C3D-C4D	-5.62	1.33	1.41
25	N	607	CHL	C3D-C4D	-5.61	1.33	1.41
25	n	607	CHL	C3D-C4D	-5.61	1.33	1.41
25	4	607	CHL	C3D-C4D	-5.60	1.33	1.41
25	6	601	CHL	C3A-C2A	-5.59	1.49	1.54
25	8	601	CHL	C3B-C2B	5.58	1.47	1.40
25	3	606	CHL	C3A-C2A	-5.58	1.49	1.54
25	3	601	CHL	C3A-C2A	-5.57	1.49	1.54
25	7	601	CHL	C3A-C2A	-5.57	1.49	1.54
25	g	607	CHL	CHB-C4A	-5.57	1.31	1.38
25	6	608	CHL	C3A-C2A	-5.56	1.49	1.54
25	1	605	CHL	C3A-C2A	-5.56	1.49	1.54
25	5	605	CHL	C3A-C2A	-5.56	1.49	1.54
25	5	606	CHL	C3A-C2A	-5.55	1.49	1.54
25	G	607	CHL	CHB-C4A	-5.54	1.31	1.38
25	4	601	CHL	C3B-C2B	5.53	1.47	1.40
25	g	605	CHL	C3D-C4D	-5.52	1.33	1.41
25	5	607	CHL	C3D-C4D	-5.52	1.33	1.41
25	2	608	CHL	C3A-C2A	-5.51	1.50	1.54
25	G	605	CHL	C3D-C4D	-5.50	1.33	1.41
25	1	609	CHL	C3A-C2A	-5.50	1.50	1.54
25	1	607	CHL	C3D-C4D	-5.49	1.33	1.41
25	Y	609	CHL	CHB-C4A	-5.48	1.32	1.38
25	R	614	CHL	C3D-C4D	-5.47	1.33	1.41
25	r	614	CHL	C3D-C4D	-5.47	1.33	1.41
25	5	609	CHL	C3A-C2A	-5.47	1.50	1.54
25	3	601	CHL	CHB-C4A	-5.45	1.32	1.38
25	7	601	CHL	CHB-C4A	-5.44	1.32	1.38
25	G	609	CHL	C3D-C4D	-5.43	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	609	CHL	C3D-C4D	-5.43	1.33	1.41
25	y	609	CHL	CHB-C4A	-5.42	1.32	1.38
25	7	605	CHL	C3D-C4D	-5.41	1.33	1.41
25	Y	601	CHL	CHB-C4A	-5.40	1.32	1.38
25	y	601	CHL	CHB-C4A	-5.40	1.32	1.38
25	3	605	CHL	C3D-C4D	-5.40	1.33	1.41
25	8	601	CHL	C3D-C4D	-5.40	1.33	1.41
25	G	605	CHL	CHC-C4B	5.39	1.48	1.39
25	6	607	CHL	C3D-C4D	-5.39	1.33	1.41
25	R	614	CHL	OBD-CAD	5.39	1.29	1.22
25	r	614	CHL	OBD-CAD	5.39	1.29	1.22
25	N	608	CHL	C3A-C2A	-5.39	1.50	1.54
25	n	608	CHL	C3A-C2A	-5.39	1.50	1.54
25	G	601	CHL	CHB-C4A	-5.37	1.32	1.38
25	r	608	CHL	C3A-C2A	-5.37	1.50	1.54
25	4	601	CHL	C3D-C4D	-5.37	1.33	1.41
25	s	606	CHL	C3D-C4D	-5.37	1.33	1.41
25	S	606	CHL	C3D-C4D	-5.36	1.33	1.41
25	g	605	CHL	CHC-C4B	5.35	1.48	1.39
25	6	606	CHL	C3A-C2A	-5.35	1.50	1.54
25	g	601	CHL	CHB-C4A	-5.34	1.32	1.38
25	2	607	CHL	C3D-C4D	-5.34	1.33	1.41
25	s	601	CHL	C3A-C2A	-5.33	1.50	1.54
25	R	608	CHL	C3A-C2A	-5.33	1.50	1.54
25	G	609	CHL	C3A-C2A	-5.30	1.50	1.54
25	g	609	CHL	C3A-C2A	-5.30	1.50	1.54
25	Y	608	CHL	C3A-C2A	-5.30	1.50	1.54
25	4	608	CHL	C3A-C2A	-5.30	1.50	1.54
25	S	606	CHL	CHC-C4B	5.29	1.48	1.39
25	s	606	CHL	CHC-C4B	5.29	1.48	1.39
25	Y	607	CHL	CHB-C4A	-5.28	1.32	1.38
25	S	601	CHL	C3A-C2A	-5.28	1.50	1.54
25	g	605	CHL	OBD-CAD	5.27	1.29	1.22
25	G	606	CHL	O2D-CGD	5.27	1.46	1.33
25	8	608	CHL	C3A-C2A	-5.27	1.50	1.54
25	2	606	CHL	C3A-C2A	-5.26	1.50	1.54
38	D	405	PL9	C7-C3	-5.26	1.44	1.51
25	y	607	CHL	CHB-C4A	-5.26	1.32	1.38
25	S	607	CHL	C3D-C4D	-5.25	1.33	1.41
25	G	609	CHL	CHB-C4A	-5.25	1.32	1.38
25	4	606	CHL	C3A-C2A	-5.25	1.50	1.54
25	y	608	CHL	C3A-C2A	-5.24	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	d	405	PL9	C7-C3	-5.24	1.44	1.51
25	G	606	CHL	C3A-C2A	-5.24	1.50	1.54
25	2	605	CHL	C3D-C4D	-5.24	1.33	1.41
25	6	605	CHL	C3D-C4D	-5.24	1.33	1.41
25	g	606	CHL	O2D-CGD	5.23	1.46	1.33
25	N	605	CHL	OBD-CAD	5.23	1.29	1.22
25	n	605	CHL	OBD-CAD	5.23	1.29	1.22
25	g	609	CHL	CHB-C4A	-5.22	1.32	1.38
25	G	605	CHL	OBD-CAD	5.21	1.29	1.22
25	8	606	CHL	C3A-C2A	-5.21	1.50	1.54
25	s	607	CHL	C3D-C4D	-5.20	1.33	1.41
25	g	605	CHL	C3A-C2A	-5.20	1.50	1.54
25	g	606	CHL	C3A-C2A	-5.19	1.50	1.54
25	G	605	CHL	C3A-C2A	-5.19	1.50	1.54
25	5	601	CHL	C3A-C2A	-5.17	1.50	1.54
25	6	605	CHL	C3B-C2B	5.12	1.47	1.40
25	1	601	CHL	C3A-C2A	-5.12	1.50	1.54
25	3	608	CHL	C3A-C2A	-5.12	1.50	1.54
25	3	605	CHL	O2D-CGD	5.11	1.45	1.33
25	7	605	CHL	O2D-CGD	5.11	1.45	1.33
25	s	601	CHL	O2D-CGD	5.09	1.45	1.33
25	2	605	CHL	C3B-C2B	5.09	1.47	1.40
25	2	605	CHL	O2D-CGD	5.09	1.45	1.33
25	5	601	CHL	O2D-CGD	5.09	1.45	1.33
25	4	609	CHL	C3A-C2A	-5.09	1.50	1.54
25	n	607	CHL	C3A-C2A	-5.08	1.50	1.54
25	2	601	CHL	O2D-CGD	5.08	1.45	1.33
25	n	601	CHL	O2D-CGD	5.08	1.45	1.33
25	S	601	CHL	O2D-CGD	5.08	1.45	1.33
25	7	608	CHL	C3A-C2A	-5.07	1.50	1.54
25	4	607	CHL	O2D-CGD	5.07	1.45	1.33
25	8	607	CHL	O2D-CGD	5.07	1.45	1.33
25	N	601	CHL	O2D-CGD	5.07	1.45	1.33
25	8	609	CHL	C3A-C2A	-5.06	1.50	1.54
25	6	605	CHL	O2D-CGD	5.06	1.45	1.33
25	1	601	CHL	O2D-CGD	5.06	1.45	1.33
25	6	606	CHL	O2D-CGD	5.06	1.45	1.33
25	S	607	CHL	O2D-CGD	5.05	1.45	1.33
25	s	607	CHL	O2D-CGD	5.05	1.45	1.33
25	N	608	CHL	CHB-C4A	-5.05	1.32	1.38
25	n	608	CHL	CHB-C4A	-5.05	1.32	1.38
25	6	601	CHL	O2D-CGD	5.05	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	606	CHL	O2D-CGD	5.05	1.45	1.33
25	N	607	CHL	C3A-C2A	-5.05	1.50	1.54
25	r	607	CHL	O2D-CGD	5.05	1.45	1.33
25	S	608	CHL	C3B-C2B	5.05	1.47	1.40
25	8	609	CHL	CHB-C4A	-5.03	1.32	1.38
25	5	606	CHL	O2D-CGD	5.03	1.45	1.33
25	6	609	CHL	CHB-C1B	5.03	1.47	1.39
25	R	607	CHL	C3A-C2A	-5.03	1.50	1.54
25	R	607	CHL	O2D-CGD	5.03	1.45	1.33
25	2	601	CHL	CHB-C4A	-5.03	1.32	1.38
25	6	601	CHL	CHB-C4A	-5.03	1.32	1.38
25	1	606	CHL	O2D-CGD	5.03	1.45	1.33
25	2	609	CHL	CHB-C1B	5.02	1.47	1.39
25	n	606	CHL	O2D-CGD	5.02	1.45	1.33
25	s	608	CHL	C3B-C2B	5.02	1.47	1.40
25	4	609	CHL	CHB-C4A	-5.01	1.32	1.38
25	G	606	CHL	OBD-CAD	5.01	1.28	1.22
25	g	606	CHL	OBD-CAD	5.01	1.28	1.22
25	N	606	CHL	C3B-C2B	5.01	1.47	1.40
25	r	607	CHL	C3A-C2A	-5.00	1.50	1.54
25	n	608	CHL	O2D-CGD	5.00	1.45	1.33
25	N	606	CHL	O2D-CGD	5.00	1.45	1.33
25	8	607	CHL	CHB-C1B	5.00	1.47	1.39
25	3	607	CHL	O2D-CGD	5.00	1.45	1.33
25	7	607	CHL	O2D-CGD	5.00	1.45	1.33
25	N	601	CHL	CHB-C4A	-4.99	1.32	1.38
25	n	601	CHL	CHB-C4A	-4.99	1.32	1.38
25	r	607	CHL	OBD-CAD	4.99	1.28	1.22
25	3	606	CHL	O2D-CGD	4.99	1.45	1.33
25	G	608	CHL	C3A-C2A	-4.99	1.50	1.54
25	n	606	CHL	C3B-C2B	4.98	1.47	1.40
25	n	609	CHL	O2D-CGD	4.98	1.45	1.33
25	7	606	CHL	O2D-CGD	4.98	1.45	1.33
25	N	608	CHL	O2D-CGD	4.98	1.45	1.33
25	5	607	CHL	CHB-C4A	-4.98	1.32	1.38
25	S	606	CHL	CHB-C1B	4.97	1.47	1.39
25	s	606	CHL	CHB-C1B	4.97	1.47	1.39
25	G	601	CHL	O2D-CGD	4.97	1.45	1.33
25	g	608	CHL	C3A-C2A	-4.97	1.50	1.54
25	R	607	CHL	OBD-CAD	4.97	1.28	1.22
25	2	607	CHL	O2D-CGD	4.97	1.45	1.33
25	4	606	CHL	O2D-CGD	4.96	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	607	CHL	CHB-C4A	-4.96	1.32	1.38
25	R	608	CHL	O2D-CGD	4.96	1.45	1.33
25	r	608	CHL	O2D-CGD	4.96	1.45	1.33
25	6	607	CHL	O2D-CGD	4.96	1.45	1.33
25	N	605	CHL	O2D-CGD	4.96	1.45	1.33
25	n	605	CHL	O2D-CGD	4.96	1.45	1.33
25	8	608	CHL	O2D-CGD	4.96	1.45	1.33
25	3	605	CHL	C3B-C2B	4.96	1.47	1.40
25	7	605	CHL	C3B-C2B	4.96	1.47	1.40
25	g	601	CHL	O2D-CGD	4.95	1.45	1.33
25	N	609	CHL	O2D-CGD	4.95	1.45	1.33
25	s	606	CHL	O2D-CGD	4.95	1.45	1.33
25	8	606	CHL	O2D-CGD	4.95	1.45	1.33
25	r	607	CHL	CHB-C4A	-4.95	1.32	1.38
25	S	606	CHL	O2D-CGD	4.95	1.45	1.33
25	4	607	CHL	CHB-C1B	4.95	1.47	1.39
25	G	608	CHL	O2D-CGD	4.94	1.45	1.33
25	g	608	CHL	O2D-CGD	4.94	1.45	1.33
25	4	608	CHL	O2D-CGD	4.94	1.45	1.33
25	1	607	CHL	CHB-C4A	-4.94	1.32	1.38
25	3	601	CHL	O2D-CGD	4.93	1.45	1.33
25	7	601	CHL	O2D-CGD	4.93	1.45	1.33
25	2	609	CHL	OBD-CAD	4.93	1.28	1.22
25	6	609	CHL	OBD-CAD	4.93	1.28	1.22
25	7	605	CHL	C3A-C2A	-4.93	1.50	1.54
25	1	605	CHL	O2D-CGD	4.93	1.45	1.33
25	4	609	CHL	O2D-CGD	4.93	1.45	1.33
25	5	605	CHL	O2D-CGD	4.93	1.45	1.33
25	3	605	CHL	C3A-C2A	-4.92	1.50	1.54
25	N	607	CHL	CHB-C4A	-4.91	1.32	1.38
25	2	605	CHL	C3A-C2A	-4.90	1.50	1.54
25	N	601	CHL	C3A-C2A	-4.90	1.50	1.54
25	8	609	CHL	O2D-CGD	4.90	1.45	1.33
25	n	607	CHL	CHB-C4A	-4.89	1.32	1.38
25	3	609	CHL	O2D-CGD	4.89	1.45	1.33
25	1	601	CHL	CHD-C4C	4.89	1.48	1.39
25	5	601	CHL	CHD-C4C	4.89	1.48	1.39
25	2	608	CHL	C3B-C2B	4.89	1.47	1.40
25	Y	605	CHL	C3A-C2A	-4.88	1.50	1.54
25	1	601	CHL	CHD-C1D	4.88	1.47	1.39
25	2	605	CHL	OBD-CAD	4.87	1.28	1.22
25	4	601	CHL	OBD-CAD	4.87	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	606	CHL	OBD-CAD	4.87	1.28	1.22
25	2	609	CHL	O2D-CGD	4.87	1.45	1.33
25	6	609	CHL	O2D-CGD	4.87	1.45	1.33
25	y	605	CHL	C3A-C2A	-4.87	1.50	1.54
25	7	609	CHL	O2D-CGD	4.87	1.45	1.33
25	6	608	CHL	C3B-C2B	4.87	1.47	1.40
25	3	605	CHL	CHC-C4B	4.87	1.47	1.39
25	7	605	CHL	CHC-C4B	4.87	1.47	1.39
25	8	601	CHL	OBD-CAD	4.86	1.28	1.22
25	3	605	CHL	OBD-CAD	4.86	1.28	1.22
25	S	607	CHL	CHB-C4A	-4.86	1.32	1.38
25	S	607	CHL	OBD-CAD	4.86	1.28	1.22
25	S	606	CHL	OBD-CAD	4.86	1.28	1.22
25	s	606	CHL	OBD-CAD	4.86	1.28	1.22
25	5	601	CHL	C3B-C2B	4.85	1.46	1.40
25	7	609	CHL	C3A-C2A	-4.85	1.50	1.54
25	1	601	CHL	C3B-C2B	4.85	1.46	1.40
25	s	607	CHL	OBD-CAD	4.85	1.28	1.22
25	5	601	CHL	CHD-C1D	4.85	1.47	1.39
25	6	605	CHL	C3A-C2A	-4.85	1.50	1.54
25	8	601	CHL	CHD-C1D	4.84	1.47	1.39
25	3	607	CHL	O2A-CGA	4.84	1.47	1.33
25	7	607	CHL	O2A-CGA	4.84	1.47	1.33
25	2	605	CHL	CHC-C4B	4.84	1.47	1.39
25	4	601	CHL	CHC-C4B	4.84	1.47	1.39
25	8	601	CHL	CHC-C4B	4.84	1.47	1.39
25	7	609	CHL	CHD-C1D	4.84	1.47	1.39
25	y	608	CHL	CHB-C4A	-4.84	1.32	1.38
25	3	609	CHL	C3A-C2A	-4.84	1.50	1.54
25	G	606	CHL	CHB-C4A	-4.84	1.32	1.38
25	Y	608	CHL	CHB-C4A	-4.84	1.32	1.38
25	Y	605	CHL	CHC-C4B	4.83	1.47	1.39
25	y	605	CHL	CHC-C4B	4.83	1.47	1.39
25	n	601	CHL	C3A-C2A	-4.83	1.50	1.54
25	1	607	CHL	O2D-CGD	4.83	1.45	1.33
25	4	606	CHL	OBD-CAD	4.82	1.28	1.22
25	8	606	CHL	OBD-CAD	4.82	1.28	1.22
25	4	607	CHL	OBD-CAD	4.82	1.28	1.22
25	3	609	CHL	CHD-C1D	4.82	1.47	1.39
25	r	608	CHL	CHB-C4A	-4.82	1.32	1.38
25	6	605	CHL	OBD-CAD	4.82	1.28	1.22
25	2	606	CHL	OBD-CAD	4.81	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	608	CHL	CHB-C4A	-4.81	1.32	1.38
25	6	605	CHL	CHC-C4B	4.81	1.47	1.39
25	G	601	CHL	C3A-C2A	-4.81	1.50	1.54
25	g	601	CHL	C3A-C2A	-4.81	1.50	1.54
25	s	607	CHL	CHB-C4A	-4.81	1.32	1.38
25	5	607	CHL	O2D-CGD	4.81	1.45	1.33
25	g	606	CHL	CHB-C4A	-4.81	1.32	1.38
25	7	607	CHL	OBD-CAD	4.80	1.28	1.22
25	G	609	CHL	O2D-CGD	4.80	1.45	1.33
25	G	607	CHL	OBD-CAD	4.80	1.28	1.22
25	8	607	CHL	OBD-CAD	4.80	1.28	1.22
25	r	614	CHL	C2A-C3A	-4.80	1.50	1.54
25	4	601	CHL	O2D-CGD	4.80	1.45	1.30
25	8	601	CHL	O2D-CGD	4.80	1.45	1.30
25	4	601	CHL	CHD-C1D	4.80	1.47	1.39
25	2	608	CHL	O2D-CGD	4.80	1.45	1.33
25	g	609	CHL	O2D-CGD	4.80	1.45	1.33
25	3	607	CHL	CHD-C1D	4.79	1.47	1.39
25	y	605	CHL	O2D-CGD	4.79	1.45	1.33
25	7	605	CHL	OBD-CAD	4.79	1.28	1.22
25	7	601	CHL	CHC-C4B	4.79	1.47	1.39
25	Y	606	CHL	O2D-CGD	4.79	1.45	1.33
25	y	606	CHL	O2D-CGD	4.79	1.45	1.33
25	g	607	CHL	OBD-CAD	4.79	1.28	1.22
25	s	608	CHL	CHB-C1B	4.78	1.47	1.39
25	Y	605	CHL	O2D-CGD	4.78	1.45	1.33
25	N	605	CHL	CHB-C4A	-4.78	1.32	1.38
25	7	607	CHL	CHB-C4A	-4.78	1.32	1.38
25	1	608	CHL	O2D-CGD	4.78	1.45	1.33
25	5	608	CHL	O2D-CGD	4.78	1.45	1.33
25	6	608	CHL	O2D-CGD	4.77	1.45	1.33
25	3	607	CHL	CHB-C4A	-4.77	1.32	1.38
25	4	601	CHL	CHB-C1B	4.77	1.47	1.39
25	8	601	CHL	CHB-C1B	4.77	1.47	1.39
25	S	608	CHL	CHB-C1B	4.77	1.47	1.39
25	8	606	CHL	CHB-C4A	-4.77	1.32	1.38
25	3	608	CHL	O2D-CGD	4.76	1.44	1.33
25	3	607	CHL	OBD-CAD	4.76	1.28	1.22
25	2	608	CHL	CHC-C4B	4.76	1.47	1.39
25	1	605	CHL	C3B-C2B	4.76	1.46	1.40
25	7	608	CHL	O2D-CGD	4.75	1.44	1.33
25	Y	601	CHL	CHD-C4C	4.75	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	601	CHL	CHD-C4C	4.75	1.48	1.39
25	2	607	CHL	OBD-CAD	4.75	1.28	1.22
25	R	614	CHL	C2A-C3A	-4.75	1.50	1.54
25	Y	606	CHL	CHB-C4A	-4.75	1.32	1.38
25	3	601	CHL	CHC-C4B	4.75	1.47	1.39
25	7	607	CHL	CHD-C1D	4.75	1.47	1.39
25	2	608	CHL	CHB-C1B	4.75	1.47	1.39
25	6	608	CHL	CHB-C1B	4.75	1.47	1.39
25	r	606	CHL	O2D-CGD	4.75	1.44	1.33
25	G	607	CHL	O2D-CGD	4.75	1.44	1.33
25	3	609	CHL	OBD-CAD	4.75	1.28	1.22
25	7	609	CHL	OBD-CAD	4.75	1.28	1.22
25	6	608	CHL	CHC-C4B	4.74	1.47	1.39
25	r	606	CHL	CHB-C4A	-4.74	1.32	1.38
25	4	601	CHL	CHD-C4C	4.74	1.48	1.39
25	1	609	CHL	O2D-CGD	4.74	1.44	1.33
25	4	608	CHL	CHB-C1B	4.74	1.47	1.39
25	8	608	CHL	CHB-C1B	4.74	1.47	1.39
25	5	605	CHL	C3B-C2B	4.74	1.46	1.40
25	3	606	CHL	CHB-C4A	-4.74	1.32	1.38
25	4	606	CHL	CHB-C4A	-4.74	1.32	1.38
25	7	606	CHL	CHB-C4A	-4.74	1.32	1.38
25	G	605	CHL	O2D-CGD	4.74	1.44	1.33
25	8	608	CHL	CHC-C4B	4.73	1.47	1.39
25	3	608	CHL	C3B-C2B	4.73	1.46	1.40
25	g	607	CHL	CHC-C1C	4.73	1.48	1.39
25	1	606	CHL	CHB-C4A	-4.73	1.32	1.38
25	5	609	CHL	O2D-CGD	4.73	1.44	1.33
25	8	601	CHL	CHD-C4C	4.72	1.48	1.39
25	R	606	CHL	O2D-CGD	4.72	1.44	1.33
25	7	609	CHL	CHB-C4A	-4.72	1.32	1.38
25	n	605	CHL	CHB-C4A	-4.72	1.32	1.38
25	Y	601	CHL	C3A-C2A	-4.72	1.50	1.54
25	8	609	CHL	CHD-C1D	4.72	1.47	1.39
25	3	609	CHL	CHB-C4A	-4.72	1.32	1.38
25	N	606	CHL	CHB-C1B	4.72	1.47	1.39
25	g	605	CHL	O2D-CGD	4.71	1.44	1.33
25	y	609	CHL	O2D-CGD	4.71	1.44	1.33
25	G	606	CHL	C3B-C2B	4.71	1.46	1.40
25	g	606	CHL	C3B-C2B	4.71	1.46	1.40
25	4	608	CHL	CHC-C4B	4.71	1.47	1.39
25	g	607	CHL	O2D-CGD	4.71	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	605	CHL	C3A-C2A	-4.71	1.50	1.54
25	n	605	CHL	C3A-C2A	-4.71	1.50	1.54
25	G	607	CHL	CHC-C1C	4.70	1.48	1.39
25	R	606	CHL	CHB-C4A	-4.70	1.33	1.38
25	7	608	CHL	C3B-C2B	4.70	1.46	1.40
25	2	605	CHL	CHB-C1B	4.70	1.47	1.39
25	6	605	CHL	CHB-C1B	4.70	1.47	1.39
25	y	606	CHL	CHB-C4A	-4.69	1.33	1.38
25	6	607	CHL	OBD-CAD	4.69	1.28	1.22
25	n	606	CHL	CHB-C1B	4.69	1.47	1.39
25	Y	609	CHL	O2D-CGD	4.69	1.44	1.33
25	5	606	CHL	CHB-C4A	-4.69	1.33	1.38
25	1	608	CHL	CHB-C1B	4.68	1.47	1.39
25	5	608	CHL	CHB-C1B	4.68	1.47	1.39
25	y	601	CHL	C3A-C2A	-4.68	1.50	1.54
25	g	606	CHL	CHC-C4B	4.68	1.47	1.39
25	5	607	CHL	OBD-CAD	4.68	1.28	1.22
25	G	606	CHL	CHC-C4B	4.68	1.47	1.39
25	1	605	CHL	OBD-CAD	4.68	1.28	1.22
25	3	607	CHL	C3B-C2B	4.68	1.46	1.40
25	4	609	CHL	CHD-C1D	4.68	1.47	1.39
25	1	607	CHL	OBD-CAD	4.67	1.28	1.22
25	3	608	CHL	CHB-C4A	-4.67	1.33	1.38
25	y	607	CHL	O2D-CGD	4.67	1.44	1.33
25	Y	606	CHL	C3A-C2A	-4.67	1.50	1.54
25	y	606	CHL	C3A-C2A	-4.67	1.50	1.54
25	r	606	CHL	OBD-CAD	4.66	1.28	1.22
25	3	607	CHL	CHD-C4C	4.66	1.48	1.39
25	5	608	CHL	CHC-C4B	4.66	1.47	1.39
25	y	601	CHL	O2D-CGD	4.66	1.44	1.33
25	4	607	CHL	CHD-C4C	4.66	1.48	1.39
25	G	607	CHL	CHC-C4B	4.66	1.47	1.39
25	g	607	CHL	CHC-C4B	4.66	1.47	1.39
25	6	607	CHL	C3A-C2A	-4.66	1.50	1.54
25	7	608	CHL	CHB-C4A	-4.66	1.33	1.38
25	2	601	CHL	CHD-C4C	4.66	1.48	1.39
25	1	608	CHL	CHC-C4B	4.66	1.47	1.39
25	y	606	CHL	C3B-C2B	4.65	1.46	1.40
25	5	605	CHL	OBD-CAD	4.65	1.28	1.22
25	7	607	CHL	CHD-C4C	4.65	1.48	1.39
25	6	601	CHL	CHD-C4C	4.65	1.48	1.39
25	G	608	CHL	CHB-C4A	-4.65	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	608	CHL	O2D-CGD	4.64	1.44	1.33
25	S	601	CHL	CHD-C1D	4.64	1.47	1.39
25	G	605	CHL	CHC-C1C	4.64	1.48	1.39
25	Y	601	CHL	O2D-CGD	4.64	1.44	1.33
25	R	614	CHL	O2D-CGD	4.64	1.44	1.33
25	r	614	CHL	O2D-CGD	4.64	1.44	1.33
25	R	614	CHL	CHB-C1B	4.64	1.47	1.39
25	7	607	CHL	C3B-C2B	4.64	1.46	1.40
25	g	608	CHL	CHB-C4A	-4.64	1.33	1.38
25	Y	607	CHL	O2D-CGD	4.64	1.44	1.33
25	6	609	CHL	C3A-C2A	-4.64	1.50	1.54
25	3	605	CHL	CHB-C1B	4.64	1.47	1.39
25	Y	606	CHL	C3B-C2B	4.63	1.46	1.40
25	G	605	CHL	CHB-C4A	-4.63	1.33	1.38
25	g	605	CHL	CHB-C4A	-4.63	1.33	1.38
25	g	605	CHL	CHC-C1C	4.63	1.48	1.39
25	8	607	CHL	CHD-C4C	4.63	1.48	1.39
25	r	614	CHL	CHB-C1B	4.63	1.47	1.39
25	2	606	CHL	CHB-C4A	-4.63	1.33	1.38
25	6	606	CHL	CHB-C4A	-4.63	1.33	1.38
25	2	609	CHL	C3A-C2A	-4.63	1.50	1.54
25	1	606	CHL	OBD-CAD	4.63	1.28	1.22
25	5	606	CHL	OBD-CAD	4.63	1.28	1.22
25	G	605	CHL	C3B-C2B	4.63	1.46	1.40
25	g	605	CHL	C3B-C2B	4.63	1.46	1.40
25	Y	608	CHL	O2D-CGD	4.62	1.44	1.33
25	5	601	CHL	CHB-C4A	-4.62	1.33	1.38
25	5	605	CHL	CHB-C4A	-4.62	1.33	1.38
25	R	606	CHL	OBD-CAD	4.62	1.28	1.22
25	3	609	CHL	CHD-C4C	4.62	1.48	1.39
25	7	609	CHL	CHD-C4C	4.62	1.48	1.39
25	7	605	CHL	CHB-C1B	4.62	1.47	1.39
25	N	601	CHL	CHC-C4B	4.62	1.47	1.39
25	n	601	CHL	CHC-C4B	4.62	1.47	1.39
25	s	601	CHL	CHD-C1D	4.62	1.47	1.39
25	N	607	CHL	O2D-CGD	4.61	1.44	1.33
25	n	607	CHL	O2D-CGD	4.61	1.44	1.33
25	N	607	CHL	OBD-CAD	4.61	1.28	1.22
25	n	607	CHL	OBD-CAD	4.61	1.28	1.22
25	3	607	CHL	C3A-C2A	-4.60	1.50	1.54
25	7	607	CHL	C3A-C2A	-4.60	1.50	1.54
25	R	606	CHL	CHC-C4B	4.60	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	606	CHL	CHC-C4B	4.60	1.47	1.39
25	1	601	CHL	CHB-C4A	-4.59	1.33	1.38
25	n	606	CHL	CHC-C4B	4.59	1.47	1.39
25	2	607	CHL	C3B-C2B	4.59	1.46	1.40
25	6	607	CHL	C3B-C2B	4.59	1.46	1.40
25	6	607	CHL	CHB-C4A	-4.59	1.33	1.38
25	4	607	CHL	C3B-C2B	4.59	1.46	1.40
25	8	607	CHL	C3B-C2B	4.59	1.46	1.40
25	1	605	CHL	CHB-C4A	-4.59	1.33	1.38
25	g	609	CHL	OBD-CAD	4.59	1.28	1.22
25	6	608	CHL	O2A-CGA	4.59	1.46	1.30
25	2	608	CHL	O2A-CGA	4.58	1.46	1.30
25	4	609	CHL	CHD-C4C	4.58	1.48	1.39
25	7	606	CHL	CHC-C4B	4.58	1.47	1.39
25	2	607	CHL	CHB-C4A	-4.58	1.33	1.38
25	n	609	CHL	OBD-CAD	4.58	1.28	1.22
25	s	608	CHL	O2D-CGD	4.58	1.44	1.33
25	3	606	CHL	CHC-C4B	4.58	1.47	1.39
25	N	607	CHL	C3B-C2B	4.58	1.46	1.40
25	5	608	CHL	O2A-CGA	4.58	1.45	1.30
25	1	609	CHL	OBD-CAD	4.58	1.28	1.22
25	5	609	CHL	OBD-CAD	4.58	1.28	1.22
25	3	601	CHL	CHD-C4C	4.58	1.48	1.39
25	7	601	CHL	CHD-C4C	4.58	1.48	1.39
25	s	606	CHL	C3B-C2B	4.58	1.46	1.40
25	1	601	CHL	CHC-C4B	4.57	1.47	1.39
25	5	601	CHL	CHC-C4B	4.57	1.47	1.39
25	G	609	CHL	OBD-CAD	4.57	1.28	1.22
25	N	606	CHL	CHC-C4B	4.57	1.47	1.39
25	4	606	CHL	CHC-C4B	4.57	1.47	1.39
25	N	608	CHL	CHC-C4B	4.57	1.47	1.39
25	S	608	CHL	O2D-CGD	4.57	1.44	1.33
25	1	601	CHL	O2A-CGA	4.57	1.45	1.30
25	5	601	CHL	O2A-CGA	4.57	1.45	1.30
25	8	606	CHL	CHC-C4B	4.57	1.47	1.39
25	3	605	CHL	O2A-CGA	4.57	1.45	1.30
25	3	606	CHL	O2A-CGA	4.57	1.45	1.30
25	1	609	CHL	CHB-C4A	-4.57	1.33	1.38
25	5	609	CHL	CHB-C4A	-4.57	1.33	1.38
25	S	606	CHL	O2A-CGA	4.56	1.45	1.30
25	2	601	CHL	C3B-C2B	4.56	1.46	1.40
25	g	605	CHL	CHB-C1B	4.56	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	608	CHL	CHC-C4B	4.56	1.47	1.39
25	8	609	CHL	CHD-C4C	4.56	1.48	1.39
25	8	609	CHL	OBD-CAD	4.56	1.28	1.22
25	1	605	CHL	CHC-C4B	4.56	1.47	1.39
25	G	605	CHL	CHB-C1B	4.56	1.47	1.39
25	1	608	CHL	O2A-CGA	4.56	1.45	1.30
25	2	607	CHL	C3A-C2A	-4.56	1.50	1.54
25	n	605	CHL	O2A-CGA	4.56	1.46	1.33
25	N	605	CHL	O2A-CGA	4.56	1.46	1.33
25	7	605	CHL	O2A-CGA	4.55	1.45	1.30
25	8	607	CHL	CHD-C1D	4.55	1.47	1.39
25	2	606	CHL	CHC-C4B	4.55	1.47	1.39
25	1	605	CHL	O2A-CGA	4.55	1.45	1.30
25	3	607	CHL	CHC-C4B	4.55	1.47	1.39
25	5	605	CHL	O2A-CGA	4.55	1.45	1.30
25	s	606	CHL	O2A-CGA	4.55	1.45	1.30
25	5	605	CHL	CHC-C4B	4.55	1.47	1.39
25	7	606	CHL	O2A-CGA	4.55	1.45	1.30
25	4	601	CHL	O2A-CGA	4.55	1.45	1.30
25	7	607	CHL	CHC-C4B	4.54	1.47	1.39
25	S	601	CHL	CHD-C4C	4.54	1.48	1.39
25	s	601	CHL	CHD-C4C	4.54	1.48	1.39
25	2	606	CHL	O2A-CGA	4.54	1.45	1.30
25	6	606	CHL	O2A-CGA	4.54	1.45	1.30
25	n	607	CHL	C3B-C2B	4.54	1.46	1.40
25	4	606	CHL	CHB-C1B	4.54	1.47	1.39
25	7	609	CHL	CHB-C1B	4.54	1.47	1.39
25	8	606	CHL	CHB-C1B	4.54	1.47	1.39
25	6	605	CHL	O2A-CGA	4.54	1.45	1.30
25	4	607	CHL	O2A-CGA	4.54	1.45	1.30
25	N	609	CHL	OBD-CAD	4.54	1.28	1.22
25	8	601	CHL	O2A-CGA	4.53	1.45	1.30
25	8	608	CHL	O2A-CGA	4.53	1.45	1.30
25	6	609	CHL	C3B-C2B	4.53	1.46	1.40
25	4	606	CHL	O2A-CGA	4.53	1.45	1.30
25	S	606	CHL	C3B-C2B	4.53	1.46	1.40
25	4	608	CHL	O2A-CGA	4.52	1.45	1.30
25	2	609	CHL	C3B-C2B	4.52	1.46	1.40
25	4	606	CHL	C3B-C2B	4.52	1.46	1.40
25	2	605	CHL	O2A-CGA	4.52	1.45	1.30
25	1	606	CHL	O2A-CGA	4.52	1.45	1.30
25	5	606	CHL	O2A-CGA	4.52	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	606	CHL	O2A-CGA	4.52	1.45	1.30
25	8	607	CHL	O2A-CGA	4.52	1.45	1.30
25	Y	605	CHL	C3B-C2B	4.52	1.46	1.40
25	1	601	CHL	OBD-CAD	4.52	1.28	1.22
25	3	608	CHL	O2A-CGA	4.52	1.45	1.30
25	6	601	CHL	C3B-C2B	4.52	1.46	1.40
25	4	609	CHL	OBD-CAD	4.52	1.28	1.22
25	4	609	CHL	O2A-CGA	4.52	1.45	1.30
25	8	609	CHL	O2A-CGA	4.52	1.45	1.30
25	6	606	CHL	CHC-C4B	4.52	1.46	1.39
25	7	608	CHL	CHB-C1B	4.52	1.46	1.39
25	7	608	CHL	O2A-CGA	4.52	1.45	1.30
25	8	606	CHL	C3B-C2B	4.52	1.46	1.40
25	3	609	CHL	CHB-C1B	4.51	1.46	1.39
25	S	608	CHL	OBD-CAD	4.51	1.28	1.22
25	s	608	CHL	OBD-CAD	4.51	1.28	1.22
25	4	607	CHL	CHD-C1D	4.51	1.46	1.39
25	Y	605	CHL	CHB-C1B	4.51	1.46	1.39
25	y	605	CHL	CHB-C1B	4.51	1.46	1.39
25	G	606	CHL	O2A-CGA	4.51	1.46	1.33
25	g	606	CHL	O2A-CGA	4.51	1.46	1.33
25	y	605	CHL	C3B-C2B	4.50	1.46	1.40
25	S	601	CHL	O2A-CGA	4.50	1.45	1.30
25	s	601	CHL	O2A-CGA	4.50	1.45	1.30
25	2	601	CHL	O2A-CGA	4.50	1.45	1.30
25	6	601	CHL	O2A-CGA	4.50	1.45	1.30
25	g	605	CHL	O2A-CGA	4.49	1.45	1.30
25	S	607	CHL	O2A-CGA	4.48	1.46	1.33
25	s	607	CHL	O2A-CGA	4.48	1.46	1.33
25	G	605	CHL	O2A-CGA	4.48	1.45	1.30
25	S	608	CHL	O2A-CGA	4.48	1.45	1.30
25	3	608	CHL	CHB-C1B	4.48	1.46	1.39
25	N	606	CHL	C3A-C2A	-4.47	1.50	1.54
25	7	609	CHL	O2A-CGA	4.47	1.46	1.33
25	3	606	CHL	C3B-C2B	4.47	1.46	1.40
25	7	606	CHL	C3B-C2B	4.47	1.46	1.40
25	4	609	CHL	CHB-C1B	4.47	1.46	1.39
25	8	609	CHL	CHB-C1B	4.47	1.46	1.39
25	8	609	CHL	CHC-C4B	4.47	1.46	1.39
25	3	609	CHL	O2A-CGA	4.47	1.46	1.33
25	G	601	CHL	CHD-C4C	4.47	1.47	1.39
25	1	601	CHL	CHB-C1B	4.46	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	607	CHL	OBD-CAD	4.46	1.28	1.22
25	4	606	CHL	CHD-C4C	4.46	1.47	1.39
25	1	608	CHL	C3B-C2B	4.46	1.46	1.40
25	5	608	CHL	C3B-C2B	4.46	1.46	1.40
25	4	601	CHL	CHC-C1C	4.46	1.47	1.39
25	g	608	CHL	CHC-C4B	4.46	1.46	1.39
25	R	614	CHL	C3B-C2B	4.46	1.46	1.40
25	r	614	CHL	C3B-C2B	4.46	1.46	1.40
25	s	608	CHL	O2A-CGA	4.46	1.45	1.30
25	8	606	CHL	CHD-C4C	4.46	1.47	1.39
25	y	605	CHL	OBD-CAD	4.46	1.28	1.22
25	2	606	CHL	C3B-C2B	4.46	1.46	1.40
25	8	601	CHL	CHC-C1C	4.46	1.47	1.39
25	1	606	CHL	CHB-C1B	4.46	1.46	1.39
25	5	601	CHL	OBD-CAD	4.45	1.28	1.22
25	Y	606	CHL	O2A-CGA	4.45	1.46	1.33
25	y	606	CHL	O2A-CGA	4.45	1.46	1.33
25	2	601	CHL	CHC-C4B	4.45	1.46	1.39
25	g	601	CHL	CHD-C4C	4.45	1.47	1.39
25	6	606	CHL	C3B-C2B	4.44	1.46	1.40
25	2	606	CHL	CHB-C1B	4.44	1.46	1.39
25	G	608	CHL	CHC-C4B	4.44	1.46	1.39
25	5	601	CHL	CHB-C1B	4.44	1.46	1.39
25	6	606	CHL	CHB-C1B	4.44	1.46	1.39
25	3	608	CHL	CHC-C4B	4.44	1.46	1.39
25	7	608	CHL	CHC-C4B	4.44	1.46	1.39
25	3	607	CHL	CHB-C1B	4.43	1.46	1.39
25	7	607	CHL	CHB-C1B	4.43	1.46	1.39
25	Y	605	CHL	OBD-CAD	4.43	1.28	1.22
25	Y	607	CHL	OBD-CAD	4.43	1.28	1.22
25	5	605	CHL	CHB-C1B	4.43	1.46	1.39
25	4	609	CHL	C3B-C2B	4.43	1.46	1.40
25	5	609	CHL	CHD-C4C	4.42	1.47	1.39
25	4	608	CHL	C3B-C2B	4.42	1.46	1.40
25	5	606	CHL	CHB-C1B	4.42	1.46	1.39
25	4	609	CHL	CHC-C4B	4.42	1.46	1.39
25	R	608	CHL	CHC-C4B	4.41	1.46	1.39
25	r	608	CHL	CHC-C4B	4.41	1.46	1.39
25	4	607	CHL	CHC-C4B	4.41	1.46	1.39
25	8	607	CHL	CHC-C4B	4.41	1.46	1.39
25	y	606	CHL	CHB-C1B	4.41	1.46	1.39
25	8	609	CHL	C3B-C2B	4.41	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	605	CHL	CHC-C4B	4.41	1.46	1.39
25	1	605	CHL	CHB-C1B	4.41	1.46	1.39
25	6	601	CHL	CHC-C4B	4.40	1.46	1.39
25	s	608	CHL	CHC-C4B	4.40	1.46	1.39
25	1	609	CHL	CHD-C4C	4.40	1.47	1.39
25	G	606	CHL	CHD-C1D	4.40	1.46	1.39
25	n	606	CHL	CHB-C4A	-4.40	1.33	1.38
25	1	609	CHL	CHB-C1B	4.40	1.46	1.39
25	n	606	CHL	C3A-C2A	-4.40	1.50	1.54
25	g	608	CHL	CHB-C1B	4.40	1.46	1.39
25	5	609	CHL	CHB-C1B	4.39	1.46	1.39
25	N	601	CHL	CHD-C4C	4.39	1.47	1.39
25	n	601	CHL	CHD-C4C	4.39	1.47	1.39
25	g	606	CHL	CHD-C4C	4.39	1.47	1.39
25	1	606	CHL	CHC-C4B	4.39	1.46	1.39
25	3	606	CHL	CHB-C1B	4.39	1.46	1.39
30	l	101	LHG	O7-C5	-4.39	1.36	1.46
25	Y	605	CHL	O2A-CGA	4.39	1.46	1.33
25	y	605	CHL	O2A-CGA	4.39	1.46	1.33
25	4	608	CHL	CHC-C1C	4.39	1.47	1.39
25	n	605	CHL	CHC-C4B	4.39	1.46	1.39
25	N	606	CHL	CHB-C4A	-4.39	1.33	1.38
25	n	606	CHL	O2A-CGA	4.39	1.46	1.33
25	8	608	CHL	CHC-C1C	4.38	1.47	1.39
25	8	601	CHL	CHB-C4A	-4.38	1.33	1.38
25	G	606	CHL	CHD-C4C	4.38	1.47	1.39
25	Y	606	CHL	CHB-C1B	4.38	1.46	1.39
25	5	606	CHL	CHC-C4B	4.38	1.46	1.39
25	8	608	CHL	C3B-C2B	4.38	1.46	1.40
25	2	607	CHL	CHD-C4C	4.38	1.47	1.39
25	6	607	CHL	CHD-C4C	4.38	1.47	1.39
25	r	606	CHL	CHB-C1B	4.38	1.46	1.39
25	N	606	CHL	O2A-CGA	4.38	1.46	1.33
25	G	608	CHL	CHB-C1B	4.37	1.46	1.39
25	R	606	CHL	CHB-C1B	4.37	1.46	1.39
25	S	608	CHL	CHC-C4B	4.37	1.46	1.39
25	6	609	CHL	CHD-C4C	4.37	1.47	1.39
25	g	606	CHL	CHD-C1D	4.37	1.46	1.39
25	2	605	CHL	CHB-C4A	-4.37	1.33	1.38
25	r	606	CHL	CHD-C1D	4.36	1.46	1.39
25	7	606	CHL	CHB-C1B	4.36	1.46	1.39
30	L	101	LHG	O7-C5	-4.35	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	605	CHL	C3B-C2B	4.35	1.46	1.40
25	1	608	CHL	CHB-C4A	-4.35	1.33	1.38
25	5	608	CHL	CHB-C4A	-4.35	1.33	1.38
25	n	601	CHL	C3B-C2B	4.34	1.46	1.40
25	4	601	CHL	CHB-C4A	-4.34	1.33	1.38
25	n	609	CHL	CHD-C1D	4.34	1.46	1.39
25	s	606	CHL	CHC-C1C	4.34	1.47	1.39
25	2	607	CHL	CHC-C4B	4.34	1.46	1.39
25	6	607	CHL	CHC-C4B	4.34	1.46	1.39
25	1	609	CHL	O2A-CGA	4.34	1.46	1.33
25	G	601	CHL	CHC-C4B	4.34	1.46	1.39
25	G	609	CHL	CHD-C4C	4.34	1.47	1.39
25	g	609	CHL	CHD-C4C	4.34	1.47	1.39
25	n	609	CHL	O2A-CGA	4.33	1.46	1.33
25	R	614	CHL	CHB-C4A	-4.33	1.33	1.38
25	r	614	CHL	CHB-C4A	-4.33	1.33	1.38
25	R	606	CHL	CHD-C1D	4.33	1.46	1.39
25	G	609	CHL	CHD-C1D	4.33	1.46	1.39
25	6	605	CHL	CHB-C4A	-4.33	1.33	1.38
25	S	606	CHL	CHC-C1C	4.33	1.47	1.39
25	2	609	CHL	CHD-C4C	4.33	1.47	1.39
25	8	607	CHL	C3A-C2A	-4.33	1.51	1.54
25	G	606	CHL	CHB-C1B	4.32	1.46	1.39
25	g	606	CHL	CHB-C1B	4.32	1.46	1.39
25	g	609	CHL	CHD-C1D	4.32	1.46	1.39
25	5	609	CHL	O2A-CGA	4.32	1.45	1.33
25	g	609	CHL	O2A-CGA	4.32	1.45	1.33
25	N	609	CHL	O2A-CGA	4.31	1.45	1.33
25	3	601	CHL	CHC-C1C	4.31	1.47	1.39
25	1	609	CHL	CHD-C1D	4.31	1.46	1.39
25	N	605	CHL	C3B-C2B	4.31	1.46	1.40
25	7	601	CHL	CHC-C1C	4.30	1.47	1.39
25	8	606	CHL	CHD-C1D	4.30	1.46	1.39
25	6	606	CHL	CHD-C1D	4.30	1.46	1.39
25	4	607	CHL	C3A-C2A	-4.30	1.51	1.54
25	5	609	CHL	C3B-C2B	4.30	1.46	1.40
38	D	405	PL9	C3-C4	-4.30	1.42	1.49
38	d	405	PL9	C3-C4	-4.30	1.42	1.49
25	2	606	CHL	CHD-C1D	4.30	1.46	1.39
25	N	601	CHL	C3B-C2B	4.30	1.46	1.40
25	7	607	CHL	CHC-C1C	4.29	1.47	1.39
25	s	601	CHL	CHC-C4B	4.29	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	601	CHL	CHC-C4B	4.29	1.46	1.39
25	3	605	CHL	CHD-C4C	4.29	1.47	1.39
25	7	605	CHL	CHD-C4C	4.29	1.47	1.39
25	5	607	CHL	CHD-C4C	4.29	1.47	1.39
25	R	608	CHL	CHB-C1B	4.29	1.46	1.39
25	r	608	CHL	CHB-C1B	4.29	1.46	1.39
25	1	607	CHL	CHD-C4C	4.29	1.47	1.39
25	7	609	CHL	CHC-C4B	4.29	1.46	1.39
25	N	609	CHL	CHD-C1D	4.29	1.46	1.39
25	G	609	CHL	O2A-CGA	4.29	1.45	1.33
25	2	601	CHL	CHD-C1D	4.29	1.46	1.39
25	3	607	CHL	CHC-C1C	4.29	1.47	1.39
25	n	606	CHL	OBD-CAD	4.28	1.27	1.22
25	R	607	CHL	O2A-CGA	4.28	1.45	1.33
25	2	609	CHL	CHC-C4B	4.28	1.46	1.39
25	2	607	CHL	CHD-C1D	4.28	1.46	1.39
25	G	608	CHL	C3B-C2B	4.28	1.46	1.40
25	6	605	CHL	CHC-C1C	4.28	1.47	1.39
25	Y	609	CHL	OBD-CAD	4.28	1.27	1.22
25	6	609	CHL	CHC-C4B	4.27	1.46	1.39
25	3	609	CHL	C3B-C2B	4.27	1.46	1.40
25	1	609	CHL	C3B-C2B	4.27	1.46	1.40
25	7	606	CHL	OBD-CAD	4.27	1.27	1.22
25	3	609	CHL	CHC-C4B	4.27	1.46	1.39
25	6	606	CHL	CHD-C4C	4.27	1.47	1.39
25	6	601	CHL	CHD-C1D	4.27	1.46	1.39
25	r	607	CHL	O2A-CGA	4.27	1.45	1.33
25	2	605	CHL	CHC-C1C	4.27	1.47	1.39
25	y	609	CHL	OBD-CAD	4.27	1.27	1.22
25	4	606	CHL	CHD-C1D	4.27	1.46	1.39
25	Y	608	CHL	CHB-C1B	4.26	1.46	1.39
25	y	608	CHL	CHB-C1B	4.26	1.46	1.39
25	4	609	CHL	CHC-C1C	4.26	1.47	1.39
25	8	609	CHL	CHC-C1C	4.26	1.47	1.39
25	S	601	CHL	CHC-C4B	4.26	1.46	1.39
25	Y	605	CHL	CHC-C1C	4.26	1.47	1.39
25	6	608	CHL	CHB-C4A	-4.26	1.33	1.38
25	N	607	CHL	O2A-CGA	4.26	1.45	1.33
25	n	607	CHL	O2A-CGA	4.26	1.45	1.33
25	2	606	CHL	CHD-C4C	4.26	1.47	1.39
25	r	606	CHL	CHC-C1C	4.25	1.47	1.39
25	2	605	CHL	CHD-C4C	4.25	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	601	CHL	CHD-C1D	4.25	1.46	1.39
25	y	601	CHL	CHD-C1D	4.25	1.46	1.39
25	2	607	CHL	CHB-C1B	4.25	1.46	1.39
25	2	607	CHL	O2A-CGA	4.25	1.45	1.33
25	7	601	CHL	C3B-C2B	4.25	1.46	1.40
25	2	608	CHL	CHB-C4A	-4.25	1.33	1.38
25	5	609	CHL	CHD-C1D	4.24	1.46	1.39
25	g	608	CHL	C3B-C2B	4.24	1.46	1.40
25	R	606	CHL	CHC-C1C	4.24	1.47	1.39
25	7	609	CHL	C3B-C2B	4.24	1.46	1.40
25	N	606	CHL	OBD-CAD	4.24	1.27	1.22
25	3	601	CHL	C3B-C2B	4.24	1.46	1.40
25	6	607	CHL	O2A-CGA	4.24	1.45	1.33
25	1	605	CHL	CHD-C1D	4.24	1.46	1.39
25	5	605	CHL	CHD-C1D	4.24	1.46	1.39
25	5	601	CHL	CHC-C1C	4.24	1.47	1.39
25	6	605	CHL	CHD-C4C	4.24	1.47	1.39
25	S	607	CHL	C3A-C2A	-4.24	1.51	1.54
25	G	608	CHL	CHC-C1C	4.24	1.47	1.39
25	g	608	CHL	CHC-C1C	4.24	1.47	1.39
25	3	606	CHL	OBD-CAD	4.23	1.27	1.22
25	G	605	CHL	CHD-C1D	4.23	1.46	1.39
25	6	607	CHL	CHB-C1B	4.23	1.46	1.39
25	g	605	CHL	CHD-C1D	4.23	1.46	1.39
25	N	608	CHL	CHB-C1B	4.23	1.46	1.39
25	Y	608	CHL	CHC-C4B	4.23	1.46	1.39
25	6	607	CHL	CHD-C1D	4.23	1.46	1.39
25	1	601	CHL	CHC-C1C	4.22	1.47	1.39
25	3	605	CHL	CHB-C4A	-4.22	1.33	1.38
25	7	605	CHL	CHB-C4A	-4.22	1.33	1.38
25	2	609	CHL	O2A-CGA	4.22	1.45	1.33
25	6	609	CHL	O2A-CGA	4.22	1.45	1.33
25	R	608	CHL	O2A-CGA	4.22	1.45	1.33
25	r	608	CHL	O2A-CGA	4.22	1.45	1.33
25	y	608	CHL	CHC-C4B	4.22	1.46	1.39
25	S	608	CHL	CHB-C4A	-4.22	1.33	1.38
25	2	607	CHL	CHC-C1C	4.21	1.47	1.39
25	g	609	CHL	C3B-C2B	4.21	1.46	1.40
25	y	605	CHL	CHC-C1C	4.21	1.47	1.39
25	2	601	CHL	OBD-CAD	4.21	1.27	1.22
25	6	601	CHL	OBD-CAD	4.21	1.27	1.22
25	Y	609	CHL	O2A-CGA	4.21	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	609	CHL	O2A-CGA	4.21	1.45	1.33
25	R	614	CHL	CHD-C4C	4.21	1.47	1.39
25	S	608	CHL	CHC-C1C	4.21	1.47	1.39
25	s	608	CHL	CHC-C1C	4.21	1.47	1.39
25	7	601	CHL	OBD-CAD	4.21	1.27	1.22
25	G	607	CHL	CHD-C4C	4.21	1.47	1.39
25	G	605	CHL	CHD-C4C	4.21	1.47	1.39
25	g	605	CHL	CHD-C4C	4.21	1.47	1.39
25	3	601	CHL	OBD-CAD	4.21	1.27	1.22
25	N	609	CHL	CHD-C4C	4.21	1.47	1.39
25	n	609	CHL	CHD-C4C	4.21	1.47	1.39
25	Y	609	CHL	CHD-C4C	4.20	1.47	1.39
25	5	606	CHL	CHD-C1D	4.20	1.46	1.39
25	N	605	CHL	CHB-C1B	4.20	1.46	1.39
25	R	606	CHL	O2A-CGA	4.20	1.45	1.33
25	4	608	CHL	CHB-C4A	-4.20	1.33	1.38
25	G	609	CHL	C3B-C2B	4.20	1.46	1.40
25	3	608	CHL	CHC-C1C	4.20	1.47	1.39
25	g	607	CHL	CHD-C4C	4.20	1.47	1.39
25	Y	605	CHL	CHB-C4A	-4.20	1.33	1.38
25	n	605	CHL	CHB-C1B	4.20	1.46	1.39
25	Y	608	CHL	CHC-C1C	4.19	1.47	1.39
25	8	608	CHL	CHB-C4A	-4.19	1.33	1.38
25	N	608	CHL	CHC-C1C	4.19	1.47	1.39
25	n	608	CHL	CHC-C1C	4.19	1.47	1.39
25	r	606	CHL	O2A-CGA	4.19	1.45	1.33
25	y	609	CHL	CHD-C4C	4.19	1.47	1.39
25	r	614	CHL	CHD-C4C	4.19	1.47	1.39
25	y	608	CHL	CHC-C1C	4.18	1.47	1.39
25	6	607	CHL	CHC-C1C	4.18	1.47	1.39
25	1	607	CHL	CHC-C4B	4.18	1.46	1.39
25	5	607	CHL	CHC-C4B	4.18	1.46	1.39
25	N	601	CHL	O2A-CGA	4.18	1.45	1.33
25	n	608	CHL	CHB-C1B	4.18	1.46	1.39
25	r	614	CHL	CHC-C1C	4.17	1.47	1.39
25	2	609	CHL	CHB-C4A	-4.17	1.33	1.38
25	7	606	CHL	CHD-C1D	4.17	1.46	1.39
25	G	601	CHL	C3B-C2B	4.17	1.46	1.40
25	s	608	CHL	CHB-C4A	-4.17	1.33	1.38
25	r	607	CHL	C3B-C2B	4.17	1.46	1.40
25	N	606	CHL	CHD-C1D	4.17	1.46	1.39
25	n	606	CHL	CHD-C1D	4.17	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	609	CHL	CHD-C1D	4.17	1.46	1.39
25	n	601	CHL	O2A-CGA	4.17	1.45	1.33
25	3	605	CHL	CHC-C1C	4.17	1.47	1.39
25	R	614	CHL	CHC-C4B	4.16	1.46	1.39
25	G	608	CHL	O2A-CGA	4.16	1.45	1.33
25	2	609	CHL	CHD-C1D	4.16	1.46	1.39
25	6	609	CHL	CHD-C1D	4.16	1.46	1.39
25	1	606	CHL	CHD-C1D	4.16	1.46	1.39
25	3	605	CHL	CHD-C1D	4.16	1.46	1.39
25	7	605	CHL	CHD-C1D	4.16	1.46	1.39
25	s	607	CHL	CHD-C4C	4.16	1.47	1.39
25	r	607	CHL	CHC-C4B	4.16	1.46	1.39
25	5	605	CHL	CHD-C4C	4.16	1.47	1.39
25	7	608	CHL	CHC-C1C	4.16	1.47	1.39
25	5	605	CHL	CHC-C1C	4.16	1.47	1.39
25	Y	608	CHL	C3B-C2B	4.16	1.46	1.40
25	R	614	CHL	CHC-C1C	4.16	1.47	1.39
25	3	601	CHL	O2A-CGA	4.15	1.45	1.33
25	3	606	CHL	CHD-C1D	4.15	1.46	1.39
25	g	601	CHL	C3B-C2B	4.15	1.46	1.40
25	4	601	CHL	C3D-C2D	4.15	1.46	1.39
25	1	608	CHL	OBD-CAD	4.15	1.27	1.22
25	5	608	CHL	OBD-CAD	4.15	1.27	1.22
25	7	605	CHL	CHC-C1C	4.15	1.47	1.39
25	2	605	CHL	CHD-C1D	4.15	1.46	1.39
25	Y	609	CHL	CHD-C1D	4.15	1.46	1.39
25	6	605	CHL	CHD-C1D	4.15	1.46	1.39
25	1	605	CHL	CHC-C1C	4.15	1.47	1.39
25	y	605	CHL	CHB-C4A	-4.15	1.33	1.38
25	1	605	CHL	CHD-C4C	4.15	1.47	1.39
25	G	608	CHL	CHD-C4C	4.14	1.47	1.39
25	S	608	CHL	C3A-C2A	-4.14	1.51	1.54
25	R	606	CHL	C3B-C2B	4.14	1.46	1.40
25	r	606	CHL	C3B-C2B	4.14	1.46	1.40
25	g	608	CHL	O2A-CGA	4.14	1.45	1.33
25	R	607	CHL	C3B-C2B	4.14	1.46	1.40
25	1	606	CHL	CHD-C4C	4.14	1.47	1.39
25	G	606	CHL	CHC-C1C	4.14	1.47	1.39
25	5	606	CHL	CHD-C4C	4.14	1.47	1.39
25	R	607	CHL	CHC-C4B	4.14	1.46	1.39
25	s	607	CHL	C3A-C2A	-4.14	1.51	1.54
25	g	608	CHL	CHD-C4C	4.13	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	601	CHL	O2A-CGA	4.13	1.45	1.33
25	Y	601	CHL	O2A-CGA	4.13	1.45	1.33
25	n	608	CHL	C3B-C2B	4.13	1.46	1.40
25	1	607	CHL	O2A-CGA	4.13	1.45	1.33
25	G	607	CHL	O2A-CGA	4.13	1.45	1.33
25	g	607	CHL	O2A-CGA	4.13	1.45	1.33
25	2	608	CHL	OBD-CAD	4.13	1.27	1.22
25	6	608	CHL	OBD-CAD	4.13	1.27	1.22
25	7	601	CHL	O2A-CGA	4.13	1.45	1.33
25	2	608	CHL	CHC-C1C	4.13	1.47	1.39
25	n	606	CHL	CHD-C4C	4.12	1.47	1.39
26	A	405	CLA	CMC-C2C	-4.12	1.42	1.50
26	a	405	CLA	CMC-C2C	-4.12	1.42	1.50
25	6	609	CHL	CHB-C4A	-4.12	1.33	1.38
25	N	608	CHL	C3B-C2B	4.12	1.46	1.40
25	y	608	CHL	C3B-C2B	4.12	1.46	1.40
25	1	606	CHL	C3B-C2B	4.12	1.45	1.40
25	5	607	CHL	O2A-CGA	4.12	1.45	1.33
25	1	607	CHL	CHC-C1C	4.11	1.47	1.39
25	5	607	CHL	CHC-C1C	4.11	1.47	1.39
25	r	614	CHL	CHC-C4B	4.11	1.46	1.39
25	g	606	CHL	CHC-C1C	4.11	1.47	1.39
25	8	601	CHL	C3D-C2D	4.11	1.46	1.39
25	S	607	CHL	CHD-C4C	4.11	1.47	1.39
25	7	606	CHL	CHD-C4C	4.11	1.47	1.39
25	S	601	CHL	CHC-C1C	4.11	1.47	1.39
25	S	607	CHL	C3B-C2B	4.11	1.45	1.40
25	s	607	CHL	C3B-C2B	4.11	1.45	1.40
25	s	608	CHL	C3A-C2A	-4.11	1.51	1.54
25	N	606	CHL	CHD-C4C	4.10	1.47	1.39
25	4	607	CHL	CHC-C1C	4.10	1.47	1.39
25	s	601	CHL	CHC-C1C	4.10	1.47	1.39
25	R	608	CHL	CHC-C1C	4.10	1.47	1.39
25	8	607	CHL	CHC-C1C	4.10	1.47	1.39
25	r	608	CHL	CHC-C1C	4.10	1.47	1.39
25	r	614	CHL	CHD-C1D	4.09	1.46	1.39
25	3	606	CHL	CHD-C4C	4.09	1.47	1.39
25	6	608	CHL	CHC-C1C	4.09	1.47	1.39
25	5	606	CHL	C3B-C2B	4.09	1.45	1.40
25	R	606	CHL	CHD-C4C	4.09	1.47	1.39
25	r	606	CHL	CHD-C4C	4.09	1.47	1.39
25	1	607	CHL	CHD-C1D	4.08	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	607	CHL	CHD-C1D	4.08	1.46	1.39
25	1	606	CHL	CHC-C1C	4.08	1.47	1.39
25	5	606	CHL	CHC-C1C	4.08	1.47	1.39
25	y	606	CHL	CHC-C4B	4.07	1.46	1.39
25	2	601	CHL	CHB-C1B	4.07	1.46	1.39
25	Y	609	CHL	C3B-C2B	4.07	1.45	1.40
25	S	607	CHL	CHB-C1B	4.07	1.46	1.39
25	s	607	CHL	CHB-C1B	4.07	1.46	1.39
25	y	609	CHL	C3B-C2B	4.07	1.45	1.40
25	s	606	CHL	CHD-C4C	4.06	1.47	1.39
25	S	606	CHL	CHB-C4A	-4.06	1.33	1.38
25	s	606	CHL	CHB-C4A	-4.06	1.33	1.38
25	R	614	CHL	CHD-C1D	4.05	1.46	1.39
25	2	608	CHL	CHD-C4C	4.05	1.47	1.39
26	B	605	CLA	CMD-C2D	-4.05	1.42	1.50
25	S	601	CHL	C3B-C2B	4.04	1.45	1.40
25	s	601	CHL	C3B-C2B	4.04	1.45	1.40
25	N	605	CHL	CHC-C1C	4.04	1.47	1.39
25	6	608	CHL	CHD-C4C	4.04	1.47	1.39
25	n	605	CHL	CHC-C1C	4.04	1.47	1.39
25	N	606	CHL	CHC-C1C	4.04	1.47	1.39
25	n	606	CHL	CHC-C1C	4.04	1.47	1.39
25	S	601	CHL	OBD-CAD	4.04	1.27	1.22
25	s	601	CHL	OBD-CAD	4.04	1.27	1.22
25	Y	606	CHL	CHC-C4B	4.03	1.46	1.39
25	6	601	CHL	CHB-C1B	4.03	1.46	1.39
25	S	606	CHL	CHD-C4C	4.03	1.47	1.39
25	8	607	CHL	CHB-C4A	-4.03	1.33	1.38
26	b	605	CLA	CMD-C2D	-4.03	1.42	1.50
25	6	609	CHL	CHC-C1C	4.02	1.47	1.39
25	7	608	CHL	CHD-C4C	4.02	1.47	1.39
25	R	607	CHL	CHC-C1C	4.01	1.47	1.39
25	3	608	CHL	CHD-C4C	4.01	1.47	1.39
38	d	405	PL9	C6-C1	-4.01	1.41	1.48
25	r	607	CHL	CHC-C1C	4.01	1.47	1.39
25	N	607	CHL	CHC-C4B	4.01	1.46	1.39
25	n	608	CHL	O2A-CGA	4.00	1.45	1.33
25	6	601	CHL	CHC-C1C	4.00	1.47	1.39
25	2	609	CHL	CHC-C1C	3.99	1.47	1.39
25	n	607	CHL	CHC-C4B	3.99	1.46	1.39
25	N	607	CHL	CHC-C1C	3.99	1.47	1.39
25	n	607	CHL	CHC-C1C	3.99	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	601	CHL	CHB-C1B	3.99	1.46	1.39
25	g	601	CHL	O2A-CGA	3.99	1.45	1.33
25	G	601	CHL	O2A-CGA	3.99	1.45	1.33
25	N	608	CHL	O2A-CGA	3.99	1.45	1.33
25	G	607	CHL	CHD-C1D	3.98	1.46	1.39
25	g	607	CHL	CHD-C1D	3.98	1.46	1.39
25	y	607	CHL	CHC-C4B	3.98	1.46	1.39
25	4	607	CHL	CHB-C4A	-3.98	1.33	1.38
38	D	405	PL9	C6-C1	-3.97	1.41	1.48
25	G	605	CHL	C3D-C2D	3.97	1.46	1.39
25	g	605	CHL	C3D-C2D	3.97	1.46	1.39
25	3	601	CHL	CHD-C1D	3.97	1.46	1.39
25	7	601	CHL	CHD-C1D	3.97	1.46	1.39
25	Y	607	CHL	CHC-C4B	3.97	1.46	1.39
25	5	609	CHL	CHC-C4B	3.97	1.46	1.39
25	4	606	CHL	CHC-C1C	3.97	1.47	1.39
25	2	601	CHL	CHC-C1C	3.96	1.47	1.39
25	n	601	CHL	CHB-C1B	3.96	1.46	1.39
25	Y	608	CHL	O2A-CGA	3.96	1.44	1.33
25	y	608	CHL	O2A-CGA	3.96	1.44	1.33
25	g	601	CHL	CHB-C1B	3.96	1.46	1.39
25	n	608	CHL	CHD-C4C	3.95	1.46	1.39
25	N	601	CHL	CHD-C1D	3.95	1.46	1.39
25	n	601	CHL	CHD-C1D	3.95	1.46	1.39
25	1	609	CHL	CHC-C4B	3.95	1.46	1.39
25	N	608	CHL	CHD-C4C	3.95	1.46	1.39
25	S	606	CHL	CHD-C1D	3.94	1.46	1.39
25	3	607	CHL	C3D-C2D	3.93	1.46	1.39
25	7	607	CHL	C3D-C2D	3.93	1.46	1.39
25	3	609	CHL	CHC-C1C	3.93	1.46	1.39
25	5	608	CHL	CHC-C1C	3.93	1.46	1.39
25	s	606	CHL	CHD-C1D	3.93	1.46	1.39
25	8	606	CHL	CHC-C1C	3.93	1.46	1.39
25	G	601	CHL	CHB-C1B	3.93	1.46	1.39
25	2	605	CHL	C3D-C2D	3.93	1.46	1.39
25	6	605	CHL	C3D-C2D	3.93	1.46	1.39
25	1	607	CHL	C3B-C2B	3.92	1.45	1.40
25	5	607	CHL	C3B-C2B	3.92	1.45	1.40
25	6	608	CHL	CHD-C1D	3.91	1.46	1.39
25	G	607	CHL	C3B-C2B	3.91	1.45	1.40
25	g	607	CHL	C3B-C2B	3.91	1.45	1.40
25	1	608	CHL	CHC-C1C	3.90	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	608	CHL	CHD-C1D	3.90	1.45	1.39
25	7	605	CHL	C3D-C2D	3.90	1.46	1.39
25	7	609	CHL	CHC-C1C	3.90	1.46	1.39
25	4	601	CHL	C3A-C2A	-3.89	1.51	1.54
25	8	608	CHL	CHD-C4C	3.89	1.46	1.39
25	3	601	CHL	CHB-C1B	3.89	1.45	1.39
25	7	601	CHL	CHB-C1B	3.89	1.45	1.39
25	8	601	CHL	C3A-C2A	-3.89	1.51	1.54
25	S	607	CHL	CHD-C1D	3.88	1.45	1.39
25	s	607	CHL	CHD-C1D	3.88	1.45	1.39
25	Y	608	CHL	CHD-C4C	3.88	1.46	1.39
25	3	605	CHL	C3D-C2D	3.88	1.46	1.39
26	b	613	CLA	CMD-C2D	-3.88	1.42	1.50
25	n	605	CHL	CHD-C1D	3.88	1.45	1.39
25	r	607	CHL	CHB-C1B	3.88	1.45	1.39
26	B	613	CLA	CMD-C2D	-3.87	1.42	1.50
25	N	605	CHL	CHD-C1D	3.87	1.45	1.39
25	y	608	CHL	CHD-C4C	3.87	1.46	1.39
25	r	607	CHL	CHD-C4C	3.86	1.46	1.39
25	5	608	CHL	CHD-C4C	3.86	1.46	1.39
25	N	601	CHL	OBD-CAD	3.86	1.27	1.22
25	R	608	CHL	C3B-C2B	3.86	1.45	1.40
25	r	608	CHL	C3B-C2B	3.86	1.45	1.40
25	4	608	CHL	CHD-C4C	3.86	1.46	1.39
25	S	607	CHL	CHC-C4B	3.86	1.45	1.39
25	s	607	CHL	CHC-C4B	3.86	1.45	1.39
25	n	605	CHL	CHD-C4C	3.86	1.46	1.39
25	G	608	CHL	OBD-CAD	3.86	1.27	1.22
25	n	601	CHL	OBD-CAD	3.86	1.27	1.22
25	R	607	CHL	CHD-C4C	3.85	1.46	1.39
25	Y	607	CHL	O2A-CGA	3.85	1.44	1.33
25	y	607	CHL	O2A-CGA	3.85	1.44	1.33
25	g	608	CHL	OBD-CAD	3.84	1.27	1.22
25	1	607	CHL	CHB-C1B	3.84	1.45	1.39
25	5	607	CHL	CHB-C1B	3.84	1.45	1.39
25	7	609	CHL	C3D-C2D	3.84	1.46	1.39
25	3	609	CHL	C3D-C2D	3.84	1.46	1.39
25	s	608	CHL	CHD-C1D	3.84	1.45	1.39
26	Y	604	CLA	CMB-C2B	-3.84	1.42	1.50
26	y	604	CLA	CMB-C2B	-3.84	1.42	1.50
25	1	608	CHL	CHD-C4C	3.84	1.46	1.39
25	S	608	CHL	CHD-C4C	3.83	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	608	CHL	CHD-C4C	3.83	1.46	1.39
25	R	607	CHL	CHB-C1B	3.83	1.45	1.39
25	3	606	CHL	CHC-C1C	3.83	1.46	1.39
25	N	605	CHL	CHD-C4C	3.82	1.46	1.39
25	4	609	CHL	C3D-C2D	3.82	1.46	1.39
25	8	609	CHL	C3D-C2D	3.82	1.46	1.39
35	A	408	PHO	C4D-ND	-3.82	1.32	1.38
35	a	408	PHO	C4D-ND	-3.82	1.32	1.38
25	Y	607	CHL	C3B-C2B	3.81	1.45	1.40
25	y	607	CHL	C3B-C2B	3.81	1.45	1.40
25	7	606	CHL	CHC-C1C	3.81	1.46	1.39
25	R	608	CHL	CHD-C1D	3.81	1.45	1.39
25	r	608	CHL	CHD-C1D	3.81	1.45	1.39
25	y	601	CHL	OBD-CAD	3.81	1.27	1.22
39	B	626	DGD	O2G-C2G	-3.80	1.37	1.46
39	b	626	DGD	O2G-C2G	-3.80	1.37	1.46
25	S	608	CHL	CHD-C1D	3.80	1.45	1.39
25	Y	601	CHL	OBD-CAD	3.79	1.27	1.22
26	S	609	CLA	C1D-ND	3.79	1.42	1.37
25	8	606	CHL	C3D-C2D	3.79	1.46	1.39
26	s	609	CLA	C1D-ND	3.78	1.42	1.37
25	Y	601	CHL	CHC-C4B	3.78	1.45	1.39
25	y	601	CHL	CHC-C4B	3.77	1.45	1.39
25	N	609	CHL	C3D-C2D	3.77	1.46	1.39
25	2	606	CHL	CHC-C1C	3.77	1.46	1.39
25	6	606	CHL	CHC-C1C	3.77	1.46	1.39
25	n	608	CHL	CHD-C1D	3.76	1.45	1.39
25	4	607	CHL	C3D-C2D	3.76	1.46	1.39
25	N	608	CHL	OBD-CAD	3.76	1.27	1.22
25	n	608	CHL	OBD-CAD	3.76	1.27	1.22
25	4	606	CHL	C3D-C2D	3.76	1.46	1.39
25	6	609	CHL	C3D-C2D	3.75	1.46	1.39
25	n	609	CHL	C3D-C2D	3.75	1.46	1.39
25	g	601	CHL	CHD-C1D	3.75	1.45	1.39
25	Y	601	CHL	C3B-C2B	3.75	1.45	1.40
25	y	601	CHL	C3B-C2B	3.75	1.45	1.40
26	B	612	CLA	CMC-C2C	-3.74	1.43	1.50
26	b	612	CLA	CMC-C2C	-3.74	1.43	1.50
25	G	601	CHL	CHD-C1D	3.74	1.45	1.39
25	N	608	CHL	CHD-C1D	3.74	1.45	1.39
25	n	601	CHL	CHC-C1C	3.73	1.46	1.39
26	N	604	CLA	CMB-C2B	-3.73	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	607	CHL	C3D-C2D	3.73	1.46	1.39
25	G	608	CHL	CHD-C1D	3.72	1.45	1.39
25	N	601	CHL	CHC-C1C	3.72	1.46	1.39
25	S	606	CHL	C3D-C2D	3.71	1.46	1.39
25	s	606	CHL	C3D-C2D	3.71	1.46	1.39
25	g	607	CHL	CHB-C1B	3.71	1.45	1.39
25	S	607	CHL	CHC-C1C	3.71	1.46	1.39
25	Y	605	CHL	C3D-C2D	3.71	1.46	1.39
25	s	607	CHL	CHC-C1C	3.71	1.46	1.39
25	2	609	CHL	C3D-C2D	3.70	1.46	1.39
25	G	601	CHL	CHC-C1C	3.70	1.46	1.39
25	g	601	CHL	CHC-C1C	3.70	1.46	1.39
25	g	608	CHL	CHD-C1D	3.70	1.45	1.39
25	1	605	CHL	C3D-C2D	3.70	1.45	1.39
25	5	605	CHL	C3D-C2D	3.70	1.45	1.39
25	Y	609	CHL	C3D-C2D	3.69	1.45	1.39
25	y	609	CHL	C3D-C2D	3.69	1.45	1.39
25	Y	608	CHL	CHD-C1D	3.69	1.45	1.39
26	n	604	CLA	CMB-C2B	-3.69	1.43	1.50
25	y	605	CHL	C3D-C2D	3.68	1.45	1.39
25	4	608	CHL	OBD-CAD	3.68	1.27	1.22
25	n	606	CHL	C3D-C2D	3.68	1.45	1.39
25	N	609	CHL	C3B-C2B	3.68	1.45	1.40
25	G	607	CHL	CHB-C1B	3.67	1.45	1.39
25	r	614	CHL	C3D-C2D	3.67	1.45	1.39
25	8	608	CHL	OBD-CAD	3.67	1.27	1.22
25	2	607	CHL	C3D-C2D	3.67	1.45	1.39
25	6	607	CHL	C3D-C2D	3.67	1.45	1.39
25	R	614	CHL	C3D-C2D	3.67	1.45	1.39
25	y	609	CHL	CHB-C1B	3.66	1.45	1.39
26	G	604	CLA	CMB-C2B	-3.66	1.43	1.50
26	g	604	CLA	CMB-C2B	-3.66	1.43	1.50
30	d	409	LHG	O7-C5	-3.66	1.38	1.46
25	7	608	CHL	OBD-CAD	3.66	1.27	1.22
25	N	606	CHL	C3D-C2D	3.65	1.45	1.39
25	n	609	CHL	CHC-C4B	3.65	1.45	1.39
30	D	409	LHG	O7-C5	-3.65	1.38	1.46
25	n	609	CHL	C3B-C2B	3.65	1.45	1.40
25	y	608	CHL	CHD-C1D	3.65	1.45	1.39
25	Y	609	CHL	CHB-C1B	3.64	1.45	1.39
26	G	614	CLA	C1D-ND	3.64	1.42	1.37
25	R	607	CHL	CHD-C1D	3.64	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	608	CHL	OBD-CAD	3.64	1.27	1.22
25	N	609	CHL	CHC-C4B	3.64	1.45	1.39
26	g	610	CLA	C1D-ND	3.64	1.42	1.37
26	d	402	CLA	CMD-C2D	-3.63	1.43	1.50
25	1	608	CHL	CHD-C1D	3.62	1.45	1.39
26	D	402	CLA	CMD-C2D	-3.61	1.43	1.50
25	g	609	CHL	CHB-C1B	3.61	1.45	1.39
26	g	614	CLA	C1D-ND	3.61	1.42	1.37
25	n	605	CHL	C3D-C2D	3.61	1.45	1.39
25	G	606	CHL	C3D-C2D	3.60	1.45	1.39
25	g	606	CHL	C3D-C2D	3.60	1.45	1.39
25	G	609	CHL	CHB-C1B	3.60	1.45	1.39
26	G	610	CLA	C1D-ND	3.60	1.42	1.37
25	r	607	CHL	CHD-C1D	3.60	1.45	1.39
25	1	609	CHL	CHC-C1C	3.60	1.46	1.39
25	Y	609	CHL	CHC-C1C	3.59	1.46	1.39
25	y	609	CHL	CHC-C1C	3.59	1.46	1.39
25	y	605	CHL	CHD-C4C	3.59	1.46	1.39
26	C	505	CLA	CMD-C2D	-3.59	1.43	1.50
26	B	617	CLA	CMC-C2C	-3.59	1.43	1.50
26	b	617	CLA	CMC-C2C	-3.59	1.43	1.50
25	5	609	CHL	CHC-C1C	3.58	1.46	1.39
26	c	505	CLA	CMD-C2D	-3.58	1.43	1.50
25	N	605	CHL	C3D-C2D	3.58	1.45	1.39
25	S	607	CHL	C3D-C2D	3.58	1.45	1.39
25	s	607	CHL	C3D-C2D	3.58	1.45	1.39
39	c	520	DGD	O5D-C6D	-3.58	1.37	1.43
25	Y	605	CHL	CHD-C4C	3.57	1.46	1.39
25	5	608	CHL	CHD-C1D	3.56	1.45	1.39
25	y	606	CHL	OBD-CAD	3.56	1.27	1.22
26	N	612	CLA	C1D-ND	3.55	1.42	1.37
26	n	612	CLA	C1D-ND	3.55	1.42	1.37
25	Y	606	CHL	OBD-CAD	3.55	1.27	1.22
39	C	520	DGD	O5D-C6D	-3.55	1.37	1.43
25	6	606	CHL	C3D-C2D	3.55	1.45	1.39
38	D	405	PL9	C7-C8	-3.55	1.45	1.50
25	G	601	CHL	OBD-CAD	3.55	1.26	1.22
25	g	601	CHL	OBD-CAD	3.55	1.26	1.22
30	d	408	LHG	O7-C5	-3.54	1.38	1.46
25	y	601	CHL	CHB-C1B	3.54	1.45	1.39
25	2	606	CHL	C3D-C2D	3.54	1.45	1.39
25	S	601	CHL	CHB-C1B	3.53	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	609	CHL	CHC-C4B	3.53	1.45	1.39
25	y	609	CHL	CHC-C4B	3.53	1.45	1.39
25	n	609	CHL	CHC-C1C	3.53	1.46	1.39
30	D	408	LHG	O7-C5	-3.52	1.38	1.46
25	N	609	CHL	CHC-C1C	3.51	1.46	1.39
29	R	623	NEX	C7-C6	-3.51	1.26	1.30
25	Y	607	CHL	CHB-C1B	3.51	1.45	1.39
25	y	607	CHL	CHB-C1B	3.51	1.45	1.39
25	Y	601	CHL	CHB-C1B	3.50	1.45	1.39
38	d	405	PL9	C7-C8	-3.50	1.45	1.50
25	G	609	CHL	C3D-C2D	3.50	1.45	1.39
25	y	607	CHL	CHC-C1C	3.49	1.46	1.39
25	s	601	CHL	CHB-C1B	3.48	1.45	1.39
25	1	606	CHL	C3D-C2D	3.48	1.45	1.39
25	5	606	CHL	C3D-C2D	3.48	1.45	1.39
25	Y	607	CHL	CHC-C1C	3.48	1.46	1.39
25	g	609	CHL	C3D-C2D	3.48	1.45	1.39
25	N	609	CHL	CHB-C1B	3.48	1.45	1.39
25	R	606	CHL	C3D-C2D	3.47	1.45	1.39
25	G	607	CHL	C3D-C2D	3.46	1.45	1.39
25	g	607	CHL	C3D-C2D	3.46	1.45	1.39
26	4	611	CLA	C1D-ND	3.46	1.42	1.37
25	3	608	CHL	CHD-C1D	3.46	1.45	1.39
25	7	608	CHL	CHD-C1D	3.46	1.45	1.39
25	R	608	CHL	CHD-C4C	3.46	1.46	1.39
26	2	612	CLA	C4B-NB	3.46	1.42	1.37
26	8	611	CLA	C1D-ND	3.45	1.42	1.37
25	r	608	CHL	CHD-C4C	3.45	1.46	1.39
25	n	609	CHL	CHB-C1B	3.45	1.45	1.39
25	Y	607	CHL	CHD-C4C	3.45	1.46	1.39
25	y	607	CHL	CHD-C4C	3.45	1.46	1.39
26	4	603	CLA	C1D-ND	3.45	1.42	1.37
25	r	606	CHL	C3D-C2D	3.44	1.45	1.39
26	R	609	CLA	C4B-NB	3.44	1.42	1.37
26	5	612	CLA	C1D-ND	3.44	1.42	1.37
26	6	612	CLA	C4B-NB	3.44	1.42	1.37
26	r	609	CLA	C4B-NB	3.44	1.42	1.37
29	r	623	NEX	C7-C6	-3.44	1.26	1.30
25	n	607	CHL	CHD-C4C	3.44	1.46	1.39
25	Y	608	CHL	OBD-CAD	3.43	1.26	1.22
25	N	607	CHL	CHD-C4C	3.43	1.45	1.39
25	1	609	CHL	C3D-C2D	3.43	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	609	CHL	C3D-C2D	3.43	1.45	1.39
25	N	607	CHL	CHD-C1D	3.42	1.45	1.39
26	2	612	CLA	C1D-ND	3.42	1.42	1.37
25	N	607	CHL	C3D-C2D	3.42	1.45	1.39
25	g	609	CHL	CHC-C1C	3.42	1.45	1.39
26	1	612	CLA	C1D-ND	3.42	1.42	1.37
25	N	607	CHL	CHB-C1B	3.42	1.45	1.39
25	n	607	CHL	CHB-C1B	3.42	1.45	1.39
26	8	603	CLA	C1D-ND	3.41	1.42	1.37
25	3	606	CHL	C3D-C2D	3.41	1.45	1.39
25	7	606	CHL	C3D-C2D	3.41	1.45	1.39
26	2	614	CLA	C1D-ND	3.41	1.42	1.37
25	y	608	CHL	OBD-CAD	3.41	1.26	1.22
25	g	609	CHL	CHC-C4B	3.41	1.45	1.39
26	n	614	CLA	C1D-ND	3.40	1.42	1.37
26	s	603	CLA	C1D-ND	3.40	1.42	1.37
25	1	607	CHL	C3D-C2D	3.39	1.45	1.39
25	5	607	CHL	C3D-C2D	3.39	1.45	1.39
25	G	609	CHL	CHC-C1C	3.39	1.45	1.39
26	G	612	CLA	C1D-ND	3.39	1.42	1.37
26	g	612	CLA	C1D-ND	3.39	1.42	1.37
25	n	607	CHL	C3D-C2D	3.39	1.45	1.39
26	6	612	CLA	C1D-ND	3.38	1.42	1.37
25	y	607	CHL	CHD-C1D	3.38	1.45	1.39
25	n	607	CHL	CHD-C1D	3.38	1.45	1.39
25	G	609	CHL	CHC-C4B	3.38	1.45	1.39
26	S	603	CLA	C1D-ND	3.37	1.42	1.37
25	Y	606	CHL	CHC-C1C	3.37	1.45	1.39
26	N	614	CLA	C1D-ND	3.37	1.42	1.37
26	6	614	CLA	C1D-ND	3.37	1.42	1.37
25	Y	607	CHL	CHD-C1D	3.37	1.45	1.39
38	D	405	PL9	C52-C5	-3.37	1.43	1.50
38	d	405	PL9	C52-C5	-3.37	1.43	1.50
26	1	614	CLA	C1D-ND	3.36	1.42	1.37
26	B	604	CLA	CMB-C2B	-3.36	1.43	1.50
26	b	604	CLA	CMB-C2B	-3.36	1.43	1.50
26	R	612	CLA	C4B-NB	3.36	1.42	1.37
26	r	612	CLA	C4B-NB	3.36	1.42	1.37
25	Y	605	CHL	CHD-C1D	3.35	1.45	1.39
25	y	605	CHL	CHD-C1D	3.35	1.45	1.39
41	f	101	HEM	FE-ND	3.35	2.05	1.94
25	4	608	CHL	CHD-C1D	3.35	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	608	CHL	CHD-C1D	3.35	1.45	1.39
35	A	409	PHO	CMD-C2D	-3.34	1.44	1.51
35	a	409	PHO	CMD-C2D	-3.34	1.44	1.51
29	N	1623	NEX	C7-C6	-3.34	1.26	1.30
29	n	1623	NEX	C7-C6	-3.34	1.26	1.30
26	c	508	CLA	CMB-C2B	-3.34	1.43	1.50
26	R	609	CLA	C1D-ND	3.34	1.42	1.37
41	F	101	HEM	FE-ND	3.34	2.05	1.94
35	A	409	PHO	C4D-ND	-3.33	1.33	1.38
35	a	409	PHO	C4D-ND	-3.33	1.33	1.38
35	A	409	PHO	CMC-C2C	-3.33	1.45	1.50
25	y	606	CHL	CHC-C1C	3.33	1.45	1.39
26	c	506	CLA	CMB-C2B	-3.33	1.44	1.50
25	1	601	CHL	C3D-C2D	3.33	1.45	1.39
26	R	616	CLA	C1D-ND	3.33	1.42	1.37
26	r	616	CLA	C1D-ND	3.33	1.42	1.37
25	5	601	CHL	C3D-C2D	3.32	1.45	1.39
26	C	508	CLA	CMB-C2B	-3.32	1.44	1.50
25	4	608	CHL	C3D-C2D	3.32	1.45	1.39
25	8	608	CHL	C3D-C2D	3.32	1.45	1.39
25	y	601	CHL	CHC-C1C	3.32	1.45	1.39
26	5	614	CLA	C1D-ND	3.32	1.42	1.37
26	8	610	CLA	C1D-ND	3.31	1.42	1.37
25	Y	601	CHL	CHC-C1C	3.31	1.45	1.39
26	C	506	CLA	CMB-C2B	-3.31	1.44	1.50
35	a	409	PHO	CMC-C2C	-3.30	1.45	1.50
41	F	101	HEM	CAB-C3B	3.29	1.56	1.47
25	r	607	CHL	C3D-C2D	3.29	1.45	1.39
26	B	605	CLA	CMB-C2B	-3.29	1.44	1.50
41	f	101	HEM	CAB-C3B	3.29	1.56	1.47
26	b	605	CLA	CMB-C2B	-3.28	1.44	1.50
26	S	610	CLA	C1D-ND	3.28	1.42	1.37
25	R	607	CHL	C3D-C2D	3.28	1.45	1.39
26	r	609	CLA	C1D-ND	3.28	1.42	1.37
26	s	610	CLA	C1D-ND	3.28	1.42	1.37
38	D	405	PL9	C53-C6	-3.28	1.44	1.50
38	d	405	PL9	C53-C6	-3.28	1.44	1.50
26	3	604	CLA	C1D-ND	3.27	1.42	1.37
26	8	612	CLA	C1D-ND	3.27	1.42	1.37
25	3	608	CHL	C3D-C2D	3.27	1.45	1.39
25	2	608	CHL	C3D-C2D	3.26	1.45	1.39
25	S	601	CHL	C3D-C2D	3.26	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	608	CHL	C3D-C2D	3.26	1.45	1.39
25	s	601	CHL	C3D-C2D	3.26	1.45	1.39
26	7	604	CLA	C1D-ND	3.26	1.42	1.37
26	r	611	CLA	C1D-ND	3.26	1.42	1.37
25	7	608	CHL	C3D-C2D	3.25	1.45	1.39
26	Y	603	CLA	C4B-NB	3.25	1.42	1.37
26	4	610	CLA	C1D-ND	3.25	1.42	1.37
26	n	611	CLA	C1D-ND	3.24	1.42	1.37
26	C	507	CLA	C1D-ND	3.24	1.42	1.37
26	c	507	CLA	C1D-ND	3.24	1.42	1.37
26	G	611	CLA	C4B-NB	3.24	1.42	1.37
26	g	611	CLA	C4B-NB	3.24	1.42	1.37
26	3	610	CLA	C1D-ND	3.24	1.42	1.37
26	7	610	CLA	C1D-ND	3.24	1.42	1.37
26	4	604	CLA	C1D-ND	3.23	1.42	1.37
26	R	612	CLA	C1D-ND	3.23	1.42	1.37
26	y	603	CLA	C4B-NB	3.23	1.42	1.37
26	R	611	CLA	C1D-ND	3.22	1.42	1.37
36	b	623	SQD	O48-C23	3.22	1.42	1.33
29	Y	1623	NEX	C7-C6	-3.22	1.26	1.30
26	G	611	CLA	CMB-C2B	-3.22	1.44	1.50
26	4	612	CLA	C1D-ND	3.21	1.42	1.37
36	B	623	SQD	O48-C23	3.21	1.42	1.33
29	1	1623	NEX	C7-C8	-3.21	1.26	1.31
39	c	520	DGD	O2G-C2G	-3.20	1.39	1.46
26	a	405	CLA	CMD-C2D	-3.20	1.44	1.50
26	8	604	CLA	C1D-ND	3.19	1.42	1.37
26	3	602	CLA	C1D-ND	3.19	1.42	1.37
26	6	614	CLA	C4B-NB	3.19	1.42	1.37
26	R	613	CLA	C1D-ND	3.19	1.42	1.37
26	r	613	CLA	C1D-ND	3.19	1.42	1.37
26	2	613	CLA	C4B-NB	3.19	1.42	1.37
26	6	613	CLA	C4B-NB	3.19	1.42	1.37
26	N	611	CLA	C1D-ND	3.18	1.42	1.37
26	g	611	CLA	CMB-C2B	-3.18	1.44	1.50
25	Y	606	CHL	CHD-C4C	3.18	1.45	1.39
26	B	606	CLA	C1D-ND	3.18	1.42	1.37
26	b	606	CLA	C1D-ND	3.18	1.42	1.37
26	B	607	CLA	CMC-C2C	-3.18	1.44	1.50
26	4	602	CLA	C1D-ND	3.18	1.42	1.37
26	8	602	CLA	C1D-ND	3.18	1.42	1.37
26	A	405	CLA	CMD-C2D	-3.17	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	613	CLA	C4B-NB	3.17	1.42	1.37
39	C	520	DGD	O2G-C2G	-3.17	1.39	1.46
26	6	611	CLA	C1D-ND	3.17	1.42	1.37
29	5	1623	NEX	C7-C8	-3.17	1.26	1.31
26	b	607	CLA	CMC-C2C	-3.17	1.44	1.50
26	7	602	CLA	C1D-ND	3.17	1.42	1.37
26	r	612	CLA	C1D-ND	3.17	1.42	1.37
29	S	1623	NEX	C7-C6	-3.16	1.26	1.30
41	F	101	HEM	CAC-C3C	3.16	1.55	1.47
41	f	101	HEM	CAC-C3C	3.16	1.55	1.47
26	B	608	CLA	CMB-C2B	-3.16	1.44	1.50
25	y	606	CHL	CHD-C4C	3.16	1.45	1.39
26	2	604	CLA	C1D-ND	3.16	1.42	1.37
26	2	614	CLA	C4B-NB	3.16	1.42	1.37
26	3	613	CLA	C1D-ND	3.16	1.42	1.37
26	7	613	CLA	C1D-ND	3.16	1.42	1.37
29	R	623	NEX	C7-C8	-3.15	1.26	1.31
29	r	623	NEX	C7-C8	-3.15	1.26	1.31
26	g	611	CLA	C1D-ND	3.15	1.42	1.37
29	y	1623	NEX	C7-C6	-3.15	1.26	1.30
26	r	613	CLA	C4B-NB	3.15	1.42	1.37
26	b	608	CLA	CMB-C2B	-3.15	1.44	1.50
26	b	602	CLA	C1D-ND	3.14	1.42	1.37
26	7	614	CLA	C1D-ND	3.14	1.42	1.37
26	R	616	CLA	C4B-NB	3.14	1.42	1.37
26	Y	611	CLA	C4B-NB	3.14	1.42	1.37
26	y	611	CLA	C4B-NB	3.14	1.42	1.37
26	5	611	CLA	C1D-ND	3.13	1.42	1.37
26	6	604	CLA	C1D-ND	3.13	1.42	1.37
26	B	605	CLA	MG-ND	-3.13	1.99	2.05
26	b	605	CLA	MG-ND	-3.13	1.99	2.05
26	B	606	CLA	CMC-C2C	-3.13	1.44	1.50
26	b	606	CLA	CMC-C2C	-3.13	1.44	1.50
26	6	610	CLA	C1D-ND	3.13	1.42	1.37
25	Y	607	CHL	C3D-C2D	3.12	1.45	1.39
25	y	607	CHL	C3D-C2D	3.12	1.45	1.39
29	s	1623	NEX	C7-C6	-3.12	1.26	1.30
26	1	611	CLA	C1D-ND	3.12	1.42	1.37
26	6	604	CLA	C4B-NB	3.11	1.41	1.37
39	c	518	DGD	O1G-C1G	-3.11	1.38	1.45
26	2	611	CLA	C1D-ND	3.11	1.41	1.37
35	a	408	PHO	CMB-C2B	-3.11	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	602	CLA	C1D-ND	3.11	1.41	1.37
29	G	1623	NEX	C7-C6	-3.11	1.27	1.30
25	Y	608	CHL	C3D-C2D	3.10	1.44	1.39
25	y	608	CHL	C3D-C2D	3.10	1.44	1.39
26	3	614	CLA	C1D-ND	3.10	1.41	1.37
26	N	604	CLA	C4B-NB	3.10	1.41	1.37
26	n	604	CLA	C4B-NB	3.10	1.41	1.37
36	B	621	SQD	O47-C7	3.10	1.43	1.34
26	2	611	CLA	C4B-NB	3.10	1.41	1.37
35	A	408	PHO	CMC-C2C	-3.10	1.45	1.50
35	a	408	PHO	CMC-C2C	-3.10	1.45	1.50
26	G	611	CLA	C1D-ND	3.10	1.41	1.37
39	C	518	DGD	O1G-C1G	-3.10	1.38	1.45
26	5	613	CLA	C1D-ND	3.09	1.41	1.37
26	r	616	CLA	C4B-NB	3.09	1.41	1.37
26	b	612	CLA	C1B-NB	-3.09	1.33	1.37
29	y	1623	NEX	C7-C8	-3.09	1.26	1.31
26	6	611	CLA	C4B-NB	3.09	1.41	1.37
26	2	604	CLA	C4B-NB	3.09	1.41	1.37
36	B	623	SQD	O47-C7	3.08	1.43	1.34
35	A	408	PHO	CMB-C2B	-3.08	1.45	1.51
30	C	522	LHG	O7-C5	-3.08	1.39	1.46
30	c	522	LHG	O7-C5	-3.08	1.39	1.46
26	1	612	CLA	C4B-NB	3.08	1.41	1.37
36	b	621	SQD	O47-C7	3.08	1.43	1.34
36	b	623	SQD	O47-C7	3.08	1.43	1.34
25	1	609	CHL	CBD-CGD	-3.07	1.48	1.52
26	G	604	CLA	C4B-NB	3.07	1.41	1.37
26	g	604	CLA	C4B-NB	3.07	1.41	1.37
25	S	608	CHL	C3D-C2D	3.07	1.44	1.39
26	5	612	CLA	C4B-NB	3.07	1.41	1.37
29	g	1623	NEX	C7-C6	-3.07	1.27	1.30
26	1	613	CLA	C1D-ND	3.06	1.41	1.37
26	B	612	CLA	C1B-NB	-3.06	1.33	1.37
26	4	611	CLA	C4B-NB	3.06	1.41	1.37
26	s	604	CLA	C1D-ND	3.06	1.41	1.37
39	c	518	DGD	O2G-C2G	-3.06	1.39	1.46
29	6	1623	NEX	C7-C8	-3.06	1.26	1.31
26	S	609	CLA	C4B-NB	3.06	1.41	1.37
26	s	609	CLA	C4B-NB	3.06	1.41	1.37
29	Y	1623	NEX	C7-C8	-3.05	1.26	1.31
25	2	601	CHL	C3D-C2D	3.05	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	601	CHL	C3D-C2D	3.05	1.44	1.39
25	5	608	CHL	C3D-C2D	3.05	1.44	1.39
26	2	610	CLA	C1D-ND	3.04	1.41	1.37
26	d	402	CLA	C1B-NB	-3.04	1.33	1.37
26	5	604	CLA	CMB-C2B	-3.04	1.44	1.50
29	2	1623	NEX	C7-C8	-3.04	1.27	1.31
25	5	609	CHL	CBD-CGD	-3.04	1.48	1.52
26	D	402	CLA	C1B-NB	-3.04	1.33	1.37
26	C	509	CLA	CMD-C2D	-3.04	1.44	1.50
26	c	509	CLA	CMD-C2D	-3.04	1.44	1.50
26	5	613	CLA	C4B-NB	3.04	1.41	1.37
26	B	615	CLA	CMD-C2D	-3.04	1.44	1.50
26	b	615	CLA	CMD-C2D	-3.04	1.44	1.50
26	S	604	CLA	C1D-ND	3.03	1.41	1.37
26	g	614	CLA	C4B-NB	3.03	1.41	1.37
26	B	614	CLA	C1B-NB	-3.03	1.33	1.37
26	b	614	CLA	C1B-NB	-3.03	1.33	1.37
26	1	604	CLA	CMB-C2B	-3.03	1.44	1.50
26	1	613	CLA	C4B-NB	3.03	1.41	1.37
26	8	611	CLA	C4B-NB	3.03	1.41	1.37
25	1	608	CHL	C3D-C2D	3.03	1.44	1.39
39	C	518	DGD	O2G-C2G	-3.02	1.39	1.46
25	N	601	CHL	C3D-C2D	3.02	1.44	1.39
39	C	519	DGD	O1G-C1G	-3.02	1.38	1.45
39	c	519	DGD	O1G-C1G	-3.02	1.38	1.45
26	N	612	CLA	C4B-NB	3.02	1.41	1.37
26	n	612	CLA	C4B-NB	3.02	1.41	1.37
30	S	2630	LHG	O7-C5	-3.01	1.39	1.46
30	s	2630	LHG	O7-C5	-3.01	1.39	1.46
25	5	607	CHL	CBD-CGD	-3.01	1.48	1.52
25	s	608	CHL	C3D-C2D	3.01	1.44	1.39
26	a	407	CLA	C1D-ND	3.01	1.41	1.37
26	B	612	CLA	CMB-C2B	-3.01	1.44	1.50
26	b	612	CLA	CMB-C2B	-3.01	1.44	1.50
26	2	602	CLA	C1D-ND	3.01	1.41	1.37
26	6	602	CLA	C1D-ND	3.01	1.41	1.37
37	D	411	LMG	O8-C9	-3.01	1.38	1.45
26	D	402	CLA	CMB-C2B	-3.01	1.44	1.50
26	d	402	CLA	CMB-C2B	-3.01	1.44	1.50
26	c	505	CLA	MG-ND	-3.01	1.99	2.05
26	N	611	CLA	C4B-NB	3.00	1.41	1.37
26	n	611	CLA	C4B-NB	3.00	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S	612	CLA	C1D-ND	3.00	1.41	1.37
25	n	601	CHL	C3D-C2D	3.00	1.44	1.39
26	3	604	CLA	C4B-NB	3.00	1.41	1.37
26	7	604	CLA	C4B-NB	3.00	1.41	1.37
26	G	610	CLA	C4B-NB	3.00	1.41	1.37
26	A	407	CLA	C1D-ND	3.00	1.41	1.37
26	g	612	CLA	C4B-NB	3.00	1.41	1.37
26	G	604	CLA	C1D-ND	2.99	1.41	1.37
26	g	604	CLA	C1D-ND	2.99	1.41	1.37
26	C	505	CLA	MG-ND	-2.99	1.99	2.05
26	4	603	CLA	C4B-NB	2.99	1.41	1.37
26	8	603	CLA	C4B-NB	2.99	1.41	1.37
26	s	612	CLA	C1D-ND	2.99	1.41	1.37
26	n	603	CLA	C1D-ND	2.98	1.41	1.37
25	2	609	CHL	CBD-CGD	-2.98	1.48	1.52
26	n	610	CLA	C1D-ND	2.98	1.41	1.37
39	C	520	DGD	O1G-C1G	-2.98	1.38	1.45
39	c	520	DGD	O1G-C1G	-2.98	1.38	1.45
26	G	614	CLA	C4B-NB	2.98	1.41	1.37
25	G	608	CHL	C3D-C2D	2.98	1.44	1.39
26	5	604	CLA	C4B-NB	2.97	1.41	1.37
37	d	411	LMG	O8-C9	-2.97	1.38	1.45
26	D	402	CLA	MG-NB	-2.97	1.99	2.05
26	d	402	CLA	MG-NB	-2.97	1.99	2.05
26	2	603	CLA	C1D-ND	2.97	1.41	1.37
26	6	603	CLA	C1D-ND	2.97	1.41	1.37
26	3	611	CLA	CMB-C2B	-2.97	1.44	1.50
26	7	611	CLA	CMB-C2B	-2.97	1.44	1.50
26	1	604	CLA	C4B-NB	2.97	1.41	1.37
26	B	604	CLA	CMD-C2D	-2.97	1.44	1.50
25	1	607	CHL	CBD-CGD	-2.97	1.48	1.52
26	1	611	CLA	C4B-NB	2.96	1.41	1.37
26	5	611	CLA	C4B-NB	2.96	1.41	1.37
26	b	604	CLA	CMD-C2D	-2.96	1.44	1.50
26	b	604	CLA	MG-NB	-2.96	1.99	2.05
26	N	603	CLA	C1D-ND	2.96	1.41	1.37
36	A	418	SQD	O47-C7	2.96	1.42	1.34
36	a	418	SQD	O47-C7	2.96	1.42	1.34
26	3	613	CLA	C4B-NB	2.96	1.41	1.37
26	7	613	CLA	C4B-NB	2.96	1.41	1.37
26	8	604	CLA	C4B-NB	2.95	1.41	1.37
25	6	609	CHL	CBD-CGD	-2.95	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g	610	CLA	C4B-NB	2.95	1.41	1.37
25	y	606	CHL	CHD-C1D	2.95	1.44	1.39
26	b	613	CLA	MG-ND	-2.95	1.99	2.05
26	4	604	CLA	C4B-NB	2.95	1.41	1.37
26	N	603	CLA	CMD-C2D	-2.95	1.44	1.50
25	N	608	CHL	C3D-C2D	2.94	1.44	1.39
26	n	603	CLA	CMD-C2D	-2.94	1.44	1.50
29	n	1623	NEX	C7-C8	-2.94	1.27	1.31
26	s	613	CLA	C1D-ND	2.94	1.41	1.37
26	C	501	CLA	C1D-ND	2.94	1.41	1.37
25	g	608	CHL	C3D-C2D	2.94	1.44	1.39
26	B	604	CLA	MG-NB	-2.94	2.00	2.05
26	c	507	CLA	CMC-C2C	-2.94	1.44	1.50
25	3	601	CHL	CBD-CGD	-2.94	1.48	1.52
25	7	601	CHL	CBD-CGD	-2.94	1.48	1.52
26	B	605	CLA	MG-NB	-2.93	2.00	2.05
26	S	613	CLA	C1D-ND	2.93	1.41	1.37
26	7	611	CLA	C1D-ND	2.93	1.41	1.37
26	B	613	CLA	MG-ND	-2.93	2.00	2.05
26	Y	602	CLA	C1D-ND	2.93	1.41	1.37
26	y	602	CLA	C1D-ND	2.93	1.41	1.37
26	g	602	CLA	C1D-ND	2.93	1.41	1.37
25	n	608	CHL	C3D-C2D	2.93	1.44	1.39
30	Y	2630	LHG	O7-C5	-2.93	1.39	1.46
30	y	2630	LHG	O7-C5	-2.93	1.39	1.46
26	S	614	CLA	C1D-ND	2.92	1.41	1.37
26	s	614	CLA	C1D-ND	2.92	1.41	1.37
26	G	612	CLA	C4B-NB	2.92	1.41	1.37
26	Y	611	CLA	CMD-C2D	-2.92	1.44	1.50
26	y	611	CLA	CMD-C2D	-2.92	1.44	1.50
29	N	1623	NEX	C7-C8	-2.92	1.27	1.31
26	b	605	CLA	CMA-C3A	-2.92	1.47	1.53
26	c	508	CLA	C1B-NB	-2.92	1.34	1.37
26	N	610	CLA	C1D-ND	2.92	1.41	1.37
26	2	603	CLA	C4B-NB	2.92	1.41	1.37
26	6	603	CLA	C4B-NB	2.92	1.41	1.37
26	C	507	CLA	CMC-C2C	-2.91	1.44	1.50
25	Y	606	CHL	CHD-C1D	2.91	1.44	1.39
35	A	409	PHO	C4D-CHA	2.91	1.43	1.39
26	g	613	CLA	C4B-NB	2.91	1.41	1.37
26	N	602	CLA	C1D-ND	2.91	1.41	1.37
26	B	605	CLA	CMA-C3A	-2.91	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	406	CLA	C1D-ND	2.91	1.41	1.37
26	a	406	CLA	C1D-ND	2.91	1.41	1.37
26	c	501	CLA	C1D-ND	2.91	1.41	1.37
35	a	409	PHO	C4D-CHA	2.90	1.43	1.39
26	b	605	CLA	MG-NB	-2.90	2.00	2.05
26	R	601	CLA	C4B-NB	2.90	1.41	1.37
26	r	601	CLA	C4B-NB	2.90	1.41	1.37
26	1	614	CLA	C4B-NB	2.90	1.41	1.37
26	B	603	CLA	C1D-ND	2.90	1.41	1.37
26	C	510	CLA	CMD-C2D	-2.90	1.44	1.50
26	G	613	CLA	C4B-NB	2.90	1.41	1.37
26	3	611	CLA	C1D-ND	2.90	1.41	1.37
26	b	603	CLA	C1D-ND	2.90	1.41	1.37
39	H	102	DGD	O5D-C6D	-2.89	1.38	1.43
39	h	102	DGD	O5D-C6D	-2.89	1.38	1.43
26	4	612	CLA	C4B-NB	2.89	1.41	1.37
26	8	612	CLA	C4B-NB	2.89	1.41	1.37
26	G	602	CLA	C1D-ND	2.89	1.41	1.37
26	c	510	CLA	CMD-C2D	-2.89	1.44	1.50
26	r	610	CLA	C1D-ND	2.89	1.41	1.37
35	A	408	PHO	CMD-C2D	-2.89	1.45	1.51
26	5	614	CLA	C4B-NB	2.89	1.41	1.37
26	S	611	CLA	C1D-ND	2.89	1.41	1.37
26	s	611	CLA	C1D-ND	2.89	1.41	1.37
26	y	603	CLA	C3B-C4B	2.88	1.51	1.42
36	A	418	SQD	O48-C23	2.88	1.41	1.33
26	C	508	CLA	C1B-NB	-2.88	1.34	1.37
26	b	604	CLA	MG-ND	-2.88	2.00	2.05
25	y	601	CHL	C3D-C2D	2.88	1.44	1.39
26	Y	603	CLA	C3B-C4B	2.87	1.51	1.42
25	Y	601	CHL	C3D-C2D	2.87	1.44	1.39
26	B	604	CLA	MG-ND	-2.87	2.00	2.05
36	a	418	SQD	O48-C23	2.87	1.41	1.33
26	b	608	CLA	CMC-C2C	-2.86	1.44	1.50
26	1	610	CLA	C1D-ND	2.86	1.41	1.37
26	5	610	CLA	C1D-ND	2.86	1.41	1.37
26	B	608	CLA	CMC-C2C	-2.86	1.44	1.50
26	Y	612	CLA	C1D-ND	2.86	1.41	1.37
26	y	612	CLA	C1D-ND	2.86	1.41	1.37
29	6	1623	NEX	C7-C6	-2.86	1.27	1.30
26	R	610	CLA	C1D-ND	2.86	1.41	1.37
26	S	602	CLA	C4B-NB	2.86	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	608	CHL	CBD-CGD	-2.85	1.48	1.52
35	a	408	PHO	CMD-C2D	-2.85	1.45	1.51
26	7	614	CLA	C4B-NB	2.85	1.41	1.37
26	n	602	CLA	C1D-ND	2.85	1.41	1.37
26	R	612	CLA	C3B-C4B	2.85	1.51	1.42
39	H	102	DGD	O3G-C3G	-2.84	1.38	1.43
39	h	102	DGD	O3G-C3G	-2.84	1.38	1.43
26	3	614	CLA	C4B-NB	2.84	1.41	1.37
35	A	408	PHO	C4D-CHA	2.84	1.43	1.39
35	a	408	PHO	C4D-CHA	2.84	1.43	1.39
26	B	607	CLA	CMD-C2D	-2.84	1.44	1.50
26	b	607	CLA	CMD-C2D	-2.84	1.44	1.50
26	G	602	CLA	CMC-C2C	-2.84	1.45	1.50
26	g	602	CLA	CMC-C2C	-2.84	1.45	1.50
26	B	609	CLA	CMD-C2D	-2.84	1.45	1.50
26	b	609	CLA	CMD-C2D	-2.84	1.45	1.50
26	s	602	CLA	C4B-NB	2.84	1.41	1.37
26	D	402	CLA	CMC-C2C	-2.84	1.45	1.50
26	d	402	CLA	CMC-C2C	-2.84	1.45	1.50
29	2	1623	NEX	C7-C6	-2.83	1.27	1.30
26	S	612	CLA	C4B-NB	2.83	1.41	1.37
26	s	612	CLA	C4B-NB	2.83	1.41	1.37
26	S	610	CLA	C4B-NB	2.83	1.41	1.37
26	6	613	CLA	C1D-ND	2.83	1.41	1.37
26	7	610	CLA	C4B-NB	2.83	1.41	1.37
26	s	610	CLA	C4B-NB	2.83	1.41	1.37
26	g	603	CLA	C4B-NB	2.83	1.41	1.37
37	D	411	LMG	O1-C7	-2.83	1.38	1.43
37	d	411	LMG	O1-C7	-2.83	1.38	1.43
26	r	612	CLA	C3B-C4B	2.83	1.51	1.42
26	B	608	CLA	C1B-NB	-2.83	1.34	1.37
26	Y	603	CLA	C1D-ND	2.83	1.41	1.37
26	c	508	CLA	C1D-ND	2.83	1.41	1.37
26	C	508	CLA	CMC-C2C	-2.83	1.45	1.50
25	8	609	CHL	CBD-CGD	-2.83	1.48	1.52
26	c	508	CLA	CMC-C2C	-2.82	1.45	1.50
26	2	613	CLA	C1D-ND	2.82	1.41	1.37
25	4	609	CHL	CBD-CGD	-2.82	1.48	1.52
25	y	606	CHL	C3D-C2D	2.82	1.44	1.39
26	C	505	CLA	MG-NB	-2.82	2.00	2.05
26	R	604	CLA	C1D-ND	2.81	1.41	1.37
26	r	604	CLA	C1D-ND	2.81	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	608	CHL	CBD-CGD	-2.81	1.49	1.52
26	3	610	CLA	C4B-NB	2.81	1.41	1.37
26	y	614	CLA	C1D-ND	2.81	1.41	1.37
26	y	603	CLA	C1D-ND	2.81	1.41	1.37
26	5	602	CLA	C1D-ND	2.81	1.41	1.37
26	y	604	CLA	C1D-ND	2.81	1.41	1.37
36	b	621	SQD	O48-C23	2.80	1.41	1.33
26	G	613	CLA	C1D-ND	2.80	1.41	1.37
26	2	610	CLA	C4B-NB	2.80	1.41	1.37
26	g	613	CLA	C1D-ND	2.80	1.41	1.37
25	6	608	CHL	CBD-CGD	-2.80	1.49	1.52
26	R	602	CLA	C1D-ND	2.80	1.41	1.37
26	r	602	CLA	C1D-ND	2.80	1.41	1.37
26	6	610	CLA	C4B-NB	2.79	1.41	1.37
36	B	621	SQD	O48-C23	2.79	1.41	1.33
26	b	608	CLA	C1B-NB	-2.79	1.34	1.37
26	r	601	CLA	C1D-ND	2.79	1.41	1.37
26	s	613	CLA	C4B-NB	2.79	1.41	1.37
26	G	603	CLA	C4B-NB	2.79	1.41	1.37
25	Y	606	CHL	C3D-C2D	2.79	1.44	1.39
26	1	604	CLA	C1D-ND	2.79	1.41	1.37
26	c	511	CLA	C1D-ND	2.79	1.41	1.37
26	B	613	CLA	C1B-NB	-2.79	1.34	1.37
26	R	601	CLA	C1D-ND	2.78	1.41	1.37
26	G	603	CLA	C1D-ND	2.78	1.41	1.37
26	C	511	CLA	C1D-ND	2.78	1.41	1.37
26	7	611	CLA	C4B-NB	2.78	1.41	1.37
26	g	603	CLA	C1D-ND	2.78	1.41	1.37
26	r	616	CLA	C1B-C2B	2.78	1.49	1.43
26	S	613	CLA	C4B-NB	2.78	1.41	1.37
41	F	101	HEM	FE-NB	2.77	2.03	1.94
26	Y	604	CLA	C4B-NB	2.77	1.41	1.37
25	2	608	CHL	CBD-CGD	-2.77	1.49	1.52
26	5	604	CLA	C1D-ND	2.77	1.41	1.37
26	Y	614	CLA	C1D-ND	2.77	1.41	1.37
26	Y	604	CLA	C1D-ND	2.77	1.41	1.37
26	y	604	CLA	C4B-NB	2.77	1.41	1.37
26	b	613	CLA	MG-NB	-2.77	2.00	2.05
26	c	505	CLA	MG-NB	-2.77	2.00	2.05
26	4	610	CLA	C4B-NB	2.77	1.41	1.37
26	1	602	CLA	C1D-ND	2.77	1.41	1.37
26	c	502	CLA	MG-NB	-2.76	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	611	CLA	C4B-NB	2.76	1.41	1.37
26	C	508	CLA	C1D-ND	2.76	1.41	1.37
26	B	606	CLA	CMD-C2D	-2.76	1.45	1.50
26	b	606	CLA	CMD-C2D	-2.76	1.45	1.50
41	f	101	HEM	FE-NB	2.76	2.03	1.94
26	Y	611	CLA	C3B-C4B	2.76	1.50	1.42
26	B	613	CLA	MG-NB	-2.76	2.00	2.05
26	Y	602	CLA	CMC-C2C	-2.76	1.45	1.50
26	y	602	CLA	CMC-C2C	-2.76	1.45	1.50
26	7	603	CLA	C1D-ND	2.76	1.41	1.37
26	y	611	CLA	C3B-C4B	2.76	1.50	1.42
26	b	607	CLA	C1D-ND	2.76	1.41	1.37
26	R	616	CLA	C1B-C2B	2.75	1.49	1.43
26	8	610	CLA	C4B-NB	2.75	1.41	1.37
26	Y	612	CLA	C4B-NB	2.75	1.41	1.37
26	s	603	CLA	C4B-NB	2.75	1.41	1.37
26	y	612	CLA	C4B-NB	2.75	1.41	1.37
26	s	614	CLA	C4B-NB	2.74	1.41	1.37
26	n	613	CLA	C1D-ND	2.74	1.41	1.37
36	A	412	SQD	O48-C23	2.74	1.41	1.33
36	a	412	SQD	O48-C23	2.74	1.41	1.33
26	C	502	CLA	CMB-C2B	-2.74	1.45	1.50
26	Y	613	CLA	CMD-C2D	-2.74	1.45	1.50
26	c	502	CLA	CMB-C2B	-2.74	1.45	1.50
26	y	613	CLA	CMD-C2D	-2.74	1.45	1.50
26	3	603	CLA	C1D-ND	2.74	1.41	1.37
26	c	512	CLA	CMD-C2D	-2.74	1.45	1.50
26	n	604	CLA	C1D-ND	2.73	1.41	1.37
25	G	601	CHL	C3D-C2D	2.73	1.44	1.39
25	g	601	CHL	C3D-C2D	2.73	1.44	1.39
26	3	612	CLA	C1D-ND	2.73	1.41	1.37
26	D	403	CLA	C1D-ND	2.73	1.41	1.37
26	d	403	CLA	C1D-ND	2.73	1.41	1.37
26	y	613	CLA	C4B-NB	2.73	1.41	1.37
26	b	613	CLA	C1B-NB	-2.73	1.34	1.37
26	1	603	CLA	C4B-NB	2.73	1.41	1.37
26	5	603	CLA	C4B-NB	2.73	1.41	1.37
26	C	502	CLA	MG-NB	-2.73	2.00	2.05
26	B	611	CLA	CMC-C2C	-2.73	1.45	1.50
26	Y	610	CLA	CMD-C2D	-2.73	1.45	1.50
26	y	610	CLA	CMD-C2D	-2.73	1.45	1.50
26	7	612	CLA	C1D-ND	2.72	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N	614	CLA	C4B-NB	2.72	1.41	1.37
26	n	614	CLA	C4B-NB	2.72	1.41	1.37
26	1	603	CLA	C1D-ND	2.72	1.41	1.37
26	5	603	CLA	C1D-ND	2.72	1.41	1.37
26	B	607	CLA	C1D-ND	2.72	1.41	1.37
26	3	612	CLA	C4B-NB	2.72	1.41	1.37
26	7	612	CLA	C4B-NB	2.72	1.41	1.37
35	A	409	PHO	CAC-C3C	-2.72	1.46	1.51
35	a	409	PHO	CAC-C3C	-2.72	1.46	1.51
26	B	617	CLA	C1D-ND	2.71	1.41	1.37
26	C	509	CLA	CMB-C2B	-2.71	1.45	1.50
26	c	509	CLA	CMB-C2B	-2.71	1.45	1.50
26	N	613	CLA	C4B-NB	2.71	1.41	1.37
26	n	613	CLA	C4B-NB	2.71	1.41	1.37
26	N	604	CLA	C1D-ND	2.71	1.41	1.37
26	b	617	CLA	C1D-ND	2.71	1.41	1.37
26	y	610	CLA	CMC-C2C	-2.71	1.45	1.50
26	2	602	CLA	C4B-NB	2.71	1.41	1.37
26	6	602	CLA	C4B-NB	2.71	1.41	1.37
39	h	102	DGD	O2G-C2G	-2.70	1.40	1.46
26	b	608	CLA	CMD-C2D	-2.70	1.45	1.50
26	8	602	CLA	C4B-NB	2.70	1.41	1.37
26	Y	610	CLA	C1D-ND	2.70	1.41	1.37
26	C	512	CLA	CMD-C2D	-2.70	1.45	1.50
29	G	1623	NEX	O4-C5	-2.70	1.38	1.43
29	g	1623	NEX	O4-C5	-2.70	1.38	1.43
30	1	2630	LHG	O7-C5	-2.70	1.40	1.46
26	S	603	CLA	C4B-NB	2.69	1.41	1.37
26	C	501	CLA	C4B-NB	2.69	1.41	1.37
26	Y	612	CLA	CMD-C2D	-2.69	1.45	1.50
26	y	612	CLA	CMD-C2D	-2.69	1.45	1.50
26	Y	610	CLA	CMC-C2C	-2.69	1.45	1.50
26	b	611	CLA	CMC-C2C	-2.69	1.45	1.50
27	N	1621	LUT	C22-C21	-2.69	1.51	1.54
39	c	519	DGD	O2G-C2G	-2.69	1.40	1.46
26	G	603	CLA	C3B-C4B	2.69	1.50	1.42
30	5	2630	LHG	O7-C5	-2.69	1.40	1.46
39	C	519	DGD	O2G-C2G	-2.69	1.40	1.46
26	N	613	CLA	C1D-ND	2.69	1.41	1.37
26	3	602	CLA	CMC-C2C	-2.69	1.45	1.50
26	7	602	CLA	CMC-C2C	-2.69	1.45	1.50
39	H	102	DGD	O2G-C2G	-2.69	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	608	CHL	CBD-CGD	-2.68	1.49	1.52
26	4	602	CLA	C4B-NB	2.68	1.41	1.37
26	8	611	CLA	C1B-C2B	2.68	1.49	1.43
26	N	613	CLA	C1B-C2B	2.68	1.49	1.43
26	4	611	CLA	C1B-C2B	2.68	1.49	1.43
26	S	614	CLA	C4B-NB	2.68	1.41	1.37
26	R	609	CLA	C3B-C4B	2.68	1.50	1.42
26	r	609	CLA	C3B-C4B	2.68	1.50	1.42
26	y	610	CLA	C1D-ND	2.68	1.41	1.37
26	g	614	CLA	C1B-C2B	2.68	1.49	1.43
26	7	602	CLA	C4B-NB	2.67	1.41	1.37
26	g	603	CLA	C3B-C4B	2.67	1.50	1.42
26	n	613	CLA	C1B-C2B	2.67	1.49	1.43
26	G	613	CLA	C1B-C2B	2.67	1.49	1.43
26	g	613	CLA	C1B-C2B	2.67	1.49	1.43
26	b	608	CLA	C1D-ND	2.67	1.41	1.37
25	8	608	CHL	CBD-CGD	-2.67	1.49	1.52
26	c	501	CLA	C4B-NB	2.66	1.41	1.37
26	B	608	CLA	CMD-C2D	-2.66	1.45	1.50
26	Y	613	CLA	C4B-NB	2.66	1.41	1.37
26	1	610	CLA	C4B-NB	2.66	1.41	1.37
26	5	610	CLA	C4B-NB	2.66	1.41	1.37
26	n	603	CLA	C4B-NB	2.65	1.41	1.37
27	g	1621	LUT	C22-C21	-2.65	1.51	1.54
25	1	608	CHL	CBD-CGD	-2.65	1.49	1.52
25	5	608	CHL	CBD-CGD	-2.65	1.49	1.52
26	s	604	CLA	CMB-C2B	-2.65	1.45	1.50
26	B	613	CLA	CMB-C2B	-2.64	1.45	1.50
26	S	604	CLA	CMB-C2B	-2.64	1.45	1.50
26	b	613	CLA	CMB-C2B	-2.64	1.45	1.50
25	3	601	CHL	C3D-C2D	2.64	1.44	1.39
26	Y	614	CLA	CMD-C2D	-2.63	1.45	1.50
26	y	614	CLA	CMD-C2D	-2.63	1.45	1.50
26	G	611	CLA	MG-NB	-2.63	2.00	2.05
26	G	614	CLA	C1B-C2B	2.63	1.49	1.43
26	c	503	CLA	C1D-ND	2.63	1.41	1.37
26	3	611	CLA	C1B-C2B	2.63	1.49	1.43
26	B	608	CLA	C1D-ND	2.63	1.41	1.37
36	A	412	SQD	O47-C7	2.63	1.41	1.34
29	S	1623	NEX	C7-C8	-2.63	1.27	1.31
29	s	1623	NEX	C7-C8	-2.63	1.27	1.31
26	C	513	CLA	C1D-ND	2.63	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	513	CLA	C1D-ND	2.63	1.41	1.37
26	R	603	CLA	C1D-ND	2.63	1.41	1.37
26	C	512	CLA	C1B-NB	-2.63	1.34	1.37
26	s	611	CLA	C4B-NB	2.63	1.41	1.37
26	B	604	CLA	C1B-NB	-2.62	1.34	1.37
26	b	604	CLA	C1B-NB	-2.62	1.34	1.37
26	C	511	CLA	CMD-C2D	-2.62	1.45	1.50
26	c	511	CLA	CMD-C2D	-2.62	1.45	1.50
36	a	412	SQD	O47-C7	2.62	1.41	1.34
25	2	607	CHL	CBD-CGD	-2.62	1.49	1.52
27	n	1621	LUT	C22-C21	-2.62	1.51	1.54
26	2	612	CLA	C3B-C4B	2.62	1.50	1.42
26	6	612	CLA	C3B-C4B	2.62	1.50	1.42
25	8	607	CHL	CBD-CGD	-2.62	1.49	1.52
37	B	622	LMG	O7-C8	-2.62	1.40	1.46
26	r	616	CLA	CMB-C2B	-2.62	1.45	1.50
26	B	602	CLA	CMC-C2C	-2.62	1.45	1.50
26	b	602	CLA	CMC-C2C	-2.62	1.45	1.50
26	c	501	CLA	CMD-C2D	-2.62	1.45	1.50
26	c	504	CLA	C1B-NB	-2.62	1.34	1.37
27	G	1621	LUT	C22-C21	-2.62	1.51	1.54
37	b	622	LMG	O7-C8	-2.62	1.40	1.46
26	B	614	CLA	CMB-C2B	-2.62	1.45	1.50
39	h	102	DGD	O1G-C1G	-2.62	1.39	1.45
26	7	611	CLA	C1B-C2B	2.62	1.49	1.43
26	3	602	CLA	C4B-NB	2.62	1.41	1.37
26	r	610	CLA	CMC-C2C	-2.61	1.45	1.50
26	b	607	CLA	C4B-NB	2.61	1.41	1.37
26	1	611	CLA	C1B-C2B	2.61	1.49	1.43
26	5	611	CLA	C1B-C2B	2.61	1.49	1.43
26	C	501	CLA	CMD-C2D	-2.61	1.45	1.50
26	N	603	CLA	C4B-NB	2.61	1.41	1.37
25	7	601	CHL	C3D-C2D	2.61	1.44	1.39
26	b	614	CLA	CMD-C2D	-2.60	1.45	1.50
26	b	608	CLA	CHC-C4B	-2.60	1.33	1.39
26	r	603	CLA	C1D-ND	2.60	1.41	1.37
26	B	602	CLA	C4B-NB	2.60	1.41	1.37
26	b	602	CLA	C4B-NB	2.60	1.41	1.37
26	B	608	CLA	CHC-C4B	-2.60	1.33	1.39
25	3	607	CHL	CBD-CGD	-2.60	1.49	1.52
26	R	610	CLA	CMC-C2C	-2.60	1.45	1.50
26	3	611	CLA	CMD-C2D	-2.60	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	611	CLA	CMD-C2D	-2.60	1.45	1.50
26	s	602	CLA	CMD-C2D	-2.60	1.45	1.50
26	c	506	CLA	MG-ND	-2.60	2.00	2.05
26	g	611	CLA	MG-NB	-2.60	2.00	2.05
27	Y	1621	LUT	C22-C21	-2.60	1.51	1.54
30	3	2630	LHG	O7-C5	-2.59	1.40	1.46
25	4	607	CHL	CBD-CGD	-2.59	1.49	1.52
26	b	605	CLA	C1B-C2B	2.59	1.49	1.43
26	A	410	CLA	CMD-C2D	-2.59	1.45	1.50
26	B	615	CLA	CMC-C2C	-2.59	1.45	1.50
26	Y	603	CLA	CMD-C2D	-2.59	1.45	1.50
26	N	611	CLA	C1B-C2B	2.59	1.49	1.43
26	n	611	CLA	C1B-C2B	2.59	1.49	1.43
26	n	604	CLA	MG-NB	-2.59	2.00	2.05
30	G	2630	LHG	O7-C5	-2.59	1.40	1.46
30	g	2630	LHG	O7-C5	-2.59	1.40	1.46
26	b	610	CLA	MG-NB	-2.59	2.00	2.05
26	B	614	CLA	CMD-C2D	-2.59	1.45	1.50
26	Y	611	CLA	C1D-ND	2.59	1.41	1.37
39	H	102	DGD	O1G-C1G	-2.59	1.39	1.45
26	B	610	CLA	MG-NB	-2.59	2.00	2.05
38	d	405	PL9	C11-C9	-2.58	1.46	1.51
26	B	605	CLA	C1B-C2B	2.58	1.49	1.43
26	C	503	CLA	C1D-ND	2.58	1.41	1.37
26	S	602	CLA	CMD-C2D	-2.58	1.45	1.50
26	B	606	CLA	CMB-C2B	-2.58	1.45	1.50
26	b	606	CLA	CMB-C2B	-2.58	1.45	1.50
26	B	609	CLA	C4B-NB	2.58	1.41	1.37
26	N	604	CLA	MG-NB	-2.58	2.00	2.05
27	y	1621	LUT	C22-C21	-2.58	1.51	1.54
25	6	607	CHL	CBD-CGD	-2.58	1.49	1.52
26	C	506	CLA	MG-ND	-2.58	2.00	2.05
26	G	611	CLA	CMD-C2D	-2.58	1.45	1.50
26	y	603	CLA	CMD-C2D	-2.58	1.45	1.50
26	S	611	CLA	C4B-NB	2.58	1.41	1.37
26	1	613	CLA	C1B-C2B	2.58	1.49	1.43
26	5	613	CLA	C1B-C2B	2.58	1.49	1.43
26	2	613	CLA	CMD-C2D	-2.58	1.45	1.50
26	6	613	CLA	CMD-C2D	-2.58	1.45	1.50
26	b	613	CLA	CMC-C2C	-2.58	1.45	1.50
26	3	612	CLA	CMD-C2D	-2.57	1.45	1.50
26	7	612	CLA	CMD-C2D	-2.57	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	614	CLA	CMB-C2B	-2.57	1.45	1.50
26	R	616	CLA	CMB-C2B	-2.57	1.45	1.50
26	S	603	CLA	CMD-C2D	-2.57	1.45	1.50
26	a	410	CLA	CMD-C2D	-2.57	1.45	1.50
26	y	604	CLA	MG-NB	-2.57	2.00	2.05
26	c	512	CLA	C1B-NB	-2.57	1.34	1.37
26	R	613	CLA	C1B-C2B	2.57	1.49	1.43
29	1	1623	NEX	C7-C6	-2.57	1.27	1.30
29	5	1623	NEX	C7-C6	-2.57	1.27	1.30
30	B	2630	LHG	O7-C5	-2.57	1.40	1.46
30	b	2630	LHG	O7-C5	-2.57	1.40	1.46
26	B	607	CLA	C4B-NB	2.57	1.41	1.37
26	C	504	CLA	C1B-NB	-2.57	1.34	1.37
26	s	603	CLA	CMD-C2D	-2.57	1.45	1.50
26	Y	610	CLA	C4B-NB	2.57	1.41	1.37
26	C	505	CLA	C1B-NB	-2.57	1.34	1.37
39	C	520	DGD	O3G-C3G	-2.57	1.39	1.43
39	c	520	DGD	O3G-C3G	-2.57	1.39	1.43
26	B	613	CLA	CMA-C3A	-2.56	1.47	1.53
39	C	519	DGD	O5D-C6D	-2.56	1.39	1.43
39	c	519	DGD	O5D-C6D	-2.56	1.39	1.43
25	7	607	CHL	CBD-CGD	-2.56	1.49	1.52
26	N	602	CLA	CMD-C2D	-2.56	1.45	1.50
39	C	518	DGD	O3E-C3E	-2.56	1.36	1.43
26	b	609	CLA	C4B-NB	2.56	1.41	1.37
26	c	505	CLA	C1B-NB	-2.56	1.34	1.37
26	r	613	CLA	C1B-C2B	2.56	1.49	1.43
26	Y	604	CLA	MG-NB	-2.56	2.00	2.05
26	B	614	CLA	MG-NB	-2.56	2.00	2.05
39	c	518	DGD	O3E-C3E	-2.56	1.36	1.43
30	7	2630	LHG	O7-C5	-2.56	1.40	1.46
26	b	614	CLA	MG-NB	-2.56	2.00	2.05
26	R	602	CLA	C4B-NB	2.56	1.41	1.37
26	r	602	CLA	C4B-NB	2.56	1.41	1.37
26	y	611	CLA	C1D-ND	2.55	1.41	1.37
26	B	613	CLA	CMC-C2C	-2.55	1.45	1.50
26	g	611	CLA	CMD-C2D	-2.55	1.45	1.50
26	n	602	CLA	CMD-C2D	-2.55	1.45	1.50
25	y	609	CHL	CBD-CGD	-2.55	1.49	1.52
38	D	405	PL9	C11-C9	-2.55	1.46	1.51
26	B	610	CLA	CMD-C2D	-2.55	1.45	1.50
26	G	604	CLA	MG-NB	-2.54	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	615	CLA	CMC-C2C	-2.54	1.45	1.50
26	b	613	CLA	CMA-C3A	-2.54	1.47	1.53
25	R	608	CHL	CBD-CGD	-2.54	1.49	1.52
25	r	608	CHL	C3D-C2D	2.54	1.44	1.39
26	N	603	CLA	C3B-C4B	2.54	1.50	1.42
26	y	610	CLA	C4B-NB	2.54	1.41	1.37
26	B	603	CLA	CMD-C2D	-2.54	1.45	1.50
26	b	603	CLA	CMD-C2D	-2.54	1.45	1.50
26	6	604	CLA	CMB-C2B	-2.54	1.45	1.50
30	B	2631	LHG	O7-C5	-2.54	1.40	1.46
26	N	602	CLA	CMC-C2C	-2.54	1.45	1.50
26	g	603	CLA	CMD-C2D	-2.54	1.45	1.50
26	n	602	CLA	CMC-C2C	-2.54	1.45	1.50
26	C	505	CLA	C1B-C2B	2.54	1.49	1.43
26	c	505	CLA	C1B-C2B	2.54	1.49	1.43
25	y	607	CHL	CBD-CGD	-2.54	1.49	1.52
26	c	506	CLA	C1D-ND	2.54	1.41	1.37
26	c	503	CLA	CMD-C2D	-2.53	1.45	1.50
26	C	513	CLA	CMC-C2C	-2.53	1.45	1.50
26	r	613	CLA	CMD-C2D	-2.53	1.45	1.50
26	C	503	CLA	CMD-C2D	-2.53	1.45	1.50
26	G	603	CLA	CMD-C2D	-2.53	1.45	1.50
30	n	2630	LHG	O7-C5	-2.53	1.40	1.46
26	G	612	CLA	C1B-C2B	2.53	1.49	1.43
26	7	613	CLA	C1B-C2B	2.53	1.49	1.43
26	C	502	CLA	MG-ND	-2.53	2.00	2.05
26	6	614	CLA	C1B-C2B	2.53	1.49	1.43
25	R	608	CHL	C3D-C2D	2.53	1.44	1.39
26	2	604	CLA	CMB-C2B	-2.53	1.45	1.50
26	s	609	CLA	C1B-C2B	2.53	1.49	1.43
26	R	610	CLA	C3B-C4B	2.53	1.50	1.42
26	r	610	CLA	C3B-C4B	2.53	1.50	1.42
26	S	604	CLA	C4B-NB	2.53	1.41	1.37
26	c	513	CLA	CMC-C2C	-2.53	1.45	1.50
30	C	2630	LHG	O7-C5	-2.53	1.40	1.46
26	b	616	CLA	C4B-NB	2.52	1.41	1.37
26	3	613	CLA	C1B-C2B	2.52	1.49	1.43
30	N	2630	LHG	O7-C5	-2.52	1.40	1.46
26	B	616	CLA	C1D-ND	2.52	1.41	1.37
26	5	613	CLA	CMD-C2D	-2.52	1.45	1.50
25	G	607	CHL	CBD-CGD	-2.52	1.49	1.52
25	g	607	CHL	CBD-CGD	-2.52	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	s	604	CLA	C4B-NB	2.52	1.41	1.37
26	S	609	CLA	C1B-C2B	2.52	1.49	1.43
26	b	616	CLA	C1D-ND	2.52	1.41	1.37
26	g	612	CLA	C1B-C2B	2.52	1.49	1.43
26	3	614	CLA	C1B-C2B	2.52	1.49	1.43
26	7	614	CLA	C1B-C2B	2.52	1.49	1.43
25	Y	609	CHL	CBD-CGD	-2.51	1.49	1.52
26	2	611	CLA	C1B-C2B	2.51	1.49	1.43
25	S	608	CHL	CBD-CGD	-2.51	1.49	1.52
25	s	608	CHL	CBD-CGD	-2.51	1.49	1.52
25	y	608	CHL	CBD-CGD	-2.51	1.49	1.52
30	R	2630	LHG	O7-C5	-2.51	1.40	1.46
26	g	604	CLA	MG-NB	-2.51	2.00	2.05
26	n	603	CLA	C3B-C4B	2.51	1.50	1.42
26	2	602	CLA	CMC-C2C	-2.51	1.45	1.50
26	2	602	CLA	CMD-C2D	-2.51	1.45	1.50
26	6	602	CLA	CMD-C2D	-2.51	1.45	1.50
26	C	512	CLA	CMB-C2B	-2.51	1.45	1.50
26	c	512	CLA	CMB-C2B	-2.51	1.45	1.50
26	s	611	CLA	C1B-C2B	2.51	1.49	1.43
30	r	2630	LHG	O7-C5	-2.51	1.40	1.46
26	y	603	CLA	CMB-C2B	-2.51	1.45	1.50
25	Y	608	CHL	CBD-CGD	-2.51	1.49	1.52
26	B	616	CLA	C4B-NB	2.51	1.41	1.37
26	C	504	CLA	CMB-C2B	-2.51	1.45	1.50
26	2	614	CLA	C1B-C2B	2.51	1.49	1.43
26	b	610	CLA	CMD-C2D	-2.51	1.45	1.50
26	6	602	CLA	CMC-C2C	-2.50	1.45	1.50
26	C	509	CLA	C1B-NB	-2.50	1.34	1.37
39	C	518	DGD	O5D-C6D	-2.50	1.39	1.43
30	b	2631	LHG	O7-C5	-2.50	1.40	1.46
30	c	2630	LHG	O7-C5	-2.50	1.40	1.46
26	C	506	CLA	C1D-ND	2.50	1.41	1.37
26	N	604	CLA	CMD-C2D	-2.50	1.45	1.50
26	1	602	CLA	CMC-C2C	-2.50	1.45	1.50
26	5	602	CLA	CMC-C2C	-2.50	1.45	1.50
26	Y	603	CLA	CMB-C2B	-2.50	1.45	1.50
26	B	614	CLA	C1D-ND	2.50	1.41	1.37
26	b	614	CLA	C1D-ND	2.50	1.41	1.37
26	r	604	CLA	C4B-NB	2.50	1.41	1.37
25	r	608	CHL	CBD-CGD	-2.50	1.49	1.52
26	2	603	CLA	CMD-C2D	-2.50	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N	612	CLA	C1B-C2B	2.50	1.49	1.43
26	n	612	CLA	C1B-C2B	2.50	1.49	1.43
26	4	612	CLA	C1B-C2B	2.50	1.49	1.43
26	B	603	CLA	CMB-C2B	-2.49	1.45	1.50
26	b	603	CLA	CMB-C2B	-2.49	1.45	1.50
26	C	501	CLA	C3B-C4B	2.49	1.50	1.42
26	c	501	CLA	C3B-C4B	2.49	1.50	1.42
26	G	610	CLA	C1B-C2B	2.49	1.49	1.43
26	c	507	CLA	CMB-C2B	-2.49	1.45	1.50
26	2	613	CLA	C1B-C2B	2.49	1.49	1.43
26	n	610	CLA	C4B-NB	2.49	1.41	1.37
26	R	613	CLA	CMD-C2D	-2.49	1.45	1.50
39	c	518	DGD	O5D-C6D	-2.49	1.39	1.43
26	B	602	CLA	CMD-C2D	-2.49	1.45	1.50
26	8	602	CLA	C1B-C2B	2.49	1.49	1.43
26	Y	602	CLA	CMD-C2D	-2.49	1.45	1.50
26	y	602	CLA	CMD-C2D	-2.49	1.45	1.50
26	c	502	CLA	MG-ND	-2.49	2.00	2.05
26	1	613	CLA	CMD-C2D	-2.49	1.45	1.50
26	s	602	CLA	CMC-C2C	-2.49	1.45	1.50
26	S	602	CLA	CMC-C2C	-2.49	1.45	1.50
26	8	612	CLA	C1B-C2B	2.49	1.49	1.43
26	y	604	CLA	MG-ND	-2.49	2.00	2.05
26	6	611	CLA	C1B-C2B	2.49	1.49	1.43
25	Y	607	CHL	CBD-CGD	-2.49	1.49	1.52
26	3	603	CLA	C4B-NB	2.48	1.41	1.37
26	3	612	CLA	CMC-C2C	-2.48	1.45	1.50
26	s	610	CLA	CMB-C2B	-2.48	1.45	1.50
26	n	604	CLA	CMD-C2D	-2.48	1.45	1.50
26	S	611	CLA	C1B-C2B	2.48	1.49	1.43
26	B	615	CLA	C1B-NB	-2.48	1.34	1.37
26	N	604	CLA	C1B-NB	-2.48	1.34	1.37
26	g	613	CLA	CMD-C2D	-2.48	1.45	1.50
26	G	613	CLA	CMD-C2D	-2.48	1.45	1.50
26	C	512	CLA	MG-NB	-2.48	2.00	2.05
26	c	512	CLA	MG-NB	-2.48	2.00	2.05
35	a	408	PHO	C3B-C2B	-2.48	1.37	1.40
26	c	509	CLA	MG-ND	-2.48	2.00	2.05
26	3	614	CLA	CMD-C2D	-2.47	1.45	1.50
26	R	604	CLA	C4B-NB	2.47	1.41	1.37
26	S	610	CLA	CMB-C2B	-2.47	1.45	1.50
26	C	509	CLA	MG-ND	-2.47	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	612	CLA	CMC-C2C	-2.47	1.45	1.50
26	B	607	CLA	C3B-C4B	2.47	1.49	1.42
26	7	603	CLA	C1B-C2B	2.47	1.48	1.43
26	y	612	CLA	C3B-C4B	2.47	1.49	1.42
26	G	604	CLA	CMD-C2D	-2.47	1.45	1.50
26	C	509	CLA	C1D-ND	2.47	1.41	1.37
26	c	509	CLA	C1D-ND	2.47	1.41	1.37
26	6	613	CLA	C1B-C2B	2.47	1.48	1.43
26	8	603	CLA	C1B-C2B	2.47	1.48	1.43
26	C	506	CLA	C1B-NB	-2.47	1.34	1.37
26	N	610	CLA	C4B-NB	2.47	1.41	1.37
26	c	506	CLA	C1B-NB	-2.47	1.34	1.37
26	3	603	CLA	C1B-C2B	2.47	1.48	1.43
26	s	614	CLA	C1B-C2B	2.47	1.48	1.43
26	5	602	CLA	C1B-C2B	2.47	1.48	1.43
25	n	607	CHL	CBD-CGD	-2.47	1.49	1.52
26	c	504	CLA	CMB-C2B	-2.47	1.45	1.50
26	g	610	CLA	C1B-C2B	2.47	1.48	1.43
35	A	408	PHO	C3B-C2B	-2.46	1.37	1.40
26	B	607	CLA	C1B-NB	-2.46	1.34	1.37
26	b	607	CLA	C1B-NB	-2.46	1.34	1.37
26	b	607	CLA	C3B-C4B	2.46	1.49	1.42
26	b	602	CLA	CMD-C2D	-2.46	1.45	1.50
26	b	615	CLA	C1B-NB	-2.46	1.34	1.37
26	b	616	CLA	CMD-C2D	-2.46	1.45	1.50
26	1	603	CLA	C1B-C2B	2.46	1.48	1.43
26	5	603	CLA	C1B-C2B	2.46	1.48	1.43
26	C	506	CLA	MG-NB	-2.46	2.00	2.05
26	c	506	CLA	MG-NB	-2.46	2.00	2.05
26	C	512	CLA	MG-ND	-2.46	2.00	2.05
26	c	512	CLA	MG-ND	-2.46	2.00	2.05
26	b	605	CLA	CMC-C2C	-2.46	1.45	1.50
26	S	603	CLA	C1B-C2B	2.46	1.48	1.43
26	s	603	CLA	C1B-C2B	2.46	1.48	1.43
39	H	102	DGD	O4D-C4D	-2.46	1.36	1.43
39	h	102	DGD	O4D-C4D	-2.46	1.36	1.43
26	n	603	CLA	CMB-C2B	-2.46	1.45	1.50
26	Y	604	CLA	MG-ND	-2.46	2.00	2.05
35	a	409	PHO	C1D-C2D	2.46	1.42	1.39
26	r	610	CLA	C4B-NB	2.46	1.41	1.37
26	6	603	CLA	CMD-C2D	-2.45	1.45	1.50
26	b	608	CLA	MG-NB	-2.45	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	616	CLA	CMD-C2D	-2.45	1.45	1.50
26	a	410	CLA	MG-ND	-2.45	2.00	2.05
26	4	604	CLA	CMB-C2B	-2.45	1.45	1.50
26	8	604	CLA	CMB-C2B	-2.45	1.45	1.50
26	4	603	CLA	C1B-C2B	2.45	1.48	1.43
26	C	507	CLA	CMB-C2B	-2.45	1.45	1.50
35	A	409	PHO	C1D-C2D	2.45	1.42	1.39
26	b	608	CLA	C4B-NB	2.45	1.41	1.37
26	c	509	CLA	C1B-NB	-2.45	1.34	1.37
26	4	602	CLA	C1B-C2B	2.45	1.48	1.43
26	1	610	CLA	CMB-C2B	-2.45	1.45	1.50
26	5	610	CLA	CMB-C2B	-2.45	1.45	1.50
26	c	504	CLA	CMD-C2D	-2.45	1.45	1.50
26	1	602	CLA	C1B-C2B	2.44	1.48	1.43
39	b	626	DGD	O3G-C3G	-2.44	1.39	1.43
26	3	610	CLA	CMB-C2B	-2.44	1.45	1.50
26	7	610	CLA	CMB-C2B	-2.44	1.45	1.50
26	7	614	CLA	CMD-C2D	-2.44	1.45	1.50
26	4	604	CLA	C1B-C2B	2.44	1.48	1.43
26	B	615	CLA	CMB-C2B	-2.44	1.45	1.50
26	S	612	CLA	CMD-C2D	-2.44	1.45	1.50
26	g	604	CLA	CMD-C2D	-2.44	1.45	1.50
26	s	612	CLA	CMD-C2D	-2.44	1.45	1.50
26	7	603	CLA	C4B-NB	2.44	1.41	1.37
26	3	604	CLA	CMB-C2B	-2.44	1.45	1.50
26	B	605	CLA	CMC-C2C	-2.44	1.45	1.50
26	c	503	CLA	MG-NB	-2.44	2.01	2.05
26	c	508	CLA	MG-NB	-2.44	2.01	2.05
26	S	614	CLA	C1B-C2B	2.44	1.48	1.43
26	1	602	CLA	C4B-NB	2.44	1.41	1.37
26	5	602	CLA	C4B-NB	2.44	1.41	1.37
26	C	505	CLA	CMB-C2B	-2.43	1.45	1.50
26	b	615	CLA	CMB-C2B	-2.43	1.45	1.50
26	c	505	CLA	CMB-C2B	-2.43	1.45	1.50
29	r	623	NEX	O24-C25	-2.43	1.43	1.46
26	B	608	CLA	C4B-NB	2.43	1.41	1.37
26	R	603	CLA	CMD-C2D	-2.43	1.45	1.50
26	5	604	CLA	CMD-C2D	-2.43	1.45	1.50
26	B	608	CLA	MG-NB	-2.43	2.01	2.05
26	R	611	CLA	C1B-C2B	2.43	1.48	1.43
26	N	603	CLA	CMB-C2B	-2.43	1.45	1.50
26	Y	612	CLA	C3B-C4B	2.43	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	503	CLA	MG-NB	-2.43	2.01	2.05
26	7	604	CLA	CMB-C2B	-2.43	1.45	1.50
26	8	604	CLA	C1B-C2B	2.43	1.48	1.43
26	Y	613	CLA	C1D-ND	2.43	1.41	1.37
26	Y	614	CLA	C4B-NB	2.43	1.41	1.37
26	y	613	CLA	C1D-ND	2.43	1.41	1.37
26	C	504	CLA	CMD-C2D	-2.43	1.45	1.50
26	r	611	CLA	MG-ND	-2.43	2.01	2.05
26	c	507	CLA	C1B-C2B	2.43	1.48	1.43
25	5	606	CHL	CBD-CGD	-2.43	1.49	1.52
26	A	405	CLA	CMB-C2B	-2.43	1.45	1.50
26	r	603	CLA	CMD-C2D	-2.43	1.45	1.50
26	B	610	CLA	CMC-C2C	-2.42	1.45	1.50
26	b	610	CLA	CMC-C2C	-2.42	1.45	1.50
27	6	1621	LUT	C22-C21	-2.42	1.51	1.54
29	R	623	NEX	O24-C25	-2.42	1.43	1.46
26	2	604	CLA	C1B-C2B	2.42	1.48	1.43
26	b	611	CLA	CMD-C2D	-2.42	1.45	1.50
26	n	603	CLA	CMC-C2C	-2.42	1.45	1.50
26	a	405	CLA	CMB-C2B	-2.42	1.45	1.50
26	A	410	CLA	CMB-C2B	-2.42	1.45	1.50
26	C	508	CLA	MG-NB	-2.42	2.01	2.05
26	6	602	CLA	C1B-C2B	2.42	1.48	1.43
26	R	611	CLA	MG-ND	-2.42	2.01	2.05
26	6	604	CLA	C1B-C2B	2.42	1.48	1.43
26	1	604	CLA	CMD-C2D	-2.42	1.45	1.50
26	B	611	CLA	CMD-C2D	-2.42	1.45	1.50
26	C	509	CLA	CMA-C3A	-2.42	1.48	1.53
26	c	509	CLA	CMA-C3A	-2.42	1.48	1.53
26	C	507	CLA	C1B-C2B	2.42	1.48	1.43
41	F	101	HEM	FE-NA	2.42	2.03	1.95
41	f	101	HEM	FE-NA	2.42	2.03	1.95
26	A	410	CLA	MG-ND	-2.41	2.01	2.05
26	n	604	CLA	C1B-NB	-2.41	1.34	1.37
26	S	609	CLA	C3B-C4B	2.41	1.49	1.42
26	B	605	CLA	C1D-ND	2.41	1.41	1.37
26	C	502	CLA	C1B-NB	-2.41	1.34	1.37
26	c	502	CLA	C1B-NB	-2.41	1.34	1.37
26	N	603	CLA	CMC-C2C	-2.41	1.45	1.50
26	b	604	CLA	CMC-C2C	-2.41	1.45	1.50
26	a	410	CLA	CMB-C2B	-2.41	1.45	1.50
27	2	1621	LUT	C22-C21	-2.41	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r	601	CLA	C3B-C4B	2.41	1.49	1.42
35	A	409	PHO	CMB-C2B	-2.41	1.46	1.51
26	1	614	CLA	C1B-C2B	2.41	1.48	1.43
26	2	602	CLA	C1B-C2B	2.41	1.48	1.43
39	B	626	DGD	O3G-C3G	-2.41	1.39	1.43
26	B	604	CLA	CMC-C2C	-2.41	1.45	1.50
26	b	617	CLA	C1B-C2B	2.41	1.48	1.43
26	y	614	CLA	C4B-NB	2.41	1.41	1.37
39	C	519	DGD	O6D-C5D	-2.41	1.38	1.44
26	B	616	CLA	CMC-C2C	-2.41	1.45	1.50
26	b	616	CLA	CMC-C2C	-2.41	1.45	1.50
26	s	609	CLA	C3B-C4B	2.40	1.49	1.42
26	s	602	CLA	MG-NB	-2.40	2.01	2.05
26	R	604	CLA	CMB-C2B	-2.40	1.45	1.50
26	r	604	CLA	CMB-C2B	-2.40	1.45	1.50
26	c	502	CLA	CMD-C2D	-2.40	1.45	1.50
26	r	611	CLA	C1B-C2B	2.40	1.48	1.43
26	n	610	CLA	C1B-C2B	2.40	1.48	1.43
26	C	508	CLA	CHC-C4B	-2.40	1.34	1.39
26	c	508	CLA	CHC-C4B	-2.40	1.34	1.39
26	C	506	CLA	CMC-C2C	-2.40	1.45	1.50
26	6	603	CLA	C1B-C2B	2.40	1.48	1.43
26	S	613	CLA	C1B-C2B	2.40	1.48	1.43
26	s	613	CLA	C1B-C2B	2.40	1.48	1.43
26	B	603	CLA	MG-NB	-2.40	2.01	2.05
26	b	603	CLA	MG-NB	-2.40	2.01	2.05
26	B	615	CLA	C1D-ND	2.40	1.41	1.37
26	b	615	CLA	C1D-ND	2.40	1.41	1.37
26	S	602	CLA	MG-NB	-2.40	2.01	2.05
26	c	506	CLA	CMC-C2C	-2.40	1.45	1.50
26	B	614	CLA	MG-ND	-2.40	2.01	2.05
35	A	408	PHO	C1D-C2D	2.40	1.42	1.39
35	a	408	PHO	C1D-C2D	2.40	1.42	1.39
26	R	603	CLA	MG-ND	-2.40	2.01	2.05
26	r	603	CLA	MG-ND	-2.40	2.01	2.05
26	Y	604	CLA	CMD-C2D	-2.39	1.45	1.50
26	y	604	CLA	CMD-C2D	-2.39	1.45	1.50
26	b	616	CLA	CMB-C2B	-2.39	1.45	1.50
39	c	519	DGD	O6D-C5D	-2.39	1.38	1.44
26	b	614	CLA	MG-ND	-2.39	2.01	2.05
26	B	616	CLA	CMB-C2B	-2.39	1.45	1.50
26	R	610	CLA	CMB-C2B	-2.39	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S	604	CLA	CMD-C2D	-2.39	1.45	1.50
26	r	610	CLA	CMB-C2B	-2.39	1.45	1.50
26	C	502	CLA	CMD-C2D	-2.39	1.45	1.50
26	R	610	CLA	CMD-C2D	-2.39	1.45	1.50
26	Y	610	CLA	CMB-C2B	-2.39	1.45	1.50
26	r	610	CLA	CMD-C2D	-2.39	1.45	1.50
26	y	610	CLA	CMB-C2B	-2.39	1.45	1.50
26	5	614	CLA	C1B-C2B	2.39	1.48	1.43
25	1	606	CHL	CBD-CGD	-2.39	1.49	1.52
26	Y	604	CLA	C1B-NB	-2.39	1.34	1.37
26	B	602	CLA	CMB-C2B	-2.39	1.45	1.50
25	N	607	CHL	CBD-CGD	-2.39	1.49	1.52
35	a	409	PHO	CMB-C2B	-2.39	1.46	1.51
26	2	610	CLA	C1B-C2B	2.39	1.48	1.43
26	N	610	CLA	C1B-C2B	2.39	1.48	1.43
26	6	610	CLA	C1B-C2B	2.39	1.48	1.43
26	A	405	CLA	C1B-NB	-2.39	1.34	1.37
26	a	405	CLA	C1B-NB	-2.39	1.34	1.37
26	R	601	CLA	C1B-C2B	2.39	1.48	1.43
26	s	614	CLA	CMD-C2D	-2.39	1.45	1.50
25	3	609	CHL	CBD-CGD	-2.39	1.49	1.52
25	7	609	CHL	CBD-CGD	-2.39	1.49	1.52
26	B	617	CLA	C1B-C2B	2.38	1.48	1.43
26	R	610	CLA	C4B-NB	2.38	1.41	1.37
26	G	602	CLA	CMD-C2D	-2.38	1.45	1.50
26	g	602	CLA	CMD-C2D	-2.38	1.45	1.50
26	b	605	CLA	C1D-ND	2.38	1.41	1.37
26	N	602	CLA	MG-ND	-2.38	2.01	2.05
26	n	602	CLA	MG-ND	-2.38	2.01	2.05
26	Y	611	CLA	CMC-C2C	-2.38	1.45	1.50
26	y	611	CLA	CMC-C2C	-2.38	1.45	1.50
26	D	402	CLA	C4B-NB	2.38	1.41	1.37
26	c	511	CLA	C4B-NB	2.38	1.41	1.37
26	d	402	CLA	C4B-NB	2.38	1.41	1.37
26	R	601	CLA	C3B-C4B	2.38	1.49	1.42
26	s	604	CLA	CMD-C2D	-2.38	1.45	1.50
26	N	602	CLA	MG-NB	-2.38	2.01	2.05
26	C	502	CLA	C1B-C2B	2.38	1.48	1.43
26	S	614	CLA	CMD-C2D	-2.38	1.45	1.50
26	b	611	CLA	C1B-NB	-2.38	1.34	1.37
26	b	602	CLA	CMB-C2B	-2.38	1.45	1.50
26	c	503	CLA	MG-ND	-2.38	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	610	CLA	CMD-C2D	-2.38	1.45	1.50
26	6	612	CLA	C1B-C2B	2.38	1.48	1.43
26	2	603	CLA	C1B-C2B	2.38	1.48	1.43
25	7	605	CHL	CBD-CGD	-2.37	1.49	1.52
26	8	610	CLA	CMD-C2D	-2.37	1.45	1.50
26	7	603	CLA	MG-ND	-2.37	2.01	2.05
26	A	406	CLA	CMD-C2D	-2.37	1.45	1.50
26	6	603	CLA	CMB-C2B	-2.37	1.45	1.50
26	a	406	CLA	CMD-C2D	-2.37	1.45	1.50
28	3	1622	XAT	O4-C5	-2.37	1.43	1.46
28	7	1622	XAT	O4-C5	-2.37	1.43	1.46
26	R	613	CLA	CMB-C2B	-2.37	1.45	1.50
26	r	613	CLA	CMB-C2B	-2.37	1.45	1.50
29	3	1623	NEX	C7-C6	-2.37	1.27	1.30
26	8	610	CLA	C1B-C2B	2.37	1.48	1.43
26	C	503	CLA	MG-ND	-2.37	2.01	2.05
26	2	612	CLA	C1B-C2B	2.37	1.48	1.43
26	R	604	CLA	CMD-C2D	-2.37	1.45	1.50
26	r	604	CLA	CMD-C2D	-2.37	1.45	1.50
26	1	604	CLA	MG-NB	-2.37	2.01	2.05
26	2	603	CLA	CMB-C2B	-2.36	1.45	1.50
26	B	610	CLA	CMB-C2B	-2.36	1.45	1.50
26	N	613	CLA	CMD-C2D	-2.36	1.45	1.50
26	n	613	CLA	CMD-C2D	-2.36	1.45	1.50
26	A	410	CLA	MG-NB	-2.36	2.01	2.05
26	r	601	CLA	C1B-C2B	2.36	1.48	1.43
26	B	611	CLA	C1B-NB	-2.36	1.34	1.37
26	G	602	CLA	C4B-NB	2.36	1.41	1.37
26	a	407	CLA	CMB-C2B	-2.36	1.45	1.50
26	C	510	CLA	MG-NB	-2.36	2.01	2.05
25	3	605	CHL	CBD-CGD	-2.36	1.49	1.52
26	7	614	CLA	C3B-C4B	2.36	1.49	1.42
26	7	610	CLA	CMC-C2C	-2.36	1.45	1.50
26	5	604	CLA	MG-NB	-2.36	2.01	2.05
26	g	602	CLA	C4B-NB	2.36	1.41	1.37
26	B	609	CLA	CMB-C2B	-2.35	1.45	1.50
29	7	1623	NEX	C7-C6	-2.35	1.27	1.30
26	b	617	CLA	C1B-NB	-2.35	1.34	1.37
26	N	604	CLA	MG-ND	-2.35	2.01	2.05
26	n	602	CLA	MG-NB	-2.35	2.01	2.05
26	n	604	CLA	MG-ND	-2.35	2.01	2.05
26	3	603	CLA	CMD-C2D	-2.35	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n	614	CLA	CMD-C2D	-2.35	1.46	1.50
26	c	510	CLA	MG-NB	-2.35	2.01	2.05
26	y	604	CLA	C1B-NB	-2.35	1.34	1.37
26	G	613	CLA	C3B-C4B	2.35	1.49	1.42
26	3	603	CLA	MG-ND	-2.35	2.01	2.05
26	C	511	CLA	C4B-NB	2.35	1.40	1.37
26	7	603	CLA	CMD-C2D	-2.34	1.46	1.50
26	C	510	CLA	C1B-NB	-2.34	1.34	1.37
26	c	510	CLA	C1B-NB	-2.34	1.34	1.37
25	R	608	CHL	OBD-CAD	2.34	1.25	1.22
26	4	610	CLA	C1B-C2B	2.34	1.48	1.43
26	1	612	CLA	CMD-C2D	-2.34	1.46	1.50
26	5	612	CLA	CMD-C2D	-2.34	1.46	1.50
26	2	613	CLA	MG-ND	-2.34	2.01	2.05
26	6	604	CLA	CMD-C2D	-2.34	1.46	1.50
26	3	614	CLA	C3B-C4B	2.34	1.49	1.42
26	c	507	CLA	CMD-C2D	-2.34	1.46	1.50
26	Y	614	CLA	C1B-C2B	2.34	1.48	1.43
26	y	614	CLA	C1B-C2B	2.34	1.48	1.43
26	A	405	CLA	C1D-ND	2.34	1.40	1.37
26	a	405	CLA	C1D-ND	2.34	1.40	1.37
28	4	622	XAT	O4-C5	-2.34	1.43	1.46
26	1	602	CLA	CMD-C2D	-2.34	1.46	1.50
26	2	604	CLA	CMD-C2D	-2.34	1.46	1.50
26	5	602	CLA	CMD-C2D	-2.34	1.46	1.50
26	B	609	CLA	MG-NB	-2.33	2.01	2.05
28	8	622	XAT	O4-C5	-2.33	1.43	1.46
30	D	410	LHG	O7-C5	-2.33	1.41	1.46
26	c	502	CLA	C1B-C2B	2.33	1.48	1.43
26	c	507	CLA	CAC-C3C	-2.33	1.45	1.51
26	c	510	CLA	C1D-ND	2.33	1.40	1.37
26	C	505	CLA	CMC-C2C	-2.33	1.46	1.50
26	C	513	CLA	C1B-NB	-2.33	1.34	1.37
26	b	609	CLA	MG-NB	-2.33	2.01	2.05
28	G	1622	XAT	O4-C5	-2.33	1.43	1.46
26	A	407	CLA	CMB-C2B	-2.33	1.46	1.50
26	B	611	CLA	MG-NB	-2.33	2.01	2.05
26	b	610	CLA	CMB-C2B	-2.33	1.46	1.50
26	B	611	CLA	CMB-C2B	-2.33	1.46	1.50
26	7	610	CLA	CMD-C2D	-2.33	1.46	1.50
26	a	410	CLA	MG-NB	-2.33	2.01	2.05
26	y	611	CLA	CMB-C2B	-2.33	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g	613	CLA	C3B-C4B	2.33	1.49	1.42
26	G	611	CLA	CHC-C1C	2.33	1.43	1.38
26	g	611	CLA	CHC-C1C	2.33	1.43	1.38
26	S	613	CLA	CMD-C2D	-2.33	1.46	1.50
26	b	617	CLA	CMD-C2D	-2.33	1.46	1.50
26	n	603	CLA	MG-ND	-2.33	2.01	2.05
26	B	614	CLA	CMC-C2C	-2.33	1.46	1.50
25	5	605	CHL	CBD-CGD	-2.33	1.49	1.52
26	G	614	CLA	CMD-C2D	-2.32	1.46	1.50
26	2	614	CLA	CMD-C2D	-2.32	1.46	1.50
26	B	611	CLA	C1D-ND	2.32	1.40	1.37
26	b	611	CLA	C1D-ND	2.32	1.40	1.37
26	c	505	CLA	CMC-C2C	-2.32	1.46	1.50
26	g	614	CLA	CMD-C2D	-2.32	1.46	1.50
26	6	613	CLA	MG-ND	-2.32	2.01	2.05
25	r	608	CHL	OBD-CAD	2.32	1.25	1.22
26	s	612	CLA	C3B-C4B	2.32	1.49	1.42
26	C	502	CLA	CHC-C4B	-2.32	1.34	1.39
26	D	403	CLA	CMD-C2D	-2.32	1.46	1.50
26	R	616	CLA	CMD-C2D	-2.32	1.46	1.50
26	r	616	CLA	CMD-C2D	-2.32	1.46	1.50
26	N	614	CLA	CMD-C2D	-2.32	1.46	1.50
30	d	410	LHG	O7-C5	-2.32	1.41	1.46
26	n	614	CLA	C1B-C2B	2.32	1.48	1.43
26	s	613	CLA	CMD-C2D	-2.32	1.46	1.50
26	Y	613	CLA	C1B-C2B	2.32	1.48	1.43
26	S	612	CLA	C3B-C4B	2.32	1.49	1.42
26	C	503	CLA	CMB-C2B	-2.32	1.46	1.50
26	c	503	CLA	CMB-C2B	-2.32	1.46	1.50
29	1	1623	NEX	O24-C25	-2.32	1.43	1.46
29	5	1623	NEX	O24-C25	-2.32	1.43	1.46
26	B	612	CLA	CMD-C2D	-2.31	1.46	1.50
26	b	612	CLA	CMD-C2D	-2.31	1.46	1.50
26	4	611	CLA	C3B-C4B	2.31	1.49	1.42
26	B	610	CLA	MG-ND	-2.31	2.01	2.05
25	4	606	CHL	CBD-CGD	-2.31	1.49	1.52
26	b	609	CLA	CMB-C2B	-2.31	1.46	1.50
26	s	602	CLA	CMB-C2B	-2.31	1.46	1.50
26	3	610	CLA	CMC-C2C	-2.31	1.46	1.50
26	3	613	CLA	CMD-C2D	-2.31	1.46	1.50
26	7	613	CLA	CMD-C2D	-2.31	1.46	1.50
26	b	611	CLA	MG-NB	-2.31	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	y	614	CLA	MG-ND	-2.31	2.01	2.05
26	D	403	CLA	C1B-NB	-2.31	1.34	1.37
28	R	622	XAT	O4-C5	-2.31	1.43	1.46
28	r	622	XAT	O4-C5	-2.31	1.43	1.46
26	b	608	CLA	MG-ND	-2.31	2.01	2.05
26	Y	602	CLA	MG-NB	-2.31	2.01	2.05
26	B	606	CLA	MG-NB	-2.31	2.01	2.05
26	N	603	CLA	MG-ND	-2.31	2.01	2.05
26	b	611	CLA	CMB-C2B	-2.31	1.46	1.50
26	5	603	CLA	CMD-C2D	-2.31	1.46	1.50
26	B	617	CLA	C1B-NB	-2.30	1.34	1.37
26	B	617	CLA	CMD-C2D	-2.30	1.46	1.50
26	N	614	CLA	C1B-C2B	2.30	1.48	1.43
26	5	614	CLA	CMD-C2D	-2.30	1.46	1.50
26	c	513	CLA	C1B-NB	-2.30	1.34	1.37
26	C	507	CLA	CMD-C2D	-2.30	1.46	1.50
26	B	607	CLA	CMB-C2B	-2.30	1.46	1.50
26	Y	611	CLA	CMB-C2B	-2.30	1.46	1.50
26	b	607	CLA	CMB-C2B	-2.30	1.46	1.50
26	d	403	CLA	C1B-NB	-2.30	1.34	1.37
26	s	602	CLA	C1D-ND	2.30	1.40	1.37
26	C	507	CLA	CAC-C3C	-2.30	1.45	1.51
26	C	510	CLA	C1D-ND	2.30	1.40	1.37
26	3	612	CLA	CMB-C2B	-2.30	1.46	1.50
26	A	407	CLA	CMD-C2D	-2.30	1.46	1.50
26	B	608	CLA	MG-ND	-2.30	2.01	2.05
26	3	613	CLA	CMC-C2C	-2.30	1.46	1.50
26	N	602	CLA	C4B-NB	2.30	1.40	1.37
26	n	602	CLA	C4B-NB	2.30	1.40	1.37
25	8	606	CHL	CBD-CGD	-2.30	1.49	1.52
26	3	610	CLA	CMD-C2D	-2.30	1.46	1.50
26	8	611	CLA	C3B-C4B	2.30	1.49	1.42
26	b	606	CLA	MG-NB	-2.30	2.01	2.05
26	S	602	CLA	CMB-C2B	-2.30	1.46	1.50
26	6	614	CLA	CMD-C2D	-2.30	1.46	1.50
26	4	604	CLA	C3B-C4B	2.30	1.49	1.42
26	8	604	CLA	C3B-C4B	2.30	1.49	1.42
26	B	609	CLA	C1B-NB	-2.30	1.34	1.37
26	b	609	CLA	C1B-NB	-2.30	1.34	1.37
29	7	1623	NEX	O24-C25	-2.30	1.43	1.46
26	B	616	CLA	C1B-C2B	2.30	1.48	1.43
26	b	616	CLA	C1B-C2B	2.30	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	y	613	CLA	C1B-C2B	2.29	1.48	1.43
38	D	405	PL9	C16-C14	-2.29	1.46	1.51
38	d	405	PL9	C16-C14	-2.29	1.46	1.51
26	y	610	CLA	C3B-C4B	2.29	1.49	1.42
26	B	603	CLA	CMC-C2C	-2.29	1.46	1.50
26	7	612	CLA	CMB-C2B	-2.29	1.46	1.50
28	g	1622	XAT	O4-C5	-2.29	1.43	1.46
26	Y	610	CLA	C3B-C4B	2.29	1.49	1.42
26	5	613	CLA	MG-ND	-2.29	2.01	2.05
26	c	513	CLA	CMD-C2D	-2.29	1.46	1.50
25	1	605	CHL	CBD-CGD	-2.29	1.49	1.52
26	c	502	CLA	CHC-C4B	-2.29	1.34	1.39
26	Y	614	CLA	MG-ND	-2.29	2.01	2.05
26	7	613	CLA	CMC-C2C	-2.29	1.46	1.50
26	r	609	CLA	CMD-C2D	-2.29	1.46	1.50
26	B	612	CLA	C1D-ND	2.29	1.40	1.37
26	b	614	CLA	CMC-C2C	-2.29	1.46	1.50
26	y	602	CLA	MG-NB	-2.29	2.01	2.05
29	3	1623	NEX	O24-C25	-2.29	1.43	1.46
26	6	611	CLA	C3B-C4B	2.29	1.49	1.42
26	C	510	CLA	C4B-NB	2.29	1.40	1.37
26	c	510	CLA	C4B-NB	2.29	1.40	1.37
26	s	602	CLA	CHC-C1C	2.29	1.43	1.38
26	3	602	CLA	C1B-C2B	2.29	1.48	1.43
26	7	602	CLA	C1B-C2B	2.29	1.48	1.43
26	1	610	CLA	CMD-C2D	-2.29	1.46	1.50
26	r	603	CLA	CMB-C2B	-2.29	1.46	1.50
26	C	504	CLA	C1D-ND	2.29	1.40	1.37
26	4	610	CLA	CMC-C2C	-2.28	1.46	1.50
26	8	610	CLA	CMC-C2C	-2.28	1.46	1.50
26	B	605	CLA	C1B-NB	-2.28	1.34	1.37
26	b	605	CLA	C1B-NB	-2.28	1.34	1.37
26	5	612	CLA	C1B-C2B	2.28	1.48	1.43
26	N	604	CLA	CMC-C2C	-2.28	1.46	1.50
26	N	611	CLA	CMD-C2D	-2.28	1.46	1.50
26	n	611	CLA	CMD-C2D	-2.28	1.46	1.50
26	1	613	CLA	MG-ND	-2.28	2.01	2.05
26	5	610	CLA	CMD-C2D	-2.28	1.46	1.50
26	S	602	CLA	CHC-C1C	2.28	1.43	1.38
26	y	613	CLA	MG-ND	-2.28	2.01	2.05
26	1	614	CLA	CMD-C2D	-2.28	1.46	1.50
26	c	508	CLA	CMD-C2D	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	602	CLA	MG-NB	-2.28	2.01	2.05
26	B	610	CLA	C1B-C2B	2.28	1.48	1.43
26	b	610	CLA	C1B-C2B	2.28	1.48	1.43
26	7	611	CLA	MG-ND	-2.28	2.01	2.05
29	Y	1623	NEX	O24-C25	-2.28	1.43	1.46
29	y	1623	NEX	O24-C25	-2.28	1.43	1.46
26	s	604	CLA	C1B-C2B	2.28	1.48	1.43
26	d	403	CLA	CMD-C2D	-2.28	1.46	1.50
26	C	513	CLA	C4B-NB	2.28	1.40	1.37
26	c	513	CLA	C4B-NB	2.28	1.40	1.37
26	a	406	CLA	CMB-C2B	-2.28	1.46	1.50
26	G	604	CLA	C1B-NB	-2.28	1.34	1.37
26	S	602	CLA	C1D-ND	2.28	1.40	1.37
26	a	407	CLA	CMD-C2D	-2.28	1.46	1.50
25	5	601	CHL	CBD-CGD	-2.28	1.49	1.52
26	b	610	CLA	MG-ND	-2.28	2.01	2.05
26	g	602	CLA	MG-ND	-2.28	2.01	2.05
26	A	406	CLA	CAC-C3C	-2.28	1.45	1.51
37	Z	101	LMG	C7-C8	2.28	1.57	1.50
37	z	101	LMG	C7-C8	2.28	1.57	1.50
37	D	411	LMG	O7-C8	-2.28	1.41	1.46
37	d	411	LMG	O7-C8	-2.28	1.41	1.46
26	A	406	CLA	C1B-C2B	2.28	1.48	1.43
26	a	406	CLA	C1B-C2B	2.28	1.48	1.43
26	g	604	CLA	C1B-NB	-2.27	1.34	1.37
26	R	603	CLA	CMB-C2B	-2.27	1.46	1.50
26	y	602	CLA	MG-ND	-2.27	2.01	2.05
26	2	611	CLA	C3B-C4B	2.27	1.49	1.42
26	S	612	CLA	C1B-C2B	2.27	1.48	1.43
26	s	612	CLA	C1B-C2B	2.27	1.48	1.43
30	b	2631	LHG	P-O6	2.27	1.68	1.59
26	S	612	CLA	CMC-C2C	-2.27	1.46	1.50
26	s	612	CLA	CMC-C2C	-2.27	1.46	1.50
26	1	612	CLA	C1B-C2B	2.27	1.48	1.43
26	6	603	CLA	MG-ND	-2.27	2.01	2.05
26	B	612	CLA	C4B-NB	2.27	1.40	1.37
26	b	612	CLA	C4B-NB	2.27	1.40	1.37
26	C	508	CLA	CMD-C2D	-2.27	1.46	1.50
36	A	412	SQD	O47-C45	-2.27	1.41	1.46
30	B	2631	LHG	P-O6	2.27	1.68	1.59
26	4	603	CLA	CMB-C2B	-2.27	1.46	1.50
26	Y	602	CLA	CMB-C2B	-2.27	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	y	602	CLA	CMB-C2B	-2.27	1.46	1.50
26	Y	603	CLA	CMC-C2C	-2.27	1.46	1.50
26	n	604	CLA	CMC-C2C	-2.27	1.46	1.50
26	y	603	CLA	CMC-C2C	-2.27	1.46	1.50
26	3	611	CLA	MG-ND	-2.27	2.01	2.05
38	D	405	PL9	C31-C29	-2.27	1.46	1.51
38	d	405	PL9	C31-C29	-2.27	1.46	1.51
26	S	611	CLA	CMD-C2D	-2.27	1.46	1.50
26	s	611	CLA	CMD-C2D	-2.27	1.46	1.50
27	1	1621	LUT	C1-C6	-2.27	1.50	1.53
26	b	612	CLA	MG-NB	-2.27	2.01	2.05
26	N	614	CLA	C3B-C4B	2.27	1.49	1.42
26	7	613	CLA	CMB-C2B	-2.27	1.46	1.50
26	C	503	CLA	C4B-NB	2.27	1.40	1.37
26	c	503	CLA	C4B-NB	2.27	1.40	1.37
26	Y	612	CLA	CMC-C2C	-2.27	1.46	1.50
26	s	611	CLA	CMC-C2C	-2.27	1.46	1.50
26	A	410	CLA	C1D-ND	2.27	1.40	1.37
26	a	410	CLA	C1D-ND	2.27	1.40	1.37
26	1	603	CLA	CMD-C2D	-2.26	1.46	1.50
26	A	410	CLA	CMC-C2C	-2.26	1.46	1.50
26	a	410	CLA	CMC-C2C	-2.26	1.46	1.50
26	S	604	CLA	C1B-C2B	2.26	1.48	1.43
25	Y	605	CHL	CBD-CGD	-2.26	1.49	1.52
25	y	605	CHL	CBD-CGD	-2.26	1.49	1.52
28	y	1622	XAT	O4-C5	-2.26	1.43	1.46
26	n	614	CLA	C3B-C4B	2.26	1.49	1.42
25	7	606	CHL	CBD-CGD	-2.26	1.49	1.52
26	N	612	CLA	CMD-C2D	-2.26	1.46	1.50
26	n	612	CLA	CMD-C2D	-2.26	1.46	1.50
26	r	602	CLA	MG-NB	-2.26	2.01	2.05
26	N	603	CLA	C1B-NB	-2.26	1.34	1.37
26	n	603	CLA	C1B-NB	-2.26	1.34	1.37
26	G	614	CLA	C3B-C4B	2.26	1.49	1.42
26	b	612	CLA	C1D-ND	2.26	1.40	1.37
26	G	602	CLA	MG-ND	-2.26	2.01	2.05
26	A	406	CLA	CMB-C2B	-2.26	1.46	1.50
26	G	602	CLA	CMB-C2B	-2.26	1.46	1.50
26	y	612	CLA	CMC-C2C	-2.26	1.46	1.50
26	Y	602	CLA	MG-ND	-2.26	2.01	2.05
26	R	612	CLA	CMD-C2D	-2.26	1.46	1.50
26	s	602	CLA	C3B-C4B	2.26	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	602	CLA	C1B-C2B	2.26	1.48	1.43
26	b	611	CLA	MG-ND	-2.26	2.01	2.05
26	D	402	CLA	CMA-C3A	-2.26	1.48	1.53
26	d	402	CLA	CMA-C3A	-2.26	1.48	1.53
26	a	406	CLA	CAC-C3C	-2.26	1.45	1.51
26	3	613	CLA	CMB-C2B	-2.26	1.46	1.50
26	R	611	CLA	C3B-C4B	2.26	1.49	1.42
26	2	614	CLA	C3B-C4B	2.25	1.49	1.42
26	b	603	CLA	CMC-C2C	-2.25	1.46	1.50
26	S	602	CLA	C3B-C4B	2.25	1.49	1.42
26	C	511	CLA	CMC-C2C	-2.25	1.46	1.50
26	c	511	CLA	CMC-C2C	-2.25	1.46	1.50
26	r	612	CLA	CMD-C2D	-2.25	1.46	1.50
26	B	602	CLA	C1B-C2B	2.25	1.48	1.43
26	b	602	CLA	C1B-C2B	2.25	1.48	1.43
26	G	603	CLA	CAC-C3C	-2.25	1.45	1.51
26	D	403	CLA	C4B-NB	2.25	1.40	1.37
26	d	403	CLA	C4B-NB	2.25	1.40	1.37
26	g	602	CLA	CMB-C2B	-2.25	1.46	1.50
25	R	607	CHL	CBD-CGD	-2.25	1.49	1.52
25	r	607	CHL	CBD-CGD	-2.25	1.49	1.52
26	Y	603	CLA	MG-ND	-2.25	2.01	2.05
26	Y	614	CLA	MG-NB	-2.25	2.01	2.05
26	y	603	CLA	MG-ND	-2.25	2.01	2.05
26	y	614	CLA	MG-NB	-2.25	2.01	2.05
26	S	611	CLA	CMC-C2C	-2.25	1.46	1.50
25	1	601	CHL	CBD-CGD	-2.25	1.49	1.52
26	g	614	CLA	C3B-C4B	2.25	1.49	1.42
26	r	611	CLA	C3B-C4B	2.25	1.49	1.42
26	A	406	CLA	C1B-NB	-2.25	1.34	1.37
26	a	406	CLA	C1B-NB	-2.25	1.34	1.37
26	g	603	CLA	CAC-C3C	-2.25	1.45	1.51
26	6	610	CLA	CMB-C2B	-2.25	1.46	1.50
26	B	612	CLA	MG-NB	-2.25	2.01	2.05
26	3	612	CLA	C1B-C2B	2.25	1.48	1.43
29	S	1623	NEX	O24-C25	-2.25	1.43	1.46
29	s	1623	NEX	O24-C25	-2.25	1.43	1.46
26	2	610	CLA	CMB-C2B	-2.25	1.46	1.50
26	R	604	CLA	C1B-NB	-2.25	1.34	1.37
26	r	604	CLA	C1B-NB	-2.25	1.34	1.37
26	2	603	CLA	MG-ND	-2.25	2.01	2.05
26	4	603	CLA	MG-ND	-2.25	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	603	CLA	MG-NB	-2.25	2.01	2.05
26	R	609	CLA	CMD-C2D	-2.25	1.46	1.50
26	1	603	CLA	MG-ND	-2.25	2.01	2.05
26	5	603	CLA	MG-ND	-2.25	2.01	2.05
26	N	610	CLA	CMD-C2D	-2.25	1.46	1.50
26	n	610	CLA	CMD-C2D	-2.25	1.46	1.50
36	a	412	SQD	O47-C45	-2.25	1.41	1.46
26	C	511	CLA	C1B-C2B	2.24	1.48	1.43
26	Y	614	CLA	CMB-C2B	-2.24	1.46	1.50
26	r	611	CLA	C4B-NB	2.24	1.40	1.37
26	C	513	CLA	CMD-C2D	-2.24	1.46	1.50
25	R	606	CHL	CBD-CGD	-2.24	1.49	1.52
25	r	606	CHL	CBD-CGD	-2.24	1.49	1.52
29	g	1623	NEX	O24-C25	-2.24	1.43	1.46
26	B	611	CLA	MG-ND	-2.24	2.01	2.05
26	Y	613	CLA	MG-ND	-2.24	2.01	2.05
26	c	504	CLA	C1D-ND	2.24	1.40	1.37
26	g	610	CLA	CMB-C2B	-2.24	1.46	1.50
26	N	612	CLA	C3B-C4B	2.23	1.49	1.42
26	n	612	CLA	C3B-C4B	2.23	1.49	1.42
26	c	503	CLA	CMC-C2C	-2.23	1.46	1.50
26	c	511	CLA	C1B-C2B	2.23	1.48	1.43
26	1	602	CLA	MG-NB	-2.23	2.01	2.05
26	1	610	CLA	CMC-C2C	-2.23	1.46	1.50
26	R	604	CLA	C1B-C2B	2.23	1.48	1.43
26	r	604	CLA	C1B-C2B	2.23	1.48	1.43
26	g	613	CLA	CHC-C1C	2.23	1.43	1.38
26	7	612	CLA	C1B-C2B	2.23	1.48	1.43
28	Y	1622	XAT	O4-C5	-2.23	1.43	1.46
37	C	521	LMG	O1-C7	-2.23	1.39	1.43
26	r	602	CLA	C1B-C2B	2.23	1.48	1.43
26	5	602	CLA	MG-NB	-2.23	2.01	2.05
26	C	503	CLA	CMC-C2C	-2.23	1.46	1.50
26	N	613	CLA	CMC-C2C	-2.23	1.46	1.50
26	8	603	CLA	CMB-C2B	-2.23	1.46	1.50
26	6	614	CLA	C3B-C4B	2.23	1.49	1.42
26	C	504	CLA	CMC-C2C	-2.23	1.46	1.50
28	2	1622	XAT	O4-C5	-2.23	1.43	1.46
28	6	1622	XAT	O4-C5	-2.23	1.43	1.46
26	c	507	CLA	MG-NB	-2.23	2.01	2.05
26	n	613	CLA	CMC-C2C	-2.23	1.46	1.50
26	C	504	CLA	MG-NB	-2.23	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	8	610	CLA	CMB-C2B	-2.23	1.46	1.50
26	y	614	CLA	CMB-C2B	-2.23	1.46	1.50
28	Y	1622	XAT	O24-C25	-2.22	1.43	1.46
26	B	603	CLA	C4B-NB	2.22	1.40	1.37
26	8	603	CLA	CMD-C2D	-2.22	1.46	1.50
26	r	603	CLA	MG-NB	-2.22	2.01	2.05
27	5	1621	LUT	C1-C6	-2.22	1.50	1.53
25	2	606	CHL	CBD-CGD	-2.22	1.49	1.52
26	5	610	CLA	CMC-C2C	-2.22	1.46	1.50
26	Y	602	CLA	C1B-C2B	2.22	1.48	1.43
26	c	504	CLA	CMC-C2C	-2.22	1.46	1.50
26	4	610	CLA	CMB-C2B	-2.22	1.46	1.50
25	r	614	CHL	CBD-CGD	-2.22	1.49	1.52
26	y	604	CLA	CMC-C2C	-2.22	1.46	1.50
26	3	610	CLA	C3B-C4B	2.22	1.49	1.42
26	7	610	CLA	C3B-C4B	2.22	1.49	1.42
26	8	603	CLA	MG-ND	-2.22	2.01	2.05
26	R	602	CLA	CMD-C2D	-2.22	1.46	1.50
26	r	602	CLA	CMD-C2D	-2.22	1.46	1.50
26	N	602	CLA	C3B-C4B	2.22	1.49	1.42
26	n	602	CLA	C3B-C4B	2.22	1.49	1.42
26	c	505	CLA	CHC-C4B	-2.22	1.34	1.39
26	a	405	CLA	C1C-NC	-2.22	1.34	1.37
26	1	611	CLA	CMD-C2D	-2.22	1.46	1.50
26	5	611	CLA	CMD-C2D	-2.22	1.46	1.50
25	R	614	CHL	CBD-CGD	-2.22	1.49	1.52
26	6	613	CLA	C3B-C4B	2.22	1.49	1.42
35	A	408	PHO	CAC-C3C	-2.22	1.47	1.51
26	6	602	CLA	MG-NB	-2.21	2.01	2.05
26	c	504	CLA	MG-NB	-2.21	2.01	2.05
26	3	602	CLA	CMB-C2B	-2.21	1.46	1.50
26	7	602	CLA	CMB-C2B	-2.21	1.46	1.50
26	3	614	CLA	CMB-C2B	-2.21	1.46	1.50
26	C	501	CLA	CMC-C2C	-2.21	1.46	1.50
26	7	614	CLA	CMB-C2B	-2.21	1.46	1.50
26	C	512	CLA	C4B-NB	2.21	1.40	1.37
25	3	606	CHL	CBD-CGD	-2.21	1.49	1.52
26	C	507	CLA	C1B-NB	-2.21	1.35	1.37
26	4	603	CLA	CMD-C2D	-2.21	1.46	1.50
26	R	601	CLA	MG-NB	-2.21	2.01	2.05
25	Y	601	CHL	CMC-C2C	2.21	1.49	1.44
25	y	601	CHL	CMC-C2C	2.21	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	2	613	CLA	C3B-C4B	2.21	1.49	1.42
26	A	405	CLA	C1B-C2B	2.21	1.48	1.43
26	C	507	CLA	MG-NB	-2.21	2.01	2.05
26	Y	612	CLA	C1B-NB	-2.21	1.35	1.37
26	b	610	CLA	C1D-ND	2.21	1.40	1.37
26	y	612	CLA	C1B-NB	-2.21	1.35	1.37
26	N	610	CLA	CMB-C2B	-2.21	1.46	1.50
26	Y	613	CLA	CMB-C2B	-2.21	1.46	1.50
26	n	610	CLA	CMB-C2B	-2.21	1.46	1.50
26	y	613	CLA	CMB-C2B	-2.21	1.46	1.50
26	b	617	CLA	MG-NB	-2.21	2.01	2.05
26	G	613	CLA	CHC-C1C	2.21	1.42	1.38
26	B	610	CLA	C1D-ND	2.21	1.40	1.37
26	C	505	CLA	CHC-C4B	-2.21	1.34	1.39
26	N	610	CLA	MG-NB	-2.21	2.01	2.05
26	r	603	CLA	C4B-NB	2.21	1.40	1.37
26	3	603	CLA	CMB-C2B	-2.20	1.46	1.50
26	7	603	CLA	CMB-C2B	-2.20	1.46	1.50
27	7	1621	LUT	C22-C21	-2.20	1.52	1.54
26	2	602	CLA	MG-NB	-2.20	2.01	2.05
26	A	406	CLA	MG-NB	-2.20	2.01	2.05
26	B	617	CLA	MG-NB	-2.20	2.01	2.05
26	a	406	CLA	MG-NB	-2.20	2.01	2.05
26	S	613	CLA	CMB-C2B	-2.20	1.46	1.50
26	s	613	CLA	CMB-C2B	-2.20	1.46	1.50
26	B	607	CLA	MG-ND	-2.20	2.01	2.05
26	b	607	CLA	MG-ND	-2.20	2.01	2.05
26	r	612	CLA	C1B-C2B	2.20	1.48	1.43
26	Y	612	CLA	CMB-C2B	-2.20	1.46	1.50
26	c	506	CLA	CMD-C2D	-2.20	1.46	1.50
26	y	612	CLA	CMB-C2B	-2.20	1.46	1.50
25	6	606	CHL	CBD-CGD	-2.20	1.49	1.52
39	B	626	DGD	O1G-C1G	-2.20	1.40	1.45
39	b	626	DGD	O1G-C1G	-2.20	1.40	1.45
29	G	1623	NEX	O24-C25	-2.20	1.43	1.46
26	c	507	CLA	C1B-NB	-2.20	1.35	1.37
26	6	610	CLA	C3B-C4B	2.20	1.49	1.42
26	c	511	CLA	CMB-C2B	-2.20	1.46	1.50
25	s	601	CHL	CBD-CGD	-2.20	1.49	1.52
26	G	610	CLA	CMB-C2B	-2.20	1.46	1.50
26	5	613	CLA	CMB-C2B	-2.20	1.46	1.50
26	7	611	CLA	CHC-C4B	-2.20	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	609	CHL	CBD-CGD	-2.20	1.49	1.52
26	Y	603	CLA	C1B-NB	-2.20	1.35	1.37
26	S	604	CLA	MG-NB	-2.20	2.01	2.05
26	2	602	CLA	CMB-C2B	-2.20	1.46	1.50
26	R	611	CLA	C4B-NB	2.20	1.40	1.37
26	2	610	CLA	C3B-C4B	2.20	1.49	1.42
29	2	1623	NEX	O24-C25	-2.20	1.43	1.46
29	6	1623	NEX	O24-C25	-2.20	1.43	1.46
26	R	603	CLA	C4B-NB	2.20	1.40	1.37
26	S	602	CLA	C1B-C2B	2.20	1.48	1.43
26	y	602	CLA	C1B-C2B	2.20	1.48	1.43
26	4	602	CLA	CMD-C2D	-2.20	1.46	1.50
26	8	602	CLA	CMD-C2D	-2.20	1.46	1.50
26	7	613	CLA	MG-ND	-2.20	2.01	2.05
26	c	511	CLA	CMA-C3A	-2.20	1.48	1.53
26	Y	613	CLA	CMC-C2C	-2.20	1.46	1.50
26	3	602	CLA	CMD-C2D	-2.19	1.46	1.50
26	Y	604	CLA	CMC-C2C	-2.19	1.46	1.50
26	7	602	CLA	CMD-C2D	-2.19	1.46	1.50
26	s	604	CLA	MG-NB	-2.19	2.01	2.05
26	C	501	CLA	CMB-C2B	-2.19	1.46	1.50
26	C	511	CLA	CMB-C2B	-2.19	1.46	1.50
27	1	1621	LUT	C22-C21	-2.19	1.52	1.54
26	C	513	CLA	C1B-C2B	2.19	1.48	1.43
26	c	513	CLA	C1B-C2B	2.19	1.48	1.43
26	c	512	CLA	C4B-NB	2.19	1.40	1.37
25	G	609	CHL	CMC-C2C	2.19	1.49	1.44
26	y	613	CLA	CMC-C2C	-2.19	1.46	1.50
26	4	602	CLA	CMC-C2C	-2.19	1.46	1.50
26	2	603	CLA	C3B-C4B	2.19	1.49	1.42
26	5	612	CLA	C3B-C4B	2.19	1.49	1.42
26	r	601	CLA	MG-NB	-2.19	2.01	2.05
26	6	612	CLA	CMD-C2D	-2.19	1.46	1.50
25	g	609	CHL	CMC-C2C	2.19	1.49	1.44
35	a	408	PHO	CAC-C3C	-2.19	1.47	1.51
26	c	501	CLA	CMC-C2C	-2.19	1.46	1.50
37	c	521	LMG	O1-C7	-2.19	1.40	1.43
26	C	512	CLA	CMC-C2C	-2.19	1.46	1.50
26	c	512	CLA	CMC-C2C	-2.19	1.46	1.50
38	D	405	PL9	C46-C44	-2.19	1.46	1.51
38	d	405	PL9	C46-C44	-2.19	1.46	1.51
26	N	611	CLA	C3B-C4B	2.19	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n	611	CLA	C3B-C4B	2.19	1.49	1.42
26	c	504	CLA	MG-ND	-2.19	2.01	2.05
26	a	405	CLA	C1B-C2B	2.19	1.48	1.43
36	a	412	SQD	O2-C2	-2.19	1.37	1.43
28	y	1622	XAT	O24-C25	-2.19	1.43	1.46
25	G	609	CHL	CBD-CGD	-2.19	1.49	1.52
25	g	609	CHL	CBD-CGD	-2.19	1.49	1.52
26	C	506	CLA	CMD-C2D	-2.19	1.46	1.50
26	2	612	CLA	CMD-C2D	-2.18	1.46	1.50
26	s	602	CLA	C1B-C2B	2.18	1.48	1.43
26	s	611	CLA	MG-NB	-2.18	2.01	2.05
26	n	610	CLA	MG-NB	-2.18	2.01	2.05
26	4	602	CLA	C3B-C4B	2.18	1.49	1.42
26	7	611	CLA	MG-NB	-2.18	2.01	2.05
27	3	1621	LUT	C22-C21	-2.18	1.52	1.54
26	5	602	CLA	MG-ND	-2.18	2.01	2.05
26	S	613	CLA	CMC-C2C	-2.18	1.46	1.50
26	S	611	CLA	MG-NB	-2.18	2.01	2.05
26	1	603	CLA	CMB-C2B	-2.18	1.46	1.50
26	5	603	CLA	CMB-C2B	-2.18	1.46	1.50
26	6	602	CLA	CMB-C2B	-2.18	1.46	1.50
26	3	602	CLA	C3B-C4B	2.18	1.49	1.42
26	7	602	CLA	C3B-C4B	2.18	1.49	1.42
26	g	602	CLA	C3B-C4B	2.18	1.49	1.42
26	S	602	CLA	MG-ND	-2.18	2.01	2.05
26	s	602	CLA	MG-ND	-2.18	2.01	2.05
26	C	505	CLA	C1D-ND	2.18	1.40	1.37
26	c	505	CLA	C1D-ND	2.18	1.40	1.37
26	y	603	CLA	C1B-NB	-2.18	1.35	1.37
26	3	611	CLA	MG-NB	-2.18	2.01	2.05
26	R	612	CLA	C1B-C2B	2.18	1.48	1.43
25	S	601	CHL	CBD-CGD	-2.18	1.49	1.52
26	6	603	CLA	C3B-C4B	2.18	1.49	1.42
26	1	612	CLA	CMB-C2B	-2.18	1.46	1.50
26	R	611	CLA	CMD-C2D	-2.18	1.46	1.50
26	5	612	CLA	CMB-C2B	-2.18	1.46	1.50
26	r	611	CLA	CMD-C2D	-2.18	1.46	1.50
26	G	602	CLA	C3B-C4B	2.18	1.49	1.42
26	8	602	CLA	C3B-C4B	2.18	1.49	1.42
26	8	602	CLA	CMC-C2C	-2.18	1.46	1.50
26	A	405	CLA	C1C-NC	-2.18	1.34	1.37
26	s	613	CLA	CMC-C2C	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	406	CLA	CHC-C4B	-2.17	1.34	1.39
36	A	412	SQD	O2-C2	-2.17	1.37	1.43
26	G	603	CLA	CMC-C2C	-2.17	1.46	1.50
26	g	603	CLA	CMC-C2C	-2.17	1.46	1.50
26	C	504	CLA	MG-ND	-2.17	2.01	2.05
26	g	604	CLA	MG-ND	-2.17	2.01	2.05
26	b	603	CLA	C4B-NB	2.17	1.40	1.37
26	1	612	CLA	C3B-C4B	2.17	1.49	1.42
26	b	606	CLA	C1B-NB	-2.17	1.35	1.37
26	3	604	CLA	C1B-C2B	2.17	1.48	1.43
26	7	604	CLA	C1B-C2B	2.17	1.48	1.43
26	8	604	CLA	CMD-C2D	-2.17	1.46	1.50
26	b	604	CLA	C4B-NB	2.17	1.40	1.37
26	8	603	CLA	CMC-C2C	-2.17	1.46	1.50
26	d	403	CLA	CMB-C2B	-2.17	1.46	1.50
26	N	603	CLA	CAC-C3C	-2.17	1.45	1.51
26	n	603	CLA	CAC-C3C	-2.17	1.45	1.51
26	N	610	CLA	CMC-C2C	-2.17	1.46	1.50
26	r	611	CLA	MG-NB	-2.17	2.01	2.05
26	3	604	CLA	C3B-C4B	2.17	1.49	1.42
26	8	603	CLA	C3B-C4B	2.17	1.49	1.42
26	B	616	CLA	CHC-C4B	-2.17	1.34	1.39
27	5	1621	LUT	C22-C21	-2.16	1.52	1.54
26	1	613	CLA	CMC-C2C	-2.16	1.46	1.50
26	4	603	CLA	C3B-C4B	2.16	1.49	1.42
26	B	606	CLA	CMA-C3A	-2.16	1.48	1.53
26	n	613	CLA	MG-ND	-2.16	2.01	2.05
26	1	604	CLA	C3B-C4B	2.16	1.49	1.42
26	g	610	CLA	CMD-C2D	-2.16	1.46	1.50
26	3	613	CLA	MG-ND	-2.16	2.01	2.05
26	G	602	CLA	MG-NB	-2.16	2.01	2.05
26	B	604	CLA	C4B-NB	2.16	1.40	1.37
39	c	518	DGD	O3G-C3G	-2.16	1.40	1.43
26	1	613	CLA	CMB-C2B	-2.16	1.46	1.50
26	N	611	CLA	MG-NB	-2.16	2.01	2.05
26	N	612	CLA	CMC-C2C	-2.16	1.46	1.50
26	5	613	CLA	CMC-C2C	-2.16	1.46	1.50
26	B	609	CLA	MG-ND	-2.16	2.01	2.05
26	b	609	CLA	MG-ND	-2.16	2.01	2.05
26	C	511	CLA	CMA-C3A	-2.16	1.48	1.53
26	Y	613	CLA	C3B-C4B	2.16	1.49	1.42
26	R	611	CLA	MG-NB	-2.16	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S	610	CLA	C3B-C4B	2.16	1.49	1.42
26	N	602	CLA	CMB-C2B	-2.16	1.46	1.50
26	n	602	CLA	CMB-C2B	-2.16	1.46	1.50
26	6	613	CLA	CMC-C2C	-2.16	1.46	1.50
26	G	610	CLA	C3B-C4B	2.16	1.49	1.42
26	8	612	CLA	C3B-C4B	2.16	1.49	1.42
26	g	610	CLA	C3B-C4B	2.16	1.49	1.42
26	5	604	CLA	C3B-C4B	2.16	1.49	1.42
26	b	616	CLA	CHC-C4B	-2.16	1.34	1.39
26	C	503	CLA	C3B-C4B	2.16	1.49	1.42
26	c	503	CLA	C3B-C4B	2.16	1.49	1.42
26	s	610	CLA	C3B-C4B	2.16	1.49	1.42
26	1	614	CLA	C3B-C4B	2.16	1.49	1.42
26	5	614	CLA	C3B-C4B	2.16	1.49	1.42
30	y	2630	LHG	O8-C6	-2.16	1.40	1.45
26	3	611	CLA	CHC-C4B	-2.16	1.34	1.39
26	c	502	CLA	C1D-ND	2.16	1.40	1.37
26	2	611	CLA	CMD-C2D	-2.15	1.46	1.50
26	6	611	CLA	CMD-C2D	-2.15	1.46	1.50
26	7	604	CLA	CMC-C2C	-2.15	1.46	1.50
26	B	606	CLA	MG-ND	-2.15	2.01	2.05
29	N	1623	NEX	O24-C25	-2.15	1.43	1.46
26	2	613	CLA	CMB-C2B	-2.15	1.46	1.50
26	3	604	CLA	CMC-C2C	-2.15	1.46	1.50
26	6	613	CLA	CMB-C2B	-2.15	1.46	1.50
25	N	609	CHL	CBD-CGD	-2.15	1.49	1.52
26	G	604	CLA	MG-ND	-2.15	2.01	2.05
26	2	613	CLA	CMC-C2C	-2.15	1.46	1.50
26	B	606	CLA	C4B-NB	2.15	1.40	1.37
26	b	606	CLA	C4B-NB	2.15	1.40	1.37
26	4	612	CLA	CMD-C2D	-2.15	1.46	1.50
26	8	612	CLA	CMD-C2D	-2.15	1.46	1.50
26	n	610	CLA	CMC-C2C	-2.15	1.46	1.50
38	d	405	PL9	C36-C34	-2.15	1.46	1.51
26	c	504	CLA	CAC-C3C	-2.15	1.45	1.51
26	c	501	CLA	CMB-C2B	-2.15	1.46	1.50
26	S	604	CLA	MG-ND	-2.15	2.01	2.05
26	R	609	CLA	C1B-C2B	2.15	1.48	1.43
26	r	609	CLA	C1B-C2B	2.15	1.48	1.43
26	r	602	CLA	CHC-C1C	2.15	1.42	1.38
26	b	606	CLA	MG-ND	-2.15	2.01	2.05
26	c	513	CLA	MG-NB	-2.15	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	611	CLA	CMB-C2B	-2.15	1.46	1.50
26	C	504	CLA	C4B-NB	2.15	1.40	1.37
26	c	504	CLA	C4B-NB	2.15	1.40	1.37
26	1	611	CLA	CMB-C2B	-2.15	1.46	1.50
26	B	606	CLA	C1B-NB	-2.15	1.35	1.37
26	C	503	CLA	C1B-NB	-2.15	1.35	1.37
26	b	614	CLA	C1B-C2B	2.15	1.48	1.43
26	1	614	CLA	CMB-C2B	-2.15	1.46	1.50
26	5	614	CLA	CMB-C2B	-2.15	1.46	1.50
26	s	604	CLA	MG-ND	-2.14	2.01	2.05
37	C	521	LMG	O7-C8	-2.14	1.41	1.46
37	c	521	LMG	O7-C8	-2.14	1.41	1.46
26	c	503	CLA	C1B-NB	-2.14	1.35	1.37
26	g	602	CLA	MG-NB	-2.14	2.01	2.05
26	3	614	CLA	CMC-C2C	-2.14	1.46	1.50
26	n	611	CLA	MG-NB	-2.14	2.01	2.05
26	7	614	CLA	CMC-C2C	-2.14	1.46	1.50
26	4	612	CLA	C3B-C4B	2.14	1.49	1.42
26	1	604	CLA	MG-ND	-2.14	2.01	2.05
26	1	604	CLA	CMC-C2C	-2.14	1.46	1.50
26	D	403	CLA	CMB-C2B	-2.14	1.46	1.50
26	5	604	CLA	CMC-C2C	-2.14	1.46	1.50
41	F	101	HEM	CMB-C2B	2.14	1.55	1.50
41	f	101	HEM	CMB-C2B	2.14	1.55	1.50
26	4	604	CLA	CMD-C2D	-2.14	1.46	1.50
26	G	610	CLA	CMD-C2D	-2.14	1.46	1.50
26	c	509	CLA	MG-NB	-2.14	2.01	2.05
26	A	406	CLA	CHC-C4B	-2.14	1.34	1.39
26	4	603	CLA	CMC-C2C	-2.14	1.46	1.50
26	N	611	CLA	CMB-C2B	-2.14	1.46	1.50
26	n	611	CLA	CMB-C2B	-2.14	1.46	1.50
31	B	620	BCR	C1-C6	-2.14	1.51	1.53
31	b	620	BCR	C1-C6	-2.14	1.51	1.53
26	n	612	CLA	CMC-C2C	-2.14	1.46	1.50
26	y	613	CLA	C3B-C4B	2.14	1.49	1.42
26	R	602	CLA	CMB-C2B	-2.14	1.46	1.50
26	r	602	CLA	CMB-C2B	-2.14	1.46	1.50
26	A	405	CLA	C3B-C4B	2.14	1.49	1.42
26	a	405	CLA	C3B-C4B	2.14	1.49	1.42
26	6	614	CLA	CMB-C2B	-2.14	1.46	1.50
26	1	602	CLA	MG-ND	-2.14	2.01	2.05
26	C	513	CLA	MG-NB	-2.14	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	504	CLA	C1B-C2B	2.13	1.48	1.43
25	3	608	CHL	CMC-C2C	2.13	1.49	1.44
26	7	604	CLA	C3B-C4B	2.13	1.49	1.42
39	C	518	DGD	O3G-C3G	-2.13	1.40	1.43
26	S	611	CLA	CMB-C2B	-2.13	1.46	1.50
26	s	611	CLA	CMB-C2B	-2.13	1.46	1.50
30	Y	2630	LHG	O8-C6	-2.13	1.40	1.45
26	6	602	CLA	C3B-C4B	2.13	1.49	1.42
26	B	614	CLA	C1B-C2B	2.13	1.48	1.43
26	C	509	CLA	CMC-C2C	-2.13	1.46	1.50
26	c	509	CLA	CMC-C2C	-2.13	1.46	1.50
26	n	613	CLA	C3B-C4B	2.13	1.49	1.42
26	N	613	CLA	MG-ND	-2.13	2.01	2.05
38	D	405	PL9	C36-C34	-2.13	1.46	1.51
27	r	620	LUT	C22-C21	-2.13	1.52	1.54
26	G	612	CLA	CMD-C2D	-2.13	1.46	1.50
26	g	612	CLA	CMD-C2D	-2.13	1.46	1.50
26	b	606	CLA	CMA-C3A	-2.13	1.48	1.53
36	b	623	SQD	O2-C2	-2.13	1.37	1.43
39	c	518	DGD	O3G-C1D	-2.13	1.36	1.40
26	s	611	CLA	MG-ND	-2.13	2.01	2.05
31	C	517	BCR	C1-C6	-2.13	1.51	1.53
31	c	517	BCR	C1-C6	-2.13	1.51	1.53
26	6	612	CLA	CMB-C2B	-2.13	1.46	1.50
28	4	622	XAT	O24-C25	-2.13	1.43	1.46
28	8	622	XAT	O24-C25	-2.13	1.43	1.46
25	7	608	CHL	CMC-C2C	2.13	1.49	1.44
26	c	507	CLA	CHC-C4B	-2.13	1.34	1.39
26	2	602	CLA	C3B-C4B	2.13	1.48	1.42
28	5	1622	XAT	O4-C5	-2.13	1.43	1.46
26	5	604	CLA	MG-ND	-2.12	2.01	2.05
26	d	403	CLA	MG-NB	-2.12	2.01	2.05
26	C	504	CLA	CAC-C3C	-2.12	1.45	1.51
26	b	610	CLA	C1B-NB	-2.12	1.35	1.37
26	1	603	CLA	CMC-C2C	-2.12	1.46	1.50
26	C	502	CLA	C1D-ND	2.12	1.40	1.37
26	c	504	CLA	C1B-C2B	2.12	1.48	1.43
26	S	610	CLA	MG-NB	-2.12	2.01	2.05
26	S	611	CLA	MG-ND	-2.12	2.01	2.05
26	y	614	CLA	CMC-C2C	-2.12	1.46	1.50
26	C	506	CLA	C4B-NB	2.12	1.40	1.37
28	1	1622	XAT	O4-C5	-2.12	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	s	610	CLA	CMD-C2D	-2.12	1.46	1.50
26	G	612	CLA	C3B-C4B	2.12	1.48	1.42
26	r	612	CLA	CHC-C1C	2.12	1.42	1.38
26	B	609	CLA	CMC-C2C	-2.12	1.46	1.50
26	g	603	CLA	CMB-C2B	-2.12	1.46	1.50
26	4	612	CLA	CMB-C2B	-2.12	1.46	1.50
26	G	603	CLA	CMB-C2B	-2.12	1.46	1.50
26	4	611	CLA	CMD-C2D	-2.12	1.46	1.50
26	G	613	CLA	CMB-C2B	-2.12	1.46	1.50
26	g	613	CLA	CMB-C2B	-2.12	1.46	1.50
26	s	614	CLA	C3B-C4B	2.12	1.48	1.42
26	C	507	CLA	CHC-C4B	-2.12	1.34	1.39
26	B	611	CLA	C4B-NB	2.12	1.40	1.37
26	b	611	CLA	C4B-NB	2.12	1.40	1.37
26	2	612	CLA	CMB-C2B	-2.12	1.46	1.50
26	R	611	CLA	CMB-C2B	-2.11	1.46	1.50
26	R	616	CLA	C3B-C4B	2.11	1.48	1.42
26	B	617	CLA	C3B-C4B	2.11	1.48	1.42
26	N	613	CLA	C3B-C4B	2.11	1.48	1.42
26	1	603	CLA	C3B-C4B	2.11	1.48	1.42
26	S	614	CLA	C3B-C4B	2.11	1.48	1.42
26	b	617	CLA	C3B-C4B	2.11	1.48	1.42
25	N	608	CHL	CBD-CGD	-2.11	1.49	1.52
36	B	623	SQD	O2-C2	-2.11	1.37	1.43
26	C	508	CLA	MG-ND	-2.11	2.01	2.05
26	1	613	CLA	C3B-C4B	2.11	1.48	1.42
26	3	604	CLA	CMD-C2D	-2.11	1.46	1.50
26	7	604	CLA	CMD-C2D	-2.11	1.46	1.50
26	G	603	CLA	C1B-NB	-2.11	1.35	1.37
26	g	603	CLA	C1B-NB	-2.11	1.35	1.37
26	C	509	CLA	MG-NB	-2.11	2.01	2.05
39	C	518	DGD	O3G-C1D	-2.11	1.36	1.40
26	1	602	CLA	CMB-C2B	-2.11	1.46	1.50
26	5	602	CLA	CMB-C2B	-2.11	1.46	1.50
26	1	612	CLA	CMC-C2C	-2.11	1.46	1.50
26	8	611	CLA	CMD-C2D	-2.11	1.46	1.50
28	N	1622	XAT	O4-C5	-2.11	1.43	1.46
28	n	1622	XAT	O4-C5	-2.11	1.43	1.46
26	B	615	CLA	MG-ND	-2.11	2.01	2.05
26	b	615	CLA	MG-ND	-2.11	2.01	2.05
30	C	523	LHG	P-O6	2.11	1.67	1.59
30	c	523	LHG	P-O6	2.11	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	y	603	CLA	CAC-C3C	-2.11	1.45	1.51
28	R	622	XAT	O24-C25	-2.11	1.43	1.46
28	r	622	XAT	O24-C25	-2.11	1.43	1.46
25	Y	607	CHL	C4A-C3A	-2.10	1.47	1.51
26	2	614	CLA	CMB-C2B	-2.10	1.46	1.50
26	Y	614	CLA	CMC-C2C	-2.10	1.46	1.50
26	s	610	CLA	MG-NB	-2.10	2.01	2.05
26	R	602	CLA	CHC-C1C	2.10	1.42	1.38
26	C	501	CLA	C1B-NB	-2.10	1.35	1.37
26	c	501	CLA	C1B-NB	-2.10	1.35	1.37
26	D	403	CLA	MG-NB	-2.10	2.01	2.05
26	G	602	CLA	C1B-C2B	2.10	1.48	1.43
26	3	613	CLA	C3B-C4B	2.10	1.48	1.42
26	7	613	CLA	C3B-C4B	2.10	1.48	1.42
26	5	613	CLA	C3B-C4B	2.10	1.48	1.42
25	y	609	CHL	CMC-C2C	2.10	1.49	1.44
26	B	603	CLA	C1B-NB	-2.10	1.35	1.37
26	b	603	CLA	C1B-NB	-2.10	1.35	1.37
26	S	610	CLA	CMD-C2D	-2.10	1.46	1.50
37	B	2633	LMG	C3-C2	2.10	1.57	1.52
37	b	2633	LMG	C3-C2	2.10	1.57	1.52
35	A	408	PHO	CAA-C2A	-2.10	1.49	1.54
26	5	603	CLA	C3B-C4B	2.10	1.48	1.42
26	6	610	CLA	CMD-C2D	-2.10	1.46	1.50
28	g	1622	XAT	O24-C25	-2.10	1.43	1.46
41	F	101	HEM	C2A-C3A	-2.10	1.33	1.38
26	r	604	CLA	CMC-C2C	-2.10	1.46	1.50
36	B	623	SQD	O4-C4	-2.10	1.37	1.43
27	8	620	LUT	C1-C6	-2.10	1.51	1.53
26	c	508	CLA	MG-ND	-2.10	2.01	2.05
26	y	602	CLA	C3B-C4B	2.10	1.48	1.42
26	R	604	CLA	CMC-C2C	-2.10	1.46	1.50
26	3	612	CLA	MG-ND	-2.10	2.01	2.05
26	7	612	CLA	MG-ND	-2.10	2.01	2.05
26	g	603	CLA	MG-ND	-2.10	2.01	2.05
26	s	603	CLA	MG-ND	-2.10	2.01	2.05
26	r	616	CLA	C3B-C4B	2.10	1.48	1.42
30	4	2630	LHG	O7-C5	-2.10	1.41	1.46
30	8	2630	LHG	O7-C5	-2.10	1.41	1.46
25	3	609	CHL	CMC-C2C	2.10	1.49	1.44
25	7	609	CHL	CMC-C2C	2.10	1.49	1.44
26	y	614	CLA	C3B-C4B	2.10	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y	603	CLA	CAC-C3C	-2.10	1.45	1.51
29	n	1623	NEX	O24-C25	-2.10	1.43	1.46
26	a	405	CLA	MG-ND	-2.09	2.01	2.05
26	C	511	CLA	C3B-C4B	2.09	1.48	1.42
26	c	511	CLA	C3B-C4B	2.09	1.48	1.42
38	D	405	PL9	C26-C24	-2.09	1.47	1.51
38	d	405	PL9	C26-C24	-2.09	1.47	1.51
26	R	604	CLA	MG-NB	-2.09	2.01	2.05
26	r	604	CLA	MG-NB	-2.09	2.01	2.05
30	C	523	LHG	O7-C5	-2.09	1.41	1.46
30	c	523	LHG	O7-C5	-2.09	1.41	1.46
26	8	610	CLA	C3B-C4B	2.09	1.48	1.42
26	3	612	CLA	C3B-C4B	2.09	1.48	1.42
26	r	602	CLA	C3B-C4B	2.09	1.48	1.42
26	2	610	CLA	CMD-C2D	-2.09	1.46	1.50
26	G	611	CLA	C1B-C2B	2.09	1.48	1.43
26	R	612	CLA	CHC-C1C	2.09	1.42	1.38
26	B	602	CLA	C3B-C4B	2.09	1.48	1.42
26	3	603	CLA	CAC-C3C	-2.09	1.45	1.51
26	4	604	CLA	CMC-C2C	-2.09	1.46	1.50
26	5	603	CLA	CMC-C2C	-2.09	1.46	1.50
26	8	604	CLA	CMC-C2C	-2.09	1.46	1.50
39	C	520	DGD	O2E-C2E	-2.09	1.37	1.43
39	c	520	DGD	O2E-C2E	-2.09	1.37	1.43
26	S	604	CLA	C3B-C4B	2.09	1.48	1.42
27	R	620	LUT	C22-C21	-2.09	1.52	1.54
26	4	610	CLA	C3B-C4B	2.09	1.48	1.42
25	n	608	CHL	CBD-CGD	-2.09	1.49	1.52
26	r	604	CLA	MG-ND	-2.09	2.01	2.05
26	Y	612	CLA	C1B-C2B	2.09	1.48	1.43
26	4	602	CLA	CMB-C2B	-2.09	1.46	1.50
26	B	615	CLA	MG-NB	-2.09	2.01	2.05
26	b	615	CLA	MG-NB	-2.09	2.01	2.05
26	y	612	CLA	MG-ND	-2.09	2.01	2.05
35	a	408	PHO	CAA-C2A	-2.09	1.49	1.54
26	r	609	CLA	CMC-C2C	-2.09	1.46	1.50
28	2	1622	XAT	O24-C25	-2.09	1.43	1.46
26	c	512	CLA	C1D-ND	2.09	1.40	1.37
26	R	610	CLA	CHC-C1C	2.08	1.42	1.38
26	C	503	CLA	C1B-C2B	2.08	1.48	1.43
26	c	503	CLA	C1B-C2B	2.08	1.48	1.43
26	A	405	CLA	MG-ND	-2.08	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	507	CLA	MG-ND	-2.08	2.01	2.05
26	6	610	CLA	CMC-C2C	-2.08	1.46	1.50
26	b	609	CLA	CMC-C2C	-2.08	1.46	1.50
26	g	612	CLA	C3B-C4B	2.08	1.48	1.42
26	8	612	CLA	CMB-C2B	-2.08	1.46	1.50
26	c	506	CLA	C4B-NB	2.08	1.40	1.37
36	b	623	SQD	O4-C4	-2.08	1.37	1.43
26	b	603	CLA	C1B-C2B	2.08	1.48	1.43
26	Y	614	CLA	C3B-C4B	2.08	1.48	1.42
39	c	520	DGD	O4D-C4D	-2.08	1.37	1.43
26	S	603	CLA	MG-ND	-2.08	2.01	2.05
26	5	611	CLA	CMC-C2C	-2.08	1.46	1.50
26	r	611	CLA	CMB-C2B	-2.08	1.46	1.50
26	S	604	CLA	C1B-NB	-2.08	1.35	1.37
39	C	520	DGD	O4D-C4D	-2.08	1.37	1.43
26	D	402	CLA	MG-ND	-2.08	2.01	2.05
26	G	603	CLA	MG-ND	-2.08	2.01	2.05
26	d	402	CLA	MG-ND	-2.08	2.01	2.05
26	g	602	CLA	C1B-C2B	2.08	1.48	1.43
26	g	611	CLA	C1B-C2B	2.08	1.48	1.43
28	G	1622	XAT	O24-C25	-2.08	1.43	1.46
26	4	610	CLA	MG-NB	-2.08	2.01	2.05
39	C	520	DGD	O3D-C3D	-2.08	1.37	1.43
39	c	520	DGD	O3D-C3D	-2.08	1.37	1.43
26	7	603	CLA	CAC-C3C	-2.08	1.45	1.51
26	s	604	CLA	C3B-C4B	2.08	1.48	1.42
26	7	603	CLA	CHC-C4B	-2.08	1.34	1.39
41	f	101	HEM	C2A-C3A	-2.08	1.33	1.38
26	C	507	CLA	O2D-CED	-2.08	1.40	1.45
26	B	615	CLA	C4B-NB	2.08	1.40	1.37
37	C	521	LMG	C4-C5	2.08	1.57	1.53
26	8	603	CLA	MG-NB	-2.08	2.01	2.05
26	8	602	CLA	CMB-C2B	-2.08	1.46	1.50
26	5	612	CLA	CMC-C2C	-2.08	1.46	1.50
26	G	611	CLA	C1B-NB	-2.08	1.35	1.37
26	5	604	CLA	C1B-NB	-2.08	1.35	1.37
26	g	611	CLA	C1B-NB	-2.08	1.35	1.37
26	c	507	CLA	O2D-CED	-2.07	1.40	1.45
26	b	602	CLA	C3B-C4B	2.07	1.48	1.42
26	B	603	CLA	C1B-C2B	2.07	1.48	1.43
26	1	604	CLA	C1B-NB	-2.07	1.35	1.37
26	s	604	CLA	C1B-NB	-2.07	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	4	620	LUT	C1-C6	-2.07	1.51	1.53
26	r	602	CLA	CMC-C2C	-2.07	1.46	1.50
26	1	602	CLA	C3B-C4B	2.07	1.48	1.42
26	B	602	CLA	MG-NB	-2.07	2.01	2.05
26	G	612	CLA	CMC-C2C	-2.07	1.46	1.50
26	6	603	CLA	CMC-C2C	-2.07	1.46	1.50
26	g	612	CLA	CMC-C2C	-2.07	1.46	1.50
25	y	607	CHL	C4A-C3A	-2.07	1.47	1.51
26	5	611	CLA	C3B-C4B	2.07	1.48	1.42
39	C	519	DGD	O3G-C1D	-2.07	1.36	1.40
26	B	610	CLA	CHC-C4B	-2.07	1.34	1.39
26	b	610	CLA	CHC-C4B	-2.07	1.34	1.39
26	g	604	CLA	CMC-C2C	-2.07	1.46	1.50
26	1	611	CLA	C3B-C4B	2.07	1.48	1.42
26	3	603	CLA	CHC-C4B	-2.07	1.34	1.39
26	R	613	CLA	C3B-C4B	2.07	1.48	1.42
26	r	613	CLA	C3B-C4B	2.07	1.48	1.42
37	c	521	LMG	C4-C5	2.07	1.57	1.53
26	6	602	CLA	MG-ND	-2.07	2.01	2.05
26	Y	602	CLA	C3B-C4B	2.07	1.48	1.42
26	b	607	CLA	CMA-C3A	-2.07	1.48	1.53
26	S	609	CLA	CMB-C2B	-2.07	1.46	1.50
26	r	610	CLA	CHC-C1C	2.07	1.42	1.38
26	B	610	CLA	C1B-NB	-2.07	1.35	1.37
26	R	603	CLA	CMC-C2C	-2.07	1.46	1.50
26	r	603	CLA	CMC-C2C	-2.07	1.46	1.50
26	c	507	CLA	MG-ND	-2.07	2.01	2.05
26	6	611	CLA	CMB-C2B	-2.07	1.46	1.50
26	2	610	CLA	CMC-C2C	-2.06	1.46	1.50
26	B	616	CLA	C1B-NB	-2.06	1.35	1.37
26	b	616	CLA	C1B-NB	-2.06	1.35	1.37
26	g	602	CLA	C1B-NB	-2.06	1.35	1.37
26	R	602	CLA	C3B-C4B	2.06	1.48	1.42
26	R	616	CLA	MG-NB	-2.06	2.01	2.05
26	B	611	CLA	C3B-C4B	2.06	1.48	1.42
26	S	610	CLA	C1B-C2B	2.06	1.48	1.43
26	s	610	CLA	C1B-C2B	2.06	1.48	1.43
26	6	612	CLA	CMC-C2C	-2.06	1.46	1.50
26	Y	612	CLA	MG-ND	-2.06	2.01	2.05
25	Y	609	CHL	CMC-C2C	2.06	1.49	1.44
26	G	604	CLA	CMC-C2C	-2.06	1.46	1.50
26	7	612	CLA	C3B-C4B	2.06	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	613	CLA	MG-ND	-2.06	2.01	2.05
26	g	613	CLA	MG-ND	-2.06	2.01	2.05
26	b	610	CLA	C4B-NB	2.06	1.40	1.37
26	b	615	CLA	C4B-NB	2.06	1.40	1.37
26	5	602	CLA	C3B-C4B	2.06	1.48	1.42
26	b	611	CLA	C3B-C4B	2.06	1.48	1.42
26	1	611	CLA	MG-ND	-2.06	2.01	2.05
26	5	611	CLA	MG-ND	-2.06	2.01	2.05
26	8	610	CLA	MG-NB	-2.06	2.01	2.05
26	3	610	CLA	CHC-C1C	2.06	1.42	1.38
26	y	611	CLA	MG-ND	-2.06	2.01	2.05
26	C	502	CLA	CAC-C3C	-2.06	1.45	1.51
26	N	602	CLA	C1B-C2B	2.06	1.48	1.43
26	n	602	CLA	C1B-C2B	2.06	1.48	1.43
26	G	611	CLA	C3B-C4B	2.06	1.48	1.42
26	g	611	CLA	C3B-C4B	2.06	1.48	1.42
36	A	418	SQD	O2-C2	-2.06	1.37	1.43
26	a	407	CLA	CAC-C3C	-2.06	1.45	1.51
26	Y	611	CLA	MG-ND	-2.06	2.01	2.05
26	7	611	CLA	CMC-C2C	-2.06	1.46	1.50
26	1	611	CLA	CMC-C2C	-2.06	1.46	1.50
26	B	612	CLA	CHC-C4B	-2.06	1.34	1.39
39	C	519	DGD	O4E-C4E	-2.06	1.37	1.43
26	R	609	CLA	CMC-C2C	-2.06	1.46	1.50
26	y	612	CLA	C1B-C2B	2.06	1.48	1.43
26	R	604	CLA	MG-ND	-2.06	2.01	2.05
26	1	603	CLA	CAC-C3C	-2.05	1.45	1.51
30	2	2630	LHG	P-O6	2.05	1.67	1.59
26	4	603	CLA	MG-NB	-2.05	2.01	2.05
26	S	603	CLA	CMB-C2B	-2.05	1.46	1.50
25	2	609	CHL	CMC-C2C	2.05	1.49	1.44
25	6	609	CHL	CMC-C2C	2.05	1.49	1.44
26	C	504	CLA	CHC-C4B	-2.05	1.34	1.39
25	2	608	CHL	CMC-C2C	2.05	1.49	1.44
25	6	608	CHL	CMC-C2C	2.05	1.49	1.44
25	n	609	CHL	CMA-C3A	-2.05	1.49	1.53
30	6	2630	LHG	P-O6	2.05	1.67	1.59
26	2	602	CLA	MG-ND	-2.05	2.01	2.05
26	S	610	CLA	CHC-C1C	2.05	1.42	1.38
26	7	603	CLA	CMC-C2C	-2.05	1.46	1.50
39	c	519	DGD	O4E-C4E	-2.05	1.37	1.43
26	S	604	CLA	CMC-C2C	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	s	604	CLA	CMC-C2C	-2.05	1.46	1.50
30	4	2630	LHG	P-O6	2.05	1.67	1.59
26	4	611	CLA	MG-ND	-2.05	2.01	2.05
26	1	612	CLA	MG-ND	-2.05	2.01	2.05
29	g	1623	NEX	C7-C8	-2.05	1.28	1.31
26	G	610	CLA	CMC-C2C	-2.05	1.46	1.50
26	g	610	CLA	CMC-C2C	-2.05	1.46	1.50
26	4	611	CLA	CMB-C2B	-2.05	1.46	1.50
26	8	611	CLA	CMB-C2B	-2.05	1.46	1.50
25	N	609	CHL	CMA-C3A	-2.05	1.49	1.53
26	R	612	CLA	CMB-C2B	-2.05	1.46	1.50
26	C	508	CLA	C1C-NC	-2.05	1.34	1.37
26	D	403	CLA	CMC-C2C	-2.05	1.46	1.50
26	d	403	CLA	CMC-C2C	-2.05	1.46	1.50
26	s	610	CLA	CHC-C1C	2.05	1.42	1.38
26	2	603	CLA	CMC-C2C	-2.05	1.46	1.50
26	2	611	CLA	CMB-C2B	-2.05	1.46	1.50
26	1	611	CLA	MG-NB	-2.05	2.01	2.05
26	5	611	CLA	MG-NB	-2.05	2.01	2.05
26	B	607	CLA	CMA-C3A	-2.05	1.48	1.53
26	7	610	CLA	C1B-C2B	2.05	1.47	1.43
26	a	407	CLA	CMC-C2C	-2.05	1.46	1.50
26	R	609	CLA	CMB-C2B	-2.05	1.46	1.50
26	s	614	CLA	MG-NB	-2.04	2.01	2.05
26	B	607	CLA	CHC-C4B	-2.04	1.34	1.39
26	b	607	CLA	CHC-C4B	-2.04	1.34	1.39
26	2	612	CLA	CMC-C2C	-2.04	1.46	1.50
26	N	604	CLA	C3B-C4B	2.04	1.48	1.42
26	c	509	CLA	C4B-NB	2.04	1.40	1.37
26	r	616	CLA	MG-NB	-2.04	2.01	2.05
39	c	519	DGD	O3G-C1D	-2.04	1.36	1.40
26	2	604	CLA	CMC-C2C	-2.04	1.46	1.50
26	G	603	CLA	CAA-C2A	-2.04	1.50	1.54
26	g	603	CLA	CAA-C2A	-2.04	1.50	1.54
26	C	510	CLA	C1B-C2B	2.04	1.47	1.43
26	N	612	CLA	CMB-C2B	-2.04	1.46	1.50
26	n	612	CLA	CMB-C2B	-2.04	1.46	1.50
26	A	407	CLA	CAC-C3C	-2.04	1.45	1.51
26	c	502	CLA	CAC-C3C	-2.04	1.45	1.51
26	b	612	CLA	CHC-C4B	-2.04	1.34	1.39
26	C	510	CLA	MG-ND	-2.04	2.01	2.05
26	c	510	CLA	MG-ND	-2.04	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	407	CLA	CMC-C2C	-2.04	1.46	1.50
36	A	412	SQD	O4-C4	-2.04	1.37	1.43
36	a	412	SQD	O4-C4	-2.04	1.37	1.43
26	b	604	CLA	C1D-ND	2.04	1.40	1.37
26	Y	610	CLA	MG-ND	-2.04	2.01	2.05
26	2	604	CLA	MG-NB	-2.04	2.01	2.05
26	6	604	CLA	MG-NB	-2.04	2.01	2.05
35	a	408	PHO	C3D-CAD	-2.04	1.43	1.47
26	8	611	CLA	MG-ND	-2.04	2.01	2.05
26	B	617	CLA	MG-ND	-2.04	2.01	2.05
26	5	612	CLA	MG-ND	-2.04	2.01	2.05
26	r	612	CLA	CMB-C2B	-2.03	1.46	1.50
26	B	610	CLA	C4B-NB	2.03	1.40	1.37
26	3	610	CLA	C1B-C2B	2.03	1.47	1.43
26	s	609	CLA	CMB-C2B	-2.03	1.46	1.50
26	G	612	CLA	CMB-C2B	-2.03	1.46	1.50
26	S	609	CLA	CMD-C2D	-2.03	1.46	1.50
26	g	612	CLA	CMB-C2B	-2.03	1.46	1.50
30	8	2630	LHG	P-O6	2.03	1.67	1.59
26	S	613	CLA	C3B-C4B	2.03	1.48	1.42
26	s	613	CLA	C3B-C4B	2.03	1.48	1.42
26	A	407	CLA	CHC-C4B	-2.03	1.34	1.39
26	a	407	CLA	CHC-C4B	-2.03	1.34	1.39
26	3	603	CLA	CMC-C2C	-2.03	1.46	1.50
26	G	613	CLA	CMC-C2C	-2.03	1.46	1.50
26	g	613	CLA	CMC-C2C	-2.03	1.46	1.50
26	C	512	CLA	C1D-ND	2.03	1.40	1.37
26	6	611	CLA	MG-ND	-2.03	2.01	2.05
26	B	617	CLA	C4B-NB	2.03	1.40	1.37
26	b	617	CLA	C4B-NB	2.03	1.40	1.37
26	b	602	CLA	MG-NB	-2.03	2.01	2.05
39	H	102	DGD	O2D-C2D	-2.03	1.37	1.43
39	h	102	DGD	O2D-C2D	-2.03	1.37	1.43
26	G	614	CLA	CMC-C2C	-2.03	1.46	1.50
26	g	614	CLA	CMC-C2C	-2.03	1.46	1.50
26	6	604	CLA	CMC-C2C	-2.03	1.46	1.50
26	s	603	CLA	CMB-C2B	-2.03	1.46	1.50
26	c	511	CLA	C1B-NB	-2.03	1.35	1.37
26	c	504	CLA	CHC-C4B	-2.03	1.34	1.39
35	A	408	PHO	C1C-NC	-2.03	1.31	1.37
35	a	408	PHO	C1C-NC	-2.03	1.31	1.37
26	5	603	CLA	CAC-C3C	-2.03	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	614	CLA	CMC-C2C	-2.03	1.46	1.50
26	7	610	CLA	CHC-C1C	2.03	1.42	1.38
26	1	610	CLA	MG-NB	-2.03	2.01	2.05
26	C	511	CLA	C1B-NB	-2.03	1.35	1.37
26	G	602	CLA	C1B-NB	-2.03	1.35	1.37
29	G	1623	NEX	C7-C8	-2.03	1.28	1.31
26	S	613	CLA	MG-NB	-2.03	2.01	2.05
26	3	611	CLA	CMC-C2C	-2.03	1.46	1.50
26	n	604	CLA	C3B-C4B	2.03	1.48	1.42
26	3	604	CLA	MG-NB	-2.03	2.01	2.05
26	S	614	CLA	MG-NB	-2.03	2.01	2.05
26	R	602	CLA	CMC-C2C	-2.03	1.46	1.50
26	C	504	CLA	CMA-C3A	-2.02	1.48	1.53
36	a	418	SQD	O2-C2	-2.02	1.37	1.43
26	s	613	CLA	MG-NB	-2.02	2.01	2.05
26	r	609	CLA	CMB-C2B	-2.02	1.46	1.50
39	H	102	DGD	O2E-C2E	-2.02	1.37	1.43
39	h	102	DGD	O2E-C2E	-2.02	1.37	1.43
26	y	610	CLA	MG-ND	-2.02	2.01	2.05
26	n	611	CLA	CMC-C2C	-2.02	1.46	1.50
26	a	407	CLA	C1B-C2B	2.02	1.47	1.43
36	A	418	SQD	O3-C3	-2.02	1.37	1.43
36	a	418	SQD	O3-C3	-2.02	1.37	1.43
26	C	502	CLA	CMC-C2C	-2.02	1.46	1.50
26	B	609	CLA	C3B-C4B	2.02	1.48	1.42
26	c	511	CLA	MG-NB	-2.02	2.01	2.05
26	B	617	CLA	C1C-NC	-2.02	1.34	1.37
26	b	617	CLA	C1C-NC	-2.02	1.34	1.37
26	c	504	CLA	CMA-C3A	-2.02	1.48	1.53
26	2	603	CLA	CAC-C3C	-2.02	1.45	1.51
26	6	603	CLA	CAC-C3C	-2.02	1.45	1.51
26	b	609	CLA	C3B-C4B	2.02	1.48	1.42
26	s	609	CLA	CMD-C2D	-2.02	1.46	1.50
26	5	614	CLA	CMC-C2C	-2.02	1.46	1.50
27	y	1620	LUT	C22-C21	-2.02	1.52	1.54
26	1	614	CLA	CMC-C2C	-2.02	1.46	1.50
26	B	603	CLA	C3B-C4B	2.02	1.48	1.42
26	b	603	CLA	C3B-C4B	2.02	1.48	1.42
25	4	601	CHL	CMC-C2C	2.02	1.49	1.44
26	4	602	CLA	CHC-C1C	2.02	1.42	1.38
26	r	612	CLA	CMC-C2C	-2.01	1.46	1.50
26	C	511	CLA	MG-NB	-2.01	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r	613	CLA	CMC-C2C	-2.01	1.46	1.50
26	B	604	CLA	C1D-ND	2.01	1.40	1.37
26	C	509	CLA	C4B-NB	2.01	1.40	1.37
26	8	602	CLA	CHC-C1C	2.01	1.42	1.38
26	R	601	CLA	CMD-C2D	-2.01	1.46	1.50
26	r	601	CLA	CMD-C2D	-2.01	1.46	1.50
26	8	604	CLA	MG-NB	-2.01	2.01	2.05
26	S	610	CLA	CMC-C2C	-2.01	1.46	1.50
26	s	610	CLA	CMC-C2C	-2.01	1.46	1.50
26	S	612	CLA	C1B-NB	-2.01	1.35	1.37
26	s	612	CLA	C1B-NB	-2.01	1.35	1.37
26	b	605	CLA	CHC-C4B	-2.01	1.34	1.39
26	c	512	CLA	C3B-C4B	2.01	1.48	1.42
26	R	611	CLA	C1B-NB	-2.01	1.35	1.37
26	c	502	CLA	CMC-C2C	-2.01	1.46	1.50
26	b	617	CLA	MG-ND	-2.01	2.01	2.05
26	d	402	CLA	CAA-C2A	-2.01	1.50	1.54
37	B	2633	LMG	C7-C8	2.01	1.57	1.50
26	1	610	CLA	C1B-C2B	2.01	1.47	1.43
26	5	610	CLA	C1B-C2B	2.01	1.47	1.43
26	A	407	CLA	C1B-C2B	2.01	1.47	1.43
26	g	604	CLA	C3B-C4B	2.01	1.48	1.42
26	1	612	CLA	CHC-C4B	-2.01	1.34	1.39
26	5	612	CLA	CHC-C4B	-2.01	1.34	1.39
26	Y	610	CLA	CHC-C1C	2.01	1.42	1.38
26	b	606	CLA	C1B-C2B	2.01	1.47	1.43
26	1	610	CLA	C3B-C4B	2.01	1.48	1.42
26	R	616	CLA	CMC-C2C	-2.01	1.46	1.50
26	C	512	CLA	C3B-C4B	2.00	1.48	1.42
26	4	602	CLA	MG-NB	-2.00	2.01	2.05
26	2	611	CLA	CMC-C2C	-2.00	1.46	1.50
25	8	601	CHL	CMC-C2C	2.00	1.49	1.44
26	8	610	CLA	CHC-C1C	2.00	1.42	1.38
35	a	409	PHO	C3D-CAD	-2.00	1.43	1.47
26	b	608	CLA	C1B-C2B	2.00	1.47	1.43
25	y	601	CHL	CBD-CGD	-2.00	1.50	1.52
26	R	613	CLA	CMC-C2C	-2.00	1.46	1.50
26	5	603	CLA	CHC-C4B	-2.00	1.34	1.39
26	6	604	CLA	C3B-C4B	2.00	1.48	1.42
26	R	610	CLA	MG-ND	-2.00	2.01	2.05
25	6	605	CHL	CMC-C2C	2.00	1.49	1.44
26	Y	610	CLA	MG-NB	-2.00	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	y	610	CLA	MG-NB	-2.00	2.01	2.05
26	4	610	CLA	CHC-C1C	2.00	1.42	1.38
38	D	405	PL9	C35-C34	-2.00	1.45	1.50
38	d	405	PL9	C35-C34	-2.00	1.45	1.50
37	b	2633	LMG	C7-C8	2.00	1.57	1.50

All (5101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	601	CHL	C1B-CHB-C4A	11.79	128.91	121.32
25	g	601	CHL	C1B-CHB-C4A	11.70	128.85	121.32
25	y	601	CHL	C1B-CHB-C4A	11.07	128.44	121.32
25	Y	601	CHL	C1B-CHB-C4A	11.02	128.41	121.32
25	6	601	CHL	C1B-CHB-C4A	10.86	128.31	121.32
25	2	601	CHL	C1B-CHB-C4A	10.79	128.26	121.32
25	Y	606	CHL	C1B-CHB-C4A	10.70	128.21	121.32
25	S	606	CHL	C1B-CHB-C4A	10.66	128.18	121.32
25	s	606	CHL	C1B-CHB-C4A	10.66	128.18	121.32
25	y	606	CHL	C1B-CHB-C4A	10.66	128.18	121.32
25	7	601	CHL	C1B-CHB-C4A	10.65	128.18	121.32
25	3	601	CHL	C1B-CHB-C4A	10.60	128.14	121.32
25	n	601	CHL	C1B-CHB-C4A	10.58	128.13	121.32
25	N	601	CHL	C1B-CHB-C4A	10.55	128.11	121.32
25	n	606	CHL	C1B-CHB-C4A	10.44	128.04	121.32
25	N	606	CHL	C1B-CHB-C4A	10.40	128.01	121.32
25	r	606	CHL	C1B-CHB-C4A	10.22	127.89	121.32
25	s	607	CHL	C1B-CHB-C4A	10.22	127.89	121.32
25	5	606	CHL	C1B-CHB-C4A	10.19	127.88	121.32
25	S	607	CHL	C1B-CHB-C4A	10.17	127.87	121.32
25	R	606	CHL	C1B-CHB-C4A	10.16	127.86	121.32
25	1	606	CHL	C1B-CHB-C4A	10.15	127.85	121.32
25	5	607	CHL	C1B-CHB-C4A	10.11	127.83	121.32
25	1	607	CHL	C1B-CHB-C4A	10.09	127.81	121.32
25	N	605	CHL	C1B-CHB-C4A	9.89	127.69	121.32
25	n	605	CHL	C1B-CHB-C4A	9.85	127.66	121.32
25	n	607	CHL	C1B-CHB-C4A	9.84	127.66	121.32
25	N	607	CHL	C1B-CHB-C4A	9.84	127.65	121.32
25	R	607	CHL	C1B-CHB-C4A	9.64	127.52	121.32
25	r	607	CHL	C1B-CHB-C4A	9.61	127.51	121.32
25	6	608	CHL	C1B-CHB-C4A	9.50	127.44	121.32
25	N	605	CHL	O2D-CGD-CBD	9.47	121.35	110.95
25	n	605	CHL	O2D-CGD-CBD	9.47	121.35	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	608	CHL	C1B-CHB-C4A	9.44	127.39	121.32
25	R	608	CHL	O2D-CGD-CBD	9.42	121.30	110.95
25	2	609	CHL	O2D-CGD-CBD	9.40	121.27	110.95
25	r	608	CHL	O2D-CGD-CBD	9.40	121.27	110.95
25	6	609	CHL	O2D-CGD-CBD	9.39	121.27	110.95
25	r	608	CHL	C1B-CHB-C4A	9.37	127.35	121.32
25	R	608	CHL	C1B-CHB-C4A	9.31	127.31	121.32
25	y	609	CHL	O2D-CGD-CBD	9.31	121.18	110.95
25	3	608	CHL	C1B-CHB-C4A	9.31	127.31	121.32
25	Y	609	CHL	O2D-CGD-CBD	9.30	121.16	110.95
25	7	608	CHL	C1B-CHB-C4A	9.26	127.28	121.32
26	s	604	CLA	C4A-NA-C1A	9.20	110.88	106.68
26	S	604	CLA	C4A-NA-C1A	9.16	110.86	106.68
25	5	605	CHL	C1B-CHB-C4A	9.09	127.17	121.32
25	1	605	CHL	C1B-CHB-C4A	9.07	127.16	121.32
25	7	609	CHL	O2D-CGD-CBD	9.05	120.89	110.95
25	G	606	CHL	C1B-CHB-C4A	9.05	127.14	121.32
25	3	609	CHL	O2D-CGD-CBD	9.03	120.87	110.95
25	g	606	CHL	C1B-CHB-C4A	8.99	127.11	121.32
25	G	605	CHL	O2D-CGD-CBD	8.95	120.78	110.95
25	g	605	CHL	O2D-CGD-CBD	8.95	120.78	110.95
25	4	606	CHL	O2D-CGD-CBD	8.94	120.77	110.95
25	Y	607	CHL	C1B-CHB-C4A	8.94	127.07	121.32
25	8	606	CHL	O2D-CGD-CBD	8.92	120.75	110.95
25	N	601	CHL	O2D-CGD-CBD	8.90	120.73	110.95
25	N	608	CHL	O2D-CGD-CBD	8.87	120.69	110.95
25	2	606	CHL	C1B-CHB-C4A	8.87	127.03	121.32
25	6	606	CHL	C1B-CHB-C4A	8.87	127.03	121.32
25	g	605	CHL	C1B-CHB-C4A	8.87	127.03	121.32
25	n	601	CHL	O2D-CGD-CBD	8.86	120.68	110.95
25	y	607	CHL	C1B-CHB-C4A	8.86	127.02	121.32
25	n	608	CHL	O2D-CGD-CBD	8.85	120.67	110.95
25	3	605	CHL	O2D-CGD-CBD	8.83	120.64	110.95
25	7	606	CHL	O2D-CGD-CBD	8.82	120.64	110.95
25	G	605	CHL	C1B-CHB-C4A	8.81	126.99	121.32
25	R	606	CHL	O2D-CGD-CBD	8.81	120.63	110.95
26	C	507	CLA	C4A-NA-C1A	8.80	110.70	106.68
25	Y	608	CHL	O2D-CGD-CBD	8.80	120.62	110.95
25	3	606	CHL	O2D-CGD-CBD	8.80	120.61	110.95
25	r	606	CHL	O2D-CGD-CBD	8.80	120.61	110.95
25	S	606	CHL	O2D-CGD-CBD	8.79	120.61	110.95
25	y	608	CHL	O2D-CGD-CBD	8.79	120.60	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	605	CHL	O2D-CGD-CBD	8.78	120.60	110.95
25	1	608	CHL	C1B-CHB-C4A	8.78	126.97	121.32
25	5	608	CHL	C1B-CHB-C4A	8.78	126.97	121.32
25	s	606	CHL	O2D-CGD-CBD	8.77	120.58	110.95
25	7	606	CHL	C1B-CHB-C4A	8.74	126.94	121.32
25	2	607	CHL	O2D-CGD-CBD	8.74	120.55	110.95
26	c	507	CLA	C4A-NA-C1A	8.72	110.66	106.68
25	y	606	CHL	O2D-CGD-CBD	8.72	120.53	110.95
25	6	607	CHL	O2D-CGD-CBD	8.72	120.53	110.95
25	Y	606	CHL	O2D-CGD-CBD	8.71	120.52	110.95
25	8	608	CHL	C1B-CHB-C4A	8.70	126.92	121.32
25	3	606	CHL	C1B-CHB-C4A	8.69	126.91	121.32
25	4	608	CHL	C1B-CHB-C4A	8.64	126.88	121.32
25	Y	601	CHL	O2D-CGD-CBD	8.63	120.43	110.95
25	y	601	CHL	O2D-CGD-CBD	8.59	120.39	110.95
26	c	505	CLA	C4A-NA-C1A	8.55	110.58	106.68
26	C	505	CLA	C4A-NA-C1A	8.52	110.56	106.68
25	n	608	CHL	C1B-CHB-C4A	8.51	126.80	121.32
26	C	502	CLA	C4A-NA-C1A	8.51	110.56	106.68
25	N	609	CHL	O2D-CGD-CBD	8.48	120.27	110.95
26	c	502	CLA	C4A-NA-C1A	8.46	110.54	106.68
25	n	609	CHL	O2D-CGD-CBD	8.46	120.24	110.95
25	s	601	CHL	C1B-CHB-C4A	8.45	126.76	121.32
25	5	609	CHL	O2D-CGD-CBD	8.45	120.23	110.95
25	G	609	CHL	O2D-CGD-CBD	8.45	120.23	110.95
25	N	608	CHL	C1B-CHB-C4A	8.44	126.75	121.32
25	g	609	CHL	O2D-CGD-CBD	8.44	120.22	110.95
25	5	605	CHL	O2D-CGD-CBD	8.43	120.20	110.95
25	1	609	CHL	O2D-CGD-CBD	8.41	120.18	110.95
25	N	606	CHL	O2D-CGD-CBD	8.40	120.18	110.95
25	S	601	CHL	C1B-CHB-C4A	8.40	126.73	121.32
25	1	605	CHL	O2D-CGD-CBD	8.40	120.17	110.95
25	G	608	CHL	C1B-CHB-C4A	8.39	126.72	121.32
25	n	606	CHL	O2D-CGD-CBD	8.39	120.17	110.95
26	b	608	CLA	C4A-NA-C1A	8.30	110.46	106.68
25	Y	609	CHL	C1B-CHB-C4A	8.29	126.66	121.32
25	g	608	CHL	C1B-CHB-C4A	8.29	126.66	121.32
26	B	608	CLA	C4A-NA-C1A	8.25	110.44	106.68
25	7	607	CHL	O2D-CGD-CBD	8.21	119.97	110.95
25	y	609	CHL	C1B-CHB-C4A	8.21	126.60	121.32
25	3	607	CHL	O2D-CGD-CBD	8.21	119.96	110.95
26	d	402	CLA	C4A-NA-C1A	8.20	110.42	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	607	CHL	O2D-CGD-CBD	8.19	119.95	110.95
25	N	609	CHL	C1B-CHB-C4A	8.17	126.58	121.32
25	G	608	CHL	O2D-CGD-CBD	8.17	119.92	110.95
25	g	608	CHL	O2D-CGD-CBD	8.17	119.92	110.95
25	4	607	CHL	O2D-CGD-CBD	8.16	119.91	110.95
28	2	1622	XAT	O24-C25-C24	8.16	121.14	113.49
25	n	609	CHL	C1B-CHB-C4A	8.15	126.56	121.32
25	g	601	CHL	O2D-CGD-CBD	8.15	119.90	110.95
26	D	402	CLA	C4A-NA-C1A	8.13	110.39	106.68
25	Y	605	CHL	C1B-CHB-C4A	8.12	126.55	121.32
25	G	601	CHL	O2D-CGD-CBD	8.10	119.85	110.95
25	y	605	CHL	C1B-CHB-C4A	8.10	126.53	121.32
28	6	1622	XAT	O24-C25-C24	8.09	121.08	113.49
25	3	601	CHL	O2D-CGD-CBD	7.99	119.73	110.95
25	7	601	CHL	O2D-CGD-CBD	7.99	119.73	110.95
25	8	609	CHL	O2D-CGD-CBD	7.96	119.70	110.95
25	4	609	CHL	O2D-CGD-CBD	7.95	119.68	110.95
25	1	601	CHL	O2D-CGD-CBD	7.92	119.65	110.95
25	5	601	CHL	O2D-CGD-CBD	7.92	119.64	110.95
25	g	609	CHL	C1B-CHB-C4A	7.91	126.41	121.32
25	G	609	CHL	C1B-CHB-C4A	7.88	126.39	121.32
25	3	608	CHL	O2D-CGD-CBD	7.87	119.59	110.95
25	6	605	CHL	O2D-CGD-CBD	7.83	119.55	110.95
25	7	608	CHL	O2D-CGD-CBD	7.83	119.55	110.95
25	2	605	CHL	O2D-CGD-CBD	7.82	119.54	110.95
25	2	606	CHL	O2D-CGD-CBD	7.79	119.50	110.95
25	6	606	CHL	O2D-CGD-CBD	7.77	119.49	110.95
25	R	607	CHL	O2D-CGD-CBD	7.75	119.47	110.95
25	r	607	CHL	O2D-CGD-CBD	7.74	119.45	110.95
25	5	606	CHL	O2D-CGD-CBD	7.69	119.40	110.95
26	b	613	CLA	C4A-NA-C1A	7.69	110.19	106.68
25	1	606	CHL	O2D-CGD-CBD	7.67	119.38	110.95
31	8	623	BCR	C24-C23-C22	-7.66	114.90	126.23
31	4	623	BCR	C24-C23-C22	-7.66	114.91	126.23
26	B	613	CLA	C4A-NA-C1A	7.65	110.17	106.68
26	A	405	CLA	C4A-NA-C1A	7.64	110.17	106.68
25	6	601	CHL	O2D-CGD-CBD	7.62	119.32	110.95
25	s	601	CHL	O2D-CGD-CBD	7.61	119.31	110.95
25	s	607	CHL	O2D-CGD-CBD	7.61	119.31	110.95
25	S	601	CHL	O2D-CGD-CBD	7.61	119.31	110.95
25	S	607	CHL	O2D-CGD-CBD	7.59	119.29	110.95
25	2	601	CHL	O2D-CGD-CBD	7.59	119.28	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	608	CHL	C1B-CHB-C4A	7.59	126.20	121.32
26	C	511	CLA	C4A-NA-C1A	7.58	110.14	106.68
25	Y	608	CHL	C1B-CHB-C4A	7.53	126.17	121.32
25	g	606	CHL	O2D-CGD-CBD	7.51	119.20	110.95
26	c	511	CLA	C4A-NA-C1A	7.51	110.11	106.68
26	a	405	CLA	C4A-NA-C1A	7.51	110.10	106.68
25	G	606	CHL	O2D-CGD-CBD	7.50	119.19	110.95
25	2	608	CHL	O2D-CGD-CBD	7.49	119.17	110.95
25	g	607	CHL	O2D-CGD-CBD	7.48	119.17	110.95
26	B	611	CLA	C4A-NA-C1A	7.48	110.09	106.68
25	6	608	CHL	O2D-CGD-CBD	7.47	119.15	110.95
25	G	607	CHL	O2D-CGD-CBD	7.45	119.13	110.95
26	b	611	CLA	C4A-NA-C1A	7.42	110.06	106.68
28	y	1622	XAT	C6-C7-C8	-7.37	110.40	125.99
28	Y	1622	XAT	C6-C7-C8	-7.37	110.41	125.99
26	B	610	CLA	C4A-NA-C1A	7.30	110.01	106.68
25	5	607	CHL	O2D-CGD-CBD	7.27	118.94	110.95
25	1	607	CHL	O2D-CGD-CBD	7.26	118.93	110.95
25	5	601	CHL	C1B-CHB-C4A	7.26	125.99	121.32
29	1	1623	NEX	O24-C25-C24	7.25	120.29	113.49
26	b	610	CLA	C4A-NA-C1A	7.23	109.98	106.68
26	N	613	CLA	C4A-NA-C1A	7.22	109.97	106.68
26	n	613	CLA	C4A-NA-C1A	7.22	109.97	106.68
29	5	1623	NEX	O24-C25-C24	7.22	120.25	113.49
28	1	1622	XAT	O24-C25-C24	7.20	120.24	113.49
25	1	601	CHL	C1B-CHB-C4A	7.19	125.95	121.32
28	5	1622	XAT	O24-C25-C24	7.19	120.23	113.49
25	Y	605	CHL	O2D-CGD-CBD	7.17	118.82	110.95
25	y	605	CHL	O2D-CGD-CBD	7.15	118.80	110.95
28	2	1622	XAT	O4-C5-C4	7.13	120.17	113.49
28	N	1622	XAT	C15-C14-C13	-7.12	117.29	127.28
28	n	1622	XAT	C15-C14-C13	-7.12	117.30	127.28
25	G	601	CHL	C4D-ND-C1D	-7.12	99.82	105.22
26	N	611	CLA	C4A-NA-C1A	7.11	109.92	106.68
25	g	601	CHL	C4D-ND-C1D	-7.10	99.83	105.22
26	n	611	CLA	C4A-NA-C1A	7.10	109.92	106.68
28	6	1622	XAT	O4-C5-C4	7.09	120.14	113.49
26	B	602	CLA	C4A-NA-C1A	7.07	109.90	106.68
31	t	101	BCR	C24-C23-C22	-7.07	115.78	126.23
29	2	1623	NEX	O24-C25-C24	7.06	120.11	113.49
26	S	603	CLA	C4A-NA-C1A	7.05	109.90	106.68
26	s	603	CLA	C4A-NA-C1A	7.05	109.90	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	R	612	CLA	C4A-NA-C1A	7.05	109.89	106.68
31	T	101	BCR	C24-C23-C22	-7.05	115.81	126.23
26	b	602	CLA	C4A-NA-C1A	7.04	109.89	106.68
29	6	1623	NEX	O24-C25-C24	7.03	120.08	113.49
26	c	509	CLA	C4A-NA-C1A	7.00	109.87	106.68
25	8	608	CHL	C4D-ND-C1D	-6.99	99.91	105.22
26	g	611	CLA	C4A-NA-C1A	6.98	109.86	106.68
29	g	1623	NEX	O24-C25-C24	6.98	120.03	113.49
26	B	606	CLA	C4A-NA-C1A	6.97	109.86	106.68
29	G	1623	NEX	O24-C25-C24	6.97	120.02	113.49
26	r	612	CLA	C4A-NA-C1A	6.97	109.86	106.68
25	S	606	CHL	C4D-ND-C1D	-6.96	99.94	105.22
25	s	606	CHL	C4D-ND-C1D	-6.96	99.94	105.22
26	C	509	CLA	C4A-NA-C1A	6.95	109.85	106.68
26	G	611	CLA	C4A-NA-C1A	6.92	109.84	106.68
25	4	608	CHL	C4D-ND-C1D	-6.92	99.97	105.22
26	r	609	CLA	C4A-NA-C1A	6.92	109.84	106.68
26	b	606	CLA	C4A-NA-C1A	6.92	109.83	106.68
26	b	617	CLA	C4A-NA-C1A	6.91	109.83	106.68
26	R	609	CLA	C4A-NA-C1A	6.90	109.83	106.68
26	B	617	CLA	C4A-NA-C1A	6.87	109.81	106.68
26	r	602	CLA	C4A-NA-C1A	6.85	109.80	106.68
28	g	1622	XAT	O24-C25-C24	6.84	119.90	113.49
25	G	607	CHL	C1B-CHB-C4A	6.82	125.71	121.32
25	g	607	CHL	C1B-CHB-C4A	6.81	125.70	121.32
26	b	609	CLA	C4A-NA-C1A	6.81	109.79	106.68
26	B	612	CLA	C4A-NA-C1A	6.81	109.78	106.68
26	R	601	CLA	C4A-NA-C1A	6.81	109.78	106.68
26	R	602	CLA	C4A-NA-C1A	6.78	109.77	106.68
28	G	1622	XAT	O24-C25-C24	6.77	119.83	113.49
26	r	601	CLA	C4A-NA-C1A	6.76	109.77	106.68
26	B	614	CLA	C4A-NA-C1A	6.76	109.76	106.68
26	b	612	CLA	C4A-NA-C1A	6.76	109.76	106.68
26	A	406	CLA	C4A-NA-C1A	6.75	109.76	106.68
25	r	614	CHL	O2D-CGD-CBD	6.75	118.37	110.95
26	R	611	CLA	C4A-NA-C1A	6.74	109.75	106.68
26	B	609	CLA	C4A-NA-C1A	6.73	109.75	106.68
25	R	614	CHL	O2D-CGD-CBD	6.72	118.33	110.95
26	b	614	CLA	C4A-NA-C1A	6.71	109.74	106.68
25	Y	605	CHL	C4D-ND-C1D	-6.71	100.13	105.22
26	a	406	CLA	C4A-NA-C1A	6.69	109.73	106.68
26	s	611	CLA	C4A-NA-C1A	6.69	109.73	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	605	CHL	C4D-ND-C1D	-6.68	100.15	105.22
26	C	504	CLA	C4A-NA-C1A	6.68	109.72	106.68
26	r	611	CLA	C4A-NA-C1A	6.67	109.72	106.68
25	3	601	CHL	C4D-ND-C1D	-6.67	100.16	105.22
26	S	611	CLA	C4A-NA-C1A	6.60	109.69	106.68
25	2	608	CHL	C4D-ND-C1D	-6.59	100.22	105.22
25	7	601	CHL	C4D-ND-C1D	-6.59	100.22	105.22
26	c	504	CLA	C4A-NA-C1A	6.58	109.68	106.68
25	6	608	CHL	C4D-ND-C1D	-6.55	100.25	105.22
25	4	608	CHL	O2D-CGD-CBD	6.54	118.13	110.95
31	C	516	BCR	C24-C23-C22	-6.54	116.56	126.23
25	1	608	CHL	O2D-CGD-CBD	6.54	118.13	110.95
25	5	608	CHL	O2D-CGD-CBD	6.54	118.13	110.95
25	1	608	CHL	C4D-ND-C1D	-6.54	100.26	105.22
31	c	516	BCR	C24-C23-C22	-6.54	116.56	126.23
25	8	608	CHL	O2D-CGD-CBD	6.53	118.12	110.95
29	Y	1623	NEX	O24-C25-C24	6.52	119.60	113.49
25	6	607	CHL	C1B-CHB-C4A	6.51	125.51	121.32
26	Y	611	CLA	C4A-NA-C1A	6.51	109.65	106.68
31	T	101	BCR	C20-C21-C22	-6.50	118.16	127.28
29	y	1623	NEX	O24-C25-C24	6.50	119.59	113.49
28	g	1622	XAT	C6-C7-C8	-6.50	112.24	125.99
25	2	607	CHL	C1B-CHB-C4A	6.50	125.50	121.32
25	5	608	CHL	C4D-ND-C1D	-6.49	100.29	105.22
28	G	1622	XAT	C6-C7-C8	-6.48	112.28	125.99
31	t	101	BCR	C20-C21-C22	-6.48	118.19	127.28
25	1	607	CHL	C4D-ND-C1D	-6.48	100.30	105.22
25	5	607	CHL	C4D-ND-C1D	-6.48	100.30	105.22
25	R	607	CHL	C4D-ND-C1D	-6.46	100.31	105.22
26	y	611	CLA	C4A-NA-C1A	6.45	109.62	106.68
25	r	607	CHL	C4D-ND-C1D	-6.44	100.33	105.22
25	y	601	CHL	C4D-ND-C1D	-6.41	100.35	105.22
31	t	101	BCR	C16-C17-C18	-6.41	118.29	127.28
25	n	601	CHL	C4D-ND-C1D	-6.41	100.36	105.22
31	T	101	BCR	C16-C17-C18	-6.40	118.30	127.28
25	N	601	CHL	C4D-ND-C1D	-6.38	100.38	105.22
25	s	607	CHL	C4D-ND-C1D	-6.37	100.38	105.22
25	8	606	CHL	C1B-CHB-C4A	6.36	125.41	121.32
25	n	607	CHL	O2D-CGD-CBD	6.34	117.91	110.95
25	Y	601	CHL	C4D-ND-C1D	-6.34	100.41	105.22
25	3	608	CHL	C4D-ND-C1D	-6.33	100.42	105.22
25	R	606	CHL	C4D-ND-C1D	-6.33	100.42	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	S	607	CHL	C4D-ND-C1D	-6.32	100.42	105.22
25	r	606	CHL	C4D-ND-C1D	-6.31	100.43	105.22
25	N	607	CHL	O2D-CGD-CBD	6.30	117.87	110.95
25	4	606	CHL	C1B-CHB-C4A	6.30	125.37	121.32
25	Y	607	CHL	O2D-CGD-CBD	6.29	117.86	110.95
25	y	607	CHL	O2D-CGD-CBD	6.29	117.86	110.95
25	7	608	CHL	C4D-ND-C1D	-6.29	100.44	105.22
26	y	603	CLA	C4A-NA-C1A	6.26	109.54	106.68
26	Y	603	CLA	C4A-NA-C1A	6.26	109.54	106.68
28	n	1622	XAT	C31-C30-C29	-6.25	118.51	127.28
25	Y	608	CHL	C4D-ND-C1D	-6.25	100.48	105.22
25	y	608	CHL	C4D-ND-C1D	-6.25	100.48	105.22
28	N	1622	XAT	C31-C30-C29	-6.25	118.52	127.28
25	2	605	CHL	C4D-ND-C1D	-6.24	100.48	105.22
25	6	605	CHL	C4D-ND-C1D	-6.24	100.48	105.22
25	n	608	CHL	C4D-ND-C1D	-6.24	100.48	105.22
25	R	614	CHL	C4D-ND-C1D	-6.24	100.49	105.22
25	S	608	CHL	O2D-CGD-CBD	6.22	117.78	110.95
31	8	623	BCR	C11-C10-C9	-6.22	118.56	127.28
26	C	510	CLA	C4A-NA-C1A	6.22	109.52	106.68
25	g	608	CHL	C4D-ND-C1D	-6.21	100.50	105.22
25	r	614	CHL	C4D-ND-C1D	-6.21	100.51	105.22
26	a	410	CLA	C4A-NA-C1A	6.21	109.51	106.68
25	N	608	CHL	C4D-ND-C1D	-6.20	100.52	105.22
31	4	623	BCR	C11-C10-C9	-6.19	118.59	127.28
28	R	622	XAT	C26-C27-C28	-6.19	112.90	125.99
25	2	601	CHL	C4D-ND-C1D	-6.19	100.52	105.22
25	s	608	CHL	O2D-CGD-CBD	6.19	117.75	110.95
26	7	611	CLA	C4A-NA-C1A	6.19	109.50	106.68
25	G	608	CHL	C4D-ND-C1D	-6.18	100.53	105.22
28	r	622	XAT	C26-C27-C28	-6.18	112.92	125.99
26	c	510	CLA	C4A-NA-C1A	6.17	109.49	106.68
26	A	410	CLA	C4A-NA-C1A	6.16	109.49	106.68
26	C	506	CLA	C4A-NA-C1A	6.15	109.49	106.68
26	c	506	CLA	C4A-NA-C1A	6.15	109.49	106.68
25	6	601	CHL	C4D-ND-C1D	-6.15	100.55	105.22
26	D	403	CLA	C4A-NA-C1A	6.14	109.48	106.68
26	3	611	CLA	C4A-NA-C1A	6.13	109.48	106.68
25	n	607	CHL	C4D-ND-C1D	-6.12	100.57	105.22
25	3	609	CHL	C1B-CHB-C4A	6.10	125.25	121.32
25	7	601	CHL	CHA-C1A-C2A	-6.10	118.99	133.31
25	3	601	CHL	CHA-C1A-C2A	-6.10	118.99	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	607	CHL	C4D-ND-C1D	-6.10	100.59	105.22
25	g	605	CHL	C4D-ND-C1D	-6.09	100.60	105.22
25	G	605	CHL	C4D-ND-C1D	-6.08	100.60	105.22
26	B	616	CLA	C4A-NA-C1A	6.08	109.45	106.68
26	B	605	CLA	CAA-C2A-C3A	-6.08	96.58	113.00
26	b	616	CLA	C4A-NA-C1A	6.07	109.45	106.68
28	y	1622	XAT	C15-C14-C13	-6.07	118.77	127.28
26	b	605	CLA	CAA-C2A-C3A	-6.06	96.61	113.00
28	Y	1622	XAT	C15-C14-C13	-6.06	118.77	127.28
25	n	609	CHL	C4D-ND-C1D	-6.06	100.62	105.22
25	7	609	CHL	C1B-CHB-C4A	6.06	125.22	121.32
26	d	403	CLA	C4A-NA-C1A	6.05	109.44	106.68
28	r	622	XAT	O4-C5-C4	6.04	119.15	113.49
28	N	1622	XAT	O4-C5-C4	6.03	119.14	113.49
29	R	623	NEX	O24-C25-C24	6.02	119.14	113.49
25	N	609	CHL	C4D-ND-C1D	-6.02	100.65	105.22
26	b	603	CLA	C4A-NA-C1A	6.02	109.43	106.68
26	g	603	CLA	C4A-NA-C1A	6.02	109.43	106.68
29	r	623	NEX	O24-C25-C24	6.02	119.13	113.49
25	N	605	CHL	C4D-ND-C1D	-6.02	100.65	105.22
35	A	408	PHO	C4D-CHA-CBD	-6.02	105.57	108.45
28	n	1622	XAT	O4-C5-C4	6.01	119.13	113.49
25	n	605	CHL	C4D-ND-C1D	-6.01	100.66	105.22
26	G	613	CLA	C4A-NA-C1A	6.01	109.42	106.68
26	g	613	CLA	C4A-NA-C1A	6.01	109.42	106.68
26	G	603	CLA	C4A-NA-C1A	6.01	109.42	106.68
25	1	605	CHL	C4D-ND-C1D	-6.00	100.67	105.22
28	R	622	XAT	O4-C5-C4	5.99	119.11	113.49
26	Y	604	CLA	C4A-NA-C1A	5.99	109.41	106.68
29	3	1623	NEX	O24-C25-C24	5.99	119.11	113.49
28	n	1622	XAT	O24-C25-C24	5.99	119.10	113.49
26	B	603	CLA	C4A-NA-C1A	5.98	109.41	106.68
25	6	601	CHL	CHA-C1A-C2A	-5.97	119.29	133.31
28	G	1622	XAT	C15-C14-C13	-5.97	118.91	127.28
31	d	404	BCR	C7-C8-C9	-5.97	117.41	126.23
31	c	517	BCR	C24-C23-C22	-5.96	117.41	126.23
28	N	1622	XAT	O24-C25-C24	5.96	119.08	113.49
31	c	517	BCR	C7-C8-C9	-5.96	117.42	126.23
31	D	404	BCR	C7-C8-C9	-5.96	117.42	126.23
31	C	517	BCR	C7-C8-C9	-5.96	117.42	126.23
25	2	601	CHL	CHA-C1A-C2A	-5.96	119.33	133.31
26	y	604	CLA	C4A-NA-C1A	5.95	109.39	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	8	622	XAT	O24-C25-C24	5.95	119.07	113.49
25	5	605	CHL	C4D-ND-C1D	-5.95	100.70	105.22
35	a	408	PHO	C4D-CHA-CBD	-5.95	105.60	108.45
26	Y	613	CLA	C4A-NA-C1A	5.94	109.39	106.68
31	C	517	BCR	C24-C23-C22	-5.94	117.45	126.23
28	g	1622	XAT	C15-C14-C13	-5.93	118.95	127.28
29	7	1623	NEX	O24-C25-C24	5.93	119.05	113.49
29	Y	1623	NEX	C35-C34-C33	-5.93	118.96	127.28
29	y	1623	NEX	C35-C34-C33	-5.93	118.97	127.28
28	4	622	XAT	O24-C25-C24	5.91	119.03	113.49
28	Y	1622	XAT	O24-C25-C24	5.91	119.03	113.49
29	n	1623	NEX	O24-C25-C24	5.90	119.02	113.49
26	c	513	CLA	C4A-NA-C1A	5.90	109.37	106.68
25	8	606	CHL	C4D-ND-C1D	-5.90	100.74	105.22
26	y	613	CLA	C4A-NA-C1A	5.89	109.37	106.68
29	N	1623	NEX	O24-C25-C24	5.89	119.01	113.49
29	3	1623	NEX	C15-C14-C13	-5.88	119.03	127.28
26	C	503	CLA	C4A-NA-C1A	5.88	109.36	106.68
26	c	503	CLA	C4A-NA-C1A	5.88	109.36	106.68
26	A	407	CLA	C4A-NA-C1A	5.88	109.36	106.68
26	C	513	CLA	C4A-NA-C1A	5.88	109.36	106.68
29	7	1623	NEX	C15-C14-C13	-5.87	119.05	127.28
25	s	606	CHL	CHA-C1A-C2A	-5.87	119.53	133.31
28	y	1622	XAT	O24-C25-C24	5.87	118.99	113.49
25	S	606	CHL	CHA-C1A-C2A	-5.85	119.56	133.31
26	N	603	CLA	C4A-NA-C1A	5.85	109.35	106.68
26	b	607	CLA	C4A-NA-C1A	5.85	109.35	106.68
28	7	1622	XAT	O4-C5-C4	5.84	118.97	113.49
25	S	608	CHL	C4D-ND-C1D	-5.84	100.79	105.22
35	a	409	PHO	C4D-CHA-CBD	-5.84	105.66	108.45
25	R	608	CHL	C4D-ND-C1D	-5.84	100.79	105.22
26	S	613	CLA	C4A-NA-C1A	5.83	109.34	106.68
25	4	606	CHL	C4D-ND-C1D	-5.83	100.80	105.22
26	B	615	CLA	C4A-NA-C1A	5.83	109.34	106.68
26	s	613	CLA	C4A-NA-C1A	5.83	109.34	106.68
25	Y	609	CHL	C4D-ND-C1D	-5.82	100.80	105.22
25	s	608	CHL	C4D-ND-C1D	-5.82	100.80	105.22
26	b	615	CLA	C4A-NA-C1A	5.82	109.33	106.68
28	3	1622	XAT	O4-C5-C4	5.81	118.94	113.49
25	r	608	CHL	C4D-ND-C1D	-5.81	100.81	105.22
35	A	409	PHO	C4D-CHA-CBD	-5.81	105.67	108.45
25	y	609	CHL	C4D-ND-C1D	-5.81	100.81	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	n	603	CLA	C4A-NA-C1A	5.80	109.33	106.68
26	1	603	CLA	C4A-NA-C1A	5.80	109.32	106.68
26	5	603	CLA	C4A-NA-C1A	5.80	109.32	106.68
26	2	611	CLA	C4A-NA-C1A	5.79	109.32	106.68
25	g	606	CHL	C4D-ND-C1D	-5.78	100.83	105.22
26	a	407	CLA	C4A-NA-C1A	5.78	109.31	106.68
25	G	606	CHL	C4D-ND-C1D	-5.77	100.84	105.22
31	t	101	BCR	C11-C10-C9	-5.77	119.19	127.28
26	B	607	CLA	C4A-NA-C1A	5.76	109.31	106.68
26	6	611	CLA	C4A-NA-C1A	5.76	109.31	106.68
25	2	608	CHL	CHA-C1A-C2A	-5.75	119.80	133.31
25	6	608	CHL	CHA-C1A-C2A	-5.75	119.80	133.31
25	1	601	CHL	CHA-C1A-C2A	-5.75	119.82	133.31
25	5	601	CHL	CHA-C1A-C2A	-5.74	119.82	133.31
25	G	606	CHL	CHA-C1A-C2A	-5.74	119.82	133.31
25	g	606	CHL	CHA-C1A-C2A	-5.74	119.84	133.31
26	C	508	CLA	C4A-NA-C1A	5.73	109.30	106.68
26	n	614	CLA	C4A-NA-C1A	5.73	109.29	106.68
31	T	101	BCR	C11-C10-C9	-5.73	119.25	127.28
28	y	1622	XAT	C31-C30-C29	-5.72	119.25	127.28
25	G	601	CHL	CHA-C1A-C2A	-5.72	119.87	133.31
25	g	601	CHL	CHA-C1A-C2A	-5.72	119.87	133.31
25	y	606	CHL	C4D-ND-C1D	-5.72	100.88	105.22
26	c	508	CLA	C4A-NA-C1A	5.71	109.28	106.68
26	R	604	CLA	C4A-NA-C1A	5.71	109.28	106.68
26	r	604	CLA	C4A-NA-C1A	5.71	109.28	106.68
28	Y	1622	XAT	C31-C30-C29	-5.71	119.28	127.28
26	C	512	CLA	C4A-NA-C1A	5.71	109.28	106.68
28	3	1622	XAT	C6-C7-C8	-5.69	113.96	125.99
28	7	1622	XAT	C6-C7-C8	-5.69	113.96	125.99
31	h	101	BCR	C11-C10-C9	-5.69	119.30	127.28
26	B	605	CLA	C4A-NA-C1A	5.69	109.27	106.68
26	b	605	CLA	C4A-NA-C1A	5.69	109.27	106.68
31	H	101	BCR	C11-C10-C9	-5.68	119.31	127.28
25	Y	606	CHL	C4D-ND-C1D	-5.68	100.91	105.22
25	n	601	CHL	CHA-C1A-C2A	-5.68	119.97	133.31
28	r	622	XAT	C38-C25-C26	-5.68	112.95	122.30
28	R	622	XAT	C38-C25-C26	-5.68	112.96	122.30
26	c	512	CLA	C4A-NA-C1A	5.67	109.27	106.68
28	R	622	XAT	O24-C25-C24	5.67	118.81	113.49
25	N	601	CHL	CHA-C1A-C2A	-5.67	120.00	133.31
25	G	607	CHL	C4D-ND-C1D	-5.66	100.92	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	r	622	XAT	O24-C25-C24	5.65	118.79	113.49
25	5	606	CHL	CHA-C1A-C2A	-5.65	120.04	133.31
25	r	606	CHL	CHA-C1A-C2A	-5.65	120.05	133.31
25	R	606	CHL	CHA-C1A-C2A	-5.64	120.06	133.31
25	g	607	CHL	C4D-ND-C1D	-5.64	100.94	105.22
25	n	606	CHL	C4D-ND-C1D	-5.63	100.94	105.22
25	7	605	CHL	C4D-ND-C1D	-5.63	100.95	105.22
25	1	606	CHL	CHA-C1A-C2A	-5.63	120.09	133.31
25	G	609	CHL	C4D-ND-C1D	-5.63	100.95	105.22
25	Y	601	CHL	CHA-C1A-C2A	-5.63	120.10	133.31
26	N	614	CLA	C4A-NA-C1A	5.63	109.25	106.68
25	Y	607	CHL	C4D-ND-C1D	-5.63	100.95	105.22
25	y	607	CHL	C4D-ND-C1D	-5.63	100.95	105.22
25	N	606	CHL	C4D-ND-C1D	-5.62	100.95	105.22
31	C	515	BCR	C7-C8-C9	-5.62	117.92	126.23
25	y	601	CHL	CHA-C1A-C2A	-5.61	120.13	133.31
25	6	606	CHL	C4D-ND-C1D	-5.61	100.96	105.22
27	5	1620	LUT	C26-C27-C28	-5.61	115.85	124.58
25	5	605	CHL	CHA-C1A-C2A	-5.61	120.14	133.31
25	1	609	CHL	C4D-ND-C1D	-5.61	100.97	105.22
25	g	608	CHL	CHA-C1A-C2A	-5.60	120.16	133.31
26	7	603	CLA	C4A-NA-C1A	5.60	109.23	106.68
25	N	609	CHL	CHA-C1A-C2A	-5.59	120.17	133.31
25	5	609	CHL	C4D-ND-C1D	-5.59	100.97	105.22
25	1	605	CHL	CHA-C1A-C2A	-5.59	120.18	133.31
27	1	1620	LUT	C26-C27-C28	-5.59	115.88	124.58
25	3	605	CHL	C4D-ND-C1D	-5.59	100.97	105.22
25	g	609	CHL	C4D-ND-C1D	-5.59	100.98	105.22
31	c	515	BCR	C7-C8-C9	-5.59	117.96	126.23
25	4	608	CHL	CHA-C1A-C2A	-5.59	120.19	133.31
25	8	608	CHL	CHA-C1A-C2A	-5.59	120.19	133.31
25	n	609	CHL	CHA-C1A-C2A	-5.59	120.19	133.31
25	G	608	CHL	CHA-C1A-C2A	-5.59	120.19	133.31
25	Y	609	CHL	CHA-C1A-C2A	-5.59	120.19	133.31
25	y	609	CHL	CHA-C1A-C2A	-5.59	120.19	133.31
25	n	606	CHL	CHA-C1A-C2A	-5.58	120.20	133.31
25	n	608	CHL	CHA-C1A-C2A	-5.58	120.21	133.31
25	1	606	CHL	C4D-ND-C1D	-5.57	100.99	105.22
26	3	603	CLA	C4A-NA-C1A	5.57	109.22	106.68
25	Y	608	CHL	CHA-C1A-C2A	-5.57	120.23	133.31
25	y	608	CHL	CHA-C1A-C2A	-5.57	120.23	133.31
25	N	608	CHL	CHA-C1A-C2A	-5.57	120.24	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	606	CHL	CHA-C1A-C2A	-5.57	120.24	133.31
25	5	606	CHL	C4D-ND-C1D	-5.56	101.00	105.22
25	S	601	CHL	C4D-ND-C1D	-5.56	101.00	105.22
25	2	606	CHL	C4D-ND-C1D	-5.55	101.00	105.22
25	s	601	CHL	C4D-ND-C1D	-5.54	101.01	105.22
28	3	1622	XAT	C31-C30-C29	-5.54	119.51	127.28
28	7	1622	XAT	C31-C30-C29	-5.54	119.51	127.28
25	4	609	CHL	C1B-CHB-C4A	5.54	124.89	121.32
28	4	622	XAT	C6-C7-C8	-5.53	114.30	125.99
28	8	622	XAT	C6-C7-C8	-5.53	114.30	125.99
25	Y	609	CHL	CBC-CAC-C3C	-5.53	104.96	112.87
25	2	606	CHL	CHA-C1A-C2A	-5.53	120.33	133.31
25	7	608	CHL	CHA-C1A-C2A	-5.52	120.34	133.31
25	y	609	CHL	CBC-CAC-C3C	-5.52	104.97	112.87
31	8	623	BCR	C16-C17-C18	-5.52	119.54	127.28
31	4	623	BCR	C16-C17-C18	-5.51	119.55	127.28
25	3	609	CHL	CHA-C1A-C2A	-5.51	120.36	133.31
25	7	609	CHL	CHA-C1A-C2A	-5.51	120.36	133.31
26	Y	614	CLA	C4A-NA-C1A	5.51	109.19	106.68
25	6	606	CHL	CHA-C1A-C2A	-5.51	120.37	133.31
25	3	608	CHL	CHA-C1A-C2A	-5.51	120.37	133.31
26	y	614	CLA	C4A-NA-C1A	5.51	109.19	106.68
26	4	603	CLA	C4A-NA-C1A	5.50	109.19	106.68
25	6	607	CHL	C4D-ND-C1D	-5.50	101.04	105.22
28	n	1622	XAT	C6-C7-C8	-5.50	114.37	125.99
28	Y	1622	XAT	O4-C5-C18	5.50	121.19	115.05
28	y	1622	XAT	O4-C5-C18	5.50	121.19	115.05
29	r	623	NEX	C15-C14-C13	-5.49	119.57	127.28
25	3	606	CHL	CHA-C1A-C2A	-5.48	120.43	133.31
28	N	1622	XAT	C6-C7-C8	-5.48	114.41	125.99
25	7	606	CHL	CHA-C1A-C2A	-5.48	120.44	133.31
25	s	601	CHL	CHA-C1A-C2A	-5.48	120.44	133.31
25	S	601	CHL	CHA-C1A-C2A	-5.48	120.44	133.31
25	8	609	CHL	C1B-CHB-C4A	5.47	124.84	121.32
28	y	1622	XAT	C11-C10-C9	-5.47	119.61	127.28
25	7	606	CHL	C4D-ND-C1D	-5.47	101.07	105.22
28	Y	1622	XAT	C11-C10-C9	-5.46	119.61	127.28
29	R	623	NEX	C15-C14-C13	-5.46	119.62	127.28
25	G	605	CHL	CHA-C1A-C2A	-5.45	120.51	133.31
25	3	606	CHL	C4D-ND-C1D	-5.45	101.09	105.22
25	g	605	CHL	CHA-C1A-C2A	-5.44	120.54	133.31
26	8	603	CLA	C4A-NA-C1A	5.43	109.16	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	607	CHL	C4D-ND-C1D	-5.43	101.10	105.22
26	r	616	CLA	C4A-NA-C1A	5.43	109.16	106.68
27	R	620	LUT	C26-C27-C28	-5.43	116.14	124.58
27	r	620	LUT	C26-C27-C28	-5.42	116.14	124.58
29	s	1623	NEX	O24-C25-C24	5.42	118.57	113.49
31	T	101	BCR	C7-C8-C9	-5.41	118.23	126.23
25	6	609	CHL	C4D-ND-C1D	-5.41	101.12	105.22
29	S	1623	NEX	O24-C25-C24	5.41	118.56	113.49
28	N	1622	XAT	C38-C25-C26	-5.41	113.41	122.30
28	3	1622	XAT	C38-C25-C26	-5.40	113.42	122.30
28	n	1622	XAT	C38-C25-C26	-5.39	113.42	122.30
28	7	1622	XAT	C38-C25-C26	-5.38	113.44	122.30
25	8	607	CHL	C4D-ND-C1D	-5.38	101.13	105.22
31	b	618	BCR	C15-C14-C13	-5.38	119.73	127.28
31	B	618	BCR	C15-C14-C13	-5.38	119.73	127.28
25	2	609	CHL	C4D-ND-C1D	-5.37	101.14	105.22
31	t	101	BCR	C7-C8-C9	-5.37	118.30	126.23
25	4	607	CHL	C4D-ND-C1D	-5.36	101.15	105.22
26	Y	612	CLA	C4A-NA-C1A	5.35	109.12	106.68
29	r	623	NEX	C11-C10-C9	-5.35	119.77	127.28
40	D	401	BCT	O2-C-O1	5.35	133.36	119.68
26	R	616	CLA	C4A-NA-C1A	5.35	109.12	106.68
28	3	1622	XAT	C15-C14-C13	-5.34	119.79	127.28
28	4	622	XAT	C18-C5-C6	-5.34	113.51	122.30
29	R	623	NEX	C11-C10-C9	-5.34	119.79	127.28
28	8	622	XAT	C18-C5-C6	-5.34	113.52	122.30
40	d	401	BCT	O2-C-O1	5.34	133.32	119.68
26	y	612	CLA	C4A-NA-C1A	5.33	109.11	106.68
28	5	1622	XAT	C31-C30-C29	-5.33	119.81	127.28
25	2	605	CHL	C1B-CHB-C4A	5.32	124.75	121.32
28	7	1622	XAT	C15-C14-C13	-5.32	119.82	127.28
25	1	607	CHL	CHA-C1A-C2A	-5.31	120.84	133.31
25	5	607	CHL	CHA-C1A-C2A	-5.31	120.84	133.31
28	4	622	XAT	O4-C5-C18	5.31	120.98	115.05
28	8	622	XAT	O4-C5-C18	5.31	120.98	115.05
28	1	1622	XAT	C31-C30-C29	-5.30	119.84	127.28
25	6	605	CHL	C1B-CHB-C4A	5.29	124.72	121.32
25	1	608	CHL	CHA-C1A-C2A	-5.29	120.90	133.31
25	5	609	CHL	CHA-C1A-C2A	-5.29	120.90	133.31
25	1	609	CHL	CHA-C1A-C2A	-5.28	120.91	133.31
26	y	602	CLA	C4A-NA-C1A	5.28	109.09	106.68
25	Y	606	CHL	CHA-C1A-C2A	-5.28	120.92	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	606	CHL	CHA-C1A-C2A	-5.28	120.92	133.31
25	8	606	CHL	CHA-C1A-C2A	-5.28	120.92	133.31
25	4	606	CHL	CHA-C1A-C2A	-5.27	120.92	133.31
25	y	605	CHL	CHA-C1A-C2A	-5.27	120.93	133.31
25	s	607	CHL	CBC-CAC-C3C	-5.27	105.33	112.87
25	5	608	CHL	CHA-C1A-C2A	-5.27	120.94	133.31
26	S	612	CLA	C4A-NA-C1A	5.27	109.08	106.68
26	r	603	CLA	C4A-NA-C1A	5.26	109.08	106.68
25	Y	605	CHL	CHA-C1A-C2A	-5.26	120.95	133.31
28	5	1622	XAT	C15-C14-C13	-5.26	119.90	127.28
25	S	607	CHL	CBC-CAC-C3C	-5.26	105.34	112.87
27	G	1620	LUT	C26-C27-C28	-5.26	116.40	124.58
26	R	603	CLA	C4A-NA-C1A	5.26	109.08	106.68
25	r	607	CHL	CHA-C1A-C2A	-5.25	120.97	133.31
28	G	1622	XAT	C31-C30-C29	-5.25	119.91	127.28
27	g	1620	LUT	C26-C27-C28	-5.25	116.41	124.58
25	R	607	CHL	CHA-C1A-C2A	-5.24	120.99	133.31
28	1	1622	XAT	C15-C14-C13	-5.24	119.92	127.28
25	4	609	CHL	CHA-C1A-C2A	-5.23	121.02	133.31
25	8	609	CHL	CHA-C1A-C2A	-5.22	121.05	133.31
27	4	620	LUT	C26-C27-C28	-5.22	116.45	124.58
29	3	1623	NEX	C38-C25-C26	-5.22	113.71	122.30
27	8	620	LUT	C26-C27-C28	-5.22	116.46	124.58
28	g	1622	XAT	C31-C30-C29	-5.22	119.96	127.28
26	s	612	CLA	C4A-NA-C1A	5.21	109.06	106.68
26	Y	602	CLA	C4A-NA-C1A	5.21	109.06	106.68
28	1	1622	XAT	C38-C25-C26	-5.21	113.72	122.30
28	5	1622	XAT	C38-C25-C26	-5.21	113.73	122.30
29	n	1623	NEX	C35-C34-C33	-5.20	119.99	127.28
29	7	1623	NEX	C38-C25-C26	-5.19	113.75	122.30
29	N	1623	NEX	C35-C34-C33	-5.19	120.00	127.28
29	6	1623	NEX	C15-C14-C13	-5.19	120.00	127.28
28	y	1622	XAT	C15-C35-C34	-5.18	112.92	123.52
29	2	1623	NEX	C15-C14-C13	-5.17	120.02	127.28
29	Y	1623	NEX	C17-C1-C6	-5.17	105.84	110.47
28	Y	1622	XAT	C15-C35-C34	-5.17	112.95	123.52
27	6	1620	LUT	C26-C27-C28	-5.16	116.55	124.58
25	8	609	CHL	C4D-ND-C1D	-5.16	101.30	105.22
31	c	515	BCR	C21-C20-C19	-5.16	108.25	123.20
31	C	515	BCR	C21-C20-C19	-5.15	108.27	123.20
31	4	623	BCR	C28-C27-C26	-5.15	104.87	114.06
31	8	623	BCR	C28-C27-C26	-5.14	104.89	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	y	1623	NEX	C17-C1-C6	-5.13	105.88	110.47
27	2	1620	LUT	C26-C27-C28	-5.13	116.60	124.58
27	3	1620	LUT	C26-C27-C28	-5.13	116.60	124.58
27	7	1620	LUT	C26-C27-C28	-5.13	116.60	124.58
26	C	508	CLA	CMB-C2B-C1B	-5.12	117.62	125.42
28	7	1622	XAT	O24-C25-C38	5.11	120.76	115.05
26	c	508	CLA	CMB-C2B-C1B	-5.11	117.64	125.42
28	g	1622	XAT	C15-C35-C34	-5.11	113.07	123.52
25	N	605	CHL	CHA-C1A-C2A	-5.10	121.32	133.31
28	3	1622	XAT	O24-C25-C38	5.10	120.75	115.05
25	G	609	CHL	CHA-C1A-C2A	-5.10	121.33	133.31
28	G	1622	XAT	C15-C35-C34	-5.09	113.10	123.52
25	n	605	CHL	CHA-C1A-C2A	-5.09	121.36	133.31
25	4	607	CHL	CHA-C1A-C2A	-5.08	121.37	133.31
25	g	609	CHL	CHA-C1A-C2A	-5.08	121.38	133.31
28	r	622	XAT	C6-C7-C8	-5.07	115.27	125.99
25	G	607	CHL	CHA-C1A-C2A	-5.07	121.40	133.31
25	4	609	CHL	C4D-ND-C1D	-5.07	101.37	105.22
26	8	602	CLA	C4A-NA-C1A	5.07	108.99	106.68
31	8	623	BCR	C15-C14-C13	-5.06	120.18	127.28
25	8	607	CHL	CHA-C1A-C2A	-5.06	121.42	133.31
28	R	622	XAT	C6-C7-C8	-5.06	115.29	125.99
28	g	1622	XAT	C38-C25-C26	-5.06	113.97	122.30
29	G	1623	NEX	C38-C25-C26	-5.06	113.97	122.30
25	4	607	CHL	C1B-CHB-C4A	5.06	124.58	121.32
25	g	607	CHL	CHA-C1A-C2A	-5.06	121.43	133.31
29	g	1623	NEX	C38-C25-C26	-5.06	113.98	122.30
26	G	602	CLA	C4A-NA-C1A	5.05	108.98	106.68
26	r	613	CLA	C4A-NA-C1A	5.05	108.98	106.68
28	G	1622	XAT	C38-C25-C26	-5.04	114.00	122.30
29	y	1623	NEX	C27-C28-C29	-5.04	117.71	125.53
29	Y	1623	NEX	C27-C28-C29	-5.04	117.71	125.53
29	s	1623	NEX	C11-C10-C9	-5.04	120.21	127.28
31	4	623	BCR	C15-C14-C13	-5.04	120.21	127.28
29	S	1623	NEX	C11-C10-C9	-5.03	120.22	127.28
28	R	622	XAT	O4-C5-C18	5.03	120.67	115.05
29	R	623	NEX	C27-C28-C29	-5.03	117.73	125.53
29	r	623	NEX	C27-C28-C29	-5.03	117.73	125.53
25	R	608	CHL	CHA-C1A-C2A	-5.02	121.51	133.31
29	5	1623	NEX	C27-C28-C29	-5.02	117.73	125.53
29	1	1623	NEX	C27-C28-C29	-5.02	117.74	125.53
25	r	608	CHL	CHA-C1A-C2A	-5.02	121.53	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	g	1623	NEX	C11-C10-C9	-5.01	120.25	127.28
25	6	605	CHL	CHA-C1A-C2A	-5.00	121.57	133.31
28	1	1622	XAT	O4-C5-C4	5.00	118.17	113.49
25	2	605	CHL	CHA-C1A-C2A	-5.00	121.58	133.31
26	7	613	CLA	C4A-NA-C1A	5.00	108.96	106.68
36	a	412	SQD	O6-C1-C2	4.99	115.85	108.27
28	r	622	XAT	O4-C5-C18	4.99	120.63	115.05
25	2	609	CHL	CHA-C1A-C2A	-4.99	121.59	133.31
25	8	607	CHL	C1B-CHB-C4A	4.99	124.53	121.32
25	6	609	CHL	CHA-C1A-C2A	-4.99	121.60	133.31
28	5	1622	XAT	O4-C5-C4	4.98	118.16	113.49
29	2	1623	NEX	C38-C25-C26	-4.98	114.10	122.30
29	G	1623	NEX	C11-C10-C9	-4.98	120.29	127.28
36	A	412	SQD	O6-C1-C2	4.98	115.83	108.27
29	6	1623	NEX	C38-C25-C26	-4.98	114.11	122.30
26	g	602	CLA	C4A-NA-C1A	4.97	108.95	106.68
25	3	605	CHL	C1B-CHB-C4A	4.97	124.52	121.32
29	n	1623	NEX	C27-C28-C29	-4.97	117.82	125.53
28	Y	1622	XAT	C38-C25-C26	-4.96	114.13	122.30
28	n	1622	XAT	C15-C35-C34	-4.96	113.36	123.52
28	G	1622	XAT	O4-C5-C18	4.96	120.59	115.05
28	y	1622	XAT	C38-C25-C26	-4.96	114.15	122.30
28	g	1622	XAT	O4-C5-C18	4.96	120.59	115.05
26	N	612	CLA	C4A-NA-C1A	4.95	108.94	106.68
26	n	612	CLA	C4A-NA-C1A	4.95	108.94	106.68
27	Y	1620	LUT	C26-C27-C28	-4.95	116.88	124.58
28	N	1622	XAT	C15-C35-C34	-4.95	113.40	123.52
29	N	1623	NEX	C27-C28-C29	-4.95	117.86	125.53
28	4	622	XAT	O4-C5-C4	4.94	118.12	113.49
25	7	605	CHL	C1B-CHB-C4A	4.94	124.50	121.32
27	y	1620	LUT	C26-C27-C28	-4.94	116.89	124.58
25	1	609	CHL	C1B-CHB-C4A	4.93	124.50	121.32
26	2	604	CLA	C4A-NA-C1A	4.93	108.93	106.68
26	R	613	CLA	C4A-NA-C1A	4.93	108.93	106.68
26	6	604	CLA	C4A-NA-C1A	4.93	108.93	106.68
31	b	620	BCR	C7-C8-C9	-4.93	118.95	126.23
27	2	1620	LUT	C35-C34-C33	-4.92	120.38	127.28
26	4	602	CLA	C4A-NA-C1A	4.92	108.92	106.68
31	B	620	BCR	C7-C8-C9	-4.91	118.97	126.23
26	3	613	CLA	C4A-NA-C1A	4.91	108.92	106.68
25	5	609	CHL	C1B-CHB-C4A	4.91	124.48	121.32
25	1	601	CHL	C4D-ND-C1D	-4.91	101.50	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	6	1620	LUT	C35-C34-C33	-4.90	120.40	127.28
28	8	622	XAT	O4-C5-C4	4.90	118.08	113.49
29	3	1623	NEX	C11-C10-C9	-4.88	120.43	127.28
28	7	1622	XAT	O24-C25-C24	4.88	118.06	113.49
26	G	604	CLA	C4A-NA-C1A	4.87	108.90	106.68
26	S	614	CLA	C4A-NA-C1A	4.87	108.90	106.68
29	n	1623	NEX	C38-C25-C26	-4.87	114.29	122.30
29	N	1623	NEX	C38-C25-C26	-4.87	114.29	122.30
28	2	1622	XAT	C38-C25-C26	-4.87	114.29	122.30
26	c	501	CLA	C4A-NA-C1A	4.87	108.90	106.68
28	3	1622	XAT	O24-C25-C24	4.86	118.05	113.49
28	6	1622	XAT	C38-C25-C26	-4.86	114.30	122.30
28	4	622	XAT	C26-C27-C28	-4.86	115.72	125.99
29	7	1623	NEX	C11-C10-C9	-4.86	120.47	127.28
26	a	410	CLA	C1-C2-C3	-4.85	118.25	126.20
29	s	1623	NEX	C38-C25-C26	-4.85	114.33	122.30
25	5	601	CHL	C4D-ND-C1D	-4.84	101.54	105.22
28	8	622	XAT	C26-C27-C28	-4.84	115.76	125.99
31	4	623	BCR	C7-C8-C9	-4.84	119.08	126.23
27	G	1621	LUT	C15-C14-C13	-4.84	120.50	127.28
26	A	410	CLA	C1-C2-C3	-4.83	118.29	126.20
31	8	623	BCR	C7-C8-C9	-4.82	119.10	126.23
26	C	501	CLA	C4A-NA-C1A	4.82	108.88	106.68
29	S	1623	NEX	C38-C25-C26	-4.82	114.37	122.30
29	S	1623	NEX	O24-C25-C38	4.81	120.43	115.05
29	s	1623	NEX	O24-C25-C38	4.81	120.43	115.05
27	S	1621	LUT	C35-C34-C33	-4.81	120.53	127.28
27	s	1621	LUT	C35-C34-C33	-4.81	120.54	127.28
26	N	604	CLA	C4A-NA-C1A	4.80	108.87	106.68
26	n	604	CLA	C4A-NA-C1A	4.80	108.87	106.68
27	g	1621	LUT	C15-C14-C13	-4.80	120.55	127.28
29	1	1623	NEX	C38-C25-C26	-4.80	114.41	122.30
28	2	1622	XAT	C31-C30-C29	-4.77	120.58	127.28
26	s	614	CLA	C4A-NA-C1A	4.77	108.86	106.68
31	C	514	BCR	C15-C14-C13	-4.77	120.59	127.28
29	5	1623	NEX	C38-C25-C26	-4.77	114.45	122.30
26	g	604	CLA	C4A-NA-C1A	4.77	108.85	106.68
28	1	1622	XAT	C6-C7-C8	-4.76	115.92	125.99
31	c	514	BCR	C15-C14-C13	-4.76	120.60	127.28
28	5	1622	XAT	C6-C7-C8	-4.76	115.93	125.99
28	3	1622	XAT	C18-C5-C6	-4.75	114.48	122.30
28	6	1622	XAT	C31-C30-C29	-4.75	120.61	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	8	611	CLA	C4A-NA-C1A	4.75	108.84	106.68
26	6	603	CLA	C4A-NA-C1A	4.74	108.84	106.68
29	n	1623	NEX	C15-C14-C13	-4.74	120.63	127.28
28	7	1622	XAT	C18-C5-C6	-4.74	114.50	122.30
28	2	1622	XAT	C18-C5-C6	-4.73	114.51	122.30
28	N	1622	XAT	C27-C28-C29	-4.73	118.19	125.53
31	c	517	BCR	C15-C14-C13	-4.73	120.65	127.28
31	C	517	BCR	C15-C14-C13	-4.72	120.65	127.28
28	n	1622	XAT	C27-C28-C29	-4.72	118.21	125.53
28	6	1622	XAT	C18-C5-C6	-4.71	114.55	122.30
29	7	1623	NEX	O24-C25-C38	4.71	120.31	115.05
26	C	508	CLA	O2D-CGD-O1D	-4.70	114.70	123.85
25	7	605	CHL	CHA-C1A-C2A	-4.70	122.28	133.31
29	3	1623	NEX	O24-C25-C38	4.70	120.30	115.05
25	3	605	CHL	CHA-C1A-C2A	-4.69	122.29	133.31
25	3	609	CHL	C4D-ND-C1D	-4.69	101.66	105.22
29	N	1623	NEX	C15-C14-C13	-4.69	120.70	127.28
26	2	603	CLA	C4A-NA-C1A	4.69	108.82	106.68
31	H	101	BCR	C16-C17-C18	-4.69	120.71	127.28
27	S	1621	LUT	C26-C27-C28	-4.67	117.31	124.58
26	c	508	CLA	O2D-CGD-O1D	-4.67	114.76	123.85
38	D	405	PL9	C7-C3-C4	4.67	120.75	116.91
25	s	607	CHL	CHA-C1A-C2A	-4.67	122.35	133.31
25	S	607	CHL	CHA-C1A-C2A	-4.66	122.36	133.31
31	h	101	BCR	C16-C17-C18	-4.66	120.74	127.28
27	s	1621	LUT	C26-C27-C28	-4.66	117.33	124.58
29	1	1623	NEX	C31-C30-C29	-4.66	120.75	127.28
25	7	609	CHL	C4D-ND-C1D	-4.66	101.69	105.22
25	Y	607	CHL	CHA-C1A-C2A	-4.65	122.38	133.31
29	y	1623	NEX	C11-C10-C9	-4.65	120.76	127.28
25	2	607	CHL	CHA-C1A-C2A	-4.64	122.41	133.31
29	Y	1623	NEX	C11-C10-C9	-4.64	120.77	127.28
29	5	1623	NEX	C31-C30-C29	-4.63	120.78	127.28
25	y	607	CHL	CHA-C1A-C2A	-4.63	122.43	133.31
39	C	518	DGD	O3G-C3G-C2G	-4.63	99.55	110.82
31	c	517	BCR	C11-C10-C9	-4.63	120.78	127.28
28	y	1622	XAT	O24-C25-C38	4.63	120.22	115.05
39	c	518	DGD	O3G-C3G-C2G	-4.63	99.56	110.82
28	8	622	XAT	C38-C25-C26	-4.63	114.69	122.30
26	4	611	CLA	C4A-NA-C1A	4.62	108.79	106.68
29	R	623	NEX	C38-C25-C26	-4.62	114.69	122.30
28	1	1622	XAT	C18-C5-C6	-4.62	114.69	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	613	CLA	C4A-NA-C1A	4.62	108.79	106.68
38	d	405	PL9	C7-C3-C4	4.62	120.72	116.91
25	6	607	CHL	CHA-C1A-C2A	-4.62	122.46	133.31
25	n	609	CHL	CBC-CAC-C3C	-4.62	106.26	112.87
29	r	623	NEX	C38-C25-C26	-4.62	114.70	122.30
26	1	613	CLA	C4A-NA-C1A	4.61	108.78	106.68
28	4	622	XAT	C38-C25-C26	-4.61	114.72	122.30
31	C	517	BCR	C11-C10-C9	-4.60	120.82	127.28
28	5	1622	XAT	C18-C5-C6	-4.60	114.74	122.30
31	B	619	BCR	C15-C14-C13	-4.60	120.83	127.28
25	N	609	CHL	CBC-CAC-C3C	-4.59	106.30	112.87
31	T	101	BCR	C20-C19-C18	-4.59	113.78	126.36
28	r	622	XAT	C18-C5-C6	-4.59	114.75	122.30
25	r	614	CHL	CBC-CAC-C3C	-4.59	106.31	112.87
28	R	622	XAT	C18-C5-C6	-4.58	114.76	122.30
28	Y	1622	XAT	O24-C25-C38	4.58	120.17	115.05
31	t	101	BCR	C20-C19-C18	-4.58	113.80	126.36
31	c	515	BCR	C15-C14-C13	-4.58	120.86	127.28
26	R	601	CLA	CAC-C3C-C4C	4.57	130.74	124.79
28	g	1622	XAT	C27-C28-C29	-4.57	118.44	125.53
26	n	604	CLA	CMB-C2B-C1B	-4.57	118.46	125.42
26	2	612	CLA	C4A-NA-C1A	4.57	108.76	106.68
25	R	614	CHL	CBC-CAC-C3C	-4.56	106.34	112.87
27	N	1620	LUT	C26-C27-C28	-4.56	117.48	124.58
29	Y	1623	NEX	C38-C25-C26	-4.56	114.80	122.30
26	r	601	CLA	CAC-C3C-C4C	4.56	130.72	124.79
29	y	1623	NEX	C38-C25-C26	-4.56	114.81	122.30
31	b	619	BCR	C15-C14-C13	-4.55	120.89	127.28
28	r	622	XAT	O24-C25-C38	4.55	120.13	115.05
28	G	1622	XAT	C27-C28-C29	-4.54	118.48	125.53
28	Y	1622	XAT	C18-C5-C6	-4.54	114.83	122.30
30	L	101	LHG	O4-P-O5	4.54	133.57	112.44
27	n	1620	LUT	C26-C27-C28	-4.54	117.51	124.58
28	y	1622	XAT	C18-C5-C6	-4.54	114.83	122.30
30	l	101	LHG	O4-P-O5	4.54	133.56	112.44
30	4	2630	LHG	O4-P-O5	4.54	133.55	112.44
26	N	604	CLA	CMB-C2B-C1B	-4.53	118.52	125.42
31	H	101	BCR	C24-C23-C22	-4.53	119.53	126.23
31	C	515	BCR	C15-C14-C13	-4.53	120.92	127.28
26	G	614	CLA	C4A-NA-C1A	4.53	108.75	106.68
30	c	523	LHG	O4-P-O5	4.53	133.52	112.44
31	h	101	BCR	C24-C23-C22	-4.53	119.53	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	523	LHG	O4-P-O5	4.53	133.51	112.44
28	N	1622	XAT	O24-C25-C38	4.53	120.11	115.05
28	n	1622	XAT	O24-C25-C38	4.53	120.11	115.05
30	8	2630	LHG	O4-P-O5	4.53	133.50	112.44
28	r	622	XAT	C35-C34-C33	-4.53	120.93	127.28
29	1	1623	NEX	C35-C34-C33	-4.53	120.93	127.28
26	g	614	CLA	C4A-NA-C1A	4.53	108.74	106.68
29	7	1623	NEX	C27-C28-C29	-4.52	118.51	125.53
27	S	1620	LUT	C35-C34-C33	-4.52	120.94	127.28
28	R	622	XAT	O24-C25-C38	4.52	120.10	115.05
28	G	1622	XAT	O4-C5-C4	4.52	117.73	113.49
26	8	612	CLA	C4A-NA-C1A	4.51	108.74	106.68
27	s	1620	LUT	C35-C34-C33	-4.51	120.95	127.28
25	S	608	CHL	CHA-C1A-C2A	-4.51	122.71	133.31
29	3	1623	NEX	C27-C28-C29	-4.51	118.53	125.53
25	s	608	CHL	CHA-C1A-C2A	-4.51	122.72	133.31
28	R	622	XAT	C35-C34-C33	-4.51	120.96	127.28
26	4	612	CLA	C4A-NA-C1A	4.51	108.73	106.68
29	5	1623	NEX	C35-C34-C33	-4.50	120.96	127.28
29	N	1623	NEX	O24-C25-C38	4.50	120.08	115.05
30	D	408	LHG	O4-P-O5	4.50	133.39	112.44
31	C	516	BCR	C16-C17-C18	-4.50	120.97	127.28
28	g	1622	XAT	O4-C5-C4	4.50	117.71	113.49
30	d	408	LHG	O4-P-O5	4.50	133.36	112.44
35	A	409	PHO	CMB-C2B-C3B	4.49	133.66	124.68
30	s	2630	LHG	O4-P-O5	4.49	133.33	112.44
26	6	612	CLA	C4A-NA-C1A	4.49	108.73	106.68
30	S	2630	LHG	O4-P-O5	4.49	133.31	112.44
29	Y	1623	NEX	C15-C14-C13	-4.48	120.99	127.28
25	8	601	CHL	C4D-ND-C1D	-4.48	101.82	105.22
29	n	1623	NEX	O24-C25-C38	4.48	120.05	115.05
35	a	409	PHO	CMB-C2B-C3B	4.47	133.62	124.68
30	Y	2630	LHG	O4-P-O5	4.47	133.25	112.44
30	y	2630	LHG	O4-P-O5	4.47	133.25	112.44
30	D	409	LHG	O4-P-O5	4.47	133.25	112.44
30	d	409	LHG	O4-P-O5	4.47	133.25	112.44
30	n	2630	LHG	O4-P-O5	4.47	133.22	112.44
29	y	1623	NEX	C15-C14-C13	-4.47	121.02	127.28
31	c	516	BCR	C16-C17-C18	-4.47	121.02	127.28
27	1	1620	LUT	C35-C34-C33	-4.46	121.02	127.28
30	N	2630	LHG	O4-P-O5	4.46	133.20	112.44
31	b	618	BCR	C16-C17-C18	-4.46	121.03	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	517	BCR	C33-C5-C6	-4.44	119.64	124.48
30	r	2630	LHG	O4-P-O5	4.44	133.11	112.44
27	3	1621	LUT	C26-C27-C28	-4.44	117.67	124.58
31	B	618	BCR	C16-C17-C18	-4.44	121.05	127.28
30	C	522	LHG	O4-P-O5	4.44	133.08	112.44
30	R	2630	LHG	O4-P-O5	4.44	133.08	112.44
25	G	609	CHL	CBC-CAC-C3C	-4.43	106.52	112.87
27	5	1620	LUT	C35-C34-C33	-4.43	121.06	127.28
30	c	522	LHG	O4-P-O5	4.43	133.06	112.44
28	6	1622	XAT	C15-C14-C13	-4.43	121.06	127.28
25	R	614	CHL	C1B-CHB-C4A	4.43	124.17	121.32
26	n	602	CLA	C4A-NA-C1A	4.43	108.70	106.68
25	N	607	CHL	CHA-C1A-C2A	-4.42	122.92	133.31
30	1	2630	LHG	O4-P-O5	4.42	133.02	112.44
39	C	519	DGD	O3G-C3G-C2G	-4.42	100.06	110.82
30	5	2630	LHG	O4-P-O5	4.42	133.01	112.44
27	Y	1621	LUT	C15-C14-C13	-4.42	121.08	127.28
30	g	2630	LHG	O4-P-O5	4.42	133.00	112.44
25	4	601	CHL	C4D-ND-C1D	-4.42	101.87	105.22
39	c	519	DGD	O3G-C3G-C2G	-4.42	100.08	110.82
30	d	410	LHG	O4-P-O5	4.42	132.99	112.44
27	7	1621	LUT	C26-C27-C28	-4.41	117.71	124.58
30	D	410	LHG	O4-P-O5	4.41	132.97	112.44
27	n	1621	LUT	C15-C14-C13	-4.41	121.09	127.28
26	R	601	CLA	CBC-CAC-C3C	4.41	124.37	112.42
30	G	2630	LHG	O4-P-O5	4.41	132.96	112.44
25	n	607	CHL	CHA-C1A-C2A	-4.41	122.96	133.31
25	r	614	CHL	C1B-CHB-C4A	4.41	124.16	121.32
26	r	601	CLA	CBC-CAC-C3C	4.41	124.36	112.42
25	g	609	CHL	CBC-CAC-C3C	-4.40	106.57	112.87
28	2	1622	XAT	C15-C14-C13	-4.40	121.10	127.28
26	5	614	CLA	C4A-NA-C1A	4.40	108.69	106.68
31	C	517	BCR	C33-C5-C6	-4.40	119.68	124.48
27	y	1621	LUT	C15-C14-C13	-4.40	121.11	127.28
26	N	602	CLA	C4A-NA-C1A	4.39	108.68	106.68
28	y	1622	XAT	O4-C5-C4	4.39	117.60	113.49
30	C	2630	LHG	O4-P-O5	4.39	132.85	112.44
27	N	1621	LUT	C15-C14-C13	-4.39	121.13	127.28
28	Y	1622	XAT	O4-C5-C4	4.39	117.60	113.49
30	c	2630	LHG	O4-P-O5	4.38	132.84	112.44
29	G	1623	NEX	C15-C14-C13	-4.38	121.14	127.28
27	G	1621	LUT	C26-C27-C28	-4.38	117.77	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	g	1623	NEX	C15-C14-C13	-4.37	121.14	127.28
25	N	605	CHL	O2D-CGD-O1D	-4.37	115.34	123.85
29	S	1623	NEX	C27-C28-C29	-4.37	118.75	125.53
25	n	605	CHL	O2D-CGD-O1D	-4.37	115.34	123.85
26	1	614	CLA	C4A-NA-C1A	4.37	108.67	106.68
25	N	601	CHL	CBC-CAC-C3C	-4.37	106.62	112.87
26	C	508	CLA	O2D-CGD-CBD	4.37	118.86	111.23
26	B	604	CLA	C4A-NA-C1A	4.36	108.67	106.68
30	B	2630	LHG	O4-P-O5	4.36	132.74	112.44
29	s	1623	NEX	C27-C28-C29	-4.36	118.76	125.53
29	r	623	NEX	C35-C34-C33	-4.36	121.16	127.28
25	n	601	CHL	CBC-CAC-C3C	-4.36	106.63	112.87
27	g	1621	LUT	C26-C27-C28	-4.36	117.80	124.58
26	c	508	CLA	O2D-CGD-CBD	4.36	118.85	111.23
26	C	504	CLA	O2D-CGD-O1D	-4.36	115.37	123.85
26	c	504	CLA	O2D-CGD-O1D	-4.36	115.37	123.85
30	b	2630	LHG	O4-P-O5	4.36	132.71	112.44
27	Y	1621	LUT	C35-C34-C33	-4.35	121.17	127.28
29	R	623	NEX	C35-C34-C33	-4.35	121.17	127.28
31	B	619	BCR	C11-C10-C9	-4.35	121.18	127.28
30	2	2630	LHG	O4-P-O5	4.35	132.67	112.44
30	6	2630	LHG	O4-P-O5	4.35	132.67	112.44
28	1	1622	XAT	C11-C10-C9	-4.34	121.19	127.28
31	b	619	BCR	C11-C10-C9	-4.34	121.19	127.28
28	7	1622	XAT	C15-C35-C34	-4.34	114.64	123.52
28	3	1622	XAT	C15-C35-C34	-4.34	114.64	123.52
28	5	1622	XAT	C11-C10-C9	-4.34	121.20	127.28
30	B	2631	LHG	O4-P-O5	4.34	132.61	112.44
30	b	2631	LHG	O4-P-O5	4.34	132.61	112.44
25	4	601	CHL	CHA-C1A-C2A	-4.33	123.15	133.31
31	c	515	BCR	C11-C10-C9	-4.32	121.22	127.28
37	D	411	LMG	C1-C2-C3	-4.32	100.92	110.01
26	b	613	CLA	CMB-C2B-C1B	-4.32	118.84	125.42
26	y	604	CLA	CMB-C2B-C1B	-4.32	118.84	125.42
25	8	601	CHL	CHA-C1A-C2A	-4.31	123.18	133.31
26	b	604	CLA	C4A-NA-C1A	4.31	108.65	106.68
27	y	1621	LUT	C35-C34-C33	-4.31	121.23	127.28
26	4	602	CLA	O2D-CGD-O1D	-4.31	115.46	123.85
26	Y	604	CLA	CMB-C2B-C1B	-4.30	118.87	125.42
29	2	1623	NEX	C27-C28-C29	-4.30	118.86	125.53
29	6	1623	NEX	C27-C28-C29	-4.30	118.86	125.53
37	d	411	LMG	C1-C2-C3	-4.30	100.97	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	d	403	CLA	O2D-CGD-O1D	-4.30	115.48	123.85
31	C	515	BCR	C11-C10-C9	-4.30	121.25	127.28
30	7	2630	LHG	O4-P-O5	4.29	132.40	112.44
26	8	602	CLA	O2D-CGD-O1D	-4.28	115.51	123.85
30	3	2630	LHG	O4-P-O5	4.28	132.36	112.44
26	D	403	CLA	O2D-CGD-O1D	-4.28	115.51	123.85
26	B	613	CLA	CMB-C2B-C1B	-4.28	118.90	125.42
26	N	610	CLA	C4A-NA-C1A	4.28	108.63	106.68
26	n	610	CLA	C4A-NA-C1A	4.28	108.63	106.68
31	C	516	BCR	C28-C27-C26	-4.28	106.43	114.06
29	S	1623	NEX	C15-C14-C13	-4.27	121.30	127.28
36	B	623	SQD	C1-O5-C5	4.25	122.03	113.72
29	Y	1623	NEX	C2-C1-C6	4.25	113.34	109.21
31	b	620	BCR	C16-C17-C18	-4.25	121.32	127.28
26	4	604	CLA	C4A-NA-C1A	4.25	108.62	106.68
31	B	620	BCR	C16-C17-C18	-4.25	121.32	127.28
29	y	1623	NEX	C2-C1-C6	4.25	113.34	109.21
31	c	516	BCR	C28-C27-C26	-4.25	106.48	114.06
29	s	1623	NEX	C15-C14-C13	-4.25	121.32	127.28
26	3	604	CLA	C4A-NA-C1A	4.25	108.62	106.68
28	G	1622	XAT	C4-C3-C2	-4.24	102.85	110.79
31	t	101	BCR	C15-C14-C13	-4.24	121.33	127.28
31	T	101	BCR	C15-C14-C13	-4.24	121.33	127.28
36	b	623	SQD	O47-C7-C8	4.24	120.65	111.48
36	b	623	SQD	C1-O5-C5	4.23	121.99	113.72
31	A	411	BCR	C7-C8-C9	-4.23	119.97	126.23
28	1	1622	XAT	O4-C5-C18	4.23	119.78	115.05
36	B	623	SQD	O47-C7-C8	4.23	120.63	111.48
28	5	1622	XAT	O4-C5-C18	4.23	119.77	115.05
25	G	605	CHL	O2D-CGD-O1D	-4.22	115.63	123.85
25	g	605	CHL	O2D-CGD-O1D	-4.22	115.64	123.85
29	6	1623	NEX	C11-C10-C9	-4.21	121.37	127.28
28	g	1622	XAT	C4-C3-C2	-4.21	102.91	110.79
36	b	621	SQD	O47-C7-C8	4.20	120.58	111.48
29	2	1623	NEX	C11-C10-C9	-4.20	121.39	127.28
26	7	604	CLA	C4A-NA-C1A	4.20	108.59	106.68
36	B	621	SQD	O47-C7-C8	4.20	120.56	111.48
27	G	1621	LUT	C35-C34-C33	-4.20	121.39	127.28
26	R	604	CLA	O2D-CGD-CBD	4.19	118.56	111.23
31	a	411	BCR	C7-C8-C9	-4.19	120.03	126.23
27	g	1621	LUT	C35-C34-C33	-4.18	121.41	127.28
26	8	604	CLA	C4A-NA-C1A	4.18	108.59	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	1	1621	LUT	C15-C14-C13	-4.18	121.41	127.28
26	r	604	CLA	O2D-CGD-CBD	4.18	118.54	111.23
26	G	604	CLA	CMB-C2B-C1B	-4.18	119.06	125.42
26	g	604	CLA	CMB-C2B-C1B	-4.17	119.06	125.42
26	s	614	CLA	O2D-CGD-O1D	-4.16	115.75	123.85
27	5	1621	LUT	C15-C14-C13	-4.16	121.44	127.28
27	2	1620	LUT	C35-C15-C14	-4.16	115.02	123.52
26	S	610	CLA	C4A-NA-C1A	4.15	108.57	106.68
26	G	612	CLA	C4A-NA-C1A	4.14	108.57	106.68
25	7	607	CHL	CHA-C1A-C2A	-4.14	123.58	133.31
28	r	622	XAT	C15-C14-C13	-4.14	121.47	127.28
26	g	612	CLA	C4A-NA-C1A	4.14	108.57	106.68
26	S	614	CLA	O2D-CGD-O1D	-4.14	115.79	123.85
31	c	515	BCR	C16-C17-C18	-4.13	121.48	127.28
27	2	1621	LUT	C15-C14-C13	-4.13	121.48	127.28
27	6	1620	LUT	C35-C15-C14	-4.13	115.06	123.52
31	D	404	BCR	C11-C10-C9	-4.13	121.49	127.28
31	d	404	BCR	C11-C10-C9	-4.13	121.49	127.28
25	3	607	CHL	CHA-C1A-C2A	-4.12	123.64	133.31
28	R	622	XAT	C15-C14-C13	-4.12	121.50	127.28
31	C	515	BCR	C16-C17-C18	-4.12	121.51	127.28
36	A	418	SQD	O9-S-O7	-4.11	100.44	113.82
36	a	418	SQD	O9-S-O7	-4.11	100.44	113.82
27	6	1621	LUT	C15-C14-C13	-4.11	121.51	127.28
27	s	1620	LUT	C26-C27-C28	-4.09	118.21	124.58
36	b	623	SQD	O9-S-O7	-4.09	100.52	113.82
26	5	612	CLA	C4A-NA-C1A	4.09	108.54	106.68
36	B	623	SQD	O9-S-O7	-4.08	100.54	113.82
26	s	610	CLA	C4A-NA-C1A	4.08	108.54	106.68
26	y	614	CLA	O2D-CGD-O1D	-4.08	115.91	123.85
27	r	620	LUT	C30-C31-C32	-4.07	111.41	123.20
31	d	404	BCR	C24-C23-C22	-4.07	120.21	126.23
27	R	620	LUT	C30-C31-C32	-4.07	111.41	123.20
31	D	404	BCR	C24-C23-C22	-4.06	120.22	126.23
26	b	609	CLA	CMB-C2B-C1B	-4.06	119.24	125.42
27	S	1620	LUT	C26-C27-C28	-4.06	118.26	124.58
29	R	623	NEX	C26-C27-C28	-4.06	117.41	125.99
29	r	623	NEX	C26-C27-C28	-4.06	117.41	125.99
26	Y	614	CLA	O2D-CGD-O1D	-4.06	115.95	123.85
26	1	611	CLA	C4A-NA-C1A	4.05	108.53	106.68
26	5	611	CLA	C4A-NA-C1A	4.05	108.53	106.68
27	y	1621	LUT	C26-C27-C28	-4.05	118.27	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	609	CLA	CMB-C2B-C1B	-4.05	119.25	125.42
39	C	520	DGD	O3G-C3G-C2G	-4.05	100.97	110.82
26	2	613	CLA	C4A-NA-C1A	4.04	108.52	106.68
26	b	615	CLA	O2D-CGD-O1D	-4.04	115.98	123.85
39	c	520	DGD	O3G-C3G-C2G	-4.04	100.99	110.82
26	1	612	CLA	C4A-NA-C1A	4.03	108.52	106.68
27	Y	1621	LUT	C26-C27-C28	-4.03	118.31	124.58
27	1	1620	LUT	C30-C31-C32	-4.03	111.53	123.20
25	2	609	CHL	CBC-CAC-C3C	-4.02	107.11	112.87
28	3	1622	XAT	C27-C28-C29	-4.02	119.30	125.53
28	7	1622	XAT	C27-C28-C29	-4.02	119.30	125.53
27	5	1620	LUT	C30-C31-C32	-4.01	111.57	123.20
28	N	1622	XAT	C11-C10-C9	-4.01	121.65	127.28
26	B	615	CLA	O2D-CGD-O1D	-4.01	116.05	123.85
26	b	605	CLA	C1D-ND-C4D	4.01	109.12	106.31
28	G	1622	XAT	O24-C25-C38	4.01	119.52	115.05
31	H	101	BCR	C15-C14-C13	-4.00	121.66	127.28
31	h	101	BCR	C15-C14-C13	-4.00	121.66	127.28
28	y	1622	XAT	C10-C11-C12	-4.00	111.60	123.20
36	a	418	SQD	O7-S-C6	4.00	112.73	106.76
28	Y	1622	XAT	C10-C11-C12	-4.00	111.62	123.20
25	6	609	CHL	CBC-CAC-C3C	-3.99	107.16	112.87
26	D	402	CLA	CAA-CBA-CGA	-3.99	101.87	113.21
26	b	605	CLA	C2D-C1D-ND	-3.99	106.18	110.13
26	d	402	CLA	CAA-CBA-CGA	-3.99	101.89	113.21
28	n	1622	XAT	C11-C10-C9	-3.98	121.69	127.28
26	B	605	CLA	C1D-ND-C4D	3.98	109.11	106.31
28	g	1622	XAT	O24-C25-C38	3.98	119.49	115.05
36	A	418	SQD	O7-S-C6	3.97	112.69	106.76
26	B	605	CLA	C2D-C1D-ND	-3.97	106.19	110.13
26	B	612	CLA	CMB-C2B-C1B	-3.97	119.37	125.42
29	N	1623	NEX	C17-C1-C6	-3.97	106.92	110.47
27	N	1620	LUT	C35-C34-C33	-3.97	121.71	127.28
31	H	101	BCR	C7-C8-C9	-3.97	120.36	126.23
28	G	1622	XAT	C10-C11-C12	-3.97	111.70	123.20
26	a	410	CLA	O2D-CGD-O1D	-3.97	116.12	123.85
31	h	101	BCR	C7-C8-C9	-3.97	120.37	126.23
36	b	621	SQD	O9-S-O7	-3.96	100.94	113.82
26	b	612	CLA	CMB-C2B-C1B	-3.96	119.39	125.42
27	6	1621	LUT	C26-C27-C28	-3.96	118.42	124.58
27	2	1621	LUT	C26-C27-C28	-3.96	118.42	124.58
28	g	1622	XAT	C10-C11-C12	-3.95	111.74	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	410	CLA	O2D-CGD-O1D	-3.95	116.15	123.85
27	n	1620	LUT	C35-C34-C33	-3.95	121.74	127.28
36	B	621	SQD	O9-S-O7	-3.95	100.98	113.82
29	2	1623	NEX	O24-C25-C38	3.95	119.46	115.05
31	c	517	BCR	C16-C17-C18	-3.95	121.74	127.28
29	g	1623	NEX	O24-C25-C38	3.95	119.46	115.05
28	Y	1622	XAT	C27-C28-C29	-3.94	119.42	125.53
28	y	1622	XAT	C27-C28-C29	-3.93	119.42	125.53
28	8	622	XAT	C35-C34-C33	-3.93	121.76	127.28
29	n	1623	NEX	C17-C1-C6	-3.93	106.95	110.47
26	C	504	CLA	CMB-C2B-C1B	-3.93	119.44	125.42
31	B	620	BCR	C11-C10-C9	-3.93	121.77	127.28
31	b	620	BCR	C11-C10-C9	-3.93	121.77	127.28
31	T	101	BCR	C33-C5-C6	-3.93	120.20	124.48
27	N	1621	LUT	C10-C11-C12	-3.93	111.83	123.20
25	4	601	CHL	C1B-CHB-C4A	-3.93	118.80	121.32
28	4	622	XAT	C35-C34-C33	-3.93	121.77	127.28
38	d	405	PL9	C7-C3-C2	-3.92	118.77	123.39
27	n	1621	LUT	C10-C11-C12	-3.92	111.84	123.20
29	G	1623	NEX	O24-C25-C38	3.92	119.43	115.05
38	D	405	PL9	C7-C3-C2	-3.92	118.77	123.39
31	C	517	BCR	C16-C17-C18	-3.92	121.78	127.28
25	8	601	CHL	C1B-CHB-C4A	-3.92	118.80	121.32
26	6	613	CLA	C4A-NA-C1A	3.91	108.47	106.68
31	C	514	BCR	C10-C11-C12	-3.91	111.86	123.20
26	c	504	CLA	CMB-C2B-C1B	-3.91	119.46	125.42
28	y	1622	XAT	C35-C34-C33	-3.91	121.79	127.28
28	g	1622	XAT	C18-C5-C6	-3.91	115.86	122.30
28	G	1622	XAT	C18-C5-C6	-3.91	115.87	122.30
29	6	1623	NEX	O24-C25-C38	3.91	119.42	115.05
26	C	505	CLA	O2D-CGD-O1D	-3.91	116.25	123.85
26	C	506	CLA	CMB-C2B-C1B	-3.90	119.47	125.42
35	A	408	PHO	C2B-C1B-NB	-3.90	106.61	109.43
31	c	514	BCR	C10-C11-C12	-3.90	111.89	123.20
25	r	608	CHL	O1D-CGD-CBD	-3.89	118.82	124.72
27	1	1621	LUT	C26-C27-C28	-3.89	118.52	124.58
25	R	608	CHL	O1D-CGD-CBD	-3.89	118.82	124.72
26	N	602	CLA	CMB-C2B-C1B	-3.89	119.50	125.42
26	n	602	CLA	CMB-C2B-C1B	-3.89	119.50	125.42
26	c	506	CLA	CMB-C2B-C1B	-3.89	119.50	125.42
31	c	516	BCR	C20-C21-C22	-3.89	121.83	127.28
28	Y	1622	XAT	C35-C34-C33	-3.89	121.83	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	3	1621	LUT	C15-C14-C13	-3.89	121.83	127.28
27	7	1621	LUT	C15-C14-C13	-3.89	121.83	127.28
26	c	505	CLA	O2D-CGD-O1D	-3.88	116.29	123.85
26	Y	611	CLA	O2D-CGD-O1D	-3.88	116.29	123.85
31	t	101	BCR	C33-C5-C6	-3.88	120.25	124.48
27	S	1620	LUT	C35-C15-C14	-3.88	115.59	123.52
27	s	1620	LUT	C35-C15-C14	-3.87	115.59	123.52
26	s	612	CLA	CMB-C2B-C1B	-3.87	119.52	125.42
26	B	605	CLA	CBC-CAC-C3C	3.87	122.92	112.42
27	Y	1620	LUT	C10-C11-C12	-3.87	111.98	123.20
27	y	1620	LUT	C10-C11-C12	-3.87	111.99	123.20
27	5	1621	LUT	C26-C27-C28	-3.87	118.56	124.58
26	3	614	CLA	C4A-NA-C1A	3.86	108.44	106.68
26	N	604	CLA	O2D-CGD-O1D	-3.86	116.33	123.85
26	S	612	CLA	CMB-C2B-C1B	-3.86	119.54	125.42
26	N	613	CLA	O2D-CGD-CBD	3.86	117.98	111.23
25	3	607	CHL	C4D-ND-C1D	-3.86	102.29	105.22
27	3	1620	LUT	C10-C11-C12	-3.86	112.01	123.20
31	b	620	BCR	C15-C14-C13	-3.86	121.86	127.28
27	7	1620	LUT	C10-C11-C12	-3.86	112.02	123.20
36	a	412	SQD	O9-S-C6	3.86	112.51	106.76
31	B	620	BCR	C15-C14-C13	-3.86	121.87	127.28
25	6	601	CHL	CBC-CAC-C3C	-3.85	107.35	112.87
26	b	605	CLA	CBC-CAC-C3C	3.85	122.87	112.42
31	C	516	BCR	C20-C21-C22	-3.85	121.87	127.28
26	y	611	CLA	O2D-CGD-O1D	-3.85	116.35	123.85
25	7	607	CHL	C4D-ND-C1D	-3.85	102.30	105.22
25	2	601	CHL	CBC-CAC-C3C	-3.85	107.36	112.87
28	n	1622	XAT	C18-C5-C6	-3.85	115.96	122.30
35	a	408	PHO	C2B-C1B-NB	-3.85	106.65	109.43
26	b	613	CLA	CMD-C2D-C1D	-3.85	117.95	124.73
36	A	412	SQD	O9-S-C6	3.85	112.50	106.76
26	S	602	CLA	C4A-NA-C1A	3.85	108.43	106.68
28	N	1622	XAT	C18-C5-C6	-3.85	115.97	122.30
26	n	604	CLA	O2D-CGD-O1D	-3.85	116.36	123.85
29	5	1623	NEX	O24-C25-C38	3.84	119.34	115.05
25	r	607	CHL	C1C-CHC-C4B	3.84	129.81	116.07
26	n	613	CLA	O2D-CGD-CBD	3.84	117.94	111.23
26	B	613	CLA	CMD-C2D-C1D	-3.84	117.97	124.73
25	R	607	CHL	C1C-CHC-C4B	3.84	129.79	116.07
26	2	614	CLA	C4A-NA-C1A	3.84	108.43	106.68
26	6	614	CLA	C4A-NA-C1A	3.84	108.43	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A	414	PL9	C7-C3-C2	-3.83	118.87	123.39
26	7	614	CLA	C4A-NA-C1A	3.83	108.43	106.68
29	G	1623	NEX	C35-C34-C33	-3.83	121.91	127.28
38	a	414	PL9	C7-C3-C2	-3.83	118.88	123.39
29	g	1623	NEX	C35-C34-C33	-3.83	121.91	127.28
28	n	1622	XAT	O4-C5-C18	3.83	119.32	115.05
28	N	1622	XAT	O4-C5-C18	3.83	119.32	115.05
36	A	412	SQD	O9-S-O7	-3.82	101.38	113.82
39	C	518	DGD	O6D-C1D-O3G	-3.82	101.02	110.04
29	1	1623	NEX	O24-C25-C38	3.82	119.32	115.05
27	G	1620	LUT	C35-C34-C33	-3.82	121.92	127.28
36	a	412	SQD	O9-S-O7	-3.82	101.40	113.82
28	3	1622	XAT	C26-C27-C28	-3.82	117.92	125.99
26	b	613	CLA	O2D-CGD-O1D	-3.81	116.42	123.85
31	C	514	BCR	C20-C21-C22	-3.81	121.93	127.28
31	C	514	BCR	C15-C16-C17	-3.81	115.72	123.52
29	Y	1623	NEX	O24-C25-C38	3.81	119.31	115.05
39	c	518	DGD	O6D-C1D-O3G	-3.81	101.05	110.04
25	y	608	CHL	C1C-CHC-C4B	3.81	129.69	116.07
27	G	1621	LUT	C10-C11-C12	-3.81	112.17	123.20
25	Y	608	CHL	C1C-CHC-C4B	3.80	129.68	116.07
27	g	1621	LUT	C10-C11-C12	-3.80	112.18	123.20
28	3	1622	XAT	O4-C5-C18	3.80	119.30	115.05
26	s	602	CLA	C4A-NA-C1A	3.80	108.41	106.68
31	T	101	BCR	C28-C27-C26	-3.80	107.28	114.06
28	7	1622	XAT	C26-C27-C28	-3.80	117.96	125.99
31	c	514	BCR	C15-C16-C17	-3.80	115.75	123.52
25	N	608	CHL	C1C-CHC-C4B	3.80	129.66	116.07
31	c	514	BCR	C20-C21-C22	-3.80	121.95	127.28
39	C	520	DGD	O6D-C1D-O3G	-3.79	101.08	110.04
31	C	516	BCR	C33-C5-C6	-3.79	120.34	124.48
26	B	606	CLA	O2D-CGD-O1D	-3.79	116.47	123.85
26	B	613	CLA	O2D-CGD-O1D	-3.79	116.47	123.85
25	n	608	CHL	C1C-CHC-C4B	3.79	129.63	116.07
29	y	1623	NEX	O24-C25-C38	3.79	119.28	115.05
39	c	520	DGD	O6D-C1D-O3G	-3.78	101.11	110.04
36	b	621	SQD	C4-C3-C2	3.78	117.47	110.83
27	g	1620	LUT	C35-C34-C33	-3.78	121.98	127.28
28	7	1622	XAT	C4-C3-C2	-3.78	103.72	110.79
27	6	1620	LUT	C30-C31-C32	-3.78	112.26	123.20
31	t	101	BCR	C28-C27-C26	-3.78	107.32	114.06
26	b	606	CLA	O2D-CGD-O1D	-3.77	116.50	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	7	1622	XAT	O4-C5-C18	3.77	119.26	115.05
31	c	516	BCR	C33-C5-C6	-3.77	120.37	124.48
27	2	1620	LUT	C30-C31-C32	-3.77	112.28	123.20
26	C	509	CLA	O2D-CGD-O1D	-3.76	116.53	123.85
28	3	1622	XAT	C4-C3-C2	-3.76	103.75	110.79
36	B	621	SQD	C4-C3-C2	3.76	117.43	110.83
31	D	404	BCR	C16-C17-C18	-3.76	122.01	127.28
27	4	620	LUT	C7-C8-C9	-3.76	120.68	126.23
26	c	512	CLA	O2D-CGD-O1D	-3.75	116.55	123.85
31	a	411	BCR	C15-C14-C13	-3.75	122.02	127.28
26	c	509	CLA	O2D-CGD-O1D	-3.75	116.55	123.85
31	d	404	BCR	C16-C17-C18	-3.74	122.03	127.28
28	5	1622	XAT	O24-C25-C38	3.74	119.23	115.05
27	4	620	LUT	C15-C14-C13	-3.74	122.03	127.28
26	B	605	CLA	CAA-C2A-C1A	3.74	124.23	111.97
27	8	620	LUT	C7-C8-C9	-3.74	120.70	126.23
26	G	611	CLA	O2D-CGD-O1D	-3.73	116.58	123.85
26	C	512	CLA	O2D-CGD-O1D	-3.73	116.58	123.85
31	A	411	BCR	C15-C14-C13	-3.73	122.05	127.28
36	A	418	SQD	C45-O47-C7	3.73	126.72	117.80
26	g	611	CLA	O2D-CGD-O1D	-3.73	116.59	123.85
36	a	418	SQD	C45-O47-C7	3.73	126.72	117.80
27	3	1620	LUT	C35-C34-C33	-3.73	122.05	127.28
26	b	605	CLA	CAA-C2A-C1A	3.73	124.18	111.97
27	N	1620	LUT	C35-C15-C14	-3.72	115.91	123.52
26	B	605	CLA	CAA-CBA-CGA	-3.72	102.65	113.21
28	5	1622	XAT	C27-C28-C29	-3.72	119.76	125.53
28	N	1622	XAT	C4-C3-C2	-3.72	103.84	110.79
29	g	1623	NEX	C27-C28-C29	-3.71	119.77	125.53
28	1	1622	XAT	O24-C25-C38	3.71	119.20	115.05
27	5	1620	LUT	C10-C11-C12	-3.71	112.44	123.20
27	7	1620	LUT	C35-C34-C33	-3.71	122.07	127.28
26	b	605	CLA	CAA-CBA-CGA	-3.71	102.67	113.21
27	3	1620	LUT	C15-C14-C13	-3.71	122.08	127.28
28	6	1622	XAT	C11-C10-C9	-3.71	122.08	127.28
27	8	620	LUT	C15-C14-C13	-3.71	122.08	127.28
28	2	1622	XAT	C11-C10-C9	-3.71	122.08	127.28
28	n	1622	XAT	C4-C3-C2	-3.71	103.86	110.79
27	2	1621	LUT	C35-C34-C33	-3.71	122.08	127.28
27	6	1621	LUT	C35-C34-C33	-3.71	122.08	127.28
36	a	412	SQD	O47-C7-C8	3.70	119.50	111.48
27	1	1620	LUT	C10-C11-C12	-3.70	112.47	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	n	1620	LUT	C35-C15-C14	-3.70	115.94	123.52
26	c	501	CLA	O2D-CGD-O1D	-3.70	116.64	123.85
26	c	513	CLA	O2D-CGD-O1D	-3.70	116.64	123.85
28	1	1622	XAT	C27-C28-C29	-3.70	119.79	125.53
36	A	412	SQD	O47-C7-C8	3.70	119.48	111.48
29	G	1623	NEX	C27-C28-C29	-3.70	119.80	125.53
26	d	403	CLA	O2D-CGD-CBD	3.69	117.69	111.23
26	C	501	CLA	O2D-CGD-O1D	-3.69	116.66	123.85
27	7	1620	LUT	C15-C14-C13	-3.69	122.10	127.28
29	6	1623	NEX	C31-C30-C29	-3.69	122.11	127.28
26	g	602	CLA	C1-C2-C3	-3.69	120.16	126.20
26	C	513	CLA	O2D-CGD-O1D	-3.69	116.67	123.85
26	G	602	CLA	C1-C2-C3	-3.68	120.16	126.20
28	N	1622	XAT	C10-C11-C12	-3.68	112.54	123.20
29	2	1623	NEX	C31-C30-C29	-3.68	122.12	127.28
28	n	1622	XAT	C10-C11-C12	-3.68	112.55	123.20
26	D	403	CLA	O2D-CGD-CBD	3.68	117.66	111.23
31	A	411	BCR	C20-C21-C22	-3.67	122.13	127.28
31	A	411	BCR	C16-C17-C18	-3.67	122.13	127.28
25	G	601	CHL	CBC-CAC-C3C	-3.67	107.62	112.87
25	g	601	CHL	CBC-CAC-C3C	-3.66	107.63	112.87
26	b	603	CLA	O2D-CGD-O1D	-3.66	116.72	123.85
31	a	411	BCR	C20-C21-C22	-3.66	122.14	127.28
31	a	411	BCR	C16-C17-C18	-3.66	122.14	127.28
37	A	413	LMG	O6-C1-O1	-3.66	101.41	110.04
31	c	517	BCR	C15-C16-C17	-3.66	116.04	123.52
31	a	411	BCR	C11-C10-C9	-3.66	122.15	127.28
31	C	517	BCR	C15-C16-C17	-3.65	116.05	123.52
31	c	514	BCR	C16-C17-C18	-3.65	122.16	127.28
37	a	413	LMG	O6-C1-O1	-3.65	101.43	110.04
31	A	411	BCR	C11-C10-C9	-3.65	122.17	127.28
29	1	1623	NEX	C15-C14-C13	-3.64	122.17	127.28
26	B	603	CLA	O2D-CGD-O1D	-3.64	116.76	123.85
31	C	514	BCR	C16-C17-C18	-3.64	122.17	127.28
26	B	605	CLA	CHB-C4A-NA	3.64	129.65	124.40
29	5	1623	NEX	C15-C14-C13	-3.63	122.19	127.28
27	g	1621	LUT	C7-C8-C9	-3.63	120.87	126.23
26	Y	611	CLA	C3B-C4B-NB	-3.63	107.29	110.53
25	G	608	CHL	C1C-CHC-C4B	3.62	129.03	116.07
26	B	607	CLA	O2D-CGD-O1D	-3.62	116.80	123.85
25	g	608	CHL	C1C-CHC-C4B	3.62	129.02	116.07
26	R	603	CLA	O2D-CGD-O1D	-3.62	116.80	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	G	1620	LUT	C15-C14-C13	-3.62	122.20	127.28
26	b	605	CLA	CHB-C4A-NA	3.62	129.62	124.40
35	a	409	PHO	C3B-C4B-NB	-3.61	105.11	107.46
27	G	1621	LUT	C7-C8-C9	-3.61	120.89	126.23
26	b	607	CLA	O2D-CGD-O1D	-3.61	116.82	123.85
31	B	619	BCR	C16-C17-C18	-3.61	122.21	127.28
31	b	619	BCR	C16-C17-C18	-3.61	122.21	127.28
26	B	604	CLA	O2D-CGD-O1D	-3.61	116.83	123.85
25	s	606	CHL	C3D-C4D-ND	3.61	118.72	112.94
25	S	606	CHL	C3D-C4D-ND	3.60	118.72	112.94
26	r	603	CLA	O2D-CGD-O1D	-3.60	116.83	123.85
39	h	102	DGD	O3G-C3G-C2G	-3.60	102.06	110.82
27	S	1620	LUT	C15-C14-C13	-3.60	122.24	127.28
26	b	604	CLA	O2D-CGD-O1D	-3.59	116.85	123.85
26	y	611	CLA	C3B-C4B-NB	-3.59	107.32	110.53
27	s	1620	LUT	C15-C14-C13	-3.59	122.24	127.28
25	R	608	CHL	C1C-CHC-C4B	3.59	128.91	116.07
25	r	608	CHL	C1C-CHC-C4B	3.59	128.91	116.07
39	H	102	DGD	O3G-C3G-C2G	-3.58	102.10	110.82
27	N	1621	LUT	C16-C1-C6	-3.58	104.63	110.24
27	g	1620	LUT	C15-C14-C13	-3.58	122.26	127.28
26	C	505	CLA	O2D-CGD-CBD	3.58	117.49	111.23
27	3	1620	LUT	C30-C31-C32	-3.58	112.84	123.20
26	B	611	CLA	O2D-CGD-O1D	-3.58	116.89	123.85
27	7	1620	LUT	C30-C31-C32	-3.57	112.85	123.20
25	S	608	CHL	C1B-CHB-C4A	3.57	123.62	121.32
26	c	505	CLA	O2D-CGD-CBD	3.57	117.47	111.23
27	n	1621	LUT	C16-C1-C6	-3.57	104.65	110.24
26	b	611	CLA	O2D-CGD-O1D	-3.57	116.91	123.85
36	B	621	SQD	O6-C1-C2	3.56	113.69	108.27
28	8	622	XAT	O24-C25-C38	3.56	119.03	115.05
35	A	409	PHO	C3B-C4B-NB	-3.56	105.14	107.46
26	C	513	CLA	CAA-C2A-C3A	-3.56	103.37	113.00
27	S	1621	LUT	C30-C31-C32	-3.56	112.89	123.20
27	g	1620	LUT	C10-C11-C12	-3.56	112.89	123.20
25	G	609	CHL	C1C-CHC-C4B	3.56	128.80	116.07
28	4	622	XAT	O24-C25-C38	3.56	119.02	115.05
27	s	1621	LUT	C30-C31-C32	-3.55	112.90	123.20
36	b	621	SQD	O6-C1-C2	3.55	113.67	108.27
26	4	602	CLA	O2D-CGD-CBD	3.55	117.44	111.23
29	g	1623	NEX	C31-C30-C29	-3.55	122.30	127.28
26	c	513	CLA	CAA-C2A-C3A	-3.55	103.41	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	r	620	LUT	C35-C15-C14	-3.55	116.26	123.52
25	g	609	CHL	C1C-CHC-C4B	3.55	128.77	116.07
27	r	620	LUT	C35-C34-C33	-3.55	122.30	127.28
27	G	1620	LUT	C10-C11-C12	-3.54	112.93	123.20
28	R	622	XAT	C10-C11-C12	-3.54	112.93	123.20
28	y	1622	XAT	C4-C3-C2	-3.54	104.17	110.79
28	r	622	XAT	C10-C11-C12	-3.54	112.94	123.20
27	R	620	LUT	C35-C15-C14	-3.54	116.28	123.52
28	Y	1622	XAT	C4-C3-C2	-3.53	104.18	110.79
29	G	1623	NEX	C31-C30-C29	-3.53	122.33	127.28
38	a	414	PL9	C7-C3-C4	3.53	121.79	117.88
26	8	602	CLA	O2D-CGD-CBD	3.53	117.39	111.23
31	b	619	BCR	C28-C27-C26	-3.53	107.77	114.06
26	s	604	CLA	CHB-C4A-NA	3.52	129.49	124.40
31	B	619	BCR	C28-C27-C26	-3.52	107.77	114.06
31	B	620	BCR	C28-C27-C26	-3.52	107.77	114.06
26	B	605	CLA	CAC-C3C-C4C	3.52	129.37	124.79
27	N	1621	LUT	C7-C8-C9	-3.52	121.03	126.23
26	C	502	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
26	c	502	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
26	r	602	CLA	O2D-CGD-O1D	-3.51	117.01	123.85
26	S	604	CLA	CHB-C4A-NA	3.51	129.47	124.40
36	B	621	SQD	O9-S-C6	3.51	112.00	106.76
26	n	614	CLA	CMB-C2B-C1B	-3.51	120.07	125.42
26	R	610	CLA	C4A-NA-C1A	3.51	108.28	106.68
36	a	412	SQD	C4-C3-C2	3.51	116.99	110.83
27	R	620	LUT	C35-C34-C33	-3.51	122.36	127.28
26	1	604	CLA	CMB-C2B-C1B	-3.51	120.08	125.42
31	b	620	BCR	C28-C27-C26	-3.50	107.81	114.06
26	b	605	CLA	CAC-C3C-C4C	3.50	129.35	124.79
26	R	602	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
28	n	1622	XAT	C35-C34-C33	-3.50	122.37	127.28
36	b	621	SQD	O9-S-C6	3.50	111.98	106.76
25	S	608	CHL	C1C-CHC-C4B	3.50	128.58	116.07
26	N	614	CLA	CMB-C2B-C1B	-3.50	120.10	125.42
26	5	604	CLA	CMB-C2B-C1B	-3.50	120.10	125.42
25	s	608	CHL	C1C-CHC-C4B	3.49	128.57	116.07
29	r	623	NEX	C15-C35-C34	-3.49	116.37	123.52
29	R	623	NEX	C15-C35-C34	-3.49	116.38	123.52
26	R	603	CLA	CMB-C2B-C1B	-3.49	120.10	125.42
38	A	414	PL9	C7-C3-C4	3.49	121.74	117.88
27	n	1621	LUT	C7-C8-C9	-3.49	121.08	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	613	CLA	CHB-C4A-NA	3.49	129.43	124.40
36	A	412	SQD	C4-C3-C2	3.48	116.94	110.83
26	G	610	CLA	C4A-NA-C1A	3.48	108.27	106.68
26	r	603	CLA	CMB-C2B-C1B	-3.48	120.12	125.42
25	s	608	CHL	C1B-CHB-C4A	3.48	123.56	121.32
27	s	1621	LUT	C35-C15-C14	-3.48	116.41	123.52
31	B	620	BCR	C1-C6-C5	-3.47	117.89	122.64
31	b	620	BCR	C1-C6-C5	-3.47	117.89	122.64
28	N	1622	XAT	C35-C34-C33	-3.47	122.41	127.28
26	r	610	CLA	C4A-NA-C1A	3.47	108.26	106.68
26	C	509	CLA	CMB-C2B-C1B	-3.47	120.14	125.42
26	c	509	CLA	CMB-C2B-C1B	-3.47	120.14	125.42
26	C	507	CLA	CHB-C4A-NA	3.47	129.41	124.40
26	B	609	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
26	c	509	CLA	CHB-C4A-NA	3.47	129.40	124.40
25	7	606	CHL	OMC-CMC-C2C	-3.47	119.10	125.12
26	B	613	CLA	CHB-C4A-NA	3.46	129.40	124.40
26	y	604	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
25	3	606	CHL	OMC-CMC-C2C	-3.46	119.11	125.12
26	N	602	CLA	C1-C2-C3	-3.46	120.53	126.20
27	s	1621	LUT	C10-C11-C12	-3.46	113.17	123.20
27	S	1621	LUT	C35-C15-C14	-3.46	116.44	123.52
35	A	408	PHO	O1D-CGD-CBD	3.46	129.97	124.72
35	a	408	PHO	O1D-CGD-CBD	3.46	129.96	124.72
28	3	1622	XAT	C24-C23-C22	-3.45	104.33	110.79
26	b	611	CLA	CAA-CBA-CGA	-3.45	103.40	113.21
27	N	1620	LUT	C10-C11-C12	-3.45	113.20	123.20
27	S	1621	LUT	C10-C11-C12	-3.45	113.20	123.20
27	n	1620	LUT	C10-C11-C12	-3.45	113.20	123.20
26	n	602	CLA	C1-C2-C3	-3.45	120.54	126.20
27	1	1620	LUT	C35-C15-C14	-3.45	116.46	123.52
26	B	611	CLA	CAA-CBA-CGA	-3.45	103.42	113.21
26	b	609	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
26	b	616	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
39	B	626	DGD	O6D-C1D-O3G	-3.45	101.90	110.04
29	g	1623	NEX	C16-C1-C6	3.44	113.56	110.47
27	r	620	LUT	C10-C11-C12	-3.44	113.22	123.20
26	B	616	CLA	O2D-CGD-O1D	-3.44	117.15	123.85
25	1	607	CHL	CMA-C3A-C4A	-3.44	107.19	114.61
25	5	607	CHL	CMA-C3A-C4A	-3.44	107.19	114.61
29	G	1623	NEX	C16-C1-C6	3.44	113.55	110.47
25	n	601	CHL	C1C-CHC-C4B	3.44	128.38	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	509	CLA	CHB-C4A-NA	3.44	129.37	124.40
26	c	507	CLA	CHB-C4A-NA	3.44	129.37	124.40
26	a	410	CLA	O2D-CGD-CBD	3.44	117.24	111.23
27	5	1620	LUT	C35-C15-C14	-3.44	116.48	123.52
28	7	1622	XAT	C24-C23-C22	-3.44	104.36	110.79
25	N	601	CHL	C1C-CHC-C4B	3.44	128.37	116.07
25	S	606	CHL	O2D-CGD-O1D	-3.44	117.16	123.85
26	Y	604	CLA	O2D-CGD-O1D	-3.43	117.16	123.85
29	N	1623	NEX	C11-C10-C9	-3.43	122.47	127.28
25	Y	601	CHL	C1C-CHC-C4B	3.43	128.35	116.07
26	S	604	CLA	CMB-C2B-C1B	-3.43	120.19	125.42
31	b	619	BCR	C20-C21-C22	-3.43	122.47	127.28
26	1	604	CLA	C4A-NA-C1A	3.43	108.24	106.68
39	b	626	DGD	O6D-C1D-O3G	-3.43	101.94	110.04
27	R	620	LUT	C10-C11-C12	-3.43	113.27	123.20
25	y	601	CHL	C1C-CHC-C4B	3.43	128.33	116.07
25	8	601	CHL	CBC-CAC-C3C	-3.43	107.97	112.87
26	A	405	CLA	CMB-C2B-C1B	-3.43	120.20	125.42
31	B	619	BCR	C20-C21-C22	-3.42	122.48	127.28
26	s	604	CLA	CMB-C2B-C1B	-3.42	120.21	125.42
25	s	606	CHL	O2D-CGD-O1D	-3.42	117.18	123.85
36	A	412	SQD	O5-C5-C4	3.42	115.86	109.70
26	A	410	CLA	O2D-CGD-CBD	3.42	117.21	111.23
29	n	1623	NEX	C11-C10-C9	-3.42	122.48	127.28
26	a	405	CLA	CMB-C2B-C1B	-3.42	120.22	125.42
25	S	601	CHL	C3D-C4D-ND	3.41	118.42	112.94
25	g	606	CHL	CMB-C2B-C3B	3.41	131.50	124.68
27	5	1621	LUT	C35-C34-C33	-3.41	122.49	127.28
35	a	409	PHO	C2B-C1B-NB	-3.41	106.96	109.43
29	2	1623	NEX	C16-C1-C6	3.41	113.52	110.47
25	6	607	CHL	O1D-CGD-CBD	-3.41	119.55	124.72
25	s	601	CHL	C3D-C4D-ND	3.41	118.41	112.94
26	7	612	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
26	y	602	CLA	C1-C2-C3	-3.41	120.61	126.20
25	3	609	CHL	CBC-CAC-C3C	-3.41	108.00	112.87
26	C	509	CLA	O2D-CGD-CBD	3.41	117.19	111.23
25	4	601	CHL	CBC-CAC-C3C	-3.40	108.00	112.87
26	g	610	CLA	C4A-NA-C1A	3.40	108.23	106.68
26	3	612	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
28	Y	1622	XAT	C26-C27-C28	-3.40	118.80	125.99
28	y	1622	XAT	C26-C27-C28	-3.40	118.81	125.99
31	C	515	BCR	C15-C16-C17	-3.40	116.56	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	607	CHL	O1D-CGD-CBD	-3.40	119.57	124.72
27	1	1621	LUT	C35-C34-C33	-3.40	122.51	127.28
26	c	509	CLA	O2D-CGD-CBD	3.40	117.17	111.23
31	c	515	BCR	C15-C16-C17	-3.40	116.57	123.52
36	a	412	SQD	O5-C5-C4	3.40	115.82	109.70
26	r	612	CLA	C3B-C4B-NB	-3.40	107.50	110.53
25	G	606	CHL	CMB-C2B-C3B	3.39	131.47	124.68
29	3	1623	NEX	C24-C23-C22	-3.39	104.44	110.79
25	2	609	CHL	O1D-CGD-CBD	-3.39	119.58	124.72
27	n	1621	LUT	C26-C27-C28	-3.39	119.30	124.58
26	s	602	CLA	C3B-C4B-NB	-3.39	107.50	110.53
25	6	609	CHL	O1D-CGD-CBD	-3.39	119.58	124.72
25	Y	607	CHL	C1C-CHC-C4B	3.39	128.19	116.07
25	3	605	CHL	CBC-CAC-C3C	-3.39	108.03	112.87
25	y	601	CHL	CMD-C2D-C3D	-3.38	117.92	124.68
25	R	614	CHL	CMA-C3A-C4A	-3.38	107.32	114.61
26	G	603	CLA	CHB-C4A-NA	3.38	129.28	124.40
31	B	620	BCR	C24-C23-C22	-3.38	121.23	126.23
26	b	613	CLA	CMB-C2B-C3B	3.38	134.51	126.55
26	Y	602	CLA	C1-C2-C3	-3.38	120.66	126.20
27	N	1621	LUT	C26-C27-C28	-3.38	119.32	124.58
26	B	604	CLA	CMB-C2B-C1B	-3.38	120.27	125.42
27	Y	1620	LUT	C30-C31-C32	-3.38	113.40	123.20
26	a	406	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
25	7	609	CHL	CBC-CAC-C3C	-3.38	108.03	112.87
38	d	405	PL9	C7-C8-C9	-3.38	121.01	126.83
25	y	607	CHL	C1C-CHC-C4B	3.38	128.16	116.07
31	b	619	BCR	C8-C7-C6	-3.38	117.98	127.00
29	7	1623	NEX	C24-C23-C22	-3.38	104.47	110.79
25	Y	609	CHL	C1C-CHC-C4B	3.38	128.15	116.07
25	y	609	CHL	C1C-CHC-C4B	3.38	128.15	116.07
27	n	1621	LUT	C21-C26-C27	-3.38	108.94	112.83
31	b	620	BCR	C24-C23-C22	-3.37	121.24	126.23
25	Y	601	CHL	CMD-C2D-C3D	-3.37	117.94	124.68
39	C	519	DGD	O6D-C1D-O3G	-3.37	102.07	110.04
25	n	608	CHL	CBC-CAC-C3C	-3.37	108.04	112.87
25	r	614	CHL	CMA-C3A-C4A	-3.37	107.34	114.61
26	S	602	CLA	C3B-C4B-NB	-3.37	107.52	110.53
38	D	405	PL9	C7-C8-C9	-3.37	121.03	126.83
39	c	519	DGD	O6D-C1D-O3G	-3.37	102.08	110.04
35	A	409	PHO	C2B-C1B-NB	-3.37	107.00	109.43
26	r	610	CLA	O2D-CGD-O1D	-3.37	117.29	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	G	603	CLA	CAA-C2A-C3A	-3.37	103.90	113.00
26	g	603	CLA	CAA-C2A-C3A	-3.37	103.90	113.00
27	y	1620	LUT	C30-C31-C32	-3.37	113.44	123.20
26	5	604	CLA	C4A-NA-C1A	3.37	108.22	106.68
31	B	619	BCR	C8-C7-C6	-3.37	118.01	127.00
26	b	613	CLA	C3B-C4B-NB	-3.37	107.53	110.53
26	A	406	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
26	R	612	CLA	C3B-C4B-NB	-3.36	107.53	110.53
29	3	1623	NEX	C11-C12-C13	-3.36	117.14	126.36
25	7	605	CHL	CBC-CAC-C3C	-3.36	108.06	112.87
29	7	1623	NEX	C11-C12-C13	-3.36	117.15	126.36
26	B	613	CLA	CMB-C2B-C3B	3.36	134.45	126.55
26	g	603	CLA	CHB-C4A-NA	3.36	129.25	124.40
29	6	1623	NEX	C16-C1-C6	3.36	113.48	110.47
25	N	608	CHL	CBC-CAC-C3C	-3.36	108.07	112.87
25	3	601	CHL	C3D-C4D-ND	3.35	118.32	112.94
26	R	610	CLA	O2D-CGD-O1D	-3.35	117.32	123.85
26	b	604	CLA	CMB-C2B-C1B	-3.35	120.32	125.42
26	B	613	CLA	C3B-C4B-NB	-3.34	107.55	110.53
26	S	613	CLA	CMB-C2B-C1B	-3.34	120.33	125.42
26	s	613	CLA	CMB-C2B-C1B	-3.34	120.33	125.42
25	n	605	CHL	C1C-CHC-C4B	3.34	128.01	116.07
25	5	605	CHL	CBC-CAC-C3C	-3.34	108.10	112.87
27	8	620	LUT	C30-C31-C32	-3.34	113.53	123.20
25	N	609	CHL	C1C-CHC-C4B	3.34	128.00	116.07
27	4	620	LUT	C30-C31-C32	-3.33	113.54	123.20
25	1	608	CHL	C1C-CHC-C4B	3.33	128.00	116.07
26	G	602	CLA	CMB-C2B-C1B	-3.33	120.34	125.42
26	D	403	CLA	CMB-C2B-C1B	-3.33	120.34	125.42
26	D	402	CLA	CMB-C2B-C1B	-3.33	120.35	125.42
26	d	402	CLA	CMB-C2B-C1B	-3.33	120.35	125.42
27	s	1620	LUT	C21-C26-C27	-3.33	109.00	112.83
26	7	602	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
25	8	608	CHL	OMC-CMC-C2C	-3.33	119.34	125.12
27	N	1621	LUT	C21-C26-C27	-3.33	109.00	112.83
25	R	607	CHL	C4-C3-C5	3.33	121.00	115.23
25	N	605	CHL	C1C-CHC-C4B	3.33	127.97	116.07
27	4	620	LUT	C11-C10-C9	-3.32	122.62	127.28
25	5	608	CHL	C1C-CHC-C4B	3.32	127.96	116.07
26	7	603	CLA	CHB-C4A-NA	3.32	129.20	124.40
25	S	606	CHL	OMC-CMC-C2C	-3.32	119.35	125.12
25	1	605	CHL	CBC-CAC-C3C	-3.32	108.12	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	617	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
25	6	601	CHL	C1C-CHC-C4B	3.32	127.94	116.07
27	S	1620	LUT	C10-C11-C12	-3.32	113.59	123.20
25	n	609	CHL	C1C-CHC-C4B	3.32	127.94	116.07
25	2	601	CHL	C1C-CHC-C4B	3.32	127.94	116.07
25	2	608	CHL	C1C-CHC-C4B	3.32	127.93	116.07
26	g	602	CLA	CMB-C2B-C1B	-3.32	120.37	125.42
26	B	617	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
25	6	608	CHL	C1C-CHC-C4B	3.31	127.93	116.07
25	r	607	CHL	C4-C3-C5	3.31	120.98	115.23
25	7	608	CHL	C1C-CHC-C4B	3.31	127.92	116.07
26	C	510	CLA	CMB-C2B-C1B	-3.31	120.38	125.42
25	g	601	CHL	C1C-CHC-C4B	3.31	127.90	116.07
25	7	601	CHL	C3D-C4D-ND	3.31	118.24	112.94
27	Y	1620	LUT	C35-C15-C14	-3.31	116.75	123.52
28	4	622	XAT	C4-C3-C2	-3.31	104.61	110.79
28	8	622	XAT	C4-C3-C2	-3.31	104.61	110.79
27	8	620	LUT	C11-C10-C9	-3.31	122.64	127.28
28	5	1622	XAT	C35-C34-C33	-3.31	122.64	127.28
26	N	604	CLA	CHB-C1B-NB	3.31	129.01	124.05
26	6	611	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
25	s	606	CHL	OMC-CMC-C2C	-3.31	119.38	125.12
25	3	608	CHL	C1C-CHC-C4B	3.30	127.89	116.07
27	s	1620	LUT	C10-C11-C12	-3.30	113.62	123.20
25	4	606	CHL	CBC-CAC-C3C	-3.30	108.14	112.87
31	T	101	BCR	C1-C6-C7	3.30	124.61	115.65
25	4	608	CHL	OMC-CMC-C2C	-3.30	119.38	125.12
28	1	1622	XAT	C35-C34-C33	-3.30	122.65	127.28
26	N	603	CLA	CHB-C4A-NA	3.30	129.16	124.40
26	n	603	CLA	CHB-C4A-NA	3.30	129.16	124.40
26	r	611	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
26	d	403	CLA	CMB-C2B-C1B	-3.30	120.39	125.42
25	G	601	CHL	C1C-CHC-C4B	3.30	127.88	116.07
31	t	101	BCR	C1-C6-C7	3.30	124.60	115.65
25	8	606	CHL	CBC-CAC-C3C	-3.30	108.15	112.87
29	r	623	NEX	C31-C30-C29	-3.30	122.65	127.28
26	s	603	CLA	CHB-C4A-NA	3.30	129.16	124.40
25	N	601	CHL	C1-C2-C3	-3.29	120.80	126.20
25	y	601	CHL	C4-C3-C5	3.29	120.95	115.23
26	R	611	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
26	n	613	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
25	y	605	CHL	C1C-CHC-C4B	3.29	127.85	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	3	602	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
25	Y	605	CHL	C1C-CHC-C4B	3.29	127.85	116.07
25	G	608	CHL	C1-C2-C3	-3.29	120.80	126.20
27	Y	1620	LUT	C15-C14-C13	-3.29	122.66	127.28
26	N	613	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
28	6	1622	XAT	C27-C28-C29	-3.29	120.43	125.53
27	S	1620	LUT	C21-C26-C27	-3.29	109.05	112.83
26	g	611	CLA	CMB-C2B-C1B	-3.29	120.41	125.42
28	2	1622	XAT	C27-C28-C29	-3.29	120.43	125.53
25	n	601	CHL	C1-C2-C3	-3.29	120.81	126.20
26	3	603	CLA	CHB-C4A-NA	3.29	129.14	124.40
26	Y	602	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
26	2	611	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
27	y	1620	LUT	C35-C15-C14	-3.29	116.80	123.52
28	2	1622	XAT	C7-C8-C9	-3.29	120.43	125.53
31	b	618	BCR	C21-C20-C19	-3.29	113.68	123.20
26	c	510	CLA	CMB-C2B-C1B	-3.29	120.42	125.42
31	b	620	BCR	C4-C5-C6	-3.29	118.27	122.70
25	3	601	CHL	CMD-C2D-C3D	-3.28	118.12	124.68
26	B	611	CLA	CAA-C2A-C3A	-3.28	104.12	113.00
26	a	410	CLA	C3B-C4B-NB	-3.28	107.60	110.53
31	B	618	BCR	C21-C20-C19	-3.28	113.69	123.20
26	n	604	CLA	CHB-C1B-NB	3.28	128.97	124.05
26	r	604	CLA	CBA-CAA-C2A	3.28	123.56	113.79
25	g	608	CHL	C1-C2-C3	-3.28	120.82	126.20
26	c	508	CLA	CMB-C2B-C3B	3.28	134.27	126.55
28	G	1622	XAT	C11-C10-C9	-3.28	122.68	127.28
25	7	601	CHL	CMD-C2D-C3D	-3.28	118.13	124.68
26	C	508	CLA	CMB-C2B-C3B	3.28	134.26	126.55
26	R	604	CLA	CBA-CAA-C2A	3.28	123.55	113.79
26	S	603	CLA	CHB-C4A-NA	3.28	129.13	124.40
26	B	606	CLA	C1-C2-C3	-3.28	120.82	126.20
26	b	611	CLA	CAA-C2A-C3A	-3.28	104.14	113.00
27	8	620	LUT	C18-C5-C6	-3.28	120.91	124.48
29	R	623	NEX	C31-C30-C29	-3.28	122.68	127.28
25	7	601	CHL	CMA-C3A-C4A	-3.28	107.55	114.61
26	b	606	CLA	C1-C2-C3	-3.28	120.83	126.20
27	r	620	LUT	C15-C14-C13	-3.28	122.68	127.28
25	R	606	CHL	C3D-C4D-ND	3.28	118.19	112.94
25	3	601	CHL	CMA-C3A-C4A	-3.27	107.56	114.61
31	c	517	BCR	C21-C20-C19	-3.27	113.71	123.20
26	B	611	CLA	CHB-C4A-NA	3.27	129.12	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	r	622	XAT	C35-C15-C14	-3.27	116.82	123.52
26	y	602	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
27	R	620	LUT	C15-C14-C13	-3.27	122.69	127.28
25	G	607	CHL	C1C-CHC-C4B	3.27	127.76	116.07
36	b	623	SQD	O9-S-C6	3.27	111.63	106.76
25	Y	601	CHL	C4-C3-C5	3.27	120.90	115.23
25	Y	601	CHL	O2D-CGD-O1D	-3.27	117.49	123.85
25	3	601	CHL	C1C-CHC-C4B	3.27	127.75	116.07
25	y	601	CHL	O2D-CGD-O1D	-3.26	117.49	123.85
25	5	609	CHL	O1D-CGD-CBD	-3.26	119.77	124.72
31	B	620	BCR	C4-C5-C6	-3.26	118.29	122.70
31	C	517	BCR	C21-C20-C19	-3.26	113.74	123.20
26	D	403	CLA	CHB-C4A-NA	3.26	129.11	124.40
25	g	605	CHL	C1C-CHC-C4B	3.26	127.74	116.07
26	G	611	CLA	CMB-C2B-C1B	-3.26	120.45	125.42
28	R	622	XAT	C35-C15-C14	-3.26	116.85	123.52
25	5	607	CHL	C3D-C4D-ND	3.26	118.17	112.94
25	g	607	CHL	C1C-CHC-C4B	3.26	127.72	116.07
27	y	1620	LUT	C15-C14-C13	-3.26	122.71	127.28
26	b	611	CLA	CHB-C4A-NA	3.26	129.10	124.40
25	1	607	CHL	C3D-C4D-ND	3.26	118.16	112.94
26	A	410	CLA	C3B-C4B-NB	-3.26	107.62	110.53
31	a	411	BCR	C24-C23-C22	-3.25	121.42	126.23
25	7	601	CHL	C1C-CHC-C4B	3.25	127.72	116.07
25	G	601	CHL	C3D-C4D-ND	3.25	118.16	112.94
36	B	623	SQD	O9-S-C6	3.25	111.61	106.76
25	2	601	CHL	C3D-C4D-ND	3.25	118.16	112.94
27	N	1621	LUT	C35-C34-C33	-3.25	122.72	127.28
25	G	605	CHL	C1C-CHC-C4B	3.25	127.71	116.07
26	g	603	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
28	6	1622	XAT	C7-C8-C9	-3.25	120.49	125.53
25	r	606	CHL	C3D-C4D-ND	3.25	118.15	112.94
26	R	610	CLA	CHB-C4A-NA	3.25	129.09	124.40
27	n	1620	LUT	C30-C31-C32	-3.25	113.78	123.20
27	N	1620	LUT	C30-C31-C32	-3.25	113.79	123.20
27	4	620	LUT	C18-C5-C6	-3.25	120.94	124.48
25	g	601	CHL	C3D-C4D-ND	3.25	118.15	112.94
25	5	601	CHL	CMD-C2D-C3D	-3.24	118.20	124.68
28	g	1622	XAT	C11-C10-C9	-3.24	122.73	127.28
25	5	605	CHL	C3D-C4D-ND	3.24	118.14	112.94
26	R	609	CLA	C3B-C4B-NB	-3.24	107.64	110.53
26	r	609	CLA	C3B-C4B-NB	-3.24	107.64	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	507	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
28	g	1622	XAT	C35-C34-C33	-3.24	122.73	127.28
27	n	1621	LUT	C35-C34-C33	-3.24	122.73	127.28
29	S	1623	NEX	C26-C27-C28	-3.24	119.14	125.99
26	c	507	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
29	6	1623	NEX	C15-C35-C34	-3.24	116.89	123.52
31	T	101	BCR	C16-C15-C14	-3.24	116.89	123.52
31	t	101	BCR	C16-C15-C14	-3.24	116.89	123.52
26	3	614	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
26	G	603	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
26	d	403	CLA	CHB-C4A-NA	3.24	129.07	124.40
25	6	601	CHL	C3D-C4D-ND	3.24	118.13	112.94
25	1	609	CHL	O1D-CGD-CBD	-3.23	119.82	124.72
25	1	605	CHL	C3D-C4D-ND	3.23	118.12	112.94
25	2	605	CHL	C3D-C4D-ND	3.23	118.12	112.94
25	6	605	CHL	C3D-C4D-ND	3.23	118.12	112.94
25	8	606	CHL	C3D-C4D-ND	3.23	118.12	112.94
26	r	610	CLA	CHB-C4A-NA	3.23	129.06	124.40
26	5	610	CLA	C3B-C4B-NB	-3.23	107.65	110.53
25	y	608	CHL	CBC-CAC-C3C	-3.23	108.25	112.87
26	s	614	CLA	O2D-CGD-CBD	3.22	116.87	111.23
31	A	411	BCR	C24-C23-C22	-3.22	121.47	126.23
26	C	511	CLA	CHB-C4A-NA	3.22	129.05	124.40
25	1	601	CHL	CMD-C2D-C3D	-3.22	118.25	124.68
26	c	511	CLA	CHB-C4A-NA	3.22	129.05	124.40
29	2	1623	NEX	C15-C35-C34	-3.22	116.93	123.52
26	7	614	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
29	S	1623	NEX	C35-C34-C33	-3.22	122.76	127.28
26	R	602	CLA	CMB-C2B-C1B	-3.22	120.52	125.42
26	S	614	CLA	O2D-CGD-CBD	3.22	116.86	111.23
29	1	1623	NEX	C11-C10-C9	-3.22	122.77	127.28
28	r	622	XAT	C4-C3-C2	-3.22	104.77	110.79
31	C	515	BCR	C24-C23-C22	-3.22	121.48	126.23
26	A	406	CLA	O2D-CGD-CBD	3.22	116.85	111.23
29	s	1623	NEX	C26-C27-C28	-3.22	119.19	125.99
27	G	1621	LUT	C30-C31-C32	-3.22	113.88	123.20
28	8	622	XAT	C15-C14-C13	-3.22	122.77	127.28
29	5	1623	NEX	C11-C10-C9	-3.21	122.77	127.28
28	4	622	XAT	C15-C14-C13	-3.21	122.77	127.28
29	s	1623	NEX	C35-C34-C33	-3.21	122.77	127.28
25	R	614	CHL	C1C-CHC-C4B	3.21	127.56	116.07
25	8	609	CHL	C3D-C4D-ND	3.21	118.09	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	r	614	CHL	C1C-CHC-C4B	3.21	127.56	116.07
28	8	622	XAT	C24-C23-C22	-3.21	104.79	110.79
25	Y	608	CHL	CBC-CAC-C3C	-3.21	108.28	112.87
26	b	610	CLA	C7-C6-C5	-3.21	104.71	113.26
26	y	603	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
28	G	1622	XAT	C35-C34-C33	-3.21	122.78	127.28
25	g	606	CHL	C3D-C4D-ND	3.21	118.08	112.94
27	8	620	LUT	C18-C5-C4	3.21	120.32	114.42
28	R	622	XAT	C4-C3-C2	-3.20	104.80	110.79
31	c	515	BCR	C24-C23-C22	-3.20	121.49	126.23
26	B	610	CLA	C7-C6-C5	-3.20	104.72	113.26
31	B	618	BCR	C7-C8-C9	-3.20	121.50	126.23
26	c	513	CLA	CMB-C2B-C1B	-3.20	120.54	125.42
25	G	606	CHL	C3D-C4D-ND	3.20	118.08	112.94
25	4	609	CHL	C3D-C4D-ND	3.20	118.07	112.94
26	C	502	CLA	CHB-C4A-NA	3.20	129.02	124.40
26	r	602	CLA	CMB-C2B-C1B	-3.20	120.55	125.42
26	S	602	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
27	S	1620	LUT	C30-C31-C32	-3.20	113.94	123.20
27	s	1620	LUT	C30-C31-C32	-3.20	113.94	123.20
27	g	1621	LUT	C30-C31-C32	-3.20	113.94	123.20
26	C	505	CLA	C7-C6-C5	-3.19	104.75	113.26
26	c	505	CLA	C7-C6-C5	-3.19	104.75	113.26
25	r	606	CHL	O2A-CGA-CBA	3.19	121.58	111.83
26	a	406	CLA	O2D-CGD-CBD	3.19	116.81	111.23
25	4	606	CHL	C3D-C4D-ND	3.19	118.06	112.94
27	4	620	LUT	C35-C34-C33	-3.19	122.80	127.28
25	S	606	CHL	C1C-CHC-C4B	3.19	127.49	116.07
28	3	1622	XAT	C11-C10-C9	-3.19	122.80	127.28
35	a	409	PHO	O1D-CGD-CBD	3.19	129.56	124.72
26	s	602	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
26	B	615	CLA	C3B-C4B-NB	-3.19	107.68	110.53
27	2	1620	LUT	C10-C11-C12	-3.19	113.96	123.20
25	R	614	CHL	C3D-C4D-ND	3.19	118.06	112.94
27	7	1621	LUT	C15-C35-C34	-3.19	116.99	123.52
26	6	602	CLA	C4A-NA-C1A	3.19	108.13	106.68
27	8	620	LUT	C35-C34-C33	-3.19	122.81	127.28
26	Y	603	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
26	b	615	CLA	O2D-CGD-CBD	3.19	116.80	111.23
25	s	606	CHL	C1C-CHC-C4B	3.19	127.47	116.07
26	B	609	CLA	O2D-CGD-CBD	3.19	116.80	111.23
26	s	612	CLA	CMB-C2B-C3B	3.19	134.04	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	610	CLA	C3B-C4B-NB	-3.19	107.69	110.53
31	b	618	BCR	C7-C8-C9	-3.19	121.52	126.23
26	n	603	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
25	R	606	CHL	O2A-CGA-CBA	3.18	121.55	111.83
27	4	620	LUT	C18-C5-C4	3.18	120.28	114.42
27	6	1620	LUT	C10-C11-C12	-3.18	113.98	123.20
26	y	603	CLA	C3B-C4B-NB	-3.18	107.69	110.53
28	4	622	XAT	C24-C23-C22	-3.18	104.84	110.79
26	B	615	CLA	O2D-CGD-CBD	3.18	116.79	111.23
26	S	612	CLA	CMB-C2B-C3B	3.18	134.03	126.55
31	d	404	BCR	C38-C26-C25	-3.18	121.01	124.48
25	1	609	CHL	C3D-C4D-ND	3.18	118.04	112.94
27	R	620	LUT	C39-C29-C28	3.18	122.95	118.09
36	a	418	SQD	O9-S-C6	3.18	111.50	106.76
26	C	513	CLA	CMB-C2B-C1B	-3.18	120.58	125.42
26	6	603	CLA	CHB-C4A-NA	3.18	128.99	124.40
36	A	418	SQD	O9-S-C6	3.18	111.50	106.76
27	r	620	LUT	C39-C29-C28	3.18	122.94	118.09
25	r	614	CHL	C3D-C4D-ND	3.18	118.04	112.94
27	s	1621	LUT	C17-C1-C6	3.18	115.22	110.24
26	N	603	CLA	O2D-CGD-O1D	-3.18	117.67	123.85
28	6	1622	XAT	C35-C34-C33	-3.18	122.82	127.28
25	5	609	CHL	C3D-C4D-ND	3.18	118.03	112.94
26	Y	603	CLA	C3B-C4B-NB	-3.18	107.69	110.53
36	A	418	SQD	O6-C1-C2	3.17	113.09	108.27
36	a	418	SQD	O6-C1-C2	3.17	113.09	108.27
27	n	1620	LUT	C15-C14-C13	-3.17	122.83	127.28
28	Y	1622	XAT	C24-C23-C22	-3.17	104.86	110.79
26	B	605	CLA	C1-C2-C3	-3.17	121.01	126.20
27	3	1621	LUT	C15-C35-C34	-3.16	117.04	123.52
26	b	609	CLA	O2D-CGD-CBD	3.16	116.76	111.23
28	2	1622	XAT	C35-C34-C33	-3.16	122.84	127.28
26	c	502	CLA	CHB-C4A-NA	3.16	128.96	124.40
25	1	601	CHL	C3D-C4D-ND	3.16	118.01	112.94
35	A	409	PHO	O1D-CGD-CBD	3.16	129.51	124.72
27	N	1620	LUT	C15-C14-C13	-3.16	122.85	127.28
26	b	605	CLA	C1-C2-C3	-3.16	121.02	126.20
27	S	1621	LUT	C17-C1-C6	3.16	115.19	110.24
26	2	603	CLA	CHB-C4A-NA	3.15	128.95	124.40
28	7	1622	XAT	C11-C10-C9	-3.15	122.85	127.28
26	c	508	CLA	CMC-C2C-C1C	-3.15	120.11	125.03
31	D	404	BCR	C38-C26-C25	-3.15	121.04	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	605	CHL	C1C-CHC-C4B	3.15	127.35	116.07
26	S	609	CLA	C4A-NA-C1A	3.15	108.12	106.68
27	2	1621	LUT	C10-C11-C12	-3.15	114.07	123.20
26	b	615	CLA	C3B-C4B-NB	-3.15	107.72	110.53
31	C	516	BCR	C10-C11-C12	-3.15	114.08	123.20
25	1	605	CHL	C1C-CHC-C4B	3.15	127.33	116.07
29	1	1623	NEX	C24-C23-C22	-3.15	104.90	110.79
28	y	1622	XAT	C24-C23-C22	-3.15	104.90	110.79
26	6	610	CLA	C4A-NA-C1A	3.15	108.11	106.68
31	c	516	BCR	C10-C11-C12	-3.15	114.08	123.20
26	y	613	CLA	O2D-CGD-CBD	3.15	116.73	111.23
26	7	603	CLA	CBC-CAC-C3C	-3.15	103.89	112.42
25	N	606	CHL	CMB-C2B-C3B	3.15	130.97	124.68
31	8	623	BCR	C11-C12-C13	-3.14	117.74	126.36
25	s	607	CHL	C1C-CHC-C4B	3.14	127.32	116.07
26	2	610	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
26	3	603	CLA	CBC-CAC-C3C	-3.14	103.90	112.42
26	R	604	CLA	CAA-C2A-C3A	-3.14	104.51	113.00
26	2	602	CLA	C4A-NA-C1A	3.14	108.11	106.68
26	Y	613	CLA	O2D-CGD-CBD	3.14	116.72	111.23
25	S	607	CHL	C1C-CHC-C4B	3.14	127.31	116.07
25	5	601	CHL	C3D-C4D-ND	3.14	117.97	112.94
26	r	604	CLA	CAA-C2A-C3A	-3.14	104.52	113.00
25	y	608	CHL	C3D-C4D-ND	3.14	117.97	112.94
26	b	608	CLA	CMB-C2B-C1B	-3.14	120.64	125.42
26	S	603	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
39	C	518	DGD	C1E-O6E-C5E	3.14	119.85	113.72
27	7	1621	LUT	C10-C11-C12	-3.14	114.11	123.20
25	5	606	CHL	C3D-C4D-ND	3.14	117.97	112.94
31	4	623	BCR	C11-C12-C13	-3.14	117.76	126.36
25	y	601	CHL	C3D-C4D-ND	3.14	117.97	112.94
25	1	606	CHL	C3D-C4D-ND	3.14	117.97	112.94
25	Y	608	CHL	O2A-CGA-CBA	3.13	121.39	111.83
25	y	608	CHL	O2A-CGA-CBA	3.13	121.39	111.83
26	S	614	CLA	CMB-C2B-C1B	-3.13	120.65	125.42
28	2	1622	XAT	O24-C25-C38	3.13	118.55	115.05
27	6	1621	LUT	C10-C11-C12	-3.13	114.12	123.20
25	N	601	CHL	C3D-C4D-ND	3.13	117.96	112.94
25	7	606	CHL	C1C-CHC-C4B	3.13	127.28	116.07
25	3	606	CHL	C1C-CHC-C4B	3.13	127.27	116.07
26	N	602	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
25	r	606	CHL	CBC-CAC-C3C	-3.13	108.39	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	606	CHL	C1C-CHC-C4B	3.13	127.26	116.07
26	C	504	CLA	CHB-C4A-NA	3.13	128.91	124.40
26	C	508	CLA	CMC-C2C-C1C	-3.13	120.15	125.03
25	6	606	CHL	C3D-C4D-ND	3.13	117.95	112.94
28	6	1622	XAT	O24-C25-C38	3.13	118.54	115.05
26	s	614	CLA	CMB-C2B-C1B	-3.12	120.66	125.42
29	5	1623	NEX	C24-C23-C22	-3.12	104.95	110.79
25	4	607	CHL	C3D-C4D-ND	3.12	117.95	112.94
25	n	606	CHL	CMB-C2B-C3B	3.12	130.92	124.68
26	B	610	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
26	6	610	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
26	b	610	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
25	R	606	CHL	C1C-CHC-C4B	3.12	127.24	116.07
27	3	1621	LUT	C10-C11-C12	-3.12	114.16	123.20
26	r	601	CLA	C3B-C4B-NB	-3.12	107.75	110.53
26	s	603	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
25	R	606	CHL	CBC-CAC-C3C	-3.12	108.41	112.87
25	Y	608	CHL	C3D-C4D-ND	3.12	117.94	112.94
26	B	608	CLA	CMB-C2B-C1B	-3.12	120.67	125.42
25	7	606	CHL	CBC-CAC-C3C	-3.12	108.41	112.87
25	n	601	CHL	C3D-C4D-ND	3.12	117.94	112.94
26	y	614	CLA	O2D-CGD-CBD	3.12	116.68	111.23
25	Y	609	CHL	O1D-CGD-CBD	-3.12	120.00	124.72
25	2	606	CHL	C1C-CHC-C4B	3.11	127.22	116.07
35	A	408	PHO	CAA-CBA-CGA	-3.11	104.36	113.21
25	r	606	CHL	C1C-CHC-C4B	3.11	127.21	116.07
25	n	609	CHL	C1-O2A-CGA	3.11	124.19	116.65
39	c	518	DGD	C1E-O6E-C5E	3.11	119.80	113.72
27	4	620	LUT	C8-C7-C6	-3.11	118.68	127.00
28	4	622	XAT	C10-C11-C12	-3.11	114.18	123.20
25	Y	601	CHL	C3D-C4D-ND	3.11	117.93	112.94
25	7	609	CHL	O1D-CGD-CBD	-3.11	120.00	124.72
25	8	607	CHL	O1D-CGD-CBD	-3.11	120.00	124.72
35	a	408	PHO	CAA-CBA-CGA	-3.11	104.37	113.21
25	3	606	CHL	CBC-CAC-C3C	-3.11	108.42	112.87
25	8	608	CHL	C3D-C4D-ND	3.11	117.93	112.94
25	2	606	CHL	C3D-C4D-ND	3.11	117.93	112.94
38	d	405	PL9	C40-C39-C41	3.11	120.63	115.23
26	n	602	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
25	4	607	CHL	O1D-CGD-CBD	-3.11	120.01	124.72
26	Y	614	CLA	O2D-CGD-CBD	3.11	116.66	111.23
25	Y	605	CHL	C3D-C4D-ND	3.11	117.92	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	2	610	CLA	C4A-NA-C1A	3.11	108.10	106.68
25	N	609	CHL	C1-O2A-CGA	3.11	124.17	116.65
31	b	618	BCR	C15-C16-C17	-3.10	117.17	123.52
25	8	607	CHL	C3D-C4D-ND	3.10	117.92	112.94
28	6	1622	XAT	O4-C5-C18	3.10	118.52	115.05
27	8	620	LUT	C8-C7-C6	-3.10	118.71	127.00
28	8	622	XAT	C10-C11-C12	-3.10	114.21	123.20
31	B	618	BCR	C15-C16-C17	-3.10	117.17	123.52
27	g	1621	LUT	C18-C5-C6	-3.10	121.10	124.48
25	G	601	CHL	CMD-C2D-C3D	-3.10	118.49	124.68
31	H	101	BCR	C20-C21-C22	-3.10	122.93	127.28
31	h	101	BCR	C20-C21-C22	-3.10	122.93	127.28
26	A	407	CLA	CHB-C4A-NA	3.10	128.87	124.40
25	g	605	CHL	C3D-C4D-ND	3.09	117.90	112.94
26	c	504	CLA	CHB-C4A-NA	3.09	128.86	124.40
25	3	609	CHL	C3D-C4D-ND	3.09	117.90	112.94
38	D	405	PL9	C40-C39-C41	3.09	120.59	115.23
25	G	605	CHL	C3D-C4D-ND	3.09	117.90	112.94
25	y	609	CHL	O1D-CGD-CBD	-3.09	120.03	124.72
27	g	1620	LUT	C30-C31-C32	-3.09	114.25	123.20
26	s	609	CLA	C4A-NA-C1A	3.09	108.09	106.68
27	G	1621	LUT	C18-C5-C6	-3.09	121.11	124.48
25	4	608	CHL	C3D-C4D-ND	3.09	117.89	112.94
27	G	1620	LUT	C30-C31-C32	-3.09	114.25	123.20
26	Y	610	CLA	C4A-NA-C1A	3.09	108.09	106.68
26	y	603	CLA	CHB-C4A-NA	3.08	128.85	124.40
25	3	609	CHL	O1D-CGD-CBD	-3.08	120.05	124.72
28	3	1622	XAT	C31-C32-C33	-3.08	117.91	126.36
25	g	601	CHL	CMD-C2D-C3D	-3.08	118.53	124.68
26	G	613	CLA	O2D-CGD-CBD	3.08	116.62	111.23
25	G	609	CHL	C1-O2A-CGA	3.08	124.11	116.65
25	G	601	CHL	C1-C2-C3	-3.08	121.15	126.20
31	d	404	BCR	C15-C14-C13	-3.08	122.96	127.28
25	y	605	CHL	C3D-C4D-ND	3.08	117.88	112.94
26	c	512	CLA	O2D-CGD-CBD	3.08	116.61	111.23
25	7	609	CHL	C3D-C4D-ND	3.07	117.87	112.94
25	S	608	CHL	C3D-C4D-ND	3.07	117.87	112.94
26	R	601	CLA	C3B-C4B-NB	-3.07	107.79	110.53
25	2	608	CHL	C3D-C4D-ND	3.07	117.87	112.94
29	S	1623	NEX	C31-C30-C29	-3.07	122.97	127.28
31	D	404	BCR	C15-C14-C13	-3.07	122.97	127.28
28	7	1622	XAT	C31-C32-C33	-3.07	117.95	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	411	BCR	C16-C15-C14	-3.07	117.24	123.52
26	s	611	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
28	2	1622	XAT	O4-C5-C18	3.07	118.48	115.05
29	r	623	NEX	O24-C25-C38	3.07	118.47	115.05
29	s	1623	NEX	C31-C30-C29	-3.07	122.98	127.28
26	b	611	CLA	C3B-C4B-NB	-3.06	107.79	110.53
26	a	407	CLA	CHB-C4A-NA	3.06	128.82	124.40
27	S	1621	LUT	C19-C9-C8	3.06	122.77	118.09
26	Y	603	CLA	CHB-C4A-NA	3.06	128.82	124.40
25	g	609	CHL	C1-O2A-CGA	3.06	124.06	116.65
25	6	608	CHL	C3D-C4D-ND	3.06	117.85	112.94
26	R	611	CLA	CHB-C4A-NA	3.06	128.82	124.40
26	Y	610	CLA	C3B-C4B-NB	-3.06	107.80	110.53
26	y	610	CLA	C3B-C4B-NB	-3.06	107.80	110.53
31	A	411	BCR	C16-C15-C14	-3.06	117.26	123.52
27	s	1621	LUT	C19-C9-C8	3.06	122.76	118.09
26	5	603	CLA	CHB-C4A-NA	3.06	128.81	124.40
25	5	609	CHL	CBC-CAC-C3C	-3.06	108.49	112.87
26	C	512	CLA	O2D-CGD-CBD	3.06	116.57	111.23
25	r	607	CHL	C3D-C4D-ND	3.06	117.84	112.94
25	g	601	CHL	C1-C2-C3	-3.06	121.19	126.20
26	g	613	CLA	O2D-CGD-CBD	3.05	116.57	111.23
27	Y	1621	LUT	C10-C11-C12	-3.05	114.36	123.20
39	B	626	DGD	O5D-C1E-C2E	3.05	112.90	108.27
26	B	609	CLA	CMB-C2B-C3B	3.05	133.72	126.55
27	y	1621	LUT	C10-C11-C12	-3.05	114.37	123.20
25	7	605	CHL	C3D-C4D-ND	3.05	117.83	112.94
25	g	607	CHL	C3D-C4D-ND	3.05	117.83	112.94
26	1	603	CLA	CHB-C4A-NA	3.05	128.80	124.40
26	b	609	CLA	CMB-C2B-C3B	3.05	133.72	126.55
25	y	606	CHL	CMB-C2B-C3B	3.05	130.77	124.68
25	N	608	CHL	O1D-CGD-CBD	-3.05	120.10	124.72
30	d	410	LHG	O8-C23-C24	3.05	121.12	111.83
39	b	626	DGD	O5D-C1E-C2E	3.05	112.90	108.27
26	N	602	CLA	CMB-C2B-C3B	3.05	133.71	126.55
26	y	610	CLA	C4A-NA-C1A	3.04	108.07	106.68
29	R	623	NEX	O24-C25-C38	3.04	118.45	115.05
25	G	607	CHL	C3D-C4D-ND	3.04	117.82	112.94
31	b	618	BCR	C20-C21-C22	-3.04	123.01	127.28
26	S	611	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
25	s	608	CHL	C3D-C4D-ND	3.04	117.81	112.94
30	D	408	LHG	O8-C23-C24	3.04	121.10	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	606	CHL	CMB-C2B-C3B	3.04	130.75	124.68
31	C	514	BCR	C21-C20-C19	-3.04	114.41	123.20
30	d	408	LHG	O8-C23-C24	3.04	121.09	111.83
25	R	607	CHL	C3D-C4D-ND	3.03	117.81	112.94
25	g	609	CHL	CMB-C2B-C3B	3.03	130.75	124.68
27	Y	1620	LUT	C35-C34-C33	-3.03	123.02	127.28
25	2	609	CHL	C1B-CHB-C4A	3.03	123.27	121.32
26	n	602	CLA	CMB-C2B-C3B	3.03	133.68	126.55
31	A	411	BCR	C38-C26-C25	-3.03	121.18	124.48
26	b	608	CLA	CHB-C4A-NA	3.03	128.77	124.40
31	c	514	BCR	C21-C20-C19	-3.03	114.42	123.20
27	y	1620	LUT	C35-C34-C33	-3.03	123.03	127.28
30	D	410	LHG	O8-C23-C24	3.03	121.06	111.83
26	c	511	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
25	1	609	CHL	CBC-CAC-C3C	-3.03	108.54	112.87
27	Y	1620	LUT	C39-C29-C28	3.03	122.71	118.09
31	T	101	BCR	C33-C5-C4	3.03	120.05	113.60
36	a	418	SQD	C4-C3-C2	3.02	116.14	110.83
25	n	608	CHL	O1D-CGD-CBD	-3.02	120.14	124.72
26	A	405	CLA	CHB-C4A-NA	3.02	128.76	124.40
26	r	611	CLA	CHB-C4A-NA	3.02	128.76	124.40
25	G	609	CHL	CMB-C2B-C3B	3.02	130.72	124.68
36	A	418	SQD	C4-C3-C2	3.02	116.13	110.83
25	7	606	CHL	O1D-CGD-CBD	-3.02	120.14	124.72
26	C	511	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
29	R	623	NEX	C38-C25-C24	3.02	117.63	114.24
29	r	623	NEX	C38-C25-C24	3.02	117.63	114.24
39	B	626	DGD	CDB-CCB-CBB	-3.02	99.12	114.37
31	a	411	BCR	C38-C26-C25	-3.02	121.19	124.48
31	B	619	BCR	C15-C16-C17	-3.01	117.35	123.52
31	t	101	BCR	C33-C5-C4	3.01	120.02	113.60
39	b	626	DGD	CDB-CCB-CBB	-3.01	99.13	114.37
25	3	605	CHL	C3D-C4D-ND	3.01	117.77	112.94
31	b	619	BCR	C15-C16-C17	-3.01	117.36	123.52
26	g	604	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
26	y	604	CLA	CHB-C1B-NB	3.01	128.57	124.05
31	b	620	BCR	C33-C5-C4	3.01	120.02	113.60
26	A	406	CLA	CMB-C2B-C1B	-3.01	120.83	125.42
25	4	609	CHL	CMA-C3A-C4A	-3.01	108.12	114.61
28	N	1622	XAT	C24-C23-C22	-3.01	105.16	110.79
28	n	1622	XAT	C24-C23-C22	-3.01	105.16	110.79
26	a	406	CLA	CMB-C2B-C1B	-3.01	120.84	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	405	CLA	CHB-C4A-NA	3.01	128.74	124.40
31	B	618	BCR	C20-C21-C22	-3.01	123.06	127.28
25	2	608	CHL	CBC-CAC-C3C	-3.01	108.57	112.87
26	Y	604	CLA	CHB-C1B-NB	3.01	128.56	124.05
26	B	611	CLA	C3B-C4B-NB	-3.01	107.85	110.53
26	B	608	CLA	CHB-C4A-NA	3.01	128.74	124.40
25	3	606	CHL	O1D-CGD-CBD	-3.00	120.17	124.72
28	1	1622	XAT	C4-C3-C2	-3.00	105.17	110.79
26	B	616	CLA	CHB-C4A-NA	3.00	128.73	124.40
26	b	616	CLA	CHB-C4A-NA	3.00	128.73	124.40
26	y	612	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
29	s	1623	NEX	C24-C23-C22	-3.00	105.18	110.79
26	R	604	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
25	6	608	CHL	CBC-CAC-C3C	-3.00	108.58	112.87
25	6	609	CHL	C1-C2-C3	-3.00	121.28	126.20
25	r	614	CHL	O2D-CGD-O1D	-3.00	118.01	123.85
25	N	607	CHL	CMB-C2B-C3B	3.00	130.68	124.68
26	C	504	CLA	O2D-CGD-CBD	3.00	116.47	111.23
26	a	406	CLA	CAC-C3C-C4C	-3.00	120.89	124.79
26	Y	612	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
25	7	609	CHL	C1C-CHC-C4B	3.00	126.79	116.07
29	S	1623	NEX	C24-C23-C22	-3.00	105.19	110.79
35	a	409	PHO	C2D-C1D-ND	-3.00	107.27	109.43
26	r	604	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
26	g	604	CLA	CHB-C1B-NB	2.99	128.54	124.05
26	G	604	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
31	B	620	BCR	C33-C5-C4	2.99	119.98	113.60
26	B	617	CLA	O2D-CGD-CBD	2.99	116.46	111.23
25	3	609	CHL	C1C-CHC-C4B	2.99	126.77	116.07
25	8	609	CHL	O1D-CGD-CBD	-2.99	120.19	124.72
28	5	1622	XAT	C4-C3-C2	-2.99	105.20	110.79
25	8	609	CHL	CMA-C3A-C4A	-2.99	108.17	114.61
25	n	607	CHL	CMB-C2B-C3B	2.99	130.66	124.68
26	G	604	CLA	CHB-C1B-NB	2.99	128.53	124.05
26	g	604	CLA	C1-C2-C3	-2.99	121.93	126.76
35	A	409	PHO	C2D-C1D-ND	-2.99	107.27	109.43
37	B	2633	LMG	O2-C2-C1	-2.99	102.95	110.08
25	N	609	CHL	C3D-C4D-ND	2.99	117.73	112.94
25	n	609	CHL	C3D-C4D-ND	2.99	117.73	112.94
26	c	504	CLA	O2D-CGD-CBD	2.99	116.45	111.23
25	2	601	CHL	CMD-C2D-C3D	-2.99	118.71	124.68
27	r	620	LUT	C28-C29-C30	-2.99	114.31	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	7	1621	LUT	C35-C34-C33	-2.99	123.09	127.28
25	R	614	CHL	O2D-CGD-O1D	-2.99	118.03	123.85
25	Y	606	CHL	O2D-CGD-O1D	-2.99	118.03	123.85
25	y	606	CHL	O2D-CGD-O1D	-2.99	118.03	123.85
26	b	609	CLA	CHB-C4A-NA	2.99	128.71	124.40
25	y	605	CHL	OMC-CMC-C2C	-2.99	119.93	125.12
28	1	1622	XAT	C31-C32-C33	-2.99	118.17	126.36
25	n	609	CHL	CMB-C2B-C3B	2.99	130.65	124.68
25	5	609	CHL	C1C-CHC-C4B	2.98	126.75	116.07
25	3	605	CHL	O1D-CGD-CBD	-2.98	120.20	124.72
26	n	614	CLA	CMB-C2B-C3B	2.98	133.57	126.55
25	1	609	CHL	C1C-CHC-C4B	2.98	126.75	116.07
26	R	603	CLA	CMB-C2B-C3B	2.98	133.57	126.55
26	A	407	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
25	3	609	CHL	CMA-C3A-C4A	-2.98	108.18	114.61
28	5	1622	XAT	C31-C32-C33	-2.98	118.18	126.36
26	G	604	CLA	C1-C2-C3	-2.98	121.94	126.76
25	y	609	CHL	C4-C3-C5	2.98	120.41	115.23
27	y	1620	LUT	C39-C29-C28	2.98	122.64	118.09
25	4	608	CHL	C1C-CHC-C4B	2.98	126.74	116.07
37	b	2633	LMG	O2-C2-C1	-2.98	102.97	110.08
25	6	601	CHL	CMD-C2D-C3D	-2.98	118.73	124.68
26	1	604	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
27	5	1621	LUT	C18-C5-C6	-2.98	121.23	124.48
25	6	609	CHL	C3D-C4D-ND	2.98	117.72	112.94
25	N	609	CHL	CMB-C2B-C3B	2.98	130.63	124.68
25	7	609	CHL	CMA-C3A-C4A	-2.98	108.19	114.61
26	b	617	CLA	O2D-CGD-CBD	2.98	116.44	111.23
25	4	606	CHL	O1D-CGD-CBD	-2.98	120.21	124.72
26	A	406	CLA	CAC-C3C-C4C	-2.98	120.91	124.79
27	n	1621	LUT	C30-C31-C32	-2.98	114.58	123.20
25	6	609	CHL	C1B-CHB-C4A	2.98	123.24	121.32
26	B	603	CLA	CMB-C2B-C1B	-2.98	120.89	125.42
30	c	523	LHG	O8-C23-C24	2.97	120.90	111.83
26	N	614	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
25	8	608	CHL	C1C-CHC-C4B	2.97	126.71	116.07
26	n	614	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
27	g	1620	LUT	C35-C15-C14	-2.97	117.44	123.52
27	G	1620	LUT	C35-C15-C14	-2.97	117.44	123.52
28	R	622	XAT	C19-C9-C8	2.97	122.63	118.09
25	2	609	CHL	C1-C2-C3	-2.97	121.33	126.20
26	r	603	CLA	CMB-C2B-C3B	2.97	133.53	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	609	CHL	C1C-CHC-C4B	2.97	126.69	116.07
31	b	619	BCR	C24-C23-C22	-2.97	121.84	126.23
25	8	606	CHL	O1D-CGD-CBD	-2.97	120.22	124.72
26	N	614	CLA	CMB-C2B-C3B	2.97	133.53	126.55
25	n	607	CHL	C1C-CHC-C4B	2.97	126.69	116.07
26	5	604	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
26	g	611	CLA	CHB-C4A-NA	2.97	128.68	124.40
30	C	523	LHG	O8-C23-C24	2.97	120.88	111.83
26	a	407	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
25	6	605	CHL	C1C-CHC-C4B	2.97	126.68	116.07
25	4	609	CHL	O1D-CGD-CBD	-2.96	120.23	124.72
25	2	605	CHL	C1C-CHC-C4B	2.96	126.67	116.07
25	8	609	CHL	C1C-CHC-C4B	2.96	126.67	116.07
25	Y	609	CHL	C4-C3-C5	2.96	120.37	115.23
26	C	506	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
27	R	620	LUT	C28-C29-C30	-2.96	114.35	119.01
27	N	1621	LUT	C30-C31-C32	-2.96	114.62	123.20
25	Y	605	CHL	OMC-CMC-C2C	-2.96	119.98	125.12
26	G	611	CLA	CHB-C4A-NA	2.96	128.67	124.40
25	Y	609	CHL	C3D-C4D-ND	2.96	117.69	112.94
31	B	619	BCR	C24-C23-C22	-2.96	121.86	126.23
39	h	102	DGD	O6D-C1D-O3G	-2.96	103.05	110.04
26	C	509	CLA	CAA-C2A-C3A	-2.96	105.00	113.00
26	B	609	CLA	CHB-C4A-NA	2.96	128.67	124.40
25	N	607	CHL	C1C-CHC-C4B	2.96	126.65	116.07
39	H	102	DGD	O6D-C1D-O3G	-2.96	103.06	110.04
30	D	409	LHG	O8-C23-C24	2.95	120.84	111.83
36	b	623	SQD	O48-C23-C24	2.95	120.84	111.83
25	8	601	CHL	C1C-CHC-C4B	2.95	126.64	116.07
28	2	1622	XAT	C6-C7-C8	-2.95	119.75	125.99
25	7	605	CHL	O1D-CGD-CBD	-2.95	120.25	124.72
36	B	623	SQD	O48-C23-C24	2.95	120.84	111.83
27	Y	1621	LUT	C30-C31-C32	-2.95	114.65	123.20
26	5	614	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
27	3	1621	LUT	C35-C34-C33	-2.95	123.14	127.28
30	d	409	LHG	O8-C23-C24	2.95	120.83	111.83
26	b	603	CLA	CMB-C2B-C1B	-2.95	120.93	125.42
26	1	614	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
28	r	622	XAT	C19-C9-C8	2.95	122.59	118.09
27	y	1621	LUT	C30-C31-C32	-2.95	114.66	123.20
35	a	409	PHO	O2D-CGD-O1D	-2.95	118.11	123.85
25	4	606	CHL	CAA-C2A-C3A	-2.95	105.03	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	S	1620	LUT	C11-C10-C9	-2.95	123.14	127.28
27	s	1620	LUT	C11-C10-C9	-2.95	123.15	127.28
26	c	509	CLA	CAA-C2A-C3A	-2.95	105.04	113.00
26	B	602	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
26	C	504	CLA	CMB-C2B-C3B	2.95	133.48	126.55
25	4	601	CHL	C1C-CHC-C4B	2.95	126.61	116.07
25	3	607	CHL	O2A-CGA-CBA	2.94	120.81	111.83
26	Y	602	CLA	CMB-C2B-C1B	-2.94	120.94	125.42
31	T	101	BCR	C11-C12-C13	-2.94	118.29	126.36
31	c	516	BCR	C16-C15-C14	-2.94	117.50	123.52
26	c	506	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
26	g	612	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
37	C	521	LMG	C1-C2-C3	-2.94	103.82	110.01
26	B	613	CLA	CMA-C3A-C4A	-2.94	103.87	111.77
25	G	606	CHL	O2A-CGA-CBA	2.94	120.80	111.83
25	8	606	CHL	CAA-C2A-C3A	-2.94	105.06	113.00
31	t	101	BCR	C11-C12-C13	-2.94	118.30	126.36
25	2	609	CHL	C3D-C4D-ND	2.94	117.65	112.94
25	4	606	CHL	C1C-CHC-C4B	2.94	126.58	116.07
31	c	517	BCR	C20-C21-C22	-2.94	123.16	127.28
25	6	609	CHL	C1C-CHC-C4B	2.94	126.58	116.07
26	G	614	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
26	5	612	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
27	1	1621	LUT	C18-C5-C6	-2.93	121.28	124.48
25	N	601	CHL	C1C-C2C-CMC	2.93	132.09	126.80
26	b	602	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
26	b	613	CLA	CMA-C3A-C4A	-2.93	103.89	111.77
26	c	504	CLA	CMB-C2B-C3B	2.93	133.45	126.55
25	2	609	CHL	C1C-CHC-C4B	2.93	126.56	116.07
25	8	606	CHL	C1C-CHC-C4B	2.93	126.56	116.07
25	y	606	CHL	C1C-CHC-C4B	2.93	126.56	116.07
26	s	604	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
31	C	516	BCR	C16-C15-C14	-2.93	117.52	123.52
38	a	414	PL9	O2-C1-C2	-2.93	117.26	121.43
28	6	1622	XAT	C6-C7-C8	-2.93	119.80	125.99
25	6	607	CHL	C3D-C4D-ND	2.93	117.64	112.94
25	y	609	CHL	C3D-C4D-ND	2.93	117.64	112.94
25	7	607	CHL	O2A-CGA-CBA	2.93	120.77	111.83
31	8	623	BCR	C29-C30-C25	2.93	114.69	110.44
25	n	601	CHL	C1C-C2C-CMC	2.93	132.08	126.80
29	r	623	NEX	C30-C31-C32	-2.93	114.72	123.20
26	c	510	CLA	O2D-CGD-O1D	-2.93	118.15	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	3	610	CLA	C3B-C4B-NB	-2.93	107.92	110.53
38	A	414	PL9	O2-C1-C2	-2.93	117.26	121.43
25	y	607	CHL	CMB-C2B-C3B	2.93	130.53	124.68
26	B	610	CLA	CMB-C2B-C1B	-2.93	120.96	125.42
26	G	612	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
25	Y	606	CHL	C1C-CHC-C4B	2.93	126.54	116.07
26	G	603	CLA	CBC-CAC-C3C	-2.93	104.49	112.42
26	g	603	CLA	CBC-CAC-C3C	-2.93	104.49	112.42
31	C	517	BCR	C20-C21-C22	-2.92	123.18	127.28
25	7	606	CHL	C3D-C4D-ND	2.92	117.63	112.94
26	R	601	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
26	b	610	CLA	CMB-C2B-C1B	-2.92	120.97	125.42
26	y	602	CLA	CMB-C2B-C1B	-2.92	120.97	125.42
26	7	610	CLA	C3B-C4B-NB	-2.92	107.92	110.53
29	R	623	NEX	C30-C31-C32	-2.92	114.73	123.20
26	r	601	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
25	g	606	CHL	O2A-CGA-CBA	2.92	120.75	111.83
31	4	623	BCR	C29-C30-C25	2.92	114.69	110.44
26	d	402	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
26	N	603	CLA	CAA-C2A-C3A	-2.92	105.10	113.00
26	g	614	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
35	A	409	PHO	O2D-CGD-O1D	-2.92	118.16	123.85
25	n	605	CHL	C3D-C4D-ND	2.92	117.62	112.94
37	c	521	LMG	C1-C2-C3	-2.92	103.86	110.01
26	S	604	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
26	1	612	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
25	N	605	CHL	C3D-C4D-ND	2.92	117.62	112.94
31	B	618	BCR	C11-C10-C9	-2.92	123.18	127.28
26	g	610	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
25	3	606	CHL	C3D-C4D-ND	2.92	117.62	112.94
25	1	607	CHL	C1C-CHC-C4B	2.92	126.51	116.07
25	5	607	CHL	C1C-CHC-C4B	2.92	126.51	116.07
26	C	510	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
28	4	622	XAT	C38-C25-C24	2.91	117.51	114.24
26	n	603	CLA	CAA-C2A-C3A	-2.91	105.13	113.00
27	8	620	LUT	C31-C30-C29	-2.91	123.19	127.28
26	A	410	CLA	CHB-C4A-NA	2.91	128.60	124.40
26	G	610	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
26	g	602	CLA	CAC-C3C-C4C	2.91	128.58	124.79
26	C	510	CLA	CMB-C2B-C3B	2.91	133.39	126.55
26	R	610	CLA	C1-C2-C3	-2.91	121.43	126.20
26	b	613	CLA	CMD-C2D-C3D	2.91	134.36	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	601	CHL	O2D-CGD-O1D	-2.91	118.19	123.85
27	4	620	LUT	C10-C11-C12	-2.91	114.78	123.20
25	7	607	CHL	C1C-CHC-C4B	2.91	126.47	116.07
26	a	410	CLA	CHB-C4A-NA	2.91	128.59	124.40
25	n	606	CHL	C3D-C4D-ND	2.90	117.60	112.94
28	8	622	XAT	C38-C25-C24	2.90	117.50	114.24
25	Y	607	CHL	CMB-C2B-C3B	2.90	130.49	124.68
25	N	608	CHL	O2A-CGA-CBA	2.90	120.69	111.83
26	b	607	CLA	CHB-C4A-NA	2.90	128.59	124.40
25	3	607	CHL	C1C-CHC-C4B	2.90	126.45	116.07
26	c	512	CLA	CMB-C2B-C1B	-2.90	121.00	125.42
26	S	609	CLA	C3B-C4B-NB	-2.90	107.94	110.53
25	6	607	CHL	C1C-CHC-C4B	2.90	126.45	116.07
31	8	623	BCR	C3-C4-C5	-2.90	108.88	114.06
25	n	608	CHL	O2A-CGA-CBA	2.90	120.68	111.83
25	2	607	CHL	C3D-C4D-ND	2.90	117.59	112.94
26	b	608	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
29	5	1623	NEX	C26-C27-C28	-2.90	119.86	125.99
29	1	1623	NEX	C26-C27-C28	-2.90	119.87	125.99
26	B	606	CLA	O2D-CGD-CBD	2.90	116.30	111.23
26	b	606	CLA	O2D-CGD-CBD	2.90	116.29	111.23
28	3	1622	XAT	C10-C11-C12	-2.90	114.81	123.20
31	B	618	BCR	C10-C11-C12	-2.90	114.81	123.20
25	n	609	CHL	C4-C3-C5	2.89	120.25	115.23
38	a	414	PL9	C8-C7-C3	2.89	119.51	112.03
28	7	1622	XAT	C10-C11-C12	-2.89	114.81	123.20
25	2	607	CHL	C1C-CHC-C4B	2.89	126.42	116.07
26	B	608	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
26	c	505	CLA	CGD-CBD-CAD	2.89	120.21	110.85
27	8	620	LUT	C10-C11-C12	-2.89	114.82	123.20
25	n	601	CHL	O2D-CGD-O1D	-2.89	118.22	123.85
26	2	612	CLA	CAA-C2A-C3A	-2.89	105.18	113.00
26	C	512	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
25	3	601	CHL	CBC-CAC-C3C	-2.89	108.73	112.87
26	B	607	CLA	CHB-C4A-NA	2.89	128.57	124.40
26	G	602	CLA	CAC-C3C-C4C	2.89	128.55	124.79
26	A	406	CLA	CHB-C4A-NA	2.89	128.57	124.40
25	Y	609	CHL	CMB-C2B-C3B	2.89	130.46	124.68
26	R	604	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
26	r	604	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
25	7	601	CHL	CBC-CAC-C3C	-2.89	108.74	112.87
26	r	610	CLA	C1-C2-C3	-2.89	121.46	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D	402	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
26	c	510	CLA	CMB-C2B-C3B	2.89	133.34	126.55
26	a	406	CLA	CHB-C4A-NA	2.89	128.57	124.40
31	4	623	BCR	C3-C4-C5	-2.89	108.91	114.06
26	C	505	CLA	CGD-CBD-CAD	2.89	120.19	110.85
28	g	1622	XAT	C24-C23-C22	-2.89	105.39	110.79
26	B	613	CLA	CMD-C2D-C3D	2.88	134.30	127.69
26	6	612	CLA	CAA-C2A-C3A	-2.88	105.22	113.00
26	B	606	CLA	CHB-C4A-NA	2.88	128.56	124.40
25	N	606	CHL	C3D-C4D-ND	2.88	117.56	112.94
27	4	620	LUT	C31-C30-C29	-2.88	123.24	127.28
25	N	609	CHL	C4-C3-C5	2.88	120.22	115.23
25	S	601	CHL	CMB-C2B-C3B	2.88	130.43	124.68
25	s	601	CHL	CMB-C2B-C3B	2.88	130.43	124.68
26	S	610	CLA	CHB-C4A-NA	2.88	128.55	124.40
31	b	618	BCR	C10-C11-C12	-2.88	114.87	123.20
38	A	414	PL9	C8-C7-C3	2.87	119.46	112.03
37	z	101	LMG	O8-C28-O10	-2.87	116.44	123.63
26	s	613	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
37	Z	101	LMG	O8-C28-O10	-2.87	116.44	123.63
25	N	606	CHL	C1C-CHC-C4B	2.87	126.35	116.07
31	b	618	BCR	C11-C10-C9	-2.87	123.25	127.28
26	b	606	CLA	CHB-C4A-NA	2.87	128.55	124.40
36	B	623	SQD	O7-S-C6	2.87	111.04	106.76
25	n	605	CHL	CMA-C3A-C4A	-2.87	108.42	114.61
25	y	609	CHL	CMB-C2B-C3B	2.87	130.42	124.68
31	a	411	BCR	C21-C20-C19	-2.87	114.88	123.20
26	S	612	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
25	n	605	CHL	O2A-CGA-CBA	2.87	120.59	111.83
27	2	1620	LUT	C15-C14-C13	-2.87	123.25	127.28
36	b	623	SQD	O7-S-C6	2.87	111.04	106.76
37	C	521	LMG	O6-C1-O1	-2.87	103.26	110.04
26	8	604	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
37	d	411	LMG	O6-C1-O1	-2.87	103.27	110.04
28	G	1622	XAT	C24-C23-C22	-2.87	105.43	110.79
26	c	503	CLA	CHB-C4A-NA	2.87	128.54	124.40
37	D	411	LMG	O6-C1-O1	-2.87	103.27	110.04
26	b	613	CLA	O2D-CGD-CBD	2.87	116.24	111.23
25	7	601	CHL	O2A-CGA-CBA	2.87	120.58	111.83
26	s	612	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
26	s	610	CLA	CMB-C2B-C1B	-2.87	121.05	125.42
26	8	612	CLA	CHB-C4A-NA	2.87	128.54	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	S	602	CLA	CMD-C2D-C1D	-2.87	119.68	124.73
25	G	608	CHL	CBC-CAC-C3C	-2.86	108.77	112.87
25	g	608	CHL	CBC-CAC-C3C	-2.86	108.77	112.87
26	B	607	CLA	CMB-C2B-C1B	-2.86	121.06	125.42
26	y	612	CLA	C3B-C4B-NB	-2.86	107.97	110.53
31	A	411	BCR	C21-C20-C19	-2.86	114.90	123.20
25	n	606	CHL	C1C-CHC-C4B	2.86	126.31	116.07
26	s	610	CLA	CHB-C4A-NA	2.86	128.53	124.40
25	s	607	CHL	C3D-C4D-ND	2.86	117.53	112.94
25	n	609	CHL	CMA-C3A-C4A	-2.86	108.44	114.61
26	s	609	CLA	C3B-C4B-NB	-2.86	107.97	110.53
26	n	602	CLA	CAC-C3C-C4C	2.86	128.51	124.79
27	6	1620	LUT	C15-C14-C13	-2.86	123.27	127.28
26	6	613	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
25	3	601	CHL	O2A-CGA-CBA	2.86	120.55	111.83
25	N	605	CHL	CMA-C3A-C4A	-2.86	108.45	114.61
25	N	605	CHL	O2A-CGA-CBA	2.86	120.55	111.83
26	R	601	CLA	CMB-C2B-C1B	-2.86	121.07	125.42
26	2	602	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
26	S	613	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
26	r	601	CLA	CMB-C2B-C1B	-2.85	121.07	125.42
25	S	607	CHL	C3D-C4D-ND	2.85	117.52	112.94
26	r	602	CLA	C3B-C4B-NB	-2.85	107.98	110.53
37	c	521	LMG	O6-C1-O1	-2.85	103.30	110.04
26	s	602	CLA	CMD-C2D-C1D	-2.85	119.70	124.73
26	6	602	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
26	N	612	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
26	4	604	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
26	S	603	CLA	C2A-C1A-CHA	2.85	128.81	123.87
26	B	613	CLA	O2D-CGD-CBD	2.85	116.21	111.23
26	r	604	CLA	CHB-C4A-NA	2.85	128.51	124.40
26	3	613	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
27	S	1621	LUT	C8-C9-C10	-2.85	114.53	119.01
26	S	611	CLA	C3B-C4B-NB	-2.85	107.99	110.53
26	g	610	CLA	C1-C2-C3	-2.85	121.53	126.20
26	S	610	CLA	CMB-C2B-C1B	-2.85	121.08	125.42
28	2	1622	XAT	C4-C3-C2	-2.85	105.46	110.79
27	2	1620	LUT	C20-C13-C12	2.85	122.44	118.09
26	2	613	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
26	8	603	CLA	CAA-C2A-C3A	-2.85	105.31	113.00
25	N	601	CHL	CMD-C2D-C3D	-2.85	119.00	124.68
26	C	501	CLA	O2D-CGD-CBD	2.85	116.21	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	607	CLA	CMB-C2B-C1B	-2.85	121.08	125.42
26	s	603	CLA	C2A-C1A-CHA	2.85	128.81	123.87
25	g	606	CHL	C1C-CHC-C4B	2.85	126.25	116.07
26	c	501	CLA	O2D-CGD-CBD	2.85	116.20	111.23
27	s	1621	LUT	C8-C9-C10	-2.84	114.53	119.01
26	5	603	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
25	N	609	CHL	CMA-C3A-C4A	-2.84	108.48	114.61
27	3	1620	LUT	C7-C8-C9	-2.84	122.03	126.23
29	N	1623	NEX	C24-C23-C22	-2.84	105.47	110.79
26	C	503	CLA	CHB-C4A-NA	2.84	128.50	124.40
26	7	613	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
25	1	608	CHL	C3D-C4D-ND	2.84	117.49	112.94
25	5	608	CHL	C3D-C4D-ND	2.84	117.49	112.94
26	N	602	CLA	CAC-C3C-C4C	2.84	128.48	124.79
28	6	1622	XAT	C4-C3-C2	-2.84	105.48	110.79
25	n	601	CHL	C1-O2A-CGA	2.84	123.52	116.65
26	Y	612	CLA	C3B-C4B-NB	-2.84	108.00	110.53
26	5	602	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
25	n	601	CHL	CMD-C2D-C3D	-2.84	119.01	124.68
25	G	608	CHL	C3D-C4D-ND	2.84	117.49	112.94
29	7	1623	NEX	C39-C29-C30	-2.84	118.22	122.82
25	g	609	CHL	CAA-C2A-C3A	-2.84	105.33	113.00
25	G	606	CHL	C1C-CHC-C4B	2.84	126.21	116.07
26	4	603	CLA	CAA-C2A-C3A	-2.83	105.34	113.00
26	1	603	CLA	CBC-CAC-C3C	-2.83	104.74	112.42
26	c	507	CLA	C2A-C1A-CHA	2.83	128.78	123.87
29	n	1623	NEX	C24-C23-C22	-2.83	105.49	110.79
26	n	613	CLA	CHB-C4A-NA	2.83	128.49	124.40
26	C	513	CLA	CMB-C2B-C3B	2.83	133.21	126.55
26	c	513	CLA	CMB-C2B-C3B	2.83	133.21	126.55
31	C	516	BCR	C29-C30-C25	2.83	114.55	110.44
36	b	623	SQD	O5-C1-C2	2.83	116.19	110.37
26	R	604	CLA	CHB-C4A-NA	2.83	128.49	124.40
26	5	603	CLA	CBC-CAC-C3C	-2.83	104.75	112.42
26	G	610	CLA	C1-C2-C3	-2.83	121.56	126.20
26	d	403	CLA	CMB-C2B-C3B	2.83	133.21	126.55
26	1	603	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
26	n	612	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
25	1	607	CHL	O1D-CGD-CBD	-2.83	120.43	124.72
36	B	623	SQD	O5-C1-C2	2.83	116.18	110.37
25	5	609	CHL	C1-C2-C3	-2.83	121.56	126.20
26	D	403	CLA	CMB-C2B-C3B	2.83	133.20	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	6	2630	LHG	O8-C23-C24	2.83	120.45	111.83
28	1	1622	XAT	C18-C5-C4	2.83	117.42	114.24
25	G	609	CHL	CAA-C2A-C3A	-2.83	105.36	113.00
30	2	2630	LHG	O8-C23-C24	2.83	120.45	111.83
26	3	603	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
26	7	603	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
25	N	601	CHL	C1-O2A-CGA	2.82	123.49	116.65
27	7	1620	LUT	C7-C8-C9	-2.82	122.06	126.23
26	G	602	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
31	C	515	BCR	C37-C22-C23	2.82	122.40	118.09
31	c	515	BCR	C37-C22-C23	2.82	122.40	118.09
26	6	603	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
26	C	507	CLA	C2A-C1A-CHA	2.82	128.76	123.87
26	4	612	CLA	CHB-C4A-NA	2.82	128.47	124.40
27	6	1620	LUT	C20-C13-C12	2.82	122.39	118.09
25	y	601	CHL	C1-O2A-CGA	2.82	123.47	116.65
26	g	602	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
25	g	608	CHL	C3D-C4D-ND	2.82	117.46	112.94
25	3	601	CHL	O1D-CGD-CBD	-2.82	120.45	124.72
25	7	601	CHL	O1D-CGD-CBD	-2.82	120.45	124.72
26	s	611	CLA	C3B-C4B-NB	-2.82	108.02	110.53
29	7	1623	NEX	C30-C31-C32	-2.81	115.04	123.20
29	3	1623	NEX	C39-C29-C30	-2.81	118.26	122.82
31	c	516	BCR	C15-C14-C13	-2.81	123.33	127.28
25	5	607	CHL	O1D-CGD-CBD	-2.81	120.45	124.72
36	A	418	SQD	O47-C7-C8	2.81	117.57	111.48
28	5	1622	XAT	C18-C5-C4	2.81	117.40	114.24
29	3	1623	NEX	C30-C31-C32	-2.81	115.05	123.20
28	3	1622	XAT	C40-C33-C32	2.81	122.39	118.09
25	Y	601	CHL	C1-O2A-CGA	2.81	123.46	116.65
26	1	602	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
25	1	609	CHL	C1-C2-C3	-2.81	121.59	126.20
27	4	620	LUT	C21-C26-C27	-2.81	109.59	112.83
26	R	602	CLA	C3B-C4B-NB	-2.81	108.02	110.53
39	B	626	DGD	C3G-C2G-C1G	-2.81	105.24	111.78
27	n	1621	LUT	C15-C35-C34	-2.81	117.77	123.52
26	b	617	CLA	CHB-C4A-NA	2.81	128.45	124.40
31	B	618	BCR	C33-C5-C6	-2.81	121.42	124.48
31	b	618	BCR	C33-C5-C6	-2.81	121.42	124.48
29	7	1623	NEX	C15-C35-C34	-2.81	117.78	123.52
29	g	1623	NEX	C26-C27-C28	-2.81	120.06	125.99
27	8	620	LUT	C21-C26-C27	-2.80	109.60	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	612	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
27	7	1621	LUT	C19-C9-C8	2.80	122.37	118.09
25	s	601	CHL	CMA-C3A-C4A	-2.80	108.57	114.61
27	N	1621	LUT	C15-C35-C34	-2.80	117.79	123.52
26	1	602	CLA	C3B-C4B-NB	-2.80	108.03	110.53
26	3	603	CLA	C2A-C1A-CHA	2.80	128.73	123.87
26	2	603	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
36	b	621	SQD	C44-O6-C1	2.80	119.80	113.80
25	7	606	CHL	CAC-C3C-C4C	2.80	131.22	124.03
25	r	607	CHL	O2A-CGA-CBA	2.80	120.37	111.83
26	7	612	CLA	CAA-C2A-C3A	-2.80	105.44	113.00
36	a	418	SQD	O47-C7-C8	2.80	117.53	111.48
39	b	626	DGD	C3G-C2G-C1G	-2.80	105.26	111.78
27	y	1621	LUT	C21-C26-C27	-2.80	109.61	112.83
28	7	1622	XAT	C40-C33-C32	2.80	122.36	118.09
31	c	516	BCR	C29-C30-C25	2.80	114.50	110.44
31	B	619	BCR	C39-C30-C25	-2.80	105.86	110.24
36	B	621	SQD	C44-O6-C1	2.80	119.79	113.80
26	B	617	CLA	CHB-C4A-NA	2.80	128.43	124.40
27	3	1621	LUT	C19-C9-C8	2.80	122.36	118.09
25	y	606	CHL	O2A-CGA-CBA	2.79	120.36	111.83
26	2	612	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
26	5	602	CLA	C3B-C4B-NB	-2.79	108.04	110.53
26	Y	610	CLA	CHB-C1B-NB	2.79	128.24	124.05
29	G	1623	NEX	C26-C27-C28	-2.79	120.09	125.99
27	G	1621	LUT	C21-C26-C27	-2.79	109.62	112.83
26	y	610	CLA	CHB-C1B-NB	2.79	128.24	124.05
29	3	1623	NEX	C15-C35-C34	-2.79	117.81	123.52
26	3	612	CLA	CAA-C2A-C3A	-2.79	105.46	113.00
26	r	611	CLA	C3B-C4B-NB	-2.79	108.04	110.53
25	3	605	CHL	CAA-C2A-C3A	-2.79	105.47	113.00
25	N	608	CHL	OBD-CAD-C3D	-2.79	123.54	127.89
25	n	608	CHL	OBD-CAD-C3D	-2.79	123.54	127.89
29	y	1623	NEX	C26-C27-C28	-2.79	120.10	125.99
25	R	607	CHL	O2A-CGA-CBA	2.79	120.33	111.83
25	Y	606	CHL	O2A-CGA-CBA	2.79	120.33	111.83
26	R	611	CLA	C3B-C4B-NB	-2.78	108.04	110.53
26	b	605	CLA	CBA-CAA-C2A	2.78	122.08	113.79
26	N	613	CLA	CHB-C4A-NA	2.78	128.42	124.40
25	7	609	CHL	O2A-CGA-CBA	2.78	120.32	111.83
25	7	607	CHL	O1D-CGD-CBD	-2.78	120.50	124.72
31	C	516	BCR	C15-C14-C13	-2.78	123.37	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	S	1620	LUT	C7-C8-C9	-2.78	122.12	126.23
31	D	404	BCR	C21-C20-C19	-2.78	115.14	123.20
31	d	404	BCR	C21-C20-C19	-2.78	115.14	123.20
25	g	601	CHL	O2D-CGD-O1D	-2.78	118.43	123.85
25	3	609	CHL	O2A-CGA-CBA	2.78	120.32	111.83
25	S	601	CHL	CMA-C3A-C4A	-2.78	108.62	114.61
25	7	605	CHL	CAA-C2A-C3A	-2.78	105.48	113.00
27	g	1621	LUT	C21-C26-C27	-2.78	109.63	112.83
26	n	603	CLA	C1-C2-C3	-2.78	121.64	126.20
25	3	607	CHL	O1D-CGD-CBD	-2.78	120.51	124.72
31	b	619	BCR	C39-C30-C25	-2.78	105.88	110.24
27	s	1620	LUT	C7-C8-C9	-2.78	122.12	126.23
25	Y	607	CHL	CAA-CBA-CGA	-2.78	105.31	113.21
25	3	606	CHL	CAC-C3C-C4C	2.78	131.17	124.03
26	7	603	CLA	C2A-C1A-CHA	2.78	128.69	123.87
26	N	610	CLA	O2A-CGA-O1A	-2.78	116.68	123.63
25	S	607	CHL	CMA-C3A-C4A	-2.78	108.63	114.61
26	r	609	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
37	c	521	LMG	O1-C7-C8	-2.78	104.06	110.82
29	Y	1623	NEX	C24-C23-C22	-2.78	105.60	110.79
39	C	518	DGD	O3E-C3E-C2E	-2.77	103.83	110.38
39	c	518	DGD	O3E-C3E-C2E	-2.77	103.83	110.38
37	C	521	LMG	O1-C7-C8	-2.77	104.07	110.82
26	a	410	CLA	CAA-CBA-CGA	-2.77	105.33	113.21
25	y	607	CHL	CAA-CBA-CGA	-2.77	105.33	113.21
25	n	606	CHL	O2A-CGA-CBA	2.77	120.29	111.83
25	s	607	CHL	CMA-C3A-C4A	-2.77	108.64	114.61
35	a	409	PHO	CBC-CAC-C3C	2.77	116.84	112.87
26	6	603	CLA	CBC-CAC-C3C	-2.77	104.90	112.42
27	Y	1621	LUT	C21-C26-C27	-2.77	109.64	112.83
29	Y	1623	NEX	C26-C27-C28	-2.77	120.14	125.99
25	G	601	CHL	O2D-CGD-O1D	-2.77	118.46	123.85
26	B	605	CLA	CBA-CAA-C2A	2.77	122.03	113.79
26	S	610	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
26	s	610	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
31	c	515	BCR	C3-C4-C5	-2.77	109.12	114.06
27	5	1621	LUT	C10-C11-C12	-2.77	115.19	123.20
26	2	603	CLA	CBC-CAC-C3C	-2.77	104.92	112.42
31	C	515	BCR	C3-C4-C5	-2.77	109.12	114.06
26	2	602	CLA	C1-C2-C3	-2.77	121.67	126.20
29	y	1623	NEX	C24-C23-C22	-2.77	105.62	110.79
26	A	410	CLA	CAA-CBA-CGA	-2.76	105.36	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	2	1621	LUT	C19-C9-C8	2.76	122.31	118.09
26	n	611	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
25	8	607	CHL	C1C-CHC-C4B	2.76	125.96	116.07
35	A	409	PHO	CBC-CAC-C3C	2.76	116.83	112.87
25	3	608	CHL	C3D-C4D-ND	2.76	117.37	112.94
27	1	1621	LUT	C10-C11-C12	-2.76	115.20	123.20
26	C	507	CLA	CAA-C2A-C3A	-2.76	105.54	113.00
25	N	606	CHL	O2A-CGA-CBA	2.76	120.25	111.83
26	N	603	CLA	C1-C2-C3	-2.76	121.67	126.20
25	R	606	CHL	O2D-CGD-O1D	-2.76	118.48	123.85
26	n	610	CLA	O2A-CGA-O1A	-2.76	116.72	123.63
26	c	507	CLA	CAA-C2A-C3A	-2.76	105.54	113.00
31	b	620	BCR	C20-C21-C22	-2.76	123.41	127.28
26	8	610	CLA	C3B-C4B-NB	-2.76	108.07	110.53
31	B	620	BCR	C20-C21-C22	-2.76	123.41	127.28
26	6	602	CLA	C1-C2-C3	-2.76	121.68	126.20
25	G	601	CHL	C1C-C2C-CMC	2.76	131.77	126.80
26	4	610	CLA	C3B-C4B-NB	-2.75	108.07	110.53
25	G	607	CHL	CAA-C2A-C3A	-2.75	105.56	113.00
25	n	607	CHL	CED-O2D-CGD	2.75	122.16	115.92
25	S	601	CHL	C1C-CHC-C4B	2.75	125.92	116.07
25	4	607	CHL	C1C-CHC-C4B	2.75	125.92	116.07
29	n	1623	NEX	C26-C27-C28	-2.75	120.17	125.99
27	G	1620	LUT	C39-C29-C28	2.75	122.29	118.09
27	6	1621	LUT	C19-C9-C8	2.75	122.29	118.09
25	r	606	CHL	O2D-CGD-O1D	-2.75	118.49	123.85
25	g	601	CHL	C1C-C2C-CMC	2.75	131.76	126.80
25	7	608	CHL	C3D-C4D-ND	2.75	117.35	112.94
26	R	609	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
26	B	614	CLA	C4-C3-C5	2.75	120.00	115.23
26	B	612	CLA	CHB-C4A-NA	2.75	128.37	124.40
26	2	612	CLA	CHB-C4A-NA	2.75	128.37	124.40
25	Y	608	CHL	O1D-CGD-CBD	-2.75	120.56	124.72
26	2	614	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
26	n	603	CLA	C2D-C1D-ND	-2.75	107.41	110.13
25	n	608	CHL	C1-C2-C3	-2.75	121.70	126.20
25	s	601	CHL	C1C-CHC-C4B	2.75	125.89	116.07
26	4	611	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
27	g	1620	LUT	C39-C29-C28	2.74	122.28	118.09
26	N	612	CLA	CHB-C4A-NA	2.74	128.36	124.40
26	n	612	CLA	CHB-C4A-NA	2.74	128.36	124.40
25	n	608	CHL	C3D-C4D-ND	2.74	117.34	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	g	607	CHL	CAA-C2A-C3A	-2.74	105.59	113.00
26	N	611	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
29	N	1623	NEX	C26-C27-C28	-2.74	120.20	125.99
25	8	608	CHL	CBC-CAC-C3C	-2.74	108.95	112.87
31	C	515	BCR	C38-C26-C25	-2.74	121.49	124.48
28	r	622	XAT	C31-C32-C33	-2.74	118.85	126.36
26	S	614	CLA	CMB-C2B-C3B	2.74	133.00	126.55
26	s	614	CLA	CMB-C2B-C3B	2.74	133.00	126.55
25	N	607	CHL	CED-O2D-CGD	2.74	122.13	115.92
28	R	622	XAT	C31-C32-C33	-2.74	118.85	126.36
39	c	518	DGD	CDB-CCB-CBB	-2.74	100.53	114.37
25	5	606	CHL	C1C-CHC-C4B	2.74	125.86	116.07
39	C	518	DGD	CDB-CCB-CBB	-2.74	100.53	114.37
26	b	614	CLA	C4-C3-C5	2.74	119.98	115.23
31	D	404	BCR	C10-C11-C12	-2.74	115.27	123.20
31	d	404	BCR	C10-C11-C12	-2.74	115.27	123.20
26	b	612	CLA	CHB-C4A-NA	2.73	128.34	124.40
39	h	102	DGD	CDB-CCB-CBB	-2.73	100.56	114.37
25	4	601	CHL	C3D-C4D-ND	2.73	117.32	112.94
25	g	606	CHL	CBC-CAC-C3C	-2.73	108.96	112.87
26	6	604	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
25	1	606	CHL	C1C-CHC-C4B	2.73	125.84	116.07
26	1	603	CLA	CAA-C2A-C3A	-2.73	105.62	113.00
26	5	603	CLA	CAA-C2A-C3A	-2.73	105.62	113.00
28	7	1622	XAT	C35-C34-C33	-2.73	123.45	127.28
25	4	608	CHL	CBC-CAC-C3C	-2.73	108.97	112.87
26	6	614	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
26	8	611	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
27	2	1620	LUT	C39-C29-C28	2.73	122.25	118.09
25	8	601	CHL	C3D-C4D-ND	2.73	117.31	112.94
39	h	102	DGD	C3D-C4D-C5D	-2.73	105.29	110.23
26	N	603	CLA	C2D-C1D-ND	-2.73	107.43	110.13
25	N	608	CHL	C1-C2-C3	-2.73	121.73	126.20
26	7	611	CLA	CHB-C4A-NA	2.72	128.33	124.40
25	g	609	CHL	C4-C3-C5	2.72	119.96	115.23
25	y	608	CHL	O1D-CGD-CBD	-2.72	120.59	124.72
25	5	609	CHL	O2A-CGA-CBA	2.72	120.14	111.83
28	2	1622	XAT	C26-C27-C28	-2.72	120.23	125.99
25	G	609	CHL	C3D-C4D-ND	2.72	117.31	112.94
25	G	606	CHL	CBC-CAC-C3C	-2.72	108.97	112.87
25	1	609	CHL	O2A-CGA-CBA	2.72	120.14	111.83
39	H	102	DGD	CDB-CCB-CBB	-2.72	100.61	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	H	101	BCR	C3-C4-C5	-2.72	109.20	114.06
31	C	514	BCR	C8-C9-C10	-2.72	114.73	119.01
28	3	1622	XAT	C35-C34-C33	-2.72	123.46	127.28
27	6	1620	LUT	C39-C29-C28	2.72	122.24	118.09
26	R	611	CLA	C2C-C1C-NC	2.72	112.84	109.98
26	r	603	CLA	CHB-C4A-NA	2.72	128.32	124.40
26	C	501	CLA	C3B-C4B-NB	-2.72	108.10	110.53
26	c	501	CLA	C3B-C4B-NB	-2.72	108.10	110.53
40	D	401	BCT	O3-C-O1	-2.72	112.72	119.68
31	c	514	BCR	C8-C9-C10	-2.72	114.73	119.01
25	G	609	CHL	C4-C3-C5	2.72	119.94	115.23
26	3	611	CLA	CHB-C4A-NA	2.72	128.32	124.40
26	y	604	CLA	C1-C2-C3	-2.72	122.37	126.76
28	r	622	XAT	C8-C9-C10	-2.71	114.74	119.01
31	h	101	BCR	C3-C4-C5	-2.71	109.22	114.06
25	R	608	CHL	OBD-CAD-C3D	-2.71	123.66	127.89
26	r	611	CLA	C2C-C1C-NC	2.71	112.83	109.98
25	N	608	CHL	C3D-C4D-ND	2.71	117.29	112.94
25	3	605	CHL	C1C-CHC-C4B	2.71	125.78	116.07
26	2	604	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
26	Y	604	CLA	C1-C2-C3	-2.71	122.37	126.76
26	C	503	CLA	C3B-C4B-NB	-2.71	108.11	110.53
26	c	503	CLA	C3B-C4B-NB	-2.71	108.11	110.53
26	n	603	CLA	C3B-C4B-NB	-2.71	108.11	110.53
26	6	612	CLA	CHB-C4A-NA	2.71	128.31	124.40
25	5	601	CHL	C1C-CHC-C4B	2.71	125.77	116.07
28	6	1622	XAT	C15-C35-C34	-2.71	117.98	123.52
31	c	515	BCR	C38-C26-C25	-2.71	121.53	124.48
26	7	610	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
26	a	406	CLA	CMB-C2B-C3B	2.71	132.92	126.55
26	3	610	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
30	C	522	LHG	O8-C23-C24	2.71	120.09	111.83
25	7	605	CHL	C1C-CHC-C4B	2.71	125.75	116.07
39	H	102	DGD	C3D-C4D-C5D	-2.71	105.33	110.23
26	c	513	CLA	CHB-C4A-NA	2.71	128.31	124.40
28	6	1622	XAT	C26-C27-C28	-2.71	120.27	125.99
26	g	603	CLA	C1-C2-C3	-2.71	121.76	126.20
25	g	609	CHL	C3D-C4D-ND	2.71	117.28	112.94
26	S	612	CLA	CHB-C4A-NA	2.70	128.30	124.40
28	2	1622	XAT	C15-C35-C34	-2.70	117.99	123.52
26	r	610	CLA	O2A-CGA-O1A	-2.70	116.86	123.63
26	3	613	CLA	CHB-C4A-NA	2.70	128.30	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	406	CLA	CMB-C2B-C3B	2.70	132.91	126.55
25	5	606	CHL	O1D-CGD-CBD	-2.70	120.62	124.72
26	8	602	CLA	CHB-C4A-NA	2.70	128.30	124.40
31	C	514	BCR	C34-C9-C8	2.70	122.22	118.09
25	1	601	CHL	C1C-CHC-C4B	2.70	125.74	116.07
40	d	401	BCT	O3-C-O1	-2.70	112.76	119.68
28	R	622	XAT	C8-C9-C10	-2.70	114.76	119.01
27	2	1620	LUT	C11-C10-C9	-2.70	123.49	127.28
25	1	606	CHL	O1D-CGD-CBD	-2.70	120.63	124.72
27	6	1621	LUT	C39-C29-C28	2.70	122.22	118.09
30	c	522	LHG	O8-C23-C24	2.70	120.07	111.83
26	Y	611	CLA	CHB-C4A-NA	2.70	128.30	124.40
26	N	603	CLA	C3B-C4B-NB	-2.70	108.12	110.53
25	y	601	CHL	C1C-C2C-CMC	2.70	131.67	126.80
26	7	613	CLA	CHB-C4A-NA	2.70	128.30	124.40
26	c	511	CLA	C1-C2-C3	-2.70	121.77	126.20
27	2	1621	LUT	C39-C29-C28	2.70	122.21	118.09
26	C	511	CLA	C1-C2-C3	-2.70	121.77	126.20
25	2	605	CHL	CBC-CAC-C3C	-2.70	109.01	112.87
26	B	604	CLA	O2D-CGD-CBD	2.70	115.95	111.23
25	y	608	CHL	C1-C2-C3	-2.70	121.78	126.20
26	5	613	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
27	R	620	LUT	C20-C13-C12	2.70	122.21	118.09
26	C	513	CLA	CHB-C4A-NA	2.70	128.29	124.40
27	G	1621	LUT	C28-C29-C30	-2.70	114.77	119.01
27	g	1621	LUT	C28-C29-C30	-2.70	114.77	119.01
25	6	605	CHL	CBC-CAC-C3C	-2.70	109.01	112.87
26	R	603	CLA	CHB-C4A-NA	2.69	128.29	124.40
26	G	603	CLA	C1-C2-C3	-2.69	121.78	126.20
26	y	611	CLA	CHB-C4A-NA	2.69	128.29	124.40
26	s	612	CLA	CHB-C4A-NA	2.69	128.29	124.40
27	r	620	LUT	C19-C9-C8	2.69	122.20	118.09
25	r	608	CHL	OBD-CAD-C3D	-2.69	123.69	127.89
26	A	405	CLA	CMB-C2B-C3B	2.69	132.88	126.55
25	G	609	CHL	O2D-CGD-O1D	-2.69	118.61	123.85
25	g	601	CHL	CMA-C3A-C4A	-2.69	108.82	114.61
27	6	1620	LUT	C21-C26-C27	-2.69	109.73	112.83
26	3	611	CLA	CAA-C2A-C3A	-2.69	105.74	113.00
26	G	602	CLA	CMB-C2B-C3B	2.69	132.87	126.55
26	R	610	CLA	O2A-CGA-O1A	-2.69	116.91	123.63
25	G	601	CHL	CMA-C3A-C4A	-2.69	108.82	114.61
25	5	607	CHL	CAA-C2A-C3A	-2.69	105.74	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	N	2630	LHG	C20-C19-C18	-2.69	100.79	114.37
27	r	620	LUT	C20-C13-C12	2.69	122.19	118.09
26	7	611	CLA	CAA-C2A-C3A	-2.69	105.74	113.00
26	N	603	CLA	CBC-CAC-C3C	-2.69	105.14	112.42
36	B	623	SQD	C44-O6-C1	2.69	119.55	113.80
25	g	607	CHL	CMA-C3A-C4A	-2.68	108.83	114.61
26	b	604	CLA	O2D-CGD-CBD	2.68	115.92	111.23
25	g	609	CHL	O2D-CGD-O1D	-2.68	118.62	123.85
25	N	607	CHL	CMA-C3A-C4A	-2.68	108.83	114.61
25	1	607	CHL	CAA-C2A-C3A	-2.68	105.75	113.00
27	R	620	LUT	C19-C9-C8	2.68	122.19	118.09
31	c	514	BCR	C34-C9-C8	2.68	122.19	118.09
26	C	509	CLA	CMB-C2B-C3B	2.68	132.86	126.55
27	2	1620	LUT	C21-C26-C27	-2.68	109.74	112.83
26	n	603	CLA	CBC-CAC-C3C	-2.68	105.16	112.42
26	c	508	CLA	CHB-C4A-NA	2.68	128.27	124.40
25	Y	601	CHL	C1C-C2C-CMC	2.68	131.63	126.80
35	A	408	PHO	O2A-CGA-O1A	-2.68	116.93	123.63
36	a	412	SQD	O48-C23-O10	-2.68	116.93	123.63
26	c	510	CLA	CHB-C4A-NA	2.68	128.27	124.40
30	n	2630	LHG	C20-C19-C18	-2.68	100.83	114.37
25	Y	608	CHL	OBD-CAD-C3D	-2.68	123.71	127.89
25	G	607	CHL	CMB-C2B-C3B	2.68	130.03	124.68
25	Y	608	CHL	C1-C2-C3	-2.68	121.81	126.20
36	b	623	SQD	C44-O6-C1	2.68	119.54	113.80
25	G	605	CHL	OMC-CMC-C2C	-2.68	120.47	125.12
26	a	405	CLA	CMB-C2B-C3B	2.68	132.84	126.55
25	5	606	CHL	CMB-C2B-C3B	2.68	130.03	124.68
26	4	602	CLA	CHB-C4A-NA	2.68	128.26	124.40
26	R	602	CLA	CHB-C4A-NA	2.68	128.26	124.40
26	r	602	CLA	CHB-C4A-NA	2.68	128.26	124.40
31	B	618	BCR	C37-C22-C23	2.67	122.17	118.09
26	b	612	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
31	B	620	BCR	C29-C30-C25	2.67	114.32	110.44
31	H	101	BCR	C38-C26-C25	-2.67	121.57	124.48
25	G	607	CHL	CMA-C3A-C4A	-2.67	108.85	114.61
28	Y	1622	XAT	C40-C33-C32	2.67	122.17	118.09
35	a	408	PHO	O2A-CGA-O1A	-2.67	116.95	123.63
26	y	603	CLA	C1-C2-C3	-2.67	121.82	126.20
26	c	512	CLA	C3B-C4B-NB	-2.67	108.15	110.53
26	y	612	CLA	CHB-C4A-NA	2.67	128.25	124.40
26	1	613	CLA	O2D-CGD-O1D	-2.67	118.65	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	612	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
25	2	607	CHL	CAA-C2A-C3A	-2.67	105.79	113.00
26	g	602	CLA	CMB-C2B-C3B	2.67	132.82	126.55
26	c	509	CLA	CMB-C2B-C3B	2.67	132.82	126.55
25	7	607	CHL	C4-C3-C5	2.66	119.85	115.23
26	5	604	CLA	CHB-C1B-NB	2.66	128.04	124.05
25	6	607	CHL	CAA-C2A-C3A	-2.66	105.80	113.00
26	C	508	CLA	CHB-C4A-NA	2.66	128.24	124.40
25	1	606	CHL	CMB-C2B-C3B	2.66	130.00	124.68
36	A	412	SQD	O48-C23-O10	-2.66	116.97	123.63
31	h	101	BCR	C38-C26-C25	-2.66	121.58	124.48
36	A	412	SQD	C3-C4-C5	2.66	115.06	110.23
26	7	604	CLA	CMB-C2B-C1B	-2.66	121.37	125.42
26	n	614	CLA	CHB-C4A-NA	2.66	128.24	124.40
25	g	607	CHL	CMB-C2B-C3B	2.66	130.00	124.68
27	6	1620	LUT	C11-C10-C9	-2.66	123.55	127.28
26	B	604	CLA	CHB-C1B-NB	2.66	128.04	124.05
28	y	1622	XAT	C40-C33-C32	2.66	122.15	118.09
28	3	1622	XAT	C18-C5-C4	2.66	117.23	114.24
26	s	611	CLA	CHB-C4A-NA	2.66	128.24	124.40
25	7	606	CHL	CMB-C2B-C3B	2.66	129.99	124.68
36	a	412	SQD	C3-C4-C5	2.66	115.05	110.23
25	g	605	CHL	OMC-CMC-C2C	-2.66	120.51	125.12
26	8	611	CLA	CHB-C4A-NA	2.66	128.23	124.40
31	b	620	BCR	C29-C30-C25	2.66	114.30	110.44
31	b	618	BCR	C37-C22-C23	2.66	122.14	118.09
26	B	602	CLA	CHB-C4A-NA	2.65	128.23	124.40
25	n	607	CHL	CMA-C3A-C4A	-2.65	108.89	114.61
26	C	510	CLA	CHB-C4A-NA	2.65	128.23	124.40
29	g	1623	NEX	C24-C23-C22	-2.65	105.83	110.79
31	H	101	BCR	C16-C15-C14	-2.65	118.09	123.52
29	6	1623	NEX	C26-C27-C28	-2.65	120.38	125.99
25	g	605	CHL	CMB-C2B-C3B	2.65	129.98	124.68
26	C	512	CLA	C3B-C4B-NB	-2.65	108.16	110.53
25	y	608	CHL	OBD-CAD-C3D	-2.65	123.75	127.89
26	3	604	CLA	CMB-C2B-C1B	-2.65	121.38	125.42
25	3	607	CHL	C4-C3-C5	2.65	119.83	115.23
31	b	619	BCR	C29-C30-C25	2.65	114.29	110.44
29	G	1623	NEX	C24-C23-C22	-2.65	105.83	110.79
25	6	605	CHL	O1D-CGD-CBD	-2.65	120.70	124.72
25	1	601	CHL	CMB-C2B-C3B	2.65	129.98	124.68
25	5	601	CHL	CMB-C2B-C3B	2.65	129.98	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	N	610	CLA	C2A-C1A-CHA	2.65	128.46	123.87
26	b	602	CLA	CHB-C4A-NA	2.65	128.22	124.40
30	L	101	LHG	C11-C10-C9	-2.65	100.98	114.37
30	l	101	LHG	C11-C10-C9	-2.65	100.98	114.37
26	G	612	CLA	CHB-C4A-NA	2.65	128.22	124.40
26	S	611	CLA	CHB-C4A-NA	2.65	128.22	124.40
26	Y	612	CLA	CHB-C4A-NA	2.65	128.22	124.40
29	2	1623	NEX	C26-C27-C28	-2.65	120.40	125.99
26	3	604	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
31	b	620	BCR	C33-C5-C6	-2.65	121.60	124.48
36	a	418	SQD	O47-C45-C44	2.65	117.83	108.34
36	A	418	SQD	O47-C45-C44	2.64	117.83	108.34
26	5	611	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
28	1	1622	XAT	C26-C27-C28	-2.64	120.41	125.99
26	4	611	CLA	CHB-C4A-NA	2.64	128.21	124.40
27	5	1621	LUT	C30-C31-C32	-2.64	115.55	123.20
28	5	1622	XAT	C26-C27-C28	-2.64	120.41	125.99
28	7	1622	XAT	C18-C5-C4	2.64	117.21	114.24
25	4	601	CHL	CMB-C2B-C3B	2.64	129.96	124.68
31	B	620	BCR	C16-C15-C14	-2.64	118.12	123.52
26	1	604	CLA	CHB-C1B-NB	2.64	128.01	124.05
26	b	604	CLA	CHB-C1B-NB	2.64	128.01	124.05
30	B	2630	LHG	O8-C23-C24	2.64	119.88	111.83
25	N	606	CHL	O2D-CGD-O1D	-2.64	118.71	123.85
26	g	603	CLA	C3B-C4B-NB	-2.64	108.17	110.53
26	g	612	CLA	CHB-C4A-NA	2.64	128.21	124.40
26	N	611	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
26	n	611	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
31	c	515	BCR	C23-C22-C21	-2.64	114.86	119.01
25	G	605	CHL	CMB-C2B-C3B	2.64	129.95	124.68
25	1	606	CHL	CBC-CAC-C3C	-2.64	109.10	112.87
36	a	412	SQD	O8-S-C6	2.63	111.06	105.97
26	Y	603	CLA	C1-C2-C3	-2.63	121.88	126.20
31	h	101	BCR	C16-C15-C14	-2.63	118.13	123.52
26	b	605	CLA	CHC-C4B-NB	2.63	128.00	124.05
31	B	619	BCR	C29-C30-C25	2.63	114.27	110.44
31	B	620	BCR	C33-C5-C6	-2.63	121.61	124.48
36	A	412	SQD	O8-S-C6	2.63	111.06	105.97
26	N	614	CLA	CHB-C4A-NA	2.63	128.20	124.40
25	n	606	CHL	O2D-CGD-O1D	-2.63	118.72	123.85
25	Y	601	CHL	CAC-C3C-C4C	2.63	130.79	124.03
25	3	606	CHL	CMB-C2B-C3B	2.63	129.94	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	2630	LHG	O8-C23-C24	2.63	119.86	111.83
31	b	620	BCR	C16-C15-C14	-2.63	118.14	123.52
26	7	604	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
25	2	605	CHL	O1D-CGD-CBD	-2.63	120.73	124.72
26	n	610	CLA	C2A-C1A-CHA	2.63	128.43	123.87
26	b	610	CLA	CHC-C4B-NB	2.63	127.99	124.05
25	g	601	CHL	C4C-CHD-C1D	2.63	125.47	116.07
25	2	607	CHL	O2A-CGA-CBA	2.63	119.85	111.83
25	5	606	CHL	CBC-CAC-C3C	-2.63	109.11	112.87
30	c	2630	LHG	C18-C17-C16	-2.63	101.09	114.37
30	n	2630	LHG	C11-C10-C9	-2.63	101.09	114.37
25	y	601	CHL	CAC-C3C-C4C	2.63	130.78	124.03
25	8	601	CHL	CMB-C2B-C3B	2.63	129.93	124.68
29	2	1623	NEX	C24-C23-C22	-2.62	105.88	110.79
31	T	101	BCR	C35-C13-C12	2.62	122.10	118.09
29	5	1623	NEX	C15-C35-C34	-2.62	118.15	123.52
31	C	515	BCR	C23-C22-C21	-2.62	114.88	119.01
30	N	2630	LHG	C11-C10-C9	-2.62	101.11	114.37
25	6	607	CHL	O2A-CGA-CBA	2.62	119.83	111.83
25	G	601	CHL	C4C-CHD-C1D	2.62	125.45	116.07
26	r	612	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
27	3	1620	LUT	C35-C15-C14	-2.62	118.16	123.52
30	C	2630	LHG	C18-C17-C16	-2.62	101.14	114.37
27	N	1620	LUT	C38-C25-C24	-2.62	117.17	123.36
36	a	412	SQD	O48-C23-C24	2.62	119.81	111.83
27	1	1621	LUT	C30-C31-C32	-2.62	115.62	123.20
26	g	612	CLA	CAA-C2A-C3A	-2.62	105.93	113.00
26	B	605	CLA	CHC-C4B-NB	2.62	127.97	124.05
26	G	612	CLA	CAA-C2A-C3A	-2.62	105.93	113.00
29	6	1623	NEX	C24-C23-C22	-2.62	105.90	110.79
25	6	608	CHL	CMB-C2B-C3B	2.61	129.91	124.68
25	1	608	CHL	OBD-CAD-C3D	-2.61	123.81	127.89
25	5	608	CHL	OBD-CAD-C3D	-2.61	123.81	127.89
26	B	610	CLA	CHC-C4B-NB	2.61	127.97	124.05
25	8	601	CHL	O2D-CGD-CBD	2.61	120.31	113.90
26	2	611	CLA	CHB-C4A-NA	2.61	128.17	124.40
25	n	608	CHL	C7-C6-C5	2.61	120.22	113.26
26	R	612	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
26	1	611	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
29	1	1623	NEX	C15-C35-C34	-2.61	118.17	123.52
25	Y	601	CHL	C4C-CHD-C1D	2.61	125.41	116.07
25	y	601	CHL	C4C-CHD-C1D	2.61	125.41	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	612	CLA	CMB-C2B-C3B	2.61	132.69	126.55
25	N	608	CHL	C7-C6-C5	2.61	120.22	113.26
26	1	612	CLA	CHB-C4A-NA	2.61	128.17	124.40
31	b	618	BCR	C3-C4-C5	-2.61	109.40	114.06
25	2	608	CHL	CMB-C2B-C3B	2.61	129.90	124.68
26	6	611	CLA	CHB-C4A-NA	2.61	128.17	124.40
27	4	620	LUT	C15-C35-C34	-2.61	118.18	123.52
26	c	510	CLA	C3B-C4B-NB	-2.61	108.20	110.53
26	C	508	CLA	CHB-C1B-NB	2.61	127.96	124.05
25	4	601	CHL	O2D-CGD-CBD	2.61	120.30	113.90
27	7	1620	LUT	C35-C15-C14	-2.61	118.19	123.52
25	R	608	CHL	O2A-CGA-CBA	2.61	119.78	111.83
25	7	609	CHL	CMB-C2B-C3B	2.61	129.89	124.68
31	B	618	BCR	C3-C4-C5	-2.61	109.41	114.06
25	n	609	CHL	O2D-CGD-O1D	-2.60	118.78	123.85
27	8	620	LUT	C15-C35-C34	-2.60	118.19	123.52
26	b	612	CLA	CMB-C2B-C3B	2.60	132.68	126.55
31	C	516	BCR	C8-C7-C6	-2.60	120.04	127.00
25	1	608	CHL	CBC-CAC-C3C	-2.60	109.15	112.87
36	A	412	SQD	O48-C23-C24	2.60	119.77	111.83
31	c	516	BCR	C8-C7-C6	-2.60	120.05	127.00
26	y	602	CLA	C6-C7-C8	-2.60	107.32	115.97
27	2	1621	LUT	C21-C26-C27	-2.60	109.83	112.83
29	y	1623	NEX	C31-C30-C29	-2.60	123.63	127.28
25	y	609	CHL	O2D-CGD-O1D	-2.60	118.79	123.85
26	3	602	CLA	C4A-NA-C1A	2.60	107.86	106.68
35	A	409	PHO	C1-C2-C3	-2.60	121.94	126.20
26	r	609	CLA	CHB-C4A-NA	2.60	128.15	124.40
25	7	608	CHL	OBD-CAD-C3D	-2.60	123.84	127.89
26	Y	602	CLA	C6-C7-C8	-2.60	107.33	115.97
25	3	609	CHL	CMB-C2B-C3B	2.60	129.87	124.68
25	s	607	CHL	O2A-CGA-CBA	2.60	119.75	111.83
26	R	601	CLA	CHB-C4A-NA	2.60	128.15	124.40
27	3	1620	LUT	C15-C35-C34	-2.60	118.21	123.52
27	G	1621	LUT	C31-C30-C29	-2.60	123.64	127.28
26	1	602	CLA	C4A-NA-C1A	2.60	107.86	106.68
26	5	602	CLA	C4A-NA-C1A	2.60	107.86	106.68
27	6	1621	LUT	C21-C26-C27	-2.59	109.84	112.83
26	Y	610	CLA	C1-C2-C3	-2.59	121.95	126.20
39	h	102	DGD	O3E-C3E-C2E	-2.59	104.26	110.38
30	c	2630	LHG	C20-C19-C18	-2.59	101.25	114.37
26	5	612	CLA	CHB-C4A-NA	2.59	128.14	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	r	608	CHL	O2A-CGA-CBA	2.59	119.75	111.83
39	c	519	DGD	O3E-C3E-C2E	-2.59	104.26	110.38
26	C	505	CLA	C2D-C1D-ND	-2.59	107.56	110.13
26	c	505	CLA	C2D-C1D-ND	-2.59	107.56	110.13
29	Y	1623	NEX	C31-C30-C29	-2.59	123.64	127.28
31	t	101	BCR	C35-C13-C12	2.59	122.05	118.09
25	N	609	CHL	O2D-CGD-O1D	-2.59	118.80	123.85
26	4	603	CLA	CHB-C4A-NA	2.59	128.14	124.40
28	4	622	XAT	C35-C15-C14	-2.59	118.22	123.52
28	5	1622	XAT	C11-C12-C13	-2.59	119.26	126.36
26	b	605	CLA	C16-C17-C18	-2.59	104.37	115.94
26	B	605	CLA	C16-C17-C18	-2.59	104.38	115.94
25	y	608	CHL	O2D-CGD-O1D	-2.59	118.81	123.85
25	n	601	CHL	CAC-C3C-C4C	2.59	130.69	124.03
30	C	2630	LHG	C20-C19-C18	-2.59	101.28	114.37
25	G	607	CHL	O2A-CGA-CBA	2.59	119.73	111.83
25	g	607	CHL	O2A-CGA-CBA	2.59	119.73	111.83
31	c	517	BCR	C33-C5-C4	2.59	119.11	113.60
26	G	603	CLA	C3B-C4B-NB	-2.59	108.22	110.53
25	S	607	CHL	O2A-CGA-CBA	2.59	119.72	111.83
39	H	102	DGD	O3E-C3E-C2E	-2.59	104.28	110.38
27	n	1620	LUT	C38-C25-C24	-2.59	117.24	123.36
25	5	607	CHL	OMC-CMC-C2C	-2.59	120.63	125.12
25	3	601	CHL	C4C-CHD-C1D	2.59	125.32	116.07
25	7	601	CHL	C4C-CHD-C1D	2.59	125.32	116.07
28	8	622	XAT	C35-C15-C14	-2.59	118.23	123.52
25	s	608	CHL	CMB-C2B-C3B	2.59	129.85	124.68
25	S	608	CHL	CMB-C2B-C3B	2.58	129.85	124.68
26	c	508	CLA	CHB-C1B-NB	2.58	127.92	124.05
27	4	620	LUT	C35-C15-C14	-2.58	118.23	123.52
26	y	610	CLA	C1-C2-C3	-2.58	121.97	126.20
25	2	608	CHL	O1D-CGD-CBD	-2.58	120.81	124.72
26	8	612	CLA	CAA-C2A-C3A	-2.58	106.02	113.00
27	7	1620	LUT	C15-C35-C34	-2.58	118.24	123.52
25	Y	608	CHL	O2D-CGD-O1D	-2.58	118.82	123.85
28	1	1622	XAT	C11-C12-C13	-2.58	119.29	126.36
30	b	2630	LHG	C11-C10-C9	-2.58	101.32	114.37
35	a	408	PHO	CMB-C2B-C3B	2.58	129.84	124.68
29	N	1623	NEX	C31-C30-C29	-2.58	123.66	127.28
26	C	510	CLA	C3B-C4B-NB	-2.58	108.23	110.53
26	S	602	CLA	CMB-C2B-C1B	-2.58	121.49	125.42
25	N	601	CHL	CAC-C3C-C4C	2.58	130.65	124.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	605	CLA	C6-C5-C3	-2.58	107.19	113.47
39	C	519	DGD	O3E-C3E-C2E	-2.58	104.30	110.38
25	S	601	CHL	CMD-C2D-C3D	-2.58	119.53	124.68
25	s	601	CHL	CMD-C2D-C3D	-2.58	119.53	124.68
29	R	623	NEX	C17-C1-C6	-2.58	108.17	110.47
26	4	612	CLA	CAA-C2A-C3A	-2.58	106.04	113.00
26	y	613	CLA	C16-C15-C13	-2.58	107.40	115.97
25	Y	609	CHL	O2D-CGD-O1D	-2.58	118.83	123.85
30	B	2630	LHG	C11-C10-C9	-2.57	101.35	114.37
26	R	609	CLA	CHB-C4A-NA	2.57	128.12	124.40
26	8	603	CLA	CHB-C4A-NA	2.57	128.12	124.40
27	g	1621	LUT	C31-C30-C29	-2.57	123.67	127.28
25	3	608	CHL	OBD-CAD-C3D	-2.57	123.88	127.89
35	a	409	PHO	C1-C2-C3	-2.57	121.98	126.20
30	3	2630	LHG	C11-C10-C9	-2.57	101.36	114.37
38	D	405	PL9	C8-C7-C3	2.57	118.68	112.03
30	7	2630	LHG	C11-C10-C9	-2.57	101.37	114.37
26	1	614	CLA	CHB-C4A-NA	2.57	128.11	124.40
30	g	2630	LHG	C11-C10-C9	-2.57	101.39	114.37
26	4	603	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
26	r	610	CLA	C3B-C4B-NB	-2.57	108.24	110.53
25	1	607	CHL	OMC-CMC-C2C	-2.57	120.66	125.12
27	8	620	LUT	C35-C15-C14	-2.57	118.27	123.52
26	s	613	CLA	CMB-C2B-C3B	2.57	132.59	126.55
25	5	608	CHL	CBC-CAC-C3C	-2.57	109.20	112.87
26	Y	613	CLA	C16-C15-C13	-2.57	107.44	115.97
26	B	612	CLA	CHB-C1B-NB	2.57	127.90	124.05
26	s	602	CLA	CMB-C2B-C1B	-2.56	121.51	125.42
31	C	517	BCR	C33-C5-C4	2.56	119.06	113.60
25	6	608	CHL	O1D-CGD-CBD	-2.56	120.83	124.72
31	B	619	BCR	C21-C20-C19	-2.56	115.77	123.20
31	c	515	BCR	C16-C15-C14	-2.56	118.27	123.52
28	4	622	XAT	C30-C31-C32	-2.56	115.77	123.20
31	b	619	BCR	C21-C20-C19	-2.56	115.77	123.20
26	R	602	CLA	CMB-C2B-C3B	2.56	132.58	126.55
26	Y	613	CLA	C3B-C4B-NB	-2.56	108.24	110.53
31	8	623	BCR	C27-C26-C25	-2.56	119.24	122.70
30	G	2630	LHG	C11-C10-C9	-2.56	101.41	114.37
25	N	605	CHL	C4C-CHD-C1D	2.56	125.24	116.07
38	d	405	PL9	C8-C7-C3	2.56	118.65	112.03
26	b	605	CLA	C6-C5-C3	-2.56	107.23	113.47
27	Y	1621	LUT	C19-C9-C8	2.56	122.00	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	8	622	XAT	C30-C31-C32	-2.56	115.78	123.20
25	5	607	CHL	O2A-CGA-CBA	2.56	119.64	111.83
39	c	519	DGD	CDB-CCB-CBB	-2.56	101.43	114.37
26	s	610	CLA	C1-C2-C3	-2.56	122.00	126.20
25	1	605	CHL	O1D-CGD-CBD	-2.56	120.84	124.72
25	1	601	CHL	O1D-CGD-CBD	-2.56	120.84	124.72
25	5	605	CHL	O1D-CGD-CBD	-2.56	120.84	124.72
26	r	601	CLA	CHB-C4A-NA	2.56	128.09	124.40
25	S	606	CHL	CMA-C3A-C2A	-2.56	104.25	114.13
35	A	408	PHO	CMB-C2B-C3B	2.56	129.79	124.68
26	R	610	CLA	C3B-C4B-NB	-2.56	108.25	110.53
26	5	614	CLA	CHB-C4A-NA	2.56	128.09	124.40
29	r	623	NEX	C17-C1-C6	-2.56	108.19	110.47
39	C	519	DGD	CDB-CCB-CBB	-2.56	101.45	114.37
26	S	613	CLA	CMB-C2B-C3B	2.56	132.56	126.55
26	b	612	CLA	CHB-C1B-NB	2.56	127.88	124.05
25	n	605	CHL	C4C-CHD-C1D	2.55	125.21	116.07
26	5	613	CLA	CHB-C4A-NA	2.55	128.09	124.40
26	c	513	CLA	CBA-CAA-C2A	2.55	121.39	113.79
26	r	616	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
26	s	610	CLA	C3B-C4B-NB	-2.55	108.25	110.53
25	g	608	CHL	O2A-CGA-CBA	2.55	119.61	111.83
25	G	608	CHL	O2A-CGA-CBA	2.55	119.61	111.83
25	7	607	CHL	C3D-C4D-ND	2.55	117.03	112.94
26	7	602	CLA	C4A-NA-C1A	2.55	107.84	106.68
26	s	602	CLA	C1-C2-C3	-2.55	122.02	126.20
25	1	607	CHL	O2A-CGA-CBA	2.55	119.61	111.83
26	b	614	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
26	r	602	CLA	CMB-C2B-C3B	2.55	132.54	126.55
29	6	1623	NEX	C11-C12-C13	-2.55	119.38	126.36
29	n	1623	NEX	C31-C30-C29	-2.55	123.70	127.28
27	y	1621	LUT	C19-C9-C8	2.55	121.98	118.09
26	C	513	CLA	CBA-CAA-C2A	2.55	121.37	113.79
31	C	515	BCR	C16-C15-C14	-2.55	118.31	123.52
27	G	1620	LUT	C38-C25-C24	-2.55	117.33	123.36
26	y	613	CLA	C3B-C4B-NB	-2.55	108.26	110.53
26	B	603	CLA	O2D-CGD-CBD	2.55	115.68	111.23
26	8	603	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
25	s	606	CHL	CMA-C3A-C2A	-2.54	104.30	114.13
26	n	610	CLA	CMB-C2B-C1B	-2.54	121.54	125.42
26	N	610	CLA	CMB-C2B-C1B	-2.54	121.55	125.42
26	N	611	CLA	C3B-C4B-NB	-2.54	108.26	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	n	611	CLA	C3B-C4B-NB	-2.54	108.26	110.53
26	s	604	CLA	CMB-C2B-C3B	2.54	132.53	126.55
27	1	1620	LUT	C15-C14-C13	-2.54	123.71	127.28
26	b	602	CLA	C3B-C4B-NB	-2.54	108.26	110.53
25	1	605	CHL	CMB-C2B-C3B	2.54	129.76	124.68
26	S	610	CLA	C1-C2-C3	-2.54	122.03	126.20
26	B	602	CLA	C3B-C4B-NB	-2.54	108.26	110.53
27	s	1621	LUT	C39-C29-C28	2.54	121.97	118.09
25	R	614	CHL	CAA-C2A-C3A	-2.54	110.40	116.23
26	b	614	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
28	g	1622	XAT	C40-C33-C32	2.54	121.97	118.09
26	Y	603	CLA	O2D-CGD-CBD	2.54	115.67	111.23
26	b	603	CLA	O2D-CGD-CBD	2.54	115.67	111.23
26	y	603	CLA	O2D-CGD-CBD	2.54	115.67	111.23
27	N	1621	LUT	C8-C9-C10	-2.54	115.02	119.01
29	2	1623	NEX	C11-C12-C13	-2.54	119.41	126.36
26	B	607	CLA	O2D-CGD-CBD	2.54	115.67	111.23
26	R	616	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
37	b	622	LMG	O6-C1-O1	-2.54	104.05	110.04
25	g	601	CHL	C4-C3-C5	2.54	119.63	115.23
27	1	1621	LUT	C7-C8-C9	-2.54	122.48	126.23
26	C	505	CLA	C1-C2-C3	-2.54	122.04	126.20
25	5	605	CHL	CMB-C2B-C3B	2.54	129.75	124.68
26	B	614	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
27	g	1620	LUT	C38-C25-C24	-2.53	117.36	123.36
27	Y	1621	LUT	C37-C21-C22	-2.53	104.68	109.41
27	S	1621	LUT	C39-C29-C28	2.53	121.96	118.09
26	b	607	CLA	O2D-CGD-CBD	2.53	115.66	111.23
31	4	623	BCR	C27-C26-C25	-2.53	119.28	122.70
26	S	602	CLA	C1-C2-C3	-2.53	122.05	126.20
31	t	101	BCR	C7-C6-C5	-2.53	115.72	121.56
25	R	606	CHL	O1D-CGD-CBD	-2.53	120.89	124.72
25	r	606	CHL	O1D-CGD-CBD	-2.53	120.89	124.72
26	b	603	CLA	CHB-C4A-NA	2.53	128.05	124.40
25	y	607	CHL	C1-O2A-CGA	2.53	122.78	116.65
25	r	614	CHL	CAA-C2A-C3A	-2.53	110.43	116.23
26	B	617	CLA	CAA-C2A-C3A	-2.53	106.17	113.00
25	5	601	CHL	O1D-CGD-CBD	-2.53	120.89	124.72
26	G	613	CLA	CHB-C4A-NA	2.53	128.05	124.40
26	g	613	CLA	CHB-C4A-NA	2.53	128.05	124.40
31	a	411	BCR	C33-C5-C6	-2.53	121.72	124.48
25	3	607	CHL	C3D-C4D-ND	2.53	116.99	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	601	CHL	C4-C3-C5	2.53	119.62	115.23
26	b	617	CLA	CAA-C2A-C3A	-2.53	106.17	113.00
26	3	604	CLA	CHB-C4A-NA	2.53	128.05	124.40
26	S	604	CLA	CMB-C2B-C3B	2.53	132.50	126.55
26	6	614	CLA	CHB-C4A-NA	2.53	128.05	124.40
26	G	611	CLA	CHB-C1B-NB	2.53	127.84	124.05
29	G	1623	NEX	C15-C35-C34	-2.53	118.35	123.52
26	1	613	CLA	CHB-C4A-NA	2.53	128.05	124.40
31	T	101	BCR	C7-C6-C5	-2.53	115.74	121.56
26	r	602	CLA	O2D-CGD-CBD	2.52	115.64	111.23
25	5	605	CHL	O2D-CGD-O1D	-2.52	118.93	123.85
26	B	614	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
27	5	1620	LUT	C15-C14-C13	-2.52	123.74	127.28
37	B	622	LMG	O6-C1-O1	-2.52	104.08	110.04
27	n	1621	LUT	C8-C9-C10	-2.52	115.04	119.01
31	A	411	BCR	C33-C5-C6	-2.52	121.73	124.48
28	G	1622	XAT	C40-C33-C32	2.52	121.94	118.09
25	6	609	CHL	C4-C3-C5	2.52	119.60	115.23
27	y	1621	LUT	C37-C21-C22	-2.52	104.71	109.41
37	D	411	LMG	C6-C5-C4	-2.52	106.83	113.02
26	2	614	CLA	CHB-C4A-NA	2.52	128.04	124.40
26	b	607	CLA	CAA-CBA-CGA	-2.52	106.06	113.21
26	b	603	CLA	CMB-C2B-C3B	2.52	132.47	126.55
25	2	609	CHL	O2A-CGA-CBA	2.52	119.52	111.83
27	6	1620	LUT	C7-C8-C9	-2.52	122.51	126.23
26	R	602	CLA	O2D-CGD-CBD	2.52	115.63	111.23
25	6	609	CHL	O2A-CGA-CBA	2.52	119.51	111.83
26	2	610	CLA	CHB-C4A-NA	2.52	128.03	124.40
26	2	613	CLA	CHB-C4A-NA	2.52	128.03	124.40
26	c	505	CLA	C1-C2-C3	-2.52	122.07	126.20
27	2	1620	LUT	C7-C8-C9	-2.52	122.51	126.23
25	2	606	CHL	O1D-CGD-CBD	-2.52	120.91	124.72
39	h	102	DGD	C1D-C2D-C3D	-2.52	104.72	110.01
26	B	603	CLA	CHB-C4A-NA	2.52	128.03	124.40
26	6	610	CLA	CHB-C4A-NA	2.52	128.03	124.40
25	Y	607	CHL	C1-O2A-CGA	2.52	122.74	116.65
26	B	603	CLA	CMB-C2B-C3B	2.52	132.47	126.55
25	2	605	CHL	CMB-C2B-C3B	2.51	129.71	124.68
26	B	607	CLA	CAA-CBA-CGA	-2.51	106.07	113.21
26	n	610	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
28	2	1622	XAT	C18-C5-C4	2.51	117.06	114.24
28	6	1622	XAT	C18-C5-C4	2.51	117.06	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	S	610	CLA	C3B-C4B-NB	-2.51	108.29	110.53
28	1	1622	XAT	C15-C35-C34	-2.51	118.38	123.52
28	5	1622	XAT	C15-C35-C34	-2.51	118.38	123.52
39	c	518	DGD	O6E-C5E-C6E	-2.51	100.22	106.44
25	1	605	CHL	O2D-CGD-O1D	-2.51	118.96	123.85
25	6	606	CHL	O1D-CGD-CBD	-2.51	120.92	124.72
39	C	518	DGD	O6E-C5E-C6E	-2.51	100.22	106.44
26	S	602	CLA	CMD-C2D-C3D	2.51	133.44	127.69
26	6	613	CLA	CHB-C4A-NA	2.51	128.02	124.40
26	s	602	CLA	CMD-C2D-C3D	2.51	133.44	127.69
27	5	1621	LUT	C7-C8-C9	-2.51	122.53	126.23
26	n	602	CLA	CHB-C4A-NA	2.51	128.02	124.40
25	r	608	CHL	C3D-C4D-ND	2.51	116.96	112.94
29	g	1623	NEX	C15-C35-C34	-2.50	118.39	123.52
37	d	411	LMG	C6-C5-C4	-2.50	106.87	113.02
30	g	2630	LHG	C20-C19-C18	-2.50	101.71	114.37
39	c	518	DGD	C3G-C2G-C1G	-2.50	105.95	111.78
30	c	2630	LHG	O8-C23-C24	2.50	119.47	111.83
26	7	604	CLA	CHB-C4A-NA	2.50	128.01	124.40
30	G	2630	LHG	C20-C19-C18	-2.50	101.72	114.37
30	C	2630	LHG	O8-C23-C24	2.50	119.47	111.83
25	r	606	CHL	C1-C2-C3	-2.50	122.10	126.20
25	4	609	CHL	CMB-C2B-C3B	2.50	129.68	124.68
39	C	518	DGD	C3G-C2G-C1G	-2.50	105.95	111.78
29	6	1623	NEX	C35-C34-C33	-2.50	123.77	127.28
27	5	1620	LUT	C39-C29-C28	2.50	121.91	118.09
25	N	609	CHL	O1D-CGD-CBD	-2.50	120.93	124.72
39	H	102	DGD	C1D-C2D-C3D	-2.50	104.75	110.01
25	6	605	CHL	CMB-C2B-C3B	2.50	129.68	124.68
27	N	1620	LUT	C39-C29-C28	2.50	121.91	118.09
25	2	609	CHL	C4-C3-C5	2.50	119.57	115.23
25	8	609	CHL	CMB-C2B-C3B	2.50	129.68	124.68
26	r	610	CLA	O1D-CGD-CBD	2.50	129.45	124.52
26	N	602	CLA	CHB-C4A-NA	2.50	128.00	124.40
26	A	406	CLA	CHD-C1D-ND	-2.50	121.29	124.80
28	7	1622	XAT	C19-C9-C8	2.50	121.90	118.09
25	N	607	CHL	CAA-C2A-C3A	-2.50	106.25	113.00
26	c	510	CLA	C6-C7-C8	-2.50	107.66	115.97
25	y	607	CHL	CED-O2D-CGD	2.50	121.58	115.92
26	b	606	CLA	CMC-C2C-C1C	-2.50	121.13	125.03
26	2	603	CLA	CAA-C2A-C3A	-2.50	106.25	113.00
26	6	603	CLA	CAA-C2A-C3A	-2.50	106.25	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	510	CLA	C6-C7-C8	-2.50	107.66	115.97
25	n	607	CHL	C3D-C4D-ND	2.50	116.94	112.94
26	4	612	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
26	6	602	CLA	CMB-C2B-C1B	-2.50	121.62	125.42
31	c	515	BCR	C11-C12-C13	-2.49	119.52	126.36
25	Y	607	CHL	CED-O2D-CGD	2.49	121.57	115.92
28	3	1622	XAT	C19-C9-C8	2.49	121.90	118.09
26	8	612	CLA	O2D-CGD-O1D	-2.49	118.99	123.85
25	g	607	CHL	O1D-CGD-CBD	-2.49	120.94	124.72
25	R	606	CHL	C1-C2-C3	-2.49	122.11	126.20
26	g	611	CLA	CHB-C1B-NB	2.49	127.79	124.05
26	N	610	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
39	c	519	DGD	O5D-C6D-C5D	-2.49	103.81	109.42
26	B	606	CLA	C3B-C4B-NB	-2.49	108.31	110.53
26	b	606	CLA	C3B-C4B-NB	-2.49	108.31	110.53
26	R	610	CLA	O1D-CGD-CBD	2.49	129.42	124.52
29	n	1623	NEX	C15-C35-C34	-2.49	118.43	123.52
25	N	601	CHL	C4C-CHD-C1D	2.49	124.97	116.07
25	n	601	CHL	C4C-CHD-C1D	2.49	124.97	116.07
27	6	1621	LUT	C16-C1-C6	-2.49	106.34	110.24
27	n	1620	LUT	C39-C29-C28	2.49	121.89	118.09
30	c	522	LHG	C11-C10-C9	-2.49	101.80	114.37
30	7	2630	LHG	O8-C23-C24	2.49	119.41	111.83
25	Y	607	CHL	C3D-C4D-ND	2.49	116.92	112.94
31	C	516	BCR	C32-C1-C6	2.49	114.14	110.24
31	c	516	BCR	C32-C1-C6	2.49	114.14	110.24
30	1	2630	LHG	O8-C23-C24	2.48	119.41	111.83
26	a	406	CLA	CHD-C1D-ND	-2.48	121.31	124.80
25	4	606	CHL	O2D-CGD-O1D	-2.48	119.01	123.85
31	C	515	BCR	C11-C12-C13	-2.48	119.55	126.36
25	Y	605	CHL	O2A-CGA-CBA	2.48	119.41	111.83
25	Y	605	CHL	CMB-C2B-C3B	2.48	129.65	124.68
26	b	609	CLA	C1-C2-C3	-2.48	122.13	126.20
39	H	102	DGD	C1E-O6E-C5E	2.48	118.57	113.72
25	y	605	CHL	O2A-CGA-CBA	2.48	119.40	111.83
26	a	407	CLA	O2D-CGD-CBD	2.48	115.57	111.23
30	5	2630	LHG	O8-C23-C24	2.48	119.40	111.83
27	1	1620	LUT	C39-C29-C28	2.48	121.88	118.09
26	r	611	CLA	C2A-C1A-CHA	2.48	128.17	123.87
25	n	607	CHL	CAA-C2A-C3A	-2.48	106.30	113.00
25	8	606	CHL	O2D-CGD-O1D	-2.48	119.02	123.85
28	r	622	XAT	C24-C23-C22	-2.48	106.15	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	522	LHG	C11-C10-C9	-2.48	101.83	114.37
25	g	601	CHL	O2A-CGA-CBA	2.48	119.39	111.83
25	y	608	CHL	CMB-C2B-C3B	2.48	129.64	124.68
26	B	606	CLA	CMC-C2C-C1C	-2.48	121.16	125.03
25	N	607	CHL	C3D-C4D-ND	2.48	116.92	112.94
25	R	608	CHL	C3D-C4D-ND	2.48	116.92	112.94
25	2	606	CHL	CBC-CAC-C3C	-2.48	109.32	112.87
25	R	607	CHL	O1D-CGD-CBD	-2.48	120.96	124.72
25	r	607	CHL	O1D-CGD-CBD	-2.48	120.96	124.72
30	b	2631	LHG	O8-C23-C24	2.48	119.39	111.83
29	N	1623	NEX	C15-C35-C34	-2.48	118.45	123.52
25	6	606	CHL	CBC-CAC-C3C	-2.48	109.33	112.87
26	y	604	CLA	CHB-C4A-NA	2.48	127.97	124.40
26	3	611	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
37	A	413	LMG	O3-C3-C2	-2.48	104.54	110.38
25	6	601	CHL	CMB-C2B-C3B	2.48	129.63	124.68
26	R	611	CLA	C2A-C1A-CHA	2.48	128.16	123.87
26	2	602	CLA	CMB-C2B-C1B	-2.48	121.65	125.42
26	C	512	CLA	CMB-C2B-C3B	2.48	132.37	126.55
26	c	512	CLA	CMB-C2B-C3B	2.47	132.37	126.55
29	2	1623	NEX	C35-C34-C33	-2.47	123.81	127.28
26	Y	610	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
25	G	601	CHL	O2A-CGA-CBA	2.47	119.38	111.83
26	s	613	CLA	CHB-C4A-NA	2.47	127.97	124.40
30	3	2630	LHG	O8-C23-C24	2.47	119.38	111.83
26	5	610	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
39	h	102	DGD	C1E-O6E-C5E	2.47	118.55	113.72
27	G	1620	LUT	C28-C29-C30	-2.47	115.12	119.01
25	N	607	CHL	O2A-CGA-CBA	2.47	119.37	111.83
25	3	609	CHL	C1-C2-C3	-2.47	122.15	126.20
27	N	1621	LUT	C19-C9-C8	2.47	121.86	118.09
25	1	609	CHL	CMA-C3A-C4A	-2.47	109.29	114.61
26	r	613	CLA	CHB-C4A-NA	2.47	127.97	124.40
25	n	607	CHL	O2A-CGA-CBA	2.47	119.36	111.83
25	n	609	CHL	O1D-CGD-CBD	-2.47	120.98	124.72
28	5	1622	XAT	C24-C23-C22	-2.47	106.17	110.79
25	7	608	CHL	CMB-C2B-C3B	2.47	129.62	124.68
25	s	607	CHL	O1D-CGD-CBD	-2.47	120.98	124.72
30	B	2631	LHG	O8-C23-C24	2.47	119.36	111.83
27	2	1621	LUT	C16-C1-C6	-2.47	106.37	110.24
39	C	519	DGD	O5D-C6D-C5D	-2.47	103.86	109.42
31	4	623	BCR	C20-C19-C18	-2.47	119.59	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	y	610	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
25	y	605	CHL	CMB-C2B-C3B	2.47	129.61	124.68
26	r	612	CLA	CAA-C2A-C3A	-2.47	106.33	113.00
25	G	607	CHL	O1D-CGD-CBD	-2.47	120.98	124.72
25	y	607	CHL	C3D-C4D-ND	2.47	116.90	112.94
27	y	1620	LUT	C38-C25-C24	-2.47	117.52	123.36
25	6	601	CHL	O1D-CGD-CBD	-2.47	120.98	124.72
31	8	623	BCR	C20-C19-C18	-2.47	119.60	126.36
27	5	1621	LUT	C21-C26-C27	-2.47	109.99	112.83
30	G	2630	LHG	O8-C23-C24	2.47	119.35	111.83
25	8	607	CHL	CBC-CAC-C3C	-2.46	109.34	112.87
25	Y	608	CHL	CMB-C2B-C3B	2.46	129.60	124.68
26	B	609	CLA	C1-C2-C3	-2.46	122.16	126.20
26	A	407	CLA	O2D-CGD-CBD	2.46	115.53	111.23
26	1	610	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
26	Y	602	CLA	CAC-C3C-C4C	2.46	127.99	124.79
25	g	608	CHL	O2D-CGD-O1D	-2.46	119.06	123.85
26	c	506	CLA	C1-C2-C3	-2.46	122.17	126.20
37	Z	101	LMG	C1-C2-C3	-2.46	104.83	110.01
25	y	606	CHL	CMA-C3A-C4A	-2.46	109.31	114.61
25	3	607	CHL	OMC-CMC-C2C	-2.46	120.85	125.12
25	3	608	CHL	O1D-CGD-CBD	-2.46	120.99	124.72
26	7	611	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
25	5	609	CHL	CMA-C3A-C4A	-2.46	109.31	114.61
26	r	603	CLA	CAA-C2A-C3A	-2.46	106.35	113.00
37	a	413	LMG	O3-C3-C2	-2.46	104.58	110.38
25	G	608	CHL	O1D-CGD-CBD	-2.46	120.99	124.72
26	R	603	CLA	CAA-C2A-C3A	-2.46	106.36	113.00
26	7	612	CLA	C4A-NA-C1A	2.46	107.80	106.68
25	3	608	CHL	CMB-C2B-C3B	2.46	129.59	124.68
25	R	608	CHL	CMB-C2B-C3B	2.46	129.59	124.68
25	r	608	CHL	CMB-C2B-C3B	2.46	129.59	124.68
25	5	609	CHL	C4-C3-C5	2.46	119.49	115.23
30	g	2630	LHG	O8-C23-C24	2.46	119.33	111.83
27	3	1621	LUT	C31-C30-C29	-2.46	123.83	127.28
31	D	404	BCR	C33-C5-C6	-2.46	121.80	124.48
25	N	608	CHL	CMB-C2B-C3B	2.46	129.59	124.68
26	B	615	CLA	C4-C3-C5	2.46	119.49	115.23
30	1	2630	LHG	C11-C10-C9	-2.46	101.96	114.37
26	Y	604	CLA	CHB-C4A-NA	2.46	127.94	124.40
27	n	1620	LUT	C8-C9-C10	-2.45	115.15	119.01
25	7	607	CHL	OMC-CMC-C2C	-2.45	120.86	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	606	CHL	CMA-C3A-C4A	-2.45	109.32	114.61
26	R	613	CLA	CHB-C4A-NA	2.45	127.94	124.40
25	y	601	CHL	CBC-CAC-C3C	-2.45	109.36	112.87
25	4	606	CHL	CAA-CBA-CGA	-2.45	105.95	112.49
26	C	506	CLA	CMB-C2B-C3B	2.45	132.32	126.55
25	2	601	CHL	CMB-C2B-C3B	2.45	129.59	124.68
28	3	1622	XAT	C32-C33-C34	-2.45	115.15	119.01
28	7	1622	XAT	C32-C33-C34	-2.45	115.15	119.01
25	5	607	CHL	C1-C2-C3	-2.45	122.18	126.20
25	N	606	CHL	OMC-CMC-C2C	-2.45	120.86	125.12
25	n	605	CHL	OMC-CMC-C2C	-2.45	120.86	125.12
25	n	608	CHL	CMB-C2B-C3B	2.45	129.58	124.68
27	r	620	LUT	C15-C35-C34	-2.45	118.50	123.52
30	5	2630	LHG	C11-C10-C9	-2.45	101.97	114.37
25	3	601	CHL	C1C-C2C-CMC	2.45	131.22	126.80
27	2	1621	LUT	C30-C31-C32	-2.45	116.10	123.20
28	1	1622	XAT	C24-C23-C22	-2.45	106.21	110.79
37	z	101	LMG	C1-C2-C3	-2.45	104.85	110.01
25	4	607	CHL	CBC-CAC-C3C	-2.45	109.36	112.87
25	3	609	CHL	O2D-CGD-O1D	-2.45	119.08	123.85
25	2	601	CHL	O1D-CGD-CBD	-2.45	121.01	124.72
27	g	1620	LUT	C28-C29-C30	-2.45	115.16	119.01
26	R	612	CLA	CAA-C2A-C3A	-2.45	106.38	113.00
25	7	601	CHL	C1C-C2C-CMC	2.45	131.22	126.80
36	A	418	SQD	O5-C5-C4	2.45	114.11	109.70
30	R	2630	LHG	O8-C23-C24	2.45	119.30	111.83
31	t	101	BCR	C39-C30-C25	-2.45	106.40	110.24
28	R	622	XAT	C24-C23-C22	-2.45	106.21	110.79
26	Y	614	CLA	CHB-C4A-NA	2.45	127.93	124.40
26	y	614	CLA	CHB-C4A-NA	2.45	127.93	124.40
25	7	608	CHL	O1D-CGD-CBD	-2.45	121.01	124.72
36	B	621	SQD	C45-O47-C7	2.45	123.65	117.80
26	S	613	CLA	CHB-C4A-NA	2.45	127.93	124.40
25	G	608	CHL	O2D-CGD-O1D	-2.45	119.09	123.85
26	3	611	CLA	C2A-C1A-CHA	2.45	128.11	123.87
26	7	611	CLA	C2A-C1A-CHA	2.45	128.11	123.87
36	b	621	SQD	C45-O47-C7	2.45	123.65	117.80
26	y	602	CLA	CAC-C3C-C4C	2.45	127.97	124.79
25	n	609	CHL	CAC-C3C-C4C	2.45	130.31	124.03
25	7	609	CHL	C1-C2-C3	-2.45	122.19	126.20
27	7	1621	LUT	C31-C30-C29	-2.45	123.85	127.28
25	1	609	CHL	C4-C3-C5	2.44	119.47	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	T	101	BCR	C39-C30-C25	-2.44	106.41	110.24
27	6	1621	LUT	C30-C31-C32	-2.44	116.12	123.20
25	Y	601	CHL	CBC-CAC-C3C	-2.44	109.37	112.87
27	N	1620	LUT	C8-C9-C10	-2.44	115.16	119.01
27	3	1620	LUT	C39-C29-C28	2.44	121.82	118.09
26	D	402	CLA	C3B-C4B-NB	-2.44	108.35	110.53
26	d	402	CLA	C3B-C4B-NB	-2.44	108.35	110.53
31	H	101	BCR	C31-C1-C6	-2.44	106.41	110.24
30	C	2630	LHG	C11-C10-C9	-2.44	102.01	114.37
26	c	506	CLA	CMB-C2B-C3B	2.44	132.30	126.55
30	c	2630	LHG	C11-C10-C9	-2.44	102.02	114.37
26	b	615	CLA	C4-C3-C5	2.44	119.47	115.23
26	C	506	CLA	C1-C2-C3	-2.44	122.19	126.20
25	n	606	CHL	OMC-CMC-C2C	-2.44	120.88	125.12
25	N	605	CHL	OMC-CMC-C2C	-2.44	120.88	125.12
25	8	606	CHL	CAA-CBA-CGA	-2.44	105.98	112.49
39	B	626	DGD	C1D-C2D-C3D	-2.44	104.88	110.01
25	N	609	CHL	CAC-C3C-C4C	2.44	130.30	124.03
27	n	1621	LUT	C19-C9-C8	2.44	121.81	118.09
25	Y	605	CHL	C4C-CHD-C1D	2.44	124.80	116.07
31	d	404	BCR	C33-C5-C6	-2.44	121.82	124.48
25	y	608	CHL	C4-C3-C5	2.44	119.46	115.23
25	g	608	CHL	O1D-CGD-CBD	-2.44	121.02	124.72
26	G	602	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	7	609	CHL	O2D-CGD-O1D	-2.44	119.10	123.85
26	7	612	CLA	CHB-C4A-NA	2.44	127.92	124.40
27	7	1620	LUT	C39-C29-C28	2.44	121.81	118.09
25	y	605	CHL	C4C-CHD-C1D	2.44	124.79	116.07
25	1	607	CHL	C1-C2-C3	-2.44	122.20	126.20
26	3	612	CLA	CHB-C4A-NA	2.44	127.92	124.40
39	b	626	DGD	C1D-C2D-C3D	-2.44	104.89	110.01
27	1	1621	LUT	C21-C26-C27	-2.44	110.03	112.83
30	D	408	LHG	C11-C10-C9	-2.44	102.06	114.37
25	S	607	CHL	O1D-CGD-CBD	-2.44	121.03	124.72
28	y	1622	XAT	O4-C5-C6	-2.43	57.00	58.93
27	Y	1620	LUT	C38-C25-C24	-2.43	117.60	123.36
30	r	2630	LHG	O8-C23-C24	2.43	119.26	111.83
30	d	408	LHG	C11-C10-C9	-2.43	102.07	114.37
38	D	405	PL9	C22-C23-C24	-2.43	122.05	127.62
38	d	405	PL9	C22-C23-C24	-2.43	122.05	127.62
36	a	418	SQD	O5-C5-C4	2.43	114.08	109.70
26	s	604	CLA	C2A-C1A-CHA	2.43	128.09	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	F	101	HEM	CMB-C2B-C1B	-2.43	121.24	125.03
41	f	101	HEM	CMB-C2B-C1B	-2.43	121.24	125.03
31	a	411	BCR	C37-C22-C23	2.43	121.80	118.09
26	Y	602	CLA	CMB-C2B-C3B	2.43	132.26	126.55
28	N	1622	XAT	C18-C5-C4	2.43	116.97	114.24
26	B	604	CLA	C3B-C4B-NB	-2.43	108.36	110.53
25	g	607	CHL	CED-O2D-CGD	2.43	121.42	115.92
27	R	620	LUT	C15-C35-C34	-2.43	118.56	123.52
25	G	606	CHL	O2D-CGD-O1D	-2.43	119.13	123.85
37	a	415	LMG	O6-C1-O1	-2.43	104.31	110.04
39	c	519	DGD	C3G-C2G-C1G	-2.42	106.13	111.78
25	Y	608	CHL	C4-C3-C5	2.42	119.44	115.23
26	r	612	CLA	CHB-C4A-NA	2.42	127.90	124.40
31	h	101	BCR	C31-C1-C6	-2.42	106.44	110.24
27	4	620	LUT	C39-C29-C28	2.42	121.79	118.09
26	5	610	CLA	CHB-C1B-NB	2.42	127.68	124.05
26	d	403	CLA	C7-C6-C5	-2.42	106.81	113.26
27	Y	1621	LUT	C7-C8-C9	-2.42	122.65	126.23
27	s	1621	LUT	C15-C14-C13	-2.42	123.88	127.28
27	G	1621	LUT	C39-C29-C28	2.42	121.79	118.09
26	D	403	CLA	C7-C6-C5	-2.42	106.81	113.26
27	g	1621	LUT	C39-C29-C28	2.42	121.78	118.09
26	R	611	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
26	R	610	CLA	CAA-CBA-CGA	-2.42	106.34	113.21
26	c	506	CLA	CHB-C1B-NB	2.42	127.68	124.05
29	Y	1623	NEX	C15-C35-C34	-2.42	118.57	123.52
26	7	614	CLA	C3B-C4B-NB	-2.42	108.37	110.53
29	y	1623	NEX	C15-C35-C34	-2.42	118.57	123.52
27	y	1621	LUT	C7-C8-C9	-2.42	122.66	126.23
25	8	607	CHL	OMC-CMC-C2C	-2.42	120.92	125.12
27	Y	1620	LUT	C28-C29-C30	-2.42	115.21	119.01
25	3	607	CHL	C1-O2A-CGA	2.42	122.50	116.65
30	Y	2630	LHG	C11-C10-C9	-2.42	102.16	114.37
30	y	2630	LHG	C11-C10-C9	-2.42	102.16	114.37
25	2	609	CHL	O2D-CGD-O1D	-2.42	119.15	123.85
25	6	609	CHL	O2D-CGD-O1D	-2.42	119.15	123.85
27	8	620	LUT	C39-C29-C28	2.41	121.78	118.09
29	r	623	NEX	O24-C25-C26	-2.41	57.02	58.93
29	g	1623	NEX	C39-C29-C30	-2.41	118.91	122.82
26	r	610	CLA	CAA-CBA-CGA	-2.41	106.36	113.21
26	y	602	CLA	CMB-C2B-C3B	2.41	132.22	126.55
31	A	411	BCR	C10-C11-C12	-2.41	116.21	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	A	415	LMG	O6-C1-O1	-2.41	104.34	110.04
29	S	1623	NEX	O4-C5-C18	-2.41	104.63	109.22
29	s	1623	NEX	O4-C5-C18	-2.41	104.63	109.22
26	R	612	CLA	CHB-C4A-NA	2.41	127.88	124.40
25	7	605	CHL	O2D-CGD-O1D	-2.41	119.16	123.85
26	1	612	CLA	C2A-C1A-CHA	2.41	128.05	123.87
26	5	612	CLA	C2A-C1A-CHA	2.41	128.05	123.87
25	3	605	CHL	O2D-CGD-O1D	-2.41	119.16	123.85
26	y	613	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
39	C	519	DGD	C3G-C2G-C1G	-2.41	106.17	111.78
26	B	615	CLA	CHB-C4A-NA	2.41	127.88	124.40
26	b	615	CLA	CHB-C4A-NA	2.41	127.88	124.40
28	n	1622	XAT	C18-C5-C4	2.41	116.95	114.24
25	7	607	CHL	C1-O2A-CGA	2.41	122.48	116.65
37	B	622	LMG	C38-C37-C36	-2.41	102.19	114.37
26	r	611	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
29	r	623	NEX	C11-C12-C13	-2.41	119.76	126.36
30	1	2630	LHG	C20-C19-C18	-2.41	102.20	114.37
26	g	602	CLA	CHB-C4A-NA	2.41	127.87	124.40
25	N	606	CHL	O1D-CGD-CBD	-2.41	121.07	124.72
25	n	606	CHL	O1D-CGD-CBD	-2.41	121.07	124.72
30	R	2630	LHG	C20-C19-C18	-2.41	102.21	114.37
31	a	411	BCR	C10-C11-C12	-2.41	116.23	123.20
30	r	2630	LHG	C20-C19-C18	-2.41	102.21	114.37
25	g	606	CHL	O2D-CGD-O1D	-2.41	119.17	123.85
27	S	1621	LUT	C15-C14-C13	-2.41	123.91	127.28
26	c	501	CLA	C7-C6-C5	-2.41	106.85	113.26
25	G	607	CHL	CED-O2D-CGD	2.41	121.37	115.92
31	8	623	BCR	C37-C22-C23	2.41	121.76	118.09
26	R	601	CLA	CMB-C2B-C3B	2.40	132.21	126.55
27	y	1620	LUT	C28-C29-C30	-2.40	115.23	119.01
37	b	622	LMG	C38-C37-C36	-2.40	102.22	114.37
29	R	623	NEX	C11-C12-C13	-2.40	119.77	126.36
39	C	520	DGD	O5D-C6D-C5D	-2.40	104.00	109.42
26	C	501	CLA	C7-C6-C5	-2.40	106.86	113.26
25	4	607	CHL	OMC-CMC-C2C	-2.40	120.95	125.12
26	1	610	CLA	CHB-C1B-NB	2.40	127.65	124.05
26	D	402	CLA	CAC-C3C-C4C	2.40	127.92	124.79
27	3	1620	LUT	C20-C13-C12	2.40	121.76	118.09
25	n	608	CHL	O2D-CGD-O1D	-2.40	119.17	123.85
28	2	1622	XAT	C10-C11-C12	-2.40	116.24	123.20
27	8	620	LUT	C1-C6-C5	-2.40	119.35	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	607	CHL	CMA-C3A-C4A	-2.40	109.44	114.61
25	S	606	CHL	CAC-C3C-C4C	2.40	130.20	124.03
25	6	608	CHL	OBD-CAD-C3D	-2.40	124.15	127.89
28	Y	1622	XAT	O4-C5-C6	-2.40	57.03	58.93
26	3	614	CLA	C3B-C4B-NB	-2.40	108.39	110.53
31	A	411	BCR	C37-C22-C23	2.40	121.75	118.09
26	C	506	CLA	CHB-C1B-NB	2.40	127.65	124.05
28	6	1622	XAT	C10-C11-C12	-2.40	116.25	123.20
26	4	610	CLA	C4A-NA-C1A	2.40	107.77	106.68
26	8	610	CLA	C4A-NA-C1A	2.40	107.77	106.68
39	c	520	DGD	O5D-C6D-C5D	-2.40	104.01	109.42
30	5	2630	LHG	C20-C19-C18	-2.40	102.24	114.37
29	G	1623	NEX	C39-C29-C30	-2.40	118.93	122.82
26	S	604	CLA	C2A-C1A-CHA	2.40	128.03	123.87
27	4	620	LUT	C1-C6-C5	-2.40	119.36	122.64
26	B	608	CLA	CMC-C2C-C1C	-2.40	121.28	125.03
26	1	610	CLA	CHB-C4A-NA	2.40	127.86	124.40
25	N	601	CHL	O1D-CGD-CBD	-2.40	121.08	124.72
26	B	610	CLA	CMB-C2B-C3B	2.40	132.19	126.55
26	3	614	CLA	CHB-C4A-NA	2.40	127.86	124.40
26	B	608	CLA	CHC-C1C-NC	2.40	127.92	124.31
26	N	610	CLA	C1-C2-C3	-2.40	122.27	126.20
26	c	513	CLA	C3B-C4B-NB	-2.40	108.39	110.53
25	4	607	CHL	CMA-C3A-C4A	-2.40	109.45	114.61
30	D	409	LHG	C18-C17-C16	-2.40	102.26	114.37
26	7	603	CLA	CHA-C1A-NA	-2.40	120.97	126.39
25	S	607	CHL	C4-C3-C5	2.39	119.39	115.23
25	s	607	CHL	C4-C3-C5	2.39	119.39	115.23
26	5	610	CLA	CHB-C4A-NA	2.39	127.86	124.40
26	r	601	CLA	CMB-C2B-C3B	2.39	132.18	126.55
26	7	602	CLA	O2D-CGD-CBD	2.39	115.41	111.23
25	N	608	CHL	O2D-CGD-O1D	-2.39	119.19	123.85
27	N	1621	LUT	C27-C28-C29	-2.39	121.18	126.32
27	n	1621	LUT	C27-C28-C29	-2.39	121.18	126.32
39	H	102	DGD	C3G-C2G-C1G	-2.39	106.21	111.78
26	d	402	CLA	CAC-C3C-C4C	2.39	127.90	124.79
25	s	606	CHL	CAC-C3C-C4C	2.39	130.18	124.03
26	B	617	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
26	7	610	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
25	5	606	CHL	CED-O2D-CGD	2.39	121.34	115.92
27	1	1620	LUT	C19-C9-C8	2.39	121.74	118.09
27	g	1620	LUT	C21-C26-C27	-2.39	110.08	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	G	1620	LUT	C7-C8-C9	-2.39	122.70	126.23
30	d	409	LHG	C18-C17-C16	-2.39	102.29	114.37
25	n	601	CHL	O1D-CGD-CBD	-2.39	121.10	124.72
27	Y	1620	LUT	C31-C30-C29	-2.39	123.93	127.28
26	n	610	CLA	C1-C2-C3	-2.39	122.28	126.20
26	b	610	CLA	CMB-C2B-C3B	2.39	132.17	126.55
26	3	603	CLA	CHA-C1A-NA	-2.39	120.98	126.39
27	5	1620	LUT	C19-C9-C8	2.39	121.73	118.09
26	s	611	CLA	O2A-CGA-O1A	-2.39	117.66	123.63
31	4	623	BCR	C37-C22-C23	2.39	121.73	118.09
26	c	501	CLA	CHB-C4A-NA	2.39	127.84	124.40
26	B	616	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
28	Y	1622	XAT	C31-C32-C33	-2.38	119.82	126.36
29	R	623	NEX	O24-C25-C26	-2.38	57.04	58.93
26	D	402	CLA	CMA-C3A-C2A	-2.38	104.76	113.98
26	d	402	CLA	CMA-C3A-C2A	-2.38	104.76	113.98
25	R	607	CHL	CMB-C2B-C3B	2.38	129.45	124.68
26	b	616	CLA	CAA-C2A-C3A	-2.38	106.56	113.00
26	Y	613	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
26	2	604	CLA	CHB-C4A-NA	2.38	127.84	124.40
27	G	1620	LUT	C21-C26-C27	-2.38	110.08	112.83
29	N	1623	NEX	C39-C29-C30	-2.38	118.96	122.82
25	8	607	CHL	CMA-C3A-C4A	-2.38	109.48	114.61
25	7	606	CHL	O2D-CGD-O1D	-2.38	119.21	123.85
36	B	621	SQD	O7-S-C6	2.38	110.31	106.76
39	h	102	DGD	C3G-C2G-C1G	-2.38	106.23	111.78
27	s	1621	LUT	C11-C10-C9	-2.38	123.94	127.28
26	S	611	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
28	y	1622	XAT	C31-C32-C33	-2.38	119.83	126.36
26	3	612	CLA	C4A-NA-C1A	2.38	107.77	106.68
39	B	626	DGD	O2G-C1B-O1B	-2.38	118.14	123.70
26	7	614	CLA	CHB-C4A-NA	2.38	127.83	124.40
25	N	609	CHL	CAA-C2A-C3A	-2.38	106.57	113.00
37	a	413	LMG	C40-C39-C38	-2.38	102.34	114.37
25	3	606	CHL	O2D-CGD-O1D	-2.38	119.22	123.85
27	2	1620	LUT	C28-C29-C30	-2.38	115.27	119.01
37	A	413	LMG	C40-C39-C38	-2.38	102.34	114.37
26	a	405	CLA	C6-C7-C8	-2.38	108.06	115.97
26	R	613	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
25	n	609	CHL	CAA-C2A-C3A	-2.38	106.57	113.00
26	b	608	CLA	CMC-C2C-C1C	-2.38	121.32	125.03
26	s	610	CLA	CMB-C2B-C3B	2.38	132.15	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	2	1622	XAT	C31-C32-C33	-2.38	119.84	126.36
26	C	501	CLA	CHB-C4A-NA	2.38	127.83	124.40
31	B	619	BCR	C10-C11-C12	-2.38	116.31	123.20
27	g	1620	LUT	C7-C8-C9	-2.38	122.72	126.23
25	r	606	CHL	O2A-CGA-O1A	-2.38	117.68	123.63
26	A	405	CLA	C6-C7-C8	-2.38	108.06	115.97
25	2	608	CHL	OBD-CAD-C3D	-2.38	124.19	127.89
26	3	610	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
30	b	2631	LHG	C20-C19-C18	-2.38	102.36	114.37
27	y	1620	LUT	C31-C30-C29	-2.38	123.95	127.28
26	3	602	CLA	O2D-CGD-CBD	2.38	115.38	111.23
35	a	408	PHO	O2D-CGD-O1D	-2.38	119.22	123.85
25	3	607	CHL	CMA-C3A-C4A	-2.38	109.49	114.61
26	c	507	CLA	CBC-CAC-C3C	-2.38	105.98	112.42
29	S	1623	NEX	O24-C25-C26	-2.37	57.05	58.93
29	n	1623	NEX	C39-C29-C30	-2.37	118.97	122.82
31	C	515	BCR	C36-C18-C19	2.37	121.71	118.09
31	c	515	BCR	C36-C18-C19	2.37	121.71	118.09
26	C	507	CLA	CBC-CAC-C3C	-2.37	105.99	112.42
30	S	2630	LHG	O8-C23-C24	2.37	119.07	111.83
30	B	2631	LHG	C20-C19-C18	-2.37	102.37	114.37
26	b	607	CLA	CAC-C3C-C4C	2.37	127.88	124.79
26	n	610	CLA	CMB-C2B-C3B	2.37	132.13	126.55
31	b	619	BCR	C10-C11-C12	-2.37	116.33	123.20
25	r	607	CHL	C5-C3-C2	-2.37	115.84	121.17
25	Y	605	CHL	O2D-CGD-O1D	-2.37	119.23	123.85
27	7	1620	LUT	C20-C13-C12	2.37	121.71	118.09
36	b	621	SQD	O7-S-C6	2.37	110.30	106.76
26	b	617	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
25	1	606	CHL	CED-O2D-CGD	2.37	121.29	115.92
26	S	614	CLA	CHB-C4A-NA	2.37	127.82	124.40
39	b	626	DGD	O2G-C1B-O1B	-2.37	118.16	123.70
25	r	607	CHL	CMB-C2B-C3B	2.37	129.42	124.68
26	4	604	CLA	CHB-C4A-NA	2.37	127.82	124.40
30	D	409	LHG	C11-C10-C9	-2.37	102.39	114.37
28	8	622	XAT	C19-C9-C8	2.37	121.71	118.09
26	b	608	CLA	CHC-C1C-NC	2.37	127.88	124.31
39	C	518	DGD	CAB-C9B-C8B	-2.37	102.39	114.37
27	S	1621	LUT	C21-C26-C27	-2.37	110.10	112.83
26	y	613	CLA	CHB-C4A-NA	2.37	127.82	124.40
30	s	2630	LHG	O8-C23-C24	2.37	119.06	111.83
26	5	604	CLA	C3B-C4B-NB	-2.37	108.42	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	S	610	CLA	CMB-C2B-C3B	2.37	132.12	126.55
26	r	613	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
29	3	1623	NEX	C35-C34-C33	-2.37	123.96	127.28
29	7	1623	NEX	C35-C34-C33	-2.37	123.96	127.28
25	R	606	CHL	O2A-CGA-O1A	-2.37	117.71	123.63
27	6	1620	LUT	C28-C29-C30	-2.37	115.29	119.01
30	d	409	LHG	C11-C10-C9	-2.37	102.40	114.37
25	y	609	CHL	C4C-CHD-C1D	2.37	124.54	116.07
25	G	607	CHL	C11-C10-C8	-2.37	108.10	115.97
28	4	622	XAT	C19-C9-C8	2.37	121.70	118.09
26	s	604	CLA	C3A-C2A-C1A	2.37	104.88	101.34
26	B	605	CLA	CHA-C4D-ND	2.37	137.43	132.55
26	b	605	CLA	CHA-C4D-ND	2.37	137.43	132.55
25	1	606	CHL	CMA-C3A-C4A	-2.37	109.52	114.61
30	N	2630	LHG	C27-C26-C25	-2.36	102.41	114.37
26	B	607	CLA	C3B-C4B-NB	-2.36	108.42	110.53
25	Y	609	CHL	C4C-CHD-C1D	2.36	124.53	116.07
25	R	607	CHL	C5-C3-C2	-2.36	115.86	121.17
28	6	1622	XAT	C31-C32-C33	-2.36	119.88	126.36
29	7	1623	NEX	C26-C27-C28	-2.36	120.99	125.99
25	N	601	CHL	CMB-C2B-C3B	2.36	129.41	124.68
25	5	606	CHL	CMA-C3A-C4A	-2.36	109.52	114.61
26	g	614	CLA	CHB-C4A-NA	2.36	127.81	124.40
37	D	411	LMG	O1-C7-C8	-2.36	105.07	110.82
26	c	503	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
39	c	518	DGD	CAB-C9B-C8B	-2.36	102.42	114.37
27	s	1621	LUT	C21-C26-C27	-2.36	110.11	112.83
26	b	607	CLA	C3B-C4B-NB	-2.36	108.42	110.53
25	2	607	CHL	CAC-C3C-C4C	2.36	130.10	124.03
29	R	623	NEX	C4-C3-C2	-2.36	106.37	110.79
26	N	611	CLA	CHB-C4A-NA	2.36	127.81	124.40
26	n	611	CLA	CHB-C4A-NA	2.36	127.81	124.40
26	b	604	CLA	C3B-C4B-NB	-2.36	108.42	110.53
25	y	605	CHL	O2D-CGD-O1D	-2.36	119.25	123.85
29	s	1623	NEX	O24-C25-C26	-2.36	57.06	58.93
25	g	607	CHL	C11-C10-C8	-2.36	108.12	115.97
26	B	607	CLA	CAC-C3C-C4C	2.36	127.86	124.79
25	Y	601	CHL	C1-C2-C3	-2.36	122.33	126.20
26	Y	614	CLA	C3B-C4B-NB	-2.36	108.42	110.53
26	g	611	CLA	O2D-CGD-CBD	2.36	115.35	111.23
30	n	2630	LHG	C27-C26-C25	-2.36	102.44	114.37
27	S	1621	LUT	C16-C1-C6	-2.36	106.55	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	604	CLA	CHB-C4A-NA	2.36	127.80	124.40
27	S	1621	LUT	C11-C10-C9	-2.36	123.97	127.28
30	d	409	LHG	C27-C26-C25	-2.36	102.45	114.37
26	N	610	CLA	CMB-C2B-C3B	2.36	132.09	126.55
31	D	404	BCR	C35-C13-C12	2.36	121.69	118.09
31	d	404	BCR	C35-C13-C12	2.36	121.69	118.09
35	A	408	PHO	O2D-CGD-O1D	-2.36	119.26	123.85
26	Y	613	CLA	CHB-C4A-NA	2.36	127.80	124.40
37	d	411	LMG	O1-C7-C8	-2.36	105.09	110.82
39	c	520	DGD	C3G-C2G-C1G	-2.36	106.29	111.78
25	Y	607	CHL	CMA-C3A-C4A	-2.35	109.54	114.61
29	r	623	NEX	C39-C29-C30	-2.35	119.00	122.82
30	D	409	LHG	C27-C26-C25	-2.35	102.47	114.37
26	c	513	CLA	CAA-CBA-CGA	-2.35	106.52	113.21
26	B	615	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
30	N	2630	LHG	C18-C17-C16	-2.35	102.47	114.37
25	7	606	CHL	CMA-C3A-C4A	-2.35	109.54	114.61
26	N	612	CLA	CAA-C2A-C3A	-2.35	106.64	113.00
29	3	1623	NEX	C26-C27-C28	-2.35	121.02	125.99
36	b	621	SQD	C1-O5-C5	2.35	118.31	113.72
29	n	1623	NEX	C4-C3-C2	-2.35	106.39	110.79
27	2	1621	LUT	C18-C5-C6	-2.35	121.92	124.48
39	c	519	DGD	CBB-CAB-C9B	-2.35	102.48	114.37
26	C	503	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
25	G	609	CHL	O1D-CGD-CBD	-2.35	121.16	124.72
25	g	609	CHL	O1D-CGD-CBD	-2.35	121.16	124.72
25	y	607	CHL	CMA-C3A-C4A	-2.35	109.55	114.61
26	C	513	CLA	C3B-C4B-NB	-2.35	108.43	110.53
26	b	617	CLA	CMB-C2B-C3B	2.35	132.07	126.55
30	Y	2630	LHG	C20-C19-C18	-2.35	102.50	114.37
36	B	621	SQD	C1-O5-C5	2.35	118.31	113.72
26	y	610	CLA	CHB-C1B-C2B	-2.35	120.61	127.43
26	B	610	CLA	CMD-C2D-C3D	2.35	133.07	127.69
29	r	623	NEX	C4-C3-C2	-2.35	106.40	110.79
26	G	614	CLA	CHB-C4A-NA	2.35	127.79	124.40
25	4	601	CHL	CMA-C3A-C4A	-2.35	109.56	114.61
26	b	610	CLA	CMD-C2D-C3D	2.35	133.07	127.69
39	C	519	DGD	CBB-CAB-C9B	-2.34	102.52	114.37
25	6	607	CHL	CAC-C3C-C4C	2.34	130.06	124.03
27	s	1621	LUT	C16-C1-C6	-2.34	106.57	110.24
29	N	1623	NEX	C4-C3-C2	-2.34	106.41	110.79
26	B	610	CLA	CHB-C4A-NA	2.34	127.78	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	y	2630	LHG	C20-C19-C18	-2.34	102.52	114.37
39	C	520	DGD	C3G-C2G-C1G	-2.34	106.32	111.78
30	n	2630	LHG	C18-C17-C16	-2.34	102.52	114.37
27	N	1620	LUT	C19-C9-C8	2.34	121.67	118.09
27	n	1620	LUT	C19-C9-C8	2.34	121.67	118.09
26	1	604	CLA	C3B-C4B-NB	-2.34	108.44	110.53
26	y	614	CLA	C3B-C4B-NB	-2.34	108.44	110.53
26	G	611	CLA	O2D-CGD-CBD	2.34	115.33	111.23
25	n	601	CHL	CMB-C2B-C3B	2.34	129.37	124.68
25	S	607	CHL	CAC-C3C-C4C	2.34	130.05	124.03
27	y	1620	LUT	C8-C9-C10	-2.34	115.32	119.01
25	6	601	CHL	C4C-CHD-C1D	2.34	124.45	116.07
27	Y	1621	LUT	C31-C30-C29	-2.34	123.99	127.28
26	s	614	CLA	CHB-C4A-NA	2.34	127.78	124.40
27	n	1621	LUT	C35-C15-C14	-2.34	118.73	123.52
30	Y	2630	LHG	O8-C23-C24	2.34	118.97	111.83
30	y	2630	LHG	O8-C23-C24	2.34	118.97	111.83
27	Y	1620	LUT	C8-C9-C10	-2.34	115.33	119.01
26	B	617	CLA	CMB-C2B-C3B	2.34	132.06	126.55
38	D	405	PL9	C27-C28-C29	-2.34	122.27	127.62
27	Y	1620	LUT	C15-C35-C34	-2.34	118.73	123.52
25	6	607	CHL	CMB-C2B-C3B	2.34	129.36	124.68
38	d	405	PL9	C27-C28-C29	-2.34	122.27	127.62
26	3	602	CLA	CHB-C4A-NA	2.34	127.78	124.40
26	7	602	CLA	CHB-C4A-NA	2.34	127.78	124.40
26	b	615	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
26	r	602	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
25	R	607	CHL	CAA-CBA-CGA	-2.34	106.57	113.21
25	3	606	CHL	CMA-C3A-C4A	-2.34	109.57	114.61
26	y	611	CLA	O2D-CGD-CBD	2.34	115.31	111.23
26	Y	610	CLA	CHB-C4A-NA	2.34	127.77	124.40
26	8	604	CLA	CHB-C4A-NA	2.34	127.77	124.40
26	y	610	CLA	CHB-C4A-NA	2.34	127.77	124.40
27	5	1620	LUT	C21-C26-C27	-2.34	110.14	112.83
27	g	1621	LUT	C19-C9-C8	2.34	121.66	118.09
26	a	406	CLA	C1C-C2C-C3C	-2.34	104.52	106.98
26	b	610	CLA	CHB-C4A-NA	2.34	127.77	124.40
26	n	612	CLA	CAA-C2A-C3A	-2.34	106.69	113.00
26	Y	610	CLA	CHB-C1B-C2B	-2.34	120.65	127.43
25	2	601	CHL	C4C-CHD-C1D	2.34	124.42	116.07
26	5	612	CLA	CHB-C1B-C2B	-2.34	120.65	127.43
25	y	601	CHL	C1-C2-C3	-2.34	122.37	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	602	CLA	CAC-C3C-C4C	2.34	127.83	124.79
27	6	1621	LUT	C18-C5-C6	-2.34	121.94	124.48
26	S	604	CLA	C3A-C2A-C1A	2.33	104.84	101.34
25	s	607	CHL	CAC-C3C-C4C	2.33	130.03	124.03
27	y	1620	LUT	C15-C35-C34	-2.33	118.74	123.52
26	2	610	CLA	C1-C2-C3	-2.33	122.98	126.76
26	Y	611	CLA	O2D-CGD-CBD	2.33	115.31	111.23
25	6	606	CHL	CMB-C2B-C3B	2.33	129.35	124.68
30	B	2630	LHG	C20-C19-C18	-2.33	102.57	114.37
25	y	607	CHL	CAC-C3C-C4C	2.33	130.03	124.03
25	5	601	CHL	C4C-CHD-C1D	2.33	124.42	116.07
26	C	513	CLA	CAA-CBA-CGA	-2.33	106.58	113.21
27	G	1621	LUT	C15-C35-C34	-2.33	118.75	123.52
25	2	606	CHL	CMB-C2B-C3B	2.33	129.34	124.68
26	R	613	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
26	G	604	CLA	O1D-CGD-CBD	2.33	129.12	124.52
27	G	1621	LUT	C19-C9-C8	2.33	121.65	118.09
25	1	607	CHL	C4-C3-C5	2.33	119.27	115.23
26	b	605	CLA	C2A-C3A-C4A	2.33	105.63	101.87
37	a	415	LMG	C40-C39-C38	-2.33	102.59	114.37
30	b	2630	LHG	C20-C19-C18	-2.33	102.59	114.37
37	A	415	LMG	C40-C39-C38	-2.33	102.59	114.37
25	Y	607	CHL	CAC-C3C-C4C	2.33	130.02	124.03
25	8	608	CHL	CMB-C2B-C3B	2.33	129.34	124.68
26	c	511	CLA	C3B-C4B-NB	-2.33	108.45	110.53
25	y	606	CHL	C3D-C4D-ND	2.33	116.67	112.94
26	S	602	CLA	CHB-C4A-NA	2.33	127.76	124.40
25	8	601	CHL	CMA-C3A-C4A	-2.33	109.59	114.61
26	1	612	CLA	CHB-C1B-C2B	-2.33	120.67	127.43
25	5	607	CHL	C4-C3-C5	2.33	119.27	115.23
25	7	605	CHL	OMC-CMC-C2C	-2.33	121.08	125.12
30	l	101	LHG	C20-C19-C18	-2.33	102.61	114.37
27	N	1621	LUT	C35-C15-C14	-2.33	118.76	123.52
29	R	623	NEX	C39-C29-C30	-2.33	119.05	122.82
27	6	1620	LUT	C12-C13-C14	-2.33	115.35	119.01
26	R	602	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
25	Y	607	CHL	CAA-C2A-C3A	-2.33	106.72	113.00
27	g	1621	LUT	C15-C35-C34	-2.33	118.76	123.52
27	1	1621	LUT	C19-C9-C8	2.33	121.64	118.09
26	1	612	CLA	CHA-C1A-NA	-2.33	121.13	126.39
25	3	605	CHL	OMC-CMC-C2C	-2.32	121.08	125.12
25	r	607	CHL	CAA-CBA-CGA	-2.32	106.61	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	N	1620	LUT	C17-C1-C6	2.32	113.89	110.24
25	2	607	CHL	CMB-C2B-C3B	2.32	129.33	124.68
26	B	611	CLA	C3A-C2A-C1A	2.32	104.82	101.34
27	y	1621	LUT	C31-C30-C29	-2.32	124.02	127.28
27	n	1620	LUT	C17-C1-C6	2.32	113.89	110.24
26	b	611	CLA	O2D-CGD-CBD	2.32	115.29	111.23
25	S	606	CHL	C4C-CHD-C1D	2.32	124.38	116.07
27	2	1620	LUT	C12-C13-C14	-2.32	115.36	119.01
30	s	2630	LHG	C11-C10-C9	-2.32	102.63	114.37
25	r	608	CHL	CAC-C3C-C4C	2.32	130.00	124.03
26	S	602	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
25	y	607	CHL	O2A-CGA-CBA	2.32	118.91	111.83
30	L	101	LHG	C20-C19-C18	-2.32	102.64	114.37
26	S	603	CLA	O2A-CGA-O1A	-2.32	117.36	123.33
25	1	601	CHL	C4C-CHD-C1D	2.32	124.37	116.07
25	y	606	CHL	OMC-CMC-C2C	-2.32	121.09	125.12
25	y	607	CHL	CAA-C2A-C3A	-2.32	106.73	113.00
30	g	2630	LHG	C27-C26-C25	-2.32	102.65	114.37
26	b	611	CLA	C3A-C2A-C1A	2.32	104.81	101.34
25	Y	607	CHL	O2A-CGA-CBA	2.32	118.90	111.83
30	S	2630	LHG	C11-C10-C9	-2.32	102.65	114.37
26	D	402	CLA	CHD-C1D-ND	-2.32	121.54	124.80
26	s	602	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
26	r	613	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
25	R	607	CHL	CED-O2D-CGD	2.32	121.17	115.92
25	s	606	CHL	C4C-CHD-C1D	2.32	124.36	116.07
25	4	608	CHL	CMB-C2B-C3B	2.32	129.31	124.68
26	B	611	CLA	O2D-CGD-CBD	2.32	115.28	111.23
28	n	1622	XAT	C7-C8-C9	-2.32	121.94	125.53
30	G	2630	LHG	C27-C26-C25	-2.32	102.66	114.37
25	Y	606	CHL	OMC-CMC-C2C	-2.32	121.10	125.12
26	5	612	CLA	CHA-C1A-NA	-2.31	121.15	126.39
25	3	605	CHL	CMB-C2B-C3B	2.31	129.31	124.68
26	C	513	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
26	3	610	CLA	CHB-C1B-NB	2.31	127.52	124.05
26	7	610	CLA	CHB-C1B-NB	2.31	127.52	124.05
26	g	604	CLA	O1D-CGD-CBD	2.31	129.08	124.52
27	3	1620	LUT	C21-C26-C27	-2.31	110.17	112.83
39	C	518	DGD	O3D-C3D-C4D	-2.31	104.92	110.38
26	C	512	CLA	CHB-C4A-NA	2.31	127.74	124.40
28	g	1622	XAT	C18-C5-C4	2.31	116.84	114.24
26	B	604	CLA	O2A-CGA-O1A	-2.31	117.85	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	1	1622	XAT	C19-C9-C8	2.31	121.62	118.09
25	Y	606	CHL	C3D-C4D-ND	2.31	116.64	112.94
26	6	610	CLA	C1-C2-C3	-2.31	123.02	126.76
25	R	608	CHL	CAC-C3C-C4C	2.31	129.97	124.03
27	y	1620	LUT	C8-C7-C6	-2.31	120.83	127.00
25	1	607	CHL	CMB-C2B-C3B	2.31	129.30	124.68
25	5	607	CHL	CMB-C2B-C3B	2.31	129.30	124.68
26	B	603	CLA	C3B-C4B-NB	-2.31	108.47	110.53
26	G	614	CLA	O2D-CGD-CBD	2.31	115.27	111.23
25	y	609	CHL	O2A-CGA-CBA	2.31	118.87	111.83
26	b	605	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
39	c	519	DGD	C5B-C4B-C3B	-2.31	102.70	114.37
25	1	605	CHL	CAA-C2A-C3A	-2.31	106.77	113.00
25	5	605	CHL	CAA-C2A-C3A	-2.31	106.77	113.00
26	1	602	CLA	CAC-C3C-C4C	2.31	127.79	124.79
26	B	605	CLA	C2A-C3A-C4A	2.31	105.59	101.87
39	c	518	DGD	O3D-C3D-C4D	-2.31	104.94	110.38
25	s	601	CHL	O2D-CGD-O1D	-2.31	119.36	123.85
26	s	602	CLA	CHB-C4A-NA	2.31	127.73	124.40
25	7	605	CHL	CMB-C2B-C3B	2.31	129.29	124.68
26	Y	604	CLA	CMB-C2B-C3B	2.31	131.97	126.55
37	b	622	LMG	C40-C39-C38	-2.30	102.73	114.37
26	c	513	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
39	C	519	DGD	C5B-C4B-C3B	-2.30	102.73	114.37
25	n	609	CHL	O2A-CGA-CBA	2.30	118.85	111.83
26	A	406	CLA	C1C-C2C-C3C	-2.30	104.56	106.98
27	7	1620	LUT	C21-C26-C27	-2.30	110.18	112.83
37	C	521	LMG	C40-C39-C38	-2.30	102.74	114.37
26	c	505	CLA	CHC-C4B-NB	2.30	127.50	124.05
26	c	512	CLA	CHB-C4A-NA	2.30	127.72	124.40
26	1	612	CLA	CAA-C2A-C3A	-2.30	106.78	113.00
26	A	406	CLA	C11-C12-C13	-2.30	108.32	115.97
27	5	1621	LUT	C19-C9-C8	2.30	121.60	118.09
25	N	609	CHL	O2A-CGA-CBA	2.30	118.84	111.83
25	N	607	CHL	C3D-C4D-CHA	2.30	112.03	108.54
25	n	607	CHL	C3D-C4D-CHA	2.30	112.03	108.54
25	n	608	CHL	CAC-C3C-C4C	2.30	129.94	124.03
26	R	604	CLA	CMB-C2B-C3B	2.30	131.96	126.55
26	n	604	CLA	CMB-C2B-C3B	2.30	131.96	126.55
25	4	606	CHL	C4C-CHD-C1D	2.30	124.29	116.07
28	4	622	XAT	C20-C13-C12	2.30	121.60	118.09
25	N	608	CHL	CAC-C3C-C4C	2.30	129.94	124.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	1	1621	LUT	C39-C29-C28	2.30	121.60	118.09
26	b	604	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
26	Y	603	CLA	CHB-C1B-C2B	-2.30	120.76	127.43
27	1	1620	LUT	C21-C26-C27	-2.30	110.19	112.83
37	c	521	LMG	C40-C39-C38	-2.30	102.76	114.37
37	B	622	LMG	C40-C39-C38	-2.30	102.76	114.37
25	7	601	CHL	CMB-C2B-C3B	2.30	129.27	124.68
26	B	605	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
26	C	507	CLA	CHC-C4B-NB	2.30	127.49	124.05
25	r	607	CHL	CED-O2D-CGD	2.30	121.12	115.92
26	5	612	CLA	CAA-C2A-C3A	-2.30	106.80	113.00
37	A	413	LMG	C38-C37-C36	-2.30	102.77	114.37
25	G	605	CHL	C4C-CHD-C1D	2.30	124.28	116.07
25	g	605	CHL	C4C-CHD-C1D	2.30	124.28	116.07
30	d	409	LHG	C20-C19-C18	-2.30	102.77	114.37
26	s	603	CLA	O2A-CGA-O1A	-2.29	117.43	123.33
27	Y	1620	LUT	C8-C7-C6	-2.29	120.87	127.00
25	N	608	CHL	C1C-C2C-CMC	2.29	130.94	126.80
25	Y	609	CHL	O2A-CGA-CBA	2.29	118.83	111.83
26	g	614	CLA	O2D-CGD-CBD	2.29	115.24	111.23
37	B	2633	LMG	C40-C39-C38	-2.29	102.78	114.37
26	y	604	CLA	CMB-C2B-C3B	2.29	131.94	126.55
29	3	1623	NEX	C28-C29-C30	2.29	122.62	119.01
39	B	626	DGD	O3G-C3G-C2G	-2.29	105.24	110.82
26	C	505	CLA	CHC-C4B-NB	2.29	127.49	124.05
28	N	1622	XAT	C7-C8-C9	-2.29	121.97	125.53
25	3	605	CHL	C4C-CHD-C1D	2.29	124.27	116.07
25	7	605	CHL	C4C-CHD-C1D	2.29	124.27	116.07
26	6	610	CLA	C3B-C4B-NB	-2.29	108.48	110.53
25	2	601	CHL	OBD-CAD-C3D	-2.29	124.32	127.89
29	Y	1623	NEX	C39-C29-C30	-2.29	119.10	122.82
27	s	1621	LUT	C15-C35-C34	-2.29	118.83	123.52
26	c	507	CLA	CHC-C4B-NB	2.29	127.48	124.05
26	a	406	CLA	C11-C12-C13	-2.29	108.35	115.97
37	b	2633	LMG	C1-O6-C5	-2.29	109.25	113.72
30	D	409	LHG	C20-C19-C18	-2.29	102.79	114.37
26	2	610	CLA	C3B-C4B-NB	-2.29	108.49	110.53
27	S	1621	LUT	C15-C35-C34	-2.29	118.83	123.52
26	y	603	CLA	CHB-C1B-C2B	-2.29	120.78	127.43
37	a	413	LMG	C38-C37-C36	-2.29	102.80	114.37
39	b	626	DGD	O3G-C3G-C2G	-2.29	105.25	110.82
25	S	601	CHL	O2D-CGD-O1D	-2.29	119.39	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	601	CHL	C1C-C2C-CMC	2.29	130.93	126.80
26	r	604	CLA	CMB-C2B-C3B	2.29	131.93	126.55
30	N	2630	LHG	O8-C23-C24	2.29	118.81	111.83
28	5	1622	XAT	C19-C9-C8	2.29	121.58	118.09
28	G	1622	XAT	C18-C5-C4	2.29	116.81	114.24
26	d	402	CLA	CHD-C1D-ND	-2.29	121.58	124.80
26	B	616	CLA	O2D-CGD-CBD	2.29	115.23	111.23
37	b	2633	LMG	C40-C39-C38	-2.29	102.81	114.37
25	8	606	CHL	C4C-CHD-C1D	2.29	124.25	116.07
26	n	602	CLA	CHB-C1B-NB	2.29	127.48	124.05
39	C	519	DGD	O2D-C2D-C1D	-2.28	104.63	110.08
39	c	519	DGD	O2D-C2D-C1D	-2.28	104.63	110.08
27	1	1621	LUT	C8-C7-C6	-2.28	120.89	127.00
27	4	620	LUT	C27-C28-C29	-2.28	121.41	126.32
37	B	2633	LMG	C38-C37-C36	-2.28	102.83	114.37
37	b	2633	LMG	C38-C37-C36	-2.28	102.83	114.37
26	C	511	CLA	C3B-C4B-NB	-2.28	108.49	110.53
27	s	1621	LUT	C27-C28-C29	-2.28	121.41	126.32
28	8	622	XAT	C20-C13-C12	2.28	121.58	118.09
26	Y	610	CLA	CMB-C2B-C1B	-2.28	121.94	125.42
26	y	610	CLA	CMB-C2B-C1B	-2.28	121.94	125.42
35	a	408	PHO	CMA-C3A-C4A	-2.28	109.70	114.61
26	N	604	CLA	CMB-C2B-C3B	2.28	131.91	126.55
26	g	612	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
27	5	1621	LUT	C39-C29-C28	2.28	121.57	118.09
27	8	620	LUT	C27-C28-C29	-2.28	121.42	126.32
26	c	505	CLA	CHB-C4A-NA	2.28	127.69	124.40
26	C	513	CLA	O2D-CGD-CBD	2.28	115.22	111.23
30	n	2630	LHG	O8-C23-C24	2.28	118.78	111.83
26	B	617	CLA	CAC-C3C-C4C	2.28	127.75	124.79
25	3	608	CHL	O2D-CGD-O1D	-2.28	119.41	123.85
29	G	1623	NEX	C30-C31-C32	-2.28	116.60	123.20
27	R	620	LUT	C21-C26-C27	-2.28	110.21	112.83
26	R	601	CLA	CAC-C3C-C2C	-2.28	123.37	127.56
26	b	616	CLA	O2D-CGD-CBD	2.28	115.21	111.23
27	G	1621	LUT	C35-C15-C14	-2.28	118.86	123.52
26	B	606	CLA	CHC-C1C-NC	2.28	127.74	124.31
26	b	606	CLA	CHC-C1C-NC	2.28	127.74	124.31
37	B	2633	LMG	C1-O6-C5	-2.28	109.27	113.72
25	3	608	CHL	O2A-CGA-CBA	2.28	121.19	114.00
31	4	623	BCR	C20-C21-C22	-2.28	124.08	127.28
26	N	602	CLA	CHB-C1B-NB	2.28	127.46	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	605	CHL	OMC-CMC-C2C	-2.28	121.17	125.12
29	7	1623	NEX	C28-C29-C30	2.27	122.59	119.01
29	y	1623	NEX	C39-C29-C30	-2.27	119.13	122.82
30	2	2630	LHG	C11-C10-C9	-2.27	102.87	114.37
25	3	601	CHL	CMB-C2B-C3B	2.27	129.23	124.68
37	A	413	LMG	C6-C5-C4	-2.27	107.44	113.02
29	g	1623	NEX	C30-C31-C32	-2.27	116.61	123.20
27	S	1621	LUT	C27-C28-C29	-2.27	121.43	126.32
26	B	607	CLA	CHB-C1B-NB	2.27	127.46	124.05
26	b	607	CLA	CHB-C1B-NB	2.27	127.46	124.05
35	A	408	PHO	C6-C7-C8	-2.27	108.41	115.97
25	2	601	CHL	C1C-C2C-CMC	2.27	130.90	126.80
29	y	1623	NEX	C11-C12-C13	-2.27	120.13	126.36
30	6	2630	LHG	C11-C10-C9	-2.27	102.88	114.37
27	5	1621	LUT	C8-C7-C6	-2.27	120.93	127.00
30	D	410	LHG	C11-C10-C9	-2.27	102.88	114.37
28	N	1622	XAT	C40-C33-C32	2.27	121.56	118.09
26	r	601	CLA	CAC-C3C-C2C	-2.27	123.39	127.56
27	g	1621	LUT	C35-C15-C14	-2.27	118.87	123.52
27	6	1621	LUT	C8-C9-C10	-2.27	115.44	119.01
31	b	618	BCR	C23-C22-C21	-2.27	115.44	119.01
31	C	516	BCR	C34-C9-C8	2.27	121.56	118.09
26	N	610	CLA	CHB-C4A-NA	2.27	127.68	124.40
26	8	602	CLA	C3B-C4B-NB	-2.27	108.50	110.53
26	b	603	CLA	C3B-C4B-NB	-2.27	108.50	110.53
35	a	408	PHO	C6-C7-C8	-2.27	108.42	115.97
35	A	408	PHO	CMA-C3A-C4A	-2.27	109.72	114.61
26	c	513	CLA	O2D-CGD-CBD	2.27	115.20	111.23
25	7	608	CHL	O2A-CGA-CBA	2.27	121.17	114.00
25	n	608	CHL	C1C-C2C-CMC	2.27	130.89	126.80
29	Y	1623	NEX	C11-C12-C13	-2.27	120.14	126.36
25	7	607	CHL	CAA-C2A-C3A	-2.27	106.87	113.00
37	a	413	LMG	C6-C5-C4	-2.27	107.45	113.02
37	z	101	LMG	C1-O6-C5	-2.27	109.29	113.72
36	A	418	SQD	O47-C7-O49	-2.27	118.40	123.70
27	G	1620	LUT	C16-C1-C6	-2.27	106.69	110.24
25	G	608	CHL	OBD-CAD-C3D	-2.27	124.36	127.89
36	a	418	SQD	O47-C7-O49	-2.27	118.40	123.70
27	2	1621	LUT	C8-C9-C10	-2.27	115.44	119.01
30	d	410	LHG	C11-C10-C9	-2.27	102.91	114.37
26	G	612	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
31	C	515	BCR	C4-C5-C6	-2.27	119.64	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	608	CHL	O2D-CGD-O1D	-2.26	119.44	123.85
26	G	610	CLA	CHB-C4A-NA	2.26	127.67	124.40
39	c	520	DGD	O3E-C3E-C2E	-2.26	105.04	110.38
37	A	415	LMG	O3-C3-C2	-2.26	105.04	110.38
37	a	415	LMG	O3-C3-C2	-2.26	105.04	110.38
26	N	603	CLA	CHD-C1D-C2D	2.26	130.19	125.49
26	a	406	CLA	CHD-C4C-NC	2.26	127.74	124.23
31	C	516	BCR	C8-C9-C10	-2.26	115.45	119.01
25	4	601	CHL	O2D-CGD-O1D	-2.26	118.95	124.08
25	8	601	CHL	O2D-CGD-O1D	-2.26	118.95	124.08
25	1	608	CHL	OMC-CMC-C2C	-2.26	121.19	125.12
39	C	520	DGD	O3E-C3E-C2E	-2.26	105.04	110.38
27	R	620	LUT	C38-C25-C24	-2.26	118.01	123.36
25	G	608	CHL	CMD-C2D-C3D	-2.26	120.16	124.68
25	6	601	CHL	OBD-CAD-C3D	-2.26	124.36	127.89
28	8	622	XAT	C39-C29-C28	2.26	121.54	118.09
26	b	617	CLA	CAC-C3C-C4C	2.26	127.73	124.79
25	g	608	CHL	OBD-CAD-C3D	-2.26	124.36	127.89
25	1	605	CHL	OMC-CMC-C2C	-2.26	121.19	125.12
30	r	2630	LHG	C11-C10-C9	-2.26	102.94	114.37
25	5	608	CHL	OMC-CMC-C2C	-2.26	121.20	125.12
39	C	518	DGD	O3G-C1D-C2D	-2.26	104.84	108.27
31	B	618	BCR	C23-C22-C21	-2.26	115.45	119.01
26	C	505	CLA	CHB-C4A-NA	2.26	127.66	124.40
25	S	601	CHL	O1D-CGD-CBD	-2.26	121.30	124.72
26	r	603	CLA	C3B-C4B-NB	-2.26	108.51	110.53
25	5	601	CHL	O2D-CGD-O1D	-2.26	119.45	123.85
25	g	608	CHL	CMD-C2D-C3D	-2.26	120.17	124.68
27	r	620	LUT	C38-C25-C24	-2.26	118.02	123.36
25	3	607	CHL	CAA-C2A-C3A	-2.26	106.90	113.00
26	n	603	CLA	CHD-C1D-C2D	2.26	130.18	125.49
25	1	609	CHL	OMC-CMC-C2C	-2.26	121.20	125.12
31	c	516	BCR	C34-C9-C8	2.26	121.53	118.09
26	7	611	CLA	CHC-C4B-NB	2.26	127.43	124.05
26	G	613	CLA	O2D-CGD-O1D	-2.26	119.46	123.85
25	N	609	CHL	C4C-CHD-C1D	2.26	124.14	116.07
26	B	607	CLA	O2A-CGA-O1A	-2.26	117.99	123.63
36	B	621	SQD	O47-C7-O49	-2.25	118.43	123.70
27	2	1621	LUT	C8-C7-C6	-2.25	120.98	127.00
25	n	609	CHL	C4C-CHD-C1D	2.25	124.13	116.07
30	R	2630	LHG	C11-C10-C9	-2.25	102.98	114.37
25	N	601	CHL	O2A-CGA-CBA	2.25	118.70	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	d	408	LHG	O8-C23-O10	-2.25	117.99	123.63
26	n	610	CLA	CHB-C4A-NA	2.25	127.65	124.40
25	Y	608	CHL	O2A-CGA-O1A	-2.25	118.00	123.63
39	c	518	DGD	O6D-C5D-C6D	-2.25	102.23	106.69
41	f	101	HEM	C2A-C1A-NA	-2.25	107.65	110.15
26	B	616	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
30	g	2630	LHG	C18-C17-C16	-2.25	102.99	114.37
26	A	406	CLA	C1-C2-C3	-2.25	122.51	126.20
31	c	516	BCR	C8-C9-C10	-2.25	115.47	119.01
26	a	406	CLA	C1-C2-C3	-2.25	122.51	126.20
31	c	515	BCR	C4-C5-C6	-2.25	119.66	122.70
26	C	509	CLA	C2D-C1D-ND	-2.25	107.90	110.13
39	C	518	DGD	O6D-C5D-C6D	-2.25	102.24	106.69
27	r	620	LUT	C21-C26-C27	-2.25	110.24	112.83
26	C	513	CLA	O2A-CGA-CBA	2.25	118.69	111.83
25	5	609	CHL	OMC-CMC-C2C	-2.25	121.22	125.12
25	n	601	CHL	O2A-CGA-CBA	2.25	118.69	111.83
31	8	623	BCR	C20-C21-C22	-2.25	124.13	127.28
30	5	2630	LHG	C27-C26-C25	-2.25	103.01	114.37
26	S	602	CLA	CMB-C2B-C3B	2.25	131.83	126.55
26	s	602	CLA	CMB-C2B-C3B	2.24	131.83	126.55
28	n	1622	XAT	C40-C33-C32	2.24	121.52	118.09
37	Z	101	LMG	C1-O6-C5	-2.24	109.34	113.72
26	Y	603	CLA	C2A-C1A-CHA	2.24	127.76	123.87
26	c	513	CLA	CHC-C4B-NB	2.24	127.42	124.05
26	n	612	CLA	C2A-C1A-CHA	2.24	127.76	123.87
30	D	409	LHG	O8-C23-O10	-2.24	118.02	123.63
28	4	622	XAT	C39-C29-C28	2.24	121.51	118.09
25	y	608	CHL	O2A-CGA-O1A	-2.24	118.02	123.63
26	y	603	CLA	C2A-C1A-CHA	2.24	127.76	123.87
30	1	2630	LHG	C18-C17-C16	-2.24	103.04	114.37
29	1	1623	NEX	C10-C11-C12	-2.24	116.71	123.20
30	1	2630	LHG	C27-C26-C25	-2.24	103.04	114.37
36	b	621	SQD	O47-C7-O49	-2.24	118.47	123.70
41	F	101	HEM	C2A-C1A-NA	-2.24	107.67	110.15
26	Y	603	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
26	c	511	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
26	n	603	CLA	C3C-C4C-NC	-2.24	107.56	110.43
26	A	405	CLA	O2D-CGD-CBD	2.24	115.14	111.23
25	s	601	CHL	O1D-CGD-CBD	-2.24	121.33	124.72
30	C	523	LHG	C20-C19-C18	-2.24	103.05	114.37
27	g	1620	LUT	C16-C1-C6	-2.24	106.73	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	c	521	LMG	O3-C3-C2	-2.24	105.10	110.38
36	B	623	SQD	O5-C5-C4	2.24	113.73	109.70
36	b	623	SQD	O5-C5-C4	2.24	113.73	109.70
30	D	408	LHG	O8-C23-O10	-2.24	118.03	123.63
30	G	2630	LHG	C18-C17-C16	-2.24	103.06	114.37
26	b	612	CLA	CMC-C2C-C1C	-2.24	121.54	125.03
27	7	1620	LUT	C18-C5-C6	-2.24	122.04	124.48
26	a	405	CLA	CBC-CAC-C3C	2.24	118.48	112.42
25	1	601	CHL	O2D-CGD-O1D	-2.24	119.50	123.85
26	g	610	CLA	CHB-C4A-NA	2.24	127.63	124.40
26	B	612	CLA	CMC-C2C-C1C	-2.24	121.54	125.03
30	c	523	LHG	C20-C19-C18	-2.24	103.07	114.37
31	B	620	BCR	C37-C22-C23	2.24	121.50	118.09
26	c	503	CLA	C7-C6-C5	-2.24	107.30	113.26
37	C	521	LMG	O3-C3-C2	-2.24	105.11	110.38
39	C	520	DGD	O6E-C1E-O5D	-2.24	104.76	110.04
26	b	616	CLA	O2A-CGA-O1A	-2.24	118.04	123.63
26	c	513	CLA	O2A-CGA-CBA	2.24	118.65	111.83
26	4	602	CLA	C3B-C4B-NB	-2.23	108.53	110.53
25	3	607	CHL	O2D-CGD-O1D	-2.23	119.50	123.85
25	7	607	CHL	O2D-CGD-O1D	-2.23	119.50	123.85
26	A	405	CLA	CBC-CAC-C3C	2.23	118.48	112.42
25	g	601	CHL	CED-O2D-CGD	2.23	120.98	115.92
26	A	406	CLA	CHD-C4C-NC	2.23	127.70	124.23
26	C	503	CLA	C7-C6-C5	-2.23	107.31	113.26
39	c	518	DGD	O3G-C1D-C2D	-2.23	104.88	108.27
27	6	1621	LUT	C8-C7-C6	-2.23	121.03	127.00
27	n	1621	LUT	C31-C30-C29	-2.23	124.14	127.28
25	n	605	CHL	CAC-C3C-C4C	2.23	129.77	124.03
26	b	607	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
30	5	2630	LHG	C18-C17-C16	-2.23	103.08	114.37
25	N	607	CHL	C4D-CHA-CBD	-2.23	106.72	108.97
30	d	410	LHG	C27-C26-C25	-2.23	103.09	114.37
26	7	603	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
26	y	603	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
26	s	610	CLA	O2D-CGD-CBD	2.23	115.13	111.23
25	8	606	CHL	CMB-C2B-C3B	2.23	129.14	124.68
27	7	1621	LUT	C38-C25-C24	-2.23	118.08	123.36
30	d	409	LHG	O8-C23-O10	-2.23	118.05	123.63
25	1	606	CHL	CBA-CAA-C2A	-2.23	107.21	113.78
39	c	520	DGD	O6E-C1E-O5D	-2.23	104.78	110.04
26	C	507	CLA	O2A-CGA-O1A	-2.23	118.05	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	2630	LHG	C27-C26-C25	-2.23	103.10	114.37
26	3	611	CLA	CHA-C1A-NA	-2.23	121.34	126.39
25	4	609	CHL	CAC-C3C-C4C	2.23	129.76	124.03
25	N	607	CHL	CAC-C3C-C4C	2.23	129.76	124.03
25	n	607	CHL	CAC-C3C-C4C	2.23	129.76	124.03
26	Y	611	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
26	B	608	CLA	CHB-C1B-NB	2.23	127.39	124.05
25	4	606	CHL	CMB-C2B-C3B	2.23	129.14	124.68
26	N	603	CLA	C3C-C4C-NC	-2.23	107.58	110.43
26	g	613	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
26	6	603	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
26	a	405	CLA	O2D-CGD-CBD	2.23	115.12	111.23
30	D	410	LHG	C27-C26-C25	-2.23	103.11	114.37
38	D	405	PL9	C20-C19-C21	2.23	119.09	115.23
29	5	1623	NEX	C10-C11-C12	-2.23	116.75	123.20
26	b	608	CLA	CHB-C1B-NB	2.23	127.39	124.05
26	G	613	CLA	C3B-C4B-NB	-2.23	108.54	110.53
26	S	610	CLA	O2D-CGD-CBD	2.23	115.12	111.23
27	N	1621	LUT	C31-C30-C29	-2.23	124.16	127.28
26	N	612	CLA	C2A-C1A-CHA	2.23	127.73	123.87
25	y	609	CHL	CAC-C3C-C4C	2.23	129.75	124.03
27	Y	1621	LUT	C35-C15-C14	-2.23	118.96	123.52
30	6	2630	LHG	C27-C26-C25	-2.23	103.12	114.37
36	a	418	SQD	O8-S-C6	2.23	110.27	105.97
27	3	1620	LUT	C18-C5-C6	-2.23	122.06	124.48
26	b	602	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
26	c	507	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
26	n	603	CLA	O2D-CGD-CBD	2.22	115.12	111.23
26	Y	603	CLA	CAA-C2A-C3A	-2.22	106.99	113.00
38	d	405	PL9	C20-C19-C21	2.22	119.09	115.23
29	S	1623	NEX	C15-C35-C34	-2.22	118.97	123.52
29	s	1623	NEX	C15-C35-C34	-2.22	118.97	123.52
26	C	513	CLA	CHC-C4B-NB	2.22	127.39	124.05
26	G	602	CLA	C3B-C4B-NB	-2.22	108.55	110.53
26	y	603	CLA	CBC-CAC-C3C	-2.22	106.39	112.42
25	5	606	CHL	CBA-CAA-C2A	-2.22	107.23	113.78
26	3	611	CLA	CHC-C4B-NB	2.22	127.38	124.05
28	g	1622	XAT	O4-C5-C6	-2.22	57.17	58.93
36	A	418	SQD	O8-S-C6	2.22	110.26	105.97
25	N	605	CHL	CAC-C3C-C4C	2.22	129.74	124.03
30	b	2631	LHG	C11-C10-C9	-2.22	103.15	114.37
26	C	511	CLA	CMB-C2B-C1B	-2.22	122.04	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y	603	CLA	CHB-C1B-NB	2.22	127.38	124.05
27	2	1620	LUT	C38-C25-C24	-2.22	118.11	123.36
26	Y	603	CLA	CBC-CAC-C3C	-2.22	106.40	112.42
26	d	403	CLA	CAA-CBA-CGA	-2.22	106.91	113.21
26	g	602	CLA	C3B-C4B-NB	-2.22	108.55	110.53
25	5	601	CHL	CAC-C3C-C4C	2.22	129.73	124.03
27	Y	1621	LUT	C8-C9-C10	-2.22	115.52	119.01
31	b	620	BCR	C37-C22-C23	2.22	121.48	118.09
26	7	611	CLA	CHA-C1A-NA	-2.22	121.37	126.39
26	B	608	CLA	CMC-C2C-C3C	2.22	132.15	126.15
26	y	611	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
29	1	1623	NEX	C11-C12-C13	-2.22	120.28	126.36
25	4	606	CHL	OMC-CMC-C2C	-2.22	121.27	125.12
26	2	603	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
25	1	601	CHL	CAC-C3C-C4C	2.22	129.73	124.03
35	A	408	PHO	C1-C2-C3	-2.22	122.56	126.20
26	y	611	CLA	C2A-C1A-CHA	2.22	127.71	123.87
30	B	2631	LHG	C11-C10-C9	-2.22	103.16	114.37
26	b	605	CLA	O2D-CGD-CBD	2.22	115.10	111.23
25	G	601	CHL	CED-O2D-CGD	2.22	120.94	115.92
29	r	623	NEX	C28-C29-C30	2.21	122.49	119.01
30	r	2630	LHG	C18-C17-C16	-2.21	103.17	114.37
26	3	603	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
26	5	611	CLA	C3B-C4B-NB	-2.21	108.55	110.53
30	b	2630	LHG	C18-C17-C16	-2.21	103.17	114.37
25	8	609	CHL	CAC-C3C-C4C	2.21	129.72	124.03
31	T	101	BCR	C29-C30-C25	2.21	113.66	110.44
27	7	1621	LUT	C30-C31-C32	-2.21	116.78	123.20
29	7	1623	NEX	C12-C13-C14	2.21	122.49	119.01
27	3	1621	LUT	C38-C25-C24	-2.21	118.12	123.36
26	c	509	CLA	C2D-C1D-ND	-2.21	107.94	110.13
26	S	603	CLA	O1A-CGA-CBA	2.21	130.11	123.09
27	y	1621	LUT	C8-C9-C10	-2.21	115.53	119.01
26	R	603	CLA	C3B-C4B-NB	-2.21	108.56	110.53
26	s	610	CLA	CHB-C1B-NB	2.21	127.37	124.05
25	Y	609	CHL	CAC-C3C-C4C	2.21	129.72	124.03
27	y	1621	LUT	C35-C15-C14	-2.21	118.99	123.52
27	3	1621	LUT	C30-C31-C32	-2.21	116.79	123.20
26	C	501	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
30	B	2630	LHG	C18-C17-C16	-2.21	103.19	114.37
27	r	620	LUT	C12-C13-C14	-2.21	115.53	119.01
25	8	606	CHL	OMC-CMC-C2C	-2.21	121.28	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	502	CLA	O2D-CGD-CBD	2.21	115.09	111.23
26	c	502	CLA	O2D-CGD-CBD	2.21	115.09	111.23
26	S	603	CLA	CHC-C1C-NC	2.21	127.64	124.31
26	s	603	CLA	CHC-C1C-NC	2.21	127.64	124.31
26	Y	611	CLA	C2A-C1A-CHA	2.21	127.70	123.87
26	y	603	CLA	CHB-C1B-NB	2.21	127.36	124.05
30	R	2630	LHG	C18-C17-C16	-2.21	103.20	114.37
26	G	614	CLA	C3B-C4B-NB	-2.21	108.56	110.53
25	r	606	CHL	CMD-C2D-C3D	-2.21	120.27	124.68
27	6	1620	LUT	C38-C25-C24	-2.21	118.13	123.36
26	B	605	CLA	O2D-CGD-CBD	2.21	115.09	111.23
31	t	101	BCR	C4-C5-C6	-2.21	119.72	122.70
26	B	607	CLA	CHC-C1C-NC	2.21	127.64	124.31
26	c	508	CLA	CMC-C2C-C3C	2.21	132.12	126.15
26	y	603	CLA	CAA-C2A-C3A	-2.21	107.04	113.00
27	6	1621	LUT	C35-C15-C14	-2.21	119.00	123.52
26	D	403	CLA	CAA-CBA-CGA	-2.21	106.94	113.21
25	R	606	CHL	CMD-C2D-C3D	-2.20	120.28	124.68
25	n	607	CHL	C4D-CHA-CBD	-2.20	106.75	108.97
29	5	1623	NEX	C11-C12-C13	-2.20	120.32	126.36
26	C	508	CLA	CMC-C2C-C3C	2.20	132.11	126.15
26	7	610	CLA	CHB-C4A-NA	2.20	127.58	124.40
26	b	608	CLA	CMC-C2C-C3C	2.20	132.11	126.15
26	g	603	CLA	O2D-CGD-CBD	2.20	115.08	111.23
26	B	616	CLA	C6-C7-C8	-2.20	108.65	115.97
25	R	607	CHL	O2D-CGD-O1D	-2.20	119.56	123.85
27	2	1621	LUT	C35-C15-C14	-2.20	119.02	123.52
26	Y	602	CLA	CHB-C4A-NA	2.20	127.58	124.40
26	y	602	CLA	CHB-C4A-NA	2.20	127.58	124.40
26	S	610	CLA	CHB-C1B-NB	2.20	127.35	124.05
26	5	604	CLA	CMB-C2B-C3B	2.20	131.72	126.55
31	8	623	BCR	C2-C1-C6	2.20	113.63	110.44
31	c	515	BCR	C2-C1-C6	2.20	113.63	110.44
39	H	102	DGD	O6E-C5E-C4E	2.20	113.66	109.70
30	C	2630	LHG	O8-C6-C5	-2.20	102.06	108.40
26	g	614	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
27	R	620	LUT	C12-C13-C14	-2.20	115.55	119.01
29	3	1623	NEX	C12-C13-C14	2.20	122.47	119.01
26	B	602	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
30	c	2630	LHG	C27-C26-C25	-2.20	103.26	114.37
26	g	603	CLA	C3C-C4C-NC	-2.20	107.61	110.43
28	r	622	XAT	C38-C25-C24	2.20	116.71	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	R	623	NEX	C28-C29-C30	2.20	122.47	119.01
26	N	603	CLA	O2D-CGD-CBD	2.20	115.07	111.23
26	C	509	CLA	CGD-CBD-CAD	2.20	117.96	110.85
25	g	608	CHL	C1C-C2C-CMC	2.20	130.76	126.80
30	R	2630	LHG	C27-C26-C25	-2.20	103.27	114.37
26	c	509	CLA	CGD-CBD-CAD	2.20	117.95	110.85
26	B	610	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
30	C	2630	LHG	C27-C26-C25	-2.20	103.27	114.37
39	h	102	DGD	O6E-C5E-C4E	2.20	113.66	109.70
31	d	404	BCR	C15-C16-C17	-2.19	119.03	123.52
25	8	609	CHL	CBC-CAC-C3C	-2.19	109.73	112.87
25	y	601	CHL	O2A-CGA-CBA	2.19	118.52	111.83
26	s	603	CLA	O1A-CGA-CBA	2.19	130.05	123.09
26	N	602	CLA	C3B-C4B-NB	-2.19	108.57	110.53
26	n	602	CLA	C3B-C4B-NB	-2.19	108.57	110.53
26	S	602	CLA	C6-C5-C3	-2.19	108.13	113.47
25	2	606	CHL	O2D-CGD-O1D	-2.19	119.58	123.85
36	A	418	SQD	O48-C23-C24	2.19	118.52	111.83
25	4	609	CHL	CBC-CAC-C3C	-2.19	109.73	112.87
26	c	502	CLA	C1-C2-C3	-2.19	122.61	126.20
36	a	418	SQD	O48-C23-C24	2.19	118.52	111.83
27	5	1620	LUT	C28-C29-C30	-2.19	115.56	119.01
30	r	2630	LHG	C27-C26-C25	-2.19	103.29	114.37
35	a	408	PHO	C1-C2-C3	-2.19	122.61	126.20
28	R	622	XAT	C20-C13-C12	2.19	121.44	118.09
28	r	622	XAT	C20-C13-C12	2.19	121.44	118.09
25	r	607	CHL	O2D-CGD-O1D	-2.19	119.58	123.85
26	c	501	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
26	b	616	CLA	C6-C7-C8	-2.19	108.68	115.97
25	6	606	CHL	O2D-CGD-O1D	-2.19	119.58	123.85
31	B	619	BCR	C16-C15-C14	-2.19	119.04	123.52
31	T	101	BCR	C1-C6-C5	-2.19	119.64	122.64
31	4	623	BCR	C2-C3-C4	-2.19	106.46	111.28
25	r	608	CHL	C4-C3-C5	2.19	119.03	115.23
31	b	619	BCR	C33-C5-C6	-2.19	122.09	124.48
25	2	605	CHL	CAA-C2A-C3A	-2.19	107.08	113.00
27	N	1620	LUT	C28-C29-C30	-2.19	115.57	119.01
26	1	614	CLA	C3B-C4B-NB	-2.19	108.58	110.53
26	G	603	CLA	C3C-C4C-NC	-2.19	107.63	110.43
26	C	509	CLA	C3B-C4B-NB	-2.19	108.58	110.53
26	c	509	CLA	C3B-C4B-NB	-2.19	108.58	110.53
25	6	605	CHL	CAA-C2A-C3A	-2.19	107.09	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	2630	LHG	O8-C6-C5	-2.19	102.09	108.40
26	G	604	CLA	CMB-C2B-C3B	2.19	131.69	126.55
31	D	404	BCR	C15-C16-C17	-2.19	119.05	123.52
26	N	610	CLA	CHA-C1A-NA	-2.19	121.44	126.39
26	1	604	CLA	CMB-C2B-C3B	2.18	131.69	126.55
26	b	610	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
26	b	607	CLA	CHC-C1C-NC	2.18	127.60	124.31
27	5	1621	LUT	C38-C25-C24	-2.18	118.19	123.36
27	G	1620	LUT	C8-C9-C10	-2.18	115.57	119.01
26	B	604	CLA	CMB-C2B-C3B	2.18	131.68	126.55
26	b	614	CLA	O1D-CGD-CBD	2.18	128.82	124.52
27	1	1620	LUT	C8-C7-C6	-2.18	121.17	127.00
26	s	602	CLA	C6-C5-C3	-2.18	108.15	113.47
26	G	603	CLA	O2D-CGD-CBD	2.18	115.04	111.23
31	C	515	BCR	C2-C1-C6	2.18	113.61	110.44
27	1	1620	LUT	C28-C29-C30	-2.18	115.58	119.01
27	g	1620	LUT	C8-C9-C10	-2.18	115.58	119.01
26	5	614	CLA	C3B-C4B-NB	-2.18	108.58	110.53
31	T	101	BCR	C4-C5-C6	-2.18	119.76	122.70
26	3	610	CLA	CHB-C4A-NA	2.18	127.55	124.40
35	a	409	PHO	OBD-CAD-CBD	-2.18	122.62	125.82
27	1	1621	LUT	C38-C25-C24	-2.18	118.20	123.36
26	c	510	CLA	CAA-C2A-C3A	-2.18	107.11	113.00
26	1	611	CLA	C3B-C4B-NB	-2.18	108.58	110.53
28	R	622	XAT	C38-C25-C24	2.18	116.69	114.24
26	G	614	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
31	t	101	BCR	C29-C30-C25	2.18	113.60	110.44
27	S	1620	LUT	C38-C25-C24	-2.18	118.21	123.36
27	s	1620	LUT	C38-C25-C24	-2.18	118.21	123.36
37	C	521	LMG	C38-C37-C36	-2.18	103.36	114.37
26	n	610	CLA	CHA-C1A-NA	-2.18	121.46	126.39
31	4	623	BCR	C2-C1-C6	2.18	113.60	110.44
26	a	405	CLA	CHC-C1C-NC	2.18	127.59	124.31
27	G	1621	LUT	C1-C2-C3	2.18	118.37	113.59
27	n	1620	LUT	C28-C29-C30	-2.18	115.59	119.01
37	A	415	LMG	C38-C37-C36	-2.18	103.37	114.37
37	a	415	LMG	C38-C37-C36	-2.18	103.37	114.37
26	C	502	CLA	C1-C2-C3	-2.18	122.63	126.20
31	c	514	BCR	C40-C30-C25	-2.18	106.83	110.24
26	g	614	CLA	C3B-C4B-NB	-2.18	108.59	110.53
25	Y	601	CHL	O2A-CGA-CBA	2.18	118.47	111.83
39	b	626	DGD	O1G-C1A-O1A	-2.18	118.19	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	619	BCR	C16-C15-C14	-2.17	119.07	123.52
31	d	404	BCR	C3-C4-C5	-2.17	110.18	114.06
26	c	503	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
25	R	608	CHL	C4-C3-C5	2.17	119.00	115.23
25	1	609	CHL	CMB-C2B-C3B	2.17	129.03	124.68
25	y	606	CHL	O1D-CGD-CBD	-2.17	121.43	124.72
25	g	606	CHL	C4C-CHD-C1D	2.17	123.84	116.07
25	G	608	CHL	C1C-C2C-CMC	2.17	130.72	126.80
31	C	514	BCR	C40-C30-C25	-2.17	106.84	110.24
25	g	601	CHL	CMB-C2B-C3B	2.17	129.02	124.68
31	t	101	BCR	C1-C6-C5	-2.17	119.67	122.64
25	4	608	CHL	O2A-CGA-CBA	2.17	120.86	114.00
27	5	1621	LUT	C15-C35-C34	-2.17	119.08	123.52
25	G	601	CHL	CMB-C2B-C3B	2.17	129.02	124.68
26	d	403	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
25	8	607	CHL	CMB-C2B-C3B	2.17	129.02	124.68
27	Y	1621	LUT	C15-C35-C34	-2.17	119.08	123.52
26	c	501	CLA	C1-C2-C3	-2.17	122.64	126.20
26	C	502	CLA	CHC-C4B-NB	2.17	127.30	124.05
31	8	623	BCR	C2-C3-C4	-2.17	106.51	111.28
31	c	517	BCR	C11-C12-C13	-2.17	120.42	126.36
35	A	409	PHO	OBD-CAD-CBD	-2.17	122.64	125.82
27	g	1621	LUT	C1-C2-C3	2.17	118.35	113.59
27	6	1620	LUT	C19-C9-C8	2.17	121.40	118.09
27	5	1620	LUT	C8-C7-C6	-2.17	121.20	127.00
39	C	520	DGD	C1E-O6E-C5E	2.17	117.95	113.72
39	c	520	DGD	C1E-O6E-C5E	2.17	117.95	113.72
31	C	517	BCR	C11-C12-C13	-2.17	120.42	126.36
37	c	521	LMG	C38-C37-C36	-2.17	103.41	114.37
26	C	510	CLA	CAA-C2A-C3A	-2.17	107.14	113.00
26	S	609	CLA	O2A-CGA-O1A	-2.17	117.76	123.33
25	7	608	CHL	C1C-C2C-CMC	2.17	130.71	126.80
26	s	609	CLA	O2A-CGA-O1A	-2.17	117.76	123.33
25	Y	606	CHL	O1D-CGD-CBD	-2.17	121.44	124.72
27	1	1621	LUT	C15-C35-C34	-2.17	119.09	123.52
26	b	611	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
26	A	406	CLA	C16-C15-C13	-2.16	108.77	115.97
25	4	608	CHL	CMA-C3A-C4A	-2.16	109.95	114.61
28	R	622	XAT	C31-C30-C29	-2.16	124.24	127.28
30	Y	2630	LHG	C27-C26-C25	-2.16	103.43	114.37
25	8	608	CHL	CMA-C3A-C4A	-2.16	109.95	114.61
25	G	609	CHL	C1-C2-C3	-2.16	122.65	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	606	CHL	C4C-CHD-C1D	2.16	123.81	116.07
26	1	611	CLA	CHB-C4A-NA	2.16	127.52	124.40
26	5	611	CLA	CHB-C4A-NA	2.16	127.52	124.40
26	g	604	CLA	CMB-C2B-C3B	2.16	131.63	126.55
26	b	604	CLA	CMB-C2B-C3B	2.16	131.63	126.55
26	B	614	CLA	O1D-CGD-CBD	2.16	128.78	124.52
27	S	1620	LUT	C8-C7-C6	-2.16	121.23	127.00
27	s	1620	LUT	C8-C7-C6	-2.16	121.23	127.00
26	a	406	CLA	C16-C15-C13	-2.16	108.78	115.97
28	R	622	XAT	O24-C25-C26	-2.16	57.22	58.93
28	r	622	XAT	O24-C25-C26	-2.16	57.22	58.93
25	g	606	CHL	CAC-C3C-C4C	2.16	129.58	124.03
30	y	2630	LHG	C27-C26-C25	-2.16	103.45	114.37
26	C	501	CLA	C1-C2-C3	-2.16	122.66	126.20
25	Y	606	CHL	OBD-CAD-C3D	-2.16	124.52	127.89
26	c	502	CLA	CHC-C4B-NB	2.16	127.29	124.05
26	2	611	CLA	O2D-CGD-CBD	2.16	115.00	111.23
26	B	611	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
26	g	613	CLA	C3B-C4B-NB	-2.16	108.60	110.53
25	8	608	CHL	O2A-CGA-CBA	2.16	120.82	114.00
25	1	601	CHL	CBC-CAC-C3C	-2.16	109.78	112.87
26	C	503	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
26	1	604	CLA	CHB-C4A-NA	2.16	127.51	124.40
25	5	609	CHL	CMB-C2B-C3B	2.16	128.99	124.68
26	S	603	CLA	CHA-C1A-NA	-2.16	121.51	126.39
26	s	603	CLA	CHA-C1A-NA	-2.16	121.51	126.39
26	n	602	CLA	C6-C7-C8	-2.16	108.80	115.97
26	n	604	CLA	O1D-CGD-CBD	2.16	128.77	124.52
30	b	2631	LHG	C18-C17-C16	-2.16	103.47	114.37
30	c	522	LHG	C27-C26-C25	-2.16	103.47	114.37
26	b	606	CLA	CHB-C1B-NB	2.16	127.28	124.05
39	B	626	DGD	O1G-C1A-O1A	-2.16	118.24	123.63
26	N	602	CLA	O2D-CGD-CBD	2.16	115.00	111.23
26	2	611	CLA	C3B-C4B-NB	-2.16	108.61	110.53
26	B	606	CLA	CHB-C1B-NB	2.16	127.28	124.05
26	6	612	CLA	C2A-C1A-CHA	2.16	127.61	123.87
30	s	2630	LHG	C27-C26-C25	-2.15	103.48	114.37
26	2	612	CLA	C2A-C1A-CHA	2.15	127.61	123.87
31	D	404	BCR	C3-C4-C5	-2.15	110.21	114.06
26	y	602	CLA	C3B-C4B-NB	-2.15	108.61	110.53
26	Y	611	CLA	C6-C5-C3	-2.15	108.22	113.47
27	1	1620	LUT	C20-C13-C12	2.15	121.38	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D	403	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
30	S	2630	LHG	C27-C26-C25	-2.15	103.48	114.37
27	S	1621	LUT	C31-C30-C29	-2.15	124.26	127.28
25	g	609	CHL	C1-C2-C3	-2.15	122.67	126.20
26	A	405	CLA	CHC-C1C-NC	2.15	127.55	124.31
25	3	608	CHL	C1C-C2C-CMC	2.15	130.68	126.80
26	N	604	CLA	O1D-CGD-CBD	2.15	128.76	124.52
26	b	605	CLA	C11-C10-C8	-2.15	108.81	115.97
26	A	405	CLA	C1C-C2C-C3C	2.15	109.24	106.98
26	G	602	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
26	4	610	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
26	8	610	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
30	C	522	LHG	C27-C26-C25	-2.15	103.50	114.37
27	2	1620	LUT	C19-C9-C8	2.15	121.37	118.09
26	6	611	CLA	O2D-CGD-CBD	2.15	114.99	111.23
31	B	619	BCR	C11-C12-C13	-2.15	120.47	126.36
26	B	606	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
25	S	607	CHL	O2D-CGD-O1D	-2.15	119.66	123.85
26	y	602	CLA	CAA-CBA-CGA	-2.15	107.11	113.21
26	B	605	CLA	C11-C10-C8	-2.15	108.82	115.97
25	4	607	CHL	CMB-C2B-C3B	2.15	128.98	124.68
31	c	516	BCR	C31-C1-C6	-2.15	106.87	110.24
25	n	605	CHL	OBD-CAD-C3D	-2.15	124.54	127.89
27	G	1621	LUT	C37-C21-C22	-2.15	105.40	109.41
30	B	2631	LHG	C18-C17-C16	-2.15	103.51	114.37
27	N	1620	LUT	C7-C8-C9	-2.15	123.06	126.23
25	G	606	CHL	CAC-C3C-C4C	2.15	129.55	124.03
28	G	1622	XAT	O4-C5-C6	-2.15	57.23	58.93
25	G	607	CHL	C1-O2A-CGA	2.15	121.85	116.65
26	R	603	CLA	O1D-CGD-CBD	2.15	128.75	124.52
26	r	603	CLA	O1D-CGD-CBD	2.15	128.75	124.52
26	6	611	CLA	C3B-C4B-NB	-2.15	108.61	110.53
41	f	101	HEM	CBA-CAA-C2A	-2.15	106.60	112.53
27	S	1621	LUT	C20-C13-C12	2.15	121.37	118.09
26	Y	602	CLA	CAA-CBA-CGA	-2.15	107.11	113.21
27	4	620	LUT	C19-C9-C8	2.15	121.37	118.09
37	z	101	LMG	O2-C2-C1	-2.15	104.96	110.08
36	B	621	SQD	O48-C23-C24	2.15	118.38	111.83
25	3	608	CHL	C4C-CHD-C1D	2.15	123.75	116.07
39	c	519	DGD	CAB-C9B-C8B	-2.15	103.53	114.37
26	B	604	CLA	C1D-ND-C4D	2.14	107.82	106.31
27	y	1621	LUT	C15-C35-C34	-2.14	119.13	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	s	2630	LHG	O8-C23-O10	-2.14	118.26	123.63
36	b	621	SQD	O48-C23-C24	2.14	118.37	111.83
31	B	619	BCR	C33-C5-C6	-2.14	122.14	124.48
28	r	622	XAT	C31-C30-C29	-2.14	124.27	127.28
26	n	602	CLA	O2D-CGD-CBD	2.14	114.98	111.23
31	b	619	BCR	C11-C12-C13	-2.14	120.49	126.36
30	S	2630	LHG	O8-C23-O10	-2.14	118.27	123.63
26	b	604	CLA	C1D-ND-C4D	2.14	107.81	106.31
26	b	606	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
29	S	1623	NEX	C11-C12-C13	-2.14	120.49	126.36
39	B	626	DGD	O2D-C2D-C3D	-2.14	105.33	110.38
26	a	407	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
30	C	522	LHG	C18-C17-C16	-2.14	103.55	114.37
26	b	602	CLA	C1-C2-C3	-2.14	122.69	126.20
25	4	606	CHL	CMA-C3A-C4A	-2.14	110.00	114.61
30	c	522	LHG	C18-C17-C16	-2.14	103.55	114.37
39	b	626	DGD	O2D-C2D-C3D	-2.14	105.33	110.38
29	s	1623	NEX	C11-C12-C13	-2.14	120.50	126.36
26	g	602	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
27	s	1621	LUT	C20-C13-C12	2.14	121.36	118.09
27	s	1621	LUT	C31-C30-C29	-2.14	124.28	127.28
25	6	601	CHL	O2D-CGD-O1D	-2.14	119.68	123.85
26	N	602	CLA	C6-C7-C8	-2.14	108.85	115.97
26	6	602	CLA	CMB-C2B-C3B	2.14	131.58	126.55
25	g	608	CHL	CMB-C2B-C3B	2.14	128.96	124.68
26	a	405	CLA	C1C-C2C-C3C	2.14	109.23	106.98
30	S	2630	LHG	C5-O7-C7	-2.14	112.68	117.80
30	s	2630	LHG	C5-O7-C7	-2.14	112.68	117.80
31	c	515	BCR	C10-C11-C12	-2.14	117.00	123.20
39	C	519	DGD	CAB-C9B-C8B	-2.14	103.56	114.37
26	c	511	CLA	CMB-C2B-C3B	2.14	131.58	126.55
26	n	603	CLA	CHB-C1B-C2B	-2.14	121.22	127.43
26	A	405	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
26	R	609	CLA	C1D-ND-C4D	-2.14	104.81	106.31
26	C	512	CLA	CAA-C2A-C3A	-2.14	107.23	113.00
26	C	512	CLA	C1-C2-C3	-2.14	122.70	126.20
25	G	601	CHL	C1-O2A-CGA	2.14	121.82	116.65
37	Z	101	LMG	O2-C2-C1	-2.14	104.99	110.08
25	s	607	CHL	O2D-CGD-O1D	-2.14	119.69	123.85
26	5	604	CLA	CHB-C4A-NA	2.13	127.48	124.40
29	y	1623	NEX	C30-C31-C32	-2.13	117.02	123.20
41	F	101	HEM	CBA-CAA-C2A	-2.13	106.63	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	c	512	CLA	CAA-C2A-C3A	-2.13	107.23	113.00
25	2	601	CHL	O2D-CGD-O1D	-2.13	119.70	123.85
25	N	605	CHL	OBD-CAD-C3D	-2.13	124.56	127.89
25	G	608	CHL	CMB-C2B-C3B	2.13	128.94	124.68
25	3	609	CHL	C4-C3-C5	2.13	118.93	115.23
25	7	609	CHL	C4-C3-C5	2.13	118.93	115.23
27	n	1620	LUT	C7-C8-C9	-2.13	123.08	126.23
26	C	508	CLA	CHC-C1C-NC	2.13	127.52	124.31
26	G	602	CLA	C6-C7-C8	-2.13	108.88	115.97
25	G	606	CHL	OMC-CMC-C2C	-2.13	121.42	125.12
39	c	520	DGD	CAB-C9B-C8B	-2.13	103.59	114.37
25	5	601	CHL	CMA-C3A-C4A	-2.13	110.02	114.61
25	8	606	CHL	CMA-C3A-C4A	-2.13	110.02	114.61
26	y	611	CLA	C6-C5-C3	-2.13	108.28	113.47
25	R	606	CHL	C4C-CHD-C1D	2.13	123.69	116.07
29	7	1623	NEX	C20-C13-C14	-2.13	119.36	122.82
25	7	608	CHL	C4C-CHD-C1D	2.13	123.69	116.07
26	A	407	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
28	N	1622	XAT	C28-C29-C30	2.13	122.36	119.01
26	3	612	CLA	CHA-C1A-NA	-2.13	121.57	126.39
26	7	612	CLA	CHA-C1A-NA	-2.13	121.57	126.39
26	g	602	CLA	C6-C7-C8	-2.13	108.89	115.97
39	C	520	DGD	CAB-C9B-C8B	-2.13	103.60	114.37
27	R	620	LUT	C18-C5-C6	-2.13	122.16	124.48
27	r	620	LUT	C18-C5-C6	-2.13	122.16	124.48
26	N	603	CLA	CHB-C1B-C2B	-2.13	121.24	127.43
26	1	612	CLA	CHB-C1B-NB	2.13	127.24	124.05
26	5	612	CLA	CHB-C1B-NB	2.13	127.24	124.05
30	C	522	LHG	C20-C19-C18	-2.13	103.61	114.37
25	g	607	CHL	C1-O2A-CGA	2.13	121.80	116.65
27	g	1621	LUT	C37-C21-C22	-2.13	105.44	109.41
29	6	1623	NEX	C39-C29-C30	-2.13	119.37	122.82
27	8	620	LUT	C19-C9-C8	2.13	121.34	118.09
31	C	516	BCR	C31-C1-C6	-2.13	106.91	110.24
29	N	1623	NEX	C30-C31-C32	-2.13	117.04	123.20
31	C	515	BCR	C10-C11-C12	-2.13	117.04	123.20
25	g	606	CHL	OMC-CMC-C2C	-2.13	121.43	125.12
30	c	522	LHG	C20-C19-C18	-2.13	103.62	114.37
30	8	2630	LHG	C5-O7-C7	-2.13	114.09	117.85
27	s	1621	LUT	C28-C29-C30	-2.13	115.67	119.01
26	B	615	CLA	C2D-C1D-ND	-2.13	108.02	110.13
26	b	615	CLA	C2D-C1D-ND	-2.13	108.02	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	1	1621	LUT	C27-C28-C29	-2.13	121.75	126.32
29	Y	1623	NEX	C30-C31-C32	-2.12	117.04	123.20
26	S	609	CLA	O1A-CGA-CBA	2.12	129.83	123.09
39	C	520	DGD	C7B-C6B-C5B	-2.12	103.63	114.37
26	C	511	CLA	CMB-C2B-C3B	2.12	131.55	126.55
25	y	606	CHL	OBD-CAD-C3D	-2.12	124.58	127.89
26	2	602	CLA	CMB-C2B-C3B	2.12	131.54	126.55
31	H	101	BCR	C2-C1-C6	2.12	113.52	110.44
31	h	101	BCR	C2-C1-C6	2.12	113.52	110.44
27	5	1620	LUT	C8-C9-C10	-2.12	115.67	119.01
39	c	520	DGD	C7B-C6B-C5B	-2.12	103.64	114.37
30	4	2630	LHG	C5-O7-C7	-2.12	114.10	117.85
39	c	520	DGD	CBB-CAB-C9B	-2.12	103.64	114.37
25	r	606	CHL	C4C-CHD-C1D	2.12	123.66	116.07
25	4	608	CHL	O1D-CGD-CBD	-2.12	121.51	124.72
26	C	502	CLA	CAA-C2A-C3A	-2.12	107.27	113.00
26	a	405	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
29	2	1623	NEX	C39-C29-C30	-2.12	119.38	122.82
26	a	406	CLA	C3C-C4C-NC	-2.12	107.71	110.43
31	C	514	BCR	C16-C15-C14	-2.12	119.18	123.52
25	2	601	CHL	CMA-C3A-C4A	-2.12	110.04	114.61
26	G	604	CLA	CHB-C4A-NA	2.12	127.46	124.40
25	2	605	CHL	O2D-CGD-O1D	-2.12	119.72	123.85
26	S	609	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
25	g	601	CHL	C1-O2A-CGA	2.12	121.78	116.65
25	5	601	CHL	CBC-CAC-C3C	-2.12	109.84	112.87
25	6	601	CHL	CED-O2D-CGD	2.12	120.72	115.92
26	3	614	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
27	6	1620	LUT	C8-C7-C6	-2.12	121.34	127.00
39	C	520	DGD	CBB-CAB-C9B	-2.12	103.66	114.37
27	5	1620	LUT	C20-C13-C12	2.12	121.32	118.09
26	A	407	CLA	CHD-C1D-ND	-2.12	121.82	124.80
26	B	616	CLA	C2A-C1A-CHA	2.12	127.54	123.87
30	s	2630	LHG	C18-C17-C16	-2.12	103.66	114.37
30	S	2630	LHG	C18-C17-C16	-2.12	103.67	114.37
30	l	101	LHG	O8-C23-C24	2.12	118.29	111.83
27	2	1620	LUT	C8-C7-C6	-2.12	121.34	127.00
25	1	601	CHL	CMA-C3A-C4A	-2.12	110.05	114.61
26	s	609	CLA	O1A-CGA-CBA	2.12	129.81	123.09
26	C	506	CLA	C2A-C1A-CHA	2.12	127.54	123.87
27	7	1620	LUT	C8-C9-C10	-2.12	115.68	119.01
39	c	520	DGD	C5B-C4B-C3B	-2.12	103.67	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	601	CHL	CMA-C3A-C4A	-2.12	110.05	114.61
26	3	602	CLA	C1-C2-C3	-2.12	122.73	126.20
26	7	614	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
31	B	620	BCR	C21-C20-C19	-2.12	117.07	123.20
26	3	610	CLA	C4A-NA-C1A	2.12	107.64	106.68
26	7	610	CLA	C4A-NA-C1A	2.12	107.64	106.68
29	n	1623	NEX	O24-C25-C26	-2.12	57.25	58.93
39	C	520	DGD	C5B-C4B-C3B	-2.12	103.68	114.37
35	A	408	PHO	CMC-C2C-C1C	-2.11	120.93	124.73
25	G	609	CHL	O2A-CGA-CBA	2.11	118.28	111.83
26	a	407	CLA	CHD-C1D-ND	-2.11	121.83	124.80
27	S	1621	LUT	C28-C29-C30	-2.11	115.68	119.01
26	Y	602	CLA	C3B-C4B-NB	-2.11	108.64	110.53
26	n	614	CLA	C3B-C4B-NB	-2.11	108.64	110.53
31	c	514	BCR	C16-C15-C14	-2.11	119.19	123.52
26	c	512	CLA	C1-C2-C3	-2.11	122.73	126.20
28	6	1622	XAT	C24-C23-C22	-2.11	106.84	110.79
26	3	602	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
26	7	602	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
26	7	612	CLA	CMD-C2D-C3D	2.11	132.53	127.69
26	C	513	CLA	C2A-C1A-CHA	2.11	127.53	123.87
26	c	513	CLA	C2A-C1A-CHA	2.11	127.53	123.87
26	1	604	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
29	n	1623	NEX	C30-C31-C32	-2.11	117.08	123.20
31	c	516	BCR	C35-C13-C12	2.11	121.31	118.09
26	C	508	CLA	CGD-CBD-CAD	2.11	117.68	110.85
26	R	611	CLA	O1D-CGD-CBD	2.11	128.68	124.52
26	7	604	CLA	CMB-C2B-C3B	2.11	131.52	126.55
26	g	614	CLA	CMB-C2B-C3B	2.11	131.52	126.55
26	c	502	CLA	CMC-C2C-C3C	2.11	131.86	126.15
26	B	602	CLA	C1-C2-C3	-2.11	122.74	126.20
26	r	611	CLA	O1D-CGD-CBD	2.11	128.68	124.52
31	B	619	BCR	C34-C9-C8	2.11	121.31	118.09
28	3	1622	XAT	O24-C25-C26	-2.11	57.26	58.93
29	3	1623	NEX	C20-C13-C14	-2.11	119.40	122.82
26	1	610	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
25	R	608	CHL	CAA-C2A-C3A	-2.11	107.30	113.00
27	5	1620	LUT	C7-C8-C9	-2.11	123.11	126.23
28	2	1622	XAT	C24-C23-C22	-2.11	106.84	110.79
31	b	620	BCR	C21-C20-C19	-2.11	117.09	123.20
26	5	610	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
27	3	1621	LUT	C3-C4-C5	-2.11	106.92	112.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	511	CLA	C2A-C1A-CHA	2.11	127.53	123.87
27	3	1620	LUT	C8-C9-C10	-2.11	115.69	119.01
25	G	609	CHL	C4C-CHD-C1D	2.11	123.61	116.07
27	1	1620	LUT	C7-C8-C9	-2.11	123.11	126.23
25	6	605	CHL	O2D-CGD-O1D	-2.11	119.74	123.85
28	g	1622	XAT	C26-C27-C28	-2.11	121.53	125.99
27	7	1621	LUT	C3-C4-C5	-2.11	106.93	112.18
25	6	605	CHL	C4C-CHD-C1D	2.11	123.61	116.07
25	g	609	CHL	O2A-CGA-CBA	2.11	118.27	111.83
26	c	502	CLA	CAA-C2A-C3A	-2.11	107.30	113.00
26	N	604	CLA	C4B-C3B-C2B	-2.11	104.68	107.30
25	7	608	CHL	CAC-C3C-C4C	2.11	129.45	124.03
25	r	608	CHL	CAA-C2A-C3A	-2.11	107.30	113.00
31	b	619	BCR	C37-C22-C23	2.11	121.31	118.09
25	g	606	CHL	CED-O2D-CGD	2.11	120.70	115.92
26	c	508	CLA	CHC-C1C-NC	2.11	127.48	124.31
25	3	608	CHL	CAC-C3C-C4C	2.11	129.45	124.03
26	c	506	CLA	C2A-C1A-CHA	2.11	127.52	123.87
28	n	1622	XAT	C28-C29-C30	2.11	122.32	119.01
26	g	610	CLA	CAA-C2A-C1A	2.11	118.88	111.97
27	5	1621	LUT	C27-C28-C29	-2.11	121.79	126.32
25	2	605	CHL	C4C-CHD-C1D	2.11	123.60	116.07
28	G	1622	XAT	C26-C27-C28	-2.11	121.54	125.99
27	5	1621	LUT	C31-C30-C29	-2.11	124.33	127.28
35	a	409	PHO	C4B-NB-C1B	2.11	111.89	108.82
25	1	605	CHL	O2A-CGA-CBA	2.11	120.65	114.00
26	s	609	CLA	O2D-CGD-O1D	-2.11	119.75	123.85
26	5	604	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
25	2	601	CHL	CED-O2D-CGD	2.10	120.69	115.92
31	B	619	BCR	C37-C22-C23	2.10	121.30	118.09
31	C	516	BCR	C35-C13-C12	2.10	121.30	118.09
39	b	626	DGD	C1E-O6E-C5E	2.10	117.83	113.72
26	d	402	CLA	O2D-CGD-CBD	2.10	114.91	111.23
25	s	601	CHL	CED-O2D-CGD	2.10	120.69	115.92
26	N	604	CLA	CHB-C4A-NA	2.10	127.43	124.40
26	c	508	CLA	CGD-CBD-CAD	2.10	117.65	110.85
25	S	607	CHL	CMB-C2B-C3B	2.10	128.88	124.68
25	s	607	CHL	CMB-C2B-C3B	2.10	128.88	124.68
28	N	1622	XAT	O24-C25-C26	-2.10	57.26	58.93
26	N	604	CLA	O2D-CGD-CBD	2.10	114.90	111.23
29	Y	1623	NEX	C4-C3-C2	-2.10	106.86	110.79
30	3	2630	LHG	C18-C17-C16	-2.10	103.75	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	2630	LHG	C18-C17-C16	-2.10	103.75	114.37
37	Z	101	LMG	C38-C37-C36	-2.10	103.75	114.37
25	N	605	CHL	CMB-C2B-C3B	2.10	128.88	124.68
27	8	620	LUT	C40-C33-C32	2.10	121.30	118.09
30	L	101	LHG	O8-C23-C24	2.10	118.24	111.83
26	b	607	CLA	CMB-C2B-C3B	2.10	131.49	126.55
39	C	519	DGD	C7B-C6B-C5B	-2.10	103.75	114.37
26	b	617	CLA	C3A-C2A-C1A	2.10	104.48	101.34
26	b	616	CLA	C2A-C1A-CHA	2.10	127.51	123.87
26	b	611	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
26	C	502	CLA	CMC-C2C-C3C	2.10	131.82	126.15
26	G	614	CLA	CMB-C2B-C3B	2.10	131.49	126.55
27	1	1620	LUT	C8-C9-C10	-2.10	115.71	119.01
26	b	611	CLA	C2A-C1A-CHA	2.10	127.51	123.87
25	G	605	CHL	CAC-C3C-C4C	2.10	129.42	124.03
26	7	603	CLA	CHC-C4B-NB	2.10	127.19	124.05
25	3	601	CHL	O2D-CGD-O1D	-2.10	119.77	123.85
25	8	608	CHL	O1D-CGD-CBD	-2.10	121.54	124.72
25	S	606	CHL	O2A-CGA-CBA	2.10	120.62	114.00
35	a	408	PHO	CMC-C2C-C1C	-2.10	120.96	124.73
25	s	606	CHL	O2A-CGA-CBA	2.10	120.62	114.00
29	1	1623	NEX	O24-C25-C26	-2.10	57.27	58.93
29	5	1623	NEX	O24-C25-C26	-2.10	57.27	58.93
26	A	406	CLA	C3C-C4C-NC	-2.10	107.75	110.43
39	c	519	DGD	C7B-C6B-C5B	-2.10	103.77	114.37
25	7	601	CHL	O2D-CGD-O1D	-2.10	119.77	123.85
26	6	602	CLA	CHB-C4A-NA	2.10	127.42	124.40
37	z	101	LMG	C38-C37-C36	-2.10	103.78	114.37
26	r	603	CLA	C1D-ND-C4D	2.10	107.78	106.31
26	r	609	CLA	C1D-ND-C4D	-2.10	104.84	106.31
28	n	1622	XAT	O24-C25-C26	-2.09	57.27	58.93
26	G	610	CLA	CAA-C2A-C1A	2.09	118.84	111.97
29	N	1623	NEX	O24-C25-C26	-2.09	57.27	58.93
25	N	606	CHL	C4C-CHD-C1D	2.09	123.56	116.07
25	g	609	CHL	C4C-CHD-C1D	2.09	123.56	116.07
25	Y	609	CHL	C6-C5-C3	-2.09	108.37	113.47
26	7	602	CLA	C1-C2-C3	-2.09	122.77	126.20
27	1	1621	LUT	C31-C30-C29	-2.09	124.34	127.28
26	N	614	CLA	C3B-C4B-NB	-2.09	108.66	110.53
25	G	606	CHL	CED-O2D-CGD	2.09	120.66	115.92
27	5	1620	LUT	C11-C10-C9	-2.09	124.34	127.28
26	b	613	CLA	C2A-C3A-C4A	2.09	105.25	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	B	622	LMG	O3-C3-C2	-2.09	105.44	110.38
25	g	605	CHL	CAC-C3C-C4C	2.09	129.41	124.03
30	Y	2630	LHG	C18-C17-C16	-2.09	103.80	114.37
25	y	609	CHL	CAA-C2A-C3A	-2.09	107.35	113.00
26	3	602	CLA	CMB-C2B-C3B	2.09	131.47	126.55
26	3	604	CLA	CMB-C2B-C3B	2.09	131.47	126.55
26	B	607	CLA	CMB-C2B-C3B	2.09	131.47	126.55
25	7	607	CHL	CMB-C2B-C3B	2.09	128.86	124.68
25	n	605	CHL	CMB-C2B-C3B	2.09	128.86	124.68
26	B	609	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
26	7	602	CLA	CMB-C2B-C3B	2.09	131.47	126.55
25	5	605	CHL	O2A-CGA-CBA	2.09	120.60	114.00
26	3	612	CLA	CMD-C2D-C3D	2.09	132.48	127.69
30	y	2630	LHG	C18-C17-C16	-2.09	103.81	114.37
27	6	1621	LUT	C28-C29-C30	-2.09	115.72	119.01
26	B	617	CLA	C3A-C2A-C1A	2.09	104.47	101.34
26	6	610	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
25	n	607	CHL	O2D-CGD-O1D	-2.09	119.78	123.85
26	8	612	CLA	CHA-C1A-NA	-2.09	121.66	126.39
26	7	604	CLA	C3B-C4B-NB	-2.09	108.67	110.53
25	S	601	CHL	CED-O2D-CGD	2.09	120.65	115.92
26	R	601	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
39	B	626	DGD	C1E-O6E-C5E	2.09	117.80	113.72
26	N	612	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
26	n	612	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
25	6	609	CHL	CAA-C2A-C3A	-2.09	107.36	113.00
26	r	603	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
27	s	1620	LUT	C40-C33-C32	2.09	121.28	118.09
25	n	608	CHL	C11-C12-C13	-2.09	109.03	115.97
26	n	604	CLA	C4B-C3B-C2B	-2.09	104.71	107.30
26	c	511	CLA	C2A-C1A-CHA	2.09	127.49	123.87
26	g	604	CLA	CHB-C4A-NA	2.09	127.41	124.40
26	3	604	CLA	C3B-C4B-NB	-2.09	108.67	110.53
26	R	603	CLA	C1D-ND-C4D	2.09	107.78	106.31
31	C	514	BCR	C36-C18-C19	2.08	121.27	118.09
26	Y	613	CLA	CMB-C2B-C3B	2.08	131.45	126.55
26	y	613	CLA	CMB-C2B-C3B	2.08	131.45	126.55
25	n	606	CHL	C4C-CHD-C1D	2.08	123.53	116.07
25	3	608	CHL	CMA-C3A-C4A	-2.08	110.12	114.61
25	7	608	CHL	CMA-C3A-C4A	-2.08	110.12	114.61
37	B	2633	LMG	C42-C41-C40	-2.08	103.84	114.37
37	a	413	LMG	O7-C10-O9	-2.08	118.84	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	S	1620	LUT	C39-C29-C28	2.08	121.27	118.09
37	A	413	LMG	O7-C10-O9	-2.08	118.84	123.70
26	n	604	CLA	CHB-C4A-NA	2.08	127.40	124.40
29	y	1623	NEX	C4-C3-C2	-2.08	106.90	110.79
25	y	609	CHL	C6-C5-C3	-2.08	108.40	113.47
25	2	607	CHL	C4-C3-C5	2.08	118.84	115.23
25	Y	609	CHL	CAA-C2A-C3A	-2.08	107.38	113.00
27	y	1620	LUT	C19-C9-C8	2.08	121.27	118.09
25	3	607	CHL	CMB-C2B-C3B	2.08	128.84	124.68
25	G	609	CHL	CAC-C3C-C4C	2.08	129.38	124.03
26	8	612	CLA	O2A-CGA-O1A	-2.08	117.98	123.33
39	C	518	DGD	C5B-C4B-C3B	-2.08	103.86	114.37
26	r	612	CLA	CHB-C1B-NB	2.08	127.17	124.05
26	4	612	CLA	CHA-C1A-NA	-2.08	121.68	126.39
25	g	609	CHL	CAC-C3C-C4C	2.08	129.37	124.03
26	R	603	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
35	A	409	PHO	C4B-NB-C1B	2.08	111.85	108.82
25	6	607	CHL	C4-C3-C5	2.08	118.84	115.23
26	8	610	CLA	CHB-C1B-NB	2.08	127.17	124.05
29	r	623	NEX	C40-C33-C32	2.08	121.26	118.09
28	5	1622	XAT	O24-C25-C26	-2.08	57.28	58.93
26	Y	614	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
25	1	601	CHL	OMC-CMC-C2C	-2.08	121.51	125.12
26	B	611	CLA	C2A-C1A-CHA	2.08	127.47	123.87
31	b	619	BCR	C34-C9-C8	2.08	121.26	118.09
30	D	408	LHG	C27-C26-C25	-2.08	103.87	114.37
25	3	601	CHL	CAC-C3C-C4C	2.08	129.37	124.03
27	S	1621	LUT	C38-C25-C24	-2.08	118.45	123.36
26	n	604	CLA	O2D-CGD-CBD	2.08	114.86	111.23
25	2	609	CHL	CAA-C2A-C3A	-2.08	107.39	113.00
26	n	612	CLA	CMB-C2B-C3B	2.08	131.43	126.55
28	G	1622	XAT	O24-C25-C26	-2.08	57.28	58.93
39	c	518	DGD	C5B-C4B-C3B	-2.08	103.88	114.37
37	b	2633	LMG	C3-C4-C5	-2.08	106.47	110.23
25	N	608	CHL	C11-C12-C13	-2.08	109.07	115.97
37	b	622	LMG	O3-C3-C2	-2.08	105.48	110.38
26	D	402	CLA	O2D-CGD-CBD	2.08	114.86	111.23
26	N	613	CLA	CMB-C2B-C3B	2.08	131.43	126.55
27	s	1620	LUT	C39-C29-C28	2.08	121.26	118.09
26	r	601	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
28	g	1622	XAT	C7-C8-C9	-2.07	122.31	125.53
28	3	1622	XAT	C38-C25-C24	2.07	116.57	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	2633	LMG	C42-C41-C40	-2.07	103.88	114.37
29	S	1623	NEX	C30-C31-C32	-2.07	117.19	123.20
25	5	601	CHL	OMC-CMC-C2C	-2.07	121.52	125.12
26	b	609	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
26	y	614	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
37	B	2633	LMG	C3-C4-C5	-2.07	106.47	110.23
28	G	1622	XAT	C7-C8-C9	-2.07	122.31	125.53
31	C	514	BCR	C37-C22-C23	2.07	121.25	118.09
31	c	514	BCR	C37-C22-C23	2.07	121.25	118.09
26	3	602	CLA	C3B-C4B-NB	-2.07	108.68	110.53
25	2	607	CHL	OMC-CMC-C2C	-2.07	121.52	125.12
25	G	608	CHL	CAC-C3C-C4C	2.07	129.36	124.03
30	d	408	LHG	C27-C26-C25	-2.07	103.89	114.37
27	2	1621	LUT	C28-C29-C30	-2.07	115.75	119.01
25	6	606	CHL	CMA-C3A-C4A	-2.07	110.15	114.61
28	7	1622	XAT	O24-C25-C26	-2.07	57.29	58.93
29	s	1623	NEX	C30-C31-C32	-2.07	117.20	123.20
31	B	618	BCR	C16-C15-C14	-2.07	119.28	123.52
26	1	604	CLA	C1-C2-C3	-2.07	123.41	126.76
25	7	601	CHL	CAC-C3C-C4C	2.07	129.35	124.03
26	2	602	CLA	CHB-C4A-NA	2.07	127.39	124.40
31	C	514	BCR	C7-C8-C9	-2.07	123.17	126.23
27	4	620	LUT	C40-C33-C32	2.07	121.25	118.09
26	B	613	CLA	C2A-C3A-C4A	2.07	105.21	101.87
37	a	415	LMG	O2-C2-C1	-2.07	105.14	110.08
26	N	603	CLA	C1D-ND-C4D	2.07	107.76	106.31
25	8	607	CHL	CAC-C3C-C4C	2.07	129.35	124.03
31	c	514	BCR	C36-C18-C19	2.07	121.25	118.09
26	c	509	CLA	C2A-C3A-C4A	2.07	105.21	101.87
31	B	620	BCR	C15-C16-C17	-2.07	119.29	123.52
26	7	602	CLA	C3B-C4B-NB	-2.07	108.69	110.53
26	n	603	CLA	C1D-ND-C4D	2.07	107.76	106.31
25	3	601	CHL	CGD-CBD-CAD	-2.07	104.16	110.85
25	7	601	CHL	CGD-CBD-CAD	-2.07	104.16	110.85
26	b	605	CLA	CHA-C1A-NA	-2.07	121.71	126.39
30	C	523	LHG	C18-C17-C16	-2.07	103.93	114.37
30	c	523	LHG	C18-C17-C16	-2.07	103.93	114.37
26	B	611	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
26	6	604	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
26	5	604	CLA	C1-C2-C3	-2.07	123.42	126.76
27	S	1620	LUT	C40-C33-C32	2.06	121.24	118.09
26	N	612	CLA	CMB-C2B-C3B	2.06	131.41	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	2	610	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
31	b	618	BCR	C16-C15-C14	-2.06	119.30	123.52
31	c	514	BCR	C7-C8-C9	-2.06	123.18	126.23
25	4	607	CHL	CAC-C3C-C4C	2.06	129.34	124.03
26	s	612	CLA	C3B-C4B-NB	-2.06	108.69	110.53
26	4	612	CLA	O2A-CGA-O1A	-2.06	118.03	123.33
26	n	613	CLA	CMB-C2B-C3B	2.06	131.40	126.55
31	C	516	BCR	C33-C5-C4	2.06	117.99	113.60
26	3	603	CLA	CHC-C4B-NB	2.06	127.14	124.05
26	B	605	CLA	CHA-C1A-NA	-2.06	121.72	126.39
27	N	1621	LUT	C28-C29-C30	-2.06	115.77	119.01
27	n	1621	LUT	C28-C29-C30	-2.06	115.77	119.01
25	2	607	CHL	O2D-CGD-O1D	-2.06	119.83	123.85
27	1	1620	LUT	C11-C10-C9	-2.06	124.39	127.28
27	Y	1620	LUT	C19-C9-C8	2.06	121.24	118.09
37	A	415	LMG	O2-C2-C1	-2.06	105.16	110.08
25	2	606	CHL	CMA-C3A-C4A	-2.06	110.17	114.61
26	B	604	CLA	CHC-C4B-NB	2.06	127.14	124.05
31	B	620	BCR	C3-C4-C5	-2.06	110.38	114.06
28	Y	1622	XAT	O24-C25-C26	-2.06	57.30	58.93
26	c	507	CLA	CMB-C2B-C3B	2.06	131.39	126.55
28	1	1622	XAT	O24-C25-C26	-2.06	57.30	58.93
26	c	507	CLA	CHA-C1A-NA	-2.06	121.73	126.39
25	g	608	CHL	CAC-C3C-C4C	2.06	129.32	124.03
31	b	620	BCR	C15-C16-C17	-2.06	119.31	123.52
28	Y	1622	XAT	C30-C31-C32	-2.06	117.23	123.20
26	B	616	CLA	C3A-C2A-C1A	2.06	104.42	101.34
26	b	616	CLA	C3A-C2A-C1A	2.06	104.42	101.34
26	R	616	CLA	C3B-C4B-NB	-2.06	108.69	110.53
26	R	611	CLA	CAC-C3C-C4C	2.06	127.47	124.79
27	6	1621	LUT	C38-C25-C24	-2.06	118.49	123.36
28	y	1622	XAT	O24-C25-C26	-2.06	57.30	58.93
27	s	1621	LUT	C38-C25-C24	-2.06	118.49	123.36
29	R	623	NEX	C40-C33-C32	2.06	121.23	118.09
26	y	603	CLA	CHD-C1D-ND	-2.06	121.91	124.80
25	N	607	CHL	O2D-CGD-O1D	-2.06	119.85	123.85
25	S	608	CHL	CMD-C2D-C3D	-2.06	120.58	124.68
31	b	620	BCR	C3-C4-C5	-2.06	110.39	114.06
26	C	506	CLA	CMC-C2C-C1C	-2.06	121.82	125.03
26	y	610	CLA	O2D-CGD-O1D	-2.05	119.85	123.85
28	y	1622	XAT	C30-C31-C32	-2.05	117.25	123.20
26	C	509	CLA	C2A-C3A-C4A	2.05	105.19	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	F	101	HEM	CAC-C3C-C4C	-2.05	119.92	124.82
26	B	612	CLA	CHC-C1C-NC	2.05	127.40	124.31
26	b	612	CLA	CHC-C1C-NC	2.05	127.40	124.31
26	c	506	CLA	CMC-C2C-C1C	-2.05	121.83	125.03
31	c	516	BCR	C33-C5-C4	2.05	117.97	113.60
25	R	614	CHL	CAC-C3C-C4C	2.05	129.31	124.03
27	3	1621	LUT	C8-C7-C6	-2.05	121.52	127.00
30	L	101	LHG	C27-C26-C25	-2.05	103.99	114.37
30	l	101	LHG	C27-C26-C25	-2.05	103.99	114.37
29	Y	1623	NEX	C28-C29-C30	2.05	122.24	119.01
25	g	607	CHL	C4C-CHD-C1D	2.05	123.41	116.07
25	R	608	CHL	O2D-CGD-O1D	-2.05	119.85	123.85
26	4	610	CLA	CHB-C1B-NB	2.05	127.13	124.05
26	B	611	CLA	CHB-C1B-NB	2.05	127.13	124.05
41	f	101	HEM	CAC-C3C-C4C	-2.05	119.92	124.82
26	C	507	CLA	CMB-C2B-C3B	2.05	131.37	126.55
27	2	1621	LUT	C38-C25-C24	-2.05	118.51	123.36
31	A	411	BCR	C15-C16-C17	-2.05	119.32	123.52
39	b	626	DGD	O6E-C1E-O5D	-2.05	105.20	110.04
25	6	607	CHL	OMC-CMC-C2C	-2.05	121.56	125.12
26	2	612	CLA	CHB-C1B-NB	2.05	127.12	124.05
25	r	614	CHL	CAC-C3C-C4C	2.05	129.30	124.03
25	R	608	CHL	CMD-C2D-C3D	-2.05	120.59	124.68
26	b	611	CLA	CHB-C1B-NB	2.05	127.12	124.05
25	n	606	CHL	CAC-C3C-C4C	2.05	129.30	124.03
39	B	626	DGD	O6E-C1E-O5D	-2.05	105.20	110.04
26	1	602	CLA	CHA-C1A-NA	-2.05	121.75	126.39
26	N	604	CLA	C1-C2-C3	-2.05	123.45	126.76
26	3	602	CLA	CHB-C1B-NB	2.05	127.12	124.05
26	4	604	CLA	C3B-C4B-NB	-2.05	108.70	110.53
27	7	1621	LUT	C8-C7-C6	-2.05	121.53	127.00
28	6	1622	XAT	O24-C25-C26	-2.05	57.31	58.93
26	y	612	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
26	r	611	CLA	CHA-C1A-NA	-2.05	121.76	126.39
28	4	622	XAT	C15-C35-C34	-2.05	119.33	123.52
26	C	507	CLA	CHA-C1A-NA	-2.05	121.76	126.39
26	R	611	CLA	CHA-C1A-NA	-2.05	121.76	126.39
26	R	612	CLA	CHB-C1B-NB	2.05	127.12	124.05
39	B	626	DGD	O6E-C5E-C6E	-2.05	101.37	106.44
26	G	603	CLA	CHB-C1B-C2B	-2.05	121.49	127.43
30	B	2630	LHG	C27-C26-C25	-2.04	104.03	114.37
25	s	608	CHL	CMD-C2D-C3D	-2.04	120.60	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	608	CHL	CAC-C3C-C4C	2.04	129.29	124.03
29	y	1623	NEX	C28-C29-C30	2.04	122.22	119.01
31	a	411	BCR	C15-C16-C17	-2.04	119.34	123.52
25	6	607	CHL	O2D-CGD-O1D	-2.04	119.87	123.85
26	2	604	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
26	c	503	CLA	O1D-CGD-CBD	2.04	128.55	124.52
29	S	1623	NEX	C39-C29-C30	-2.04	119.50	122.82
25	4	606	CHL	O2A-CGA-CBA	2.04	120.46	114.00
25	r	608	CHL	CMD-C2D-C3D	-2.04	120.60	124.68
28	N	1622	XAT	C26-C27-C28	-2.04	121.67	125.99
25	G	607	CHL	O2D-CGD-O1D	-2.04	119.87	123.85
28	7	1622	XAT	C38-C25-C24	2.04	116.54	114.24
26	G	610	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
26	S	611	CLA	CHC-C4B-NB	2.04	127.11	124.05
26	r	610	CLA	CHB-C1B-C2B	-2.04	121.50	127.43
36	A	418	SQD	O49-C7-C8	-2.04	115.79	123.78
26	5	602	CLA	C1-C2-C3	-2.04	122.85	126.20
26	b	604	CLA	CHC-C4B-NB	2.04	127.11	124.05
26	A	405	CLA	C11-C10-C8	-2.04	109.18	115.97
25	g	607	CHL	O2D-CGD-O1D	-2.04	119.87	123.85
26	S	612	CLA	C3B-C4B-NB	-2.04	108.71	110.53
25	G	607	CHL	C4C-CHD-C1D	2.04	123.37	116.07
36	a	418	SQD	O49-C7-C8	-2.04	115.80	123.78
36	b	621	SQD	O48-C23-O10	-2.04	118.52	123.63
25	n	607	CHL	C11-C10-C8	-2.04	109.18	115.97
30	b	2630	LHG	C27-C26-C25	-2.04	104.05	114.37
30	L	101	LHG	C18-C17-C16	-2.04	104.05	114.37
28	g	1622	XAT	O24-C25-C26	-2.04	57.31	58.93
26	Y	603	CLA	CHD-C1D-ND	-2.04	121.93	124.80
26	s	604	CLA	CAA-CBA-CGA	2.04	119.00	113.21
27	Y	1620	LUT	C21-C26-C27	-2.04	110.48	112.83
26	S	603	CLA	O1D-CGD-CBD	2.04	128.54	124.52
25	3	605	CHL	O2A-CGA-CBA	2.04	120.44	114.00
29	s	1623	NEX	C39-C29-C30	-2.04	119.51	122.82
28	4	622	XAT	O4-C5-C6	-2.04	57.31	58.93
25	g	606	CHL	O1D-CGD-CBD	-2.04	121.63	124.72
26	C	506	CLA	CMC-C2C-C3C	2.04	131.66	126.15
28	8	622	XAT	C15-C35-C34	-2.04	119.35	123.52
26	A	410	CLA	CMB-C2B-C3B	2.04	131.34	126.55
36	B	621	SQD	O48-C23-O10	-2.04	118.53	123.63
26	B	611	CLA	C1-C2-C3	-2.04	122.86	126.20
30	C	523	LHG	C11-C10-C9	-2.04	104.07	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	s	601	CHL	C4C-CHD-C1D	2.04	123.36	116.07
30	l	101	LHG	C18-C17-C16	-2.04	104.07	114.37
26	6	612	CLA	CHB-C1B-NB	2.04	127.10	124.05
25	1	605	CHL	C4C-CHD-C1D	2.04	123.35	116.07
26	g	603	CLA	CHB-C1B-C2B	-2.04	121.52	127.43
25	S	601	CHL	C4C-CHD-C1D	2.04	123.35	116.07
26	S	604	CLA	CAA-CBA-CGA	2.04	118.99	113.21
25	G	607	CHL	O2A-CGA-O1A	-2.04	118.54	123.63
26	3	612	CLA	CMD-C2D-C1D	-2.04	121.14	124.73
26	7	612	CLA	CMD-C2D-C1D	-2.04	121.14	124.73
26	a	405	CLA	C11-C10-C8	-2.03	109.20	115.97
25	r	608	CHL	O2D-CGD-O1D	-2.03	119.89	123.85
26	B	608	CLA	CHC-C1C-C2C	-2.03	121.17	126.95
30	b	2631	LHG	C29-C28-C27	-2.03	104.09	114.37
30	c	523	LHG	C11-C10-C9	-2.03	104.09	114.37
39	b	626	DGD	O6E-C5E-C6E	-2.03	101.40	106.44
25	7	605	CHL	O2A-CGA-CBA	2.03	120.42	114.00
26	s	611	CLA	CHC-C4B-NB	2.03	127.10	124.05
26	a	410	CLA	CMB-C2B-C3B	2.03	131.33	126.55
29	5	1623	NEX	C35-C15-C14	-2.03	119.36	123.52
26	7	602	CLA	CHB-C1B-NB	2.03	127.10	124.05
25	R	607	CHL	CMA-C3A-C4A	-2.03	110.23	114.61
25	N	606	CHL	CAC-C3C-C4C	2.03	129.25	124.03
28	n	1622	XAT	C26-C27-C28	-2.03	121.70	125.99
29	2	1623	NEX	O24-C25-C26	-2.03	57.32	58.93
29	6	1623	NEX	O24-C25-C26	-2.03	57.32	58.93
25	r	606	CHL	C6-C7-C8	-2.03	109.21	115.97
38	d	405	PL9	C12-C13-C14	-2.03	122.97	127.62
25	5	605	CHL	CAC-C3C-C4C	2.03	129.25	124.03
26	b	607	CLA	CHB-C1B-C2B	-2.03	121.53	127.43
26	n	604	CLA	C1-C2-C3	-2.03	123.48	126.76
30	3	2630	LHG	C27-C26-C25	-2.03	104.10	114.37
26	b	608	CLA	CHC-C1C-C2C	-2.03	121.18	126.95
25	R	606	CHL	C6-C7-C8	-2.03	109.22	115.97
30	B	2631	LHG	C29-C28-C27	-2.03	104.10	114.37
26	B	617	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
25	6	607	CHL	C4C-CHD-C1D	2.03	123.33	116.07
27	s	1620	LUT	C27-C28-C29	-2.03	121.96	126.32
26	s	603	CLA	O1D-CGD-CBD	2.03	128.52	124.52
26	R	610	CLA	CHB-C1B-C2B	-2.03	121.53	127.43
27	7	1621	LUT	C1-C2-C3	2.03	118.05	113.59
26	Y	612	CLA	O2A-CGA-O1A	-2.03	118.55	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	8	622	XAT	O4-C5-C6	-2.03	57.32	58.93
28	N	1622	XAT	C39-C29-C30	-2.03	119.53	122.82
25	g	607	CHL	O2A-CGA-O1A	-2.03	118.55	123.63
25	8	606	CHL	O2A-CGA-CBA	2.03	120.41	114.00
26	b	617	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
26	Y	610	CLA	O2D-CGD-O1D	-2.03	119.90	123.85
26	c	502	CLA	CBC-CAC-C3C	-2.03	106.92	112.42
25	N	607	CHL	C11-C10-C8	-2.03	109.22	115.97
25	r	606	CHL	C4-C3-C5	2.03	118.75	115.23
31	B	620	BCR	C10-C11-C12	-2.03	117.33	123.20
25	y	608	CHL	CAC-C3C-C4C	2.03	129.24	124.03
26	C	506	CLA	CHA-C1A-NA	-2.03	121.80	126.39
26	g	610	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
26	1	602	CLA	CHB-C4A-NA	2.03	127.33	124.40
26	Y	604	CLA	C3B-C4B-NB	-2.03	108.72	110.53
25	1	608	CHL	O1D-CGD-CBD	-2.03	121.65	124.72
25	6	609	CHL	OMC-CMC-C2C	-2.03	121.60	125.12
25	1	606	CHL	C4C-CHD-C1D	2.03	123.31	116.07
30	7	2630	LHG	C27-C26-C25	-2.03	104.13	114.37
26	1	612	CLA	CHC-C4B-NB	2.03	127.09	124.05
38	D	405	PL9	O1-C4-C3	-2.02	118.60	120.73
38	d	405	PL9	O1-C4-C3	-2.02	118.60	120.73
26	r	611	CLA	CAC-C3C-C4C	2.02	127.42	124.79
26	c	506	CLA	CMC-C2C-C3C	2.02	131.62	126.15
26	b	611	CLA	C1-C2-C3	-2.02	122.88	126.20
26	c	510	CLA	C11-C10-C8	-2.02	109.24	115.97
39	C	520	DGD	C3D-C4D-C5D	-2.02	106.56	110.23
39	c	520	DGD	C3D-C4D-C5D	-2.02	106.56	110.23
25	4	608	CHL	OBD-CAD-C3D	-2.02	124.73	127.89
26	5	602	CLA	CHA-C1A-NA	-2.02	121.81	126.39
26	4	611	CLA	O2A-CGA-O1A	-2.02	118.13	123.33
26	8	603	CLA	C2A-C1A-CHA	2.02	127.38	123.87
39	C	519	DGD	C3D-C4D-C5D	-2.02	106.56	110.23
26	S	609	CLA	CHB-C4A-NA	2.02	127.32	124.40
25	2	608	CHL	O2A-CGA-CBA	2.02	120.39	114.00
31	c	514	BCR	C8-C7-C6	-2.02	121.59	127.00
25	g	608	CHL	C4C-CHD-C1D	2.02	123.31	116.07
31	b	620	BCR	C10-C11-C12	-2.02	117.34	123.20
25	1	605	CHL	CAC-C3C-C4C	2.02	129.23	124.03
28	2	1622	XAT	O24-C25-C26	-2.02	57.33	58.93
36	b	623	SQD	O8-S-C6	2.02	109.88	105.97
38	D	405	PL9	C12-C13-C14	-2.02	123.00	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	605	CHL	C4C-CHD-C1D	2.02	123.30	116.07
25	2	609	CHL	OMC-CMC-C2C	-2.02	121.61	125.12
25	r	607	CHL	CMA-C3A-C4A	-2.02	110.25	114.61
26	B	607	CLA	CHB-C1B-C2B	-2.02	121.56	127.43
26	C	506	CLA	CHB-C4A-NA	2.02	127.32	124.40
25	1	607	CHL	C4C-CHD-C1D	2.02	123.30	116.07
29	R	623	NEX	C24-C23-C22	-2.02	107.01	110.79
26	8	604	CLA	C3B-C4B-NB	-2.02	108.73	110.53
25	r	614	CHL	CMD-C2D-C3D	-2.02	120.64	124.68
25	2	607	CHL	C4C-CHD-C1D	2.02	123.30	116.07
29	r	623	NEX	C24-C23-C22	-2.02	107.01	110.79
39	c	519	DGD	C3D-C4D-C5D	-2.02	106.57	110.23
25	R	614	CHL	CMD-C2D-C3D	-2.02	120.65	124.68
25	5	608	CHL	CMB-C2B-C3B	2.02	128.72	124.68
31	A	411	BCR	C36-C18-C19	2.02	121.17	118.09
25	4	607	CHL	C4C-CHD-C1D	2.02	123.29	116.07
25	G	608	CHL	C4C-CHD-C1D	2.02	123.29	116.07
29	1	1623	NEX	C35-C15-C14	-2.02	119.39	123.52
26	r	616	CLA	C3B-C4B-NB	-2.02	108.73	110.53
25	r	607	CHL	C1-C2-C3	-2.02	122.89	126.20
26	C	510	CLA	C11-C10-C8	-2.02	109.26	115.97
31	C	514	BCR	C8-C7-C6	-2.02	121.61	127.00
26	5	602	CLA	CHB-C4A-NA	2.02	127.31	124.40
26	A	406	CLA	CMC-C2C-C3C	2.02	131.60	126.15
25	5	606	CHL	C4C-CHD-C1D	2.02	123.29	116.07
26	C	503	CLA	O1D-CGD-CBD	2.02	128.50	124.52
25	R	606	CHL	C4-C3-C5	2.02	118.73	115.23
26	y	603	CLA	CHA-C1A-NA	-2.02	121.83	126.39
37	B	2633	LMG	C24-C23-C22	-2.02	104.18	114.37
25	g	601	CHL	O1D-CGD-CBD	-2.02	121.67	124.72
25	6	608	CHL	O2A-CGA-CBA	2.02	120.37	114.00
26	n	604	CLA	C3B-C2B-C1B	2.02	109.55	107.17
27	y	1620	LUT	C21-C26-C27	-2.02	110.51	112.83
28	n	1622	XAT	C39-C29-C30	-2.02	119.55	122.82
25	5	607	CHL	C4C-CHD-C1D	2.02	123.28	116.07
26	B	605	CLA	C3D-C2D-C1D	2.02	108.58	105.83
26	b	605	CLA	C3D-C2D-C1D	2.02	108.58	105.83
25	3	609	CHL	C4C-CHD-C1D	2.02	123.28	116.07
26	3	611	CLA	CAA-C2A-C1A	2.01	118.58	111.97
26	7	611	CLA	CAA-C2A-C1A	2.01	118.58	111.97
30	C	522	LHG	C5-O7-C7	-2.01	112.98	117.80
26	4	603	CLA	C2A-C1A-CHA	2.01	127.36	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	y	610	CLA	CMB-C2B-C3B	2.01	131.28	126.55
26	s	609	CLA	CHB-C4A-NA	2.01	127.30	124.40
26	c	506	CLA	CHA-C1A-NA	-2.01	121.83	126.39
31	a	411	BCR	C36-C18-C19	2.01	121.16	118.09
27	3	1621	LUT	C1-C2-C3	2.01	118.01	113.59
26	s	604	CLA	C1-C2-C3	-2.01	123.51	126.76
26	a	406	CLA	CMC-C2C-C3C	2.01	131.59	126.15
26	4	612	CLA	C2A-C1A-CHA	2.01	127.36	123.87
28	N	1622	XAT	O4-C5-C6	-2.01	57.34	58.93
25	7	605	CHL	CAC-C3C-C4C	2.01	129.20	124.03
25	1	608	CHL	CMB-C2B-C3B	2.01	128.70	124.68
26	1	602	CLA	C1-C2-C3	-2.01	122.90	126.20
25	3	601	CHL	O2A-CGA-O1A	-2.01	118.60	123.63
37	b	2633	LMG	C24-C23-C22	-2.01	104.21	114.37
37	z	101	LMG	O8-C28-C29	2.01	117.96	111.83
25	8	607	CHL	C4C-CHD-C1D	2.01	123.26	116.07
26	S	612	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
25	7	609	CHL	C4C-CHD-C1D	2.01	123.26	116.07
38	d	405	PL9	O2-C1-C6	2.01	123.68	120.48
29	1	1623	NEX	C31-C32-C33	-2.01	120.86	126.36
25	G	605	CHL	OBD-CAD-C3D	-2.01	124.76	127.89
26	5	612	CLA	CHC-C4B-NB	2.01	127.06	124.05
27	S	1620	LUT	C27-C28-C29	-2.01	122.00	126.32
25	G	606	CHL	O1D-CGD-CBD	-2.01	121.68	124.72
26	C	502	CLA	CBC-CAC-C3C	-2.01	106.98	112.42
31	B	620	BCR	C35-C13-C12	2.01	121.15	118.09
26	b	604	CLA	C4-C3-C5	2.01	118.71	115.23
39	H	102	DGD	CBB-CAB-C9B	-2.01	104.23	114.37
25	2	605	CHL	O2A-CGA-CBA	2.01	120.34	114.00
25	8	608	CHL	OBD-CAD-C3D	-2.01	124.76	127.89
26	D	403	CLA	C3B-C4B-NB	-2.01	108.74	110.53
26	A	407	CLA	CMB-C2B-C1B	-2.01	122.37	125.42
26	Y	603	CLA	CHA-C1A-NA	-2.00	121.85	126.39
26	B	604	CLA	C4-C3-C5	2.00	118.71	115.23
31	b	618	BCR	C29-C28-C27	-2.00	106.87	111.28
26	8	611	CLA	O2A-CGA-O1A	-2.00	118.18	123.33
25	N	608	CHL	C4C-CHD-C1D	2.00	123.24	116.07
25	6	605	CHL	O2A-CGA-CBA	2.00	120.33	114.00
25	4	607	CHL	O2A-CGA-CBA	2.00	120.33	114.00
31	C	517	BCR	C38-C26-C25	-2.00	122.30	124.48
26	3	611	CLA	CHC-C1C-C2C	-2.00	121.25	126.95
26	Y	604	CLA	CHC-C4B-NB	2.00	127.05	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	6	1623	NEX	C30-C31-C32	-2.00	117.40	123.20
38	d	405	PL9	O2-C1-C2	-2.00	117.28	121.83
36	B	623	SQD	C45-O47-C7	2.00	122.59	117.80
26	N	610	CLA	O2A-CGA-CBA	2.00	117.94	111.83
37	A	415	LMG	O8-C28-O10	-2.00	118.62	123.63
37	a	415	LMG	O8-C28-O10	-2.00	118.62	123.63
31	B	618	BCR	C29-C28-C27	-2.00	106.88	111.28
39	h	102	DGD	CBB-CAB-C9B	-2.00	104.25	114.37
25	5	608	CHL	O1D-CGD-CBD	-2.00	121.69	124.72
27	3	1621	LUT	C16-C1-C6	-2.00	107.10	110.24
27	7	1621	LUT	C16-C1-C6	-2.00	107.10	110.24
27	3	1620	LUT	C31-C30-C29	-2.00	124.47	127.28
29	2	1623	NEX	C30-C31-C32	-2.00	117.40	123.20
26	N	604	CLA	C3B-C2B-C1B	2.00	109.53	107.17
25	1	606	CHL	O2A-CGA-CBA	2.00	120.32	114.00
35	a	408	PHO	CMD-C2D-C3D	2.00	128.68	124.68
27	3	1621	LUT	C1-C6-C5	-2.00	119.90	122.64
27	7	1621	LUT	C1-C6-C5	-2.00	119.90	122.64
26	G	603	CLA	CHB-C1B-NB	2.00	127.05	124.05
25	R	607	CHL	C4C-CHD-C1D	2.00	123.23	116.07
25	n	608	CHL	C4C-CHD-C1D	2.00	123.23	116.07
25	s	608	CHL	O2A-CGA-CBA	2.00	120.32	114.00
27	1	1621	LUT	C35-C15-C14	-2.00	119.42	123.52
25	7	601	CHL	O2A-CGA-O1A	-2.00	118.62	123.63
26	s	612	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
29	Y	1623	NEX	O24-C25-C26	-2.00	57.34	58.93
29	y	1623	NEX	O24-C25-C26	-2.00	57.34	58.93
38	D	405	PL9	O2-C1-C6	2.00	123.66	120.48

All (532) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	1	601	CHL	ND
25	1	601	CHL	NC
25	1	601	CHL	NA
25	1	605	CHL	ND
25	1	605	CHL	NC
25	1	605	CHL	NA
25	1	606	CHL	ND
25	1	606	CHL	NC
25	1	606	CHL	NA
25	1	607	CHL	ND

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Mol	Chain	Res	Type	Atom
25	1	607	CHL	NC
25	1	607	CHL	NA
25	1	607	CHL	C8
25	1	608	CHL	ND
25	1	608	CHL	NC
25	1	608	CHL	NA
25	1	609	CHL	ND
25	1	609	CHL	NC
25	1	609	CHL	NA
25	1	609	CHL	C8
25	2	601	CHL	ND
25	2	601	CHL	NC
25	2	601	CHL	NA
25	2	605	CHL	ND
25	2	605	CHL	NC
25	2	605	CHL	NA
25	2	606	CHL	ND
25	2	606	CHL	NC
25	2	606	CHL	NA
25	2	607	CHL	ND
25	2	607	CHL	NC
25	2	607	CHL	NA
25	2	607	CHL	C8
25	2	608	CHL	ND
25	2	608	CHL	NC
25	2	608	CHL	NA
25	2	609	CHL	ND
25	2	609	CHL	NC
25	2	609	CHL	NA
25	2	609	CHL	C8
25	3	601	CHL	ND
25	3	601	CHL	NC
25	3	601	CHL	NA
25	3	601	CHL	C8
25	3	605	CHL	ND
25	3	605	CHL	NC
25	3	605	CHL	NA
25	3	606	CHL	ND
25	3	606	CHL	NC
25	3	606	CHL	NA
25	3	607	CHL	ND
25	3	607	CHL	NC

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Mol	Chain	Res	Type	Atom
25	3	607	CHL	NA
25	3	608	CHL	ND
25	3	608	CHL	NC
25	3	608	CHL	NA
25	3	609	CHL	ND
25	3	609	CHL	NC
25	3	609	CHL	NA
25	3	609	CHL	C8
25	4	601	CHL	ND
25	4	601	CHL	NC
25	4	601	CHL	NA
25	4	606	CHL	ND
25	4	606	CHL	NC
25	4	606	CHL	NA
25	4	607	CHL	ND
25	4	607	CHL	NC
25	4	607	CHL	NA
25	4	608	CHL	ND
25	4	608	CHL	NC
25	4	608	CHL	NA
25	4	609	CHL	ND
25	4	609	CHL	NC
25	4	609	CHL	NA
25	G	601	CHL	ND
25	G	601	CHL	NC
25	G	601	CHL	NA
25	G	601	CHL	C8
25	G	605	CHL	ND
25	G	605	CHL	NC
25	G	605	CHL	NA
25	G	606	CHL	ND
25	G	606	CHL	NC
25	G	606	CHL	NA
25	G	607	CHL	ND
25	G	607	CHL	NC
25	G	607	CHL	NA
25	G	607	CHL	C8
25	G	608	CHL	ND
25	G	608	CHL	NC
25	G	608	CHL	NA
25	G	608	CHL	C8
25	G	609	CHL	ND

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Mol	Chain	Res	Type	Atom
25	G	609	CHL	NC
25	G	609	CHL	NA
25	G	609	CHL	C8
25	N	601	CHL	ND
25	N	601	CHL	NC
25	N	601	CHL	NA
25	N	601	CHL	C8
25	N	605	CHL	ND
25	N	605	CHL	NC
25	N	605	CHL	NA
25	N	606	CHL	ND
25	N	606	CHL	NC
25	N	606	CHL	NA
25	N	607	CHL	ND
25	N	607	CHL	NC
25	N	607	CHL	NA
25	N	607	CHL	C8
25	N	608	CHL	ND
25	N	608	CHL	NC
25	N	608	CHL	NA
25	N	608	CHL	C8
25	N	609	CHL	ND
25	N	609	CHL	NC
25	N	609	CHL	NA
25	N	609	CHL	C8
25	R	606	CHL	ND
25	R	606	CHL	NC
25	R	606	CHL	NA
25	R	606	CHL	C8
25	R	607	CHL	ND
25	R	607	CHL	NC
25	R	607	CHL	NA
25	R	607	CHL	C8
25	R	608	CHL	ND
25	R	608	CHL	NC
25	R	608	CHL	NA
25	R	608	CHL	C8
25	R	614	CHL	ND
25	R	614	CHL	NC
25	R	614	CHL	NA
25	S	601	CHL	ND
25	S	601	CHL	NC

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Mol	Chain	Res	Type	Atom
25	S	601	CHL	NA
25	S	606	CHL	ND
25	S	606	CHL	NC
25	S	606	CHL	NA
25	S	607	CHL	ND
25	S	607	CHL	NC
25	S	607	CHL	NA
25	S	607	CHL	C8
25	S	608	CHL	ND
25	S	608	CHL	NC
25	S	608	CHL	NA
25	Y	601	CHL	ND
25	Y	601	CHL	NC
25	Y	601	CHL	NA
25	Y	601	CHL	C8
25	Y	605	CHL	ND
25	Y	605	CHL	NC
25	Y	605	CHL	NA
25	Y	606	CHL	ND
25	Y	606	CHL	NC
25	Y	606	CHL	NA
25	Y	607	CHL	ND
25	Y	607	CHL	NC
25	Y	607	CHL	NA
25	Y	607	CHL	C8
25	Y	608	CHL	ND
25	Y	608	CHL	NC
25	Y	608	CHL	NA
25	Y	608	CHL	C8
25	Y	609	CHL	ND
25	Y	609	CHL	NC
25	Y	609	CHL	NA
25	Y	609	CHL	C8
25	5	601	CHL	ND
25	5	601	CHL	NC
25	5	601	CHL	NA
25	5	605	CHL	ND
25	5	605	CHL	NC
25	5	605	CHL	NA
25	5	606	CHL	ND
25	5	606	CHL	NC
25	5	606	CHL	NA

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Mol	Chain	Res	Type	Atom
25	5	607	CHL	ND
25	5	607	CHL	NC
25	5	607	CHL	NA
25	5	607	CHL	C8
25	5	608	CHL	ND
25	5	608	CHL	NC
25	5	608	CHL	NA
25	5	609	CHL	ND
25	5	609	CHL	NC
25	5	609	CHL	NA
25	5	609	CHL	C8
25	6	601	CHL	ND
25	6	601	CHL	NC
25	6	601	CHL	NA
25	6	605	CHL	ND
25	6	605	CHL	NC
25	6	605	CHL	NA
25	6	606	CHL	ND
25	6	606	CHL	NC
25	6	606	CHL	NA
25	6	607	CHL	ND
25	6	607	CHL	NC
25	6	607	CHL	NA
25	6	607	CHL	C8
25	6	608	CHL	ND
25	6	608	CHL	NC
25	6	608	CHL	NA
25	6	609	CHL	ND
25	6	609	CHL	NC
25	6	609	CHL	NA
25	6	609	CHL	C8
25	7	601	CHL	ND
25	7	601	CHL	NC
25	7	601	CHL	NA
25	7	601	CHL	C8
25	7	605	CHL	ND
25	7	605	CHL	NC
25	7	605	CHL	NA
25	7	606	CHL	ND
25	7	606	CHL	NC
25	7	606	CHL	NA
25	7	607	CHL	ND

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Mol	Chain	Res	Type	Atom
25	7	607	CHL	NC
25	7	607	CHL	NA
25	7	608	CHL	ND
25	7	608	CHL	NC
25	7	608	CHL	NA
25	7	609	CHL	ND
25	7	609	CHL	NC
25	7	609	CHL	NA
25	7	609	CHL	C8
25	8	601	CHL	ND
25	8	601	CHL	NC
25	8	601	CHL	NA
25	8	606	CHL	ND
25	8	606	CHL	NC
25	8	606	CHL	NA
25	8	607	CHL	ND
25	8	607	CHL	NC
25	8	607	CHL	NA
25	8	608	CHL	ND
25	8	608	CHL	NC
25	8	608	CHL	NA
25	8	609	CHL	ND
25	8	609	CHL	NC
25	8	609	CHL	NA
25	g	601	CHL	ND
25	g	601	CHL	NC
25	g	601	CHL	NA
25	g	601	CHL	C8
25	g	605	CHL	ND
25	g	605	CHL	NC
25	g	605	CHL	NA
25	g	606	CHL	ND
25	g	606	CHL	NC
25	g	606	CHL	NA
25	g	607	CHL	ND
25	g	607	CHL	NC
25	g	607	CHL	NA
25	g	607	CHL	C8
25	g	608	CHL	ND
25	g	608	CHL	NC
25	g	608	CHL	NA
25	g	608	CHL	C8

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Mol	Chain	Res	Type	Atom
25	g	609	CHL	ND
25	g	609	CHL	NC
25	g	609	CHL	NA
25	g	609	CHL	C8
25	n	601	CHL	ND
25	n	601	CHL	NC
25	n	601	CHL	NA
25	n	601	CHL	C8
25	n	605	CHL	ND
25	n	605	CHL	NC
25	n	605	CHL	NA
25	n	606	CHL	ND
25	n	606	CHL	NC
25	n	606	CHL	NA
25	n	607	CHL	ND
25	n	607	CHL	NC
25	n	607	CHL	NA
25	n	607	CHL	C8
25	n	608	CHL	ND
25	n	608	CHL	NC
25	n	608	CHL	NA
25	n	608	CHL	C8
25	n	609	CHL	ND
25	n	609	CHL	NC
25	n	609	CHL	NA
25	n	609	CHL	C8
25	r	606	CHL	ND
25	r	606	CHL	NC
25	r	606	CHL	NA
25	r	606	CHL	C8
25	r	607	CHL	ND
25	r	607	CHL	NC
25	r	607	CHL	NA
25	r	607	CHL	C8
25	r	608	CHL	ND
25	r	608	CHL	NC
25	r	608	CHL	NA
25	r	608	CHL	C8
25	r	614	CHL	ND
25	r	614	CHL	NC
25	r	614	CHL	NA
25	s	601	CHL	ND

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Mol	Chain	Res	Type	Atom
25	s	601	CHL	NC
25	s	601	CHL	NA
25	s	606	CHL	ND
25	s	606	CHL	NC
25	s	606	CHL	NA
25	s	607	CHL	ND
25	s	607	CHL	NC
25	s	607	CHL	NA
25	s	607	CHL	C8
25	s	608	CHL	ND
25	s	608	CHL	NC
25	s	608	CHL	NA
25	y	601	CHL	ND
25	y	601	CHL	NC
25	y	601	CHL	NA
25	y	601	CHL	C8
25	y	605	CHL	ND
25	y	605	CHL	NC
25	y	605	CHL	NA
25	y	606	CHL	ND
25	y	606	CHL	NC
25	y	606	CHL	NA
25	y	607	CHL	ND
25	y	607	CHL	NC
25	y	607	CHL	NA
25	y	607	CHL	C8
25	y	608	CHL	ND
25	y	608	CHL	NC
25	y	608	CHL	NA
25	y	608	CHL	C8
25	y	609	CHL	ND
25	y	609	CHL	NC
25	y	609	CHL	NA
25	y	609	CHL	C8
26	1	602	CLA	ND
26	1	603	CLA	ND
26	1	610	CLA	ND
26	1	611	CLA	ND
26	1	612	CLA	ND
26	1	614	CLA	ND
26	2	602	CLA	ND
26	2	603	CLA	ND

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Mol	Chain	Res	Type	Atom
26	2	604	CLA	ND
26	2	610	CLA	ND
26	2	612	CLA	ND
26	2	614	CLA	ND
26	3	602	CLA	ND
26	3	603	CLA	ND
26	3	604	CLA	ND
26	3	610	CLA	ND
26	3	611	CLA	ND
26	3	612	CLA	ND
26	3	613	CLA	ND
26	3	614	CLA	ND
26	4	602	CLA	ND
26	4	603	CLA	ND
26	4	610	CLA	ND
26	4	611	CLA	ND
26	4	612	CLA	ND
26	A	405	CLA	ND
26	A	406	CLA	ND
26	A	410	CLA	ND
26	B	602	CLA	ND
26	B	603	CLA	ND
26	B	604	CLA	ND
26	B	605	CLA	ND
26	B	606	CLA	ND
26	B	607	CLA	ND
26	B	608	CLA	ND
26	B	611	CLA	ND
26	B	612	CLA	ND
26	B	613	CLA	ND
26	B	614	CLA	ND
26	B	615	CLA	ND
26	B	616	CLA	ND
26	B	617	CLA	ND
26	C	501	CLA	ND
26	C	502	CLA	ND
26	C	503	CLA	ND
26	C	504	CLA	ND
26	C	505	CLA	ND
26	C	506	CLA	ND
26	C	507	CLA	ND
26	C	508	CLA	ND

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Mol	Chain	Res	Type	Atom
26	C	509	CLA	ND
26	C	510	CLA	ND
26	C	511	CLA	ND
26	C	512	CLA	ND
26	D	402	CLA	ND
26	G	602	CLA	ND
26	G	603	CLA	ND
26	G	604	CLA	ND
26	G	610	CLA	ND
26	G	611	CLA	ND
26	G	612	CLA	ND
26	G	613	CLA	ND
26	G	614	CLA	ND
26	N	602	CLA	ND
26	N	603	CLA	ND
26	N	604	CLA	ND
26	N	610	CLA	ND
26	N	611	CLA	ND
26	N	612	CLA	ND
26	N	613	CLA	ND
26	N	614	CLA	ND
26	R	601	CLA	ND
26	R	602	CLA	ND
26	R	603	CLA	ND
26	R	604	CLA	ND
26	R	609	CLA	ND
26	R	610	CLA	ND
26	R	611	CLA	ND
26	R	612	CLA	ND
26	R	613	CLA	ND
26	S	602	CLA	ND
26	S	603	CLA	ND
26	S	604	CLA	ND
26	S	609	CLA	ND
26	S	610	CLA	ND
26	S	611	CLA	ND
26	S	612	CLA	ND
26	S	613	CLA	ND
26	S	614	CLA	ND
26	Y	602	CLA	ND
26	Y	603	CLA	ND
26	Y	604	CLA	ND

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Mol	Chain	Res	Type	Atom
26	Y	610	CLA	ND
26	Y	611	CLA	ND
26	Y	612	CLA	ND
26	Y	613	CLA	ND
26	Y	614	CLA	ND
26	5	602	CLA	ND
26	5	603	CLA	ND
26	5	610	CLA	ND
26	5	611	CLA	ND
26	5	612	CLA	ND
26	5	614	CLA	ND
26	6	602	CLA	ND
26	6	603	CLA	ND
26	6	604	CLA	ND
26	6	610	CLA	ND
26	6	612	CLA	ND
26	6	614	CLA	ND
26	7	602	CLA	ND
26	7	603	CLA	ND
26	7	604	CLA	ND
26	7	610	CLA	ND
26	7	611	CLA	ND
26	7	612	CLA	ND
26	7	613	CLA	ND
26	7	614	CLA	ND
26	8	602	CLA	ND
26	8	603	CLA	ND
26	8	610	CLA	ND
26	8	611	CLA	ND
26	8	612	CLA	ND
26	a	405	CLA	ND
26	a	406	CLA	ND
26	a	410	CLA	ND
26	b	602	CLA	ND
26	b	603	CLA	ND
26	b	604	CLA	ND
26	b	605	CLA	ND
26	b	606	CLA	ND
26	b	607	CLA	ND
26	b	608	CLA	ND
26	b	611	CLA	ND
26	b	612	CLA	ND

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Mol	Chain	Res	Type	Atom
26	b	613	CLA	ND
26	b	614	CLA	ND
26	b	615	CLA	ND
26	b	616	CLA	ND
26	b	617	CLA	ND
26	c	501	CLA	ND
26	c	502	CLA	ND
26	c	503	CLA	ND
26	c	504	CLA	ND
26	c	505	CLA	ND
26	c	506	CLA	ND
26	c	507	CLA	ND
26	c	508	CLA	ND
26	c	509	CLA	ND
26	c	510	CLA	ND
26	c	511	CLA	ND
26	c	512	CLA	ND
26	d	402	CLA	ND
26	g	602	CLA	ND
26	g	603	CLA	ND
26	g	604	CLA	ND
26	g	610	CLA	ND
26	g	611	CLA	ND
26	g	612	CLA	ND
26	g	613	CLA	ND
26	g	614	CLA	ND
26	n	602	CLA	ND
26	n	603	CLA	ND
26	n	604	CLA	ND
26	n	610	CLA	ND
26	n	611	CLA	ND
26	n	612	CLA	ND
26	n	613	CLA	ND
26	n	614	CLA	ND
26	r	601	CLA	ND
26	r	602	CLA	ND
26	r	603	CLA	ND
26	r	604	CLA	ND
26	r	609	CLA	ND
26	r	610	CLA	ND
26	r	611	CLA	ND
26	r	612	CLA	ND

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Mol	Chain	Res	Type	Atom
26	r	613	CLA	ND
26	s	602	CLA	ND
26	s	603	CLA	ND
26	s	604	CLA	ND
26	s	609	CLA	ND
26	s	610	CLA	ND
26	s	611	CLA	ND
26	s	612	CLA	ND
26	s	613	CLA	ND
26	s	614	CLA	ND
26	y	602	CLA	ND
26	y	603	CLA	ND
26	y	604	CLA	ND
26	y	610	CLA	ND
26	y	611	CLA	ND
26	y	612	CLA	ND
26	y	613	CLA	ND
26	y	614	CLA	ND

All (4926) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	1	601	CHL	C1C-C2C-CMC-OMC
25	1	601	CHL	C3C-C2C-CMC-OMC
25	1	605	CHL	C1A-C2A-CAA-CBA
25	1	605	CHL	C1C-C2C-CMC-OMC
25	1	605	CHL	C3C-C2C-CMC-OMC
25	1	606	CHL	C1C-C2C-CMC-OMC
25	1	607	CHL	C1C-C2C-CMC-OMC
25	1	607	CHL	C3C-C2C-CMC-OMC
25	1	607	CHL	C4C-C3C-CAC-CBC
25	1	607	CHL	CHA-CBD-CGD-O2D
25	1	608	CHL	C1A-C2A-CAA-CBA
25	1	608	CHL	C1C-C2C-CMC-OMC
25	1	608	CHL	C3C-C2C-CMC-OMC
25	1	608	CHL	CBD-CGD-O2D-CED
25	1	609	CHL	C1C-C2C-CMC-OMC
25	1	609	CHL	C3C-C2C-CMC-OMC
25	1	609	CHL	C4C-C3C-CAC-CBC
25	2	601	CHL	C1A-C2A-CAA-CBA
25	2	605	CHL	C1A-C2A-CAA-CBA
25	2	605	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
25	2	605	CHL	C3C-C2C-CMC-OMC
25	2	607	CHL	C1C-C2C-CMC-OMC
25	2	607	CHL	C3C-C2C-CMC-OMC
25	2	607	CHL	CHA-CBD-CGD-O2D
25	2	608	CHL	C1A-C2A-CAA-CBA
25	2	608	CHL	C1C-C2C-CMC-OMC
25	2	608	CHL	C3C-C2C-CMC-OMC
25	2	608	CHL	CBD-CGD-O2D-CED
25	2	609	CHL	C1C-C2C-CMC-OMC
25	2	609	CHL	C3C-C2C-CMC-OMC
25	3	605	CHL	C1A-C2A-CAA-CBA
25	3	605	CHL	C1C-C2C-CMC-OMC
25	3	605	CHL	C3C-C2C-CMC-OMC
25	3	606	CHL	C1A-C2A-CAA-CBA
25	3	606	CHL	C1C-C2C-CMC-OMC
25	3	606	CHL	C3C-C2C-CMC-OMC
25	3	607	CHL	C1C-C2C-CMC-OMC
25	3	607	CHL	C3C-C2C-CMC-OMC
25	3	608	CHL	CBD-CGD-O2D-CED
25	3	609	CHL	C1C-C2C-CMC-OMC
25	3	609	CHL	C3C-C2C-CMC-OMC
25	3	609	CHL	C4C-C3C-CAC-CBC
25	4	601	CHL	C1C-C2C-CMC-OMC
25	4	601	CHL	C3C-C2C-CMC-OMC
25	4	606	CHL	C1A-C2A-CAA-CBA
25	4	606	CHL	C1C-C2C-CMC-OMC
25	4	606	CHL	C3C-C2C-CMC-OMC
25	4	607	CHL	C1C-C2C-CMC-OMC
25	4	607	CHL	C3C-C2C-CMC-OMC
25	4	608	CHL	C1A-C2A-CAA-CBA
25	4	608	CHL	C1C-C2C-CMC-OMC
25	4	608	CHL	C3C-C2C-CMC-OMC
25	4	608	CHL	CBD-CGD-O2D-CED
25	4	609	CHL	C1C-C2C-CMC-OMC
25	4	609	CHL	C3C-C2C-CMC-OMC
25	G	605	CHL	C1C-C2C-CMC-OMC
25	G	605	CHL	C3C-C2C-CMC-OMC
25	G	605	CHL	CAD-CBD-CGD-O1D
25	G	605	CHL	CAD-CBD-CGD-O2D
25	G	605	CHL	CBD-CGD-O2D-CED
25	G	606	CHL	C1C-C2C-CMC-OMC
25	G	609	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	N	605	CHL	C1C-C2C-CMC-OMC
25	N	605	CHL	C3C-C2C-CMC-OMC
25	N	605	CHL	CAD-CBD-CGD-O1D
25	N	605	CHL	CAD-CBD-CGD-O2D
25	N	606	CHL	C1C-C2C-CMC-OMC
25	N	607	CHL	C1C-C2C-CMC-OMC
25	N	607	CHL	C3C-C2C-CMC-OMC
25	N	609	CHL	C1C-C2C-CMC-OMC
25	N	609	CHL	C3C-C2C-CMC-OMC
25	R	606	CHL	C1A-C2A-CAA-CBA
25	R	606	CHL	C11-C10-C8-C9
25	R	608	CHL	CBD-CGD-O2D-CED
25	R	614	CHL	CAD-CBD-CGD-O1D
25	R	614	CHL	CAD-CBD-CGD-O2D
25	R	614	CHL	CBD-CGD-O2D-CED
25	S	606	CHL	C1C-C2C-CMC-OMC
25	S	606	CHL	C3C-C2C-CMC-OMC
25	S	606	CHL	CAD-CBD-CGD-O1D
25	S	606	CHL	CAD-CBD-CGD-O2D
25	S	607	CHL	C1C-C2C-CMC-OMC
25	S	607	CHL	C3C-C2C-CMC-OMC
25	S	608	CHL	C1A-C2A-CAA-CBA
25	Y	605	CHL	C1A-C2A-CAA-CBA
25	Y	605	CHL	C1C-C2C-CMC-OMC
25	Y	605	CHL	C3C-C2C-CMC-OMC
25	Y	606	CHL	C1C-C2C-CMC-OMC
25	Y	607	CHL	C1C-C2C-CMC-OMC
25	Y	607	CHL	C3C-C2C-CMC-OMC
25	Y	608	CHL	C1A-C2A-CAA-CBA
25	Y	608	CHL	C1C-C2C-CMC-OMC
25	Y	608	CHL	C3C-C2C-CMC-OMC
25	5	601	CHL	C1C-C2C-CMC-OMC
25	5	601	CHL	C3C-C2C-CMC-OMC
25	5	605	CHL	C1A-C2A-CAA-CBA
25	5	605	CHL	C1C-C2C-CMC-OMC
25	5	605	CHL	C3C-C2C-CMC-OMC
25	5	606	CHL	C1C-C2C-CMC-OMC
25	5	607	CHL	C1C-C2C-CMC-OMC
25	5	607	CHL	C3C-C2C-CMC-OMC
25	5	607	CHL	C4C-C3C-CAC-CBC
25	5	607	CHL	CHA-CBD-CGD-O2D
25	5	608	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	5	608	CHL	C1C-C2C-CMC-OMC
25	5	608	CHL	C3C-C2C-CMC-OMC
25	5	608	CHL	CBD-CGD-O2D-CED
25	5	609	CHL	C1C-C2C-CMC-OMC
25	5	609	CHL	C3C-C2C-CMC-OMC
25	5	609	CHL	C4C-C3C-CAC-CBC
25	6	601	CHL	C1A-C2A-CAA-CBA
25	6	605	CHL	C1A-C2A-CAA-CBA
25	6	605	CHL	C1C-C2C-CMC-OMC
25	6	605	CHL	C3C-C2C-CMC-OMC
25	6	607	CHL	C1C-C2C-CMC-OMC
25	6	607	CHL	C3C-C2C-CMC-OMC
25	6	607	CHL	CHA-CBD-CGD-O2D
25	6	608	CHL	C1A-C2A-CAA-CBA
25	6	608	CHL	C1C-C2C-CMC-OMC
25	6	608	CHL	C3C-C2C-CMC-OMC
25	6	608	CHL	CBD-CGD-O2D-CED
25	6	609	CHL	C1C-C2C-CMC-OMC
25	6	609	CHL	C3C-C2C-CMC-OMC
25	7	605	CHL	C1A-C2A-CAA-CBA
25	7	605	CHL	C1C-C2C-CMC-OMC
25	7	605	CHL	C3C-C2C-CMC-OMC
25	7	606	CHL	C1A-C2A-CAA-CBA
25	7	606	CHL	C1C-C2C-CMC-OMC
25	7	606	CHL	C3C-C2C-CMC-OMC
25	7	607	CHL	C1C-C2C-CMC-OMC
25	7	607	CHL	C3C-C2C-CMC-OMC
25	7	608	CHL	CBD-CGD-O2D-CED
25	7	609	CHL	C1C-C2C-CMC-OMC
25	7	609	CHL	C3C-C2C-CMC-OMC
25	7	609	CHL	C4C-C3C-CAC-CBC
25	8	601	CHL	C1C-C2C-CMC-OMC
25	8	601	CHL	C3C-C2C-CMC-OMC
25	8	606	CHL	C1A-C2A-CAA-CBA
25	8	606	CHL	C1C-C2C-CMC-OMC
25	8	606	CHL	C3C-C2C-CMC-OMC
25	8	607	CHL	C1C-C2C-CMC-OMC
25	8	607	CHL	C3C-C2C-CMC-OMC
25	8	608	CHL	C1A-C2A-CAA-CBA
25	8	608	CHL	C1C-C2C-CMC-OMC
25	8	608	CHL	C3C-C2C-CMC-OMC
25	8	608	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	8	609	CHL	C1C-C2C-CMC-OMC
25	8	609	CHL	C3C-C2C-CMC-OMC
25	g	605	CHL	C1C-C2C-CMC-OMC
25	g	605	CHL	C3C-C2C-CMC-OMC
25	g	605	CHL	CAD-CBD-CGD-O1D
25	g	605	CHL	CAD-CBD-CGD-O2D
25	g	605	CHL	CBD-CGD-O2D-CED
25	g	606	CHL	C1C-C2C-CMC-OMC
25	g	609	CHL	CBD-CGD-O2D-CED
25	n	605	CHL	C1C-C2C-CMC-OMC
25	n	605	CHL	C3C-C2C-CMC-OMC
25	n	605	CHL	CAD-CBD-CGD-O1D
25	n	605	CHL	CAD-CBD-CGD-O2D
25	n	606	CHL	C1C-C2C-CMC-OMC
25	n	607	CHL	C1C-C2C-CMC-OMC
25	n	607	CHL	C3C-C2C-CMC-OMC
25	n	609	CHL	C1C-C2C-CMC-OMC
25	n	609	CHL	C3C-C2C-CMC-OMC
25	r	606	CHL	C1A-C2A-CAA-CBA
25	r	606	CHL	C11-C10-C8-C9
25	r	608	CHL	CBD-CGD-O2D-CED
25	r	614	CHL	CAD-CBD-CGD-O1D
25	r	614	CHL	CAD-CBD-CGD-O2D
25	r	614	CHL	CBD-CGD-O2D-CED
25	s	606	CHL	C1C-C2C-CMC-OMC
25	s	606	CHL	C3C-C2C-CMC-OMC
25	s	606	CHL	CAD-CBD-CGD-O1D
25	s	606	CHL	CAD-CBD-CGD-O2D
25	s	607	CHL	C1C-C2C-CMC-OMC
25	s	607	CHL	C3C-C2C-CMC-OMC
25	s	608	CHL	C1A-C2A-CAA-CBA
25	y	605	CHL	C1A-C2A-CAA-CBA
25	y	605	CHL	C1C-C2C-CMC-OMC
25	y	605	CHL	C3C-C2C-CMC-OMC
25	y	606	CHL	C1C-C2C-CMC-OMC
25	y	607	CHL	C1C-C2C-CMC-OMC
25	y	607	CHL	C3C-C2C-CMC-OMC
25	y	608	CHL	C1A-C2A-CAA-CBA
25	y	608	CHL	C1C-C2C-CMC-OMC
25	y	608	CHL	C3C-C2C-CMC-OMC
26	1	603	CLA	CBD-CGD-O2D-CED
26	1	604	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
26	1	604	CLA	CAD-CBD-CGD-O2D
26	1	610	CLA	C2B-C3B-CAB-CBB
26	1	610	CLA	C4B-C3B-CAB-CBB
26	1	611	CLA	C2B-C3B-CAB-CBB
26	1	611	CLA	C4B-C3B-CAB-CBB
26	1	612	CLA	C2B-C3B-CAB-CBB
26	1	612	CLA	C4B-C3B-CAB-CBB
26	2	603	CLA	C2B-C3B-CAB-CBB
26	2	603	CLA	C4B-C3B-CAB-CBB
26	2	603	CLA	CBD-CGD-O2D-CED
26	2	604	CLA	C1A-C2A-CAA-CBA
26	2	604	CLA	CBD-CGD-O2D-CED
26	2	610	CLA	C4B-C3B-CAB-CBB
26	2	611	CLA	C2B-C3B-CAB-CBB
26	2	611	CLA	C4B-C3B-CAB-CBB
26	2	612	CLA	CHA-CBD-CGD-O2D
26	2	614	CLA	C1A-C2A-CAA-CBA
26	2	614	CLA	C3A-C2A-CAA-CBA
26	2	614	CLA	CBD-CGD-O2D-CED
26	3	602	CLA	CHA-CBD-CGD-O1D
26	3	602	CLA	CHA-CBD-CGD-O2D
26	3	610	CLA	C2B-C3B-CAB-CBB
26	3	610	CLA	C4B-C3B-CAB-CBB
26	3	611	CLA	C1A-C2A-CAA-CBA
26	3	611	CLA	C2B-C3B-CAB-CBB
26	3	611	CLA	C4B-C3B-CAB-CBB
26	3	612	CLA	C4B-C3B-CAB-CBB
26	3	612	CLA	CAD-CBD-CGD-O1D
26	3	612	CLA	CAD-CBD-CGD-O2D
26	3	613	CLA	CBD-CGD-O2D-CED
26	4	602	CLA	CHA-CBD-CGD-O1D
26	4	602	CLA	CHA-CBD-CGD-O2D
26	4	602	CLA	CBD-CGD-O2D-CED
26	4	603	CLA	C2B-C3B-CAB-CBB
26	4	603	CLA	C4B-C3B-CAB-CBB
26	4	603	CLA	CBD-CGD-O2D-CED
26	4	604	CLA	CBD-CGD-O2D-CED
26	4	610	CLA	C2B-C3B-CAB-CBB
26	4	610	CLA	C4B-C3B-CAB-CBB
26	4	611	CLA	C2B-C3B-CAB-CBB
26	4	611	CLA	C4B-C3B-CAB-CBB
26	4	612	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	4	612	CLA	C4B-C3B-CAB-CBB
26	A	406	CLA	C1A-C2A-CAA-CBA
26	A	407	CLA	C2B-C3B-CAB-CBB
26	A	407	CLA	C4B-C3B-CAB-CBB
26	B	602	CLA	C4B-C3B-CAB-CBB
26	B	602	CLA	CAD-CBD-CGD-O2D
26	B	613	CLA	C1A-C2A-CAA-CBA
26	B	613	CLA	C3A-C2A-CAA-CBA
26	B	615	CLA	CBD-CGD-O2D-CED
26	B	616	CLA	C4B-C3B-CAB-CBB
26	C	502	CLA	CAD-CBD-CGD-O1D
26	C	502	CLA	CAD-CBD-CGD-O2D
26	C	506	CLA	C4-C3-C5-C6
26	C	507	CLA	C1A-C2A-CAA-CBA
26	C	507	CLA	C3A-C2A-CAA-CBA
26	C	507	CLA	CHA-CBD-CGD-O1D
26	C	507	CLA	CHA-CBD-CGD-O2D
26	C	507	CLA	C11-C10-C8-C9
26	D	403	CLA	CBD-CGD-O2D-CED
26	G	610	CLA	C1A-C2A-CAA-CBA
26	G	611	CLA	C1A-C2A-CAA-CBA
26	G	611	CLA	C3A-C2A-CAA-CBA
26	G	611	CLA	C4B-C3B-CAB-CBB
26	N	610	CLA	C1A-C2A-CAA-CBA
26	N	610	CLA	C3A-C2A-CAA-CBA
26	N	611	CLA	C4B-C3B-CAB-CBB
26	R	601	CLA	C1A-C2A-CAA-CBA
26	R	601	CLA	C3A-C2A-CAA-CBA
26	R	601	CLA	CBD-CGD-O2D-CED
26	R	604	CLA	CHA-CBD-CGD-O1D
26	R	604	CLA	CHA-CBD-CGD-O2D
26	R	611	CLA	C1A-C2A-CAA-CBA
26	R	611	CLA	C3A-C2A-CAA-CBA
26	R	611	CLA	CBA-CGA-O2A-C1
26	R	612	CLA	CBD-CGD-O2D-CED
26	R	613	CLA	C2B-C3B-CAB-CBB
26	R	613	CLA	C4B-C3B-CAB-CBB
26	R	616	CLA	C1A-C2A-CAA-CBA
26	R	616	CLA	C3A-C2A-CAA-CBA
26	S	602	CLA	C1A-C2A-CAA-CBA
26	S	602	CLA	C3A-C2A-CAA-CBA
26	S	603	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
26	S	603	CLA	CHA-CBD-CGD-O2D
26	S	604	CLA	C1A-C2A-CAA-CBA
26	S	609	CLA	C1A-C2A-CAA-CBA
26	S	611	CLA	C2B-C3B-CAB-CBB
26	S	611	CLA	C4B-C3B-CAB-CBB
26	S	612	CLA	CBD-CGD-O2D-CED
26	5	603	CLA	CBD-CGD-O2D-CED
26	5	604	CLA	CAD-CBD-CGD-O1D
26	5	604	CLA	CAD-CBD-CGD-O2D
26	5	610	CLA	C2B-C3B-CAB-CBB
26	5	610	CLA	C4B-C3B-CAB-CBB
26	5	611	CLA	C2B-C3B-CAB-CBB
26	5	611	CLA	C4B-C3B-CAB-CBB
26	5	612	CLA	C2B-C3B-CAB-CBB
26	5	612	CLA	C4B-C3B-CAB-CBB
26	6	603	CLA	C2B-C3B-CAB-CBB
26	6	603	CLA	C4B-C3B-CAB-CBB
26	6	603	CLA	CBD-CGD-O2D-CED
26	6	604	CLA	C1A-C2A-CAA-CBA
26	6	604	CLA	CBD-CGD-O2D-CED
26	6	611	CLA	C2B-C3B-CAB-CBB
26	6	611	CLA	C4B-C3B-CAB-CBB
26	6	612	CLA	CHA-CBD-CGD-O2D
26	6	614	CLA	C1A-C2A-CAA-CBA
26	6	614	CLA	C3A-C2A-CAA-CBA
26	6	614	CLA	CBD-CGD-O2D-CED
26	7	602	CLA	CHA-CBD-CGD-O1D
26	7	602	CLA	CHA-CBD-CGD-O2D
26	7	610	CLA	C2B-C3B-CAB-CBB
26	7	610	CLA	C4B-C3B-CAB-CBB
26	7	611	CLA	C1A-C2A-CAA-CBA
26	7	611	CLA	C2B-C3B-CAB-CBB
26	7	611	CLA	C4B-C3B-CAB-CBB
26	7	612	CLA	C4B-C3B-CAB-CBB
26	7	612	CLA	CAD-CBD-CGD-O1D
26	7	612	CLA	CAD-CBD-CGD-O2D
26	7	613	CLA	CBD-CGD-O2D-CED
26	8	602	CLA	CHA-CBD-CGD-O1D
26	8	602	CLA	CHA-CBD-CGD-O2D
26	8	602	CLA	CBD-CGD-O2D-CED
26	8	603	CLA	C2B-C3B-CAB-CBB
26	8	603	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	8	603	CLA	CBD-CGD-O2D-CED
26	8	604	CLA	CBD-CGD-O2D-CED
26	8	610	CLA	C2B-C3B-CAB-CBB
26	8	610	CLA	C4B-C3B-CAB-CBB
26	8	611	CLA	C2B-C3B-CAB-CBB
26	8	611	CLA	C4B-C3B-CAB-CBB
26	8	612	CLA	C2B-C3B-CAB-CBB
26	8	612	CLA	C4B-C3B-CAB-CBB
26	a	406	CLA	C1A-C2A-CAA-CBA
26	a	407	CLA	C2B-C3B-CAB-CBB
26	a	407	CLA	C4B-C3B-CAB-CBB
26	b	602	CLA	C4B-C3B-CAB-CBB
26	b	602	CLA	CAD-CBD-CGD-O2D
26	b	613	CLA	C1A-C2A-CAA-CBA
26	b	613	CLA	C3A-C2A-CAA-CBA
26	b	615	CLA	CBD-CGD-O2D-CED
26	b	616	CLA	C4B-C3B-CAB-CBB
26	c	502	CLA	CAD-CBD-CGD-O1D
26	c	502	CLA	CAD-CBD-CGD-O2D
26	c	506	CLA	C4-C3-C5-C6
26	c	506	CLA	C11-C12-C13-C14
26	c	507	CLA	C1A-C2A-CAA-CBA
26	c	507	CLA	C3A-C2A-CAA-CBA
26	c	507	CLA	CHA-CBD-CGD-O1D
26	c	507	CLA	CHA-CBD-CGD-O2D
26	c	507	CLA	C11-C10-C8-C9
26	d	403	CLA	CBD-CGD-O2D-CED
26	g	610	CLA	C1A-C2A-CAA-CBA
26	g	611	CLA	C1A-C2A-CAA-CBA
26	g	611	CLA	C3A-C2A-CAA-CBA
26	g	611	CLA	C4B-C3B-CAB-CBB
26	n	610	CLA	C1A-C2A-CAA-CBA
26	n	610	CLA	C3A-C2A-CAA-CBA
26	n	611	CLA	C4B-C3B-CAB-CBB
26	r	601	CLA	C1A-C2A-CAA-CBA
26	r	601	CLA	C3A-C2A-CAA-CBA
26	r	601	CLA	CBD-CGD-O2D-CED
26	r	604	CLA	CHA-CBD-CGD-O1D
26	r	604	CLA	CHA-CBD-CGD-O2D
26	r	611	CLA	C1A-C2A-CAA-CBA
26	r	611	CLA	C3A-C2A-CAA-CBA
26	r	611	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	r	612	CLA	CBD-CGD-O2D-CED
26	r	613	CLA	C2B-C3B-CAB-CBB
26	r	613	CLA	C4B-C3B-CAB-CBB
26	r	616	CLA	C1A-C2A-CAA-CBA
26	r	616	CLA	C3A-C2A-CAA-CBA
26	s	602	CLA	C1A-C2A-CAA-CBA
26	s	602	CLA	C3A-C2A-CAA-CBA
26	s	603	CLA	CHA-CBD-CGD-O1D
26	s	603	CLA	CHA-CBD-CGD-O2D
26	s	604	CLA	C1A-C2A-CAA-CBA
26	s	609	CLA	C1A-C2A-CAA-CBA
26	s	611	CLA	C2B-C3B-CAB-CBB
26	s	611	CLA	C4B-C3B-CAB-CBB
26	s	612	CLA	CBD-CGD-O2D-CED
28	1	1622	XAT	C31-C32-C33-C34
28	1	1622	XAT	C31-C32-C33-C40
28	2	1622	XAT	O4-C6-C7-C8
28	2	1622	XAT	C31-C32-C33-C34
28	G	1622	XAT	C11-C12-C13-C14
28	N	1622	XAT	C11-C12-C13-C14
28	N	1622	XAT	C11-C12-C13-C20
28	Y	1622	XAT	C11-C12-C13-C14
28	5	1622	XAT	C31-C32-C33-C34
28	5	1622	XAT	C31-C32-C33-C40
28	6	1622	XAT	O4-C6-C7-C8
28	6	1622	XAT	C31-C32-C33-C34
28	g	1622	XAT	C11-C12-C13-C14
28	n	1622	XAT	C11-C12-C13-C14
28	n	1622	XAT	C11-C12-C13-C20
28	y	1622	XAT	C11-C12-C13-C14
29	1	1623	NEX	C11-C12-C13-C14
29	G	1623	NEX	C11-C12-C13-C14
29	5	1623	NEX	C11-C12-C13-C14
29	g	1623	NEX	C11-C12-C13-C14
30	1	2630	LHG	C4-O6-P-O5
30	1	2630	LHG	O7-C5-C6-O8
30	2	2630	LHG	C4-O6-P-O5
30	3	2630	LHG	C3-O3-P-O6
30	3	2630	LHG	C4-O6-P-O3
30	3	2630	LHG	C4-O6-P-O4
30	3	2630	LHG	C4-O6-P-O5
30	4	2630	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
30	4	2630	LHG	C3-O3-P-O6
30	B	2630	LHG	C1-C2-C3-O3
30	B	2630	LHG	C3-O3-P-O5
30	B	2630	LHG	C4-O6-P-O3
30	B	2631	LHG	O1-C1-C2-O2
30	B	2631	LHG	O1-C1-C2-C3
30	C	2630	LHG	O1-C1-C2-O2
30	C	2630	LHG	O1-C1-C2-C3
30	C	522	LHG	C3-O3-P-O4
30	C	522	LHG	C3-O3-P-O6
30	C	523	LHG	C3-O3-P-O5
30	C	523	LHG	C4-O6-P-O4
30	C	523	LHG	C8-C7-O7-C5
30	D	408	LHG	C4-O6-P-O5
30	D	409	LHG	C4-O6-P-O3
30	D	409	LHG	C4-O6-P-O4
30	D	409	LHG	C4-O6-P-O5
30	D	410	LHG	C4-O6-P-O3
30	G	2630	LHG	C4-O6-P-O3
30	G	2630	LHG	C4-O6-P-O5
30	L	101	LHG	C3-O3-P-O4
30	L	101	LHG	C4-O6-P-O3
30	L	101	LHG	C4-O6-P-O4
30	N	2630	LHG	C3-O3-P-O6
30	N	2630	LHG	C4-O6-P-O5
30	S	2630	LHG	O1-C1-C2-C3
30	S	2630	LHG	C4-O6-P-O5
30	Y	2630	LHG	C4-O6-P-O3
30	Y	2630	LHG	C4-O6-P-O5
30	5	2630	LHG	C4-O6-P-O5
30	5	2630	LHG	O7-C5-C6-O8
30	6	2630	LHG	C4-O6-P-O5
30	7	2630	LHG	C3-O3-P-O6
30	7	2630	LHG	C4-O6-P-O3
30	7	2630	LHG	C4-O6-P-O4
30	7	2630	LHG	C4-O6-P-O5
30	8	2630	LHG	C3-O3-P-O5
30	8	2630	LHG	C3-O3-P-O6
30	b	2630	LHG	C1-C2-C3-O3
30	b	2630	LHG	C3-O3-P-O5
30	b	2630	LHG	C4-O6-P-O3
30	b	2631	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
30	b	2631	LHG	O1-C1-C2-C3
30	c	2630	LHG	O1-C1-C2-O2
30	c	2630	LHG	O1-C1-C2-C3
30	c	522	LHG	C3-O3-P-O4
30	c	522	LHG	C3-O3-P-O6
30	c	523	LHG	C3-O3-P-O5
30	c	523	LHG	C4-O6-P-O4
30	c	523	LHG	C8-C7-O7-C5
30	d	408	LHG	C4-O6-P-O5
30	d	409	LHG	C4-O6-P-O3
30	d	409	LHG	C4-O6-P-O4
30	d	409	LHG	C4-O6-P-O5
30	d	410	LHG	C4-O6-P-O3
30	g	2630	LHG	C4-O6-P-O3
30	g	2630	LHG	C4-O6-P-O5
30	l	101	LHG	C3-O3-P-O4
30	l	101	LHG	C4-O6-P-O3
30	l	101	LHG	C4-O6-P-O4
30	n	2630	LHG	C3-O3-P-O6
30	n	2630	LHG	C4-O6-P-O5
30	s	2630	LHG	O1-C1-C2-C3
30	s	2630	LHG	C4-O6-P-O5
30	y	2630	LHG	C4-O6-P-O3
30	y	2630	LHG	C4-O6-P-O5
31	4	623	BCR	C7-C8-C9-C10
31	4	623	BCR	C7-C8-C9-C34
31	4	623	BCR	C21-C22-C23-C24
31	4	623	BCR	C37-C22-C23-C24
31	B	618	BCR	C5-C6-C7-C8
31	B	619	BCR	C7-C8-C9-C10
31	B	619	BCR	C7-C8-C9-C34
31	B	620	BCR	C7-C8-C9-C10
31	B	620	BCR	C7-C8-C9-C34
31	C	516	BCR	C7-C8-C9-C10
31	C	517	BCR	C7-C8-C9-C10
31	C	517	BCR	C7-C8-C9-C34
31	D	404	BCR	C7-C8-C9-C10
31	H	101	BCR	C7-C8-C9-C10
31	H	101	BCR	C7-C8-C9-C34
31	T	101	BCR	C1-C6-C7-C8
31	T	101	BCR	C5-C6-C7-C8
31	T	101	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
31	T	101	BCR	C7-C8-C9-C34
31	T	101	BCR	C17-C18-C19-C20
31	T	101	BCR	C36-C18-C19-C20
31	T	101	BCR	C21-C22-C23-C24
31	8	623	BCR	C7-C8-C9-C10
31	8	623	BCR	C7-C8-C9-C34
31	8	623	BCR	C21-C22-C23-C24
31	8	623	BCR	C37-C22-C23-C24
31	b	618	BCR	C5-C6-C7-C8
31	b	619	BCR	C7-C8-C9-C10
31	b	619	BCR	C7-C8-C9-C34
31	b	620	BCR	C7-C8-C9-C10
31	b	620	BCR	C7-C8-C9-C34
31	c	516	BCR	C7-C8-C9-C10
31	c	517	BCR	C7-C8-C9-C10
31	c	517	BCR	C7-C8-C9-C34
31	d	404	BCR	C7-C8-C9-C10
31	h	101	BCR	C7-C8-C9-C10
31	h	101	BCR	C7-C8-C9-C34
31	t	101	BCR	C1-C6-C7-C8
31	t	101	BCR	C5-C6-C7-C8
31	t	101	BCR	C7-C8-C9-C10
31	t	101	BCR	C7-C8-C9-C34
31	t	101	BCR	C17-C18-C19-C20
31	t	101	BCR	C36-C18-C19-C20
31	t	101	BCR	C21-C22-C23-C24
35	A	408	PHO	CBA-CGA-O2A-C1
35	A	408	PHO	O1A-CGA-O2A-C1
35	a	408	PHO	CBA-CGA-O2A-C1
35	a	408	PHO	O1A-CGA-O2A-C1
36	A	412	SQD	O49-C7-O47-C45
36	A	412	SQD	O5-C5-C6-S
36	A	418	SQD	C2-C1-O6-C44
36	A	418	SQD	O5-C5-C6-S
36	B	621	SQD	O5-C1-O6-C44
36	B	621	SQD	O49-C7-O47-C45
36	B	621	SQD	C8-C7-O47-C45
36	B	621	SQD	C5-C6-S-O7
36	B	623	SQD	C8-C7-O47-C45
36	B	623	SQD	C5-C6-S-O7
36	a	412	SQD	O49-C7-O47-C45
36	a	412	SQD	O5-C5-C6-S

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Mol	Chain	Res	Type	Atoms
36	a	418	SQD	C2-C1-O6-C44
36	a	418	SQD	O5-C5-C6-S
36	b	621	SQD	O5-C1-O6-C44
36	b	621	SQD	O49-C7-O47-C45
36	b	621	SQD	C8-C7-O47-C45
36	b	621	SQD	C5-C6-S-O7
36	b	623	SQD	C8-C7-O47-C45
36	b	623	SQD	C5-C6-S-O7
37	A	413	LMG	O6-C1-O1-C7
37	B	2633	LMG	O9-C10-O7-C8
37	C	521	LMG	C2-C1-O1-C7
37	Z	101	LMG	O10-C28-O8-C9
37	Z	101	LMG	C29-C28-O8-C9
37	a	413	LMG	O6-C1-O1-C7
37	b	2633	LMG	O9-C10-O7-C8
37	c	521	LMG	C2-C1-O1-C7
37	z	101	LMG	O10-C28-O8-C9
37	z	101	LMG	C29-C28-O8-C9
39	B	626	DGD	O1A-C1A-O1G-C1G
39	C	519	DGD	O1G-C1G-C2G-O2G
39	b	626	DGD	O1A-C1A-O1G-C1G
39	c	519	DGD	O1G-C1G-C2G-O2G
25	Y	608	CHL	O1D-CGD-O2D-CED
25	y	608	CHL	O1D-CGD-O2D-CED
26	2	612	CLA	O1D-CGD-O2D-CED
26	2	613	CLA	O1D-CGD-O2D-CED
26	A	405	CLA	O1D-CGD-O2D-CED
26	B	606	CLA	O1D-CGD-O2D-CED
26	6	612	CLA	O1D-CGD-O2D-CED
26	6	613	CLA	O1D-CGD-O2D-CED
26	a	405	CLA	O1D-CGD-O2D-CED
26	b	606	CLA	O1D-CGD-O2D-CED
26	R	601	CLA	C2C-C3C-CAC-CBC
26	r	601	CLA	C2C-C3C-CAC-CBC
25	G	606	CHL	O1D-CGD-O2D-CED
25	S	608	CHL	O1D-CGD-O2D-CED
25	g	606	CHL	O1D-CGD-O2D-CED
25	s	608	CHL	O1D-CGD-O2D-CED
26	1	614	CLA	O1D-CGD-O2D-CED
26	4	604	CLA	O1D-CGD-O2D-CED
26	R	601	CLA	O1D-CGD-O2D-CED
26	R	612	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	5	614	CLA	O1D-CGD-O2D-CED
26	8	604	CLA	O1D-CGD-O2D-CED
26	r	601	CLA	O1D-CGD-O2D-CED
26	r	612	CLA	O1D-CGD-O2D-CED
25	2	605	CHL	CBD-CGD-O2D-CED
25	G	601	CHL	CBD-CGD-O2D-CED
25	G	606	CHL	CBD-CGD-O2D-CED
25	G	608	CHL	CBD-CGD-O2D-CED
25	N	601	CHL	CBD-CGD-O2D-CED
25	N	605	CHL	CBD-CGD-O2D-CED
25	N	608	CHL	CBD-CGD-O2D-CED
25	R	607	CHL	CBD-CGD-O2D-CED
25	S	608	CHL	CBD-CGD-O2D-CED
25	Y	608	CHL	CBD-CGD-O2D-CED
25	6	605	CHL	CBD-CGD-O2D-CED
25	g	601	CHL	CBD-CGD-O2D-CED
25	g	606	CHL	CBD-CGD-O2D-CED
25	g	608	CHL	CBD-CGD-O2D-CED
25	n	601	CHL	CBD-CGD-O2D-CED
25	n	605	CHL	CBD-CGD-O2D-CED
25	n	608	CHL	CBD-CGD-O2D-CED
25	r	607	CHL	CBD-CGD-O2D-CED
25	s	608	CHL	CBD-CGD-O2D-CED
25	y	608	CHL	CBD-CGD-O2D-CED
26	1	614	CLA	CBD-CGD-O2D-CED
26	2	612	CLA	CBD-CGD-O2D-CED
26	2	613	CLA	CBD-CGD-O2D-CED
26	3	603	CLA	CBD-CGD-O2D-CED
26	3	614	CLA	CBD-CGD-O2D-CED
26	4	611	CLA	CBD-CGD-O2D-CED
26	4	612	CLA	CBD-CGD-O2D-CED
26	A	405	CLA	CBD-CGD-O2D-CED
26	B	606	CLA	CBD-CGD-O2D-CED
26	B	608	CLA	CBD-CGD-O2D-CED
26	C	502	CLA	CBD-CGD-O2D-CED
26	C	503	CLA	CBD-CGD-O2D-CED
26	C	506	CLA	CBD-CGD-O2D-CED
26	G	612	CLA	CBD-CGD-O2D-CED
26	G	613	CLA	CBD-CGD-O2D-CED
26	N	612	CLA	CBD-CGD-O2D-CED
26	N	614	CLA	CBD-CGD-O2D-CED
26	R	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	S	602	CLA	CBD-CGD-O2D-CED
26	S	603	CLA	CBD-CGD-O2D-CED
26	Y	604	CLA	CBD-CGD-O2D-CED
26	5	614	CLA	CBD-CGD-O2D-CED
26	6	612	CLA	CBD-CGD-O2D-CED
26	6	613	CLA	CBD-CGD-O2D-CED
26	7	603	CLA	CBD-CGD-O2D-CED
26	7	614	CLA	CBD-CGD-O2D-CED
26	8	611	CLA	CBD-CGD-O2D-CED
26	8	612	CLA	CBD-CGD-O2D-CED
26	a	405	CLA	CBD-CGD-O2D-CED
26	b	606	CLA	CBD-CGD-O2D-CED
26	b	608	CLA	CBD-CGD-O2D-CED
26	c	502	CLA	CBD-CGD-O2D-CED
26	c	503	CLA	CBD-CGD-O2D-CED
26	c	506	CLA	CBD-CGD-O2D-CED
26	g	612	CLA	CBD-CGD-O2D-CED
26	g	613	CLA	CBD-CGD-O2D-CED
26	n	612	CLA	CBD-CGD-O2D-CED
26	n	614	CLA	CBD-CGD-O2D-CED
26	r	603	CLA	CBD-CGD-O2D-CED
26	s	602	CLA	CBD-CGD-O2D-CED
26	s	603	CLA	CBD-CGD-O2D-CED
26	y	604	CLA	CBD-CGD-O2D-CED
26	C	510	CLA	O1A-CGA-O2A-C1
26	N	611	CLA	O1A-CGA-O2A-C1
26	R	611	CLA	O1A-CGA-O2A-C1
26	Y	611	CLA	O1A-CGA-O2A-C1
26	c	510	CLA	O1A-CGA-O2A-C1
26	n	611	CLA	O1A-CGA-O2A-C1
26	r	611	CLA	O1A-CGA-O2A-C1
26	y	611	CLA	O1A-CGA-O2A-C1
25	G	608	CHL	O1D-CGD-O2D-CED
25	N	608	CHL	O1D-CGD-O2D-CED
25	g	608	CHL	O1D-CGD-O2D-CED
25	n	608	CHL	O1D-CGD-O2D-CED
26	3	603	CLA	O1D-CGD-O2D-CED
26	4	611	CLA	O1D-CGD-O2D-CED
26	C	503	CLA	O1D-CGD-O2D-CED
26	G	613	CLA	O1D-CGD-O2D-CED
26	N	612	CLA	O1D-CGD-O2D-CED
26	7	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	8	611	CLA	O1D-CGD-O2D-CED
26	c	503	CLA	O1D-CGD-O2D-CED
26	g	613	CLA	O1D-CGD-O2D-CED
26	n	612	CLA	O1D-CGD-O2D-CED
26	C	510	CLA	CBA-CGA-O2A-C1
26	N	611	CLA	CBA-CGA-O2A-C1
26	Y	611	CLA	CBA-CGA-O2A-C1
26	c	510	CLA	CBA-CGA-O2A-C1
26	n	611	CLA	CBA-CGA-O2A-C1
26	y	611	CLA	CBA-CGA-O2A-C1
39	B	626	DGD	C2A-C1A-O1G-C1G
39	b	626	DGD	C2A-C1A-O1G-C1G
26	N	604	CLA	CBD-CGD-O2D-CED
26	n	604	CLA	CBD-CGD-O2D-CED
26	3	603	CLA	O1A-CGA-O2A-C1
26	7	603	CLA	O1A-CGA-O2A-C1
30	S	2630	LHG	O10-C23-O8-C6
30	s	2630	LHG	O10-C23-O8-C6
26	3	613	CLA	O1D-CGD-O2D-CED
26	4	603	CLA	O1D-CGD-O2D-CED
26	7	613	CLA	O1D-CGD-O2D-CED
26	8	603	CLA	O1D-CGD-O2D-CED
26	R	601	CLA	C4C-C3C-CAC-CBC
26	r	601	CLA	C4C-C3C-CAC-CBC
25	2	608	CHL	O1D-CGD-O2D-CED
25	3	608	CHL	O1D-CGD-O2D-CED
25	4	608	CHL	O1D-CGD-O2D-CED
25	6	608	CHL	O1D-CGD-O2D-CED
25	7	608	CHL	O1D-CGD-O2D-CED
25	8	608	CHL	O1D-CGD-O2D-CED
26	2	603	CLA	O1D-CGD-O2D-CED
26	2	604	CLA	O1D-CGD-O2D-CED
26	2	614	CLA	O1D-CGD-O2D-CED
26	B	615	CLA	O1D-CGD-O2D-CED
26	D	403	CLA	O1D-CGD-O2D-CED
26	S	612	CLA	O1D-CGD-O2D-CED
26	6	603	CLA	O1D-CGD-O2D-CED
26	6	604	CLA	O1D-CGD-O2D-CED
26	6	614	CLA	O1D-CGD-O2D-CED
26	b	615	CLA	O1D-CGD-O2D-CED
26	d	403	CLA	O1D-CGD-O2D-CED
26	s	612	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	C	513	CLA	CBD-CGD-O2D-CED
26	c	513	CLA	CBD-CGD-O2D-CED
26	S	611	CLA	O1A-CGA-O2A-C1
26	s	611	CLA	O1A-CGA-O2A-C1
30	C	523	LHG	O9-C7-O7-C5
30	c	523	LHG	O9-C7-O7-C5
36	B	623	SQD	O49-C7-O47-C45
36	b	623	SQD	O49-C7-O47-C45
26	1	603	CLA	O1D-CGD-O2D-CED
26	5	603	CLA	O1D-CGD-O2D-CED
25	2	607	CHL	C3-C5-C6-C7
25	G	607	CHL	C3-C5-C6-C7
25	R	606	CHL	C3-C5-C6-C7
25	6	607	CHL	C3-C5-C6-C7
25	g	607	CHL	C3-C5-C6-C7
25	r	606	CHL	C3-C5-C6-C7
26	3	611	CLA	C3-C5-C6-C7
26	B	615	CLA	C3-C5-C6-C7
26	B	617	CLA	C3-C5-C6-C7
26	C	512	CLA	C3-C5-C6-C7
26	G	613	CLA	C3-C5-C6-C7
26	R	603	CLA	C3-C5-C6-C7
26	R	613	CLA	C3-C5-C6-C7
26	5	613	CLA	C3-C5-C6-C7
26	7	611	CLA	C3-C5-C6-C7
26	b	615	CLA	C3-C5-C6-C7
26	b	617	CLA	C3-C5-C6-C7
26	c	512	CLA	C3-C5-C6-C7
26	g	613	CLA	C3-C5-C6-C7
26	r	603	CLA	C3-C5-C6-C7
26	r	613	CLA	C3-C5-C6-C7
25	1	608	CHL	O1D-CGD-O2D-CED
25	5	608	CHL	O1D-CGD-O2D-CED
26	N	614	CLA	O1D-CGD-O2D-CED
26	n	614	CLA	O1D-CGD-O2D-CED
26	1	603	CLA	CBA-CGA-O2A-C1
26	3	603	CLA	CBA-CGA-O2A-C1
26	N	603	CLA	CBA-CGA-O2A-C1
26	5	603	CLA	CBA-CGA-O2A-C1
26	7	603	CLA	CBA-CGA-O2A-C1
26	n	603	CLA	CBA-CGA-O2A-C1
25	1	606	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	S	606	CHL	CBD-CGD-O2D-CED
25	Y	609	CHL	CBD-CGD-O2D-CED
25	5	606	CHL	CBD-CGD-O2D-CED
25	s	606	CHL	CBD-CGD-O2D-CED
25	y	609	CHL	CBD-CGD-O2D-CED
26	1	602	CLA	CBD-CGD-O2D-CED
26	2	602	CLA	CBD-CGD-O2D-CED
26	2	610	CLA	CBD-CGD-O2D-CED
26	3	612	CLA	CBD-CGD-O2D-CED
26	C	508	CLA	CBD-CGD-O2D-CED
26	C	512	CLA	CBD-CGD-O2D-CED
26	Y	612	CLA	CBD-CGD-O2D-CED
26	Y	614	CLA	CBD-CGD-O2D-CED
26	5	602	CLA	CBD-CGD-O2D-CED
26	6	602	CLA	CBD-CGD-O2D-CED
26	6	610	CLA	CBD-CGD-O2D-CED
26	7	612	CLA	CBD-CGD-O2D-CED
26	c	508	CLA	CBD-CGD-O2D-CED
26	c	512	CLA	CBD-CGD-O2D-CED
26	y	612	CLA	CBD-CGD-O2D-CED
26	y	614	CLA	CBD-CGD-O2D-CED
36	A	412	SQD	C8-C7-O47-C45
36	a	412	SQD	C8-C7-O47-C45
37	B	2633	LMG	C11-C10-O7-C8
37	b	2633	LMG	C11-C10-O7-C8
39	B	626	DGD	C2B-C1B-O2G-C2G
39	b	626	DGD	C2B-C1B-O2G-C2G
25	G	605	CHL	O1D-CGD-O2D-CED
25	G	609	CHL	O1D-CGD-O2D-CED
25	R	608	CHL	O1D-CGD-O2D-CED
25	R	614	CHL	O1D-CGD-O2D-CED
25	g	605	CHL	O1D-CGD-O2D-CED
25	g	609	CHL	O1D-CGD-O2D-CED
25	r	608	CHL	O1D-CGD-O2D-CED
25	r	614	CHL	O1D-CGD-O2D-CED
26	4	602	CLA	O1D-CGD-O2D-CED
26	8	602	CLA	O1D-CGD-O2D-CED
25	R	607	CHL	O1D-CGD-O2D-CED
25	r	607	CHL	O1D-CGD-O2D-CED
25	G	601	CHL	C4-C3-C5-C6
25	Y	601	CHL	C4-C3-C5-C6
25	g	601	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	y	601	CHL	C4-C3-C5-C6
26	B	615	CLA	C4-C3-C5-C6
26	C	504	CLA	C4-C3-C5-C6
26	G	610	CLA	C4-C3-C5-C6
26	S	610	CLA	C4-C3-C5-C6
26	b	615	CLA	C4-C3-C5-C6
26	c	504	CLA	C4-C3-C5-C6
26	g	610	CLA	C4-C3-C5-C6
26	s	610	CLA	C4-C3-C5-C6
25	G	601	CHL	C2-C3-C5-C6
25	g	601	CHL	C2-C3-C5-C6
26	B	604	CLA	C2-C3-C5-C6
26	B	615	CLA	C2-C3-C5-C6
26	C	504	CLA	C2-C3-C5-C6
26	C	506	CLA	C2-C3-C5-C6
26	S	610	CLA	C2-C3-C5-C6
26	b	604	CLA	C2-C3-C5-C6
26	b	615	CLA	C2-C3-C5-C6
26	c	504	CLA	C2-C3-C5-C6
26	c	506	CLA	C2-C3-C5-C6
26	s	610	CLA	C2-C3-C5-C6
26	B	610	CLA	CBD-CGD-O2D-CED
26	b	610	CLA	CBD-CGD-O2D-CED
26	B	608	CLA	O1D-CGD-O2D-CED
26	b	608	CLA	O1D-CGD-O2D-CED
25	N	601	CHL	C2A-CAA-CBA-CGA
25	n	601	CHL	C2A-CAA-CBA-CGA
26	4	604	CLA	C2A-CAA-CBA-CGA
26	C	507	CLA	C2A-CAA-CBA-CGA
26	8	604	CLA	C2A-CAA-CBA-CGA
26	c	507	CLA	C2A-CAA-CBA-CGA
25	N	607	CHL	C3-C5-C6-C7
25	Y	607	CHL	C3-C5-C6-C7
25	n	607	CHL	C3-C5-C6-C7
25	y	607	CHL	C3-C5-C6-C7
26	1	613	CLA	C3-C5-C6-C7
26	2	602	CLA	C3-C5-C6-C7
26	N	613	CLA	C3-C5-C6-C7
26	S	611	CLA	C3-C5-C6-C7
26	S	613	CLA	C3-C5-C6-C7
26	6	602	CLA	C3-C5-C6-C7
26	n	613	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	s	611	CLA	C3-C5-C6-C7
26	s	613	CLA	C3-C5-C6-C7
35	A	408	PHO	C3-C5-C6-C7
35	a	408	PHO	C3-C5-C6-C7
25	G	601	CHL	CBA-CGA-O2A-C1
25	Y	601	CHL	CBA-CGA-O2A-C1
25	g	601	CHL	CBA-CGA-O2A-C1
25	y	601	CHL	CBA-CGA-O2A-C1
26	2	603	CLA	CBA-CGA-O2A-C1
26	G	603	CLA	CBA-CGA-O2A-C1
26	S	611	CLA	CBA-CGA-O2A-C1
26	6	603	CLA	CBA-CGA-O2A-C1
26	g	603	CLA	CBA-CGA-O2A-C1
26	s	611	CLA	CBA-CGA-O2A-C1
39	C	520	DGD	C2A-C1A-O1G-C1G
39	c	520	DGD	C2A-C1A-O1G-C1G
30	4	2630	LHG	C24-C23-O8-C6
30	8	2630	LHG	C24-C23-O8-C6
39	B	626	DGD	C4E-C5E-C6E-O5E
39	b	626	DGD	C4E-C5E-C6E-O5E
31	C	516	BCR	C19-C20-C21-C22
31	c	516	BCR	C19-C20-C21-C22
26	2	603	CLA	O1A-CGA-O2A-C1
26	G	603	CLA	O1A-CGA-O2A-C1
26	N	603	CLA	O1A-CGA-O2A-C1
26	6	603	CLA	O1A-CGA-O2A-C1
26	g	603	CLA	O1A-CGA-O2A-C1
26	n	603	CLA	O1A-CGA-O2A-C1
36	A	418	SQD	O49-C7-O47-C45
36	a	418	SQD	O49-C7-O47-C45
25	G	601	CHL	O1D-CGD-O2D-CED
25	N	605	CHL	O1D-CGD-O2D-CED
25	g	601	CHL	O1D-CGD-O2D-CED
25	n	605	CHL	O1D-CGD-O2D-CED
26	4	612	CLA	O1D-CGD-O2D-CED
26	C	506	CLA	O1D-CGD-O2D-CED
26	8	612	CLA	O1D-CGD-O2D-CED
26	c	506	CLA	O1D-CGD-O2D-CED
25	R	608	CHL	C3-C5-C6-C7
25	r	608	CHL	C3-C5-C6-C7
26	B	608	CLA	C3-C5-C6-C7
26	b	608	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	S	607	CHL	CBD-CGD-O2D-CED
25	s	607	CHL	CBD-CGD-O2D-CED
26	1	604	CLA	CBD-CGD-O2D-CED
26	C	501	CLA	CBD-CGD-O2D-CED
26	G	604	CLA	CBD-CGD-O2D-CED
26	R	602	CLA	CBD-CGD-O2D-CED
26	5	604	CLA	CBD-CGD-O2D-CED
26	c	501	CLA	CBD-CGD-O2D-CED
26	g	604	CLA	CBD-CGD-O2D-CED
26	r	602	CLA	CBD-CGD-O2D-CED
30	B	2630	LHG	O2-C2-C3-O3
30	B	2631	LHG	O2-C2-C3-O3
30	b	2630	LHG	O2-C2-C3-O3
30	b	2631	LHG	O2-C2-C3-O3
25	N	601	CHL	O1D-CGD-O2D-CED
25	n	601	CHL	O1D-CGD-O2D-CED
26	C	502	CLA	O1D-CGD-O2D-CED
26	S	603	CLA	O1D-CGD-O2D-CED
26	c	502	CLA	O1D-CGD-O2D-CED
26	s	603	CLA	O1D-CGD-O2D-CED
25	S	607	CHL	CBA-CGA-O2A-C1
25	s	607	CHL	CBA-CGA-O2A-C1
26	b	617	CLA	CBA-CGA-O2A-C1
30	B	2631	LHG	C24-C23-O8-C6
30	S	2630	LHG	C24-C23-O8-C6
30	b	2631	LHG	C24-C23-O8-C6
30	s	2630	LHG	C24-C23-O8-C6
36	B	623	SQD	C24-C23-O48-C46
36	b	623	SQD	C24-C23-O48-C46
39	h	102	DGD	O6E-C5E-C6E-O5E
25	Y	601	CHL	O1A-CGA-O2A-C1
25	y	601	CHL	O1A-CGA-O2A-C1
26	1	603	CLA	O1A-CGA-O2A-C1
26	B	617	CLA	O1A-CGA-O2A-C1
26	5	603	CLA	O1A-CGA-O2A-C1
26	b	617	CLA	O1A-CGA-O2A-C1
30	3	2630	LHG	O10-C23-O8-C6
30	7	2630	LHG	O10-C23-O8-C6
25	2	605	CHL	O1D-CGD-O2D-CED
25	6	605	CHL	O1D-CGD-O2D-CED
26	R	603	CLA	O1D-CGD-O2D-CED
26	r	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
37	Z	101	LMG	O6-C5-C6-O5
37	z	101	LMG	O6-C5-C6-O5
39	H	102	DGD	O6E-C5E-C6E-O5E
26	B	617	CLA	CBD-CGD-O2D-CED
26	C	510	CLA	CBD-CGD-O2D-CED
26	b	617	CLA	CBD-CGD-O2D-CED
26	c	510	CLA	CBD-CGD-O2D-CED
26	Y	604	CLA	O1D-CGD-O2D-CED
26	y	604	CLA	O1D-CGD-O2D-CED
26	C	513	CLA	C3-C5-C6-C7
26	Y	613	CLA	C3-C5-C6-C7
26	c	513	CLA	C3-C5-C6-C7
26	y	613	CLA	C3-C5-C6-C7
26	3	604	CLA	CBD-CGD-O2D-CED
26	7	604	CLA	CBD-CGD-O2D-CED
26	y	603	CLA	CBD-CGD-O2D-CED
26	S	602	CLA	O1D-CGD-O2D-CED
26	s	602	CLA	O1D-CGD-O2D-CED
26	B	617	CLA	CBA-CGA-O2A-C1
36	B	621	SQD	C24-C23-O48-C46
36	b	621	SQD	C24-C23-O48-C46
26	B	604	CLA	C4-C3-C5-C6
26	B	614	CLA	C4-C3-C5-C6
26	G	611	CLA	C4-C3-C5-C6
26	b	604	CLA	C4-C3-C5-C6
26	b	614	CLA	C4-C3-C5-C6
26	g	611	CLA	C4-C3-C5-C6
26	B	614	CLA	C2-C3-C5-C6
26	G	610	CLA	C2-C3-C5-C6
26	b	614	CLA	C2-C3-C5-C6
26	g	610	CLA	C2-C3-C5-C6
25	G	601	CHL	O1A-CGA-O2A-C1
25	g	601	CHL	O1A-CGA-O2A-C1
37	Z	101	LMG	C4-C5-C6-O5
37	z	101	LMG	C4-C5-C6-O5
26	B	611	CLA	CBD-CGD-O2D-CED
26	Y	603	CLA	CBD-CGD-O2D-CED
26	b	611	CLA	CBD-CGD-O2D-CED
26	1	611	CLA	C2A-CAA-CBA-CGA
26	5	611	CLA	C2A-CAA-CBA-CGA
30	4	2630	LHG	O10-C23-O8-C6
30	8	2630	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
26	3	614	CLA	O1D-CGD-O2D-CED
26	G	612	CLA	O1D-CGD-O2D-CED
26	7	614	CLA	O1D-CGD-O2D-CED
25	S	607	CHL	O1A-CGA-O2A-C1
25	s	607	CHL	O1A-CGA-O2A-C1
30	B	2631	LHG	O10-C23-O8-C6
30	b	2631	LHG	O10-C23-O8-C6
36	A	418	SQD	O5-C1-O6-C44
36	a	418	SQD	O5-C1-O6-C44
37	C	521	LMG	O6-C1-O1-C7
37	c	521	LMG	O6-C1-O1-C7
39	B	626	DGD	O6D-C1D-O3G-C3G
39	b	626	DGD	O6D-C1D-O3G-C3G
26	g	612	CLA	O1D-CGD-O2D-CED
25	R	608	CHL	CBA-CGA-O2A-C1
25	r	608	CHL	CBA-CGA-O2A-C1
25	3	605	CHL	CBD-CGD-O2D-CED
25	R	606	CHL	CBD-CGD-O2D-CED
25	S	601	CHL	CBD-CGD-O2D-CED
25	7	605	CHL	CBD-CGD-O2D-CED
25	r	606	CHL	CBD-CGD-O2D-CED
25	s	601	CHL	CBD-CGD-O2D-CED
26	3	602	CLA	CBD-CGD-O2D-CED
26	B	604	CLA	CBD-CGD-O2D-CED
26	B	612	CLA	CBD-CGD-O2D-CED
26	G	602	CLA	CBD-CGD-O2D-CED
26	7	602	CLA	CBD-CGD-O2D-CED
26	b	604	CLA	CBD-CGD-O2D-CED
26	b	612	CLA	CBD-CGD-O2D-CED
26	g	602	CLA	CBD-CGD-O2D-CED
37	a	415	LMG	O6-C5-C6-O5
39	B	626	DGD	O6E-C5E-C6E-O5E
39	b	626	DGD	O6E-C5E-C6E-O5E
26	C	513	CLA	O1D-CGD-O2D-CED
26	c	513	CLA	O1D-CGD-O2D-CED
25	Y	601	CHL	CBD-CGD-O2D-CED
25	y	601	CHL	CBD-CGD-O2D-CED
26	C	507	CLA	CBD-CGD-O2D-CED
26	c	507	CLA	CBD-CGD-O2D-CED
37	A	415	LMG	O6-C5-C6-O5
25	R	608	CHL	O1A-CGA-O2A-C1
25	r	608	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	B	2631	LHG	C1-C2-C3-O3
30	b	2631	LHG	C1-C2-C3-O3
26	3	613	CLA	CBA-CGA-O2A-C1
26	D	403	CLA	CBA-CGA-O2A-C1
26	R	612	CLA	CBA-CGA-O2A-C1
26	S	604	CLA	CBA-CGA-O2A-C1
26	Y	612	CLA	CBA-CGA-O2A-C1
26	7	613	CLA	CBA-CGA-O2A-C1
26	d	403	CLA	CBA-CGA-O2A-C1
26	r	612	CLA	CBA-CGA-O2A-C1
26	s	604	CLA	CBA-CGA-O2A-C1
26	y	612	CLA	CBA-CGA-O2A-C1
30	3	2630	LHG	C24-C23-O8-C6
30	7	2630	LHG	C24-C23-O8-C6
37	B	622	LMG	C29-C28-O8-C9
37	b	622	LMG	C29-C28-O8-C9
25	3	609	CHL	CBD-CGD-O2D-CED
25	7	609	CHL	CBD-CGD-O2D-CED
26	N	613	CLA	CBD-CGD-O2D-CED
26	n	613	CLA	CBD-CGD-O2D-CED
26	N	604	CLA	O1D-CGD-O2D-CED
26	Y	612	CLA	O1D-CGD-O2D-CED
26	n	604	CLA	O1D-CGD-O2D-CED
26	y	612	CLA	O1D-CGD-O2D-CED
25	Y	601	CHL	C2-C3-C5-C6
25	y	601	CHL	C2-C3-C5-C6
26	G	611	CLA	C2-C3-C5-C6
26	g	611	CLA	C2-C3-C5-C6
25	3	601	CHL	C3-C5-C6-C7
25	7	601	CHL	C3-C5-C6-C7
25	Y	605	CHL	CBD-CGD-O2D-CED
25	1	607	CHL	C11-C10-C8-C9
25	3	601	CHL	C6-C7-C8-C9
25	3	601	CHL	C14-C13-C15-C16
25	G	608	CHL	C14-C13-C15-C16
25	N	601	CHL	C11-C10-C8-C9
25	N	608	CHL	C14-C13-C15-C16
25	Y	608	CHL	C14-C13-C15-C16
25	Y	609	CHL	C14-C13-C15-C16
25	5	607	CHL	C11-C10-C8-C9
25	7	601	CHL	C6-C7-C8-C9
25	7	601	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	g	608	CHL	C14-C13-C15-C16
25	n	601	CHL	C11-C10-C8-C9
25	n	608	CHL	C14-C13-C15-C16
25	y	608	CHL	C14-C13-C15-C16
25	y	609	CHL	C14-C13-C15-C16
26	B	602	CLA	C14-C13-C15-C16
26	B	606	CLA	C6-C7-C8-C9
26	B	611	CLA	C14-C13-C15-C16
26	B	615	CLA	C6-C7-C8-C9
26	B	616	CLA	C11-C10-C8-C9
26	C	502	CLA	C6-C7-C8-C9
26	C	504	CLA	C11-C12-C13-C14
26	C	506	CLA	C11-C12-C13-C14
26	C	507	CLA	C11-C12-C13-C14
26	C	509	CLA	C6-C7-C8-C9
26	C	511	CLA	C11-C10-C8-C9
26	N	612	CLA	C6-C7-C8-C9
26	R	610	CLA	C11-C12-C13-C14
26	Y	611	CLA	C6-C7-C8-C9
26	b	602	CLA	C14-C13-C15-C16
26	b	606	CLA	C6-C7-C8-C9
26	b	611	CLA	C14-C13-C15-C16
26	b	615	CLA	C6-C7-C8-C9
26	b	616	CLA	C11-C10-C8-C9
26	c	502	CLA	C6-C7-C8-C9
26	c	504	CLA	C11-C12-C13-C14
26	c	507	CLA	C11-C12-C13-C14
26	c	509	CLA	C6-C7-C8-C9
26	c	511	CLA	C11-C10-C8-C9
26	n	612	CLA	C6-C7-C8-C9
26	r	610	CLA	C11-C12-C13-C14
26	y	611	CLA	C6-C7-C8-C9
35	A	408	PHO	C14-C13-C15-C16
35	a	408	PHO	C14-C13-C15-C16
25	Y	609	CHL	O1D-CGD-O2D-CED
25	y	609	CHL	O1D-CGD-O2D-CED
26	6	610	CLA	O1D-CGD-O2D-CED
37	A	413	LMG	C2-C1-O1-C7
37	a	413	LMG	C2-C1-O1-C7
39	B	626	DGD	C2D-C1D-O3G-C3G
39	b	626	DGD	C2D-C1D-O3G-C3G
30	B	2630	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
30	b	2630	LHG	C23-C24-C25-C26
30	R	2630	LHG	O2-C2-C3-O3
30	r	2630	LHG	O2-C2-C3-O3
26	2	610	CLA	O1D-CGD-O2D-CED
37	A	415	LMG	C4-C5-C6-O5
37	a	415	LMG	C4-C5-C6-O5
25	3	606	CHL	CBD-CGD-O2D-CED
25	7	606	CHL	CBD-CGD-O2D-CED
25	y	605	CHL	CBD-CGD-O2D-CED
25	S	606	CHL	O1D-CGD-O2D-CED
25	s	606	CHL	O1D-CGD-O2D-CED
26	3	612	CLA	O1D-CGD-O2D-CED
26	Y	614	CLA	O1D-CGD-O2D-CED
26	7	612	CLA	O1D-CGD-O2D-CED
26	y	614	CLA	O1D-CGD-O2D-CED
28	2	1622	XAT	C31-C32-C33-C40
28	G	1622	XAT	C11-C12-C13-C20
28	Y	1622	XAT	C11-C12-C13-C20
28	6	1622	XAT	C31-C32-C33-C40
28	g	1622	XAT	C11-C12-C13-C20
28	y	1622	XAT	C11-C12-C13-C20
29	1	1623	NEX	C11-C12-C13-C20
29	G	1623	NEX	C11-C12-C13-C20
29	5	1623	NEX	C11-C12-C13-C20
29	6	1623	NEX	C31-C32-C33-C40
29	g	1623	NEX	C11-C12-C13-C20
31	B	620	BCR	C37-C22-C23-C24
31	C	516	BCR	C7-C8-C9-C34
31	C	516	BCR	C37-C22-C23-C24
31	D	404	BCR	C7-C8-C9-C34
31	D	404	BCR	C37-C22-C23-C24
31	T	101	BCR	C11-C12-C13-C35
31	T	101	BCR	C37-C22-C23-C24
31	b	620	BCR	C37-C22-C23-C24
31	c	516	BCR	C7-C8-C9-C34
31	c	516	BCR	C37-C22-C23-C24
31	d	404	BCR	C7-C8-C9-C34
31	d	404	BCR	C37-C22-C23-C24
31	t	101	BCR	C11-C12-C13-C35
31	t	101	BCR	C37-C22-C23-C24
31	C	516	BCR	C21-C22-C23-C24
31	T	101	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	c	516	BCR	C21-C22-C23-C24
31	t	101	BCR	C11-C12-C13-C14
37	A	413	LMG	C4-C5-C6-O5
37	a	413	LMG	C4-C5-C6-O5
25	1	606	CHL	C2A-CAA-CBA-CGA
25	5	606	CHL	C2A-CAA-CBA-CGA
26	3	604	CLA	C2A-CAA-CBA-CGA
26	3	611	CLA	C2A-CAA-CBA-CGA
26	B	602	CLA	C2A-CAA-CBA-CGA
26	7	604	CLA	C2A-CAA-CBA-CGA
26	7	611	CLA	C2A-CAA-CBA-CGA
26	b	602	CLA	C2A-CAA-CBA-CGA
26	C	506	CLA	C3-C5-C6-C7
26	c	506	CLA	C3-C5-C6-C7
30	3	2630	LHG	O7-C5-C6-O8
30	B	2631	LHG	O7-C5-C6-O8
30	7	2630	LHG	O7-C5-C6-O8
30	b	2631	LHG	O7-C5-C6-O8
36	B	623	SQD	O6-C44-C45-O47
36	b	623	SQD	O6-C44-C45-O47
26	B	609	CLA	C8-C10-C11-C12
26	N	602	CLA	C10-C11-C12-C13
26	b	609	CLA	C8-C10-C11-C12
26	c	503	CLA	C5-C6-C7-C8
26	n	602	CLA	C10-C11-C12-C13
30	D	408	LHG	C23-C24-C25-C26
30	D	409	LHG	C23-C24-C25-C26
30	G	2630	LHG	C23-C24-C25-C26
30	d	408	LHG	C23-C24-C25-C26
30	d	409	LHG	C23-C24-C25-C26
30	g	2630	LHG	C23-C24-C25-C26
26	C	512	CLA	O1D-CGD-O2D-CED
26	c	512	CLA	O1D-CGD-O2D-CED
38	D	405	PL9	C7-C8-C9-C10
38	d	405	PL9	C7-C8-C9-C10
26	B	615	CLA	C15-C16-C17-C18
26	B	617	CLA	C13-C15-C16-C17
26	C	503	CLA	C5-C6-C7-C8
26	b	615	CLA	C15-C16-C17-C18
26	b	617	CLA	C13-C15-C16-C17
30	2	2630	LHG	O1-C1-C2-O2
30	6	2630	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
26	A	410	CLA	C3-C5-C6-C7
26	a	410	CLA	C3-C5-C6-C7
36	A	418	SQD	C7-C8-C9-C10
36	a	418	SQD	C7-C8-C9-C10
25	1	606	CHL	O1D-CGD-O2D-CED
25	5	606	CHL	O1D-CGD-O2D-CED
26	1	602	CLA	O1D-CGD-O2D-CED
26	5	602	CLA	O1D-CGD-O2D-CED
26	B	616	CLA	CBD-CGD-O2D-CED
26	b	616	CLA	CBD-CGD-O2D-CED
25	G	601	CHL	C6-C7-C8-C10
25	Y	601	CHL	C6-C7-C8-C10
25	g	601	CHL	C6-C7-C8-C10
25	y	601	CHL	C6-C7-C8-C10
26	B	612	CLA	C11-C10-C8-C7
26	B	612	CLA	C12-C13-C15-C16
26	b	612	CLA	C11-C10-C8-C7
26	b	612	CLA	C12-C13-C15-C16
25	N	609	CHL	CBA-CGA-O2A-C1
25	n	609	CHL	CBA-CGA-O2A-C1
26	B	602	CLA	CBA-CGA-O2A-C1
26	b	602	CLA	CBA-CGA-O2A-C1
39	C	519	DGD	C2A-C1A-O1G-C1G
39	c	519	DGD	C2A-C1A-O1G-C1G
26	N	610	CLA	C4-C3-C5-C6
26	n	610	CLA	C4-C3-C5-C6
26	N	612	CLA	C10-C11-C12-C13
26	n	612	CLA	C10-C11-C12-C13
30	N	2630	LHG	C23-C24-C25-C26
30	n	2630	LHG	C23-C24-C25-C26
39	C	520	DGD	C1B-C2B-C3B-C4B
39	c	520	DGD	C1B-C2B-C3B-C4B
39	C	519	DGD	O6E-C5E-C6E-O5E
39	c	519	DGD	O6E-C5E-C6E-O5E
25	3	601	CHL	C5-C6-C7-C8
25	Y	601	CHL	C5-C6-C7-C8
25	7	601	CHL	C5-C6-C7-C8
25	y	601	CHL	C5-C6-C7-C8
26	B	614	CLA	C13-C15-C16-C17
26	b	614	CLA	C13-C15-C16-C17
37	B	2633	LMG	C10-C11-C12-C13
37	b	2633	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	3	613	CLA	O1A-CGA-O2A-C1
26	7	613	CLA	O1A-CGA-O2A-C1
26	r	612	CLA	O1A-CGA-O2A-C1
26	2	602	CLA	O1D-CGD-O2D-CED
26	6	602	CLA	O1D-CGD-O2D-CED
26	G	614	CLA	CBA-CGA-O2A-C1
26	g	614	CLA	CBA-CGA-O2A-C1
25	3	601	CHL	C10-C11-C12-C13
25	N	609	CHL	C15-C16-C17-C18
25	R	606	CHL	C15-C16-C17-C18
25	S	607	CHL	C5-C6-C7-C8
25	Y	608	CHL	C15-C16-C17-C18
25	7	601	CHL	C10-C11-C12-C13
25	n	609	CHL	C15-C16-C17-C18
25	r	606	CHL	C15-C16-C17-C18
25	s	607	CHL	C5-C6-C7-C8
25	y	608	CHL	C15-C16-C17-C18
26	A	410	CLA	C10-C11-C12-C13
26	B	603	CLA	C5-C6-C7-C8
26	B	607	CLA	C13-C15-C16-C17
26	B	608	CLA	C5-C6-C7-C8
26	B	611	CLA	C13-C15-C16-C17
26	B	614	CLA	C8-C10-C11-C12
26	B	616	CLA	C8-C10-C11-C12
26	C	507	CLA	C13-C15-C16-C17
26	C	510	CLA	C15-C16-C17-C18
26	G	602	CLA	C10-C11-C12-C13
26	G	603	CLA	C15-C16-C17-C18
26	Y	602	CLA	C10-C11-C12-C13
26	a	410	CLA	C10-C11-C12-C13
26	b	607	CLA	C13-C15-C16-C17
26	b	608	CLA	C5-C6-C7-C8
26	b	611	CLA	C13-C15-C16-C17
26	b	614	CLA	C8-C10-C11-C12
26	b	616	CLA	C8-C10-C11-C12
26	c	507	CLA	C13-C15-C16-C17
26	c	510	CLA	C15-C16-C17-C18
26	g	603	CLA	C15-C16-C17-C18
26	y	602	CLA	C10-C11-C12-C13
41	F	101	HEM	C3D-CAD-CBD-CGD
41	f	101	HEM	C3D-CAD-CBD-CGD
25	2	605	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	3	605	CHL	C2A-CAA-CBA-CGA
25	N	607	CHL	C2A-CAA-CBA-CGA
25	R	608	CHL	C2A-CAA-CBA-CGA
25	S	607	CHL	C2A-CAA-CBA-CGA
25	Y	607	CHL	C2A-CAA-CBA-CGA
25	6	605	CHL	C2A-CAA-CBA-CGA
25	7	605	CHL	C2A-CAA-CBA-CGA
25	n	607	CHL	C2A-CAA-CBA-CGA
25	r	608	CHL	C2A-CAA-CBA-CGA
25	s	607	CHL	C2A-CAA-CBA-CGA
25	y	607	CHL	C2A-CAA-CBA-CGA
26	2	604	CLA	C2A-CAA-CBA-CGA
26	3	603	CLA	C2A-CAA-CBA-CGA
26	B	607	CLA	C2A-CAA-CBA-CGA
26	B	611	CLA	C2A-CAA-CBA-CGA
26	G	611	CLA	C2A-CAA-CBA-CGA
26	R	604	CLA	C2A-CAA-CBA-CGA
26	R	611	CLA	C2A-CAA-CBA-CGA
26	6	604	CLA	C2A-CAA-CBA-CGA
26	7	603	CLA	C2A-CAA-CBA-CGA
26	b	607	CLA	C2A-CAA-CBA-CGA
26	b	611	CLA	C2A-CAA-CBA-CGA
26	g	611	CLA	C2A-CAA-CBA-CGA
26	r	604	CLA	C2A-CAA-CBA-CGA
26	r	611	CLA	C2A-CAA-CBA-CGA
25	1	609	CHL	C8-C10-C11-C12
25	3	609	CHL	C10-C11-C12-C13
25	5	609	CHL	C8-C10-C11-C12
25	7	609	CHL	C10-C11-C12-C13
26	B	615	CLA	C13-C15-C16-C17
26	D	402	CLA	C15-C16-C17-C18
26	G	603	CLA	C13-C15-C16-C17
26	b	603	CLA	C5-C6-C7-C8
26	b	615	CLA	C13-C15-C16-C17
26	d	402	CLA	C15-C16-C17-C18
26	g	602	CLA	C10-C11-C12-C13
26	g	603	CLA	C13-C15-C16-C17
37	B	2633	LMG	O6-C5-C6-O5
37	b	2633	LMG	O6-C5-C6-O5
39	C	518	DGD	O6E-C5E-C6E-O5E
39	c	518	DGD	O6E-C5E-C6E-O5E
30	1	2630	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
30	5	2630	LHG	C23-C24-C25-C26
37	C	521	LMG	C28-C29-C30-C31
37	c	521	LMG	C28-C29-C30-C31
26	G	604	CLA	O1D-CGD-O2D-CED
26	g	604	CLA	O1D-CGD-O2D-CED
26	D	403	CLA	O1A-CGA-O2A-C1
26	R	612	CLA	O1A-CGA-O2A-C1
26	Y	612	CLA	O1A-CGA-O2A-C1
26	d	403	CLA	O1A-CGA-O2A-C1
26	y	612	CLA	O1A-CGA-O2A-C1
25	N	608	CHL	C3-C5-C6-C7
25	n	608	CHL	C3-C5-C6-C7
30	Y	2630	LHG	C26-C27-C28-C29
37	B	2633	LMG	O6-C1-O1-C7
37	b	2633	LMG	O6-C1-O1-C7
39	C	519	DGD	O6E-C1E-O5D-C6D
39	c	519	DGD	O6E-C1E-O5D-C6D
30	y	2630	LHG	C26-C27-C28-C29
25	3	601	CHL	C8-C10-C11-C12
25	G	608	CHL	C15-C16-C17-C18
25	Y	601	CHL	C8-C10-C11-C12
25	Y	601	CHL	C13-C15-C16-C17
25	7	601	CHL	C8-C10-C11-C12
25	g	608	CHL	C15-C16-C17-C18
25	y	601	CHL	C8-C10-C11-C12
25	y	601	CHL	C13-C15-C16-C17
26	A	406	CLA	C15-C16-C17-C18
26	B	604	CLA	C5-C6-C7-C8
26	B	617	CLA	C5-C6-C7-C8
26	C	504	CLA	C13-C15-C16-C17
26	C	512	CLA	C8-C10-C11-C12
26	G	602	CLA	C8-C10-C11-C12
26	N	603	CLA	C5-C6-C7-C8
26	a	406	CLA	C15-C16-C17-C18
26	b	604	CLA	C5-C6-C7-C8
26	b	617	CLA	C5-C6-C7-C8
26	c	504	CLA	C13-C15-C16-C17
26	c	512	CLA	C8-C10-C11-C12
26	g	602	CLA	C8-C10-C11-C12
26	n	603	CLA	C5-C6-C7-C8
30	C	2630	LHG	O2-C2-C3-O3
30	D	408	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
30	N	2630	LHG	O2-C2-C3-O3
30	c	2630	LHG	O2-C2-C3-O3
30	d	408	LHG	O2-C2-C3-O3
30	n	2630	LHG	O2-C2-C3-O3
26	C	511	CLA	CBA-CGA-O2A-C1
26	c	511	CLA	CBA-CGA-O2A-C1
30	C	522	LHG	C24-C23-O8-C6
30	c	522	LHG	C24-C23-O8-C6
37	A	413	LMG	O6-C5-C6-O5
37	a	413	LMG	O6-C5-C6-O5
26	S	604	CLA	O1A-CGA-O2A-C1
26	s	604	CLA	O1A-CGA-O2A-C1
39	C	520	DGD	O1A-C1A-O1G-C1G
39	c	520	DGD	O1A-C1A-O1G-C1G
30	D	408	LHG	C7-C8-C9-C10
30	d	408	LHG	C7-C8-C9-C10
36	B	621	SQD	C7-C8-C9-C10
36	b	621	SQD	C7-C8-C9-C10
37	Z	101	LMG	C10-C11-C12-C13
37	z	101	LMG	C10-C11-C12-C13
25	R	606	CHL	C8-C10-C11-C12
25	Y	609	CHL	C13-C15-C16-C17
25	r	606	CHL	C8-C10-C11-C12
25	y	609	CHL	C13-C15-C16-C17
26	3	602	CLA	C10-C11-C12-C13
26	B	608	CLA	C13-C15-C16-C17
26	C	503	CLA	C15-C16-C17-C18
26	b	608	CLA	C13-C15-C16-C17
26	c	503	CLA	C15-C16-C17-C18
26	c	508	CLA	O1D-CGD-O2D-CED
39	H	102	DGD	C4E-C5E-C6E-O5E
39	h	102	DGD	C4E-C5E-C6E-O5E
26	B	610	CLA	O1D-CGD-O2D-CED
26	C	508	CLA	O1D-CGD-O2D-CED
26	b	610	CLA	O1D-CGD-O2D-CED
25	2	609	CHL	C8-C10-C11-C12
25	Y	607	CHL	C15-C16-C17-C18
25	Y	609	CHL	C15-C16-C17-C18
25	6	609	CHL	C8-C10-C11-C12
25	y	607	CHL	C15-C16-C17-C18
25	y	609	CHL	C15-C16-C17-C18
26	7	602	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	R	609	CLA	CBD-CGD-O2D-CED
26	r	609	CLA	CBD-CGD-O2D-CED
37	B	622	LMG	O10-C28-O8-C9
37	b	622	LMG	O10-C28-O8-C9
25	3	601	CHL	C13-C15-C16-C17
25	7	601	CHL	C13-C15-C16-C17
26	D	403	CLA	C8-C10-C11-C12
26	Y	610	CLA	C5-C6-C7-C8
26	d	403	CLA	C8-C10-C11-C12
26	y	610	CLA	C5-C6-C7-C8
25	N	601	CHL	CBA-CGA-O2A-C1
25	n	601	CHL	CBA-CGA-O2A-C1
26	C	502	CLA	CBA-CGA-O2A-C1
26	c	502	CLA	CBA-CGA-O2A-C1
26	3	614	CLA	O2A-C1-C2-C3
26	7	614	CLA	O2A-C1-C2-C3
26	1	612	CLA	CBD-CGD-O2D-CED
26	5	612	CLA	CBD-CGD-O2D-CED
25	n	609	CHL	O1A-CGA-O2A-C1
30	D	409	LHG	C7-C8-C9-C10
30	d	409	LHG	C7-C8-C9-C10
39	H	102	DGD	C1A-C2A-C3A-C4A
39	h	102	DGD	C1A-C2A-C3A-C4A
26	B	614	CLA	C3-C5-C6-C7
26	b	614	CLA	C3-C5-C6-C7
31	T	101	BCR	C19-C20-C21-C22
31	t	101	BCR	C19-C20-C21-C22
26	g	610	CLA	C5-C6-C7-C8
25	N	609	CHL	O1A-CGA-O2A-C1
37	Z	101	LMG	C28-C29-C30-C31
37	z	101	LMG	C28-C29-C30-C31
30	B	2630	LHG	O9-C7-O7-C5
30	S	2630	LHG	O9-C7-O7-C5
30	b	2630	LHG	O9-C7-O7-C5
30	s	2630	LHG	O9-C7-O7-C5
30	C	2630	LHG	C1-C2-C3-O3
30	D	408	LHG	C1-C2-C3-O3
30	N	2630	LHG	C1-C2-C3-O3
30	c	2630	LHG	C1-C2-C3-O3
30	d	408	LHG	C1-C2-C3-O3
30	n	2630	LHG	C1-C2-C3-O3
25	G	607	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	R	607	CHL	C2A-CAA-CBA-CGA
25	g	607	CHL	C2A-CAA-CBA-CGA
25	r	607	CHL	C2A-CAA-CBA-CGA
26	B	605	CLA	C2A-CAA-CBA-CGA
26	b	605	CLA	C2A-CAA-CBA-CGA
26	3	614	CLA	CBA-CGA-O2A-C1
26	B	613	CLA	CBA-CGA-O2A-C1
26	N	614	CLA	CBA-CGA-O2A-C1
26	R	603	CLA	CBA-CGA-O2A-C1
26	7	614	CLA	CBA-CGA-O2A-C1
26	b	613	CLA	CBA-CGA-O2A-C1
26	n	614	CLA	CBA-CGA-O2A-C1
26	r	603	CLA	CBA-CGA-O2A-C1
30	1	2630	LHG	C24-C23-O8-C6
30	5	2630	LHG	C24-C23-O8-C6
25	G	607	CHL	C10-C11-C12-C13
25	R	608	CHL	C10-C11-C12-C13
25	g	607	CHL	C10-C11-C12-C13
25	r	608	CHL	C10-C11-C12-C13
26	C	511	CLA	C8-C10-C11-C12
26	G	610	CLA	C5-C6-C7-C8
26	N	602	CLA	C8-C10-C11-C12
26	Y	602	CLA	C8-C10-C11-C12
26	c	511	CLA	C8-C10-C11-C12
26	n	602	CLA	C8-C10-C11-C12
26	y	602	CLA	C8-C10-C11-C12
26	C	501	CLA	O1D-CGD-O2D-CED
26	c	501	CLA	O1D-CGD-O2D-CED
26	B	606	CLA	C15-C16-C17-C18
26	B	608	CLA	C8-C10-C11-C12
26	N	612	CLA	C5-C6-C7-C8
26	R	603	CLA	C10-C11-C12-C13
26	Y	613	CLA	C8-C10-C11-C12
26	b	606	CLA	C15-C16-C17-C18
26	b	608	CLA	C8-C10-C11-C12
26	n	612	CLA	C5-C6-C7-C8
26	r	603	CLA	C10-C11-C12-C13
26	y	613	CLA	C8-C10-C11-C12
26	b	617	CLA	O1D-CGD-O2D-CED
25	2	607	CHL	C5-C6-C7-C8
25	N	601	CHL	C13-C15-C16-C17
25	N	607	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	N	607	CHL	C13-C15-C16-C17
25	6	607	CHL	C5-C6-C7-C8
25	n	601	CHL	C13-C15-C16-C17
25	n	607	CHL	C5-C6-C7-C8
25	n	607	CHL	C13-C15-C16-C17
26	A	406	CLA	C13-C15-C16-C17
26	B	607	CLA	C8-C10-C11-C12
26	B	617	CLA	C15-C16-C17-C18
26	C	508	CLA	C5-C6-C7-C8
26	a	406	CLA	C13-C15-C16-C17
26	b	607	CLA	C8-C10-C11-C12
26	b	617	CLA	C15-C16-C17-C18
26	c	508	CLA	C5-C6-C7-C8
26	b	602	CLA	O1A-CGA-O2A-C1
26	B	617	CLA	O1D-CGD-O2D-CED
25	1	607	CHL	C13-C15-C16-C17
25	S	607	CHL	C8-C10-C11-C12
25	5	607	CHL	C13-C15-C16-C17
25	s	607	CHL	C8-C10-C11-C12
39	C	519	DGD	C4E-C5E-C6E-O5E
26	5	604	CLA	O1D-CGD-O2D-CED
25	S	607	CHL	C3-C5-C6-C7
25	s	607	CHL	C3-C5-C6-C7
36	A	418	SQD	C8-C7-O47-C45
36	a	418	SQD	C8-C7-O47-C45
25	S	607	CHL	O1D-CGD-O2D-CED
25	s	607	CHL	O1D-CGD-O2D-CED
26	1	604	CLA	O1D-CGD-O2D-CED
26	C	510	CLA	O1D-CGD-O2D-CED
26	R	602	CLA	O1D-CGD-O2D-CED
26	c	510	CLA	O1D-CGD-O2D-CED
26	r	602	CLA	O1D-CGD-O2D-CED
26	B	602	CLA	O1A-CGA-O2A-C1
30	C	2630	LHG	O9-C7-O7-C5
30	c	2630	LHG	O9-C7-O7-C5
37	B	2633	LMG	C2-C1-O1-C7
37	b	2633	LMG	C2-C1-O1-C7
39	C	519	DGD	C2E-C1E-O5D-C6D
39	c	519	DGD	C2E-C1E-O5D-C6D
39	c	519	DGD	C4E-C5E-C6E-O5E
25	R	607	CHL	CBA-CGA-O2A-C1
25	r	607	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	B	611	CLA	CBA-CGA-O2A-C1
26	b	611	CLA	CBA-CGA-O2A-C1
37	D	411	LMG	C29-C28-O8-C9
37	d	411	LMG	C29-C28-O8-C9
37	A	413	LMG	C28-C29-C30-C31
37	a	413	LMG	C28-C29-C30-C31
25	N	608	CHL	C15-C16-C17-C18
25	n	608	CHL	C15-C16-C17-C18
27	4	620	LUT	C27-C28-C29-C39
27	8	620	LUT	C27-C28-C29-C39
28	3	1622	XAT	C31-C32-C33-C40
28	7	1622	XAT	C31-C32-C33-C40
29	2	1623	NEX	C31-C32-C33-C40
29	Y	1623	NEX	C11-C12-C13-C20
29	y	1623	NEX	C11-C12-C13-C20
28	3	1622	XAT	C31-C32-C33-C34
28	7	1622	XAT	C31-C32-C33-C34
31	D	404	BCR	C21-C22-C23-C24
31	d	404	BCR	C21-C22-C23-C24
25	N	601	CHL	O1A-CGA-O2A-C1
25	n	601	CHL	O1A-CGA-O2A-C1
25	1	607	CHL	C2A-CAA-CBA-CGA
25	2	607	CHL	C2A-CAA-CBA-CGA
25	3	608	CHL	C2A-CAA-CBA-CGA
25	G	605	CHL	C2A-CAA-CBA-CGA
25	Y	601	CHL	C2A-CAA-CBA-CGA
25	5	607	CHL	C2A-CAA-CBA-CGA
25	6	607	CHL	C2A-CAA-CBA-CGA
25	7	608	CHL	C2A-CAA-CBA-CGA
25	g	605	CHL	C2A-CAA-CBA-CGA
25	y	601	CHL	C2A-CAA-CBA-CGA
26	B	613	CLA	C2A-CAA-CBA-CGA
26	N	610	CLA	C2A-CAA-CBA-CGA
26	b	613	CLA	C2A-CAA-CBA-CGA
26	n	610	CLA	C2A-CAA-CBA-CGA
25	2	607	CHL	C8-C10-C11-C12
25	6	607	CHL	C8-C10-C11-C12
26	B	614	CLA	C10-C11-C12-C13
26	b	614	CLA	C10-C11-C12-C13
30	D	409	LHG	C32-C33-C34-C35
30	2	2630	LHG	O1-C1-C2-C3
30	4	2630	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
30	D	408	LHG	O1-C1-C2-C3
30	D	410	LHG	O1-C1-C2-C3
30	R	2630	LHG	O1-C1-C2-C3
30	Y	2630	LHG	O1-C1-C2-C3
30	6	2630	LHG	O1-C1-C2-C3
30	8	2630	LHG	O1-C1-C2-C3
30	d	408	LHG	O1-C1-C2-C3
30	d	410	LHG	O1-C1-C2-C3
30	r	2630	LHG	O1-C1-C2-C3
30	y	2630	LHG	O1-C1-C2-C3
26	3	604	CLA	O1D-CGD-O2D-CED
26	7	604	CLA	O1D-CGD-O2D-CED
25	2	609	CHL	C11-C12-C13-C15
25	Y	607	CHL	C16-C17-C18-C19
25	6	609	CHL	C11-C12-C13-C15
25	y	607	CHL	C16-C17-C18-C19
26	1	613	CLA	C6-C7-C8-C10
26	B	605	CLA	C16-C17-C18-C20
26	C	502	CLA	C16-C17-C18-C19
26	5	613	CLA	C6-C7-C8-C10
26	b	605	CLA	C16-C17-C18-C20
26	c	502	CLA	C16-C17-C18-C19
30	d	409	LHG	C32-C33-C34-C35
25	R	606	CHL	O1D-CGD-O2D-CED
25	r	606	CHL	O1D-CGD-O2D-CED
26	B	612	CLA	O1D-CGD-O2D-CED
26	b	612	CLA	O1D-CGD-O2D-CED
26	C	502	CLA	O1A-CGA-O2A-C1
26	G	614	CLA	O1A-CGA-O2A-C1
26	c	502	CLA	O1A-CGA-O2A-C1
26	g	614	CLA	O1A-CGA-O2A-C1
26	1	603	CLA	C3-C5-C6-C7
26	5	603	CLA	C3-C5-C6-C7
37	D	411	LMG	O6-C5-C6-O5
37	d	411	LMG	O6-C5-C6-O5
26	N	613	CLA	C8-C10-C11-C12
26	n	613	CLA	C8-C10-C11-C12
37	Z	101	LMG	O6-C1-O1-C7
37	z	101	LMG	O6-C1-O1-C7
26	Y	603	CLA	O1D-CGD-O2D-CED
26	y	603	CLA	O1D-CGD-O2D-CED
25	G	609	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	g	609	CHL	CBA-CGA-O2A-C1
25	G	601	CHL	C13-C15-C16-C17
25	g	601	CHL	C13-C15-C16-C17
26	1	603	CLA	C5-C6-C7-C8
26	C	504	CLA	C10-C11-C12-C13
26	N	611	CLA	C5-C6-C7-C8
26	5	603	CLA	C5-C6-C7-C8
26	b	610	CLA	C15-C16-C17-C18
26	b	612	CLA	C8-C10-C11-C12
26	c	504	CLA	C10-C11-C12-C13
26	n	611	CLA	C5-C6-C7-C8
30	2	2630	LHG	C23-C24-C25-C26
30	6	2630	LHG	C23-C24-C25-C26
26	R	602	CLA	C3-C5-C6-C7
25	R	608	CHL	C2-C1-O2A-CGA
25	r	608	CHL	C2-C1-O2A-CGA
26	C	501	CLA	C16-C17-C18-C19
26	C	502	CLA	C16-C17-C18-C20
26	C	508	CLA	C16-C17-C18-C19
26	c	501	CLA	C16-C17-C18-C19
26	c	502	CLA	C16-C17-C18-C20
26	c	508	CLA	C16-C17-C18-C19
26	3	614	CLA	O1A-CGA-O2A-C1
26	B	613	CLA	O1A-CGA-O2A-C1
26	N	614	CLA	O1A-CGA-O2A-C1
26	7	614	CLA	O1A-CGA-O2A-C1
26	b	613	CLA	O1A-CGA-O2A-C1
26	n	614	CLA	O1A-CGA-O2A-C1
36	B	623	SQD	O10-C23-O48-C46
36	b	623	SQD	O10-C23-O48-C46
26	B	610	CLA	C15-C16-C17-C18
26	B	612	CLA	C8-C10-C11-C12
26	N	611	CLA	C8-C10-C11-C12
26	n	611	CLA	C8-C10-C11-C12
26	b	611	CLA	O1D-CGD-O2D-CED
30	b	2630	LHG	C25-C26-C27-C28
37	C	521	LMG	C11-C12-C13-C14
37	c	521	LMG	C11-C12-C13-C14
25	1	607	CHL	CBD-CGD-O2D-CED
25	5	607	CHL	CBD-CGD-O2D-CED
30	1	2630	LHG	C12-C13-C14-C15
30	B	2630	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
30	B	2630	LHG	C25-C26-C27-C28
30	D	408	LHG	C26-C27-C28-C29
30	b	2630	LHG	C11-C10-C9-C8
30	d	408	LHG	C26-C27-C28-C29
30	n	2630	LHG	C25-C26-C27-C28
37	D	411	LMG	C19-C20-C21-C22
37	d	411	LMG	C19-C20-C21-C22
26	B	611	CLA	O1D-CGD-O2D-CED
26	B	613	CLA	C10-C11-C12-C13
26	b	613	CLA	C10-C11-C12-C13
26	b	615	CLA	C5-C6-C7-C8
30	N	2630	LHG	C25-C26-C27-C28
30	5	2630	LHG	C12-C13-C14-C15
37	C	521	LMG	C12-C13-C14-C15
37	c	521	LMG	C12-C13-C14-C15
39	B	626	DGD	CCB-CDB-CEB-CFB
39	b	626	DGD	CCB-CDB-CEB-CFB
25	2	609	CHL	CBA-CGA-O2A-C1
25	6	609	CHL	CBA-CGA-O2A-C1
39	B	626	DGD	O6D-C5D-C6D-O5D
39	b	626	DGD	O6D-C5D-C6D-O5D
30	C	2630	LHG	C31-C32-C33-C34
30	D	410	LHG	C15-C16-C17-C18
30	c	2630	LHG	C31-C32-C33-C34
30	d	410	LHG	C15-C16-C17-C18
37	c	521	LMG	C32-C33-C34-C35
39	c	519	DGD	C4A-C5A-C6A-C7A
30	D	410	LHG	O1-C1-C2-O2
30	R	2630	LHG	O1-C1-C2-O2
30	Y	2630	LHG	O1-C1-C2-O2
30	d	410	LHG	O1-C1-C2-O2
30	r	2630	LHG	O1-C1-C2-O2
30	y	2630	LHG	O1-C1-C2-O2
26	r	602	CLA	C3-C5-C6-C7
30	B	2631	LHG	C27-C28-C29-C30
30	L	101	LHG	C32-C33-C34-C35
30	b	2631	LHG	C27-C28-C29-C30
30	g	2630	LHG	C25-C26-C27-C28
30	l	101	LHG	C32-C33-C34-C35
36	A	412	SQD	C13-C14-C15-C16
36	a	412	SQD	C13-C14-C15-C16
37	C	521	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
39	C	519	DGD	C4A-C5A-C6A-C7A
26	B	615	CLA	C5-C6-C7-C8
26	N	603	CLA	C10-C11-C12-C13
26	n	603	CLA	C10-C11-C12-C13
26	1	614	CLA	C4B-C3B-CAB-CBB
26	3	603	CLA	C4B-C3B-CAB-CBB
26	A	410	CLA	C4B-C3B-CAB-CBB
26	R	610	CLA	C4B-C3B-CAB-CBB
26	R	616	CLA	C4B-C3B-CAB-CBB
26	S	610	CLA	C4B-C3B-CAB-CBB
26	Y	614	CLA	C4B-C3B-CAB-CBB
26	5	614	CLA	C4B-C3B-CAB-CBB
26	6	610	CLA	C4B-C3B-CAB-CBB
26	7	603	CLA	C4B-C3B-CAB-CBB
26	a	410	CLA	C4B-C3B-CAB-CBB
26	r	610	CLA	C4B-C3B-CAB-CBB
26	r	616	CLA	C4B-C3B-CAB-CBB
26	s	610	CLA	C4B-C3B-CAB-CBB
26	y	614	CLA	C4B-C3B-CAB-CBB
30	2	2630	LHG	C7-C8-C9-C10
30	6	2630	LHG	C7-C8-C9-C10
30	G	2630	LHG	C25-C26-C27-C28
37	D	411	LMG	C17-C18-C19-C20
37	d	411	LMG	C17-C18-C19-C20
25	2	609	CHL	C11-C12-C13-C14
25	6	609	CHL	C11-C12-C13-C14
26	C	505	CLA	C16-C17-C18-C20
26	R	613	CLA	C11-C12-C13-C15
26	c	505	CLA	C16-C17-C18-C20
26	r	613	CLA	C11-C12-C13-C15
25	S	601	CHL	O1D-CGD-O2D-CED
25	s	601	CHL	O1D-CGD-O2D-CED
26	C	501	CLA	C2A-CAA-CBA-CGA
26	G	610	CLA	C2A-CAA-CBA-CGA
26	S	602	CLA	C2A-CAA-CBA-CGA
26	c	501	CLA	C2A-CAA-CBA-CGA
26	g	610	CLA	C2A-CAA-CBA-CGA
26	s	602	CLA	C2A-CAA-CBA-CGA
25	G	601	CHL	C10-C11-C12-C13
25	Y	608	CHL	C8-C10-C11-C12
25	g	601	CHL	C10-C11-C12-C13
25	y	608	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	B	604	CLA	C15-C16-C17-C18
26	C	506	CLA	C13-C15-C16-C17
26	Y	612	CLA	C10-C11-C12-C13
26	b	604	CLA	C15-C16-C17-C18
26	c	506	CLA	C13-C15-C16-C17
26	y	612	CLA	C10-C11-C12-C13
30	S	2630	LHG	C8-C7-O7-C5
30	s	2630	LHG	C8-C7-O7-C5
37	C	521	LMG	C11-C10-O7-C8
37	c	521	LMG	C11-C10-O7-C8
37	C	521	LMG	C35-C36-C37-C38
26	Y	612	CLA	C6-C7-C8-C10
26	y	612	CLA	C6-C7-C8-C10
37	c	521	LMG	C35-C36-C37-C38
30	d	410	LHG	O2-C2-C3-O3
36	A	418	SQD	C23-C24-C25-C26
36	a	418	SQD	C23-C24-C25-C26
26	G	613	CLA	C8-C10-C11-C12
26	R	602	CLA	C8-C10-C11-C12
26	g	613	CLA	C8-C10-C11-C12
26	r	602	CLA	C8-C10-C11-C12
30	3	2630	LHG	C31-C32-C33-C34
30	C	523	LHG	C15-C16-C17-C18
30	c	523	LHG	C15-C16-C17-C18
30	d	410	LHG	C13-C14-C15-C16
37	B	2633	LMG	C30-C31-C32-C33
37	a	413	LMG	C30-C31-C32-C33
37	b	2633	LMG	C30-C31-C32-C33
26	C	511	CLA	O1A-CGA-O2A-C1
26	c	511	CLA	O1A-CGA-O2A-C1
25	1	605	CHL	C3A-C2A-CAA-CBA
25	1	607	CHL	C3A-C2A-CAA-CBA
25	2	601	CHL	C3A-C2A-CAA-CBA
25	2	605	CHL	C3A-C2A-CAA-CBA
25	3	605	CHL	C3A-C2A-CAA-CBA
25	3	606	CHL	C3A-C2A-CAA-CBA
25	4	606	CHL	C3A-C2A-CAA-CBA
25	R	606	CHL	C3A-C2A-CAA-CBA
25	S	608	CHL	C3A-C2A-CAA-CBA
25	Y	605	CHL	C3A-C2A-CAA-CBA
25	Y	608	CHL	C3A-C2A-CAA-CBA
25	5	605	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	5	607	CHL	C3A-C2A-CAA-CBA
25	6	601	CHL	C3A-C2A-CAA-CBA
25	6	605	CHL	C3A-C2A-CAA-CBA
25	7	605	CHL	C3A-C2A-CAA-CBA
25	7	606	CHL	C3A-C2A-CAA-CBA
25	8	606	CHL	C3A-C2A-CAA-CBA
25	r	606	CHL	C3A-C2A-CAA-CBA
25	s	608	CHL	C3A-C2A-CAA-CBA
25	y	605	CHL	C3A-C2A-CAA-CBA
25	y	608	CHL	C3A-C2A-CAA-CBA
26	1	611	CLA	C3A-C2A-CAA-CBA
26	3	611	CLA	C3A-C2A-CAA-CBA
26	G	610	CLA	C3A-C2A-CAA-CBA
26	R	604	CLA	C3A-C2A-CAA-CBA
26	S	609	CLA	C3A-C2A-CAA-CBA
26	5	611	CLA	C3A-C2A-CAA-CBA
26	7	611	CLA	C3A-C2A-CAA-CBA
26	g	610	CLA	C3A-C2A-CAA-CBA
26	r	604	CLA	C3A-C2A-CAA-CBA
26	s	609	CLA	C3A-C2A-CAA-CBA
26	3	602	CLA	O1D-CGD-O2D-CED
26	7	602	CLA	O1D-CGD-O2D-CED
30	D	410	LHG	C13-C14-C15-C16
30	7	2630	LHG	C31-C32-C33-C34
36	a	412	SQD	C12-C13-C14-C15
37	A	413	LMG	C30-C31-C32-C33
39	H	102	DGD	C6A-C7A-C8A-C9A
30	C	522	LHG	C27-C28-C29-C30
30	c	522	LHG	C27-C28-C29-C30
36	A	412	SQD	C12-C13-C14-C15
37	A	415	LMG	C30-C31-C32-C33
37	a	415	LMG	C30-C31-C32-C33
39	h	102	DGD	C6A-C7A-C8A-C9A
25	N	607	CHL	C8-C10-C11-C12
25	N	608	CHL	C13-C15-C16-C17
25	n	607	CHL	C8-C10-C11-C12
25	n	608	CHL	C13-C15-C16-C17
26	2	602	CLA	C10-C11-C12-C13
26	6	602	CLA	C10-C11-C12-C13
30	L	101	LHG	C10-C11-C12-C13
30	l	101	LHG	C10-C11-C12-C13
25	N	607	CHL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	N	608	CHL	C16-C17-C18-C20
25	N	609	CHL	C16-C17-C18-C20
25	Y	607	CHL	C16-C17-C18-C20
25	n	607	CHL	C16-C17-C18-C19
25	n	608	CHL	C16-C17-C18-C20
25	n	609	CHL	C16-C17-C18-C20
25	y	607	CHL	C16-C17-C18-C20
26	R	613	CLA	C11-C12-C13-C14
26	r	613	CLA	C11-C12-C13-C14
26	R	603	CLA	O1A-CGA-O2A-C1
26	r	603	CLA	O1A-CGA-O2A-C1
30	3	2630	LHG	C28-C29-C30-C31
30	C	522	LHG	C24-C25-C26-C27
30	D	409	LHG	C34-C35-C36-C37
30	7	2630	LHG	C28-C29-C30-C31
30	c	522	LHG	C24-C25-C26-C27
30	d	408	LHG	C29-C30-C31-C32
36	A	412	SQD	C18-C19-C20-C21
39	B	626	DGD	C5A-C6A-C7A-C8A
39	B	626	DGD	C5B-C6B-C7B-C8B
39	b	626	DGD	C5B-C6B-C7B-C8B
30	D	408	LHG	C25-C26-C27-C28
30	D	408	LHG	C28-C29-C30-C31
30	D	408	LHG	C29-C30-C31-C32
30	L	101	LHG	C11-C12-C13-C14
30	d	408	LHG	C25-C26-C27-C28
30	d	408	LHG	C28-C29-C30-C31
30	d	409	LHG	C34-C35-C36-C37
30	l	101	LHG	C11-C12-C13-C14
36	a	412	SQD	C18-C19-C20-C21
37	a	415	LMG	C37-C38-C39-C40
39	B	626	DGD	C2A-C3A-C4A-C5A
39	C	519	DGD	C4B-C5B-C6B-C7B
39	b	626	DGD	C2A-C3A-C4A-C5A
39	b	626	DGD	C5A-C6A-C7A-C8A
36	A	412	SQD	C24-C23-O48-C46
36	a	412	SQD	C24-C23-O48-C46
30	C	2630	LHG	C32-C33-C34-C35
30	7	2630	LHG	C27-C28-C29-C30
30	c	2630	LHG	C32-C33-C34-C35
37	A	415	LMG	C37-C38-C39-C40
37	b	622	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
39	C	518	DGD	C4B-C5B-C6B-C7B
39	c	518	DGD	C4B-C5B-C6B-C7B
39	c	519	DGD	C4B-C5B-C6B-C7B
30	1	2630	LHG	C7-C8-C9-C10
30	C	2630	LHG	C23-C24-C25-C26
30	Y	2630	LHG	C23-C24-C25-C26
30	5	2630	LHG	C7-C8-C9-C10
30	c	2630	LHG	C23-C24-C25-C26
30	y	2630	LHG	C23-C24-C25-C26
30	3	2630	LHG	C27-C28-C29-C30
30	S	2630	LHG	C32-C33-C34-C35
30	s	2630	LHG	C32-C33-C34-C35
36	a	418	SQD	C25-C26-C27-C28
37	B	622	LMG	C37-C38-C39-C40
37	D	411	LMG	C20-C21-C22-C23
37	d	411	LMG	C20-C21-C22-C23
39	C	520	DGD	C8B-C9B-CAB-CBB
39	H	102	DGD	C9A-CAA-CBA-CCA
39	c	520	DGD	C8B-C9B-CAB-CBB
26	B	611	CLA	O1A-CGA-O2A-C1
26	b	611	CLA	O1A-CGA-O2A-C1
36	A	418	SQD	C11-C10-C9-C8
36	A	418	SQD	C25-C26-C27-C28
36	B	621	SQD	C10-C11-C12-C13
36	b	621	SQD	C10-C11-C12-C13
37	B	2633	LMG	C16-C17-C18-C19
37	b	2633	LMG	C16-C17-C18-C19
25	3	605	CHL	O1D-CGD-O2D-CED
25	7	605	CHL	O1D-CGD-O2D-CED
36	B	621	SQD	C18-C19-C20-C21
36	a	418	SQD	C11-C10-C9-C8
39	C	520	DGD	CCA-CDA-CEA-CFA
39	c	520	DGD	CCA-CDA-CEA-CFA
39	h	102	DGD	C9A-CAA-CBA-CCA
25	Y	601	CHL	O1D-CGD-O2D-CED
25	y	601	CHL	O1D-CGD-O2D-CED
26	B	604	CLA	O1D-CGD-O2D-CED
26	b	604	CLA	O1D-CGD-O2D-CED
26	g	602	CLA	O1D-CGD-O2D-CED
30	G	2630	LHG	C27-C28-C29-C30
30	g	2630	LHG	C27-C28-C29-C30
36	b	621	SQD	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
39	C	519	DGD	C3A-C4A-C5A-C6A
39	c	519	DGD	C3A-C4A-C5A-C6A
25	R	606	CHL	C16-C17-C18-C19
25	r	606	CHL	C16-C17-C18-C19
30	L	101	LHG	C7-C8-C9-C10
30	l	101	LHG	C7-C8-C9-C10
36	B	623	SQD	C23-C24-C25-C26
36	b	623	SQD	C23-C24-C25-C26
25	R	607	CHL	O1A-CGA-O2A-C1
30	C	522	LHG	O10-C23-O8-C6
30	c	522	LHG	O10-C23-O8-C6
36	B	621	SQD	O10-C23-O48-C46
36	b	621	SQD	O10-C23-O48-C46
26	3	612	CLA	C2B-C3B-CAB-CBB
26	B	602	CLA	C2B-C3B-CAB-CBB
26	B	616	CLA	C2B-C3B-CAB-CBB
26	G	611	CLA	C2B-C3B-CAB-CBB
26	N	611	CLA	C2B-C3B-CAB-CBB
26	R	616	CLA	C2B-C3B-CAB-CBB
26	7	612	CLA	C2B-C3B-CAB-CBB
26	b	602	CLA	C2B-C3B-CAB-CBB
26	b	616	CLA	C2B-C3B-CAB-CBB
26	g	611	CLA	C2B-C3B-CAB-CBB
26	n	611	CLA	C2B-C3B-CAB-CBB
26	r	616	CLA	C2B-C3B-CAB-CBB
27	3	1620	LUT	C1-C6-C7-C8
27	R	620	LUT	C1-C6-C7-C8
27	R	620	LUT	C5-C6-C7-C8
27	Y	1620	LUT	C1-C6-C7-C8
27	7	1620	LUT	C1-C6-C7-C8
27	r	620	LUT	C1-C6-C7-C8
27	r	620	LUT	C5-C6-C7-C8
27	y	1620	LUT	C1-C6-C7-C8
31	A	411	BCR	C23-C24-C25-C26
31	A	411	BCR	C23-C24-C25-C30
31	B	618	BCR	C1-C6-C7-C8
31	a	411	BCR	C23-C24-C25-C26
31	a	411	BCR	C23-C24-C25-C30
31	b	618	BCR	C1-C6-C7-C8
30	2	2630	LHG	C12-C13-C14-C15
30	N	2630	LHG	C24-C25-C26-C27
30	6	2630	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
30	n	2630	LHG	C24-C25-C26-C27
26	G	602	CLA	O1D-CGD-O2D-CED
37	C	521	LMG	C4-C5-C6-O5
37	c	521	LMG	C4-C5-C6-O5
26	C	513	CLA	CBA-CGA-O2A-C1
26	R	613	CLA	CBA-CGA-O2A-C1
26	Y	603	CLA	CBA-CGA-O2A-C1
26	c	513	CLA	CBA-CGA-O2A-C1
26	r	613	CLA	CBA-CGA-O2A-C1
26	y	603	CLA	CBA-CGA-O2A-C1
30	R	2630	LHG	C24-C23-O8-C6
30	r	2630	LHG	C24-C23-O8-C6
25	N	607	CHL	C15-C16-C17-C18
25	n	607	CHL	C15-C16-C17-C18
26	C	510	CLA	C3-C5-C6-C7
26	c	510	CLA	C3-C5-C6-C7
30	C	523	LHG	C24-C25-C26-C27
30	Y	2630	LHG	C12-C13-C14-C15
30	c	523	LHG	C24-C25-C26-C27
30	y	2630	LHG	C12-C13-C14-C15
39	c	518	DGD	C4A-C5A-C6A-C7A
30	D	408	LHG	C27-C28-C29-C30
30	D	410	LHG	C14-C15-C16-C17
30	D	410	LHG	C27-C28-C29-C30
30	b	2630	LHG	C27-C28-C29-C30
30	d	408	LHG	C27-C28-C29-C30
30	d	410	LHG	C14-C15-C16-C17
30	d	410	LHG	C27-C28-C29-C30
30	l	101	LHG	C29-C30-C31-C32
30	n	2630	LHG	C11-C10-C9-C8
36	B	621	SQD	C24-C25-C26-C27
36	b	621	SQD	C24-C25-C26-C27
39	C	518	DGD	C4A-C5A-C6A-C7A
25	3	601	CHL	C2A-CAA-CBA-CGA
25	3	607	CHL	C2A-CAA-CBA-CGA
25	7	601	CHL	C2A-CAA-CBA-CGA
25	7	607	CHL	C2A-CAA-CBA-CGA
26	S	611	CLA	C2A-CAA-CBA-CGA
26	s	611	CLA	C2A-CAA-CBA-CGA
25	1	607	CHL	C5-C6-C7-C8
25	5	607	CHL	C5-C6-C7-C8
30	B	2630	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
30	B	2630	LHG	C27-C28-C29-C30
30	L	101	LHG	C29-C30-C31-C32
30	N	2630	LHG	C11-C10-C9-C8
30	b	2630	LHG	C26-C27-C28-C29
36	A	418	SQD	C15-C16-C17-C18
36	a	418	SQD	C15-C16-C17-C18
25	G	609	CHL	O1A-CGA-O2A-C1
25	g	609	CHL	O1A-CGA-O2A-C1
25	r	607	CHL	O1A-CGA-O2A-C1
30	S	2630	LHG	C24-C25-C26-C27
30	s	2630	LHG	C24-C25-C26-C27
36	A	412	SQD	C9-C10-C11-C12
36	a	412	SQD	C9-C10-C11-C12
26	S	602	CLA	C12-C13-C15-C16
26	s	602	CLA	C12-C13-C15-C16
35	A	408	PHO	C4-C3-C5-C6
35	a	408	PHO	C4-C3-C5-C6
37	A	413	LMG	C37-C38-C39-C40
37	a	413	LMG	C37-C38-C39-C40
26	N	610	CLA	C2-C3-C5-C6
26	n	610	CLA	C2-C3-C5-C6
30	S	2630	LHG	C29-C30-C31-C32
30	s	2630	LHG	C29-C30-C31-C32
39	C	520	DGD	C7A-C8A-C9A-CAA
39	c	520	DGD	C7A-C8A-C9A-CAA
30	B	2630	LHG	C12-C13-C14-C15
30	b	2630	LHG	C12-C13-C14-C15
37	D	411	LMG	C33-C34-C35-C36
37	d	411	LMG	C33-C34-C35-C36
25	G	607	CHL	C15-C16-C17-C18
25	g	607	CHL	C15-C16-C17-C18
30	C	2630	LHG	C14-C15-C16-C17
30	c	2630	LHG	C14-C15-C16-C17
36	B	621	SQD	C28-C29-C30-C31
36	b	621	SQD	C28-C29-C30-C31
30	2	2630	LHG	C24-C25-C26-C27
30	D	409	LHG	C26-C27-C28-C29
30	6	2630	LHG	C24-C25-C26-C27
30	d	409	LHG	C26-C27-C28-C29
37	Z	101	LMG	C18-C19-C20-C21
37	z	101	LMG	C18-C19-C20-C21
26	C	505	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	c	505	CLA	C5-C6-C7-C8
25	2	609	CHL	O1A-CGA-O2A-C1
30	L	101	LHG	C34-C35-C36-C37
30	l	101	LHG	C34-C35-C36-C37
30	3	2630	LHG	C15-C16-C17-C18
30	7	2630	LHG	C15-C16-C17-C18
37	B	2633	LMG	C15-C16-C17-C18
37	b	2633	LMG	C15-C16-C17-C18
39	C	519	DGD	C5B-C6B-C7B-C8B
30	D	410	LHG	O2-C2-C3-O3
30	Y	2630	LHG	C32-C33-C34-C35
30	y	2630	LHG	C32-C33-C34-C35
36	A	418	SQD	C10-C11-C12-C13
36	B	623	SQD	C9-C10-C11-C12
36	a	418	SQD	C10-C11-C12-C13
36	b	623	SQD	C9-C10-C11-C12
39	c	519	DGD	C5B-C6B-C7B-C8B
25	1	607	CHL	C8-C10-C11-C12
25	5	607	CHL	C8-C10-C11-C12
26	B	606	CLA	C5-C6-C7-C8
26	b	606	CLA	C5-C6-C7-C8
26	1	613	CLA	C6-C7-C8-C9
26	B	605	CLA	C16-C17-C18-C19
26	R	603	CLA	C11-C12-C13-C14
26	5	613	CLA	C6-C7-C8-C9
26	b	605	CLA	C16-C17-C18-C19
26	c	508	CLA	C16-C17-C18-C20
26	r	603	CLA	C11-C12-C13-C14
30	2	2630	LHG	C8-C7-O7-C5
30	B	2630	LHG	C8-C7-O7-C5
30	C	2630	LHG	C8-C7-O7-C5
30	6	2630	LHG	C8-C7-O7-C5
30	b	2630	LHG	C8-C7-O7-C5
30	c	2630	LHG	C8-C7-O7-C5
25	6	609	CHL	O1A-CGA-O2A-C1
39	C	520	DGD	C1A-C2A-C3A-C4A
39	c	520	DGD	C1A-C2A-C3A-C4A
30	B	2630	LHG	C32-C33-C34-C35
30	b	2630	LHG	C32-C33-C34-C35
39	C	519	DGD	C3B-C4B-C5B-C6B
39	c	519	DGD	C3B-C4B-C5B-C6B
25	Y	607	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	y	607	CHL	C13-C15-C16-C17
30	G	2630	LHG	C24-C25-C26-C27
30	g	2630	LHG	C24-C25-C26-C27
37	B	622	LMG	C19-C20-C21-C22
37	b	622	LMG	C19-C20-C21-C22
39	H	102	DGD	C3B-C4B-C5B-C6B
39	h	102	DGD	C3B-C4B-C5B-C6B
30	R	2630	LHG	C12-C13-C14-C15
30	r	2630	LHG	C12-C13-C14-C15
26	3	610	CLA	C10-C11-C12-C13
26	7	610	CLA	C10-C11-C12-C13
28	R	622	XAT	C27-C28-C29-C39
28	r	622	XAT	C27-C28-C29-C39
30	C	2630	LHG	C24-C25-C26-C27
30	c	2630	LHG	C24-C25-C26-C27
37	B	622	LMG	C29-C30-C31-C32
25	1	609	CHL	C3-C5-C6-C7
25	5	609	CHL	C3-C5-C6-C7
26	A	405	CLA	C3-C5-C6-C7
26	a	405	CLA	C3-C5-C6-C7
31	B	620	BCR	C21-C22-C23-C24
31	b	620	BCR	C21-C22-C23-C24
25	Y	609	CHL	CBA-CGA-O2A-C1
25	y	609	CHL	CBA-CGA-O2A-C1
36	A	412	SQD	C29-C30-C31-C32
36	a	412	SQD	C29-C30-C31-C32
37	C	521	LMG	C31-C32-C33-C34
37	b	622	LMG	C29-C30-C31-C32
37	c	521	LMG	C31-C32-C33-C34
26	G	612	CLA	C8-C10-C11-C12
25	3	606	CHL	C2A-CAA-CBA-CGA
25	7	606	CHL	C2A-CAA-CBA-CGA
25	1	609	CHL	C2C-C3C-CAC-CBC
25	N	608	CHL	C16-C17-C18-C19
25	R	607	CHL	C6-C7-C8-C9
25	n	608	CHL	C16-C17-C18-C19
25	r	607	CHL	C6-C7-C8-C9
26	B	604	CLA	C16-C17-C18-C20
26	B	610	CLA	C16-C17-C18-C19
26	C	508	CLA	C16-C17-C18-C20
26	b	604	CLA	C16-C17-C18-C20
26	b	610	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
37	B	622	LMG	C21-C22-C23-C24
37	b	622	LMG	C21-C22-C23-C24
25	3	601	CHL	C4-C3-C5-C6
25	7	601	CHL	C4-C3-C5-C6
26	C	510	CLA	C4-C3-C5-C6
26	6	602	CLA	C4-C3-C5-C6
26	c	510	CLA	C4-C3-C5-C6
26	C	510	CLA	C2-C3-C5-C6
26	c	510	CLA	C2-C3-C5-C6
38	D	405	PL9	C13-C14-C16-C17
38	d	405	PL9	C13-C14-C16-C17
30	R	2630	LHG	C23-C24-C25-C26
30	r	2630	LHG	C23-C24-C25-C26
25	5	609	CHL	C2C-C3C-CAC-CBC
37	B	622	LMG	C13-C14-C15-C16
37	B	2633	LMG	C32-C33-C34-C35
37	b	622	LMG	C13-C14-C15-C16
37	b	2633	LMG	C32-C33-C34-C35
26	g	612	CLA	C8-C10-C11-C12
38	A	414	PL9	C7-C8-C9-C10
38	a	414	PL9	C7-C8-C9-C10
30	S	2630	LHG	C34-C35-C36-C37
30	s	2630	LHG	C34-C35-C36-C37
37	C	521	LMG	C17-C18-C19-C20
37	D	411	LMG	C14-C15-C16-C17
37	c	521	LMG	C17-C18-C19-C20
37	d	411	LMG	C14-C15-C16-C17
25	Y	601	CHL	C10-C11-C12-C13
25	y	601	CHL	C10-C11-C12-C13
26	3	602	CLA	C8-C10-C11-C12
26	B	605	CLA	C8-C10-C11-C12
26	b	605	CLA	C8-C10-C11-C12
30	3	2630	LHG	C30-C31-C32-C33
30	Y	2630	LHG	C28-C29-C30-C31
30	7	2630	LHG	C30-C31-C32-C33
30	C	522	LHG	O9-C7-O7-C5
30	c	522	LHG	O9-C7-O7-C5
30	y	2630	LHG	C28-C29-C30-C31
37	B	622	LMG	C11-C10-O7-C8
37	b	622	LMG	C11-C10-O7-C8
25	N	601	CHL	C15-C16-C17-C18
25	n	601	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	C	506	CLA	C15-C16-C17-C18
26	7	602	CLA	C8-C10-C11-C12
26	c	506	CLA	C15-C16-C17-C18
26	B	610	CLA	C16-C17-C18-C20
26	b	610	CLA	C16-C17-C18-C20
30	C	2630	LHG	C12-C13-C14-C15
30	G	2630	LHG	C18-C19-C20-C21
30	c	2630	LHG	C12-C13-C14-C15
30	g	2630	LHG	C18-C19-C20-C21
30	Y	2630	LHG	C16-C17-C18-C19
30	y	2630	LHG	C16-C17-C18-C19
25	R	608	CHL	C8-C10-C11-C12
25	r	608	CHL	C8-C10-C11-C12
26	D	402	CLA	C8-C10-C11-C12
26	d	402	CLA	C8-C10-C11-C12
25	3	606	CHL	O1D-CGD-O2D-CED
25	7	606	CHL	O1D-CGD-O2D-CED
37	C	521	LMG	C29-C30-C31-C32
37	c	521	LMG	C29-C30-C31-C32
39	C	519	DGD	C9A-CAA-CBA-CCA
39	c	519	DGD	C9A-CAA-CBA-CCA
30	S	2630	LHG	O7-C5-C6-O8
30	s	2630	LHG	O7-C5-C6-O8
30	L	101	LHG	C16-C17-C18-C19
30	l	101	LHG	C16-C17-C18-C19
39	C	520	DGD	C4B-C5B-C6B-C7B
39	c	520	DGD	C4B-C5B-C6B-C7B
25	1	609	CHL	CBA-CGA-O2A-C1
25	5	609	CHL	CBA-CGA-O2A-C1
26	S	614	CLA	CBA-CGA-O2A-C1
26	s	614	CLA	CBA-CGA-O2A-C1
30	N	2630	LHG	C30-C31-C32-C33
30	S	2630	LHG	C11-C12-C13-C14
30	c	522	LHG	C28-C29-C30-C31
30	n	2630	LHG	C30-C31-C32-C33
30	s	2630	LHG	C11-C12-C13-C14
30	b	2630	LHG	C10-C11-C12-C13
37	A	413	LMG	C32-C33-C34-C35
37	a	413	LMG	C32-C33-C34-C35
30	1	2630	LHG	C11-C12-C13-C14
30	B	2630	LHG	C10-C11-C12-C13
30	C	522	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
30	C	522	LHG	C32-C33-C34-C35
30	G	2630	LHG	C29-C30-C31-C32
30	5	2630	LHG	C11-C12-C13-C14
30	c	522	LHG	C32-C33-C34-C35
30	g	2630	LHG	C29-C30-C31-C32
36	B	621	SQD	C33-C34-C35-C36
36	b	621	SQD	C33-C34-C35-C36
39	C	519	DGD	C6B-C7B-C8B-C9B
39	H	102	DGD	C7A-C8A-C9A-CAA
39	c	519	DGD	C6B-C7B-C8B-C9B
39	h	102	DGD	C7A-C8A-C9A-CAA
26	C	501	CLA	C16-C17-C18-C20
26	c	501	CLA	C16-C17-C18-C20
30	N	2630	LHG	C27-C28-C29-C30
30	n	2630	LHG	C27-C28-C29-C30
37	A	415	LMG	C32-C33-C34-C35
37	a	415	LMG	C32-C33-C34-C35
26	2	602	CLA	C4-C3-C5-C6
38	D	405	PL9	C30-C29-C31-C32
38	d	405	PL9	C30-C29-C31-C32
25	3	601	CHL	C2-C3-C5-C6
25	R	608	CHL	C2-C3-C5-C6
25	7	601	CHL	C2-C3-C5-C6
25	r	608	CHL	C2-C3-C5-C6
35	A	408	PHO	C2-C3-C5-C6
35	a	408	PHO	C2-C3-C5-C6
30	G	2630	LHG	O9-C7-O7-C5
39	b	626	DGD	O1B-C1B-O2G-C2G
30	C	523	LHG	O2-C2-C3-O3
30	c	523	LHG	O2-C2-C3-O3
39	C	520	DGD	C2B-C3B-C4B-C5B
25	2	606	CHL	C2A-CAA-CBA-CGA
25	N	606	CHL	C2A-CAA-CBA-CGA
25	6	606	CHL	C2A-CAA-CBA-CGA
25	n	606	CHL	C2A-CAA-CBA-CGA
26	1	602	CLA	C2A-CAA-CBA-CGA
26	3	602	CLA	C2A-CAA-CBA-CGA
26	3	613	CLA	C2A-CAA-CBA-CGA
26	4	602	CLA	C2A-CAA-CBA-CGA
26	5	602	CLA	C2A-CAA-CBA-CGA
26	7	602	CLA	C2A-CAA-CBA-CGA
26	7	613	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	8	602	CLA	C2A-CAA-CBA-CGA
25	Y	605	CHL	CBA-CGA-O2A-C1
25	y	605	CHL	CBA-CGA-O2A-C1
37	A	413	LMG	C29-C28-O8-C9
37	a	413	LMG	C29-C28-O8-C9
30	C	522	LHG	C11-C10-C9-C8
30	c	522	LHG	C11-C10-C9-C8
39	c	520	DGD	C2B-C3B-C4B-C5B
39	B	626	DGD	C4D-C5D-C6D-O5D
39	b	626	DGD	C4D-C5D-C6D-O5D
30	L	101	LHG	C11-C10-C9-C8
30	l	101	LHG	C11-C10-C9-C8
25	G	601	CHL	C15-C16-C17-C18
25	G	607	CHL	C8-C10-C11-C12
25	g	601	CHL	C15-C16-C17-C18
25	g	607	CHL	C8-C10-C11-C12
26	B	614	CLA	C15-C16-C17-C18
26	b	614	CLA	C15-C16-C17-C18
30	S	2630	LHG	O1-C1-C2-O2
30	s	2630	LHG	O1-C1-C2-O2
26	C	513	CLA	O1A-CGA-O2A-C1
26	c	513	CLA	O1A-CGA-O2A-C1
30	C	2630	LHG	O10-C23-O8-C6
30	c	2630	LHG	O10-C23-O8-C6
37	B	2633	LMG	O10-C28-O8-C9
37	b	2633	LMG	O10-C28-O8-C9
30	g	2630	LHG	C17-C18-C19-C20
30	B	2630	LHG	C29-C30-C31-C32
30	G	2630	LHG	C17-C18-C19-C20
30	b	2630	LHG	C29-C30-C31-C32
39	h	102	DGD	C3A-C4A-C5A-C6A
26	1	602	CLA	C1A-C2A-CAA-CBA
26	1	604	CLA	C1A-C2A-CAA-CBA
26	1	610	CLA	C1A-C2A-CAA-CBA
26	1	611	CLA	C1A-C2A-CAA-CBA
26	3	604	CLA	C1A-C2A-CAA-CBA
26	3	614	CLA	C1A-C2A-CAA-CBA
26	4	604	CLA	C1A-C2A-CAA-CBA
26	4	610	CLA	C1A-C2A-CAA-CBA
26	A	407	CLA	C1A-C2A-CAA-CBA
26	A	410	CLA	C1A-C2A-CAA-CBA
26	B	610	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	B	612	CLA	C1A-C2A-CAA-CBA
26	C	501	CLA	C1A-C2A-CAA-CBA
26	C	506	CLA	C1A-C2A-CAA-CBA
26	C	508	CLA	C1A-C2A-CAA-CBA
26	C	511	CLA	C1A-C2A-CAA-CBA
26	G	602	CLA	C1A-C2A-CAA-CBA
26	N	602	CLA	C1A-C2A-CAA-CBA
26	R	604	CLA	C1A-C2A-CAA-CBA
26	R	610	CLA	C1A-C2A-CAA-CBA
26	Y	602	CLA	C1A-C2A-CAA-CBA
26	Y	610	CLA	C1A-C2A-CAA-CBA
26	Y	614	CLA	C1A-C2A-CAA-CBA
26	5	602	CLA	C1A-C2A-CAA-CBA
26	5	604	CLA	C1A-C2A-CAA-CBA
26	5	610	CLA	C1A-C2A-CAA-CBA
26	5	611	CLA	C1A-C2A-CAA-CBA
26	7	604	CLA	C1A-C2A-CAA-CBA
26	7	614	CLA	C1A-C2A-CAA-CBA
26	8	604	CLA	C1A-C2A-CAA-CBA
26	8	610	CLA	C1A-C2A-CAA-CBA
26	a	407	CLA	C1A-C2A-CAA-CBA
26	a	410	CLA	C1A-C2A-CAA-CBA
26	b	610	CLA	C1A-C2A-CAA-CBA
26	b	612	CLA	C1A-C2A-CAA-CBA
26	c	501	CLA	C1A-C2A-CAA-CBA
26	c	506	CLA	C1A-C2A-CAA-CBA
26	c	508	CLA	C1A-C2A-CAA-CBA
26	c	511	CLA	C1A-C2A-CAA-CBA
26	g	602	CLA	C1A-C2A-CAA-CBA
26	n	602	CLA	C1A-C2A-CAA-CBA
26	r	604	CLA	C1A-C2A-CAA-CBA
26	r	610	CLA	C1A-C2A-CAA-CBA
26	y	602	CLA	C1A-C2A-CAA-CBA
26	y	610	CLA	C1A-C2A-CAA-CBA
26	y	614	CLA	C1A-C2A-CAA-CBA
37	A	415	LMG	C36-C37-C38-C39
37	Z	101	LMG	C20-C21-C22-C23
37	z	101	LMG	C20-C21-C22-C23
39	H	102	DGD	C3A-C4A-C5A-C6A
37	B	2633	LMG	C17-C18-C19-C20
37	a	415	LMG	C36-C37-C38-C39
37	b	2633	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
37	z	101	LMG	C32-C33-C34-C35
25	1	607	CHL	C2C-C3C-CAC-CBC
25	5	607	CHL	C2C-C3C-CAC-CBC
37	Z	101	LMG	C32-C33-C34-C35
30	Y	2630	LHG	O9-C7-O7-C5
30	g	2630	LHG	O9-C7-O7-C5
30	y	2630	LHG	O9-C7-O7-C5
39	B	626	DGD	O1B-C1B-O2G-C2G
25	1	607	CHL	C6-C7-C8-C10
25	3	601	CHL	C11-C10-C8-C7
25	3	601	CHL	C12-C13-C15-C16
25	G	608	CHL	C12-C13-C15-C16
25	5	607	CHL	C6-C7-C8-C10
25	7	601	CHL	C11-C10-C8-C7
25	7	601	CHL	C12-C13-C15-C16
25	g	608	CHL	C12-C13-C15-C16
26	1	602	CLA	C6-C7-C8-C10
26	B	616	CLA	C12-C13-C15-C16
26	C	507	CLA	C11-C10-C8-C7
26	C	507	CLA	C12-C13-C15-C16
26	C	510	CLA	C12-C13-C15-C16
26	C	512	CLA	C12-C13-C15-C16
26	G	603	CLA	C11-C10-C8-C7
26	G	610	CLA	C11-C12-C13-C15
26	G	610	CLA	C12-C13-C15-C16
26	G	612	CLA	C11-C10-C8-C7
26	G	613	CLA	C11-C12-C13-C15
26	N	602	CLA	C6-C7-C8-C10
26	N	612	CLA	C6-C7-C8-C10
26	R	610	CLA	C11-C10-C8-C7
26	S	602	CLA	C6-C7-C8-C10
26	Y	602	CLA	C6-C7-C8-C10
26	Y	613	CLA	C12-C13-C15-C16
26	5	602	CLA	C6-C7-C8-C10
26	b	616	CLA	C12-C13-C15-C16
26	c	507	CLA	C11-C10-C8-C7
26	c	507	CLA	C12-C13-C15-C16
26	c	510	CLA	C12-C13-C15-C16
26	c	512	CLA	C12-C13-C15-C16
26	g	603	CLA	C11-C10-C8-C7
26	g	610	CLA	C11-C12-C13-C15
26	g	610	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	g	612	CLA	C11-C10-C8-C7
26	g	613	CLA	C11-C12-C13-C15
26	n	602	CLA	C6-C7-C8-C10
26	n	612	CLA	C6-C7-C8-C10
26	r	610	CLA	C11-C10-C8-C7
26	s	602	CLA	C6-C7-C8-C10
26	y	602	CLA	C6-C7-C8-C10
26	y	613	CLA	C12-C13-C15-C16
39	C	520	DGD	C5A-C6A-C7A-C8A
39	c	520	DGD	C5A-C6A-C7A-C8A
26	R	603	CLA	C11-C12-C13-C15
26	r	603	CLA	C11-C12-C13-C15
25	Y	609	CHL	C8-C10-C11-C12
25	y	609	CHL	C8-C10-C11-C12
26	Y	603	CLA	O1A-CGA-O2A-C1
26	y	603	CLA	O1A-CGA-O2A-C1
37	B	622	LMG	C35-C36-C37-C38
37	b	622	LMG	C35-C36-C37-C38
37	B	622	LMG	C28-C29-C30-C31
37	b	622	LMG	C28-C29-C30-C31
30	C	2630	LHG	C28-C29-C30-C31
25	2	607	CHL	C4-C3-C5-C6
25	6	607	CHL	C4-C3-C5-C6
38	D	405	PL9	C45-C44-C46-C47
38	d	405	PL9	C45-C44-C46-C47
38	D	405	PL9	C43-C44-C46-C47
38	d	405	PL9	C43-C44-C46-C47
30	c	2630	LHG	C28-C29-C30-C31
37	A	415	LMG	C35-C36-C37-C38
37	a	415	LMG	C35-C36-C37-C38
26	R	613	CLA	O1A-CGA-O2A-C1
26	r	613	CLA	O1A-CGA-O2A-C1
30	B	2631	LHG	C32-C33-C34-C35
30	b	2631	LHG	C32-C33-C34-C35
25	1	609	CHL	C10-C11-C12-C13
25	N	607	CHL	C10-C11-C12-C13
25	5	609	CHL	C10-C11-C12-C13
25	n	607	CHL	C10-C11-C12-C13
26	B	617	CLA	C10-C11-C12-C13
26	N	603	CLA	C15-C16-C17-C18
26	b	617	CLA	C10-C11-C12-C13
26	n	603	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	Y	606	CHL	C2A-CAA-CBA-CGA
25	y	606	CHL	C2A-CAA-CBA-CGA
26	G	603	CLA	C2A-CAA-CBA-CGA
26	g	603	CLA	C2A-CAA-CBA-CGA
25	G	607	CHL	C14-C13-C15-C16
25	N	607	CHL	C14-C13-C15-C16
25	g	607	CHL	C14-C13-C15-C16
25	n	607	CHL	C14-C13-C15-C16
26	1	602	CLA	C6-C7-C8-C9
26	3	602	CLA	C6-C7-C8-C9
26	B	609	CLA	C14-C13-C15-C16
26	C	510	CLA	C14-C13-C15-C16
26	G	610	CLA	C11-C12-C13-C14
26	S	602	CLA	C6-C7-C8-C9
26	Y	602	CLA	C6-C7-C8-C9
26	Y	611	CLA	C11-C10-C8-C9
26	Y	612	CLA	C11-C10-C8-C9
26	5	602	CLA	C6-C7-C8-C9
26	7	602	CLA	C6-C7-C8-C9
26	b	609	CLA	C14-C13-C15-C16
26	c	510	CLA	C14-C13-C15-C16
26	g	610	CLA	C11-C12-C13-C14
26	s	602	CLA	C6-C7-C8-C9
26	y	602	CLA	C6-C7-C8-C9
26	y	611	CLA	C11-C10-C8-C9
26	y	612	CLA	C11-C10-C8-C9
30	B	2631	LHG	C33-C34-C35-C36
30	b	2631	LHG	C33-C34-C35-C36
36	a	412	SQD	C10-C11-C12-C13
39	H	102	DGD	CBA-CCA-CDA-CEA
28	R	622	XAT	C29-C30-C31-C32
28	r	622	XAT	C29-C30-C31-C32
36	A	412	SQD	C10-C11-C12-C13
39	h	102	DGD	CBA-CCA-CDA-CEA
25	3	609	CHL	O1D-CGD-O2D-CED
25	7	609	CHL	O1D-CGD-O2D-CED
25	3	609	CHL	CBA-CGA-O2A-C1
25	7	609	CHL	CBA-CGA-O2A-C1
30	1	2630	LHG	O9-C7-O7-C5
30	5	2630	LHG	O9-C7-O7-C5
26	N	612	CLA	C8-C10-C11-C12
26	n	612	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	S	602	CLA	C14-C13-C15-C16
26	s	602	CLA	C14-C13-C15-C16
30	C	2630	LHG	C4-C5-C6-O8
30	R	2630	LHG	C4-C5-C6-O8
30	Y	2630	LHG	C4-C5-C6-O8
30	c	2630	LHG	C4-C5-C6-O8
30	r	2630	LHG	C4-C5-C6-O8
30	y	2630	LHG	C4-C5-C6-O8
36	B	623	SQD	O6-C44-C45-C46
36	b	623	SQD	O6-C44-C45-C46
37	A	413	LMG	C7-C8-C9-O8
37	Z	101	LMG	O1-C7-C8-C9
37	a	413	LMG	C7-C8-C9-O8
37	z	101	LMG	O1-C7-C8-C9
39	C	519	DGD	O1G-C1G-C2G-C3G
39	c	519	DGD	O1G-C1G-C2G-C3G
26	N	613	CLA	O1D-CGD-O2D-CED
26	n	613	CLA	O1D-CGD-O2D-CED
30	b	2631	LHG	C31-C32-C33-C34
30	c	523	LHG	C26-C27-C28-C29
36	A	412	SQD	C30-C31-C32-C33
25	Y	609	CHL	C10-C11-C12-C13
25	y	609	CHL	C10-C11-C12-C13
26	B	606	CLA	C8-C10-C11-C12
26	b	606	CLA	C8-C10-C11-C12
30	B	2631	LHG	C31-C32-C33-C34
30	C	523	LHG	C26-C27-C28-C29
30	s	2630	LHG	C27-C28-C29-C30
36	a	412	SQD	C30-C31-C32-C33
26	C	507	CLA	O1D-CGD-O2D-CED
26	c	507	CLA	O1D-CGD-O2D-CED
30	D	409	LHG	C17-C18-C19-C20
30	S	2630	LHG	C27-C28-C29-C30
25	3	609	CHL	C8-C10-C11-C12
30	d	409	LHG	C17-C18-C19-C20
36	B	621	SQD	C34-C35-C36-C37
30	B	2631	LHG	C28-C29-C30-C31
30	b	2631	LHG	C28-C29-C30-C31
36	b	621	SQD	C34-C35-C36-C37
25	N	606	CHL	CHA-CBD-CGD-O1D
25	Y	607	CHL	CHA-CBD-CGD-O1D
25	n	606	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	y	607	CHL	CHA-CBD-CGD-O1D
30	N	2630	LHG	C14-C15-C16-C17
30	S	2630	LHG	C26-C27-C28-C29
30	n	2630	LHG	C14-C15-C16-C17
30	s	2630	LHG	C26-C27-C28-C29
37	B	2633	LMG	C31-C32-C33-C34
37	b	2633	LMG	C31-C32-C33-C34
26	S	614	CLA	O1A-CGA-O2A-C1
26	s	614	CLA	O1A-CGA-O2A-C1
39	H	102	DGD	CCA-CDA-CEA-CFA
39	h	102	DGD	CCA-CDA-CEA-CFA
37	C	521	LMG	C16-C17-C18-C19
37	z	101	LMG	C30-C31-C32-C33
25	G	601	CHL	C8-C10-C11-C12
25	Y	607	CHL	C5-C6-C7-C8
25	7	609	CHL	C8-C10-C11-C12
25	g	601	CHL	C8-C10-C11-C12
25	y	607	CHL	C5-C6-C7-C8
26	B	612	CLA	C13-C15-C16-C17
26	b	612	CLA	C13-C15-C16-C17
28	4	622	XAT	C27-C28-C29-C39
28	8	622	XAT	C27-C28-C29-C39
30	D	409	LHG	O9-C7-O7-C5
37	c	521	LMG	C16-C17-C18-C19
25	R	606	CHL	C16-C17-C18-C20
25	r	606	CHL	C16-C17-C18-C20
26	N	603	CLA	C16-C17-C18-C19
26	n	603	CLA	C16-C17-C18-C19
30	S	2630	LHG	C13-C14-C15-C16
30	b	2631	LHG	C14-C15-C16-C17
30	s	2630	LHG	C13-C14-C15-C16
37	Z	101	LMG	C30-C31-C32-C33
29	Y	1623	NEX	C11-C12-C13-C14
29	y	1623	NEX	C11-C12-C13-C14
25	G	608	CHL	C13-C15-C16-C17
25	g	608	CHL	C13-C15-C16-C17
26	B	602	CLA	C5-C6-C7-C8
26	B	614	CLA	C5-C6-C7-C8
26	b	602	CLA	C5-C6-C7-C8
26	b	614	CLA	C5-C6-C7-C8
30	B	2631	LHG	C14-C15-C16-C17
26	2	613	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	G	602	CLA	C2A-CAA-CBA-CGA
26	6	613	CLA	C2A-CAA-CBA-CGA
26	g	602	CLA	C2A-CAA-CBA-CGA
37	B	622	LMG	C18-C19-C20-C21
37	b	622	LMG	C18-C19-C20-C21
39	C	520	DGD	C4A-C5A-C6A-C7A
39	c	520	DGD	C4A-C5A-C6A-C7A
26	C	506	CLA	CBA-CGA-O2A-C1
26	c	506	CLA	CBA-CGA-O2A-C1
36	A	418	SQD	C44-C45-O47-C7
36	B	621	SQD	C46-C45-O47-C7
36	a	418	SQD	C44-C45-O47-C7
36	b	621	SQD	C46-C45-O47-C7
37	B	622	LMG	C16-C17-C18-C19
37	B	622	LMG	C17-C18-C19-C20
37	D	411	LMG	C32-C33-C34-C35
37	b	622	LMG	C16-C17-C18-C19
37	d	411	LMG	C32-C33-C34-C35
39	H	102	DGD	C5B-C6B-C7B-C8B
39	h	102	DGD	C5B-C6B-C7B-C8B
30	G	2630	LHG	C13-C14-C15-C16
30	g	2630	LHG	C13-C14-C15-C16
37	b	622	LMG	C17-C18-C19-C20
39	B	626	DGD	C6A-C7A-C8A-C9A
39	b	626	DGD	C6A-C7A-C8A-C9A
25	1	606	CHL	C3C-C2C-CMC-OMC
25	G	606	CHL	C3C-C2C-CMC-OMC
25	N	606	CHL	C3C-C2C-CMC-OMC
25	Y	606	CHL	C3C-C2C-CMC-OMC
25	5	606	CHL	C3C-C2C-CMC-OMC
25	g	606	CHL	C3C-C2C-CMC-OMC
25	n	606	CHL	C3C-C2C-CMC-OMC
25	y	606	CHL	C3C-C2C-CMC-OMC
27	1	1621	LUT	C29-C30-C31-C32
27	2	1621	LUT	C29-C30-C31-C32
27	N	1621	LUT	C29-C30-C31-C32
27	5	1621	LUT	C29-C30-C31-C32
27	6	1621	LUT	C29-C30-C31-C32
27	n	1621	LUT	C29-C30-C31-C32
30	C	2630	LHG	C26-C27-C28-C29
30	R	2630	LHG	C18-C19-C20-C21
30	c	2630	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
30	r	2630	LHG	C18-C19-C20-C21
36	B	623	SQD	C11-C10-C9-C8
36	b	623	SQD	C11-C10-C9-C8
25	Y	605	CHL	O1A-CGA-O2A-C1
25	y	605	CHL	O1A-CGA-O2A-C1
30	3	2630	LHG	C13-C14-C15-C16
30	7	2630	LHG	C13-C14-C15-C16
30	3	2630	LHG	C24-C25-C26-C27
30	Y	2630	LHG	C18-C19-C20-C21
30	7	2630	LHG	C24-C25-C26-C27
30	y	2630	LHG	C18-C19-C20-C21
30	d	409	LHG	O9-C7-O7-C5
30	D	410	LHG	O6-C4-C5-O7
30	d	410	LHG	O6-C4-C5-O7
26	B	607	CLA	C15-C16-C17-C18
26	B	613	CLA	C13-C15-C16-C17
26	b	607	CLA	C15-C16-C17-C18
26	b	613	CLA	C13-C15-C16-C17
30	D	410	LHG	C10-C11-C12-C13
30	d	410	LHG	C10-C11-C12-C13
39	C	519	DGD	C2B-C3B-C4B-C5B
39	c	519	DGD	C2B-C3B-C4B-C5B
26	b	616	CLA	O1D-CGD-O2D-CED
26	C	501	CLA	CBA-CGA-O2A-C1
26	G	604	CLA	CBA-CGA-O2A-C1
26	c	501	CLA	CBA-CGA-O2A-C1
26	g	604	CLA	CBA-CGA-O2A-C1
26	B	616	CLA	O1D-CGD-O2D-CED
39	h	102	DGD	CAB-CBB-CCB-CDB
25	R	608	CHL	C4-C3-C5-C6
25	r	608	CHL	C4-C3-C5-C6
26	B	603	CLA	C4-C3-C5-C6
26	C	507	CLA	C4-C3-C5-C6
26	b	603	CLA	C4-C3-C5-C6
38	D	405	PL9	C15-C14-C16-C17
38	d	405	PL9	C15-C14-C16-C17
25	2	607	CHL	C2-C3-C5-C6
25	6	607	CHL	C2-C3-C5-C6
26	C	505	CLA	C2-C3-C5-C6
26	c	505	CLA	C2-C3-C5-C6
30	D	410	LHG	C25-C26-C27-C28
30	Y	2630	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
30	d	410	LHG	C25-C26-C27-C28
30	y	2630	LHG	C27-C28-C29-C30
37	A	413	LMG	C29-C30-C31-C32
37	a	413	LMG	C29-C30-C31-C32
39	H	102	DGD	CAB-CBB-CCB-CDB
26	c	511	CLA	CBD-CGD-O2D-CED
30	B	2630	LHG	C11-C12-C13-C14
30	b	2631	LHG	C13-C14-C15-C16
30	n	2630	LHG	C29-C30-C31-C32
30	B	2631	LHG	C13-C14-C15-C16
30	D	409	LHG	C14-C15-C16-C17
30	N	2630	LHG	C29-C30-C31-C32
30	b	2630	LHG	C11-C12-C13-C14
30	d	409	LHG	C14-C15-C16-C17
37	A	413	LMG	C18-C19-C20-C21
37	a	413	LMG	C18-C19-C20-C21
30	N	2630	LHG	C13-C14-C15-C16
30	n	2630	LHG	C13-C14-C15-C16
36	a	418	SQD	C32-C33-C34-C35
37	B	622	LMG	C22-C23-C24-C25
37	b	622	LMG	C22-C23-C24-C25
30	n	2630	LHG	C34-C35-C36-C37
36	A	418	SQD	C32-C33-C34-C35
30	N	2630	LHG	C34-C35-C36-C37
30	d	409	LHG	C19-C20-C21-C22
26	B	602	CLA	C13-C15-C16-C17
26	b	602	CLA	C13-C15-C16-C17
30	D	409	LHG	C19-C20-C21-C22
37	a	413	LMG	C19-C20-C21-C22
30	G	2630	LHG	C14-C15-C16-C17
30	7	2630	LHG	C10-C11-C12-C13
30	g	2630	LHG	C14-C15-C16-C17
25	1	609	CHL	O1A-CGA-O2A-C1
30	7	2630	LHG	C35-C36-C37-C38
37	A	413	LMG	C19-C20-C21-C22
39	b	626	DGD	CDB-CEB-CFB-CGB
30	3	2630	LHG	C10-C11-C12-C13
37	B	2633	LMG	C21-C22-C23-C24
37	b	2633	LMG	C21-C22-C23-C24
39	B	626	DGD	C4B-C5B-C6B-C7B
39	b	626	DGD	C4B-C5B-C6B-C7B
26	r	609	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	C	505	CLA	CBA-CGA-O2A-C1
26	G	613	CLA	CBA-CGA-O2A-C1
26	c	505	CLA	CBA-CGA-O2A-C1
26	g	613	CLA	CBA-CGA-O2A-C1
30	3	2630	LHG	C35-C36-C37-C38
39	B	626	DGD	CDB-CEB-CFB-CGB
37	a	413	LMG	C12-C13-C14-C15
25	2	606	CHL	C1C-C2C-CMC-OMC
25	6	606	CHL	C1C-C2C-CMC-OMC
26	C	511	CLA	CBD-CGD-O2D-CED
37	A	413	LMG	C12-C13-C14-C15
25	Y	608	CHL	C13-C15-C16-C17
25	y	608	CHL	C13-C15-C16-C17
26	N	610	CLA	C5-C6-C7-C8
26	n	610	CLA	C5-C6-C7-C8
25	5	609	CHL	O1A-CGA-O2A-C1
25	N	601	CHL	C3-C5-C6-C7
25	n	601	CHL	C3-C5-C6-C7
26	R	609	CLA	O1D-CGD-O2D-CED
30	1	2630	LHG	C27-C28-C29-C30
30	5	2630	LHG	C27-C28-C29-C30
30	g	2630	LHG	C28-C29-C30-C31
30	b	2630	LHG	C19-C20-C21-C22
26	c	502	CLA	C8-C10-C11-C12
26	N	602	CLA	C16-C17-C18-C20
26	Y	610	CLA	C11-C12-C13-C14
26	n	602	CLA	C16-C17-C18-C20
26	y	610	CLA	C11-C12-C13-C14
25	1	607	CHL	C4-C3-C5-C6
25	1	609	CHL	C4-C3-C5-C6
25	5	607	CHL	C4-C3-C5-C6
25	5	609	CHL	C4-C3-C5-C6
26	1	603	CLA	C4-C3-C5-C6
26	5	603	CLA	C4-C3-C5-C6
26	c	507	CLA	C4-C3-C5-C6
30	3	2630	LHG	C17-C18-C19-C20
30	7	2630	LHG	C17-C18-C19-C20
26	Y	603	CLA	C2-C3-C5-C6
26	y	603	CLA	C2-C3-C5-C6
30	C	523	LHG	C33-C34-C35-C36
30	G	2630	LHG	C28-C29-C30-C31
30	c	523	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
26	G	612	CLA	CBA-CGA-O2A-C1
26	g	612	CLA	CBA-CGA-O2A-C1
26	C	502	CLA	C8-C10-C11-C12
30	B	2630	LHG	C19-C20-C21-C22
30	L	101	LHG	C35-C36-C37-C38
30	d	408	LHG	C16-C17-C18-C19
30	l	101	LHG	C35-C36-C37-C38
30	7	2630	LHG	C29-C30-C31-C32
30	D	410	LHG	O9-C7-O7-C5
30	d	410	LHG	O9-C7-O7-C5
39	C	520	DGD	O1B-C1B-O2G-C2G
39	c	520	DGD	O1B-C1B-O2G-C2G
25	1	607	CHL	C6-C7-C8-C9
25	2	607	CHL	C6-C7-C8-C9
25	3	601	CHL	C11-C10-C8-C9
25	5	607	CHL	C6-C7-C8-C9
25	6	607	CHL	C6-C7-C8-C9
25	7	601	CHL	C11-C10-C8-C9
26	B	612	CLA	C14-C13-C15-C16
26	B	616	CLA	C11-C12-C13-C14
26	B	616	CLA	C14-C13-C15-C16
26	C	507	CLA	C14-C13-C15-C16
26	C	509	CLA	C11-C12-C13-C14
26	C	512	CLA	C14-C13-C15-C16
26	G	603	CLA	C11-C10-C8-C9
26	G	610	CLA	C14-C13-C15-C16
26	G	612	CLA	C11-C10-C8-C9
26	G	613	CLA	C11-C12-C13-C14
26	N	602	CLA	C6-C7-C8-C9
26	R	610	CLA	C11-C10-C8-C9
26	Y	613	CLA	C14-C13-C15-C16
26	b	612	CLA	C14-C13-C15-C16
26	b	616	CLA	C11-C12-C13-C14
26	b	616	CLA	C14-C13-C15-C16
26	c	507	CLA	C14-C13-C15-C16
26	c	509	CLA	C11-C12-C13-C14
26	c	512	CLA	C14-C13-C15-C16
26	g	603	CLA	C11-C10-C8-C9
26	g	610	CLA	C14-C13-C15-C16
26	g	612	CLA	C11-C10-C8-C9
26	g	613	CLA	C11-C12-C13-C14
26	n	602	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	r	610	CLA	C11-C10-C8-C9
26	y	613	CLA	C14-C13-C15-C16
26	1	612	CLA	O1D-CGD-O2D-CED
26	A	405	CLA	C15-C16-C17-C18
26	C	505	CLA	C15-C16-C17-C18
26	D	402	CLA	C13-C15-C16-C17
26	Y	602	CLA	C13-C15-C16-C17
26	a	405	CLA	C15-C16-C17-C18
26	c	505	CLA	C15-C16-C17-C18
26	d	402	CLA	C13-C15-C16-C17
26	y	602	CLA	C13-C15-C16-C17
30	D	408	LHG	C16-C17-C18-C19
25	3	609	CHL	O1A-CGA-O2A-C1
39	C	518	DGD	C4D-C5D-C6D-O5D
26	1	602	CLA	C4B-C3B-CAB-CBB
26	1	603	CLA	C4B-C3B-CAB-CBB
26	1	604	CLA	C4B-C3B-CAB-CBB
26	2	613	CLA	C4B-C3B-CAB-CBB
26	2	614	CLA	C4B-C3B-CAB-CBB
26	4	602	CLA	C4B-C3B-CAB-CBB
26	4	604	CLA	C4B-C3B-CAB-CBB
26	B	606	CLA	C4B-C3B-CAB-CBB
26	C	503	CLA	C4B-C3B-CAB-CBB
26	S	603	CLA	C4B-C3B-CAB-CBB
26	S	609	CLA	C4B-C3B-CAB-CBB
26	Y	610	CLA	C4B-C3B-CAB-CBB
26	5	602	CLA	C4B-C3B-CAB-CBB
26	5	603	CLA	C4B-C3B-CAB-CBB
26	5	604	CLA	C4B-C3B-CAB-CBB
26	6	613	CLA	C4B-C3B-CAB-CBB
26	6	614	CLA	C4B-C3B-CAB-CBB
26	8	602	CLA	C4B-C3B-CAB-CBB
26	8	604	CLA	C4B-C3B-CAB-CBB
26	b	606	CLA	C4B-C3B-CAB-CBB
26	c	503	CLA	C4B-C3B-CAB-CBB
26	s	603	CLA	C4B-C3B-CAB-CBB
26	s	609	CLA	C4B-C3B-CAB-CBB
26	y	610	CLA	C4B-C3B-CAB-CBB
30	3	2630	LHG	C29-C30-C31-C32
37	A	413	LMG	C33-C34-C35-C36
26	5	612	CLA	O1D-CGD-O2D-CED
26	C	510	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	c	510	CLA	C13-C15-C16-C17
36	b	623	SQD	C25-C26-C27-C28
37	a	413	LMG	C33-C34-C35-C36
25	7	609	CHL	O1A-CGA-O2A-C1
26	Y	613	CLA	C2A-CAA-CBA-CGA
26	y	613	CLA	C2A-CAA-CBA-CGA
30	D	409	LHG	C25-C26-C27-C28
30	N	2630	LHG	C28-C29-C30-C31
36	B	623	SQD	C25-C26-C27-C28
25	Y	605	CHL	O1D-CGD-O2D-CED
30	S	2630	LHG	C9-C10-C11-C12
30	d	409	LHG	C25-C26-C27-C28
30	n	2630	LHG	C28-C29-C30-C31
30	s	2630	LHG	C9-C10-C11-C12
30	D	409	LHG	O6-C4-C5-C6
30	d	409	LHG	O6-C4-C5-C6
39	c	518	DGD	C4D-C5D-C6D-O5D
25	2	607	CHL	C6-C7-C8-C10
25	G	607	CHL	C11-C10-C8-C7
25	N	601	CHL	C12-C13-C15-C16
25	N	607	CHL	C12-C13-C15-C16
25	R	606	CHL	C6-C7-C8-C10
25	Y	601	CHL	C12-C13-C15-C16
25	Y	609	CHL	C12-C13-C15-C16
25	6	607	CHL	C6-C7-C8-C10
25	g	607	CHL	C11-C10-C8-C7
25	n	601	CHL	C12-C13-C15-C16
25	n	607	CHL	C12-C13-C15-C16
25	r	606	CHL	C6-C7-C8-C10
25	y	601	CHL	C12-C13-C15-C16
25	y	609	CHL	C12-C13-C15-C16
26	2	602	CLA	C11-C12-C13-C15
26	3	602	CLA	C6-C7-C8-C10
26	B	609	CLA	C12-C13-C15-C16
26	B	613	CLA	C11-C10-C8-C7
26	B	616	CLA	C11-C10-C8-C7
26	C	502	CLA	C6-C7-C8-C10
26	C	502	CLA	C11-C10-C8-C7
26	C	506	CLA	C6-C7-C8-C10
26	C	507	CLA	C11-C12-C13-C15
26	C	509	CLA	C11-C12-C13-C15
26	R	610	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
26	6	602	CLA	C11-C12-C13-C15
26	7	602	CLA	C6-C7-C8-C10
26	b	609	CLA	C12-C13-C15-C16
26	b	613	CLA	C11-C10-C8-C7
26	b	616	CLA	C11-C10-C8-C7
26	c	502	CLA	C6-C7-C8-C10
26	c	502	CLA	C11-C10-C8-C7
26	c	506	CLA	C6-C7-C8-C10
26	c	507	CLA	C6-C7-C8-C10
26	c	507	CLA	C11-C12-C13-C15
26	c	509	CLA	C11-C12-C13-C15
26	r	610	CLA	C11-C12-C13-C15
25	y	605	CHL	O1D-CGD-O2D-CED
26	G	610	CLA	C15-C16-C17-C18
26	g	610	CLA	C15-C16-C17-C18
30	D	408	LHG	C11-C12-C13-C14
30	C	2630	LHG	C30-C31-C32-C33
30	D	408	LHG	C13-C14-C15-C16
30	c	2630	LHG	C30-C31-C32-C33
30	d	408	LHG	C11-C12-C13-C14
30	d	408	LHG	C13-C14-C15-C16
37	B	622	LMG	C33-C34-C35-C36
37	b	622	LMG	C33-C34-C35-C36
25	y	609	CHL	O1A-CGA-O2A-C1
30	S	2630	LHG	C35-C36-C37-C38
25	4	601	CHL	C3A-C2A-CAA-CBA
25	R	608	CHL	C3A-C2A-CAA-CBA
25	8	601	CHL	C3A-C2A-CAA-CBA
25	r	608	CHL	C3A-C2A-CAA-CBA
26	2	604	CLA	C3A-C2A-CAA-CBA
26	N	612	CLA	C4-C3-C5-C6
26	6	604	CLA	C3A-C2A-CAA-CBA
30	s	2630	LHG	C35-C36-C37-C38
25	Y	609	CHL	O1A-CGA-O2A-C1
26	D	402	CLA	C10-C11-C12-C13
26	d	402	CLA	C10-C11-C12-C13
30	r	2630	LHG	C14-C15-C16-C17
36	b	621	SQD	C11-C12-C13-C14
26	Y	613	CLA	CBA-CGA-O2A-C1
26	y	613	CLA	CBA-CGA-O2A-C1
30	R	2630	LHG	C14-C15-C16-C17
36	B	621	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
37	B	622	LMG	C40-C41-C42-C43
37	b	622	LMG	C40-C41-C42-C43
27	3	1621	LUT	C29-C30-C31-C32
27	G	1621	LUT	C29-C30-C31-C32
27	Y	1621	LUT	C29-C30-C31-C32
27	7	1621	LUT	C29-C30-C31-C32
27	g	1621	LUT	C29-C30-C31-C32
27	y	1621	LUT	C29-C30-C31-C32
28	N	1622	XAT	C29-C30-C31-C32
28	n	1622	XAT	C29-C30-C31-C32
29	1	1623	NEX	C29-C30-C31-C32
29	5	1623	NEX	C29-C30-C31-C32
31	4	623	BCR	C19-C20-C21-C22
31	D	404	BCR	C9-C10-C11-C12
31	8	623	BCR	C19-C20-C21-C22
31	d	404	BCR	C9-C10-C11-C12
39	C	518	DGD	O6D-C5D-C6D-O5D
39	c	518	DGD	O6D-C5D-C6D-O5D
39	C	518	DGD	C6A-C7A-C8A-C9A
39	c	518	DGD	C6A-C7A-C8A-C9A
30	c	522	LHG	C33-C34-C35-C36
39	c	519	DGD	C2A-C3A-C4A-C5A
30	C	522	LHG	C33-C34-C35-C36
39	C	519	DGD	C2A-C3A-C4A-C5A
26	C	503	CLA	C2A-CAA-CBA-CGA
26	R	601	CLA	C2A-CAA-CBA-CGA
26	c	503	CLA	C2A-CAA-CBA-CGA
26	r	601	CLA	C2A-CAA-CBA-CGA
26	R	601	CLA	CBA-CGA-O2A-C1
26	r	601	CLA	CBA-CGA-O2A-C1
30	3	2630	LHG	C4-C5-C6-O8
30	B	2631	LHG	C4-C5-C6-O8
30	G	2630	LHG	C4-C5-C6-O8
30	7	2630	LHG	C4-C5-C6-O8
30	b	2631	LHG	C4-C5-C6-O8
30	g	2630	LHG	C4-C5-C6-O8
36	A	418	SQD	C44-C45-C46-O48
36	a	418	SQD	C44-C45-C46-O48
37	B	2633	LMG	C7-C8-C9-O8
37	D	411	LMG	C7-C8-C9-O8
37	b	2633	LMG	C7-C8-C9-O8
37	d	411	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
39	C	520	DGD	O1G-C1G-C2G-C3G
39	c	520	DGD	O1G-C1G-C2G-C3G
26	C	505	CLA	C16-C17-C18-C19
26	c	505	CLA	C16-C17-C18-C19
30	C	523	LHG	C12-C13-C14-C15
30	R	2630	LHG	C13-C14-C15-C16
30	r	2630	LHG	C13-C14-C15-C16
25	G	608	CHL	C1A-C2A-CAA-CBA
25	N	605	CHL	C1A-C2A-CAA-CBA
25	N	608	CHL	C1A-C2A-CAA-CBA
25	g	608	CHL	C1A-C2A-CAA-CBA
25	n	605	CHL	C1A-C2A-CAA-CBA
25	n	608	CHL	C1A-C2A-CAA-CBA
30	c	523	LHG	C12-C13-C14-C15
39	C	518	DGD	CCB-CDB-CEB-CFB
39	c	518	DGD	CCB-CDB-CEB-CFB
37	c	521	LMG	O6-C5-C6-O5
26	2	603	CLA	C4-C3-C5-C6
26	C	505	CLA	C4-C3-C5-C6
26	Y	603	CLA	C4-C3-C5-C6
26	6	603	CLA	C4-C3-C5-C6
26	c	505	CLA	C4-C3-C5-C6
26	n	612	CLA	C4-C3-C5-C6
26	y	603	CLA	C4-C3-C5-C6
30	Y	2630	LHG	C34-C35-C36-C37
30	y	2630	LHG	C34-C35-C36-C37
39	H	102	DGD	CCB-CDB-CEB-CFB
39	h	102	DGD	CCB-CDB-CEB-CFB
25	1	609	CHL	C2-C3-C5-C6
25	5	609	CHL	C2-C3-C5-C6
30	B	2630	LHG	C31-C32-C33-C34
30	b	2630	LHG	C31-C32-C33-C34
26	A	406	CLA	C16-C17-C18-C20
26	Y	610	CLA	C11-C12-C13-C15
26	a	406	CLA	C16-C17-C18-C20
26	y	610	CLA	C11-C12-C13-C15
37	C	521	LMG	O9-C10-O7-C8
37	c	521	LMG	O9-C10-O7-C8
25	G	607	CHL	C13-C15-C16-C17
25	g	607	CHL	C13-C15-C16-C17
30	Y	2630	LHG	C25-C26-C27-C28
30	y	2630	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
26	2	610	CLA	C2B-C3B-CAB-CBB
26	S	609	CLA	C2B-C3B-CAB-CBB
26	6	610	CLA	C2B-C3B-CAB-CBB
26	s	609	CLA	C2B-C3B-CAB-CBB
27	1	1620	LUT	C1-C6-C7-C8
27	2	1620	LUT	C1-C6-C7-C8
27	3	1620	LUT	C5-C6-C7-C8
27	5	1620	LUT	C1-C6-C7-C8
27	6	1620	LUT	C1-C6-C7-C8
27	7	1620	LUT	C5-C6-C7-C8
31	B	620	BCR	C23-C24-C25-C30
31	C	514	BCR	C1-C6-C7-C8
31	C	515	BCR	C23-C24-C25-C30
31	C	516	BCR	C1-C6-C7-C8
31	D	404	BCR	C1-C6-C7-C8
31	b	620	BCR	C23-C24-C25-C30
31	c	514	BCR	C1-C6-C7-C8
31	c	515	BCR	C23-C24-C25-C30
31	c	516	BCR	C1-C6-C7-C8
31	d	404	BCR	C1-C6-C7-C8
25	1	609	CHL	C14-C13-C15-C16
25	5	609	CHL	C14-C13-C15-C16
37	C	521	LMG	O6-C5-C6-O5
37	c	521	LMG	C40-C41-C42-C43
30	C	2630	LHG	C34-C35-C36-C37
30	S	2630	LHG	C31-C32-C33-C34
30	c	2630	LHG	C34-C35-C36-C37
36	B	621	SQD	C9-C10-C11-C12
36	b	621	SQD	C9-C10-C11-C12
26	1	602	CLA	C10-C11-C12-C13
26	5	602	CLA	C10-C11-C12-C13
30	1	2630	LHG	C18-C19-C20-C21
30	5	2630	LHG	C18-C19-C20-C21
30	l	101	LHG	C26-C27-C28-C29
30	s	2630	LHG	C31-C32-C33-C34
37	C	521	LMG	C40-C41-C42-C43
30	L	101	LHG	C26-C27-C28-C29
26	A	406	CLA	C16-C17-C18-C19
26	N	602	CLA	C16-C17-C18-C19
26	a	406	CLA	C16-C17-C18-C19
26	n	602	CLA	C16-C17-C18-C19
25	S	601	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	s	601	CHL	C2A-CAA-CBA-CGA
30	4	2630	LHG	O7-C5-C6-O8
30	C	2630	LHG	O7-C5-C6-O8
30	G	2630	LHG	O7-C5-C6-O8
30	R	2630	LHG	O7-C5-C6-O8
30	Y	2630	LHG	O7-C5-C6-O8
30	8	2630	LHG	O7-C5-C6-O8
30	c	2630	LHG	O7-C5-C6-O8
30	g	2630	LHG	O7-C5-C6-O8
30	r	2630	LHG	O7-C5-C6-O8
30	y	2630	LHG	O7-C5-C6-O8
36	B	623	SQD	O47-C45-C46-O48
36	b	623	SQD	O47-C45-C46-O48
37	C	521	LMG	O7-C8-C9-O8
37	D	411	LMG	O7-C8-C9-O8
37	c	521	LMG	O7-C8-C9-O8
37	d	411	LMG	O7-C8-C9-O8
39	C	520	DGD	O1G-C1G-C2G-O2G
39	c	520	DGD	O1G-C1G-C2G-O2G
26	B	612	CLA	C4-C3-C5-C6
26	b	612	CLA	C4-C3-C5-C6
30	D	409	LHG	C27-C28-C29-C30
30	d	409	LHG	C27-C28-C29-C30
26	2	603	CLA	C2-C3-C5-C6
26	N	612	CLA	C2-C3-C5-C6
26	6	603	CLA	C2-C3-C5-C6
26	n	612	CLA	C2-C3-C5-C6
30	D	408	LHG	C30-C31-C32-C33
30	R	2630	LHG	C26-C27-C28-C29
30	d	408	LHG	C30-C31-C32-C33
30	r	2630	LHG	C26-C27-C28-C29
36	B	621	SQD	C12-C13-C14-C15
25	N	609	CHL	C16-C17-C18-C19
25	n	609	CHL	C16-C17-C18-C19
30	s	2630	LHG	C16-C17-C18-C19
36	b	621	SQD	C12-C13-C14-C15
26	A	410	CLA	C5-C6-C7-C8
26	a	410	CLA	C5-C6-C7-C8
39	B	626	DGD	C1A-C2A-C3A-C4A
39	b	626	DGD	C1A-C2A-C3A-C4A
26	G	604	CLA	O1A-CGA-O2A-C1
30	G	2630	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
30	g	2630	LHG	C8-C7-O7-C5
25	R	606	CHL	C6-C7-C8-C9
25	r	606	CHL	C6-C7-C8-C9
26	C	502	CLA	C11-C10-C8-C9
26	c	502	CLA	C11-C10-C8-C9
30	S	2630	LHG	C16-C17-C18-C19
26	g	604	CLA	O1A-CGA-O2A-C1
39	C	520	DGD	CBB-CCB-CDB-CEB
39	c	520	DGD	CBB-CCB-CDB-CEB
30	b	2630	LHG	C13-C14-C15-C16
26	B	604	CLA	C16-C17-C18-C19
26	b	604	CLA	C16-C17-C18-C19
30	B	2630	LHG	C13-C14-C15-C16
30	D	410	LHG	C32-C33-C34-C35
30	d	410	LHG	C32-C33-C34-C35
26	R	604	CLA	O2A-C1-C2-C3
26	r	604	CLA	O2A-C1-C2-C3
26	r	610	CLA	CBD-CGD-O2D-CED
30	l	101	LHG	C30-C31-C32-C33
30	L	101	LHG	C30-C31-C32-C33
26	C	506	CLA	O1A-CGA-O2A-C1
26	c	506	CLA	O1A-CGA-O2A-C1
26	B	605	CLA	CBA-CGA-O2A-C1
26	C	503	CLA	CBA-CGA-O2A-C1
26	b	605	CLA	CBA-CGA-O2A-C1
25	1	607	CHL	C2-C3-C5-C6
25	5	607	CHL	C2-C3-C5-C6
26	1	603	CLA	C2-C3-C5-C6
26	B	612	CLA	C2-C3-C5-C6
26	5	603	CLA	C2-C3-C5-C6
26	b	612	CLA	C2-C3-C5-C6
25	N	607	CHL	C16-C17-C18-C20
25	n	607	CHL	C16-C17-C18-C20
26	C	504	CLA	CBD-CGD-O2D-CED
26	c	504	CLA	CBD-CGD-O2D-CED
26	A	405	CLA	C5-C6-C7-C8
26	C	501	CLA	C10-C11-C12-C13
26	a	405	CLA	C5-C6-C7-C8
26	c	501	CLA	C10-C11-C12-C13
30	Y	2630	LHG	C1-C2-C3-O3
30	y	2630	LHG	C1-C2-C3-O3
30	1	2630	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
30	5	2630	LHG	C24-C25-C26-C27
36	b	621	SQD	C32-C33-C34-C35
26	C	512	CLA	CBA-CGA-O2A-C1
26	c	503	CLA	CBA-CGA-O2A-C1
26	c	512	CLA	CBA-CGA-O2A-C1
25	1	609	CHL	C5-C6-C7-C8
25	5	609	CHL	C5-C6-C7-C8
26	1	602	CLA	C8-C10-C11-C12
26	Y	611	CLA	C5-C6-C7-C8
26	5	602	CLA	C8-C10-C11-C12
26	y	611	CLA	C5-C6-C7-C8
36	B	621	SQD	C32-C33-C34-C35
30	B	2630	LHG	O6-C4-C5-C6
30	b	2630	LHG	O6-C4-C5-C6
26	3	610	CLA	C11-C12-C13-C14
26	B	602	CLA	C16-C17-C18-C20
26	Y	603	CLA	C16-C17-C18-C20
26	7	610	CLA	C11-C12-C13-C14
26	b	602	CLA	C16-C17-C18-C20
26	y	603	CLA	C16-C17-C18-C20
37	a	413	LMG	C39-C40-C41-C42
25	G	607	CHL	C12-C13-C15-C16
25	N	601	CHL	C11-C10-C8-C7
25	R	606	CHL	C12-C13-C15-C16
25	Y	607	CHL	C12-C13-C15-C16
25	g	607	CHL	C12-C13-C15-C16
25	n	601	CHL	C11-C10-C8-C7
25	r	606	CHL	C12-C13-C15-C16
25	y	607	CHL	C12-C13-C15-C16
26	A	406	CLA	C6-C7-C8-C10
26	B	608	CLA	C12-C13-C15-C16
26	B	616	CLA	C11-C12-C13-C15
26	C	506	CLA	C11-C12-C13-C15
26	C	507	CLA	C6-C7-C8-C10
26	C	509	CLA	C6-C7-C8-C10
26	C	511	CLA	C11-C12-C13-C15
26	D	403	CLA	C11-C12-C13-C15
26	S	611	CLA	C6-C7-C8-C10
26	Y	603	CLA	C12-C13-C15-C16
26	Y	612	CLA	C11-C10-C8-C7
26	a	406	CLA	C6-C7-C8-C10
26	b	608	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	b	616	CLA	C11-C12-C13-C15
26	c	506	CLA	C11-C12-C13-C15
26	c	509	CLA	C6-C7-C8-C10
26	c	511	CLA	C11-C12-C13-C15
26	d	403	CLA	C11-C12-C13-C15
26	s	611	CLA	C6-C7-C8-C10
26	y	603	CLA	C12-C13-C15-C16
26	y	612	CLA	C11-C10-C8-C7
30	C	522	LHG	C15-C16-C17-C18
30	c	522	LHG	C15-C16-C17-C18
37	A	413	LMG	C39-C40-C41-C42
39	H	102	DGD	C4A-C5A-C6A-C7A
39	h	102	DGD	C4A-C5A-C6A-C7A
36	B	621	SQD	C25-C26-C27-C28
36	b	621	SQD	C25-C26-C27-C28
26	R	610	CLA	CBD-CGD-O2D-CED
26	c	505	CLA	CBD-CGD-O2D-CED
27	4	620	LUT	C27-C28-C29-C30
27	8	620	LUT	C27-C28-C29-C30
29	2	1623	NEX	C31-C32-C33-C34
29	6	1623	NEX	C31-C32-C33-C34
30	N	2630	LHG	C26-C27-C28-C29
30	n	2630	LHG	C26-C27-C28-C29
39	C	520	DGD	C2A-C3A-C4A-C5A
39	c	520	DGD	C2A-C3A-C4A-C5A
26	G	613	CLA	O1A-CGA-O2A-C1
26	g	613	CLA	O1A-CGA-O2A-C1
36	B	623	SQD	C5-C6-S-O8
36	b	623	SQD	C5-C6-S-O8
37	Z	101	LMG	C8-C7-O1-C1
37	z	101	LMG	C8-C7-O1-C1
26	C	505	CLA	CBD-CGD-O2D-CED
30	2	2630	LHG	O9-C7-O7-C5
30	6	2630	LHG	O9-C7-O7-C5
37	C	521	LMG	C39-C40-C41-C42
37	c	521	LMG	C39-C40-C41-C42
39	H	102	DGD	O2G-C1B-C2B-C3B
39	h	102	DGD	O2G-C1B-C2B-C3B
26	C	501	CLA	O1A-CGA-O2A-C1
26	C	505	CLA	O1A-CGA-O2A-C1
26	c	501	CLA	O1A-CGA-O2A-C1
26	c	505	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	r	601	CLA	O1A-CGA-O2A-C1
30	B	2630	LHG	C28-C29-C30-C31
30	C	2630	LHG	C27-C28-C29-C30
30	G	2630	LHG	C12-C13-C14-C15
30	c	2630	LHG	C27-C28-C29-C30
30	g	2630	LHG	C12-C13-C14-C15
25	3	601	CHL	C15-C16-C17-C18
25	7	601	CHL	C15-C16-C17-C18
30	S	2630	LHG	C19-C20-C21-C22
30	s	2630	LHG	C19-C20-C21-C22
30	b	2630	LHG	C28-C29-C30-C31
35	A	408	PHO	C13-C15-C16-C17
35	a	408	PHO	C13-C15-C16-C17
25	Y	607	CHL	O2A-C1-C2-C3
25	y	607	CHL	O2A-C1-C2-C3
26	R	601	CLA	O1A-CGA-O2A-C1
25	N	608	CHL	C10-C11-C12-C13
25	n	608	CHL	C10-C11-C12-C13
25	R	607	CHL	C6-C7-C8-C10
25	r	607	CHL	C6-C7-C8-C10
26	C	511	CLA	C16-C17-C18-C20
37	B	622	LMG	C30-C31-C32-C33
37	b	622	LMG	C30-C31-C32-C33
26	G	612	CLA	O1A-CGA-O2A-C1
26	g	612	CLA	O1A-CGA-O2A-C1
30	D	410	LHG	C31-C32-C33-C34
30	d	410	LHG	C31-C32-C33-C34
37	Z	101	LMG	O9-C10-O7-C8
37	z	101	LMG	O9-C10-O7-C8
30	B	2630	LHG	O6-C4-C5-O7
30	C	522	LHG	O6-C4-C5-O7
30	b	2630	LHG	O6-C4-C5-O7
30	c	522	LHG	O6-C4-C5-O7
26	G	614	CLA	O2A-C1-C2-C3
26	g	614	CLA	O2A-C1-C2-C3
39	B	626	DGD	C7B-C8B-C9B-CAB
30	1	2630	LHG	C4-C5-C6-O8
30	B	2630	LHG	C4-C5-C6-O8
30	D	410	LHG	C4-C5-C6-O8
30	5	2630	LHG	C4-C5-C6-O8
30	b	2630	LHG	C4-C5-C6-O8
30	d	410	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
36	B	621	SQD	O6-C44-C45-C46
36	b	621	SQD	O6-C44-C45-C46
37	A	413	LMG	O1-C7-C8-C9
37	A	415	LMG	C7-C8-C9-O8
37	a	413	LMG	O1-C7-C8-C9
37	a	415	LMG	C7-C8-C9-O8
25	N	609	CHL	CBD-CGD-O2D-CED
30	1	2630	LHG	C8-C7-O7-C5
30	C	522	LHG	C8-C7-O7-C5
30	5	2630	LHG	C8-C7-O7-C5
30	c	522	LHG	C8-C7-O7-C5
35	A	409	PHO	C5-C6-C7-C8
35	a	409	PHO	C5-C6-C7-C8
26	b	613	CLA	C16-C17-C18-C19
26	c	511	CLA	C16-C17-C18-C20
39	b	626	DGD	C7B-C8B-C9B-CAB
26	c	505	CLA	O1D-CGD-O2D-CED
37	D	411	LMG	C16-C17-C18-C19
37	d	411	LMG	C16-C17-C18-C19
30	L	101	LHG	C24-C25-C26-C27
30	l	101	LHG	C24-C25-C26-C27
29	S	1623	NEX	C7-C8-C9-C19
29	s	1623	NEX	C7-C8-C9-C19
26	b	605	CLA	C13-C15-C16-C17
26	C	505	CLA	O1D-CGD-O2D-CED
26	B	612	CLA	C3-C5-C6-C7
26	b	612	CLA	C3-C5-C6-C7
30	B	2630	LHG	O7-C5-C6-O8
30	D	410	LHG	O7-C5-C6-O8
30	b	2630	LHG	O7-C5-C6-O8
30	d	410	LHG	O7-C5-C6-O8
36	B	621	SQD	O47-C45-C46-O48
36	b	621	SQD	O47-C45-C46-O48
37	A	413	LMG	O1-C7-C8-O7
37	A	415	LMG	O7-C8-C9-O8
37	B	2633	LMG	O7-C8-C9-O8
37	a	413	LMG	O1-C7-C8-O7
37	a	415	LMG	O7-C8-C9-O8
37	b	2633	LMG	O7-C8-C9-O8
25	G	608	CHL	C10-C11-C12-C13
25	g	608	CHL	C10-C11-C12-C13
26	B	605	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	C	507	CLA	C15-C16-C17-C18
26	D	403	CLA	C10-C11-C12-C13
25	R	606	CHL	C14-C13-C15-C16
25	Y	607	CHL	C14-C13-C15-C16
25	r	606	CHL	C14-C13-C15-C16
25	y	607	CHL	C14-C13-C15-C16
26	A	406	CLA	C6-C7-C8-C9
26	B	606	CLA	C14-C13-C15-C16
26	B	613	CLA	C11-C10-C8-C9
26	C	502	CLA	C14-C13-C15-C16
26	C	506	CLA	C11-C10-C8-C9
26	Y	603	CLA	C14-C13-C15-C16
26	a	406	CLA	C6-C7-C8-C9
26	b	606	CLA	C14-C13-C15-C16
26	b	613	CLA	C11-C10-C8-C9
26	c	506	CLA	C11-C10-C8-C9
26	y	603	CLA	C14-C13-C15-C16
26	B	613	CLA	C16-C17-C18-C19
30	3	2630	LHG	O9-C7-O7-C5
30	7	2630	LHG	O9-C7-O7-C5
30	3	2630	LHG	C26-C27-C28-C29
30	G	2630	LHG	C9-C10-C11-C12
30	7	2630	LHG	C26-C27-C28-C29
26	C	512	CLA	O1A-CGA-O2A-C1
26	c	512	CLA	O1A-CGA-O2A-C1
26	y	613	CLA	O1A-CGA-O2A-C1
30	g	2630	LHG	C9-C10-C11-C12
37	B	622	LMG	C38-C39-C40-C41
26	c	507	CLA	C15-C16-C17-C18
26	d	403	CLA	C10-C11-C12-C13
37	b	622	LMG	C38-C39-C40-C41
26	C	508	CLA	C15-C16-C17-C18
26	c	508	CLA	C15-C16-C17-C18
26	Y	613	CLA	O1A-CGA-O2A-C1
25	G	606	CHL	CBA-CGA-O2A-C1
25	g	606	CHL	CBA-CGA-O2A-C1
26	N	603	CLA	C16-C17-C18-C20
26	n	603	CLA	C16-C17-C18-C20
26	c	505	CLA	C10-C11-C12-C13
25	n	609	CHL	CBD-CGD-O2D-CED
26	C	505	CLA	C10-C11-C12-C13
37	B	2633	LMG	C8-C9-O8-C28

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Mol	Chain	Res	Type	Atoms
37	b	2633	LMG	C8-C9-O8-C28
30	C	2630	LHG	C11-C10-C9-C8
30	c	2630	LHG	C11-C10-C9-C8
26	6	602	CLA	C2-C3-C5-C6
25	G	609	CHL	C8-C10-C11-C12
25	g	609	CHL	C8-C10-C11-C12
26	3	611	CLA	C5-C6-C7-C8
26	7	611	CLA	C5-C6-C7-C8
26	y	610	CLA	C10-C11-C12-C13
39	C	519	DGD	O1A-C1A-O1G-C1G
26	G	613	CLA	C2A-CAA-CBA-CGA
26	Y	602	CLA	C2A-CAA-CBA-CGA
26	g	613	CLA	C2A-CAA-CBA-CGA
26	y	602	CLA	C2A-CAA-CBA-CGA
26	B	616	CLA	C16-C17-C18-C20
26	N	610	CLA	C16-C17-C18-C19
26	b	616	CLA	C16-C17-C18-C20
26	n	610	CLA	C16-C17-C18-C19
25	R	607	CHL	C5-C6-C7-C8
26	Y	610	CLA	C10-C11-C12-C13
26	B	605	CLA	O1A-CGA-O2A-C1
26	b	605	CLA	O1A-CGA-O2A-C1
26	g	611	CLA	O1A-CGA-O2A-C1
30	1	2630	LHG	O10-C23-O8-C6
30	5	2630	LHG	O10-C23-O8-C6
39	c	519	DGD	O1A-C1A-O1G-C1G
30	D	409	LHG	C12-C13-C14-C15
30	D	410	LHG	C29-C30-C31-C32
30	N	2630	LHG	C31-C32-C33-C34
30	d	409	LHG	C12-C13-C14-C15
30	d	410	LHG	C29-C30-C31-C32
25	2	607	CHL	C4C-C3C-CAC-CBC
25	2	609	CHL	C4C-C3C-CAC-CBC
25	3	607	CHL	C4C-C3C-CAC-CBC
25	4	609	CHL	C4C-C3C-CAC-CBC
25	G	607	CHL	C4C-C3C-CAC-CBC
25	G	609	CHL	C4C-C3C-CAC-CBC
25	N	605	CHL	C4C-C3C-CAC-CBC
25	N	607	CHL	C4C-C3C-CAC-CBC
25	N	609	CHL	C4C-C3C-CAC-CBC
25	R	607	CHL	C4C-C3C-CAC-CBC
25	Y	607	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
25	6	607	CHL	C4C-C3C-CAC-CBC
25	6	609	CHL	C4C-C3C-CAC-CBC
25	7	607	CHL	C4C-C3C-CAC-CBC
25	8	609	CHL	C4C-C3C-CAC-CBC
25	g	607	CHL	C4C-C3C-CAC-CBC
25	g	609	CHL	C4C-C3C-CAC-CBC
25	n	605	CHL	C4C-C3C-CAC-CBC
25	n	607	CHL	C4C-C3C-CAC-CBC
25	n	609	CHL	C4C-C3C-CAC-CBC
25	r	607	CHL	C4C-C3C-CAC-CBC
25	y	607	CHL	C4C-C3C-CAC-CBC
26	G	611	CLA	O1A-CGA-O2A-C1
25	r	607	CHL	C5-C6-C7-C8
30	n	2630	LHG	C31-C32-C33-C34
30	D	408	LHG	O1-C1-C2-O2
30	d	408	LHG	O1-C1-C2-O2
26	2	602	CLA	C1A-C2A-CAA-CBA
26	2	610	CLA	C1A-C2A-CAA-CBA
26	3	614	CLA	C4B-C3B-CAB-CBB
26	B	611	CLA	C4B-C3B-CAB-CBB
26	G	604	CLA	C1A-C2A-CAA-CBA
26	R	601	CLA	C4B-C3B-CAB-CBB
26	R	611	CLA	C4B-C3B-CAB-CBB
26	S	610	CLA	C1A-C2A-CAA-CBA
26	6	602	CLA	C1A-C2A-CAA-CBA
26	6	610	CLA	C1A-C2A-CAA-CBA
26	7	614	CLA	C4B-C3B-CAB-CBB
26	b	611	CLA	C4B-C3B-CAB-CBB
26	g	604	CLA	C1A-C2A-CAA-CBA
26	r	601	CLA	C4B-C3B-CAB-CBB
26	r	611	CLA	C4B-C3B-CAB-CBB
26	s	610	CLA	C1A-C2A-CAA-CBA
30	D	409	LHG	C33-C34-C35-C36
30	d	409	LHG	C33-C34-C35-C36
30	B	2630	LHG	C33-C34-C35-C36
30	b	2630	LHG	C33-C34-C35-C36
26	Y	612	CLA	C4-C3-C5-C6
26	y	612	CLA	C4-C3-C5-C6
26	C	501	CLA	C15-C16-C17-C18
26	c	501	CLA	C15-C16-C17-C18
26	2	602	CLA	C2-C3-C5-C6
25	7	609	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
37	A	413	LMG	C36-C37-C38-C39
37	a	413	LMG	C36-C37-C38-C39
26	C	503	CLA	O1A-CGA-O2A-C1
26	c	503	CLA	O1A-CGA-O2A-C1
25	8	606	CHL	O1D-CGD-O2D-CED
30	C	2630	LHG	C13-C14-C15-C16
25	3	609	CHL	C2C-C3C-CAC-CBC
30	C	522	LHG	O6-C4-C5-C6
30	C	523	LHG	O6-C4-C5-C6
30	c	522	LHG	O6-C4-C5-C6
30	c	523	LHG	O6-C4-C5-C6
30	c	2630	LHG	C13-C14-C15-C16
30	L	101	LHG	C25-C26-C27-C28
30	l	101	LHG	C25-C26-C27-C28
39	C	519	DGD	C8B-C9B-CAB-CBB
39	c	519	DGD	C8B-C9B-CAB-CBB
25	4	606	CHL	O1D-CGD-O2D-CED
26	C	504	CLA	O1D-CGD-O2D-CED
26	c	504	CLA	O1D-CGD-O2D-CED
25	1	607	CHL	C11-C10-C8-C7
25	G	601	CHL	C12-C13-C15-C16
25	G	608	CHL	C11-C12-C13-C15
25	Y	608	CHL	C6-C7-C8-C10
25	Y	608	CHL	C11-C10-C8-C7
25	5	607	CHL	C11-C10-C8-C7
25	g	601	CHL	C12-C13-C15-C16
25	g	608	CHL	C11-C12-C13-C15
25	y	608	CHL	C6-C7-C8-C10
25	y	608	CHL	C11-C10-C8-C7
25	y	608	CHL	C12-C13-C15-C16
26	B	615	CLA	C6-C7-C8-C10
26	B	617	CLA	C6-C7-C8-C10
26	C	504	CLA	C12-C13-C15-C16
26	C	509	CLA	C11-C10-C8-C7
26	C	510	CLA	C11-C10-C8-C7
26	G	613	CLA	C12-C13-C15-C16
26	N	603	CLA	C12-C13-C15-C16
26	b	614	CLA	C11-C12-C13-C15
26	b	615	CLA	C6-C7-C8-C10
26	b	617	CLA	C6-C7-C8-C10
26	c	504	CLA	C12-C13-C15-C16
26	c	509	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
26	c	510	CLA	C11-C10-C8-C7
26	g	613	CLA	C12-C13-C15-C16
26	n	603	CLA	C12-C13-C15-C16
26	C	511	CLA	C16-C17-C18-C19
26	c	511	CLA	C16-C17-C18-C19
35	A	409	PHO	C16-C17-C18-C20
35	a	409	PHO	C16-C17-C18-C20
36	b	621	SQD	C13-C14-C15-C16
26	R	602	CLA	CBA-CGA-O2A-C1
26	r	602	CLA	CBA-CGA-O2A-C1
30	D	409	LHG	C24-C23-O8-C6
30	d	409	LHG	C24-C23-O8-C6
30	B	2631	LHG	C12-C13-C14-C15
36	B	621	SQD	C13-C14-C15-C16
25	N	601	CHL	C8-C10-C11-C12
25	n	601	CHL	C8-C10-C11-C12
30	b	2631	LHG	C12-C13-C14-C15
39	h	102	DGD	C8A-C9A-CAA-CBA
26	C	504	CLA	O1A-CGA-O2A-C1
26	c	504	CLA	O1A-CGA-O2A-C1
37	C	521	LMG	C14-C15-C16-C17
37	c	521	LMG	C14-C15-C16-C17
39	H	102	DGD	C8A-C9A-CAA-CBA
26	3	610	CLA	C11-C12-C13-C15
26	7	610	CLA	C11-C12-C13-C15
30	D	410	LHG	C28-C29-C30-C31
30	C	523	LHG	O6-C4-C5-O7
30	D	409	LHG	O6-C4-C5-O7
30	c	523	LHG	O6-C4-C5-O7
30	d	409	LHG	O6-C4-C5-O7
30	d	410	LHG	C28-C29-C30-C31
25	G	607	CHL	C11-C10-C8-C9
25	N	601	CHL	C14-C13-C15-C16
25	Y	601	CHL	C14-C13-C15-C16
25	g	607	CHL	C11-C10-C8-C9
25	n	601	CHL	C14-C13-C15-C16
25	y	601	CHL	C14-C13-C15-C16
26	B	608	CLA	C14-C13-C15-C16
26	C	506	CLA	C6-C7-C8-C9
26	S	611	CLA	C6-C7-C8-C9
26	b	608	CLA	C14-C13-C15-C16
26	c	502	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	c	506	CLA	C6-C7-C8-C9
26	s	611	CLA	C6-C7-C8-C9
25	G	606	CHL	O1A-CGA-O2A-C1
25	g	606	CHL	O1A-CGA-O2A-C1
26	Y	610	CLA	C8-C10-C11-C12
29	Y	1623	NEX	C33-C34-C35-C15
29	y	1623	NEX	C33-C34-C35-C15
26	Y	603	CLA	C16-C17-C18-C19
26	y	603	CLA	C16-C17-C18-C19
26	y	610	CLA	C8-C10-C11-C12
39	c	519	DGD	CBA-CCA-CDA-CEA
25	G	606	CHL	C1-C2-C3-C4
25	N	606	CHL	C1-C2-C3-C4
25	Y	606	CHL	C1-C2-C3-C4
25	g	606	CHL	C1-C2-C3-C4
25	n	606	CHL	C1-C2-C3-C4
25	y	606	CHL	C1-C2-C3-C4
26	R	601	CLA	C1-C2-C3-C4
26	R	611	CLA	C1-C2-C3-C4
26	R	612	CLA	C1-C2-C3-C4
26	S	612	CLA	C1-C2-C3-C4
26	r	601	CLA	C1-C2-C3-C4
26	r	611	CLA	C1-C2-C3-C4
26	r	612	CLA	C1-C2-C3-C4
26	s	612	CLA	C1-C2-C3-C4
39	C	519	DGD	CBA-CCA-CDA-CEA
39	C	520	DGD	C3B-C4B-C5B-C6B
39	c	520	DGD	C3B-C4B-C5B-C6B
36	A	418	SQD	O47-C45-C46-O48
36	B	621	SQD	O6-C44-C45-O47
36	a	418	SQD	O47-C45-C46-O48
36	b	621	SQD	O6-C44-C45-O47
37	A	413	LMG	O7-C8-C9-O8
37	Z	101	LMG	O1-C7-C8-O7
37	a	413	LMG	O7-C8-C9-O8
37	z	101	LMG	O1-C7-C8-O7
30	D	410	LHG	C1-C2-C3-O3
30	d	410	LHG	C1-C2-C3-O3
26	B	612	CLA	C15-C16-C17-C18
26	C	503	CLA	C10-C11-C12-C13
26	b	612	CLA	C15-C16-C17-C18
26	c	503	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
39	C	518	DGD	C5A-C6A-C7A-C8A
36	B	621	SQD	C44-C45-C46-O48
36	B	623	SQD	C44-C45-C46-O48
36	b	621	SQD	C44-C45-C46-O48
36	b	623	SQD	C44-C45-C46-O48
37	C	521	LMG	C7-C8-C9-O8
37	c	521	LMG	C7-C8-C9-O8
37	A	413	LMG	O10-C28-O8-C9
37	a	413	LMG	O10-C28-O8-C9
39	h	102	DGD	CDA-CEA-CFA-CGA
39	c	518	DGD	C5A-C6A-C7A-C8A
39	H	102	DGD	CDA-CEA-CFA-CGA
26	1	603	CLA	CAD-CBD-CGD-O2D
26	2	603	CLA	CAD-CBD-CGD-O2D
26	3	603	CLA	CAD-CBD-CGD-O2D
26	3	604	CLA	CAD-CBD-CGD-O2D
26	3	614	CLA	CAD-CBD-CGD-O2D
26	B	605	CLA	CAD-CBD-CGD-O2D
26	B	606	CLA	CAD-CBD-CGD-O2D
26	C	504	CLA	CAD-CBD-CGD-O2D
26	C	513	CLA	CAD-CBD-CGD-O2D
26	5	603	CLA	CAD-CBD-CGD-O2D
26	6	603	CLA	CAD-CBD-CGD-O2D
26	7	603	CLA	CAD-CBD-CGD-O2D
26	7	604	CLA	CAD-CBD-CGD-O2D
26	7	614	CLA	CAD-CBD-CGD-O2D
26	b	605	CLA	CAD-CBD-CGD-O2D
26	b	606	CLA	CAD-CBD-CGD-O2D
26	c	504	CLA	CAD-CBD-CGD-O2D
26	c	513	CLA	CAD-CBD-CGD-O2D
26	C	509	CLA	C8-C10-C11-C12
26	N	610	CLA	C13-C15-C16-C17
26	c	509	CLA	C8-C10-C11-C12
26	n	610	CLA	C13-C15-C16-C17
26	c	511	CLA	O1D-CGD-O2D-CED
26	G	611	CLA	CBA-CGA-O2A-C1
26	g	611	CLA	CBA-CGA-O2A-C1
25	R	606	CHL	C5-C6-C7-C8
25	r	606	CHL	C5-C6-C7-C8
26	G	603	CLA	CBD-CGD-O2D-CED
26	2	602	CLA	C2A-CAA-CBA-CGA
26	C	506	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	N	602	CLA	C2A-CAA-CBA-CGA
26	N	603	CLA	C2A-CAA-CBA-CGA
26	6	602	CLA	C2A-CAA-CBA-CGA
26	c	506	CLA	C2A-CAA-CBA-CGA
26	n	602	CLA	C2A-CAA-CBA-CGA
26	n	603	CLA	C2A-CAA-CBA-CGA
26	g	603	CLA	CBD-CGD-O2D-CED
30	C	523	LHG	C11-C10-C9-C8
30	c	523	LHG	C11-C10-C9-C8
30	d	409	LHG	C16-C17-C18-C19
30	D	409	LHG	C16-C17-C18-C19
25	1	607	CHL	CHA-CBD-CGD-O1D
25	1	608	CHL	CHA-CBD-CGD-O2D
25	2	607	CHL	CHA-CBD-CGD-O1D
25	4	601	CHL	CHA-CBD-CGD-O2D
25	4	601	CHL	CAD-CBD-CGD-O2D
25	N	606	CHL	CHA-CBD-CGD-O2D
25	N	607	CHL	CHA-CBD-CGD-O1D
25	N	607	CHL	CHA-CBD-CGD-O2D
25	S	608	CHL	CHA-CBD-CGD-O2D
25	Y	601	CHL	CHA-CBD-CGD-O2D
25	Y	607	CHL	CHA-CBD-CGD-O2D
25	5	607	CHL	CHA-CBD-CGD-O1D
25	5	608	CHL	CHA-CBD-CGD-O2D
25	6	607	CHL	CHA-CBD-CGD-O1D
25	8	601	CHL	CHA-CBD-CGD-O2D
25	8	601	CHL	CAD-CBD-CGD-O2D
25	n	606	CHL	CHA-CBD-CGD-O2D
25	n	607	CHL	CHA-CBD-CGD-O1D
25	n	607	CHL	CHA-CBD-CGD-O2D
25	s	608	CHL	CHA-CBD-CGD-O2D
25	y	601	CHL	CHA-CBD-CGD-O2D
25	y	607	CHL	CHA-CBD-CGD-O2D
26	1	603	CLA	CAD-CBD-CGD-O1D
26	2	602	CLA	CHA-CBD-CGD-O1D
26	2	602	CLA	CHA-CBD-CGD-O2D
26	2	603	CLA	CAD-CBD-CGD-O1D
26	2	610	CLA	CHA-CBD-CGD-O1D
26	2	612	CLA	CHA-CBD-CGD-O1D
26	3	603	CLA	CAD-CBD-CGD-O1D
26	3	604	CLA	CAD-CBD-CGD-O1D
26	3	614	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
26	B	602	CLA	CAD-CBD-CGD-O1D
26	B	605	CLA	CAD-CBD-CGD-O1D
26	B	606	CLA	CAD-CBD-CGD-O1D
26	C	504	CLA	CAD-CBD-CGD-O1D
26	C	513	CLA	CAD-CBD-CGD-O1D
26	G	612	CLA	CHA-CBD-CGD-O1D
26	G	612	CLA	CHA-CBD-CGD-O2D
26	N	602	CLA	CHA-CBD-CGD-O2D
26	Y	602	CLA	CHA-CBD-CGD-O1D
26	Y	602	CLA	CHA-CBD-CGD-O2D
26	5	603	CLA	CAD-CBD-CGD-O1D
26	6	602	CLA	CHA-CBD-CGD-O1D
26	6	602	CLA	CHA-CBD-CGD-O2D
26	6	603	CLA	CAD-CBD-CGD-O1D
26	6	610	CLA	CHA-CBD-CGD-O1D
26	6	612	CLA	CHA-CBD-CGD-O1D
26	7	603	CLA	CAD-CBD-CGD-O1D
26	7	604	CLA	CAD-CBD-CGD-O1D
26	7	614	CLA	CAD-CBD-CGD-O1D
26	b	602	CLA	CAD-CBD-CGD-O1D
26	b	605	CLA	CAD-CBD-CGD-O1D
26	b	606	CLA	CAD-CBD-CGD-O1D
26	c	504	CLA	CAD-CBD-CGD-O1D
26	c	513	CLA	CAD-CBD-CGD-O1D
26	g	612	CLA	CHA-CBD-CGD-O1D
26	g	612	CLA	CHA-CBD-CGD-O2D
26	n	602	CLA	CHA-CBD-CGD-O2D
26	y	602	CLA	CHA-CBD-CGD-O1D
26	y	602	CLA	CHA-CBD-CGD-O2D
29	1	1623	NEX	C33-C34-C35-C15
29	N	1623	NEX	C33-C34-C35-C15
29	5	1623	NEX	C33-C34-C35-C15
29	n	1623	NEX	C33-C34-C35-C15
30	2	2630	LHG	C4-O6-P-O3
30	3	2630	LHG	C3-O3-P-O5
30	B	2630	LHG	C4-O6-P-O5
30	B	2631	LHG	C4-O6-P-O5
30	D	409	LHG	C3-O3-P-O5
30	D	410	LHG	C3-O3-P-O4
30	D	410	LHG	C3-O3-P-O5
30	D	410	LHG	C4-O6-P-O5
30	G	2630	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
30	N	2630	LHG	C3-O3-P-O5
30	R	2630	LHG	C3-O3-P-O5
30	S	2630	LHG	C4-O6-P-O3
30	Y	2630	LHG	C4-O6-P-O4
30	6	2630	LHG	C4-O6-P-O3
30	7	2630	LHG	C3-O3-P-O5
30	b	2630	LHG	C4-O6-P-O5
30	b	2631	LHG	C4-O6-P-O5
30	d	409	LHG	C3-O3-P-O5
30	d	410	LHG	C3-O3-P-O4
30	d	410	LHG	C3-O3-P-O5
30	d	410	LHG	C4-O6-P-O5
30	g	2630	LHG	C4-O6-P-O4
30	n	2630	LHG	C3-O3-P-O5
30	r	2630	LHG	C3-O3-P-O5
30	s	2630	LHG	C4-O6-P-O3
30	y	2630	LHG	C4-O6-P-O4
35	A	409	PHO	CHA-CBD-CGD-O2D
35	a	409	PHO	CHA-CBD-CGD-O2D
26	C	501	CLA	C4-C3-C5-C6
26	c	501	CLA	C4-C3-C5-C6
26	1	614	CLA	C2B-C3B-CAB-CBB
26	2	613	CLA	C2B-C3B-CAB-CBB
26	3	603	CLA	C2B-C3B-CAB-CBB
26	4	604	CLA	C2B-C3B-CAB-CBB
26	A	410	CLA	C2B-C3B-CAB-CBB
26	R	610	CLA	C2B-C3B-CAB-CBB
26	S	610	CLA	C2B-C3B-CAB-CBB
26	Y	614	CLA	C2B-C3B-CAB-CBB
26	5	614	CLA	C2B-C3B-CAB-CBB
26	6	613	CLA	C2B-C3B-CAB-CBB
26	7	603	CLA	C2B-C3B-CAB-CBB
26	8	604	CLA	C2B-C3B-CAB-CBB
26	a	410	CLA	C2B-C3B-CAB-CBB
26	r	610	CLA	C2B-C3B-CAB-CBB
26	s	610	CLA	C2B-C3B-CAB-CBB
26	y	614	CLA	C2B-C3B-CAB-CBB
31	C	516	BCR	C5-C6-C7-C8
31	c	516	BCR	C5-C6-C7-C8
25	R	608	CHL	C5-C6-C7-C8
26	C	506	CLA	C10-C11-C12-C13
26	C	508	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	c	506	CLA	C10-C11-C12-C13
26	c	508	CLA	C10-C11-C12-C13
29	S	1623	NEX	C11-C12-C13-C20
29	s	1623	NEX	C11-C12-C13-C20
30	L	101	LHG	C28-C29-C30-C31
30	l	101	LHG	C28-C29-C30-C31
26	C	511	CLA	O1D-CGD-O2D-CED
25	4	606	CHL	CBD-CGD-O2D-CED
25	r	608	CHL	C5-C6-C7-C8
37	b	622	LMG	C39-C40-C41-C42
37	B	622	LMG	C39-C40-C41-C42
26	G	611	CLA	C5-C6-C7-C8
25	8	606	CHL	CBD-CGD-O2D-CED
30	D	409	LHG	C28-C29-C30-C31
30	d	409	LHG	C28-C29-C30-C31
36	A	412	SQD	C17-C18-C19-C20
36	a	412	SQD	C17-C18-C19-C20
30	4	2630	LHG	O1-C1-C2-O2
30	8	2630	LHG	O1-C1-C2-O2
26	R	602	CLA	O1A-CGA-O2A-C1
26	r	602	CLA	O1A-CGA-O2A-C1
30	b	2630	LHG	C17-C18-C19-C20
30	B	2630	LHG	O1-C1-C2-C3
30	b	2630	LHG	O1-C1-C2-C3
30	B	2630	LHG	C17-C18-C19-C20
26	Y	612	CLA	C8-C10-C11-C12
26	g	611	CLA	C5-C6-C7-C8
26	y	612	CLA	C8-C10-C11-C12
35	A	408	PHO	C10-C11-C12-C13
35	a	408	PHO	C10-C11-C12-C13
26	1	610	CLA	C11-C10-C8-C7
26	5	610	CLA	C11-C10-C8-C7
26	R	612	CLA	O2A-C1-C2-C3
26	r	612	CLA	O2A-C1-C2-C3
39	H	102	DGD	CBB-CCB-CDB-CEB
39	h	102	DGD	CBB-CCB-CDB-CEB
38	D	405	PL9	C18-C19-C21-C22
25	2	606	CHL	C3C-C2C-CMC-OMC
25	6	606	CHL	C3C-C2C-CMC-OMC
31	C	515	BCR	C19-C20-C21-C22
31	c	515	BCR	C19-C20-C21-C22
26	R	610	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	r	610	CLA	O1D-CGD-O2D-CED
26	B	602	CLA	C16-C17-C18-C19
26	B	607	CLA	C16-C17-C18-C20
26	B	613	CLA	C16-C17-C18-C20
26	b	602	CLA	C16-C17-C18-C19
26	b	607	CLA	C16-C17-C18-C20
26	b	613	CLA	C16-C17-C18-C20
30	R	2630	LHG	C15-C16-C17-C18
30	r	2630	LHG	C15-C16-C17-C18
39	C	520	DGD	C9B-CAB-CBB-CCB
39	c	520	DGD	C9B-CAB-CBB-CCB
26	2	602	CLA	C11-C12-C13-C14
26	C	504	CLA	C11-C10-C8-C9
26	C	510	CLA	C11-C10-C8-C9
26	C	511	CLA	C11-C12-C13-C14
26	N	603	CLA	C14-C13-C15-C16
26	Y	613	CLA	C11-C12-C13-C14
26	6	602	CLA	C11-C12-C13-C14
26	c	504	CLA	C11-C10-C8-C9
26	c	510	CLA	C11-C10-C8-C9
26	c	511	CLA	C11-C12-C13-C14
26	n	603	CLA	C14-C13-C15-C16
26	y	613	CLA	C11-C12-C13-C14
30	G	2630	LHG	C34-C35-C36-C37
25	N	601	CHL	C6-C7-C8-C10
25	Y	608	CHL	C12-C13-C15-C16
25	n	601	CHL	C6-C7-C8-C10
26	B	614	CLA	C11-C12-C13-C15
26	C	502	CLA	C11-C12-C13-C15
26	C	502	CLA	C12-C13-C15-C16
26	C	504	CLA	C11-C10-C8-C7
26	c	502	CLA	C12-C13-C15-C16
26	c	504	CLA	C11-C10-C8-C7
35	A	408	PHO	C12-C13-C15-C16
35	a	408	PHO	C12-C13-C15-C16
30	g	2630	LHG	C34-C35-C36-C37
37	A	415	LMG	C29-C30-C31-C32
37	a	415	LMG	C29-C30-C31-C32
26	1	603	CLA	C2A-CAA-CBA-CGA
26	B	616	CLA	C16-C17-C18-C19
26	N	610	CLA	C16-C17-C18-C20
26	b	603	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
26	b	616	CLA	C16-C17-C18-C19
26	n	610	CLA	C16-C17-C18-C20
25	G	608	CHL	C8-C10-C11-C12
25	g	608	CHL	C8-C10-C11-C12
26	1	604	CLA	CBA-CGA-O2A-C1
26	5	604	CLA	CBA-CGA-O2A-C1
26	7	611	CLA	CBA-CGA-O2A-C1
30	G	2630	LHG	C30-C31-C32-C33
25	S	607	CHL	C4-C3-C5-C6
25	s	607	CHL	C4-C3-C5-C6
26	Y	611	CLA	C4-C3-C5-C6
26	y	611	CLA	C4-C3-C5-C6
26	C	507	CLA	C2-C3-C5-C6
26	c	507	CLA	C2-C3-C5-C6
38	d	405	PL9	C18-C19-C21-C22
30	C	522	LHG	C29-C30-C31-C32
30	c	522	LHG	C29-C30-C31-C32
30	g	2630	LHG	C30-C31-C32-C33
36	a	418	SQD	C13-C14-C15-C16
26	3	611	CLA	CBA-CGA-O2A-C1
30	L	101	LHG	C31-C32-C33-C34
30	l	101	LHG	C31-C32-C33-C34
36	A	418	SQD	C13-C14-C15-C16
39	H	102	DGD	C2A-C3A-C4A-C5A
25	N	609	CHL	O1D-CGD-O2D-CED
30	N	2630	LHG	C11-C12-C13-C14
30	n	2630	LHG	C11-C12-C13-C14
39	h	102	DGD	C2A-C3A-C4A-C5A
35	A	409	PHO	CAA-CBA-CGA-O2A
35	a	409	PHO	CAA-CBA-CGA-O2A
30	S	2630	LHG	O2-C2-C3-O3
30	s	2630	LHG	O2-C2-C3-O3
26	C	504	CLA	CBA-CGA-O2A-C1
26	c	504	CLA	CBA-CGA-O2A-C1
37	a	415	LMG	C29-C28-O8-C9
30	C	2630	LHG	C7-C8-C9-C10
30	c	2630	LHG	C7-C8-C9-C10
31	C	515	BCR	C9-C10-C11-C12
31	c	515	BCR	C9-C10-C11-C12
26	B	603	CLA	C16-C17-C18-C19
26	8	610	CLA	O1D-CGD-O2D-CED
26	g	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	5	603	CLA	C2A-CAA-CBA-CGA
37	A	415	LMG	C29-C28-O8-C9
26	4	610	CLA	O1D-CGD-O2D-CED
30	G	2630	LHG	C26-C27-C28-C29
26	C	507	CLA	C5-C6-C7-C8
26	c	507	CLA	C5-C6-C7-C8
25	n	609	CHL	O1D-CGD-O2D-CED
30	S	2630	LHG	C4-C5-C6-O8
30	s	2630	LHG	C4-C5-C6-O8
39	B	626	DGD	C1B-C2B-C3B-C4B
39	b	626	DGD	C1B-C2B-C3B-C4B
30	d	408	LHG	C10-C11-C12-C13
30	g	2630	LHG	C26-C27-C28-C29
31	4	623	BCR	C36-C18-C19-C20
31	C	515	BCR	C36-C18-C19-C20
31	8	623	BCR	C36-C18-C19-C20
31	c	515	BCR	C36-C18-C19-C20
30	D	408	LHG	C10-C11-C12-C13
37	d	411	LMG	C31-C32-C33-C34
26	B	608	CLA	C16-C17-C18-C20
26	b	608	CLA	C16-C17-C18-C20
26	G	603	CLA	O1D-CGD-O2D-CED
37	D	411	LMG	C31-C32-C33-C34
30	N	2630	LHG	C35-C36-C37-C38
39	C	518	DGD	C5D-C6D-O5D-C1E
39	c	518	DGD	C5D-C6D-O5D-C1E
26	4	612	CLA	C2A-CAA-CBA-CGA
26	C	513	CLA	C2A-CAA-CBA-CGA
26	N	613	CLA	C2A-CAA-CBA-CGA
26	R	602	CLA	C2A-CAA-CBA-CGA
26	Y	610	CLA	C2A-CAA-CBA-CGA
26	8	612	CLA	C2A-CAA-CBA-CGA
26	c	513	CLA	C2A-CAA-CBA-CGA
26	n	613	CLA	C2A-CAA-CBA-CGA
26	r	602	CLA	C2A-CAA-CBA-CGA
26	y	610	CLA	C2A-CAA-CBA-CGA
29	2	1623	NEX	C13-C14-C15-C35
29	6	1623	NEX	C13-C14-C15-C35
30	n	2630	LHG	C35-C36-C37-C38
26	3	602	CLA	C4-C3-C5-C6
26	7	602	CLA	C4-C3-C5-C6
26	Y	611	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	y	611	CLA	C2-C3-C5-C6
36	a	418	SQD	C18-C19-C20-C21
37	A	413	LMG	C15-C16-C17-C18
37	a	413	LMG	C15-C16-C17-C18
26	A	405	CLA	C4C-C3C-CAC-CBC
26	a	405	CLA	C4C-C3C-CAC-CBC
36	A	418	SQD	C18-C19-C20-C21
26	1	604	CLA	O1A-CGA-O2A-C1
26	5	604	CLA	O1A-CGA-O2A-C1
30	r	2630	LHG	O9-C7-O7-C5
30	R	2630	LHG	C1-C2-C3-O3
30	r	2630	LHG	C1-C2-C3-O3
25	Y	608	CHL	C6-C7-C8-C9
25	y	608	CHL	C6-C7-C8-C9
26	B	617	CLA	C6-C7-C8-C9
26	D	403	CLA	C11-C12-C13-C14
26	b	617	CLA	C6-C7-C8-C9
26	d	403	CLA	C11-C12-C13-C14
39	b	626	DGD	C9B-CAB-CBB-CCB
30	Y	2630	LHG	C5-C4-O6-P
30	y	2630	LHG	C5-C4-O6-P
30	Y	2630	LHG	C9-C10-C11-C12
37	A	415	LMG	C33-C34-C35-C36
37	B	2633	LMG	C35-C36-C37-C38
37	a	415	LMG	C33-C34-C35-C36
26	1	613	CLA	C4B-C3B-CAB-CBB
26	2	604	CLA	C4B-C3B-CAB-CBB
26	3	604	CLA	C4B-C3B-CAB-CBB
26	5	613	CLA	C4B-C3B-CAB-CBB
26	6	604	CLA	C4B-C3B-CAB-CBB
26	7	604	CLA	C4B-C3B-CAB-CBB
30	y	2630	LHG	C9-C10-C11-C12
37	b	2633	LMG	C35-C36-C37-C38
39	B	626	DGD	C9B-CAB-CBB-CCB
30	R	2630	LHG	O10-C23-O8-C6
30	C	523	LHG	C24-C23-O8-C6
30	c	523	LHG	C24-C23-O8-C6
26	R	613	CLA	C5-C6-C7-C8
26	r	613	CLA	C5-C6-C7-C8
30	r	2630	LHG	O10-C23-O8-C6
25	2	609	CHL	C4-C3-C5-C6
25	3	609	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	G	608	CHL	C4-C3-C5-C6
25	6	609	CHL	C4-C3-C5-C6
25	7	609	CHL	C4-C3-C5-C6
25	g	608	CHL	C4-C3-C5-C6
26	S	612	CLA	O2A-C1-C2-C3
26	s	612	CLA	O2A-C1-C2-C3
30	D	410	LHG	C12-C13-C14-C15
26	4	603	CLA	CAA-CBA-CGA-O2A
26	8	603	CLA	CAA-CBA-CGA-O2A
39	c	518	DGD	C3B-C4B-C5B-C6B
26	r	610	CLA	C10-C11-C12-C13
26	y	611	CLA	C8-C10-C11-C12
30	d	410	LHG	C12-C13-C14-C15
37	Z	101	LMG	C29-C30-C31-C32
39	C	518	DGD	C3B-C4B-C5B-C6B
30	B	2631	LHG	C35-C36-C37-C38
30	b	2631	LHG	C35-C36-C37-C38
37	z	101	LMG	C29-C30-C31-C32
39	C	518	DGD	C5B-C6B-C7B-C8B
25	1	605	CHL	O1D-CGD-O2D-CED
25	1	607	CHL	O1D-CGD-O2D-CED
37	A	413	LMG	C17-C18-C19-C20
37	a	413	LMG	C17-C18-C19-C20
26	3	613	CLA	C6-C7-C8-C10
26	A	406	CLA	C11-C12-C13-C15
26	B	614	CLA	C6-C7-C8-C10
26	7	613	CLA	C6-C7-C8-C10
26	a	406	CLA	C11-C12-C13-C15
26	b	614	CLA	C6-C7-C8-C10
26	c	502	CLA	C11-C12-C13-C15
26	1	610	CLA	C5-C6-C7-C8
26	D	403	CLA	C5-C6-C7-C8
26	R	610	CLA	C10-C11-C12-C13
26	5	610	CLA	C5-C6-C7-C8
26	d	403	CLA	C5-C6-C7-C8
39	c	518	DGD	C5B-C6B-C7B-C8B
25	5	607	CHL	O1D-CGD-O2D-CED
26	7	611	CLA	O1A-CGA-O2A-C1
30	R	2630	LHG	O9-C7-O7-C5
39	h	102	DGD	CAA-CBA-CCA-CDA
26	B	607	CLA	C16-C17-C18-C19
26	b	607	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
39	C	520	DGD	C6A-C7A-C8A-C9A
39	H	102	DGD	CAA-CBA-CCA-CDA
39	c	520	DGD	C6A-C7A-C8A-C9A
39	C	519	DGD	C1B-C2B-C3B-C4B
39	c	519	DGD	C1B-C2B-C3B-C4B
25	4	607	CHL	O1D-CGD-O2D-CED
25	5	605	CHL	O1D-CGD-O2D-CED
26	Y	611	CLA	C8-C10-C11-C12
26	r	609	CLA	C8-C10-C11-C12
26	3	611	CLA	O1A-CGA-O2A-C1
39	c	519	DGD	C7A-C8A-C9A-CAA
25	Y	609	CHL	C4-C3-C5-C6
25	y	609	CHL	C4-C3-C5-C6
26	B	610	CLA	C3A-C2A-CAA-CBA
26	C	513	CLA	C3A-C2A-CAA-CBA
26	S	604	CLA	C3A-C2A-CAA-CBA
26	b	610	CLA	C3A-C2A-CAA-CBA
26	c	513	CLA	C3A-C2A-CAA-CBA
26	s	604	CLA	C3A-C2A-CAA-CBA
39	C	519	DGD	C7A-C8A-C9A-CAA
26	Y	612	CLA	C2-C3-C5-C6
26	y	612	CLA	C2-C3-C5-C6
26	R	609	CLA	C8-C10-C11-C12
29	1	1623	NEX	C39-C29-C30-C31
29	2	1623	NEX	C39-C29-C30-C31
29	3	1623	NEX	C39-C29-C30-C31
29	G	1623	NEX	C39-C29-C30-C31
29	N	1623	NEX	C39-C29-C30-C31
29	R	623	NEX	C39-C29-C30-C31
29	S	1623	NEX	C39-C29-C30-C31
29	Y	1623	NEX	C39-C29-C30-C31
29	5	1623	NEX	C39-C29-C30-C31
29	6	1623	NEX	C39-C29-C30-C31
29	7	1623	NEX	C39-C29-C30-C31
29	g	1623	NEX	C39-C29-C30-C31
29	n	1623	NEX	C39-C29-C30-C31
29	r	623	NEX	C39-C29-C30-C31
29	s	1623	NEX	C39-C29-C30-C31
29	y	1623	NEX	C39-C29-C30-C31
37	B	622	LMG	O6-C1-O1-C7
37	b	622	LMG	O6-C1-O1-C7
25	R	606	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	r	606	CHL	C13-C15-C16-C17
26	C	512	CLA	C10-C11-C12-C13
26	R	603	CLA	C5-C6-C7-C8
26	Y	602	CLA	C15-C16-C17-C18
26	r	603	CLA	C5-C6-C7-C8
26	y	602	CLA	C15-C16-C17-C18
30	D	409	LHG	C11-C12-C13-C14
26	c	512	CLA	C10-C11-C12-C13
30	d	409	LHG	C11-C12-C13-C14
30	d	409	LHG	C29-C30-C31-C32
37	B	2633	LMG	C34-C35-C36-C37
37	b	2633	LMG	C34-C35-C36-C37
25	8	607	CHL	O1D-CGD-O2D-CED
30	D	409	LHG	C29-C30-C31-C32
25	2	609	CHL	C2-C1-O2A-CGA
25	6	609	CHL	C2-C1-O2A-CGA
26	G	603	CLA	C2-C1-O2A-CGA
26	g	603	CLA	C2-C1-O2A-CGA
36	A	418	SQD	C24-C25-C26-C27
36	a	418	SQD	C24-C25-C26-C27
27	4	620	LUT	C7-C8-C9-C19
29	3	1623	NEX	C11-C12-C13-C20
29	7	1623	NEX	C11-C12-C13-C20
30	2	2630	LHG	C5-C4-O6-P
30	G	2630	LHG	C5-C4-O6-P
30	6	2630	LHG	C5-C4-O6-P
30	g	2630	LHG	C5-C4-O6-P
31	A	411	BCR	C7-C8-C9-C34
31	a	411	BCR	C7-C8-C9-C34
26	N	604	CLA	CBA-CGA-O2A-C1
26	n	604	CLA	CBA-CGA-O2A-C1
26	4	603	CLA	CAA-CBA-CGA-O1A
26	8	603	CLA	CAA-CBA-CGA-O1A
26	G	602	CLA	C15-C16-C17-C18
26	g	602	CLA	C15-C16-C17-C18
25	N	608	CHL	C4-C3-C5-C6
26	B	602	CLA	CAA-CBA-CGA-O2A
26	b	602	CLA	CAA-CBA-CGA-O2A
26	g	610	CLA	C16-C17-C18-C19
37	Z	101	LMG	C11-C12-C13-C14
25	G	601	CHL	C14-C13-C15-C16
25	G	607	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	Y	607	CHL	C11-C12-C13-C14
25	Y	608	CHL	C11-C10-C8-C9
25	g	601	CHL	C14-C13-C15-C16
25	g	607	CHL	C11-C12-C13-C14
25	y	607	CHL	C11-C12-C13-C14
25	y	608	CHL	C11-C10-C8-C9
26	3	613	CLA	C6-C7-C8-C9
26	B	602	CLA	C6-C7-C8-C9
26	B	603	CLA	C6-C7-C8-C9
26	B	617	CLA	C11-C10-C8-C9
26	C	501	CLA	C11-C10-C8-C9
26	G	611	CLA	C6-C7-C8-C9
26	R	610	CLA	C6-C7-C8-C9
26	Y	603	CLA	C6-C7-C8-C9
26	7	613	CLA	C6-C7-C8-C9
26	b	602	CLA	C6-C7-C8-C9
26	b	603	CLA	C6-C7-C8-C9
26	b	617	CLA	C11-C10-C8-C9
26	c	501	CLA	C11-C10-C8-C9
26	g	611	CLA	C6-C7-C8-C9
26	r	610	CLA	C6-C7-C8-C9
26	y	603	CLA	C6-C7-C8-C9
37	z	101	LMG	C11-C12-C13-C14
26	G	610	CLA	C16-C17-C18-C19
26	B	606	CLA	CBA-CGA-O2A-C1
30	G	2630	LHG	C11-C12-C13-C14
30	g	2630	LHG	C11-C12-C13-C14
37	B	2633	LMG	C7-C8-O7-C10
37	b	2633	LMG	C7-C8-O7-C10
26	G	612	CLA	C3-C5-C6-C7
26	g	612	CLA	C3-C5-C6-C7
25	1	607	CHL	C1A-C2A-CAA-CBA
25	1	609	CHL	C1A-C2A-CAA-CBA
25	3	609	CHL	C1A-C2A-CAA-CBA
25	4	607	CHL	C1A-C2A-CAA-CBA
25	G	609	CHL	C1A-C2A-CAA-CBA
25	N	609	CHL	C1A-C2A-CAA-CBA
25	5	607	CHL	C1A-C2A-CAA-CBA
25	5	609	CHL	C1A-C2A-CAA-CBA
25	7	609	CHL	C1A-C2A-CAA-CBA
25	8	607	CHL	C1A-C2A-CAA-CBA
25	g	609	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	n	609	CHL	C1A-C2A-CAA-CBA
35	A	409	PHO	C1A-C2A-CAA-CBA
35	a	409	PHO	C1A-C2A-CAA-CBA
25	n	608	CHL	C4-C3-C5-C6
26	b	606	CLA	CBA-CGA-O2A-C1
30	C	523	LHG	C30-C31-C32-C33
30	c	523	LHG	C30-C31-C32-C33
26	s	602	CLA	O1A-CGA-O2A-C1
30	C	2630	LHG	C19-C20-C21-C22
26	3	604	CLA	CAA-CBA-CGA-O2A
26	7	604	CLA	CAA-CBA-CGA-O2A
30	c	2630	LHG	C19-C20-C21-C22
25	1	608	CHL	C2A-CAA-CBA-CGA
26	R	613	CLA	C2A-CAA-CBA-CGA
26	S	614	CLA	C2A-CAA-CBA-CGA
26	r	613	CLA	C2A-CAA-CBA-CGA
26	s	614	CLA	C2A-CAA-CBA-CGA
26	S	602	CLA	O1A-CGA-O2A-C1
26	3	602	CLA	C1A-C2A-CAA-CBA
26	3	610	CLA	C1A-C2A-CAA-CBA
26	7	602	CLA	C1A-C2A-CAA-CBA
26	7	610	CLA	C1A-C2A-CAA-CBA
29	1	1623	NEX	C28-C29-C30-C31
29	2	1623	NEX	C28-C29-C30-C31
29	3	1623	NEX	C28-C29-C30-C31
29	G	1623	NEX	C28-C29-C30-C31
29	N	1623	NEX	C28-C29-C30-C31
29	R	623	NEX	C28-C29-C30-C31
29	S	1623	NEX	C28-C29-C30-C31
29	Y	1623	NEX	C28-C29-C30-C31
29	5	1623	NEX	C28-C29-C30-C31
29	6	1623	NEX	C28-C29-C30-C31
29	7	1623	NEX	C28-C29-C30-C31
29	g	1623	NEX	C28-C29-C30-C31
29	n	1623	NEX	C28-C29-C30-C31
29	r	623	NEX	C28-C29-C30-C31
29	s	1623	NEX	C28-C29-C30-C31
29	y	1623	NEX	C28-C29-C30-C31
30	N	2630	LHG	C24-C23-O8-C6
26	1	602	CLA	C2B-C3B-CAB-CBB
26	2	614	CLA	C2B-C3B-CAB-CBB
26	3	602	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	3	614	CLA	C2B-C3B-CAB-CBB
26	B	606	CLA	C2B-C3B-CAB-CBB
26	B	611	CLA	C2B-C3B-CAB-CBB
26	C	503	CLA	C2B-C3B-CAB-CBB
26	G	610	CLA	C2B-C3B-CAB-CBB
26	R	601	CLA	C2B-C3B-CAB-CBB
26	S	603	CLA	C2B-C3B-CAB-CBB
26	Y	610	CLA	C2B-C3B-CAB-CBB
26	5	602	CLA	C2B-C3B-CAB-CBB
26	6	614	CLA	C2B-C3B-CAB-CBB
26	7	602	CLA	C2B-C3B-CAB-CBB
26	7	614	CLA	C2B-C3B-CAB-CBB
26	b	606	CLA	C2B-C3B-CAB-CBB
26	b	611	CLA	C2B-C3B-CAB-CBB
26	c	503	CLA	C2B-C3B-CAB-CBB
26	g	610	CLA	C2B-C3B-CAB-CBB
26	r	601	CLA	C2B-C3B-CAB-CBB
26	s	603	CLA	C2B-C3B-CAB-CBB
26	y	610	CLA	C2B-C3B-CAB-CBB
27	1	1620	LUT	C5-C6-C7-C8
27	2	1620	LUT	C5-C6-C7-C8
27	3	1621	LUT	C1-C6-C7-C8
27	G	1620	LUT	C1-C6-C7-C8
27	N	1620	LUT	C1-C6-C7-C8
27	S	1620	LUT	C1-C6-C7-C8
27	S	1621	LUT	C1-C6-C7-C8
27	Y	1620	LUT	C5-C6-C7-C8
27	5	1620	LUT	C5-C6-C7-C8
27	6	1620	LUT	C5-C6-C7-C8
27	7	1621	LUT	C1-C6-C7-C8
27	g	1620	LUT	C1-C6-C7-C8
27	n	1620	LUT	C1-C6-C7-C8
27	s	1620	LUT	C1-C6-C7-C8
27	s	1621	LUT	C1-C6-C7-C8
27	y	1620	LUT	C5-C6-C7-C8
31	A	411	BCR	C1-C6-C7-C8
31	A	411	BCR	C5-C6-C7-C8
31	B	620	BCR	C23-C24-C25-C26
31	C	514	BCR	C5-C6-C7-C8
31	C	515	BCR	C23-C24-C25-C26
31	D	404	BCR	C5-C6-C7-C8
31	T	101	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
31	T	101	BCR	C23-C24-C25-C30
31	a	411	BCR	C1-C6-C7-C8
31	a	411	BCR	C5-C6-C7-C8
31	b	620	BCR	C23-C24-C25-C26
31	c	514	BCR	C5-C6-C7-C8
31	c	515	BCR	C23-C24-C25-C26
31	d	404	BCR	C5-C6-C7-C8
31	t	101	BCR	C23-C24-C25-C26
31	t	101	BCR	C23-C24-C25-C30
25	4	606	CHL	CAA-CBA-CGA-O1A
30	n	2630	LHG	C24-C23-O8-C6
26	n	604	CLA	O1A-CGA-O2A-C1
26	1	610	CLA	C11-C10-C8-C9
26	5	610	CLA	C11-C10-C8-C9
25	8	606	CHL	CAA-CBA-CGA-O1A
26	4	602	CLA	CAA-CBA-CGA-O2A
26	8	602	CLA	CAA-CBA-CGA-O2A
39	C	518	DGD	CAB-CBB-CCB-CDB
25	3	609	CHL	C2-C3-C5-C6
25	S	607	CHL	C2-C3-C5-C6
25	Y	609	CHL	C2-C3-C5-C6
25	7	609	CHL	C2-C3-C5-C6
25	s	607	CHL	C2-C3-C5-C6
25	y	609	CHL	C2-C3-C5-C6
39	c	518	DGD	CAB-CBB-CCB-CDB
25	Y	606	CHL	O2A-C1-C2-C3
25	y	606	CHL	O2A-C1-C2-C3
25	4	601	CHL	CAA-CBA-CGA-O2A
25	4	606	CHL	CAA-CBA-CGA-O2A
25	8	601	CHL	CAA-CBA-CGA-O2A
25	8	606	CHL	CAA-CBA-CGA-O2A
26	N	604	CLA	O1A-CGA-O2A-C1
25	G	608	CHL	C11-C10-C8-C7
25	N	608	CHL	C12-C13-C15-C16
25	R	606	CHL	C11-C10-C8-C7
25	g	608	CHL	C11-C10-C8-C7
25	n	608	CHL	C12-C13-C15-C16
25	r	606	CHL	C11-C10-C8-C7
26	C	501	CLA	C11-C10-C8-C7
26	D	403	CLA	C11-C10-C8-C7
26	N	613	CLA	C11-C10-C8-C7
26	Y	613	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
26	c	501	CLA	C11-C10-C8-C7
26	d	403	CLA	C11-C10-C8-C7
26	n	613	CLA	C11-C10-C8-C7
26	y	613	CLA	C11-C12-C13-C15
37	A	413	LMG	C14-C15-C16-C17
25	5	608	CHL	C2A-CAA-CBA-CGA
26	1	613	CLA	C2A-CAA-CBA-CGA
26	5	613	CLA	C2A-CAA-CBA-CGA
37	Z	101	LMG	C19-C20-C21-C22
37	a	413	LMG	C14-C15-C16-C17
37	z	101	LMG	C19-C20-C21-C22
30	R	2630	LHG	C24-C25-C26-C27
30	S	2630	LHG	C33-C34-C35-C36
30	r	2630	LHG	C24-C25-C26-C27
30	s	2630	LHG	C33-C34-C35-C36
37	C	521	LMG	C36-C37-C38-C39
37	c	521	LMG	C36-C37-C38-C39
25	4	607	CHL	CAA-CBA-CGA-O2A
25	8	607	CHL	CAA-CBA-CGA-O2A
26	S	609	CLA	CAA-CBA-CGA-O2A
30	C	523	LHG	C27-C28-C29-C30
37	B	2633	LMG	C41-C42-C43-C44
37	b	2633	LMG	C41-C42-C43-C44
25	1	609	CHL	C12-C13-C15-C16
25	5	609	CHL	C12-C13-C15-C16
27	8	620	LUT	C7-C8-C9-C19
26	s	609	CLA	CAA-CBA-CGA-O2A
26	R	613	CLA	C4-C3-C5-C6
26	r	613	CLA	C4-C3-C5-C6
30	b	2631	LHG	C11-C12-C13-C14
25	2	609	CHL	C2-C3-C5-C6
25	G	608	CHL	C2-C3-C5-C6
25	6	609	CHL	C2-C3-C5-C6
25	g	608	CHL	C2-C3-C5-C6
30	B	2631	LHG	C11-C12-C13-C14
36	B	621	SQD	C14-C15-C16-C17
36	b	621	SQD	C14-C15-C16-C17
30	c	523	LHG	C27-C28-C29-C30
26	B	603	CLA	C16-C17-C18-C20
26	b	603	CLA	C16-C17-C18-C20
25	7	607	CHL	C2C-C3C-CAC-CBC
26	S	603	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	s	603	CLA	C2A-CAA-CBA-CGA
26	3	604	CLA	CAA-CBA-CGA-O1A
26	7	604	CLA	CAA-CBA-CGA-O1A
26	A	406	CLA	C11-C12-C13-C14
26	C	507	CLA	C6-C7-C8-C9
26	N	603	CLA	C11-C10-C8-C9
26	a	406	CLA	C11-C12-C13-C14
26	n	603	CLA	C11-C10-C8-C9
30	B	2630	LHG	C18-C19-C20-C21
36	B	621	SQD	C29-C30-C31-C32
36	b	621	SQD	C29-C30-C31-C32
30	b	2630	LHG	C18-C19-C20-C21
37	B	2633	LMG	C23-C24-C25-C26
37	b	2633	LMG	C23-C24-C25-C26
25	3	607	CHL	C2C-C3C-CAC-CBC
25	S	601	CHL	CAA-CBA-CGA-O2A
25	s	601	CHL	CAA-CBA-CGA-O2A
26	G	602	CLA	CBA-CGA-O2A-C1
26	S	602	CLA	CBA-CGA-O2A-C1
26	g	602	CLA	CBA-CGA-O2A-C1
39	C	518	DGD	CDB-CEB-CFB-CGB
39	c	518	DGD	CDB-CEB-CFB-CGB
26	1	602	CLA	C4-C3-C5-C6
26	3	603	CLA	C4-C3-C5-C6
26	B	607	CLA	C4-C3-C5-C6
26	5	602	CLA	C4-C3-C5-C6
26	7	603	CLA	C4-C3-C5-C6
26	b	607	CLA	C4-C3-C5-C6
26	4	602	CLA	CAA-CBA-CGA-O1A
26	8	602	CLA	CAA-CBA-CGA-O1A
30	3	2630	LHG	C5-C4-O6-P
30	7	2630	LHG	C5-C4-O6-P
37	B	622	LMG	C32-C33-C34-C35
26	B	603	CLA	C2-C3-C5-C6
26	b	603	CLA	C2-C3-C5-C6
26	4	610	CLA	CBD-CGD-O2D-CED
37	b	622	LMG	C32-C33-C34-C35
26	s	602	CLA	CBA-CGA-O2A-C1
30	C	2630	LHG	C24-C23-O8-C6
30	c	2630	LHG	C24-C23-O8-C6
25	2	605	CHL	CAA-CBA-CGA-O2A
25	4	601	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	6	605	CHL	CAA-CBA-CGA-O2A
25	8	601	CHL	CAA-CBA-CGA-O1A
37	z	101	LMG	C17-C18-C19-C20
26	R	611	CLA	O2A-C1-C2-C3
26	r	611	CLA	O2A-C1-C2-C3
26	8	610	CLA	CBD-CGD-O2D-CED
37	Z	101	LMG	C17-C18-C19-C20
30	2	2630	LHG	C4-C5-C6-O8
30	6	2630	LHG	C4-C5-C6-O8
37	D	411	LMG	O1-C7-C8-C9
37	d	411	LMG	O1-C7-C8-C9
26	B	609	CLA	C15-C16-C17-C18
26	b	609	CLA	C15-C16-C17-C18
26	B	617	CLA	C2A-CAA-CBA-CGA
26	C	505	CLA	C2A-CAA-CBA-CGA
26	b	617	CLA	C2A-CAA-CBA-CGA
26	c	505	CLA	C2A-CAA-CBA-CGA
26	G	612	CLA	C10-C11-C12-C13
26	g	612	CLA	C10-C11-C12-C13
25	4	607	CHL	CAA-CBA-CGA-O1A
25	8	607	CHL	CAA-CBA-CGA-O1A
25	G	609	CHL	C4-C3-C5-C6
25	g	609	CHL	C4-C3-C5-C6
26	R	602	CLA	C4-C3-C5-C6
26	r	602	CLA	C4-C3-C5-C6
30	d	409	LHG	C24-C25-C26-C27
25	N	608	CHL	C2-C3-C5-C6
25	n	608	CHL	C2-C3-C5-C6
30	D	409	LHG	C24-C25-C26-C27
37	Z	101	LMG	C16-C17-C18-C19
25	g	609	CHL	C2C-C3C-CAC-CBC
37	z	101	LMG	C16-C17-C18-C19
39	C	518	DGD	CBB-CCB-CDB-CEB
39	c	518	DGD	CBB-CCB-CDB-CEB
26	3	602	CLA	C4B-C3B-CAB-CBB
26	7	602	CLA	C4B-C3B-CAB-CBB
26	g	613	CLA	C4B-C3B-CAB-CBB
26	B	606	CLA	O1A-CGA-O2A-C1
26	b	606	CLA	O1A-CGA-O2A-C1
36	a	418	SQD	C16-C17-C18-C19
36	A	418	SQD	C16-C17-C18-C19
25	3	605	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	4	611	CLA	CAA-CBA-CGA-O2A
26	8	611	CLA	CAA-CBA-CGA-O2A
30	C	523	LHG	C1-C2-C3-O3
30	c	523	LHG	C1-C2-C3-O3
25	G	609	CHL	C2C-C3C-CAC-CBC
25	2	606	CHL	CHA-CBD-CGD-O2D
25	G	601	CHL	CHA-CBD-CGD-O1D
25	G	601	CHL	CHA-CBD-CGD-O2D
25	N	601	CHL	CHA-CBD-CGD-O1D
25	N	601	CHL	CHA-CBD-CGD-O2D
25	N	605	CHL	CHA-CBD-CGD-O2D
25	S	607	CHL	CHA-CBD-CGD-O2D
25	S	608	CHL	CHA-CBD-CGD-O1D
25	Y	601	CHL	CHA-CBD-CGD-O1D
25	6	606	CHL	CHA-CBD-CGD-O2D
25	g	601	CHL	CHA-CBD-CGD-O1D
25	g	601	CHL	CHA-CBD-CGD-O2D
25	n	601	CHL	CHA-CBD-CGD-O1D
25	n	601	CHL	CHA-CBD-CGD-O2D
25	n	605	CHL	CHA-CBD-CGD-O2D
25	s	607	CHL	CHA-CBD-CGD-O2D
25	s	608	CHL	CHA-CBD-CGD-O1D
25	y	601	CHL	CHA-CBD-CGD-O1D
35	A	409	PHO	CHA-CBD-CGD-O1D
35	a	409	PHO	CHA-CBD-CGD-O1D
25	7	605	CHL	CAA-CBA-CGA-O1A
26	2	611	CLA	CAA-CBA-CGA-O2A
26	6	611	CLA	CAA-CBA-CGA-O2A
30	2	2630	LHG	O7-C5-C6-O8
30	6	2630	LHG	O7-C5-C6-O8
25	N	609	CHL	C10-C11-C12-C13
25	n	609	CHL	C10-C11-C12-C13
26	B	609	CLA	C5-C6-C7-C8
26	b	609	CLA	C5-C6-C7-C8
25	2	608	CHL	CAA-CBA-CGA-O2A
25	S	601	CHL	CAA-CBA-CGA-O1A
25	6	608	CHL	CAA-CBA-CGA-O2A
25	s	601	CHL	CAA-CBA-CGA-O1A
30	d	410	LHG	C8-C7-O7-C5
25	G	609	CHL	C10-C11-C12-C13
25	g	609	CHL	C10-C11-C12-C13
26	B	613	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	b	613	CLA	C15-C16-C17-C18
25	S	607	CHL	C6-C7-C8-C10
25	s	607	CHL	C6-C7-C8-C10
26	C	504	CLA	C11-C12-C13-C15
26	N	603	CLA	C11-C10-C8-C7
26	c	504	CLA	C11-C12-C13-C15
26	n	603	CLA	C11-C10-C8-C7
39	C	519	DGD	CDB-CEB-CFB-CGB
39	c	519	DGD	CDB-CEB-CFB-CGB
26	1	611	CLA	CAA-CBA-CGA-O2A
26	4	612	CLA	CAA-CBA-CGA-O1A
26	5	611	CLA	CAA-CBA-CGA-O2A
26	8	612	CLA	CAA-CBA-CGA-O1A
36	B	623	SQD	C27-C28-C29-C30
36	b	623	SQD	C27-C28-C29-C30
26	C	506	CLA	C8-C10-C11-C12
25	2	605	CHL	CAA-CBA-CGA-O1A
25	6	605	CHL	CAA-CBA-CGA-O1A
25	S	607	CHL	C11-C10-C8-C9
25	s	607	CHL	C11-C10-C8-C9
26	B	605	CLA	C6-C7-C8-C9
26	C	505	CLA	C14-C13-C15-C16
26	C	509	CLA	C11-C10-C8-C9
26	C	513	CLA	C11-C12-C13-C14
26	G	602	CLA	C6-C7-C8-C9
26	R	603	CLA	C11-C10-C8-C9
26	R	610	CLA	C14-C13-C15-C16
26	b	605	CLA	C6-C7-C8-C9
26	c	505	CLA	C14-C13-C15-C16
26	c	507	CLA	C6-C7-C8-C9
26	c	509	CLA	C11-C10-C8-C9
26	c	513	CLA	C11-C12-C13-C14
26	g	602	CLA	C6-C7-C8-C9
26	r	603	CLA	C11-C10-C8-C9
26	r	610	CLA	C14-C13-C15-C16
26	c	506	CLA	C8-C10-C11-C12
36	B	621	SQD	C5-C6-S-O8
36	b	621	SQD	C5-C6-S-O8
25	6	606	CHL	CAA-CBA-CGA-O2A
26	4	612	CLA	CAA-CBA-CGA-O2A
26	S	609	CLA	CAA-CBA-CGA-O1A
26	8	612	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
26	s	609	CLA	CAA-CBA-CGA-O1A
26	R	603	CLA	C2A-CAA-CBA-CGA
26	R	610	CLA	C2A-CAA-CBA-CGA
26	S	613	CLA	C2A-CAA-CBA-CGA
26	r	603	CLA	C2A-CAA-CBA-CGA
26	r	610	CLA	C2A-CAA-CBA-CGA
26	s	613	CLA	C2A-CAA-CBA-CGA
26	3	610	CLA	C2-C1-O2A-CGA
26	B	609	CLA	C2-C1-O2A-CGA
26	7	610	CLA	C2-C1-O2A-CGA
26	b	609	CLA	C2-C1-O2A-CGA
26	G	613	CLA	C16-C17-C18-C20
26	g	613	CLA	C16-C17-C18-C20
30	1	2630	LHG	C13-C14-C15-C16
30	5	2630	LHG	C13-C14-C15-C16
25	1	608	CHL	C3A-C2A-CAA-CBA
25	2	607	CHL	C3A-C2A-CAA-CBA
25	G	607	CHL	C4-C3-C5-C6
25	5	608	CHL	C3A-C2A-CAA-CBA
25	6	607	CHL	C3A-C2A-CAA-CBA
25	g	607	CHL	C4-C3-C5-C6
26	3	603	CLA	C3A-C2A-CAA-CBA
26	A	406	CLA	C3A-C2A-CAA-CBA
26	7	603	CLA	C3A-C2A-CAA-CBA
26	a	406	CLA	C3A-C2A-CAA-CBA
25	2	606	CHL	CAA-CBA-CGA-O2A
25	3	605	CHL	CAA-CBA-CGA-O2A
25	7	605	CHL	CAA-CBA-CGA-O2A
37	B	622	LMG	C20-C21-C22-C23
26	G	602	CLA	O1A-CGA-O2A-C1
26	C	501	CLA	C2-C3-C5-C6
26	c	501	CLA	C2-C3-C5-C6
37	b	622	LMG	C20-C21-C22-C23
25	1	601	CHL	CAA-CBA-CGA-O2A
25	5	601	CHL	CAA-CBA-CGA-O2A
26	2	611	CLA	CAA-CBA-CGA-O1A
26	6	611	CLA	CAA-CBA-CGA-O1A
30	3	2630	LHG	O8-C23-C24-C25
30	7	2630	LHG	O8-C23-C24-C25
25	G	607	CHL	O2A-C1-C2-C3
25	g	607	CHL	O2A-C1-C2-C3
26	g	602	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	1	606	CHL	CAA-CBA-CGA-O2A
25	5	606	CHL	CAA-CBA-CGA-O2A
25	s	606	CHL	CAA-CBA-CGA-O2A
26	2	612	CLA	CAA-CBA-CGA-O2A
26	4	604	CLA	CAA-CBA-CGA-O2A
26	R	616	CLA	CAA-CBA-CGA-O2A
26	6	612	CLA	CAA-CBA-CGA-O2A
26	8	604	CLA	CAA-CBA-CGA-O2A
26	r	616	CLA	CAA-CBA-CGA-O2A
30	C	522	LHG	C30-C31-C32-C33
30	c	522	LHG	C30-C31-C32-C33
39	c	520	DGD	C6B-C7B-C8B-C9B
39	C	520	DGD	C6B-C7B-C8B-C9B
25	R	608	CHL	C3C-C2C-CMC-OMC
25	r	608	CHL	C3C-C2C-CMC-OMC
29	R	623	NEX	C13-C14-C15-C35
25	6	608	CHL	CAA-CBA-CGA-O1A
26	B	608	CLA	C2A-CAA-CBA-CGA
26	b	608	CLA	C2A-CAA-CBA-CGA
26	B	609	CLA	C4-C3-C5-C6
26	b	609	CLA	C4-C3-C5-C6
25	2	608	CHL	CAA-CBA-CGA-O1A
25	S	606	CHL	CAA-CBA-CGA-O2A
25	5	606	CHL	CAA-CBA-CGA-O1A
26	4	611	CLA	CAA-CBA-CGA-O1A
38	D	405	PL9	C28-C29-C31-C32
38	d	405	PL9	C28-C29-C31-C32
29	2	1623	NEX	O24-C26-C27-C28
29	G	1623	NEX	O24-C26-C27-C28
29	N	1623	NEX	O24-C26-C27-C28
29	R	623	NEX	O24-C26-C27-C28
29	Y	1623	NEX	O24-C26-C27-C28
29	6	1623	NEX	O24-C26-C27-C28
29	g	1623	NEX	O24-C26-C27-C28
29	n	1623	NEX	O24-C26-C27-C28
29	r	623	NEX	O24-C26-C27-C28
29	y	1623	NEX	O24-C26-C27-C28
25	1	606	CHL	CAA-CBA-CGA-O1A
26	8	611	CLA	CAA-CBA-CGA-O1A
38	D	405	PL9	C34-C36-C37-C38
38	d	405	PL9	C34-C36-C37-C38
25	N	609	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	n	609	CHL	C8-C10-C11-C12
25	2	601	CHL	CAA-CBA-CGA-O1A
25	6	601	CHL	CAA-CBA-CGA-O1A
26	6	612	CLA	CAA-CBA-CGA-O1A
39	h	102	DGD	CDB-CEB-CFB-CGB
39	H	102	DGD	CDB-CEB-CFB-CGB
26	B	606	CLA	C2A-CAA-CBA-CGA
26	b	606	CLA	C2A-CAA-CBA-CGA
26	B	614	CLA	CAA-CBA-CGA-O2A
26	b	614	CLA	CAA-CBA-CGA-O2A
25	1	601	CHL	CAA-CBA-CGA-O1A
25	2	606	CHL	CAA-CBA-CGA-O1A
25	6	606	CHL	CAA-CBA-CGA-O1A
26	2	612	CLA	CAA-CBA-CGA-O1A
29	2	1623	NEX	C9-C10-C11-C12
29	6	1623	NEX	C9-C10-C11-C12
29	r	623	NEX	C13-C14-C15-C35
37	Z	101	LMG	C15-C16-C17-C18
37	z	101	LMG	C15-C16-C17-C18
36	B	621	SQD	C27-C28-C29-C30
36	b	621	SQD	C27-C28-C29-C30
37	C	521	LMG	C37-C38-C39-C40
37	c	521	LMG	C37-C38-C39-C40
30	c	2630	LHG	C25-C26-C27-C28
25	4	609	CHL	CAA-CBA-CGA-O1A
25	5	601	CHL	CAA-CBA-CGA-O1A
25	8	609	CHL	CAA-CBA-CGA-O1A
26	4	604	CLA	CAA-CBA-CGA-O1A
26	8	604	CLA	CAA-CBA-CGA-O1A
30	C	2630	LHG	C25-C26-C27-C28
30	C	523	LHG	C16-C17-C18-C19
30	D	410	LHG	C23-C24-C25-C26
30	D	410	LHG	C8-C7-O7-C5
25	N	609	CHL	C14-C13-C15-C16
25	n	609	CHL	C14-C13-C15-C16
26	B	604	CLA	C6-C7-C8-C9
26	G	613	CLA	C14-C13-C15-C16
26	Y	612	CLA	C6-C7-C8-C9
26	b	604	CLA	C6-C7-C8-C9
26	g	613	CLA	C14-C13-C15-C16
26	y	612	CLA	C6-C7-C8-C9
30	d	410	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
30	c	523	LHG	C16-C17-C18-C19
26	Y	612	CLA	CAA-CBA-CGA-O2A
26	y	612	CLA	CAA-CBA-CGA-O2A
37	d	411	LMG	O10-C28-O8-C9
30	D	410	LHG	O6-C4-C5-C6
30	d	410	LHG	O6-C4-C5-C6
27	4	620	LUT	C7-C8-C9-C10
27	8	620	LUT	C7-C8-C9-C10
28	4	622	XAT	C27-C28-C29-C30
28	8	622	XAT	C27-C28-C29-C30
36	A	418	SQD	C28-C29-C30-C31
26	B	610	CLA	C4-C3-C5-C6
26	b	610	CLA	C4-C3-C5-C6
37	D	411	LMG	O10-C28-O8-C9
36	a	418	SQD	C28-C29-C30-C31
26	C	504	CLA	C16-C17-C18-C19
26	c	504	CLA	C16-C17-C18-C19
26	1	611	CLA	CAA-CBA-CGA-O1A
26	5	611	CLA	CAA-CBA-CGA-O1A
25	4	607	CHL	C2A-CAA-CBA-CGA
25	8	607	CHL	C2A-CAA-CBA-CGA
25	3	601	CHL	C6-C7-C8-C10
25	7	601	CHL	C6-C7-C8-C10
26	B	602	CLA	C11-C10-C8-C7
26	B	602	CLA	C12-C13-C15-C16
26	B	611	CLA	C12-C13-C15-C16
26	C	508	CLA	C11-C12-C13-C15
26	G	602	CLA	C6-C7-C8-C10
26	b	602	CLA	C11-C10-C8-C7
26	b	602	CLA	C12-C13-C15-C16
26	b	611	CLA	C12-C13-C15-C16
26	c	508	CLA	C11-C12-C13-C15
26	g	602	CLA	C6-C7-C8-C10
26	C	502	CLA	C3-C5-C6-C7
25	1	605	CHL	CAA-CBA-CGA-O2A
25	5	605	CHL	CAA-CBA-CGA-O2A
26	1	603	CLA	C2B-C3B-CAB-CBB
26	1	604	CLA	C2B-C3B-CAB-CBB
26	1	613	CLA	C2B-C3B-CAB-CBB
26	2	604	CLA	C2B-C3B-CAB-CBB
26	3	604	CLA	C2B-C3B-CAB-CBB
26	3	613	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	4	602	CLA	C2B-C3B-CAB-CBB
26	B	604	CLA	C2B-C3B-CAB-CBB
26	G	612	CLA	C2B-C3B-CAB-CBB
26	G	613	CLA	C2B-C3B-CAB-CBB
26	N	612	CLA	C2B-C3B-CAB-CBB
26	S	614	CLA	C2B-C3B-CAB-CBB
26	5	603	CLA	C2B-C3B-CAB-CBB
26	5	604	CLA	C2B-C3B-CAB-CBB
26	5	613	CLA	C2B-C3B-CAB-CBB
26	6	604	CLA	C2B-C3B-CAB-CBB
26	7	604	CLA	C2B-C3B-CAB-CBB
26	7	613	CLA	C2B-C3B-CAB-CBB
26	8	602	CLA	C2B-C3B-CAB-CBB
26	b	604	CLA	C2B-C3B-CAB-CBB
26	g	612	CLA	C2B-C3B-CAB-CBB
26	g	613	CLA	C2B-C3B-CAB-CBB
26	n	612	CLA	C2B-C3B-CAB-CBB
26	s	614	CLA	C2B-C3B-CAB-CBB
27	1	1621	LUT	C1-C6-C7-C8
27	1	1621	LUT	C5-C6-C7-C8
27	2	1621	LUT	C1-C6-C7-C8
27	3	1621	LUT	C5-C6-C7-C8
27	G	1620	LUT	C5-C6-C7-C8
27	N	1620	LUT	C5-C6-C7-C8
27	N	1621	LUT	C1-C6-C7-C8
27	N	1621	LUT	C5-C6-C7-C8
27	S	1620	LUT	C5-C6-C7-C8
27	S	1621	LUT	C5-C6-C7-C8
27	5	1621	LUT	C1-C6-C7-C8
27	5	1621	LUT	C5-C6-C7-C8
27	6	1621	LUT	C1-C6-C7-C8
27	7	1621	LUT	C5-C6-C7-C8
27	g	1620	LUT	C5-C6-C7-C8
27	n	1620	LUT	C5-C6-C7-C8
27	n	1621	LUT	C1-C6-C7-C8
27	n	1621	LUT	C5-C6-C7-C8
27	s	1620	LUT	C5-C6-C7-C8
27	s	1621	LUT	C5-C6-C7-C8
31	4	623	BCR	C1-C6-C7-C8
31	4	623	BCR	C5-C6-C7-C8
31	C	517	BCR	C23-C24-C25-C26
31	C	517	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
31	8	623	BCR	C1-C6-C7-C8
31	8	623	BCR	C5-C6-C7-C8
31	c	517	BCR	C23-C24-C25-C26
31	c	517	BCR	C23-C24-C25-C30
25	Y	606	CHL	C2-C1-O2A-CGA
25	y	606	CHL	C2-C1-O2A-CGA
26	B	603	CLA	C2-C1-O2A-CGA
26	S	602	CLA	C2-C1-O2A-CGA
26	b	603	CLA	C2-C1-O2A-CGA
26	s	602	CLA	C2-C1-O2A-CGA
35	A	409	PHO	C8-C10-C11-C12
35	a	409	PHO	C8-C10-C11-C12
36	b	621	SQD	C31-C32-C33-C34
26	S	604	CLA	CAA-CBA-CGA-O2A
26	s	604	CLA	CAA-CBA-CGA-O2A
30	d	409	LHG	O8-C23-C24-C25
39	c	518	DGD	O6E-C1E-O5D-C6D
30	d	408	LHG	C33-C34-C35-C36
30	D	408	LHG	C33-C34-C35-C36
30	C	523	LHG	C13-C14-C15-C16
36	B	621	SQD	C31-C32-C33-C34
26	7	610	CLA	C3-C5-C6-C7
26	c	502	CLA	C3-C5-C6-C7
25	G	607	CHL	C2-C3-C5-C6
25	g	607	CHL	C2-C3-C5-C6
26	B	610	CLA	C2-C3-C5-C6
26	b	610	CLA	C2-C3-C5-C6
30	c	523	LHG	C13-C14-C15-C16
26	3	610	CLA	C2A-CAA-CBA-CGA
26	7	610	CLA	C2A-CAA-CBA-CGA
25	3	606	CHL	CAA-CBA-CGA-O2A
25	7	606	CHL	CAA-CBA-CGA-O2A
26	3	612	CLA	CAA-CBA-CGA-O2A
26	7	612	CLA	CAA-CBA-CGA-O2A
26	C	507	CLA	CAA-CBA-CGA-O2A
30	D	409	LHG	O8-C23-C24-C25
26	3	610	CLA	C3-C5-C6-C7
30	s	2630	LHG	C12-C13-C14-C15
37	A	413	LMG	C31-C32-C33-C34
37	a	413	LMG	C31-C32-C33-C34
30	S	2630	LHG	C12-C13-C14-C15
25	Y	607	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	y	607	CHL	C8-C10-C11-C12
26	3	603	CLA	C5-C6-C7-C8
26	A	410	CLA	C8-C10-C11-C12
26	c	507	CLA	CAA-CBA-CGA-O2A
30	G	2630	LHG	C31-C32-C33-C34
30	g	2630	LHG	C31-C32-C33-C34
25	1	607	CHL	CAA-CBA-CGA-O2A
25	5	607	CHL	CAA-CBA-CGA-O2A
30	L	101	LHG	O7-C7-C8-C9
30	l	101	LHG	O7-C7-C8-C9
26	7	603	CLA	C5-C6-C7-C8
26	3	602	CLA	C2-C3-C5-C6
26	7	602	CLA	C2-C3-C5-C6
26	n	602	CLA	CBD-CGD-O2D-CED
25	S	606	CHL	CAA-CBA-CGA-O1A
25	s	606	CHL	CAA-CBA-CGA-O1A
26	a	410	CLA	C8-C10-C11-C12
30	2	2630	LHG	C16-C17-C18-C19
30	6	2630	LHG	C16-C17-C18-C19
37	a	413	LMG	C35-C36-C37-C38
37	A	413	LMG	C35-C36-C37-C38
26	2	604	CLA	CAA-CBA-CGA-O1A
26	R	616	CLA	CAA-CBA-CGA-O1A
26	6	604	CLA	CAA-CBA-CGA-O1A
26	r	616	CLA	CAA-CBA-CGA-O1A
30	C	2630	LHG	O8-C23-C24-C25
30	c	2630	LHG	O8-C23-C24-C25
30	C	522	LHG	C14-C15-C16-C17
30	c	522	LHG	C14-C15-C16-C17
30	B	2630	LHG	O1-C1-C2-O2
30	b	2630	LHG	O1-C1-C2-O2
30	Y	2630	LHG	O10-C23-O8-C6
30	y	2630	LHG	O10-C23-O8-C6
26	N	614	CLA	O2A-C1-C2-C3
26	n	614	CLA	O2A-C1-C2-C3
25	G	608	CHL	C11-C10-C8-C9
25	g	608	CHL	C11-C10-C8-C9
26	C	506	CLA	C14-C13-C15-C16
26	C	508	CLA	C11-C12-C13-C14
26	c	506	CLA	C14-C13-C15-C16
26	c	508	CLA	C11-C12-C13-C14
27	R	620	LUT	C27-C28-C29-C39

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Mol	Chain	Res	Type	Atoms
26	1	602	CLA	CAA-CBA-CGA-O2A
26	1	613	CLA	CAA-CBA-CGA-O2A
30	D	410	LHG	O8-C23-C24-C25
30	d	410	LHG	O8-C23-C24-C25
30	4	2630	LHG	C4-C5-C6-O8
30	8	2630	LHG	C4-C5-C6-O8
26	3	603	CLA	C1A-C2A-CAA-CBA
26	3	613	CLA	C4B-C3B-CAB-CBB
26	B	604	CLA	C4B-C3B-CAB-CBB
26	C	512	CLA	C1A-C2A-CAA-CBA
26	G	610	CLA	C4B-C3B-CAB-CBB
26	G	613	CLA	C4B-C3B-CAB-CBB
26	7	603	CLA	C1A-C2A-CAA-CBA
26	7	613	CLA	C4B-C3B-CAB-CBB
26	b	604	CLA	C4B-C3B-CAB-CBB
26	c	512	CLA	C1A-C2A-CAA-CBA
26	g	610	CLA	C4B-C3B-CAB-CBB
26	2	604	CLA	CAA-CBA-CGA-O2A
26	6	604	CLA	CAA-CBA-CGA-O2A
36	a	418	SQD	C11-C12-C13-C14
39	B	626	DGD	O6E-C1E-O5D-C6D
39	C	518	DGD	O6E-C1E-O5D-C6D
39	b	626	DGD	O6E-C1E-O5D-C6D
25	7	601	CHL	CAA-CBA-CGA-O2A
26	2	603	CLA	CAA-CBA-CGA-O2A
26	C	501	CLA	CAA-CBA-CGA-O2A
26	R	603	CLA	CAA-CBA-CGA-O2A
26	5	602	CLA	CAA-CBA-CGA-O2A
26	6	603	CLA	CAA-CBA-CGA-O2A
26	c	501	CLA	CAA-CBA-CGA-O2A
26	r	603	CLA	CAA-CBA-CGA-O2A
27	R	620	LUT	C27-C28-C29-C30
27	r	620	LUT	C27-C28-C29-C30
28	R	622	XAT	C27-C28-C29-C30
28	r	622	XAT	C27-C28-C29-C30
29	3	1623	NEX	C11-C12-C13-C14
29	S	1623	NEX	C11-C12-C13-C14
29	7	1623	NEX	C11-C12-C13-C14
29	s	1623	NEX	C11-C12-C13-C14
31	A	411	BCR	C7-C8-C9-C10
31	a	411	BCR	C7-C8-C9-C10
26	N	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	A	418	SQD	C11-C12-C13-C14
25	3	601	CHL	CAA-CBA-CGA-O2A
25	N	606	CHL	CAA-CBA-CGA-O2A
26	B	617	CLA	CAA-CBA-CGA-O2A
26	G	611	CLA	CAA-CBA-CGA-O2A
26	5	613	CLA	CAA-CBA-CGA-O2A
26	b	617	CLA	CAA-CBA-CGA-O2A
26	g	611	CLA	CAA-CBA-CGA-O2A
37	A	415	LMG	O8-C28-C29-C30
26	1	612	CLA	C2A-CAA-CBA-CGA
26	5	612	CLA	C2A-CAA-CBA-CGA
26	S	610	CLA	C5-C6-C7-C8
26	s	610	CLA	C5-C6-C7-C8
39	b	626	DGD	C3B-C4B-C5B-C6B
25	n	606	CHL	CAA-CBA-CGA-O2A
37	a	415	LMG	O8-C28-C29-C30
26	B	607	CLA	C10-C11-C12-C13
25	8	607	CHL	CBD-CGD-O2D-CED
39	B	626	DGD	C3B-C4B-C5B-C6B
36	B	623	SQD	C5-C6-S-O9
36	b	623	SQD	C5-C6-S-O9
26	B	606	CLA	C13-C15-C16-C17
26	G	603	CLA	C5-C6-C7-C8
26	b	606	CLA	C13-C15-C16-C17
26	b	607	CLA	C10-C11-C12-C13
25	1	609	CHL	C2-C1-O2A-CGA
25	G	606	CHL	C2-C1-O2A-CGA
25	5	609	CHL	C2-C1-O2A-CGA
25	g	606	CHL	C2-C1-O2A-CGA
26	1	604	CLA	C2-C1-O2A-CGA
26	C	502	CLA	C2-C1-O2A-CGA
26	Y	603	CLA	C2-C1-O2A-CGA
26	5	604	CLA	C2-C1-O2A-CGA
26	c	502	CLA	C2-C1-O2A-CGA
26	y	603	CLA	C2-C1-O2A-CGA
26	A	410	CLA	C11-C10-C8-C7
26	B	604	CLA	C6-C7-C8-C10
26	B	609	CLA	C11-C12-C13-C15
26	N	602	CLA	C11-C12-C13-C15
26	Y	613	CLA	C11-C10-C8-C7
26	a	410	CLA	C11-C10-C8-C7
26	b	604	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
26	b	609	CLA	C11-C12-C13-C15
26	n	602	CLA	C11-C12-C13-C15
26	y	613	CLA	C11-C10-C8-C7
30	D	408	LHG	C24-C23-O8-C6
30	d	408	LHG	C24-C23-O8-C6
37	B	2633	LMG	C29-C28-O8-C9
37	b	2633	LMG	C29-C28-O8-C9
35	A	408	PHO	C16-C17-C18-C19
35	a	408	PHO	C16-C17-C18-C19
37	B	2633	LMG	C9-C8-O7-C10
37	b	2633	LMG	C9-C8-O7-C10
25	4	607	CHL	CBD-CGD-O2D-CED
26	3	612	CLA	CAA-CBA-CGA-O1A
26	7	612	CLA	CAA-CBA-CGA-O1A
26	G	612	CLA	CAA-CBA-CGA-O2A
26	g	612	CLA	CAA-CBA-CGA-O2A
36	B	623	SQD	O47-C7-C8-C9
36	b	623	SQD	O47-C7-C8-C9
37	B	622	LMG	C31-C32-C33-C34
37	b	622	LMG	C31-C32-C33-C34
26	C	503	CLA	C13-C15-C16-C17
26	g	603	CLA	C5-C6-C7-C8
25	R	606	CHL	C2A-CAA-CBA-CGA
25	r	606	CHL	C2A-CAA-CBA-CGA
26	S	609	CLA	C2A-CAA-CBA-CGA
26	8	610	CLA	C2A-CAA-CBA-CGA
26	s	609	CLA	C2A-CAA-CBA-CGA
26	c	503	CLA	C13-C15-C16-C17
26	B	617	CLA	C16-C17-C18-C20
26	b	617	CLA	C16-C17-C18-C20
30	N	2630	LHG	C16-C17-C18-C19
25	1	605	CHL	CAA-CBA-CGA-O1A
25	5	605	CHL	CAA-CBA-CGA-O1A
38	D	405	PL9	C46-C47-C48-C49
38	d	405	PL9	C46-C47-C48-C49
26	G	610	CLA	C13-C15-C16-C17
26	g	610	CLA	C13-C15-C16-C17
30	n	2630	LHG	C16-C17-C18-C19
25	2	601	CHL	CAA-CBA-CGA-O2A
25	4	609	CHL	CAA-CBA-CGA-O2A
25	6	601	CHL	CAA-CBA-CGA-O2A
25	8	609	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
26	B	605	CLA	C3A-C2A-CAA-CBA
26	C	512	CLA	C3A-C2A-CAA-CBA
26	b	605	CLA	C3A-C2A-CAA-CBA
26	c	512	CLA	C3A-C2A-CAA-CBA
26	C	501	CLA	CAA-CBA-CGA-O1A
26	C	507	CLA	CAA-CBA-CGA-O1A
26	C	507	CLA	C16-C17-C18-C20
26	c	507	CLA	C16-C17-C18-C20
37	a	413	LMG	C34-C35-C36-C37
25	1	607	CHL	CAA-CBA-CGA-O1A
25	5	607	CHL	CAA-CBA-CGA-O1A
26	c	501	CLA	CAA-CBA-CGA-O1A
26	c	507	CLA	CAA-CBA-CGA-O1A
36	B	623	SQD	O49-C7-C8-C9
36	b	623	SQD	O49-C7-C8-C9
30	Y	2630	LHG	C11-C12-C13-C14
30	Y	2630	LHG	C11-C10-C9-C8
30	y	2630	LHG	C11-C12-C13-C14
37	A	413	LMG	C34-C35-C36-C37
39	C	519	DGD	O1G-C1A-C2A-C3A
30	y	2630	LHG	C11-C10-C9-C8
26	4	610	CLA	C2A-CAA-CBA-CGA
25	3	606	CHL	CAA-CBA-CGA-O1A
25	7	606	CHL	CAA-CBA-CGA-O1A
25	G	608	CHL	C11-C12-C13-C14
25	S	607	CHL	C6-C7-C8-C9
25	g	608	CHL	C11-C12-C13-C14
25	s	607	CHL	C6-C7-C8-C9
26	B	614	CLA	C11-C12-C13-C14
26	C	504	CLA	C14-C13-C15-C16
26	C	511	CLA	C14-C13-C15-C16
26	N	613	CLA	C11-C10-C8-C9
26	b	614	CLA	C11-C12-C13-C14
26	c	504	CLA	C14-C13-C15-C16
26	c	511	CLA	C14-C13-C15-C16
26	n	613	CLA	C11-C10-C8-C9
39	c	519	DGD	O1G-C1A-C2A-C3A
30	S	2630	LHG	O10-C23-C24-C25
36	A	418	SQD	C17-C18-C19-C20
30	B	2631	LHG	C23-C24-C25-C26
30	b	2631	LHG	C23-C24-C25-C26
39	C	520	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
39	c	520	DGD	C3A-C4A-C5A-C6A
25	2	609	CHL	C5-C6-C7-C8
25	6	609	CHL	C5-C6-C7-C8
25	N	606	CHL	CAA-CBA-CGA-O1A
25	n	606	CHL	CAA-CBA-CGA-O1A
26	B	614	CLA	CAA-CBA-CGA-O1A
26	b	614	CLA	CAA-CBA-CGA-O1A
30	s	2630	LHG	O10-C23-C24-C25
30	B	2630	LHG	C9-C10-C11-C12
30	b	2630	LHG	C9-C10-C11-C12
36	a	418	SQD	C17-C18-C19-C20
26	C	509	CLA	C13-C15-C16-C17
26	c	509	CLA	C13-C15-C16-C17
26	R	603	CLA	CAA-CBA-CGA-O1A
26	r	603	CLA	CAA-CBA-CGA-O1A
26	y	612	CLA	CAA-CBA-CGA-O1A
26	b	605	CLA	C5-C6-C7-C8
25	R	608	CHL	C11-C12-C13-C14
25	r	608	CHL	C11-C12-C13-C14
26	B	605	CLA	C5-C6-C7-C8
31	C	515	BCR	C17-C18-C19-C20
31	c	515	BCR	C17-C18-C19-C20
26	1	602	CLA	CAA-CBA-CGA-O1A
26	Y	612	CLA	CAA-CBA-CGA-O1A
26	5	602	CLA	CAA-CBA-CGA-O1A
30	D	410	LHG	O10-C23-C24-C25
30	d	410	LHG	O10-C23-C24-C25
37	A	415	LMG	O10-C28-C29-C30
37	Z	101	LMG	O10-C28-C29-C30
37	a	415	LMG	O10-C28-C29-C30
37	B	622	LMG	C8-C7-O1-C1
37	b	622	LMG	C8-C7-O1-C1
26	5	611	CLA	CBD-CGD-O2D-CED
30	G	2630	LHG	O10-C23-C24-C25
30	N	2630	LHG	O10-C23-C24-C25
30	g	2630	LHG	O10-C23-C24-C25
37	z	101	LMG	O10-C28-C29-C30
25	G	607	CHL	C2C-C3C-CAC-CBC
39	B	626	DGD	O1G-C1G-C2G-C3G
39	b	626	DGD	O1G-C1G-C2G-C3G
26	S	604	CLA	CAA-CBA-CGA-O1A
26	b	617	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	s	604	CLA	CAA-CBA-CGA-O1A
30	n	2630	LHG	O10-C23-C24-C25
36	b	621	SQD	O49-C7-C8-C9
25	g	607	CHL	C2C-C3C-CAC-CBC
26	S	611	CLA	C5-C6-C7-C8
26	n	610	CLA	C8-C10-C11-C12
26	s	611	CLA	C5-C6-C7-C8
30	N	2630	LHG	C2-C3-O3-P
30	d	410	LHG	C2-C3-O3-P
30	n	2630	LHG	C2-C3-O3-P
26	C	510	CLA	CAA-CBA-CGA-O2A
26	c	510	CLA	CAA-CBA-CGA-O2A
30	C	523	LHG	O7-C7-C8-C9
30	c	523	LHG	O7-C7-C8-C9
36	A	412	SQD	O47-C7-C8-C9
36	a	412	SQD	O47-C7-C8-C9
37	A	413	LMG	O7-C10-C11-C12
37	a	413	LMG	O7-C10-C11-C12
26	N	610	CLA	C8-C10-C11-C12
26	B	617	CLA	CAA-CBA-CGA-O1A
26	g	612	CLA	CAA-CBA-CGA-O1A
36	B	621	SQD	O49-C7-C8-C9
25	N	609	CHL	C2C-C3C-CAC-CBC
25	1	606	CHL	CAD-CBD-CGD-O2D
25	5	606	CHL	CAD-CBD-CGD-O2D
26	1	602	CLA	CAD-CBD-CGD-O2D
26	1	610	CLA	CAD-CBD-CGD-O2D
26	B	615	CLA	CAD-CBD-CGD-O2D
26	G	602	CLA	CAD-CBD-CGD-O2D
26	R	603	CLA	CAD-CBD-CGD-O2D
26	5	602	CLA	CAD-CBD-CGD-O2D
26	5	610	CLA	CAD-CBD-CGD-O2D
26	b	615	CLA	CAD-CBD-CGD-O2D
26	g	602	CLA	CAD-CBD-CGD-O2D
26	r	603	CLA	CAD-CBD-CGD-O2D
26	3	603	CLA	C3-C5-C6-C7
26	7	603	CLA	C3-C5-C6-C7
26	G	612	CLA	CAA-CBA-CGA-O1A
30	C	522	LHG	O2-C2-C3-O3
30	c	522	LHG	O2-C2-C3-O3
25	Y	609	CHL	C2-C1-O2A-CGA
25	y	609	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
25	n	609	CHL	C2C-C3C-CAC-CBC
26	G	611	CLA	CAA-CBA-CGA-O1A
25	4	601	CHL	C1A-C2A-CAA-CBA
25	8	601	CHL	C1A-C2A-CAA-CBA
26	B	615	CLA	C16-C17-C18-C20
26	b	615	CLA	C16-C17-C18-C20
25	2	609	CHL	C10-C11-C12-C13
25	6	609	CHL	C10-C11-C12-C13
26	1	613	CLA	CAA-CBA-CGA-O1A
26	C	510	CLA	CAA-CBA-CGA-O1A
26	5	613	CLA	CAA-CBA-CGA-O1A
39	c	519	DGD	O1B-C1B-C2B-C3B
25	N	601	CHL	CAA-CBA-CGA-O2A
26	3	602	CLA	CAA-CBA-CGA-O2A
26	7	602	CLA	CAA-CBA-CGA-O2A
30	B	2631	LHG	O7-C7-C8-C9
30	b	2631	LHG	O7-C7-C8-C9
36	B	621	SQD	O47-C7-C8-C9
36	b	621	SQD	O47-C7-C8-C9
37	Z	101	LMG	O8-C28-C29-C30
37	z	101	LMG	O8-C28-C29-C30
26	1	611	CLA	CBD-CGD-O2D-CED
30	Y	2630	LHG	C8-C7-O7-C5
30	y	2630	LHG	C8-C7-O7-C5
25	3	601	CHL	CAA-CBA-CGA-O1A
39	C	519	DGD	O1B-C1B-C2B-C3B
26	b	610	CLA	C5-C6-C7-C8
25	G	601	CHL	CAA-CBA-CGA-O2A
25	g	601	CHL	CAA-CBA-CGA-O2A
26	B	610	CLA	C5-C6-C7-C8
25	7	601	CHL	CAA-CBA-CGA-O1A
26	6	603	CLA	CAA-CBA-CGA-O1A
26	c	510	CLA	CAA-CBA-CGA-O1A
26	g	611	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

434 monomers are involved in 1103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	g	602	CLA	2	0
25	4	606	CHL	2	0
26	C	511	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	d	405	PL9	1	0
30	N	2630	LHG	4	0
31	c	514	BCR	4	0
26	6	614	CLA	1	0
28	Y	1622	XAT	6	0
30	D	410	LHG	3	0
26	R	612	CLA	2	0
25	1	608	CHL	1	0
26	b	612	CLA	4	0
25	5	607	CHL	5	0
25	7	609	CHL	6	0
31	A	411	BCR	4	0
31	h	101	BCR	6	0
25	N	608	CHL	1	0
26	1	610	CLA	1	0
28	G	1622	XAT	5	0
26	s	613	CLA	1	0
31	D	404	BCR	3	0
30	b	2631	LHG	3	0
29	r	623	NEX	4	0
25	4	609	CHL	1	0
26	A	407	CLA	1	0
26	B	611	CLA	2	0
26	Y	613	CLA	4	0
36	B	623	SQD	4	0
28	5	1622	XAT	3	0
25	7	607	CHL	4	0
26	S	611	CLA	1	0
25	g	605	CHL	1	0
26	g	603	CLA	3	0
25	1	601	CHL	1	0
31	8	623	BCR	8	0
30	L	101	LHG	3	0
25	s	607	CHL	3	0
26	r	612	CLA	2	0
31	T	101	BCR	10	0
25	8	608	CHL	2	0
27	N	1621	LUT	6	0
38	D	405	PL9	2	0
31	C	514	BCR	4	0
41	f	101	HEM	1	0
35	a	409	PHO	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	506	CLA	3	0
25	5	608	CHL	1	0
26	R	602	CLA	4	0
26	S	604	CLA	2	0
26	B	605	CLA	7	0
30	g	2630	LHG	4	0
39	C	519	DGD	3	0
31	b	618	BCR	5	0
31	b	619	BCR	6	0
26	R	610	CLA	1	0
25	Y	608	CHL	2	0
30	4	2630	LHG	1	0
39	H	102	DGD	3	0
26	b	606	CLA	4	0
30	C	523	LHG	2	0
26	G	611	CLA	1	0
25	y	601	CHL	3	0
25	7	606	CHL	3	0
25	G	607	CHL	8	0
25	2	605	CHL	1	0
39	c	518	DGD	2	0
26	B	615	CLA	2	0
26	s	611	CLA	1	0
26	G	602	CLA	2	0
31	t	101	BCR	8	0
30	Y	2630	LHG	4	0
26	5	610	CLA	1	0
26	a	410	CLA	5	0
26	Y	602	CLA	6	0
26	C	503	CLA	3	0
26	a	405	CLA	6	0
26	g	611	CLA	2	0
26	n	603	CLA	5	0
26	B	612	CLA	4	0
27	5	1621	LUT	6	0
38	A	414	PL9	1	0
26	R	611	CLA	4	0
26	c	504	CLA	1	0
37	Z	101	LMG	5	0
29	7	1623	NEX	3	0
29	Y	1623	NEX	2	0
27	2	1620	LUT	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	G	2630	LHG	4	0
25	y	608	CHL	2	0
25	8	601	CHL	2	0
31	H	101	BCR	6	0
27	S	1621	LUT	2	0
26	r	604	CLA	2	0
30	B	2631	LHG	3	0
26	B	614	CLA	6	0
30	7	2630	LHG	2	0
26	1	603	CLA	2	0
25	5	609	CHL	3	0
26	b	611	CLA	3	0
31	c	517	BCR	7	0
31	b	620	BCR	5	0
27	1	1620	LUT	4	0
28	6	1622	XAT	4	0
29	N	1623	NEX	1	0
25	y	607	CHL	3	0
26	1	604	CLA	1	0
27	7	1621	LUT	3	0
25	Y	605	CHL	3	0
25	8	606	CHL	2	0
25	G	608	CHL	2	0
25	s	608	CHL	1	0
39	B	626	DGD	5	0
26	3	614	CLA	1	0
26	Y	611	CLA	1	0
25	S	606	CHL	2	0
36	b	623	SQD	4	0
26	c	511	CLA	2	0
31	B	620	BCR	4	0
25	N	607	CHL	4	0
25	6	609	CHL	3	0
26	N	604	CLA	1	0
28	g	1622	XAT	5	0
26	c	510	CLA	5	0
25	7	601	CHL	2	0
26	2	612	CLA	2	0
26	3	612	CLA	1	0
25	5	601	CHL	1	0
30	C	522	LHG	4	0
30	s	2630	LHG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	c	502	CLA	4	0
39	h	102	DGD	4	0
41	F	101	HEM	1	0
25	n	605	CHL	1	0
30	c	2630	LHG	5	0
28	r	622	XAT	5	0
25	r	607	CHL	1	0
26	c	512	CLA	3	0
26	G	610	CLA	4	0
26	d	403	CLA	2	0
26	a	407	CLA	1	0
26	C	504	CLA	2	0
30	d	408	LHG	1	0
38	a	414	PL9	1	0
26	b	605	CLA	6	0
26	r	616	CLA	3	0
26	N	613	CLA	3	0
37	b	622	LMG	5	0
29	5	1623	NEX	2	0
27	G	1621	LUT	7	0
26	6	612	CLA	2	0
26	8	610	CLA	1	0
25	2	609	CHL	2	0
26	s	603	CLA	1	0
26	n	604	CLA	1	0
27	1	1621	LUT	6	0
26	6	611	CLA	1	0
26	6	602	CLA	2	0
29	S	1623	NEX	2	0
37	c	521	LMG	1	0
25	g	608	CHL	2	0
26	N	610	CLA	8	0
26	A	405	CLA	9	0
25	Y	607	CHL	3	0
28	3	1622	XAT	3	0
25	8	609	CHL	1	0
25	N	606	CHL	1	0
26	R	603	CLA	3	0
26	c	501	CLA	4	0
27	S	1620	LUT	3	0
26	c	513	CLA	4	0
26	8	612	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	Y	610	CLA	1	0
26	C	502	CLA	5	0
25	r	608	CHL	3	0
26	S	612	CLA	1	0
26	b	613	CLA	7	0
25	S	607	CHL	4	0
26	2	603	CLA	1	0
27	6	1620	LUT	4	0
37	A	415	LMG	1	0
26	2	611	CLA	1	0
26	C	512	CLA	3	0
26	3	602	CLA	2	0
26	b	614	CLA	7	0
37	A	413	LMG	2	0
26	D	403	CLA	3	0
26	5	613	CLA	2	0
27	y	1621	LUT	5	0
31	C	517	BCR	8	0
26	C	507	CLA	5	0
26	7	614	CLA	1	0
30	r	2630	LHG	4	0
26	C	505	CLA	4	0
25	R	608	CHL	3	0
39	b	626	DGD	5	0
25	1	609	CHL	4	0
26	S	613	CLA	1	0
26	B	613	CLA	8	0
27	Y	1620	LUT	5	0
26	5	604	CLA	1	0
26	7	612	CLA	1	0
30	B	2630	LHG	2	0
26	b	609	CLA	2	0
25	N	601	CHL	3	0
27	N	1620	LUT	4	0
26	7	602	CLA	3	0
26	N	603	CLA	5	0
26	y	610	CLA	1	0
29	1	1623	NEX	2	0
26	n	612	CLA	4	0
26	c	508	CLA	3	0
26	4	612	CLA	2	0
26	D	402	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	G	604	CLA	2	0
25	R	607	CHL	1	0
26	3	611	CLA	3	0
39	c	519	DGD	2	0
31	c	516	BCR	5	0
26	B	616	CLA	2	0
26	7	604	CLA	1	0
26	b	602	CLA	4	0
26	s	604	CLA	3	0
31	B	619	BCR	3	0
26	Y	603	CLA	7	0
27	6	1621	LUT	4	0
35	A	408	PHO	6	0
26	b	608	CLA	1	0
26	5	602	CLA	2	0
28	2	1622	XAT	6	0
30	1	2630	LHG	2	0
31	C	515	BCR	4	0
30	l	101	LHG	2	0
26	R	604	CLA	3	0
31	a	411	BCR	5	0
28	7	1622	XAT	3	0
28	4	622	XAT	3	0
26	r	609	CLA	2	0
29	y	1623	NEX	1	0
26	G	613	CLA	6	0
26	5	603	CLA	2	0
37	z	101	LMG	5	0
28	n	1622	XAT	7	0
25	n	608	CHL	1	0
25	n	601	CHL	3	0
30	d	409	LHG	12	0
26	A	410	CLA	5	0
35	A	409	PHO	4	0
25	g	607	CHL	9	0
30	C	2630	LHG	6	0
27	r	620	LUT	5	0
26	b	610	CLA	2	0
27	g	1620	LUT	8	0
36	B	621	SQD	5	0
25	s	606	CHL	2	0
28	8	622	XAT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	607	CLA	5	0
29	3	1623	NEX	3	0
39	c	520	DGD	1	0
26	Y	604	CLA	1	0
26	S	614	CLA	2	0
26	A	406	CLA	3	0
29	G	1623	NEX	5	0
26	1	602	CLA	3	0
26	n	611	CLA	2	0
26	C	501	CLA	5	0
36	a	412	SQD	1	0
25	7	608	CHL	4	0
27	R	620	LUT	4	0
26	y	612	CLA	1	0
26	n	602	CLA	8	0
27	3	1621	LUT	4	0
26	R	616	CLA	3	0
26	B	603	CLA	6	0
28	1	1622	XAT	4	0
30	b	2630	LHG	2	0
25	G	606	CHL	6	0
30	8	2630	LHG	1	0
27	2	1621	LUT	4	0
37	b	2633	LMG	3	0
30	5	2630	LHG	2	0
26	y	611	CLA	1	0
25	n	609	CHL	4	0
27	y	1620	LUT	4	0
30	c	522	LHG	4	0
26	y	604	CLA	1	0
26	g	610	CLA	4	0
30	R	2630	LHG	4	0
26	7	603	CLA	3	0
36	b	621	SQD	5	0
26	b	607	CLA	4	0
26	b	616	CLA	1	0
26	G	603	CLA	3	0
25	G	609	CHL	7	0
26	6	604	CLA	1	0
26	B	608	CLA	2	0
25	2	606	CHL	1	0
37	a	415	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	Y	1621	LUT	5	0
25	S	608	CHL	1	0
25	Y	601	CHL	2	0
26	5	614	CLA	1	0
39	C	520	DGD	1	0
26	n	613	CLA	4	0
26	c	506	CLA	2	0
37	B	622	LMG	5	0
28	y	1622	XAT	5	0
25	n	607	CHL	3	0
25	4	601	CHL	2	0
26	B	604	CLA	3	0
26	6	613	CLA	1	0
30	S	2630	LHG	4	0
26	R	609	CLA	2	0
25	G	601	CHL	6	0
25	G	605	CHL	2	0
25	R	606	CHL	2	0
26	s	609	CLA	6	0
28	R	622	XAT	4	0
27	g	1621	LUT	7	0
27	s	1620	LUT	3	0
30	D	409	LHG	13	0
29	n	1623	NEX	1	0
26	C	508	CLA	3	0
26	N	612	CLA	4	0
26	y	613	CLA	3	0
26	s	610	CLA	3	0
25	g	601	CHL	6	0
29	2	1623	NEX	1	0
27	5	1620	LUT	4	0
25	g	609	CHL	7	0
37	C	521	LMG	1	0
27	n	1621	LUT	5	0
31	B	618	BCR	4	0
25	Y	609	CHL	2	0
39	C	518	DGD	2	0
25	N	605	CHL	1	0
26	B	606	CLA	4	0
25	R	614	CHL	2	0
31	c	515	BCR	3	0
26	2	604	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	3	604	CLA	1	0
26	r	603	CLA	3	0
37	d	411	LMG	2	0
26	n	610	CLA	7	0
25	g	606	CHL	6	0
26	y	602	CLA	6	0
25	3	606	CHL	3	0
26	b	603	CLA	8	0
25	n	606	CHL	1	0
29	g	1623	NEX	2	0
37	B	2633	LMG	3	0
26	G	614	CLA	2	0
25	3	607	CHL	4	0
26	r	602	CLA	4	0
27	G	1620	LUT	6	0
26	2	602	CLA	2	0
37	a	413	LMG	2	0
25	1	607	CHL	4	0
27	7	1620	LUT	3	0
26	3	613	CLA	1	0
28	N	1622	XAT	6	0
26	r	601	CLA	3	0
26	B	617	CLA	3	0
26	r	613	CLA	5	0
25	y	609	CHL	3	0
27	8	620	LUT	3	0
25	3	609	CHL	5	0
25	6	607	CHL	2	0
25	6	606	CHL	1	0
26	N	602	CLA	6	0
26	S	610	CLA	2	0
36	A	418	SQD	11	0
26	C	513	CLA	4	0
26	N	611	CLA	2	0
26	R	613	CLA	4	0
25	y	605	CHL	3	0
26	y	603	CLA	5	0
29	s	1623	NEX	3	0
26	r	611	CLA	4	0
26	b	604	CLA	2	0
36	A	412	SQD	2	0
26	b	617	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	6	605	CHL	1	0
26	6	603	CLA	1	0
30	d	410	LHG	2	0
37	D	411	LMG	2	0
25	3	608	CHL	4	0
26	g	614	CLA	2	0
35	a	408	PHO	7	0
26	c	507	CLA	4	0
25	N	609	CHL	4	0
26	C	510	CLA	5	0
30	c	523	LHG	2	0
30	n	2630	LHG	3	0
29	R	623	NEX	5	0
26	g	604	CLA	2	0
26	c	505	CLA	3	0
26	4	610	CLA	1	0
30	y	2630	LHG	4	0
26	R	601	CLA	3	0
26	s	614	CLA	2	0
31	d	404	BCR	3	0
26	b	615	CLA	3	0
26	1	613	CLA	1	0
27	4	620	LUT	2	0
25	r	614	CHL	2	0
30	2	2630	LHG	1	0
30	3	2630	LHG	3	0
26	g	613	CLA	6	0
26	r	610	CLA	1	0
25	4	608	CHL	2	0
30	D	408	LHG	1	0
26	a	406	CLA	4	0
26	s	612	CLA	1	0
25	r	606	CHL	3	0
25	3	605	CHL	1	0
26	3	603	CLA	4	0
26	S	609	CLA	5	0
26	B	609	CLA	2	0
26	7	611	CLA	2	0
26	2	613	CLA	1	0
26	c	503	CLA	3	0
26	Y	612	CLA	2	0
31	4	623	BCR	7	0

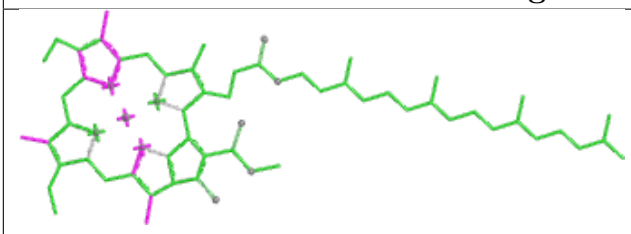
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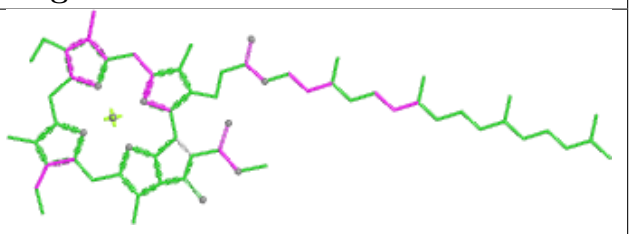
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	a	418	SQD	11	0
26	d	402	CLA	6	0
31	C	516	BCR	6	0
25	3	601	CHL	1	0
27	3	1620	LUT	4	0
26	S	603	CLA	1	0
25	2	607	CHL	2	0
27	s	1621	LUT	3	0
27	n	1620	LUT	4	0
26	B	602	CLA	5	0
30	6	2630	LHG	1	0

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

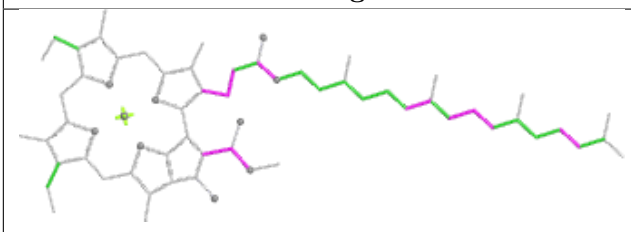
Ligand CLA g 602



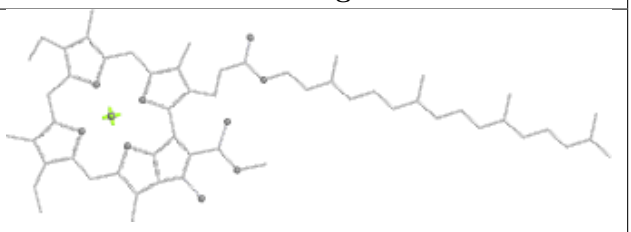
Bond lengths



Bond angles

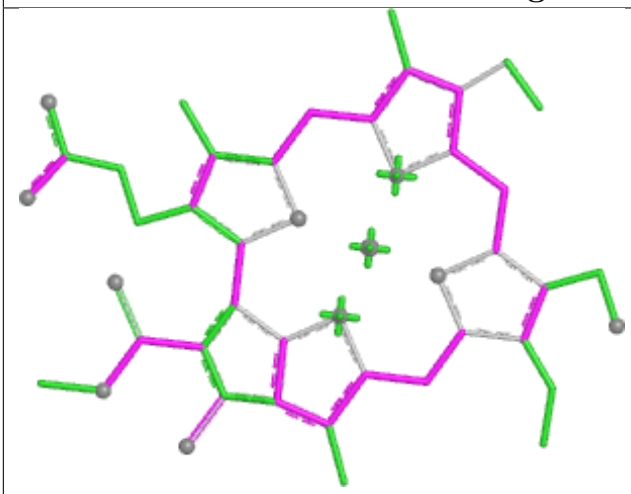


Torsions

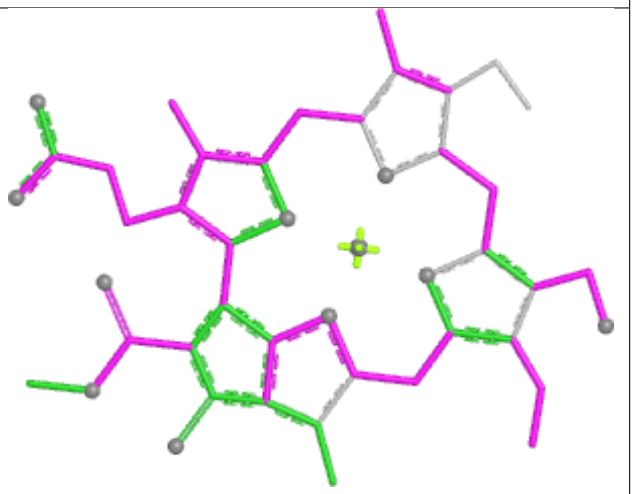


Rings

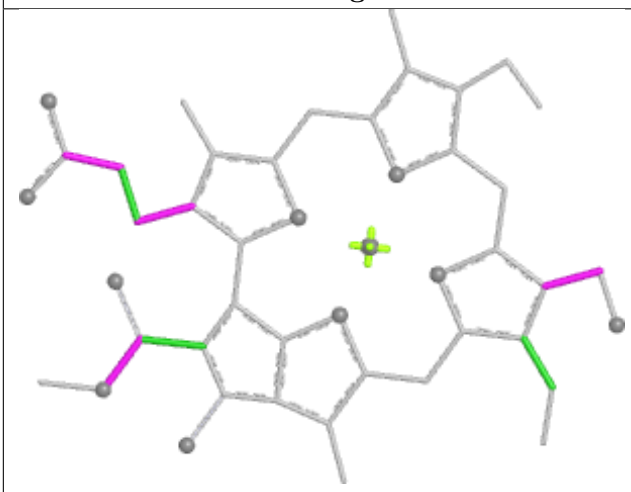
Ligand CHL 4 606



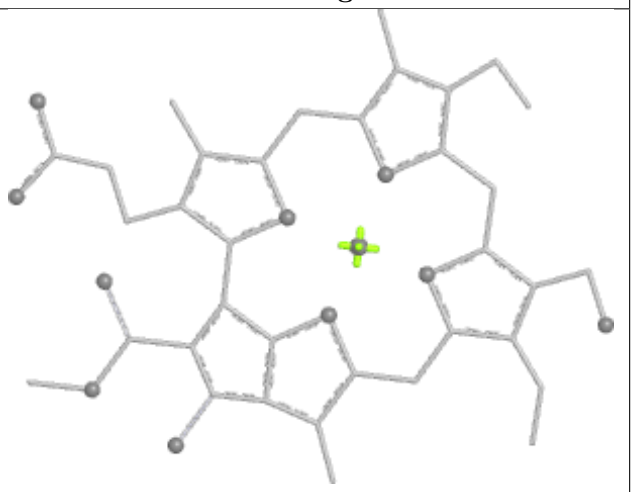
Bond lengths



Bond angles

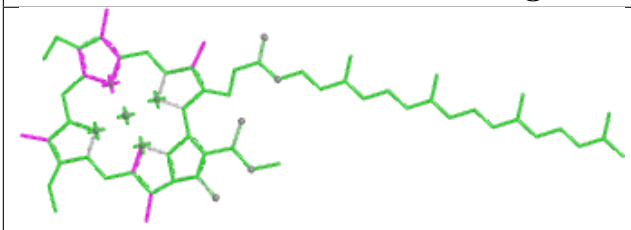


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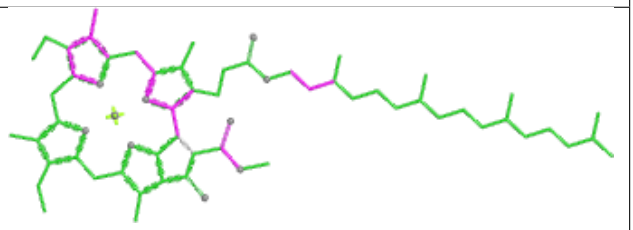


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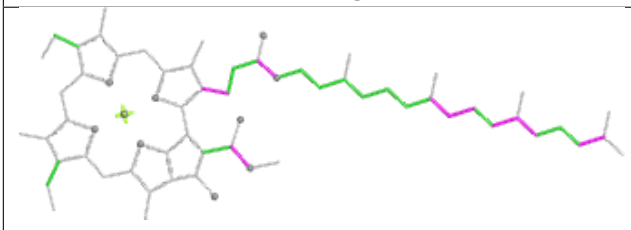
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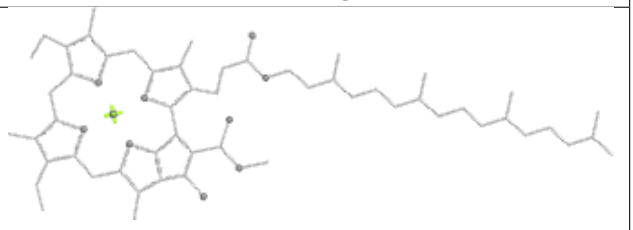
Bond lengths



Bond angles



Torsions

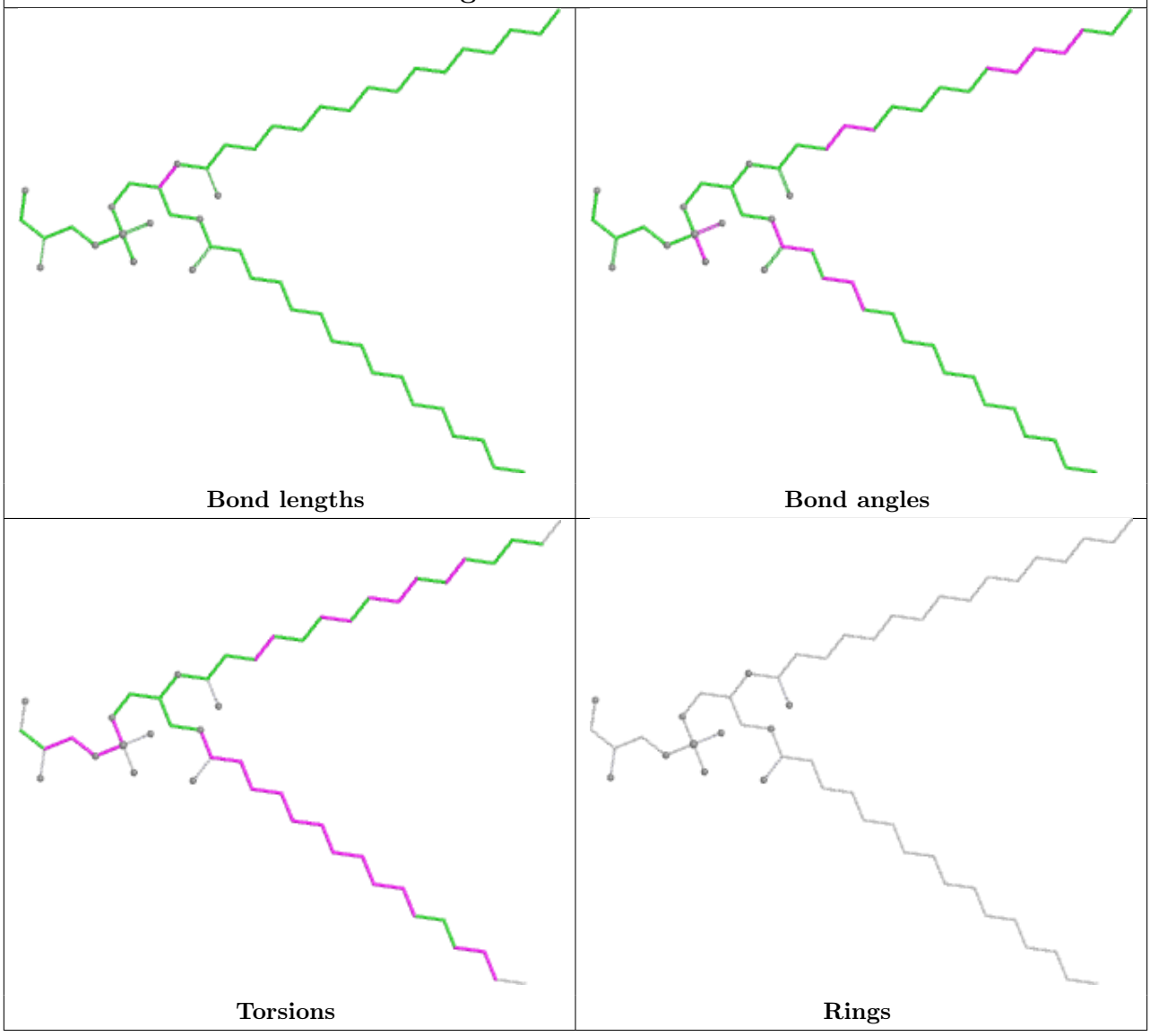


Rings

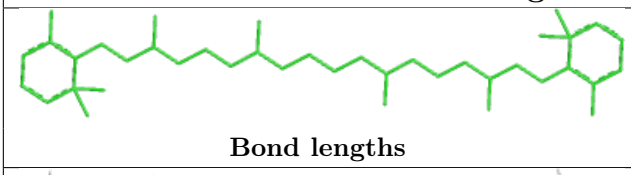
Ligand PL9 d 405



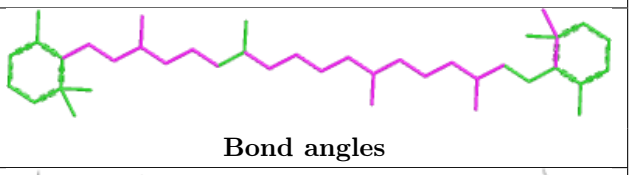
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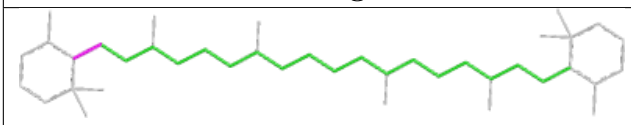
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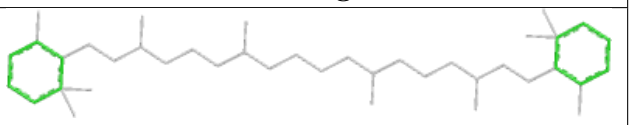
Bond lengths



Bond angles

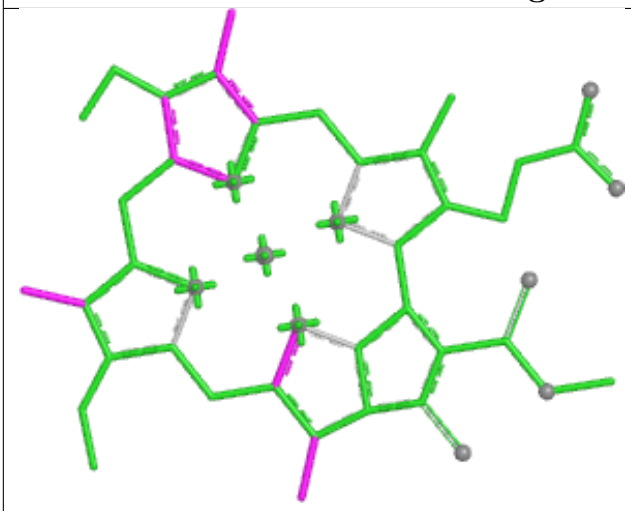


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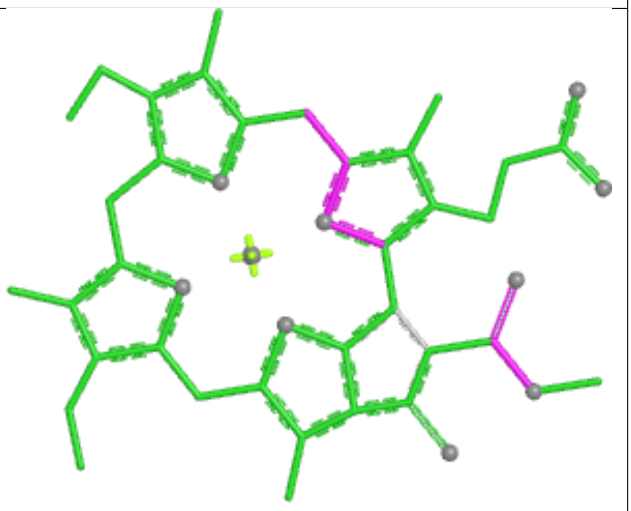


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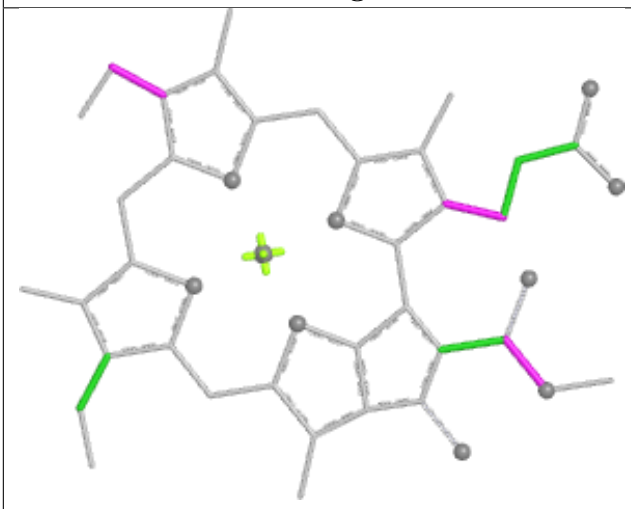
Ligand CLA 6 614



Bond lengths



Bond angles

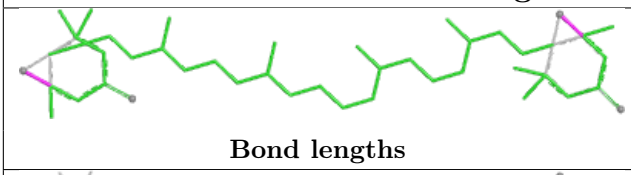


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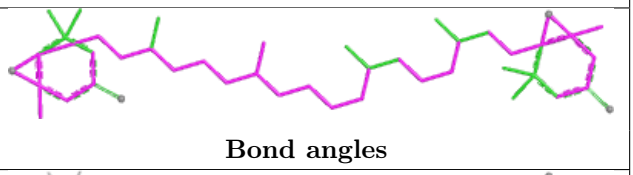


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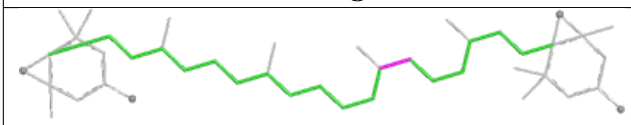
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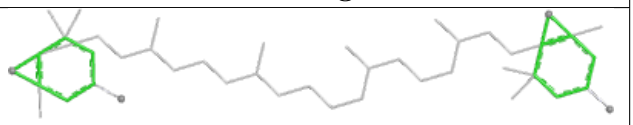
Bond lengths



Bond angles

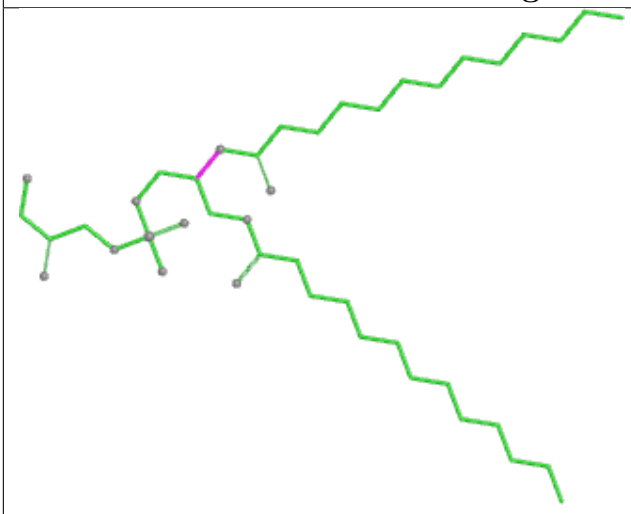


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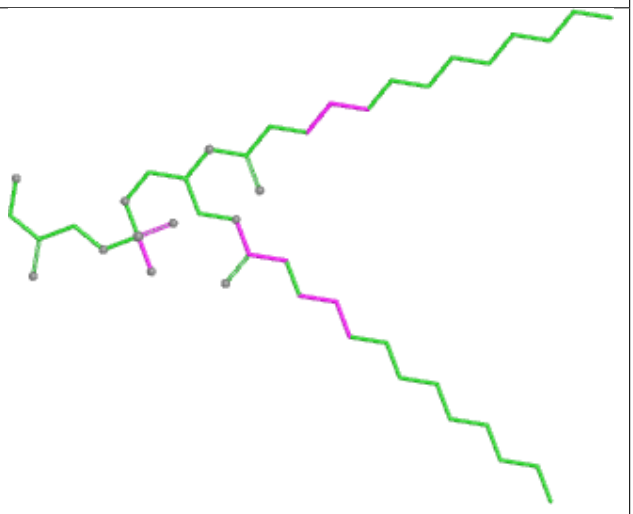


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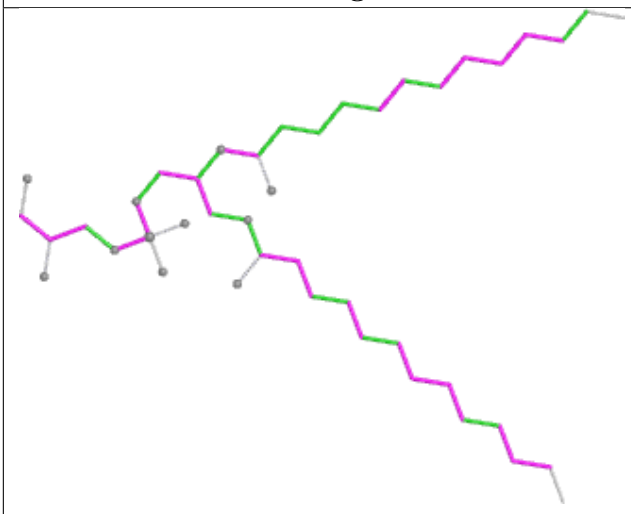
Ligand LHG D 410



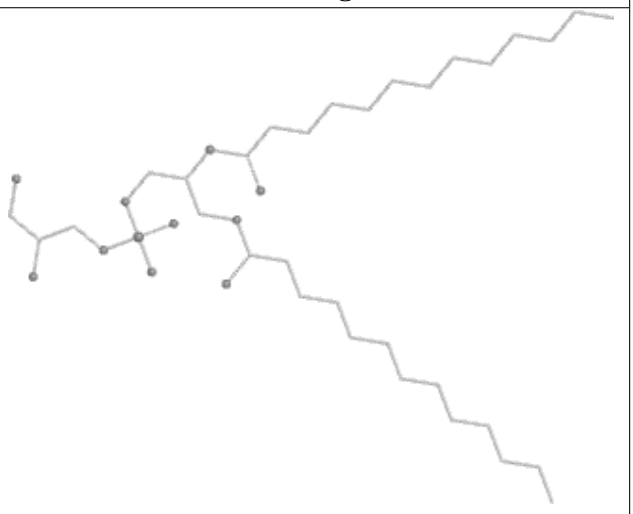
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Bond angles

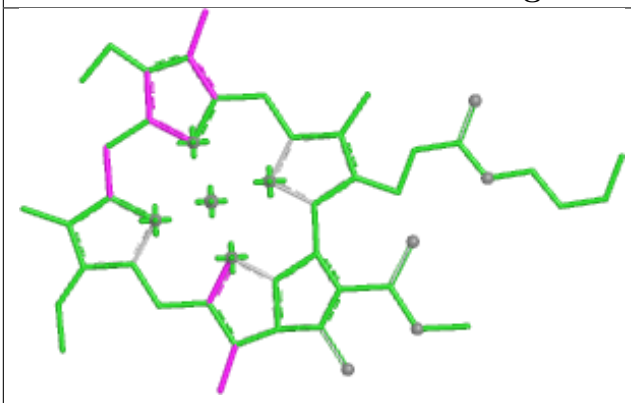


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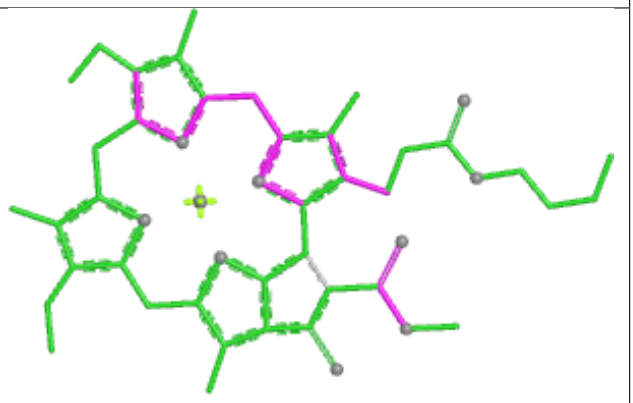


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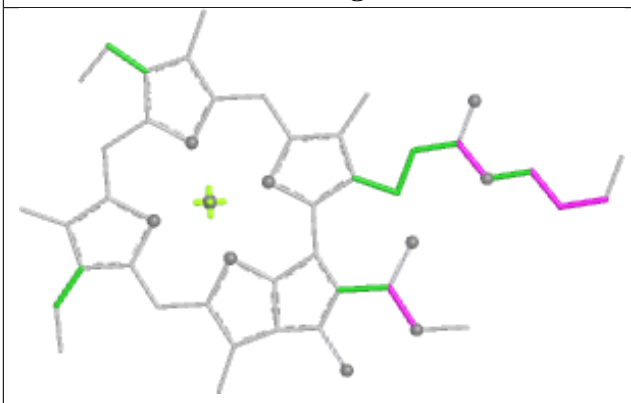
Ligand CLA R 612



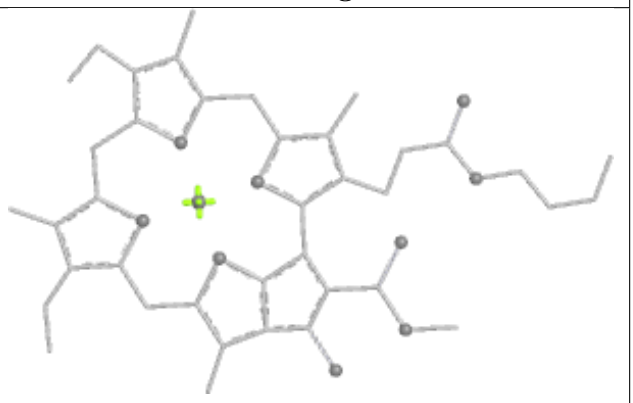
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Bond angles

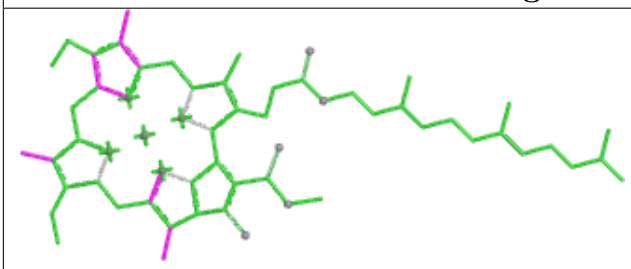


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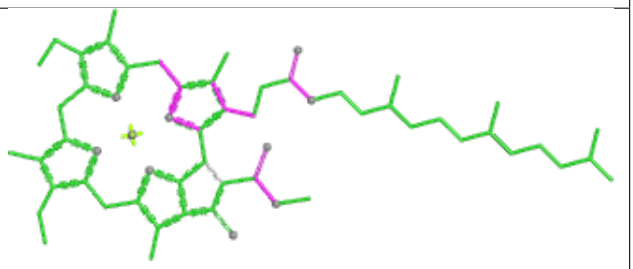


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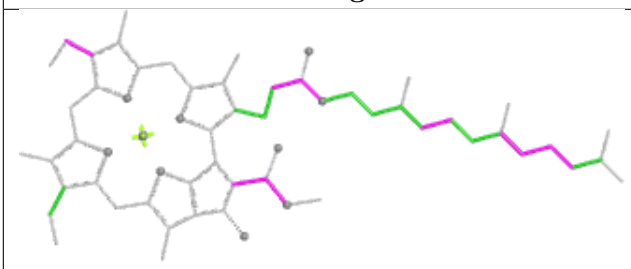
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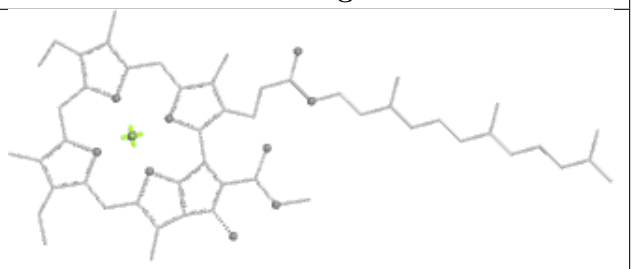
Bond lengths



Bond angles

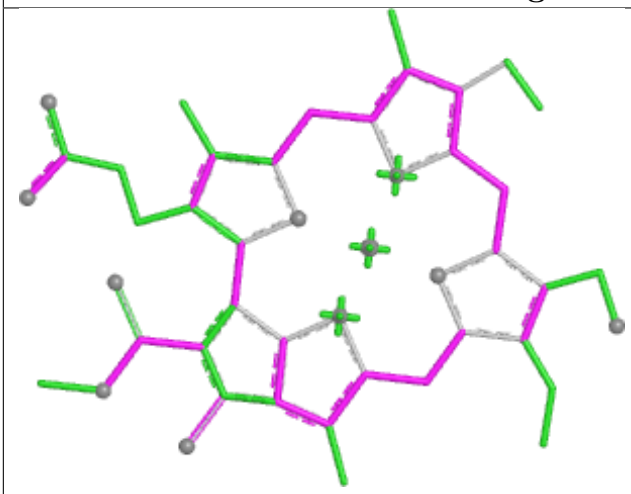


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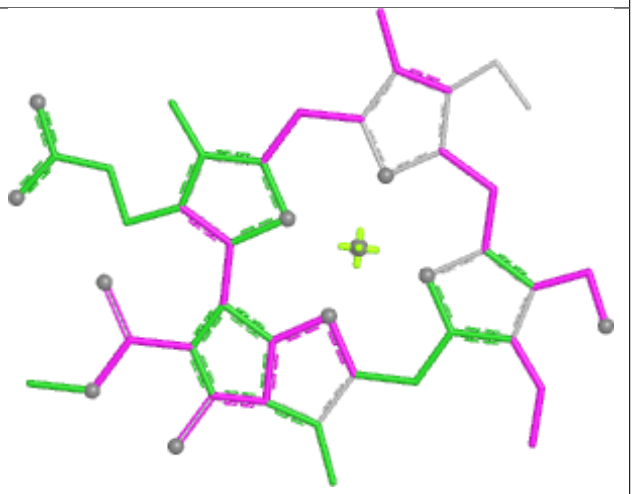


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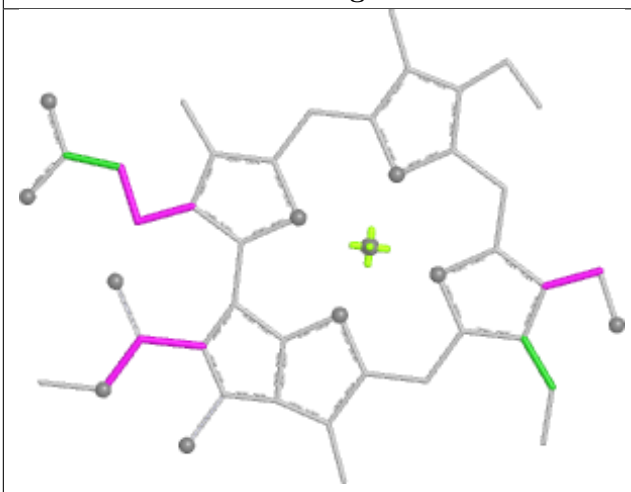
Ligand CHL 1 608



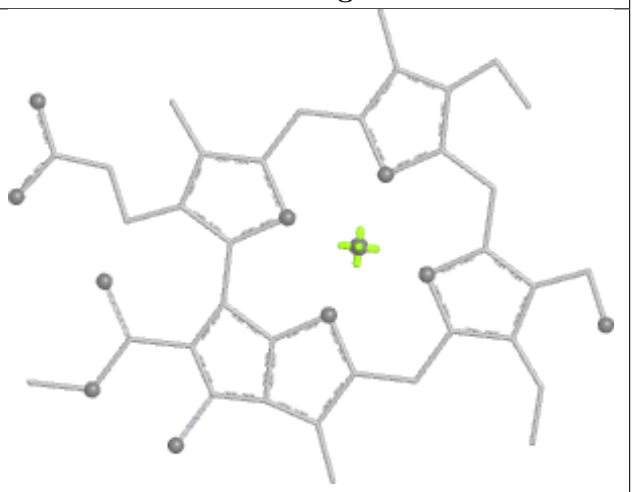
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Bond angles

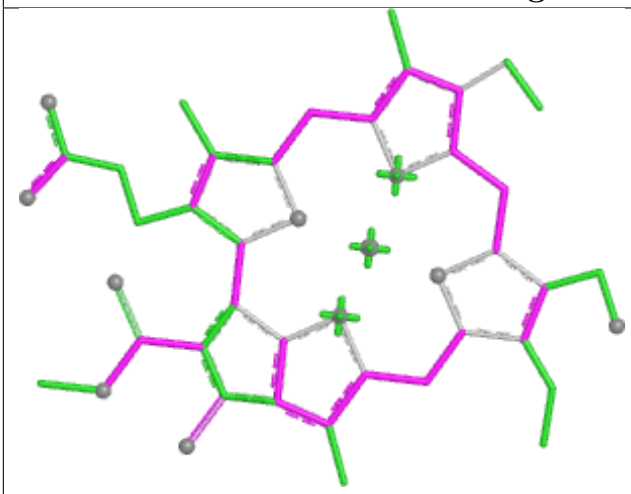


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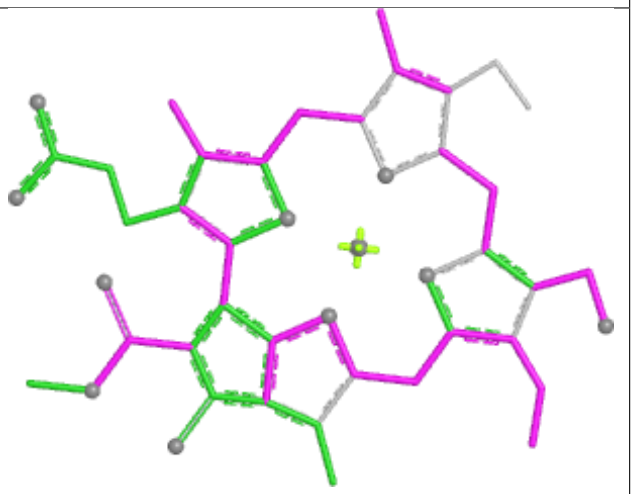


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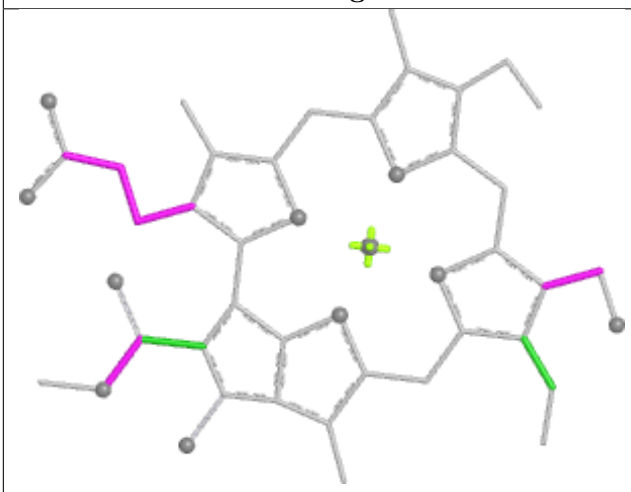
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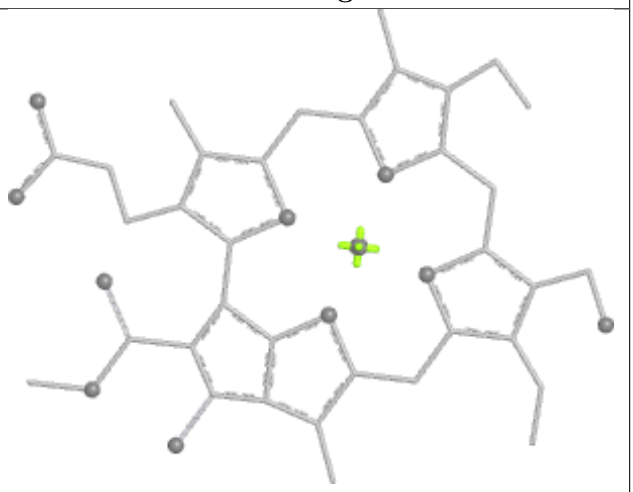
Bond lengths



Bond angles

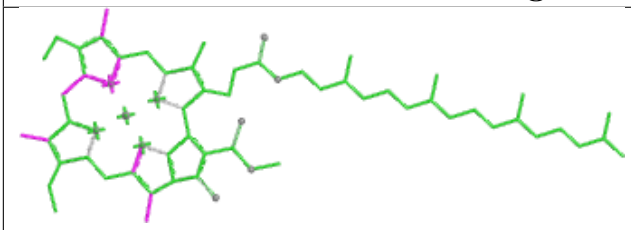


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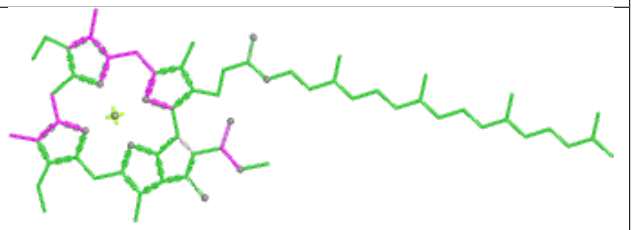


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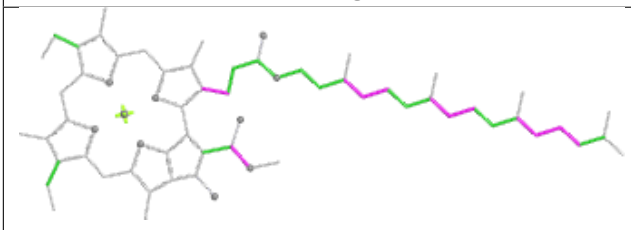
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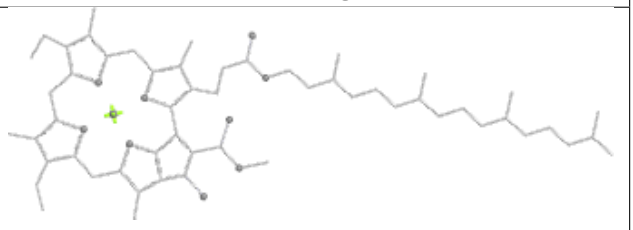
Bond lengths



Bond angles

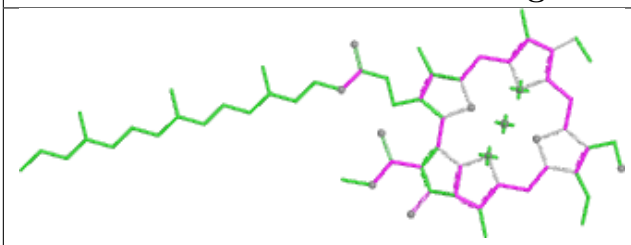


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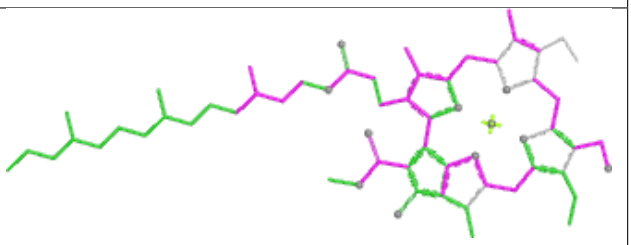


Rings

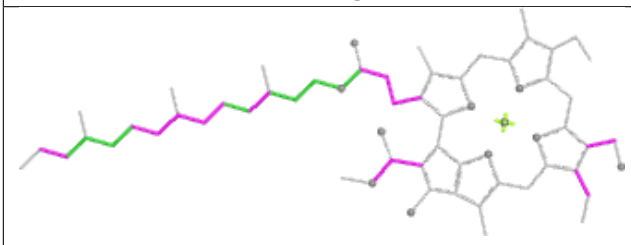
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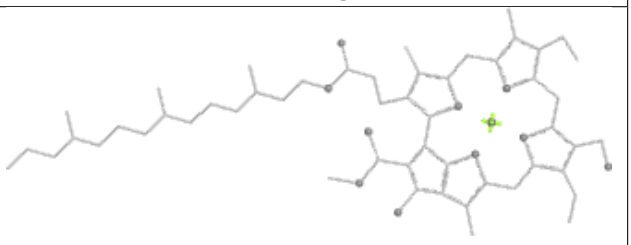
Bond lengths



Bond angles

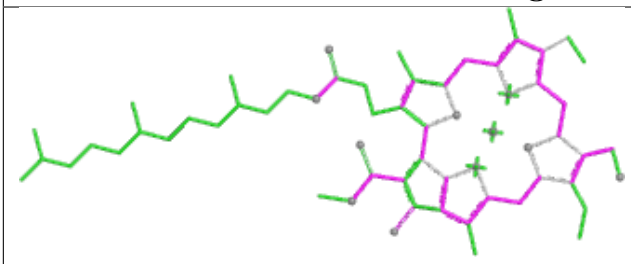


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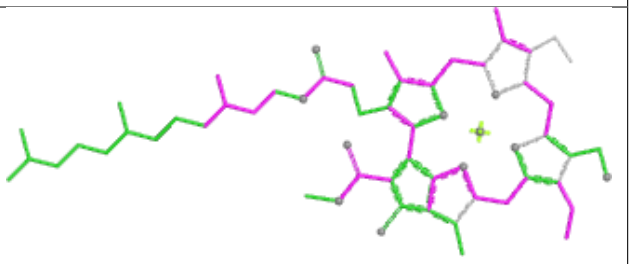


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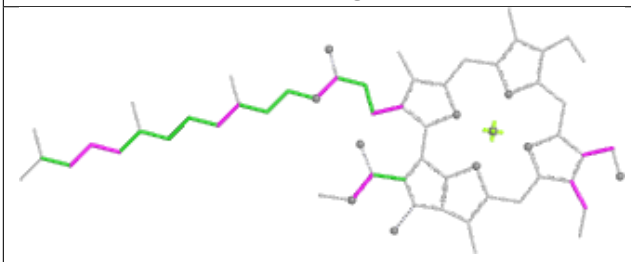
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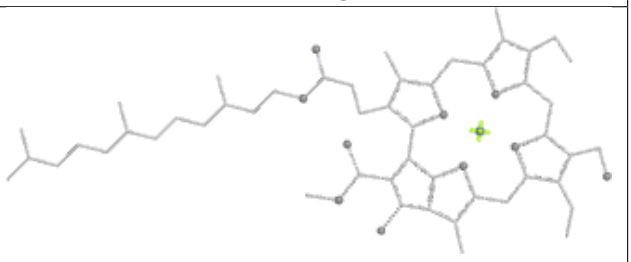
Bond lengths



Bond angles

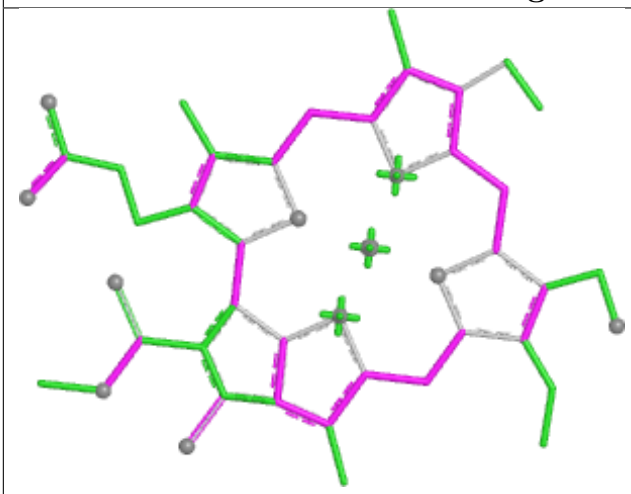


Torsions

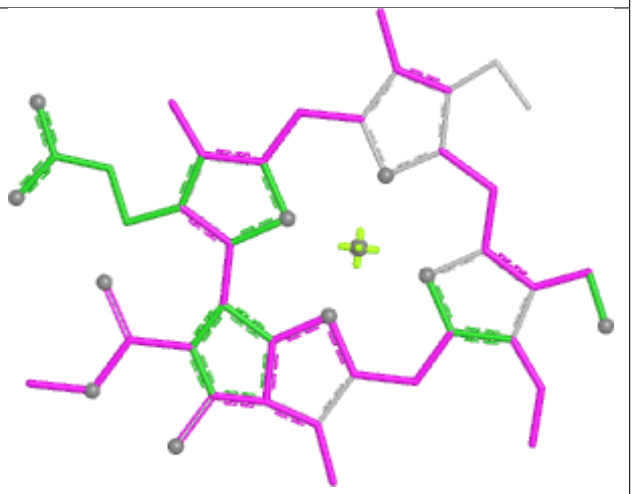


Rings

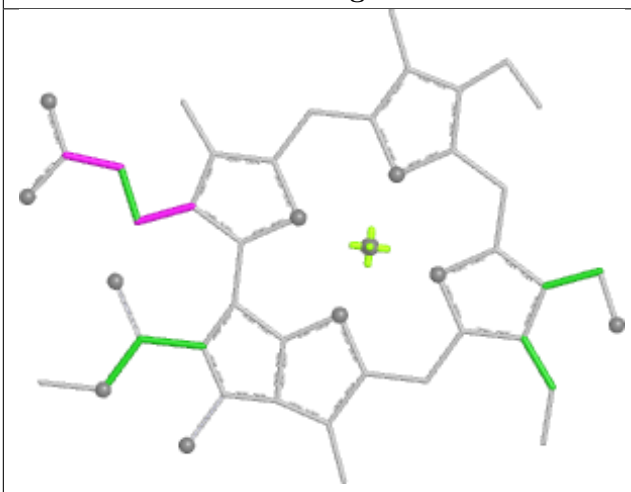
Ligand CHL 6 601



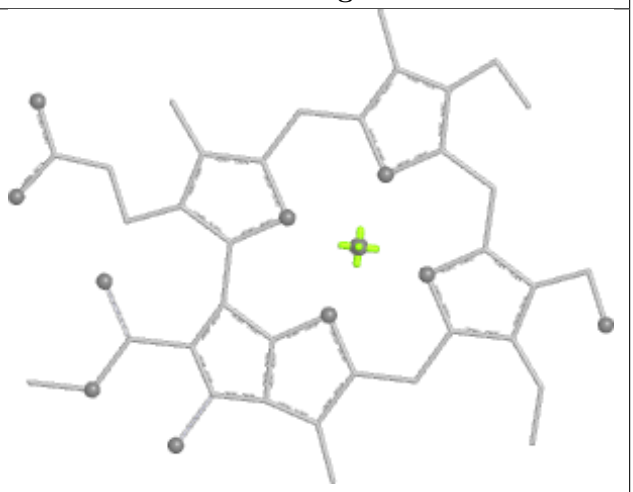
Bond lengths



Bond angles



Torsions



Rings

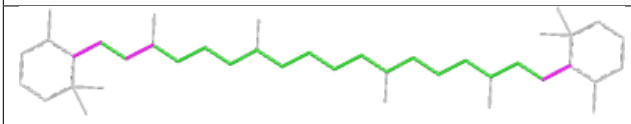
Ligand BCR A 411



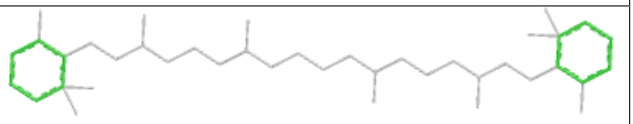
Bond lengths



Bond angles

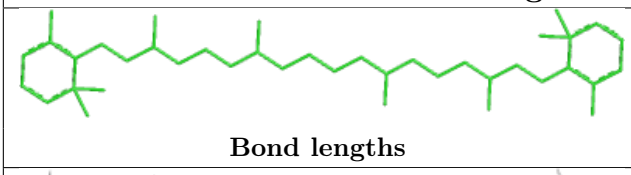


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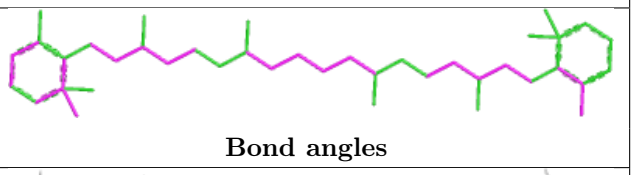


Rings

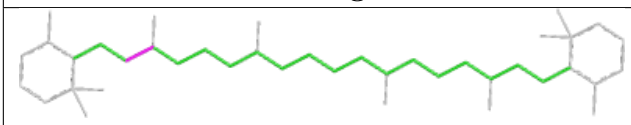
Ligand BCR h 101



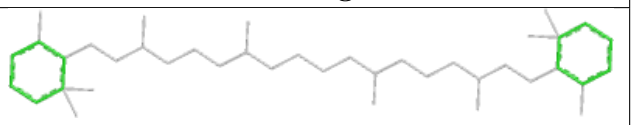
Bond lengths



Bond angles

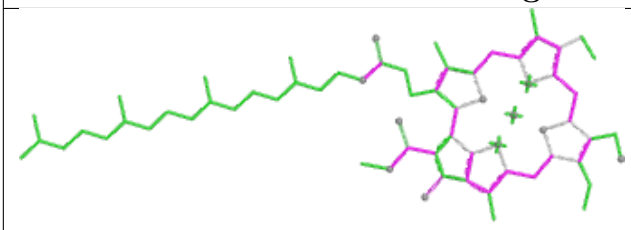


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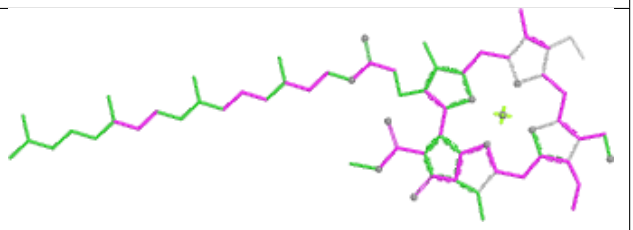


Rings

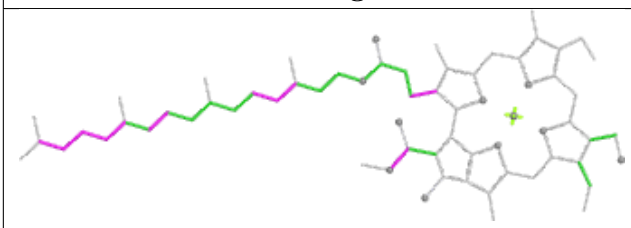
Ligand CHL N 608



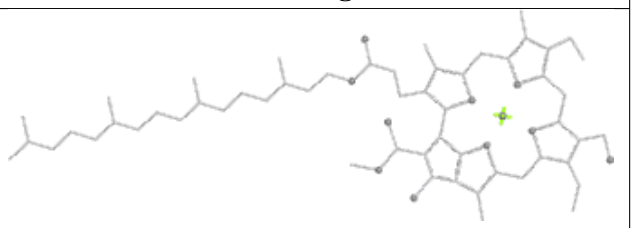
Bond lengths



Bond angles

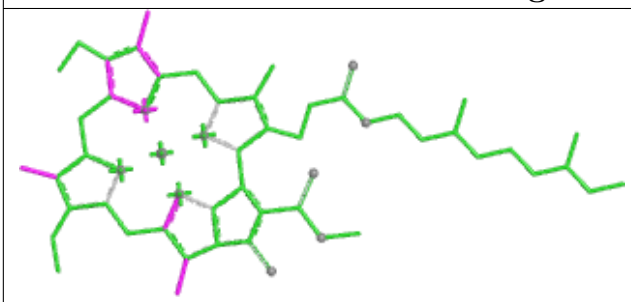


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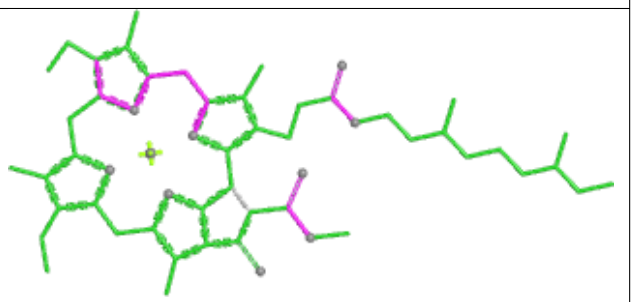


Rings

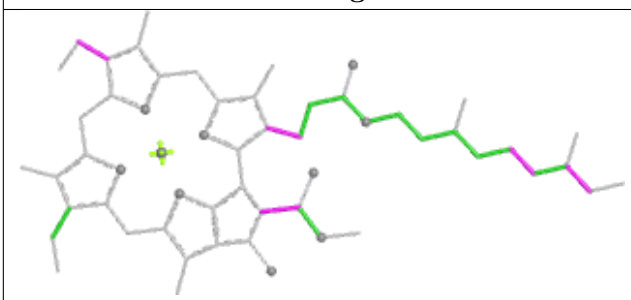
Ligand CLA 1 610



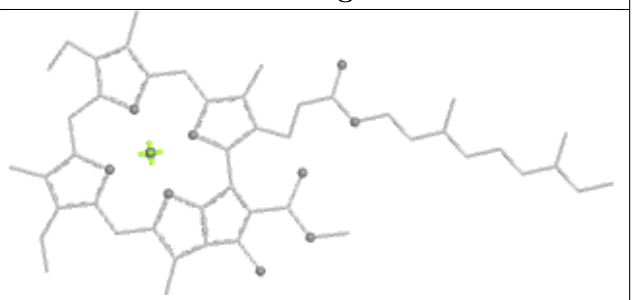
Bond lengths



Bond angles

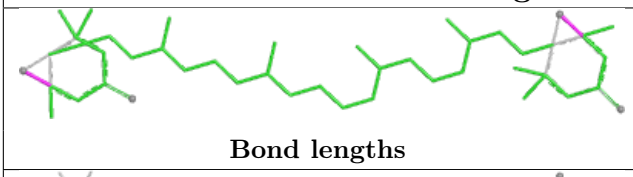


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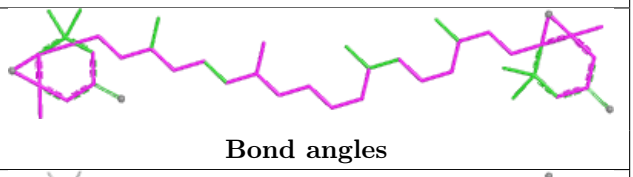


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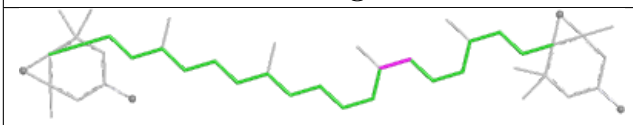
Ligand XAT G 1622



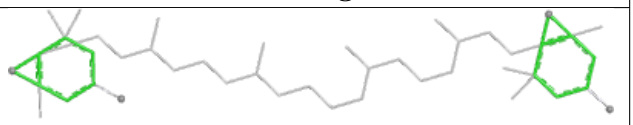
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Bond angles

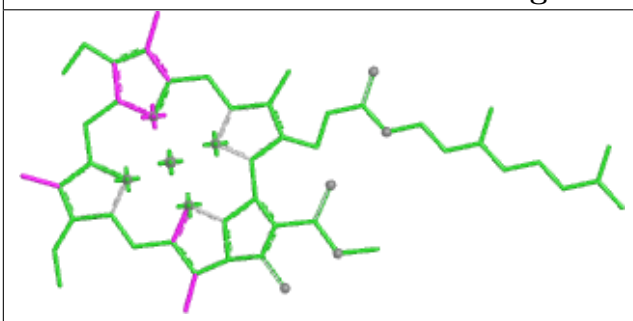


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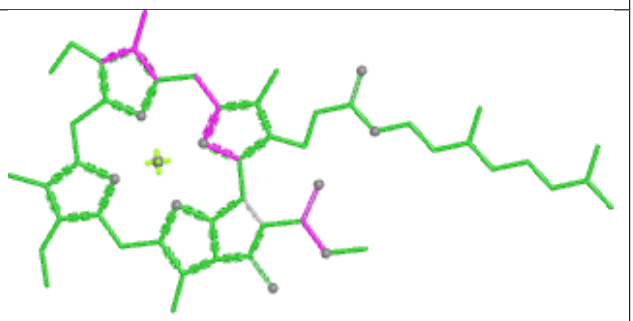


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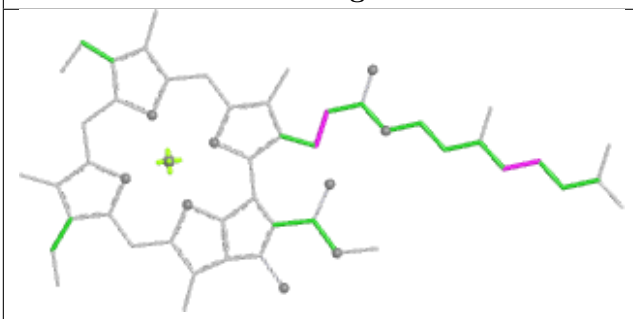
Ligand CLA s 613



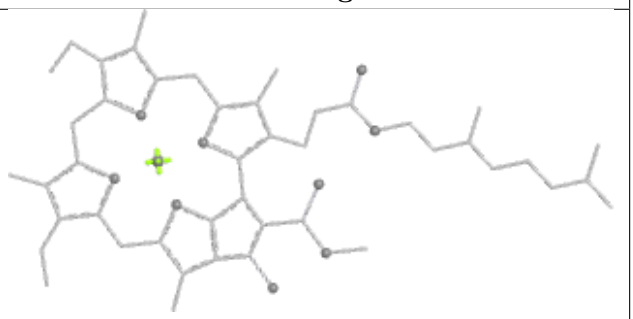
Bond lengths



Bond angles



Torsions

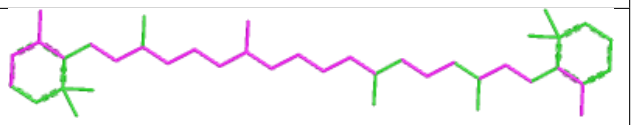


Rings

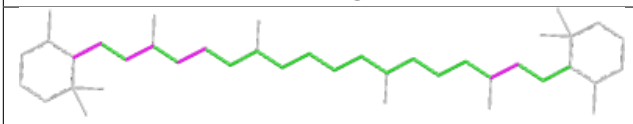
Ligand BCR D 404



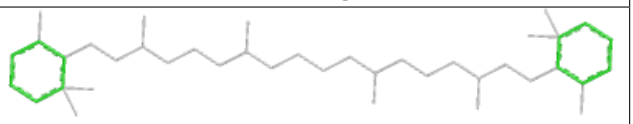
Bond lengths



Bond angles

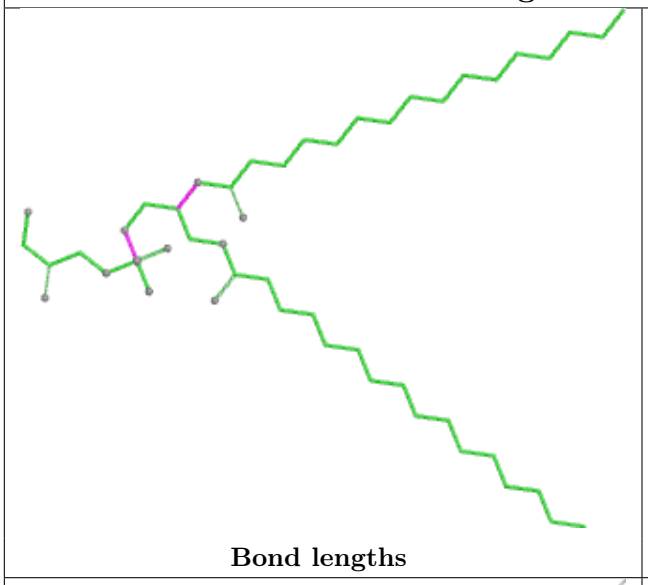


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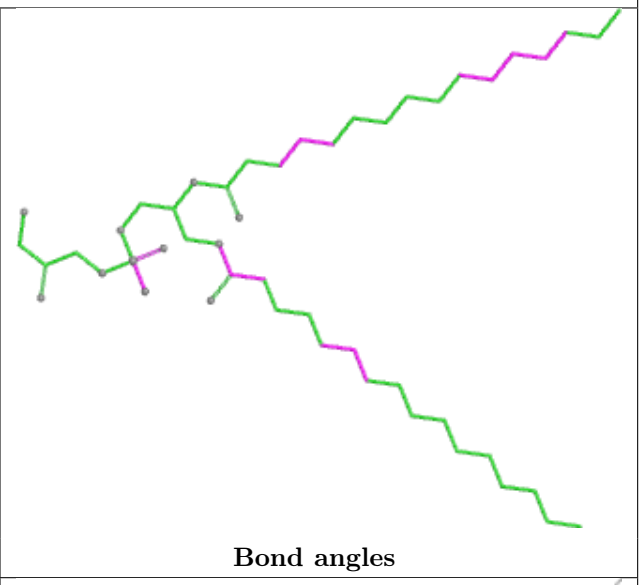


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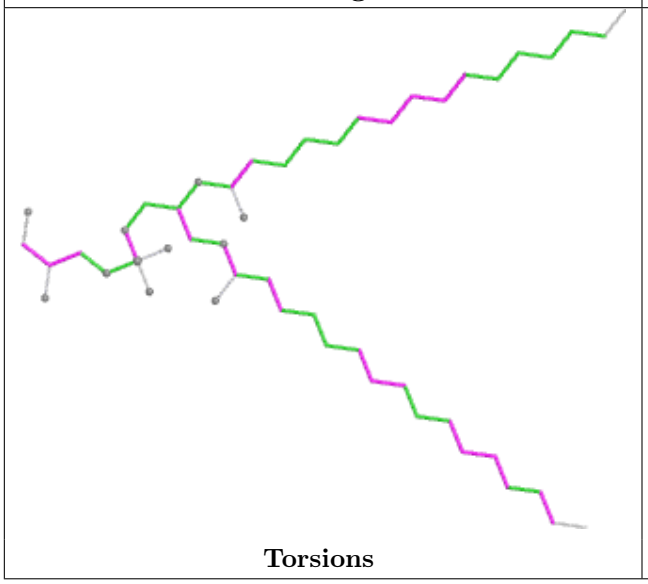
Ligand LHG b 2631



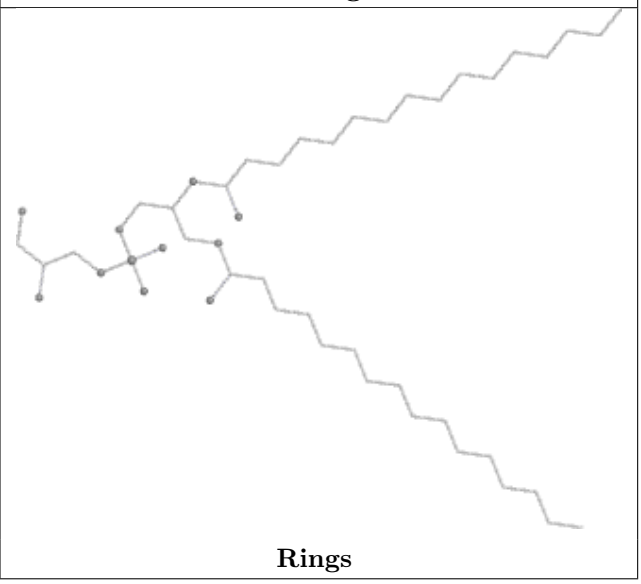
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Bond angles

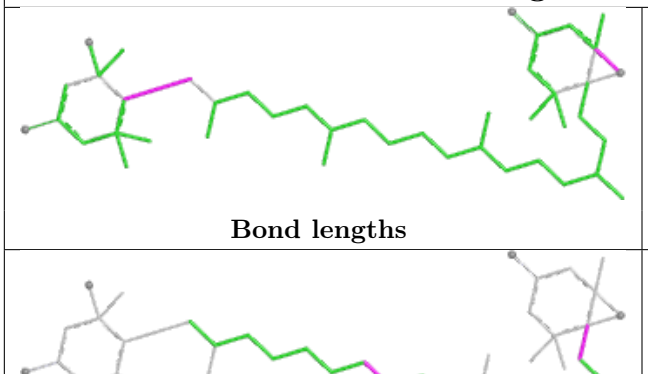


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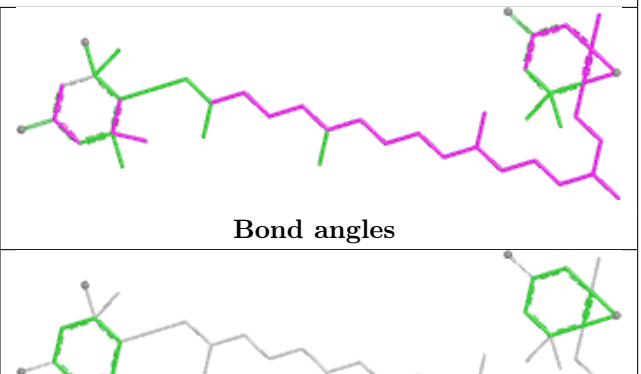


Rings

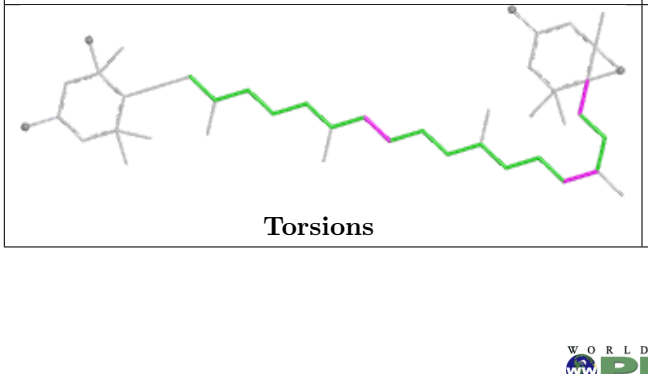
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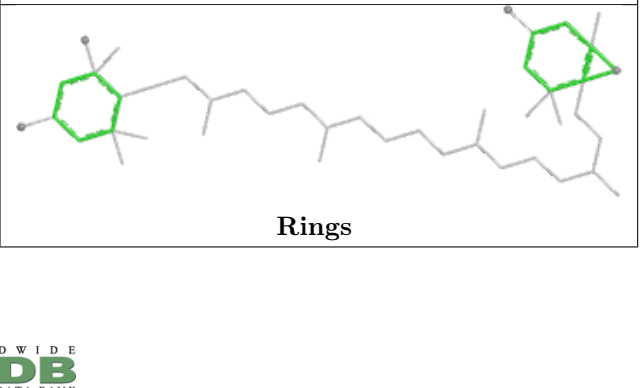
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Bond angles

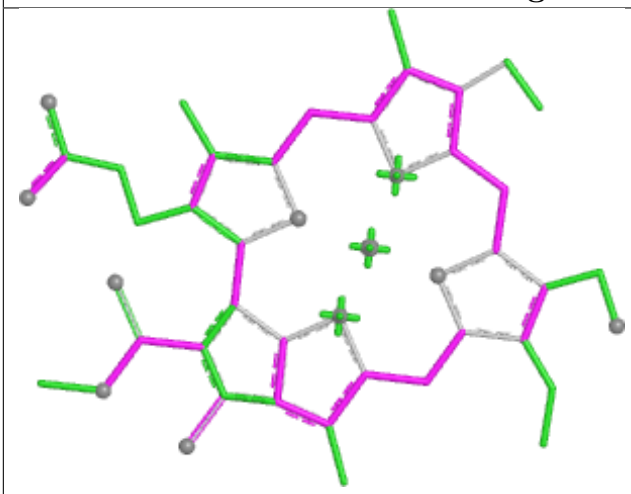


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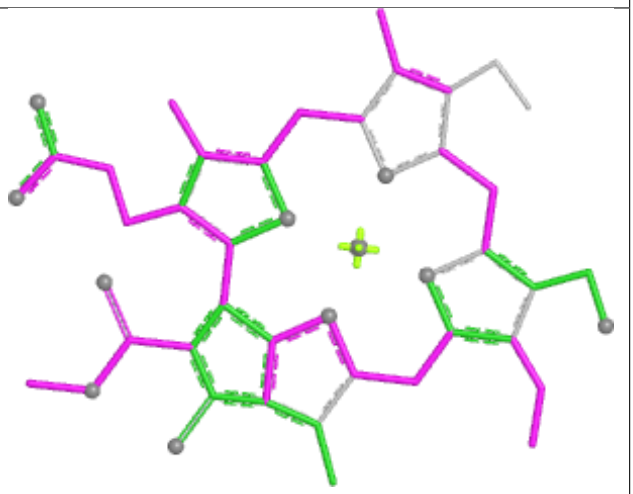


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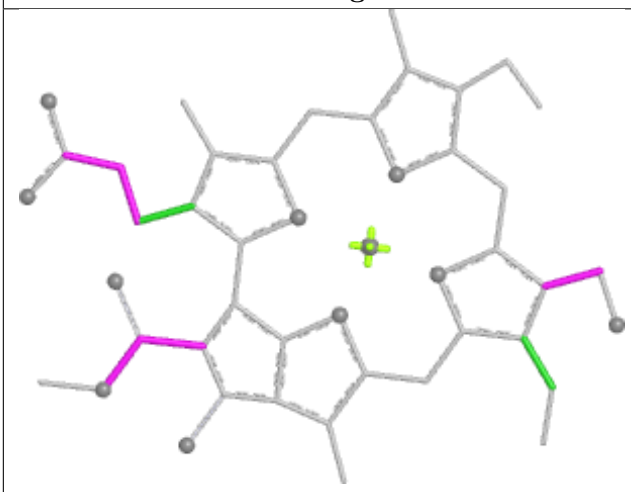
Ligand CHL 1 606



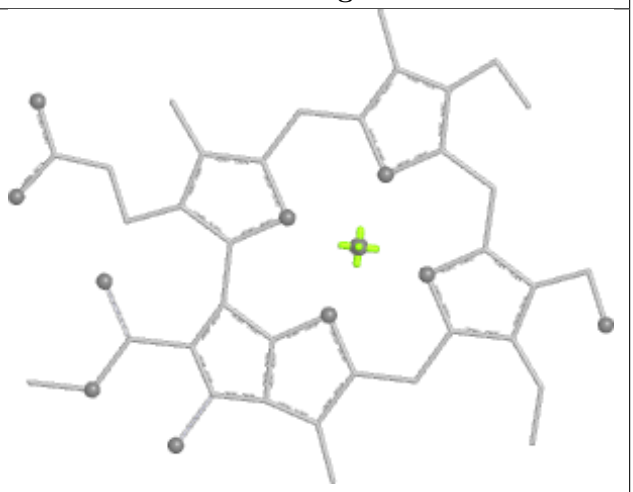
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Bond angles

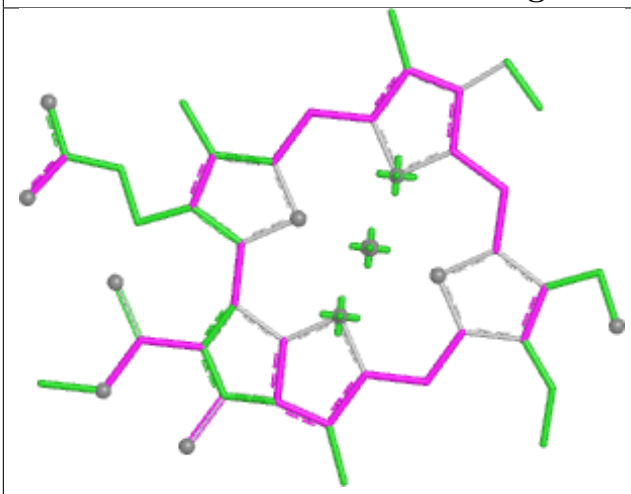


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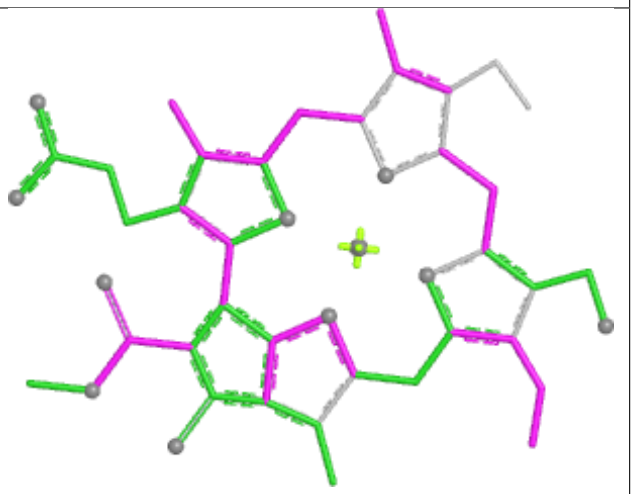


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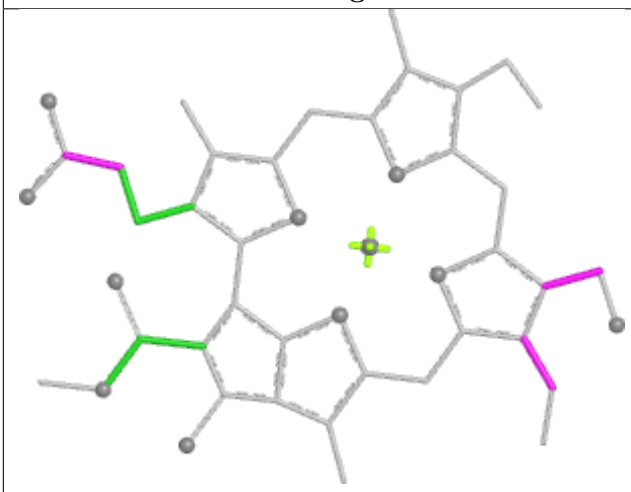
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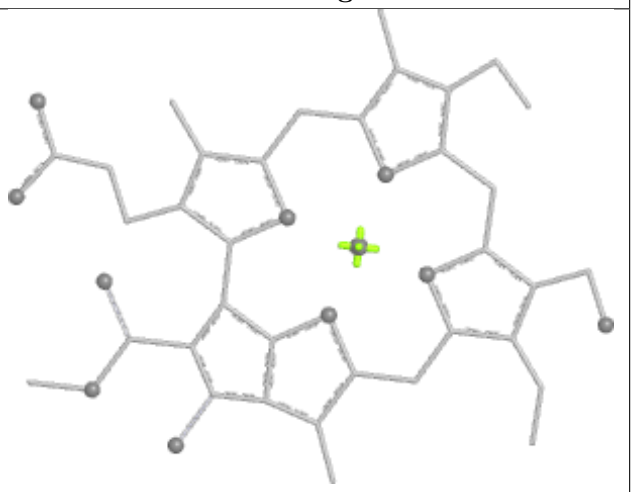
Bond lengths



Bond angles

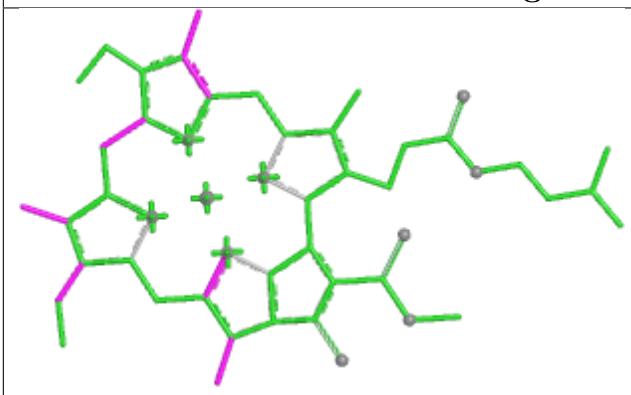


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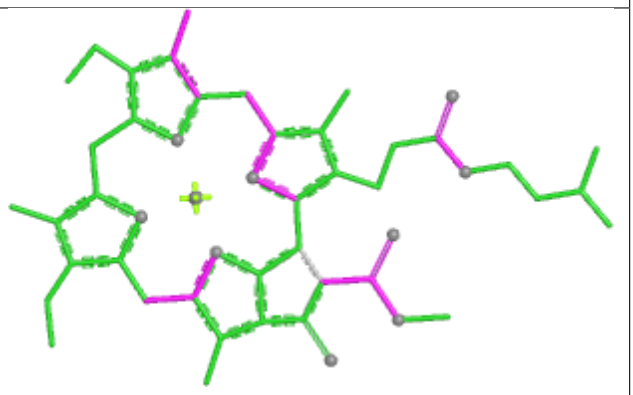


Rings

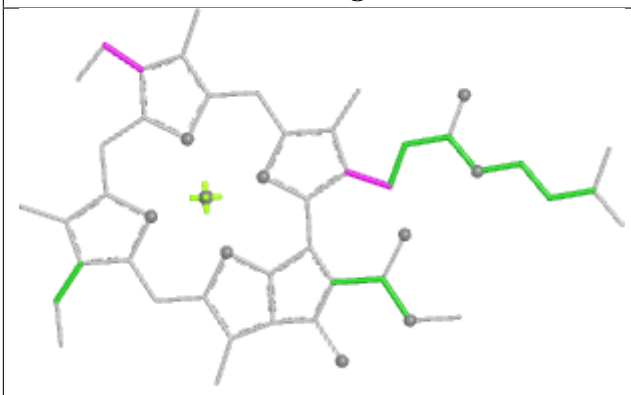
Ligand CLA A 407



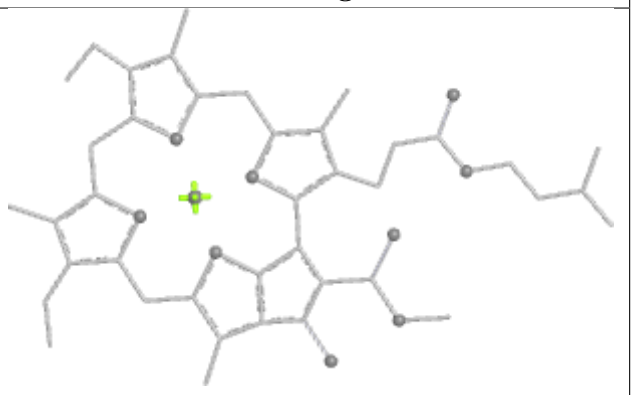
Bond lengths



Bond angles

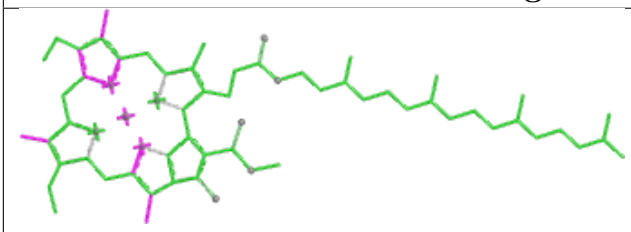


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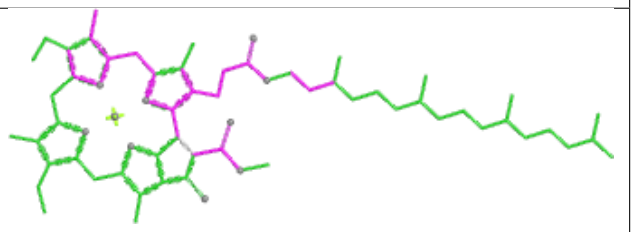


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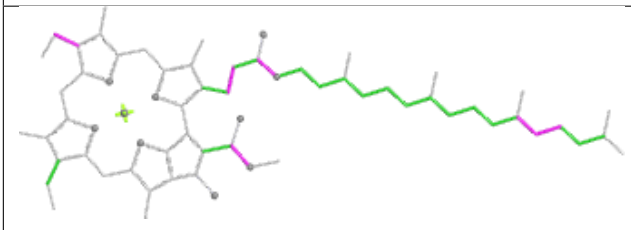
Ligand CLA B 611



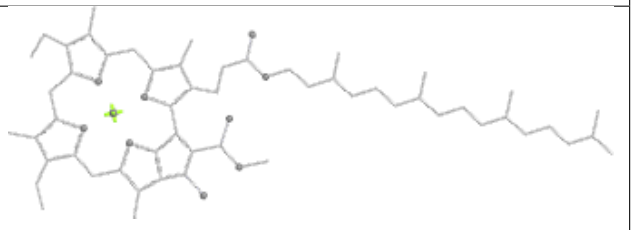
Bond lengths



Bond angles

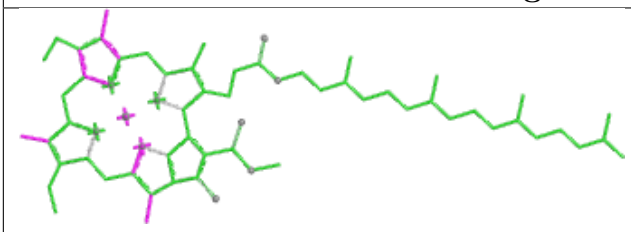


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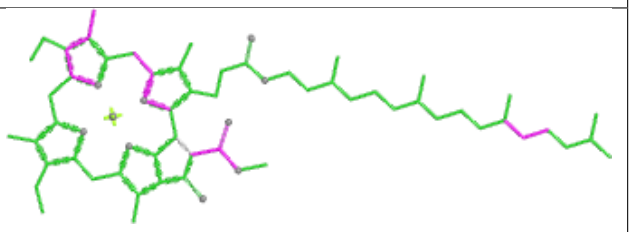


Rings

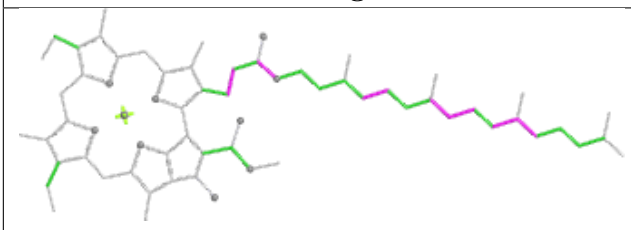
Ligand CLA Y 613



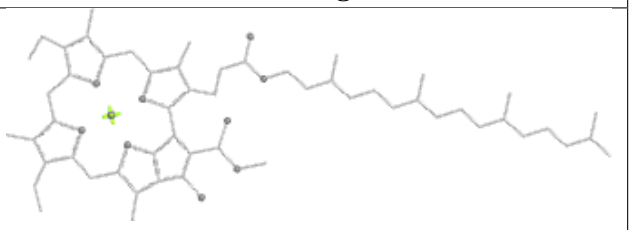
Bond lengths



Bond angles

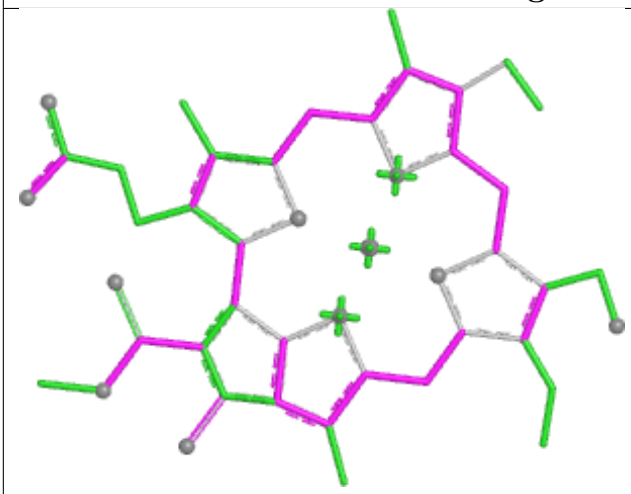


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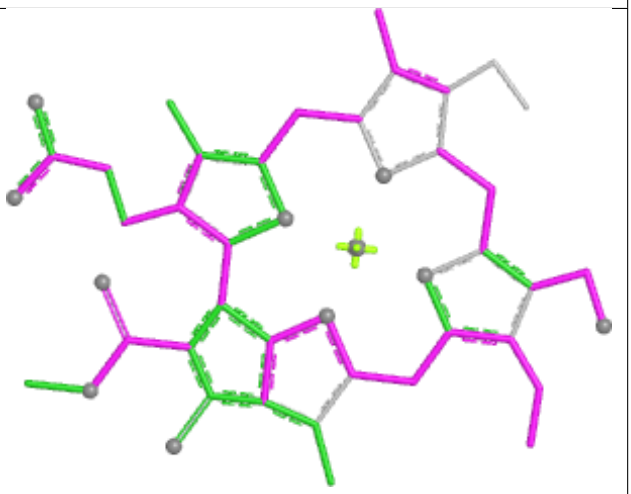


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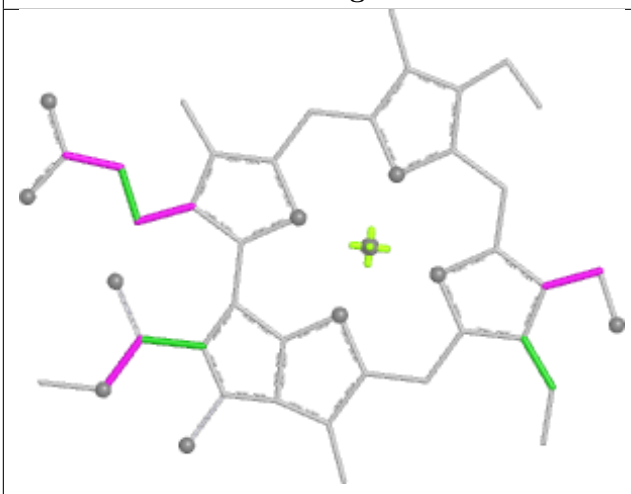
Ligand CHL 1 605



Bond lengths



Bond angles

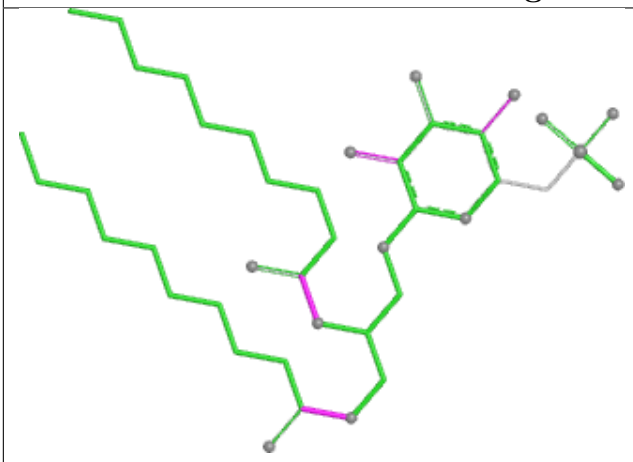


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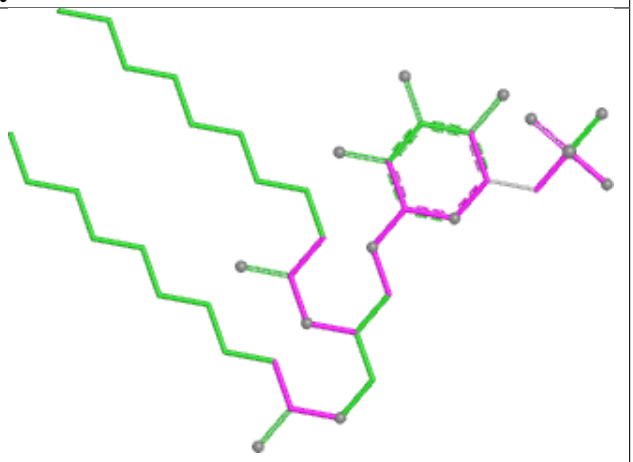


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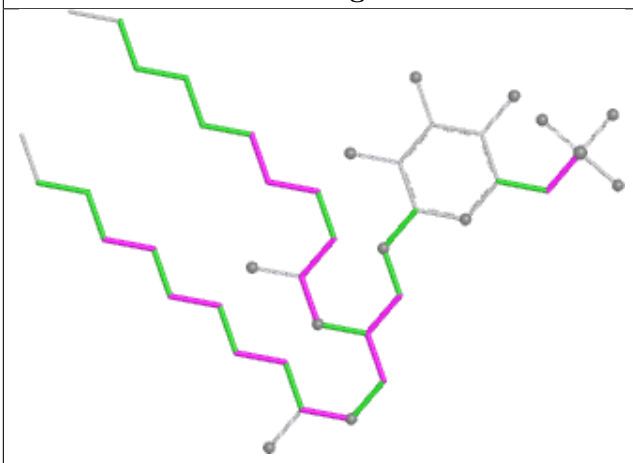
Ligand SQD B 623



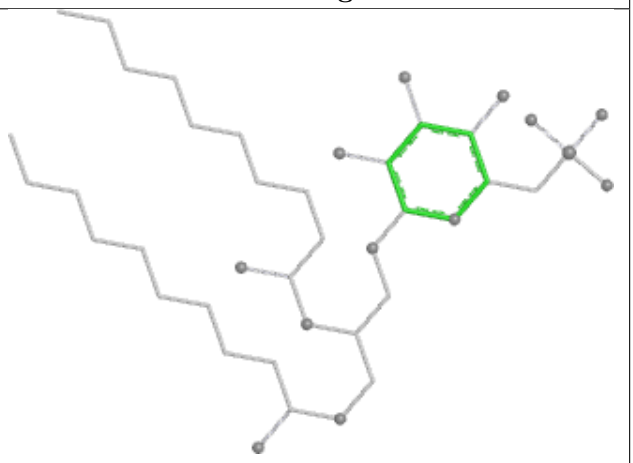
Bond lengths



Bond angles

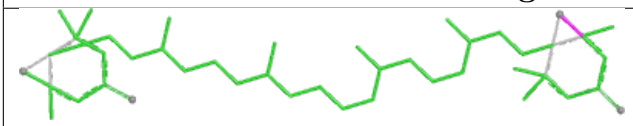


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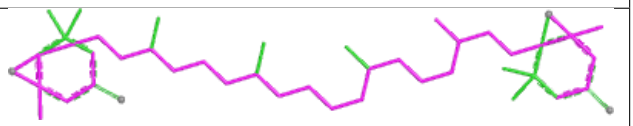


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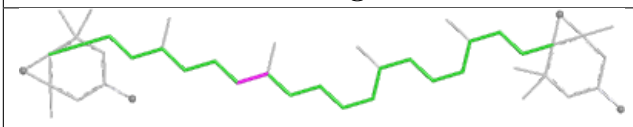
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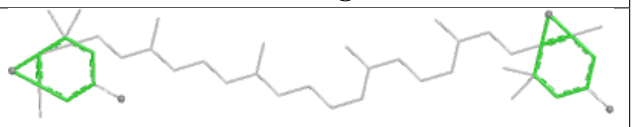
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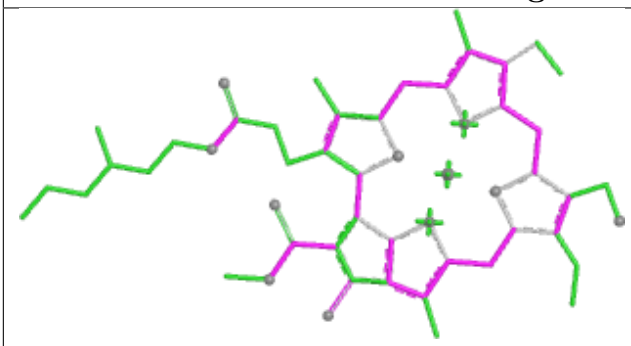


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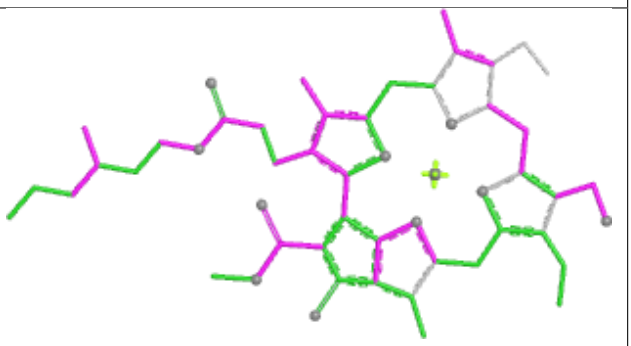


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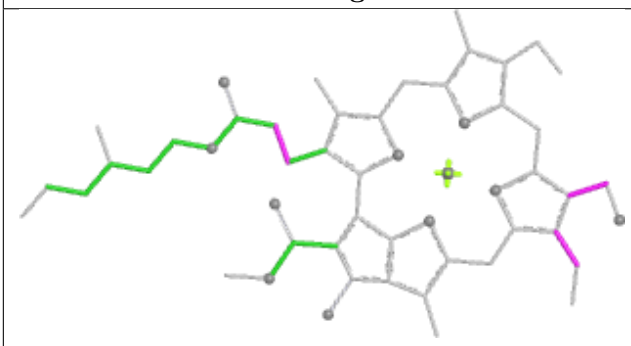
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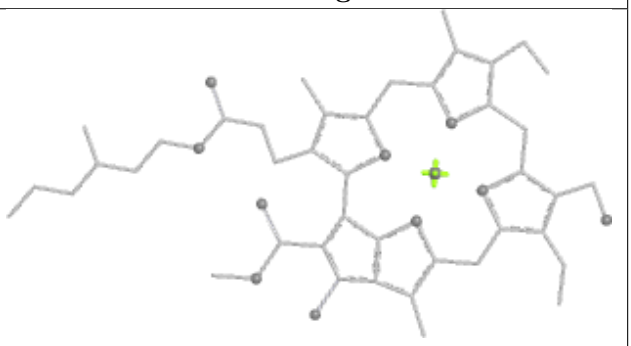
Bond lengths



Bond angles

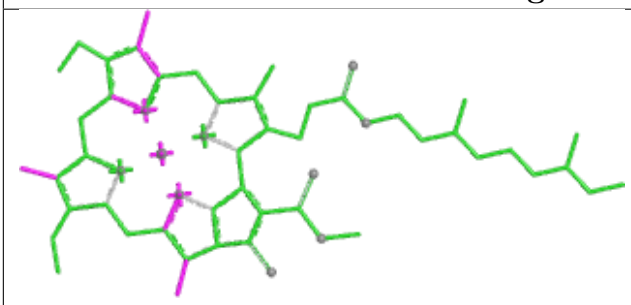


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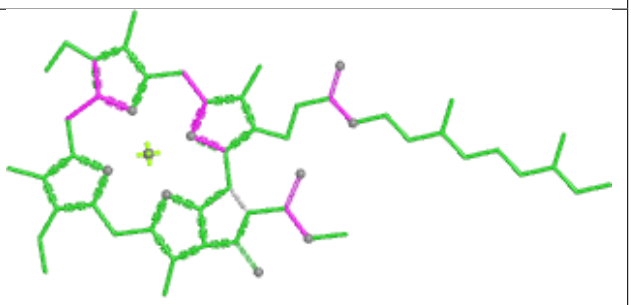


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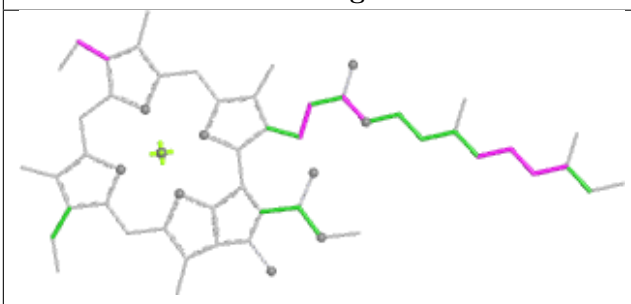
Ligand CLA S 611



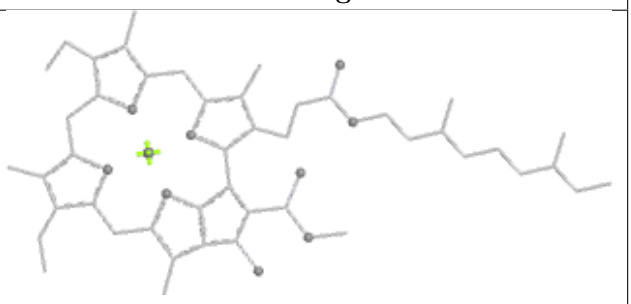
Bond lengths



Bond angles

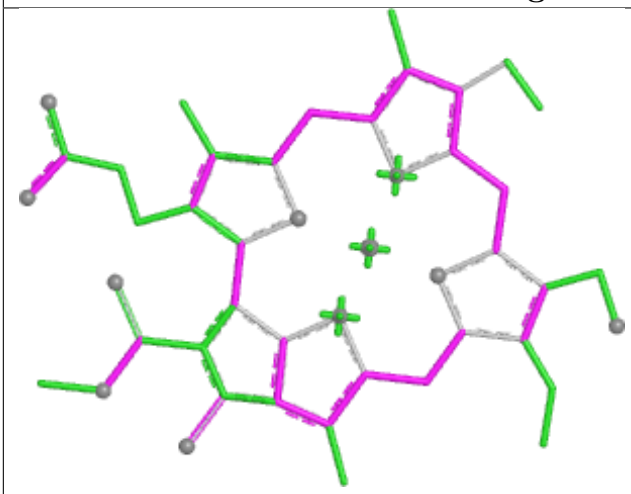


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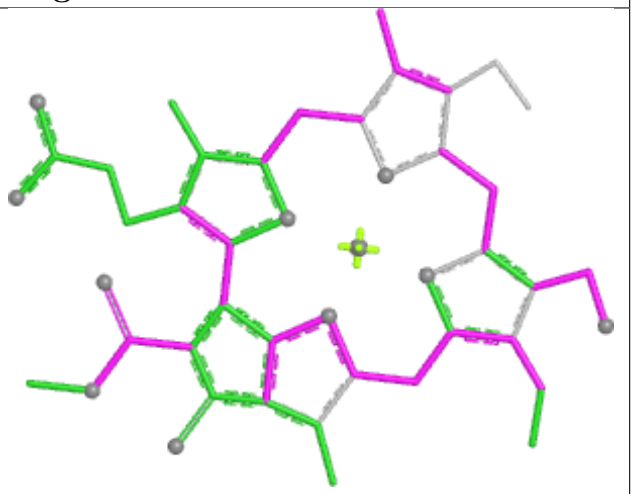


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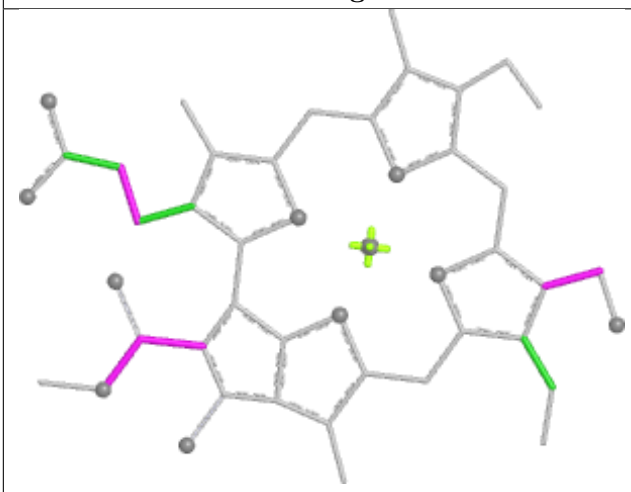
Ligand CHL g 605



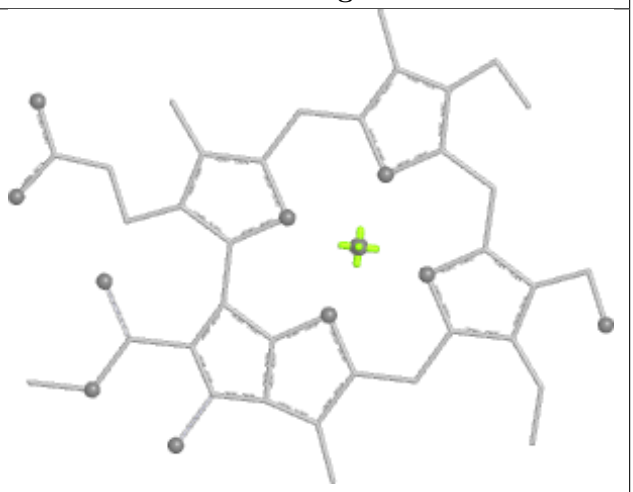
Bond lengths



Bond angles

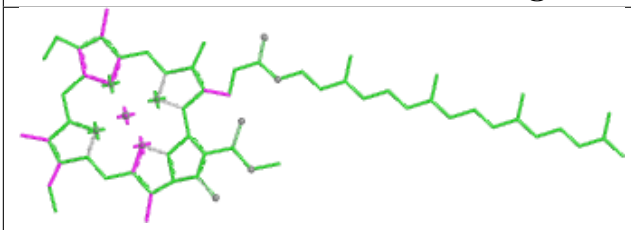


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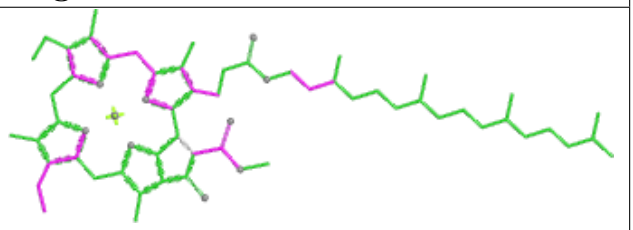


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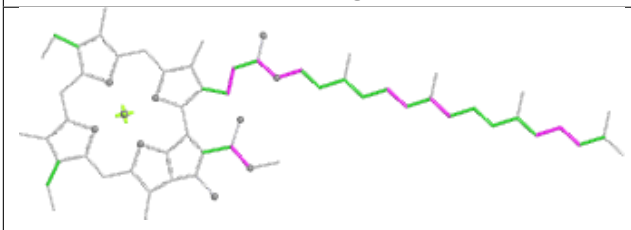
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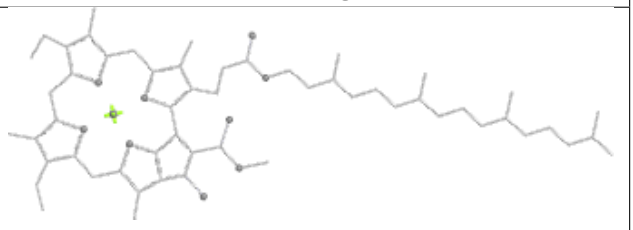
Bond lengths



Bond angles

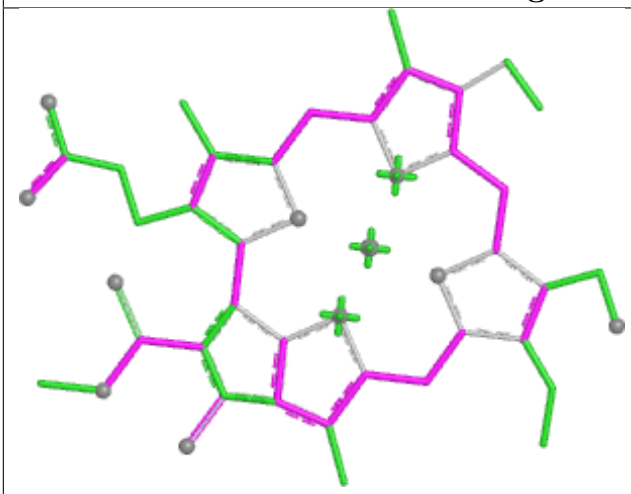


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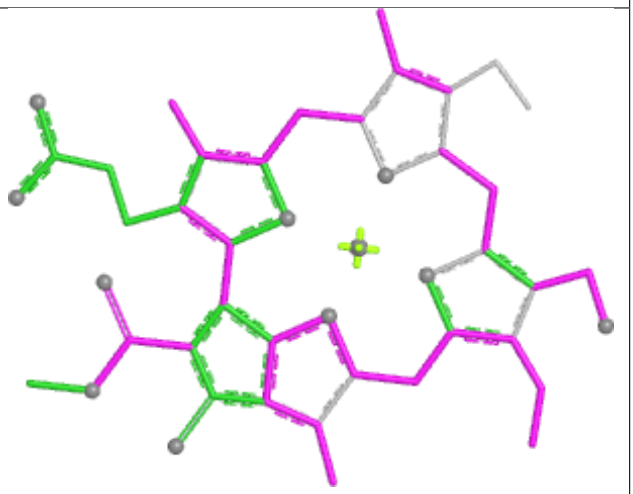


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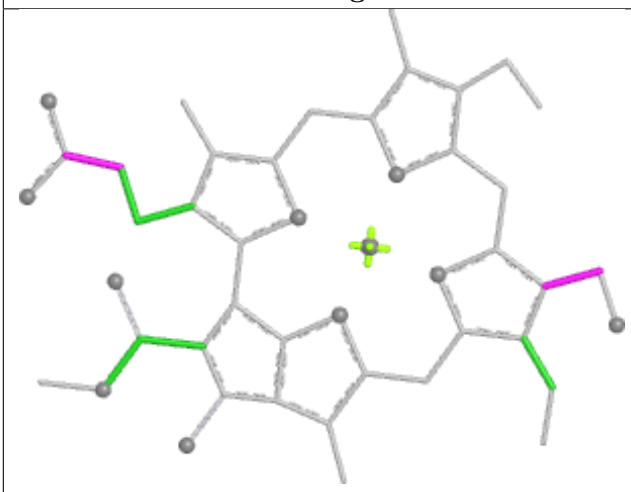
Ligand CHL 1 601



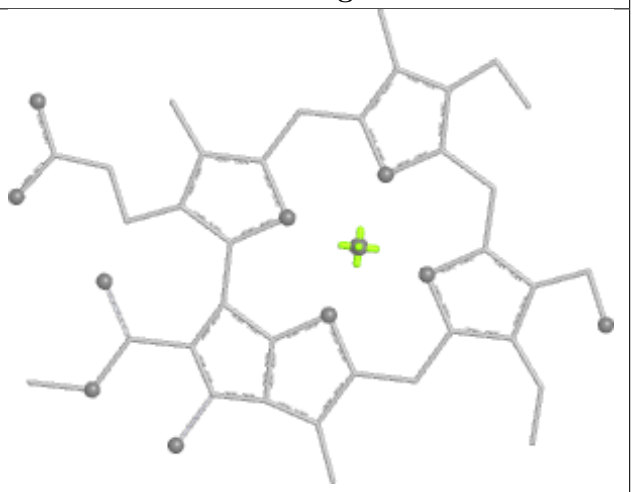
Bond lengths



Bond angles



Torsions

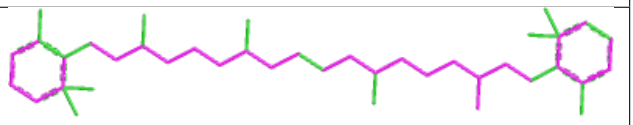


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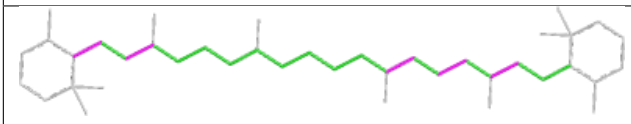
Ligand BCR 8 623



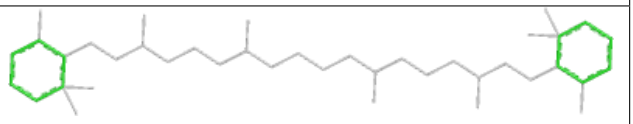
Bond lengths



Bond angles

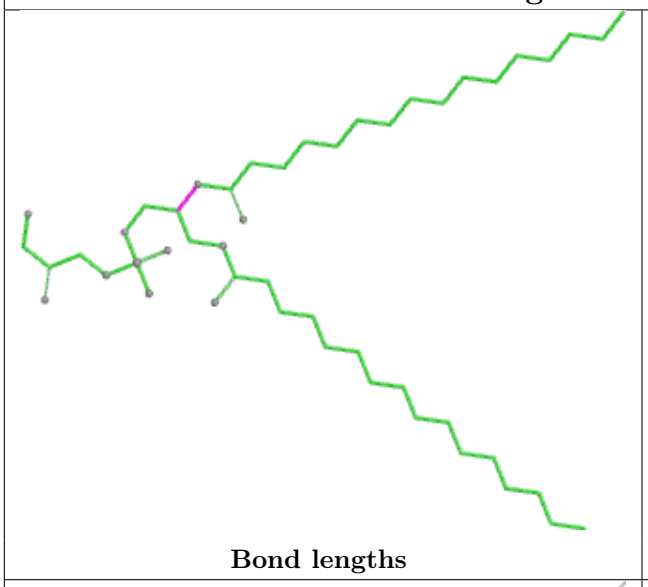


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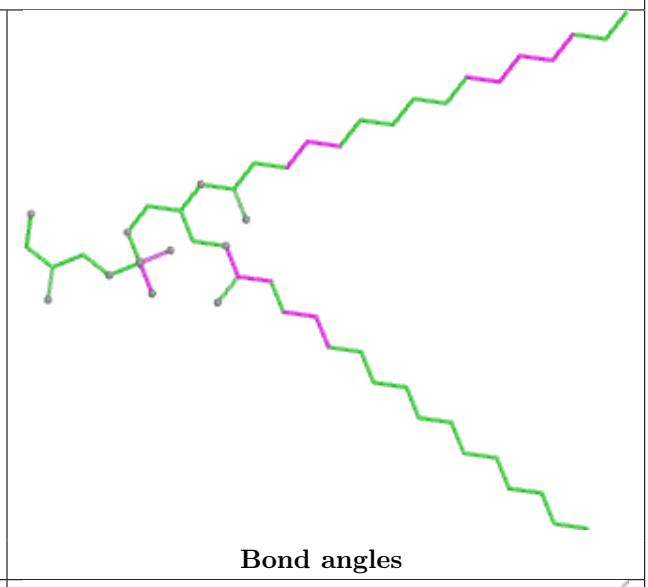


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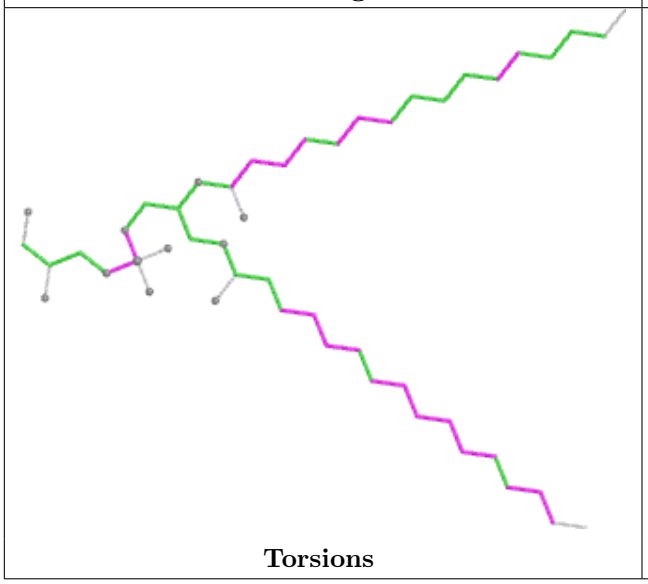
Ligand LHG L 101



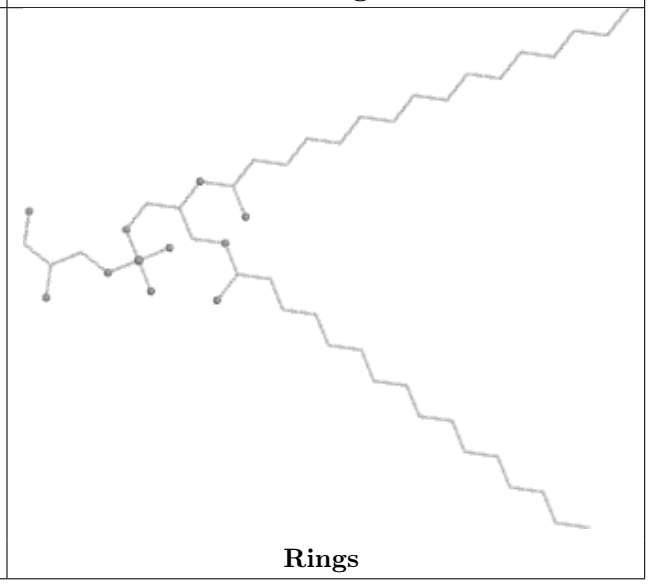
Bond lengths



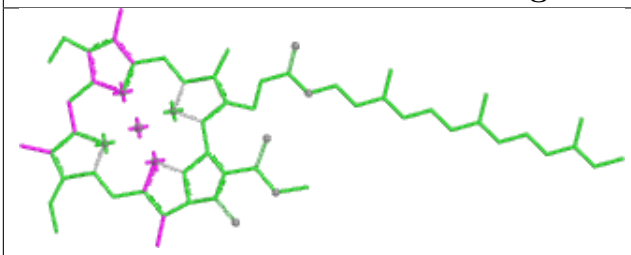
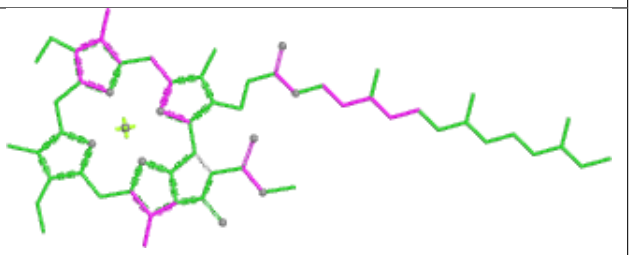
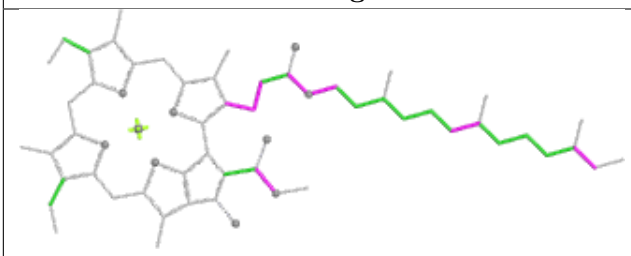
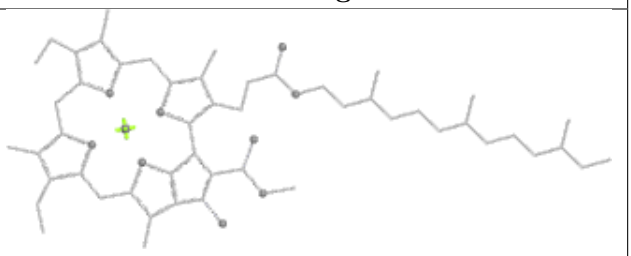
Bond angles

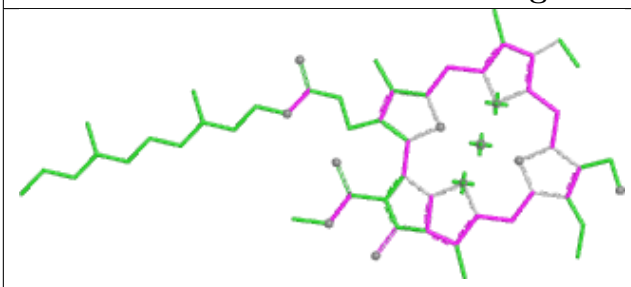
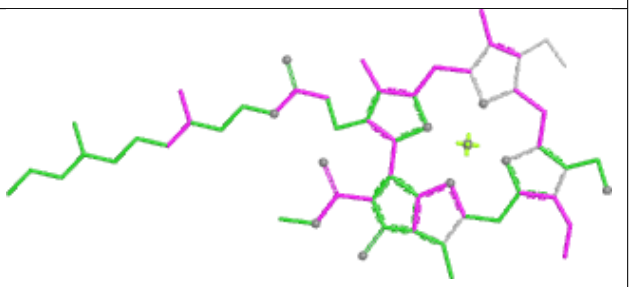
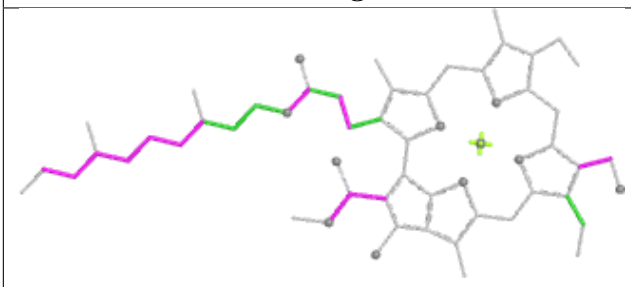
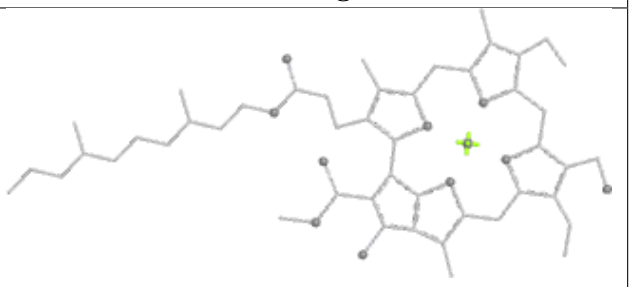


Torsions

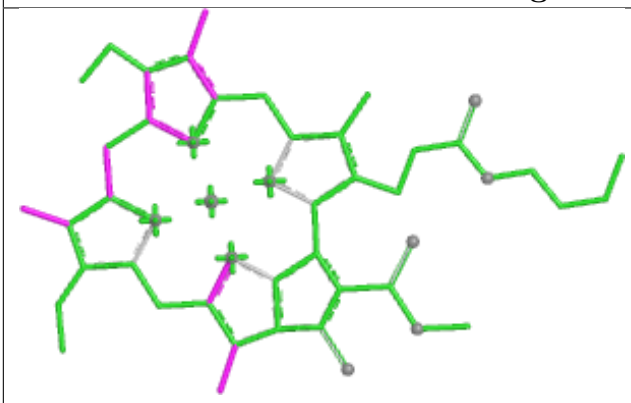


Rings

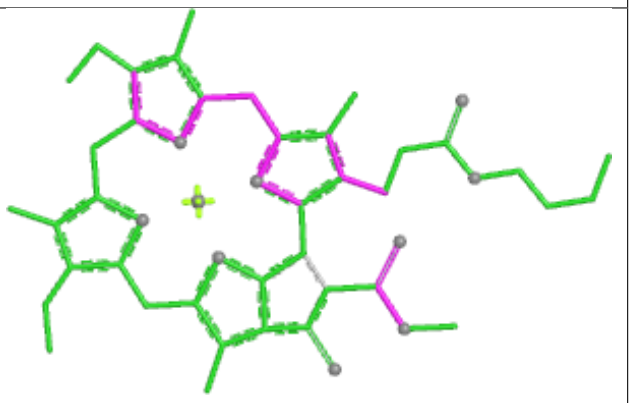
Ligand CLA s 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL s 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

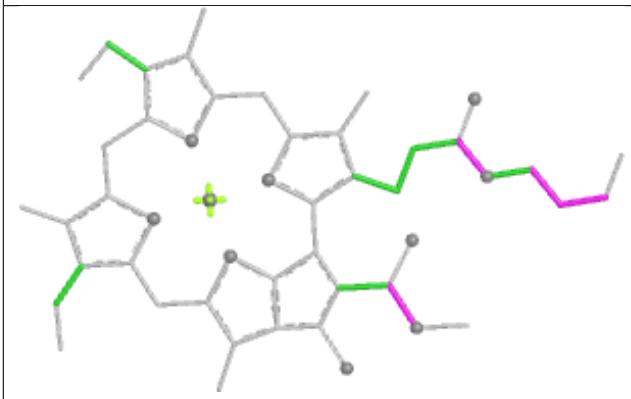
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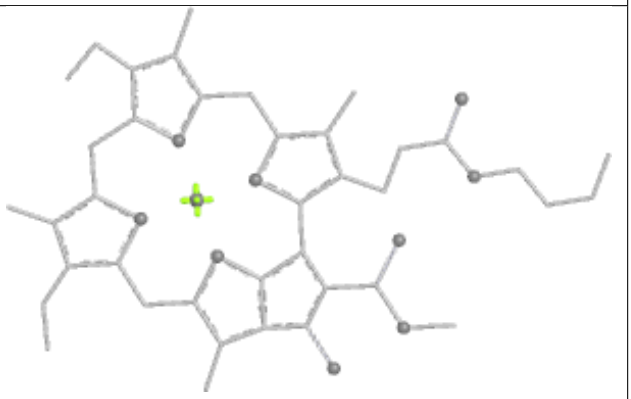
Bond lengths



Bond angles



Torsions

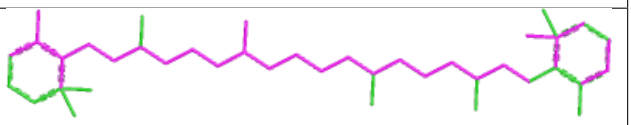


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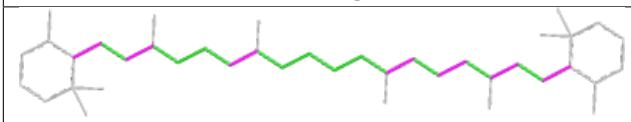
Ligand BCR T 101



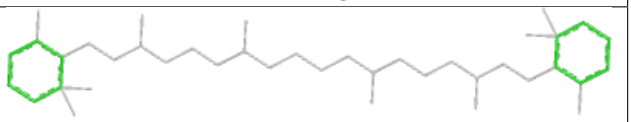
Bond lengths



Bond angles

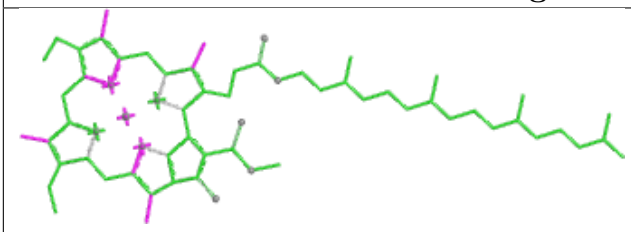


Torsions

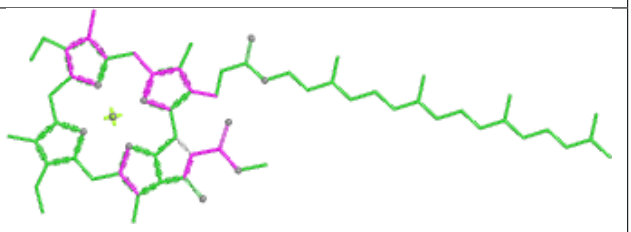


Rings

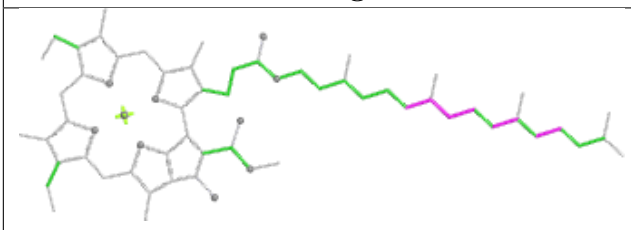
Ligand CLA c 509



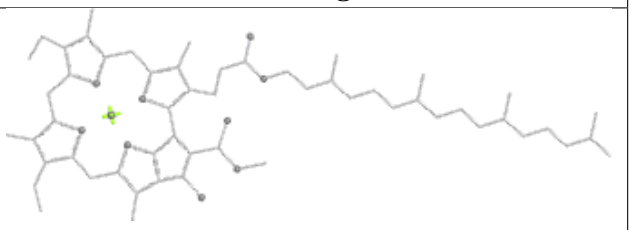
Bond lengths



Bond angles

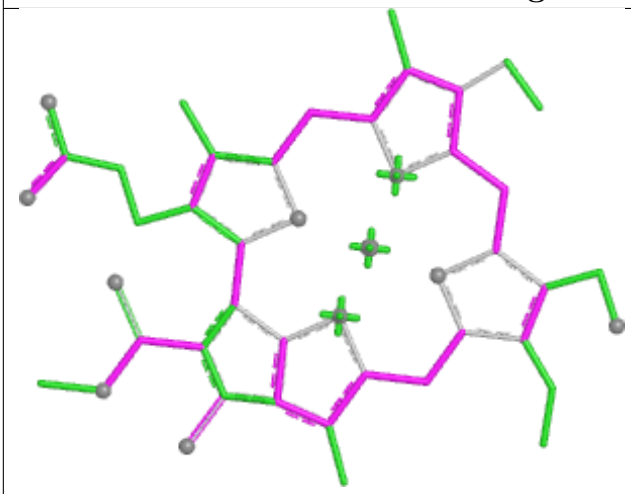


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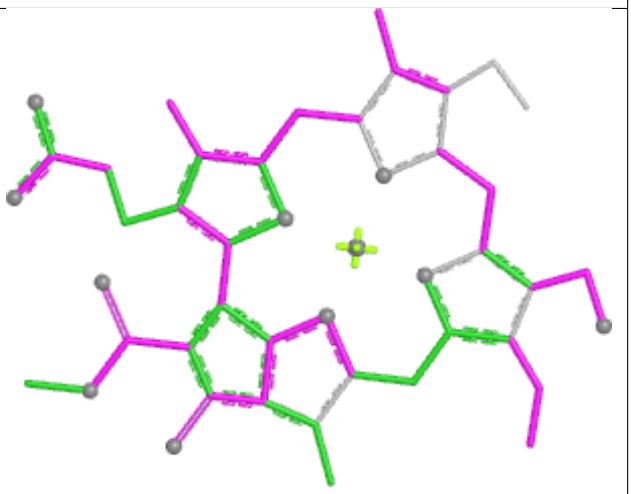


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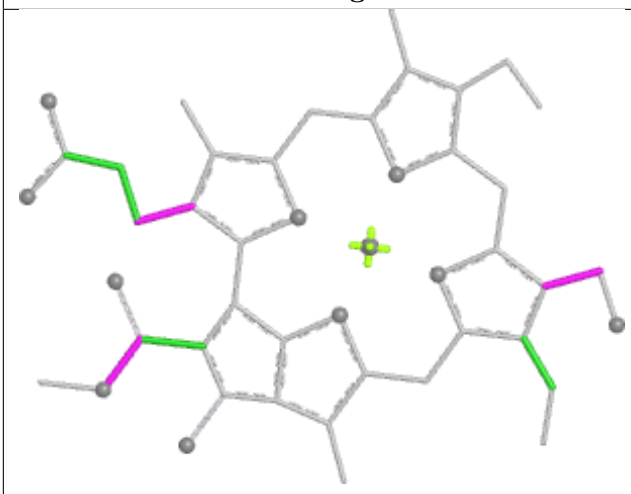
Ligand CHL 8 608



Bond lengths



Bond angles

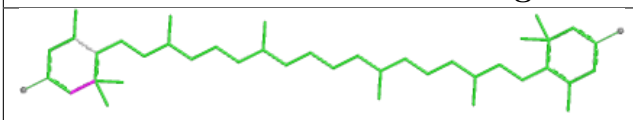


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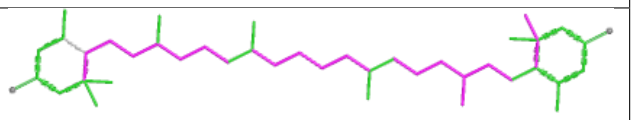


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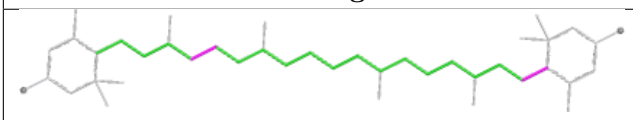
Ligand LUT N 1621



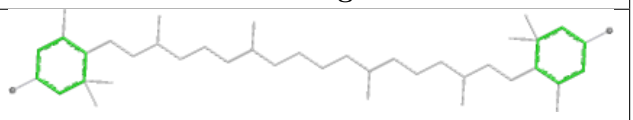
Bond lengths



Bond angles



Torsions



Rings

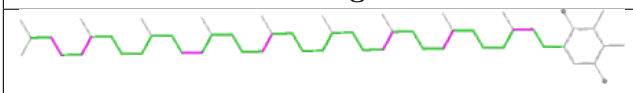
Ligand PL9 D 405



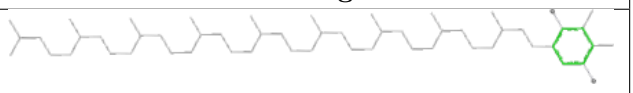
Bond lengths



Bond angles

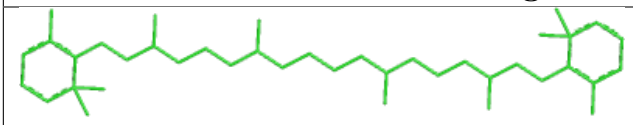


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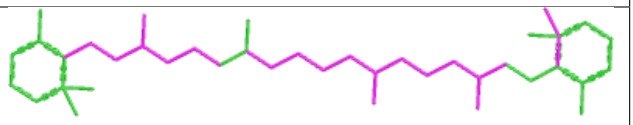


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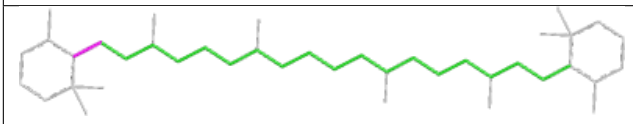
Ligand BCR C 514



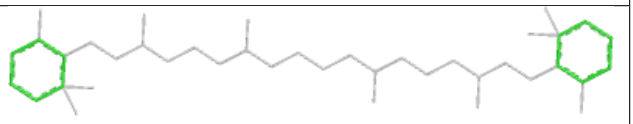
Bond lengths



Bond angles

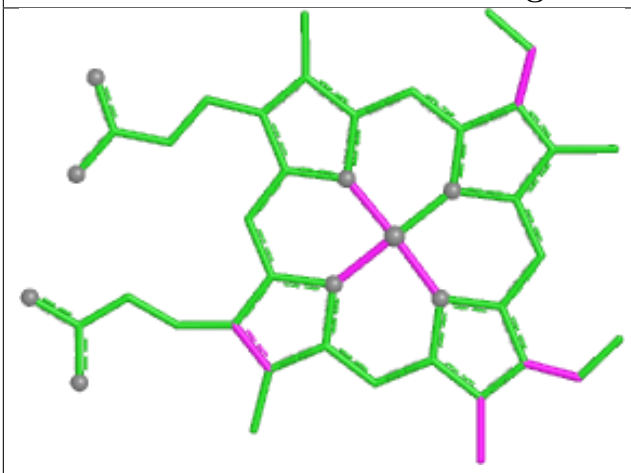


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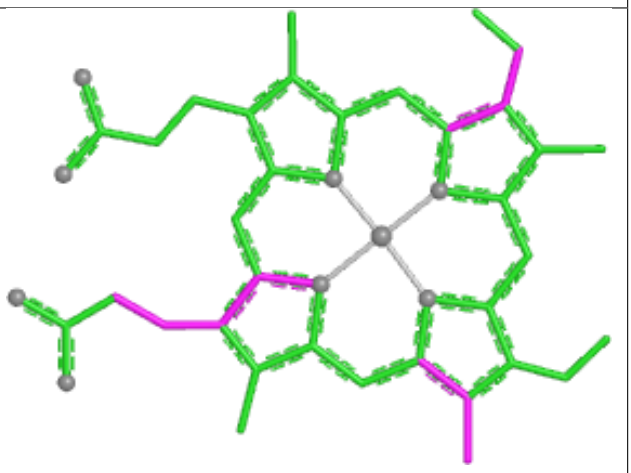


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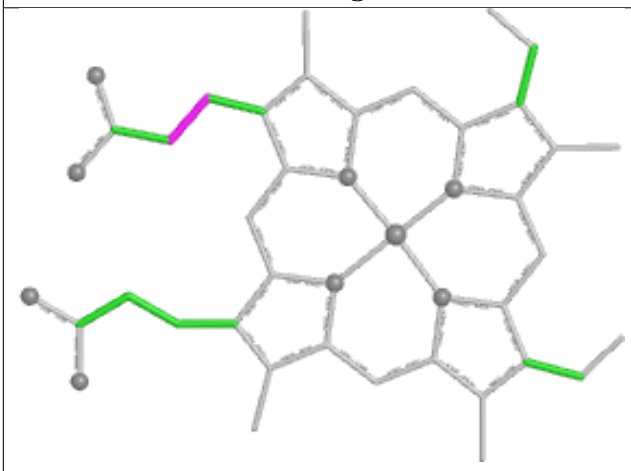
Ligand HEM f 101



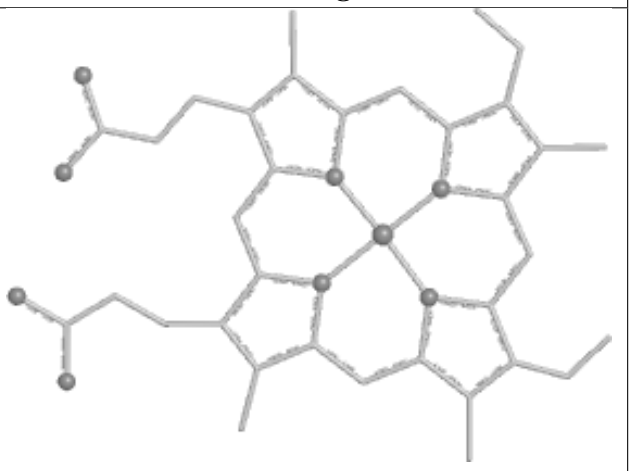
Bond lengths



Bond angles

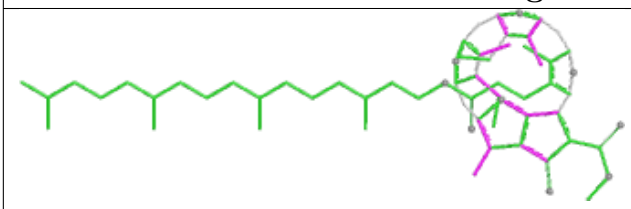


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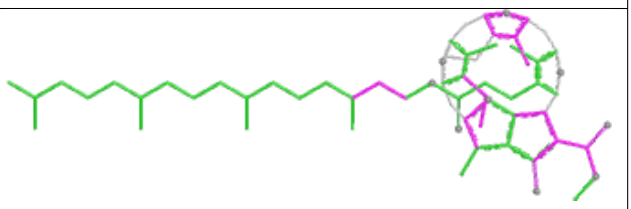


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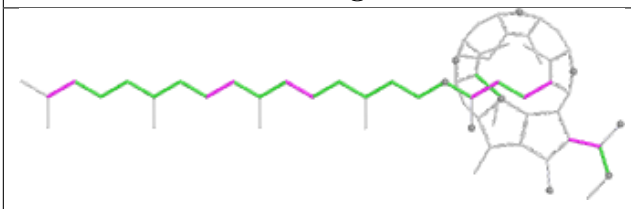
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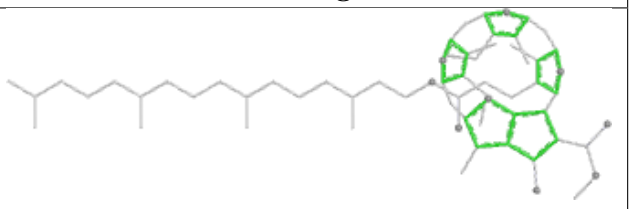
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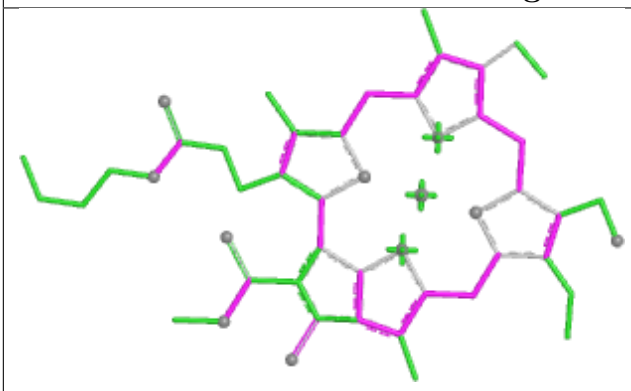


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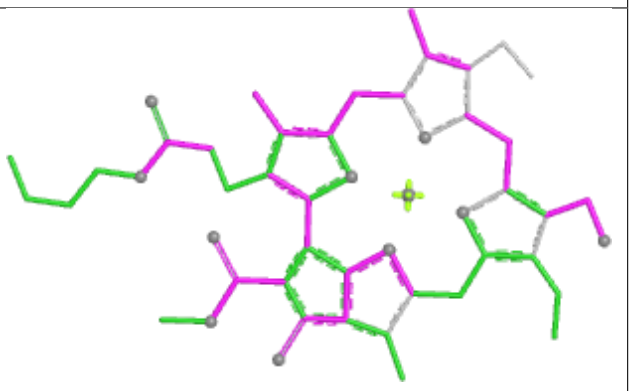


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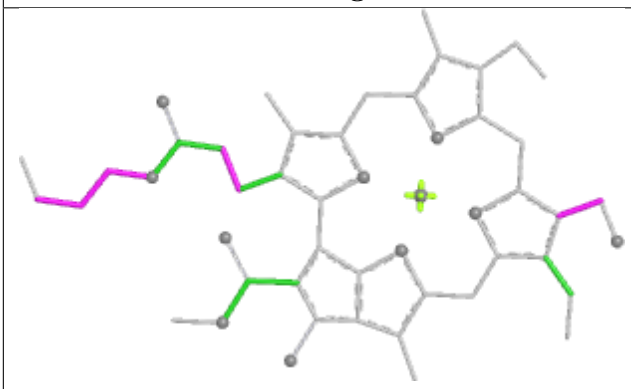
Ligand CHL Y 606



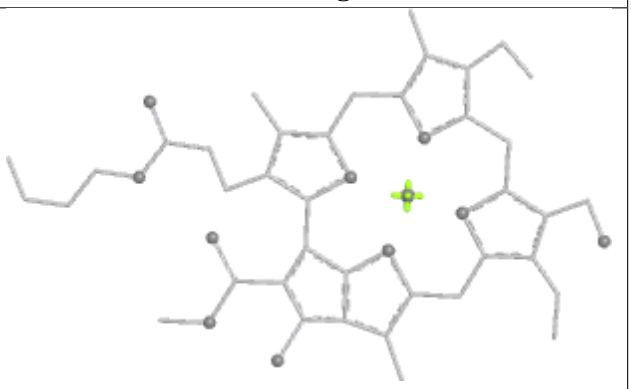
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Bond angles

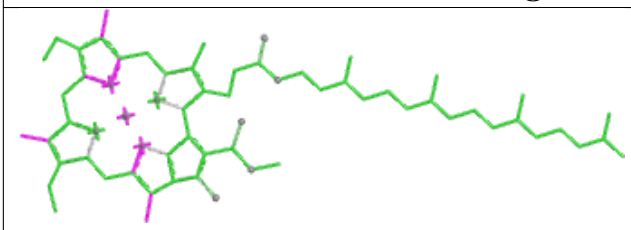


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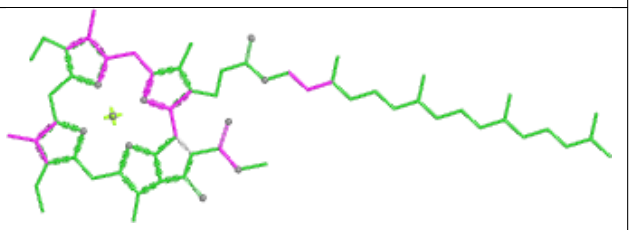


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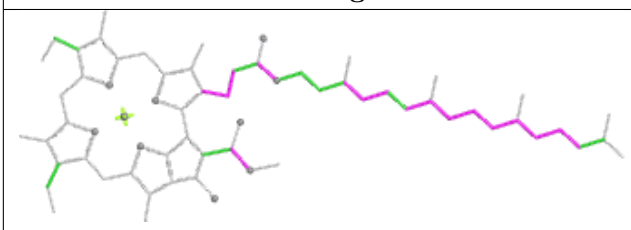
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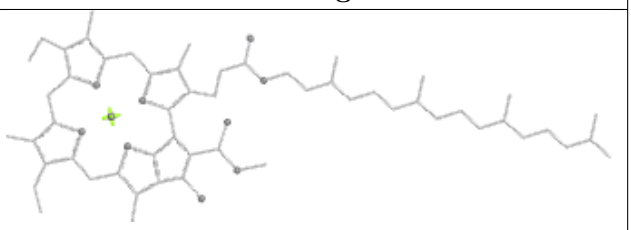
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Bond angles

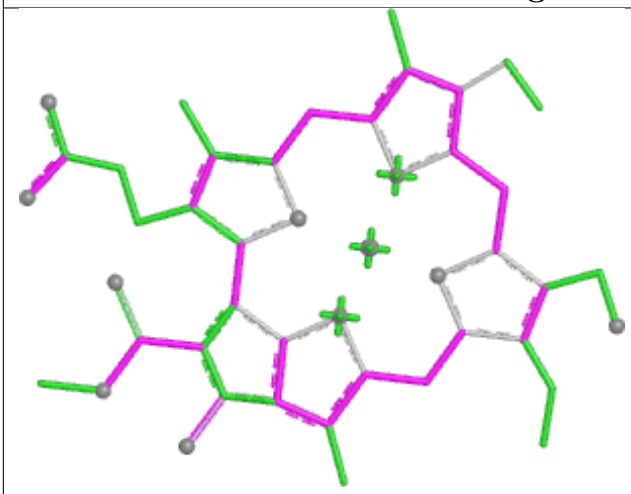


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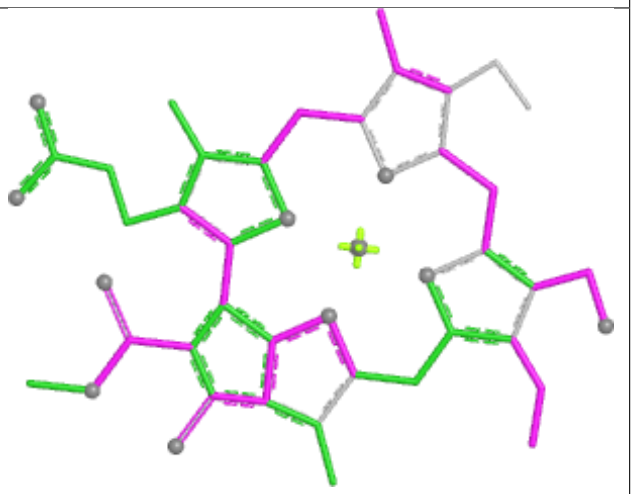


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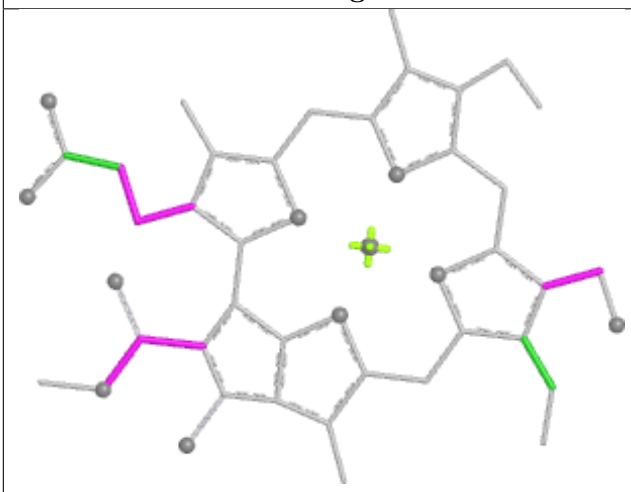
Ligand CHL 5 608



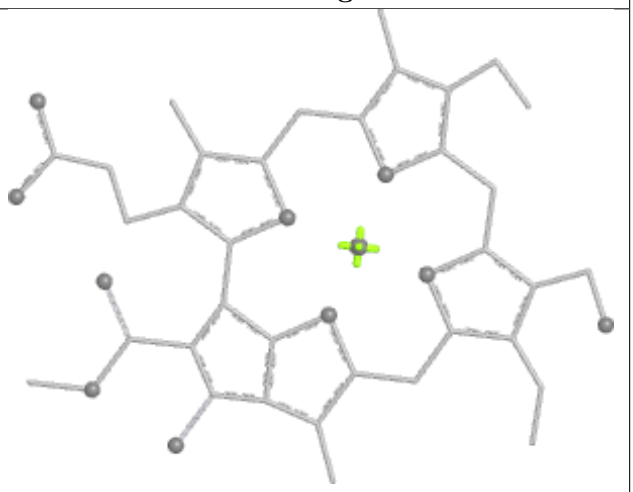
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Bond angles

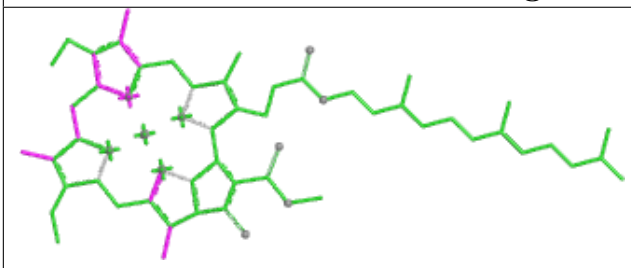


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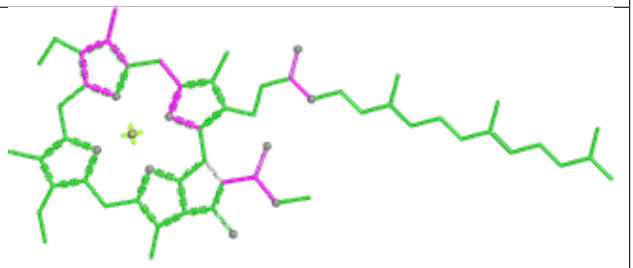


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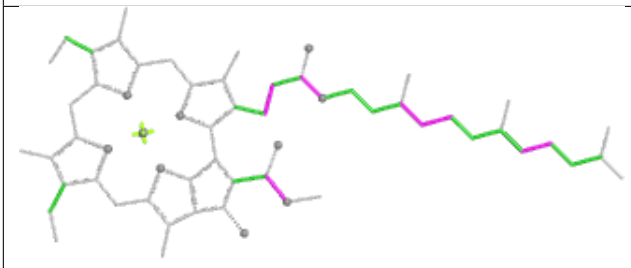
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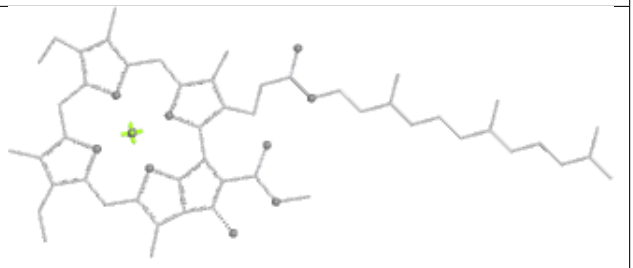
Bond lengths



Bond angles

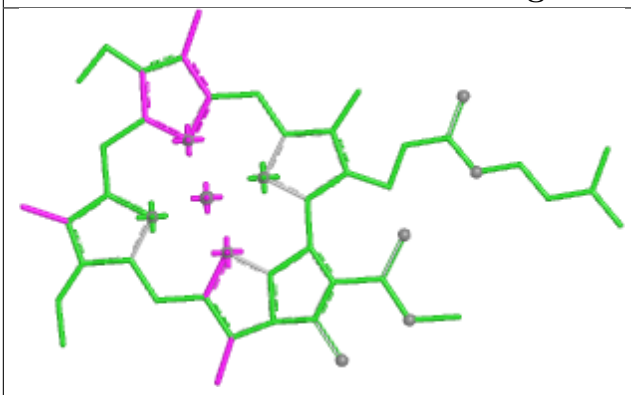


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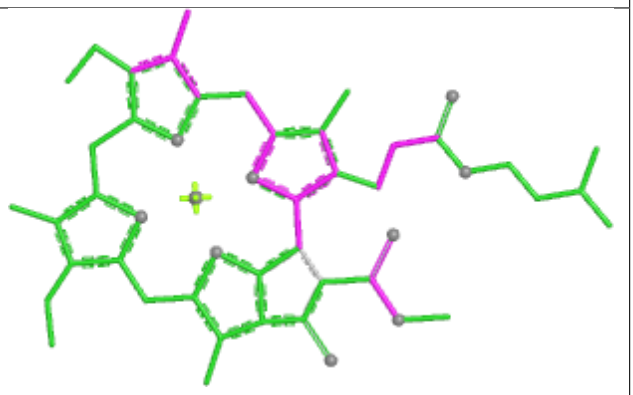


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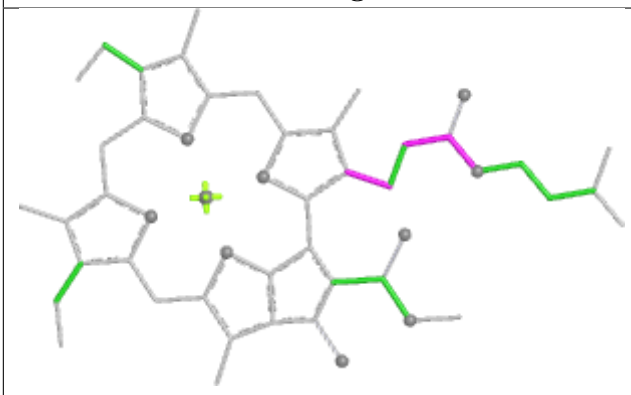
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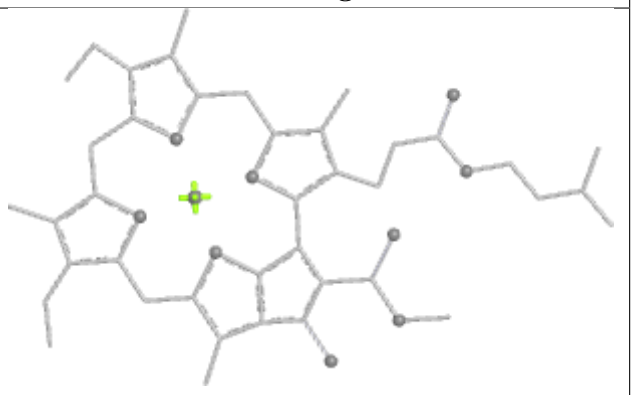
Bond lengths



Bond angles

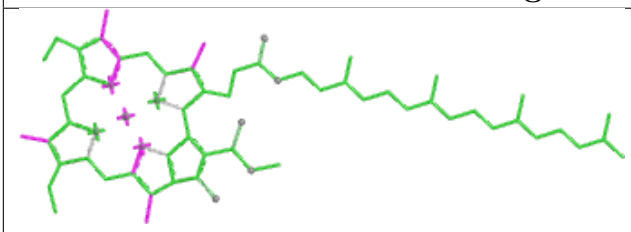


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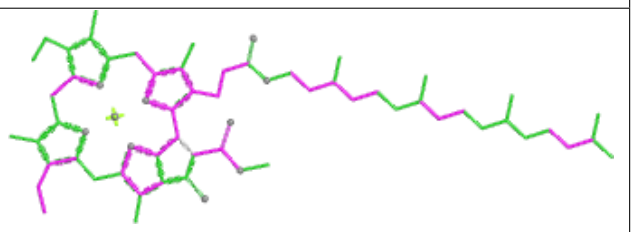


Rings

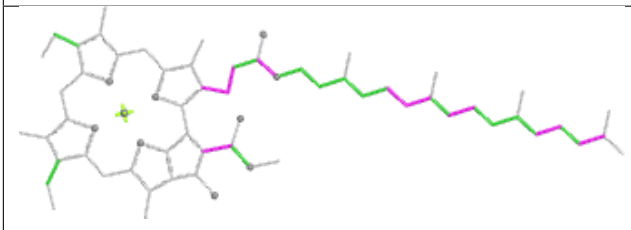
Ligand CLA B 605



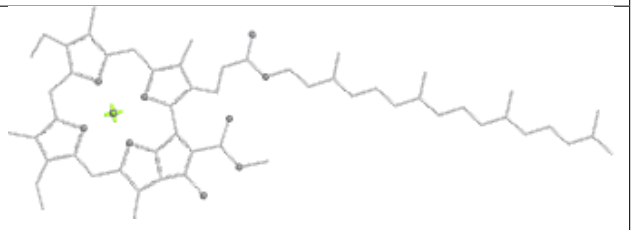
Bond lengths



Bond angles

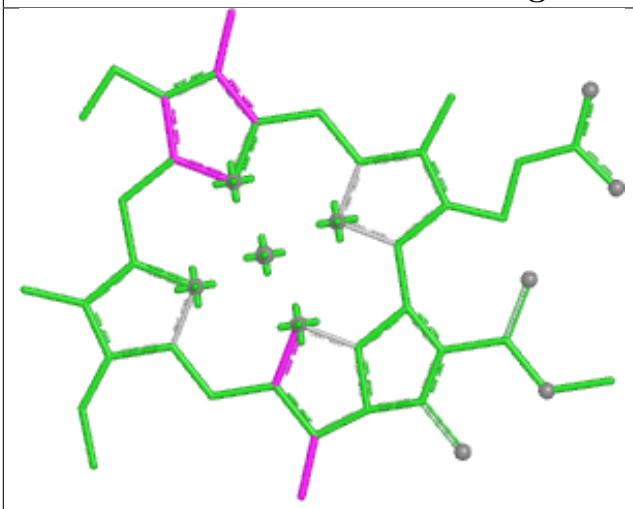


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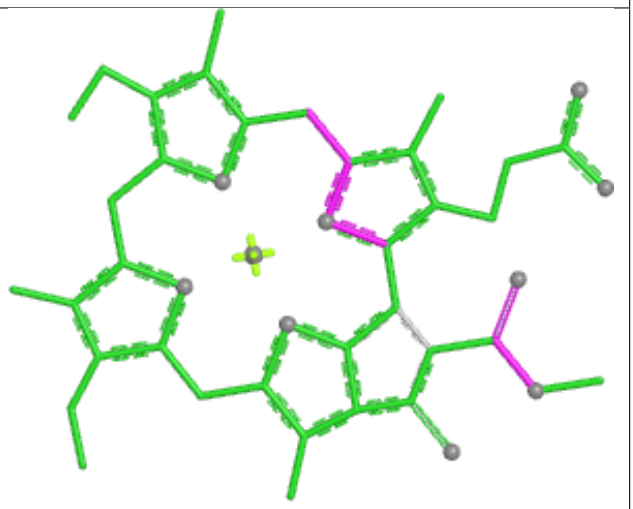


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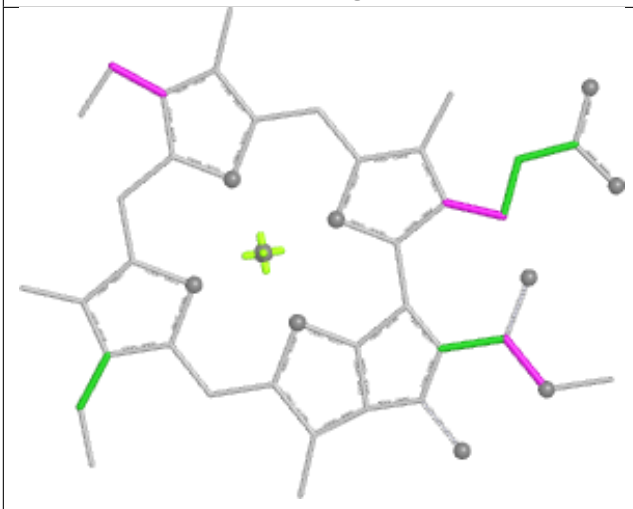
Ligand CLA 2 614



Bond lengths



Bond angles

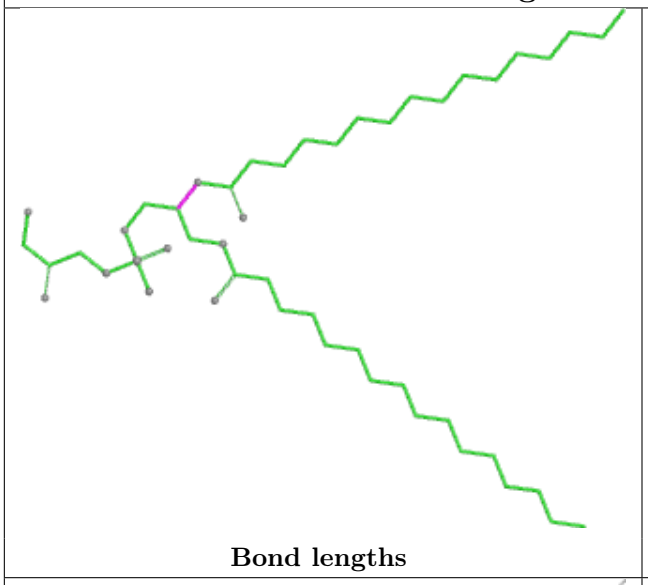


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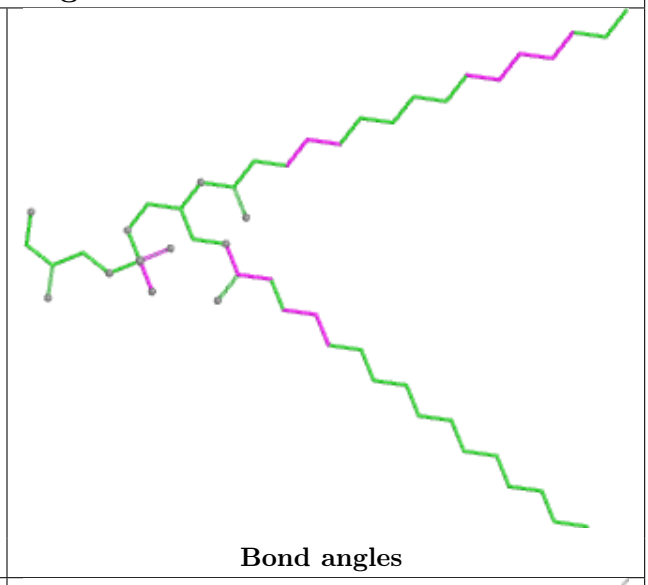


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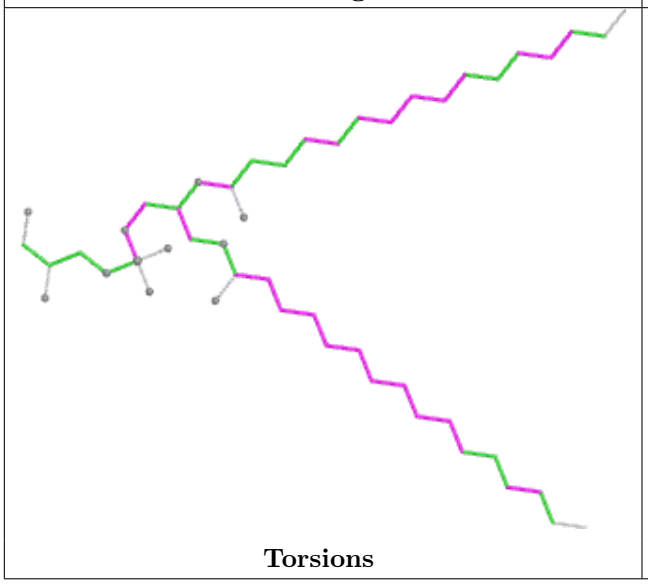
Ligand LHG g 2630



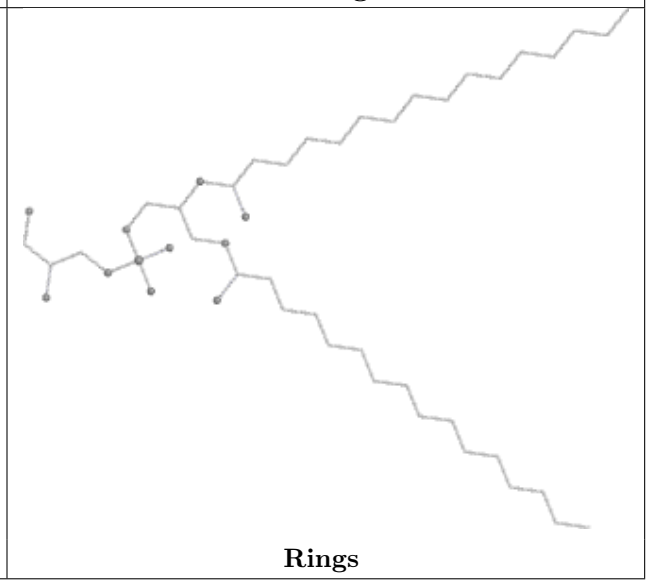
Bond lengths



Bond angles

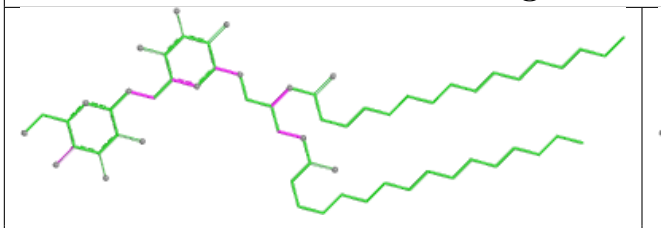


Torsions

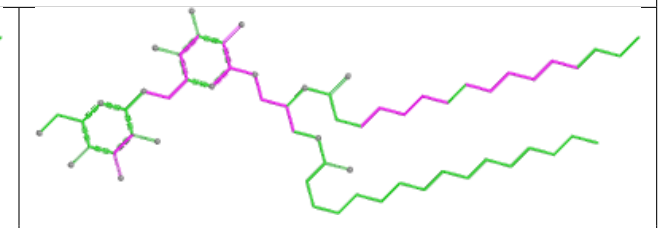


Rings

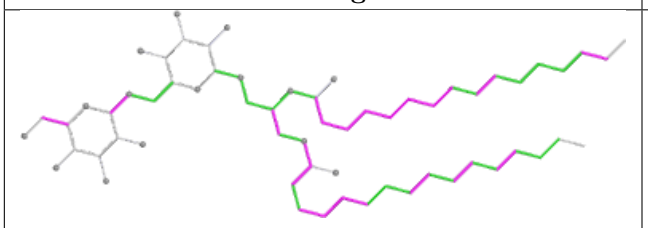
Ligand DGD C 519



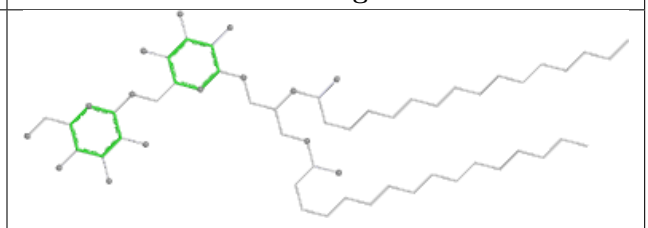
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Bond angles

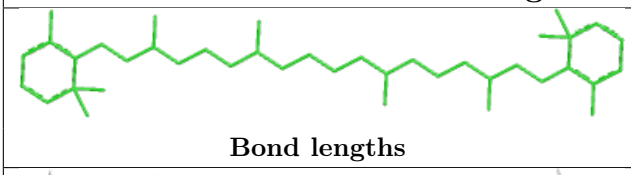


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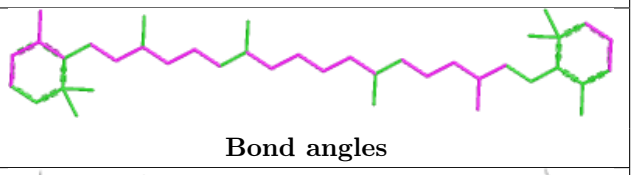


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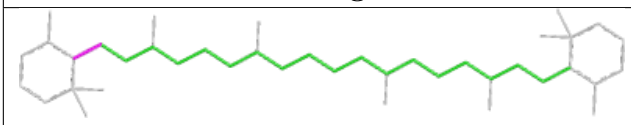
Ligand BCR b 618



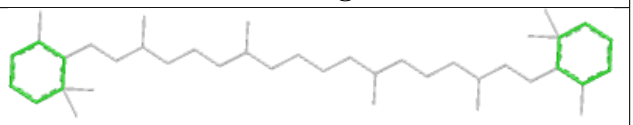
Bond lengths



Bond angles

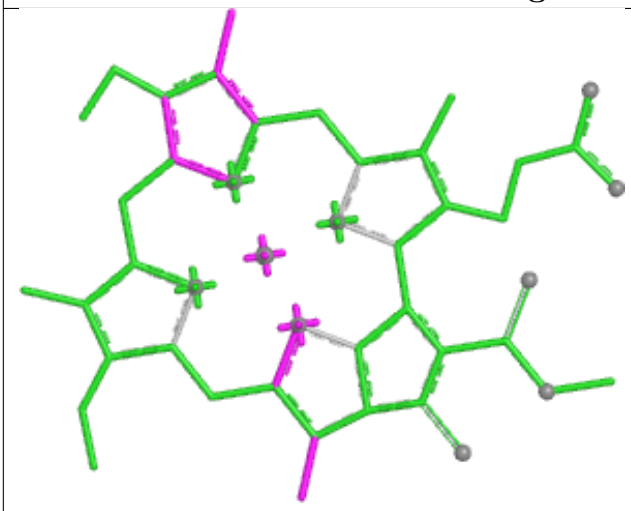


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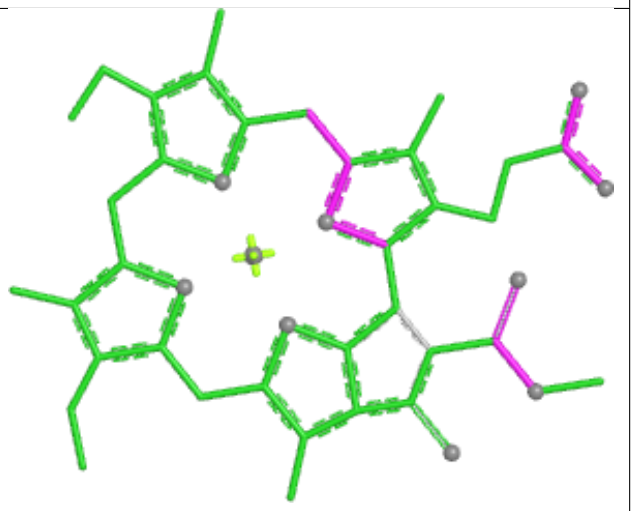


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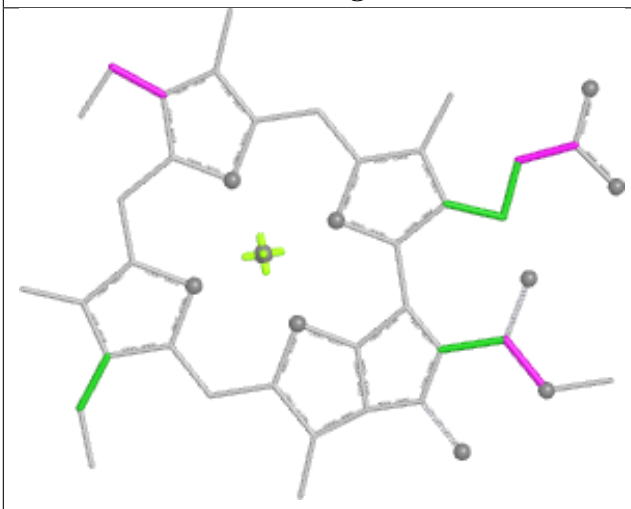
Ligand CLA 4 611



Bond lengths



Bond angles

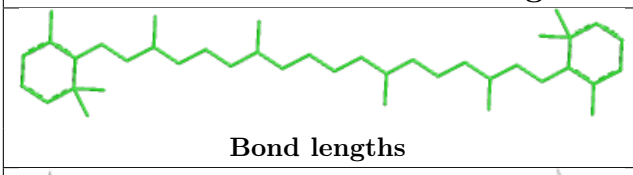


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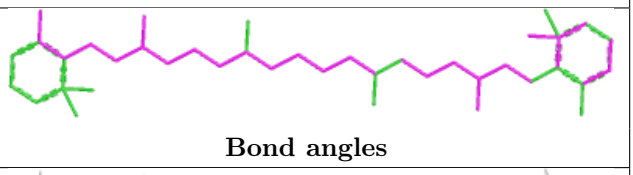


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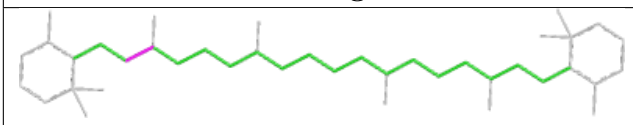
Ligand BCR b 619



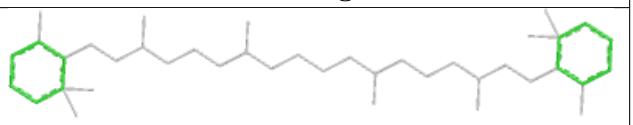
Bond lengths



Bond angles

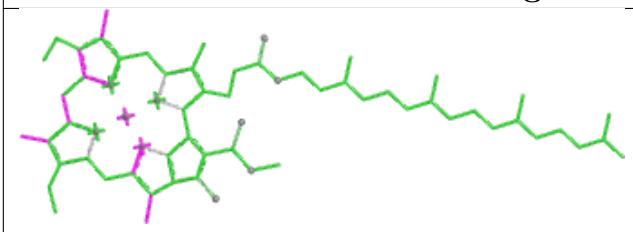


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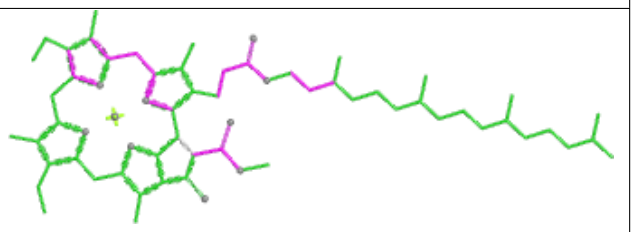


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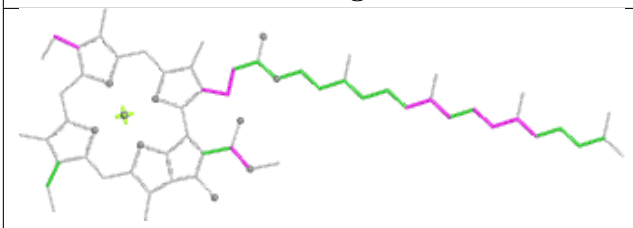
Ligand CLA R 610



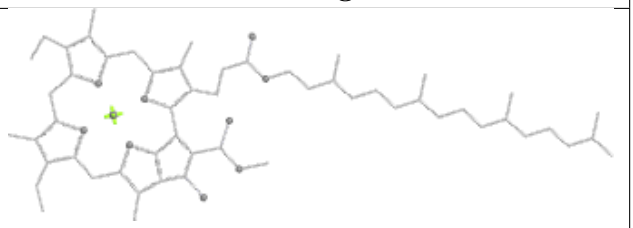
Bond lengths



Bond angles

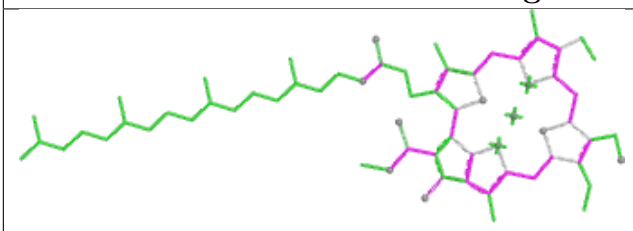


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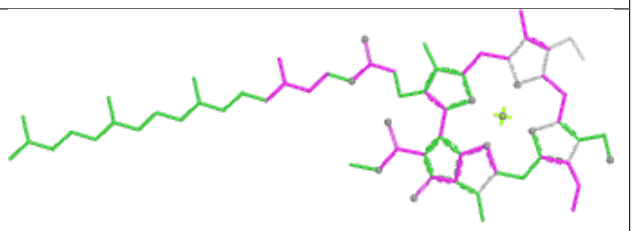


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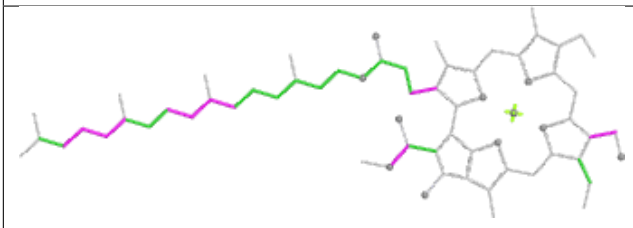
Ligand CHL Y 608



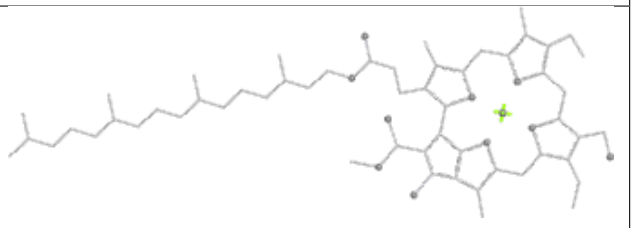
Bond lengths



Bond angles

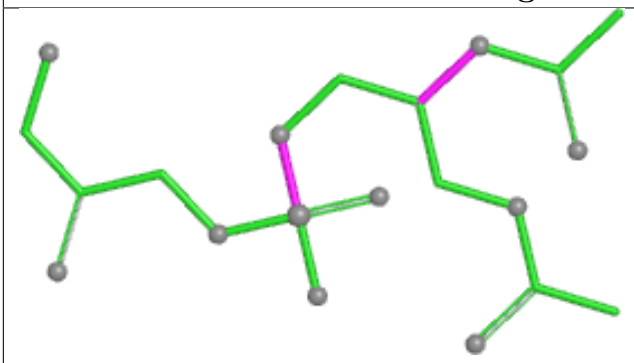


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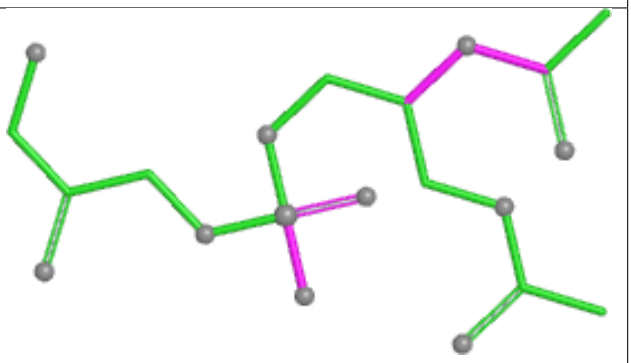


Rings

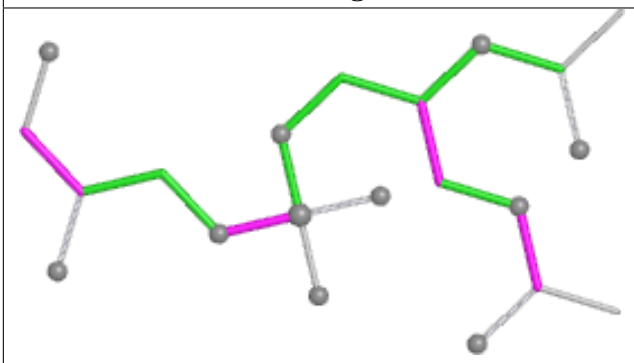
Ligand LHG 4 2630



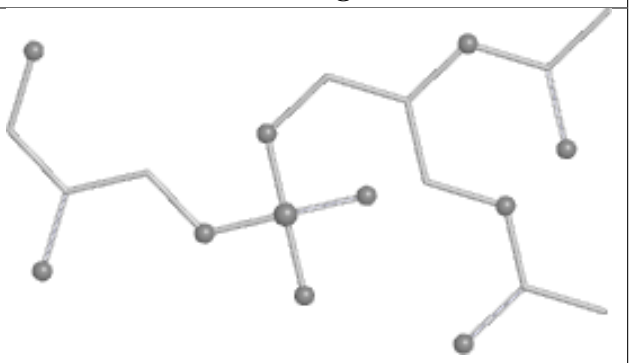
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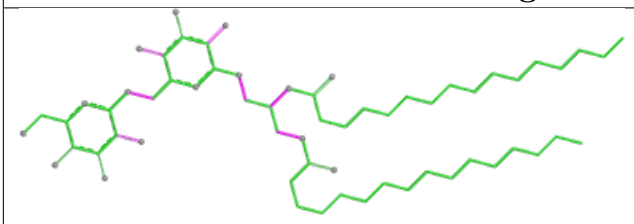


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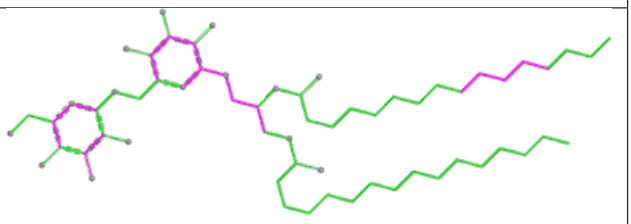


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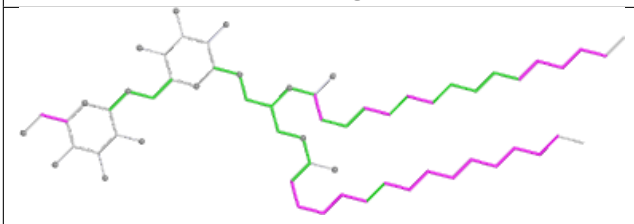
Ligand DGD H 102



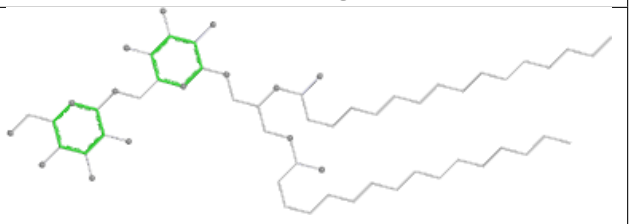
Bond lengths



Bond angles

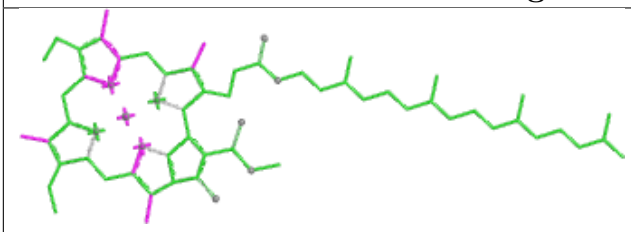


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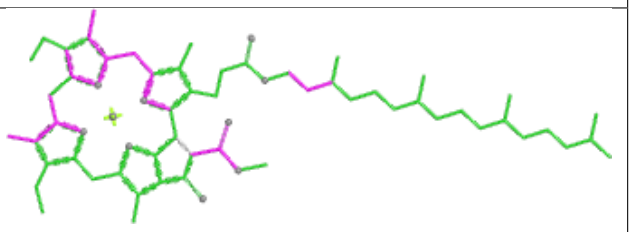


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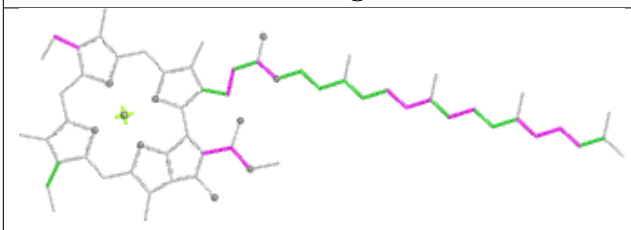
Ligand CLA b 606



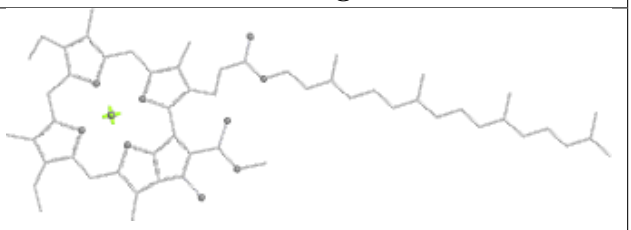
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Bond angles

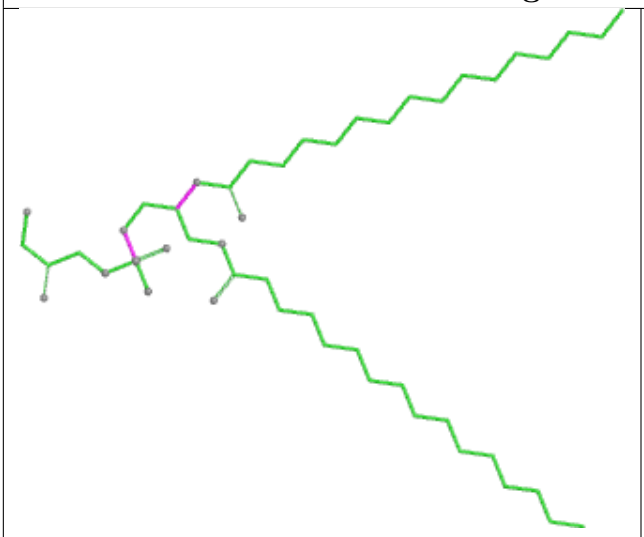


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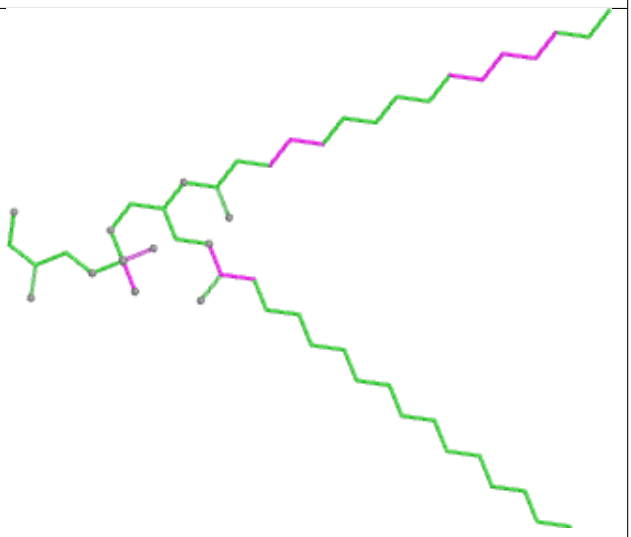


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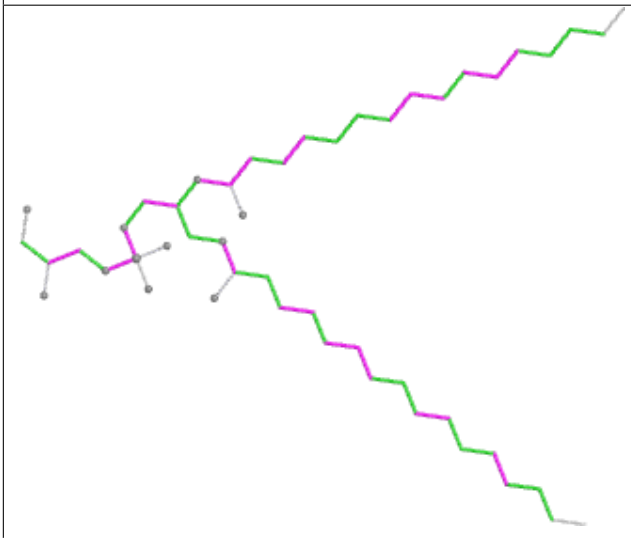
Ligand LHG C 523



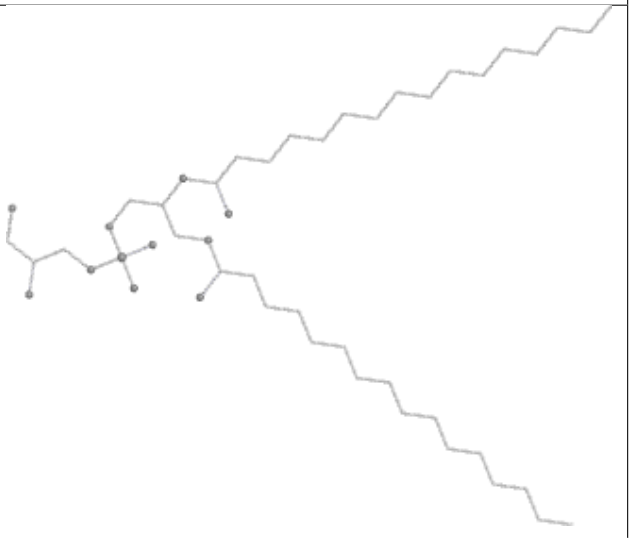
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Bond angles

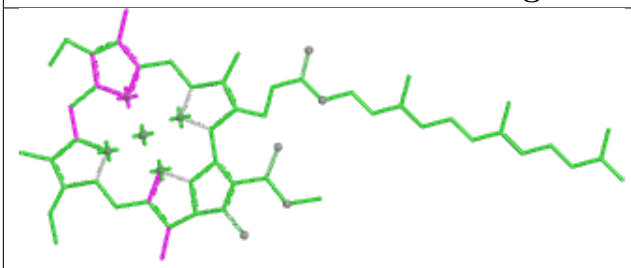


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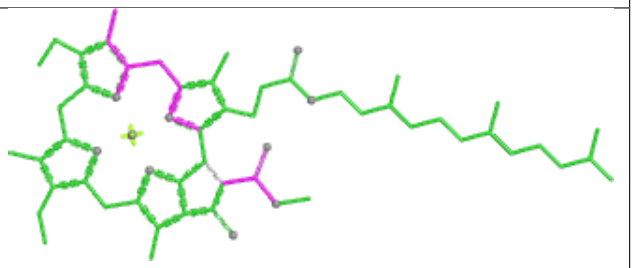


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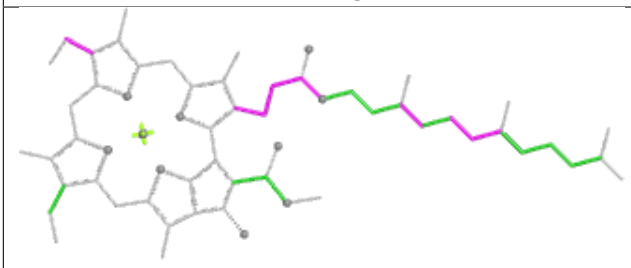
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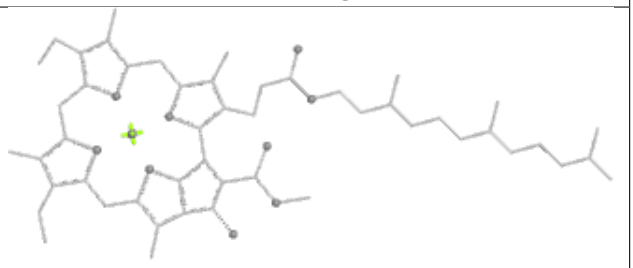
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Bond angles

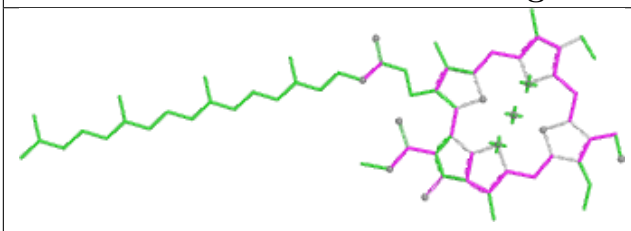


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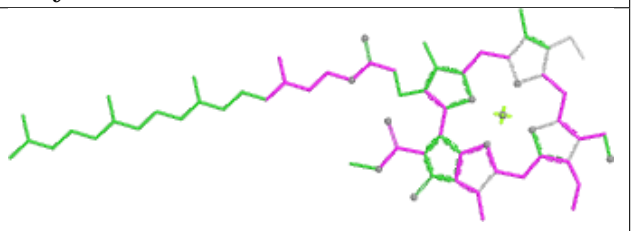


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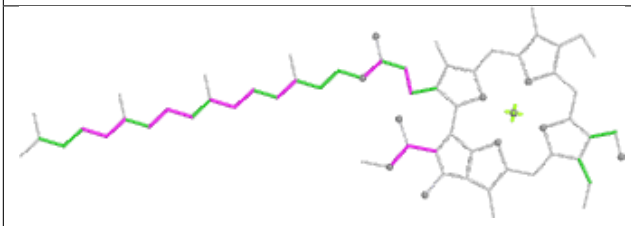
Ligand CHL y 601



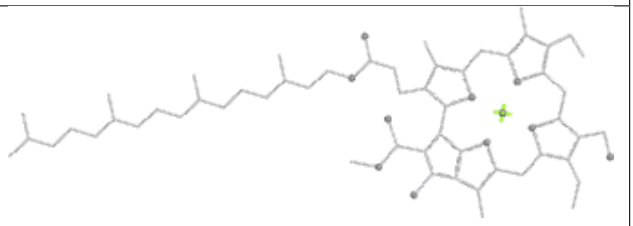
Bond lengths



Bond angles

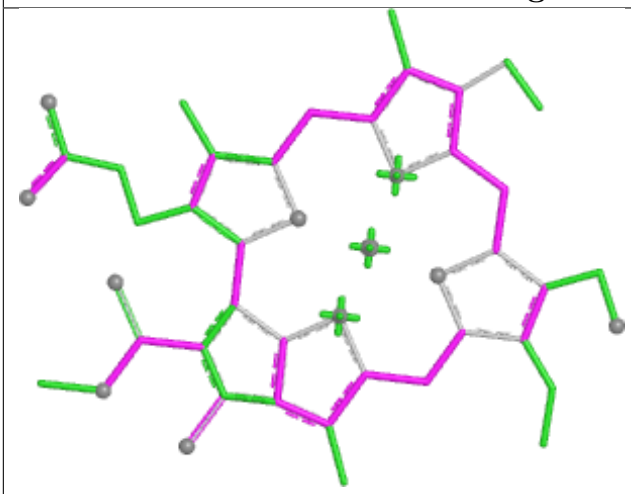


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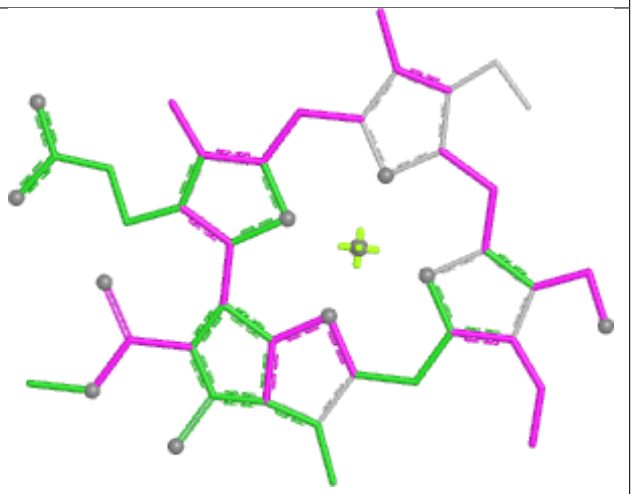


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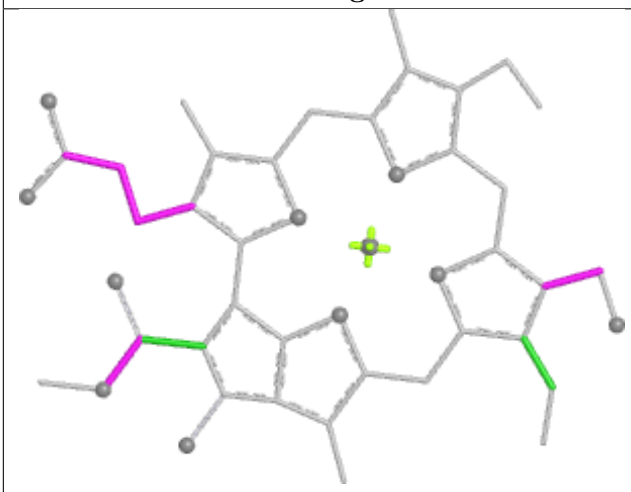
Ligand CHL 7 606



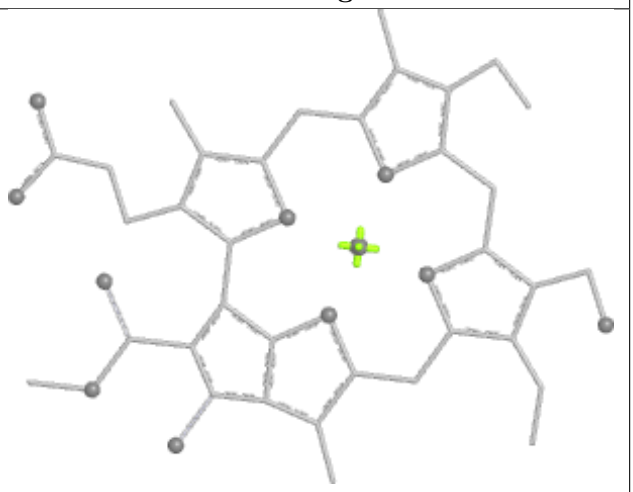
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Bond angles

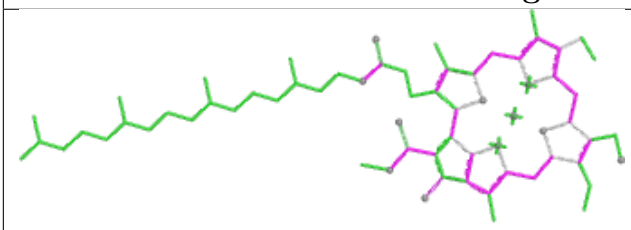


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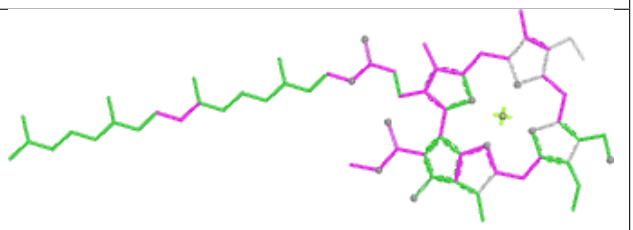


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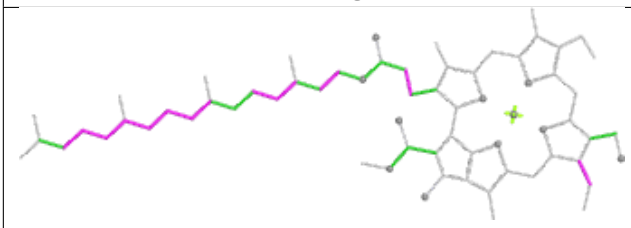
Ligand CHL G 607



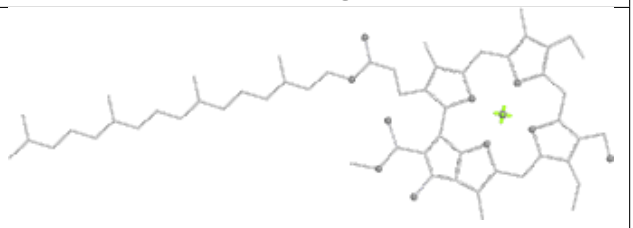
Bond lengths



Bond angles

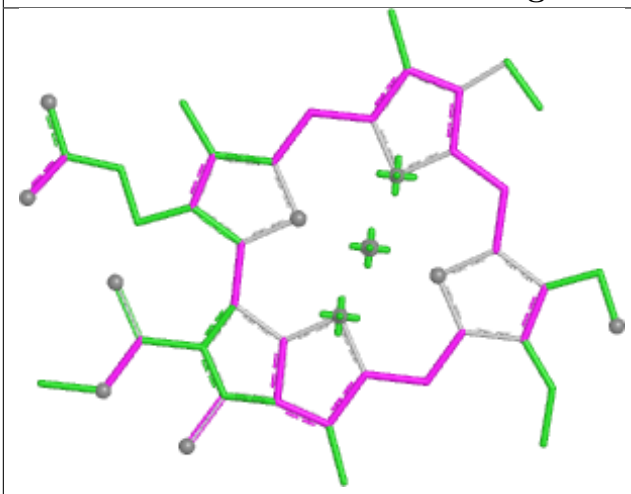


Torsions

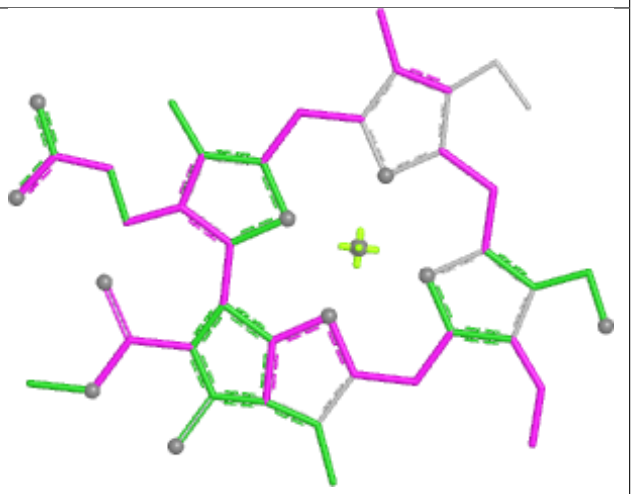


Rings

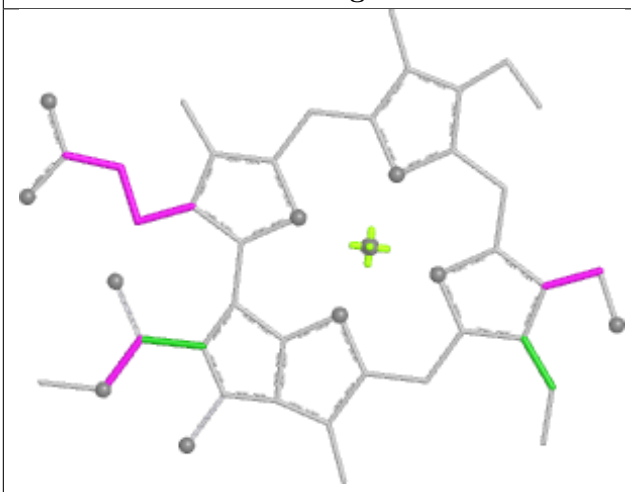
Ligand CHL 2 605



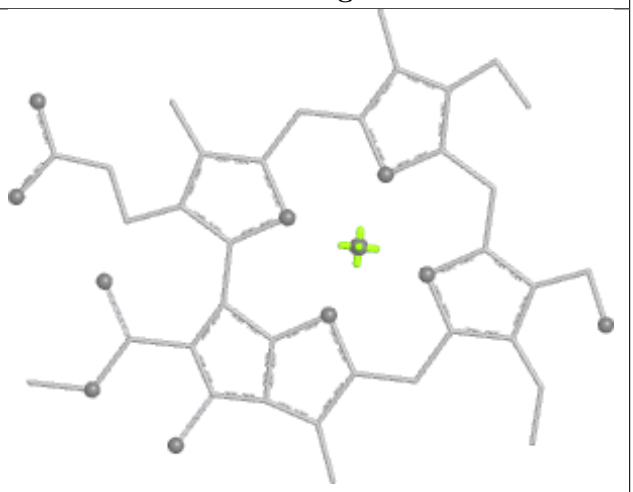
Bond lengths



Bond angles

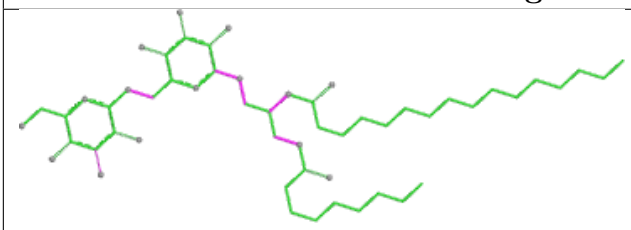


Torsions

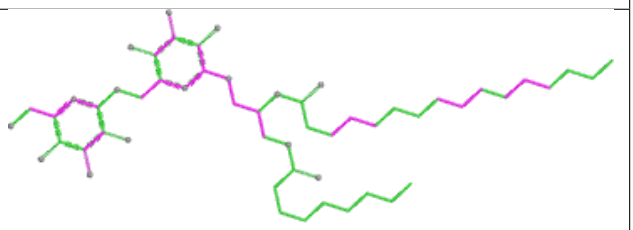


Rings

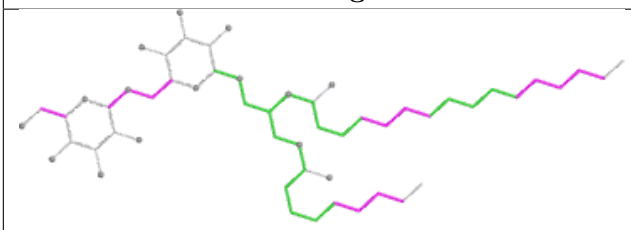
Ligand DGD c 518



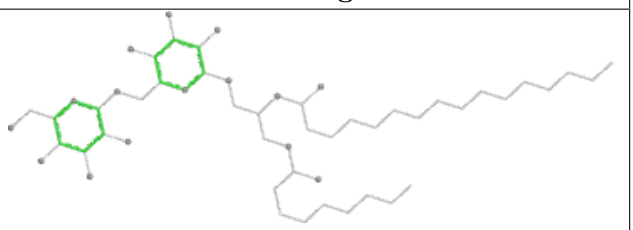
Bond lengths



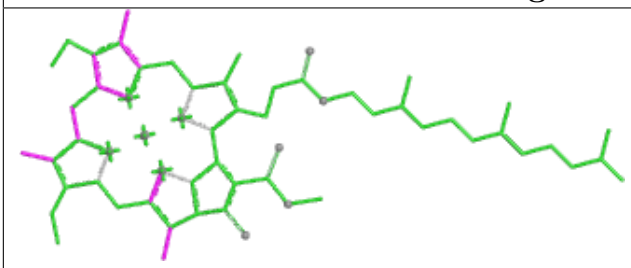
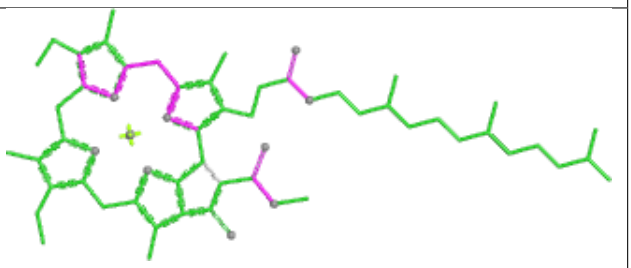
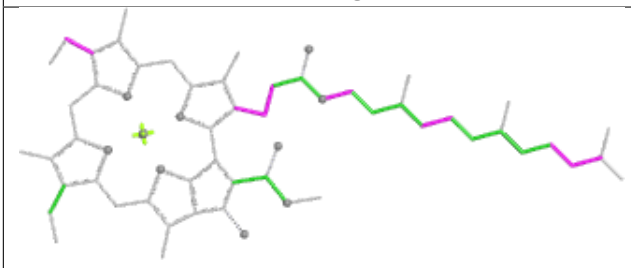
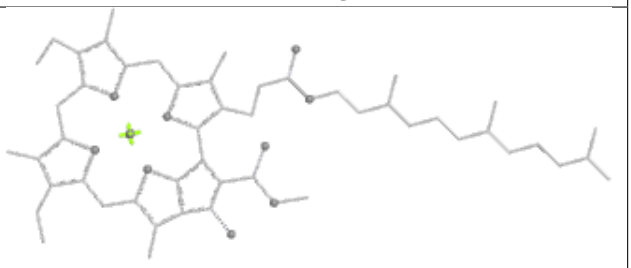
Bond angles

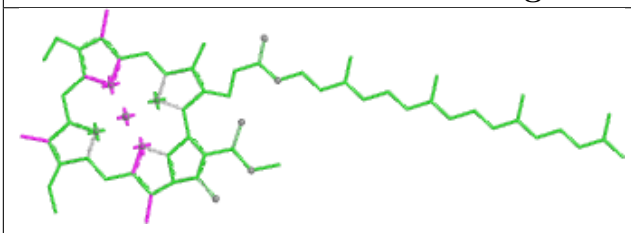
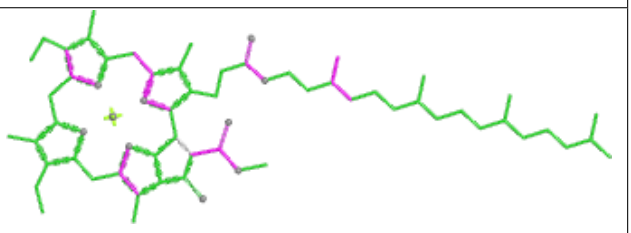
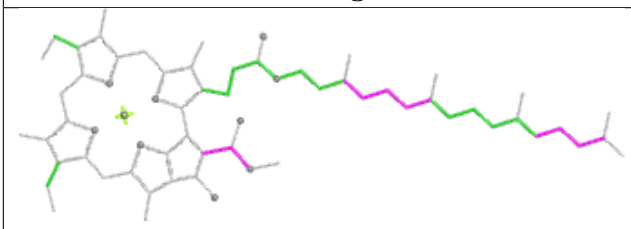
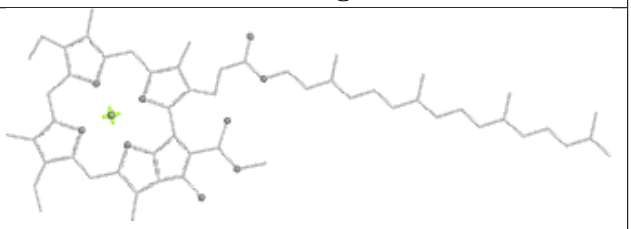


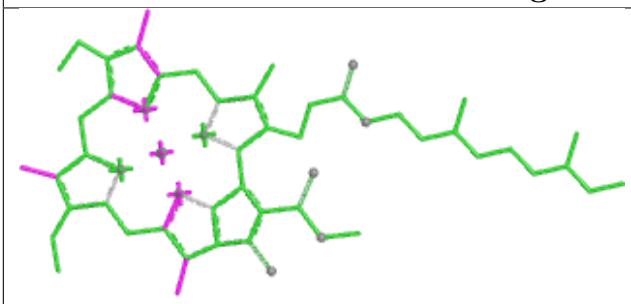
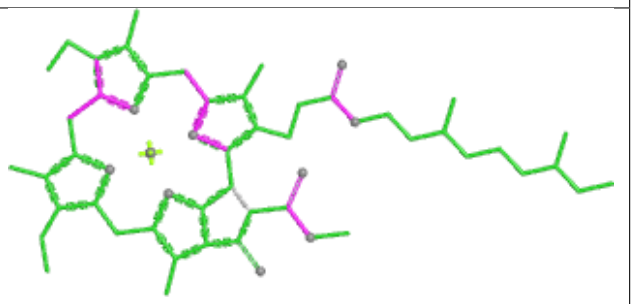
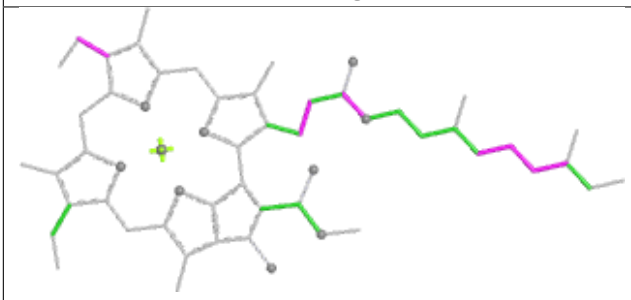
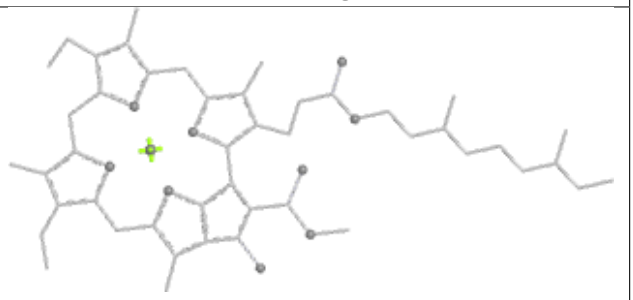
Torsions



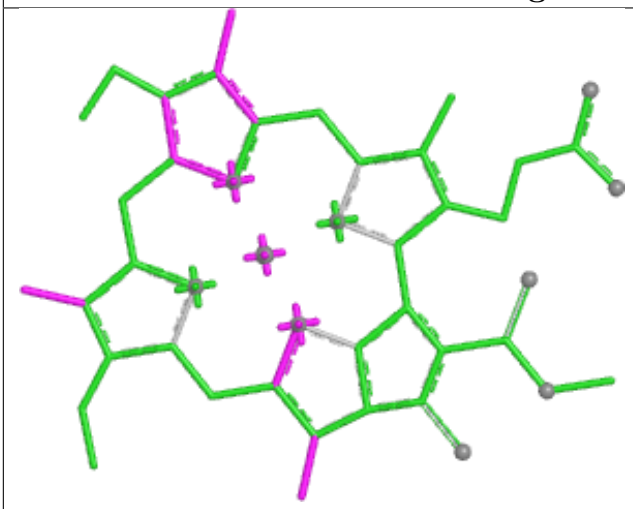
Rings

Ligand CLA 3 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

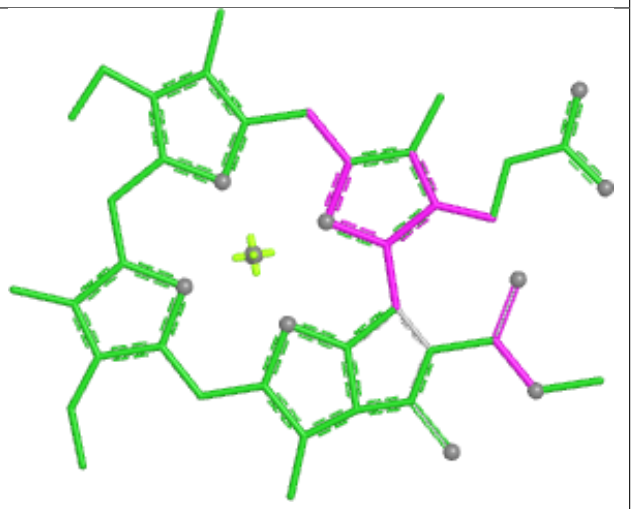
Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA s 611	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

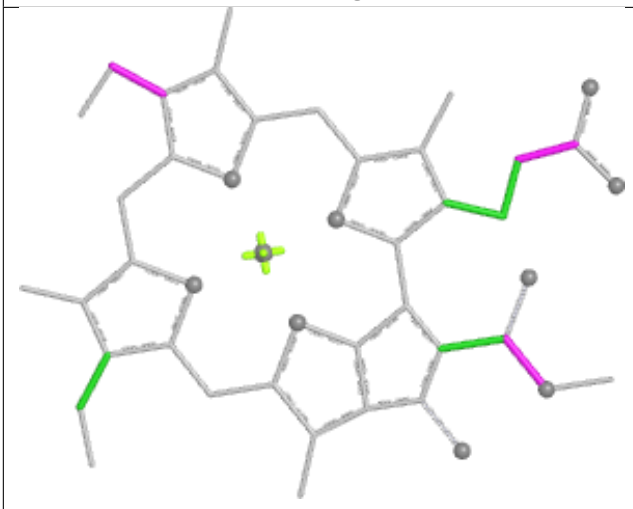
Ligand CLA 4 603



Bond lengths



Bond angles

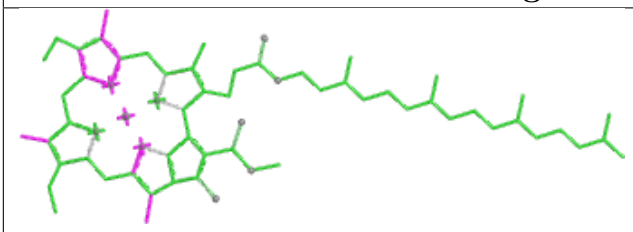


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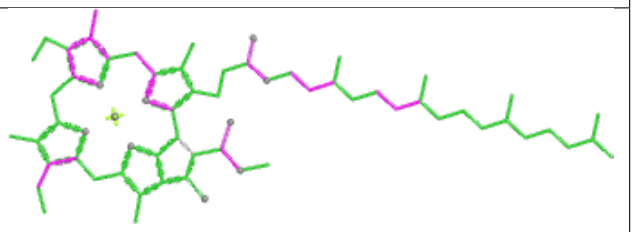


Rings

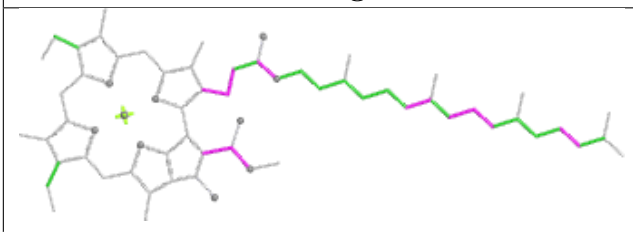
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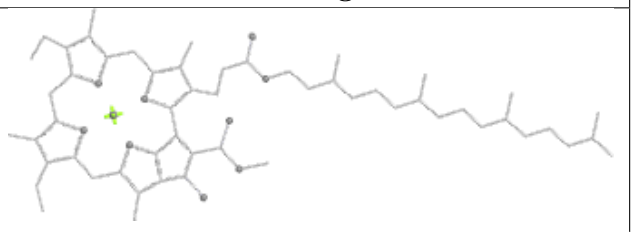
Bond lengths



Bond angles

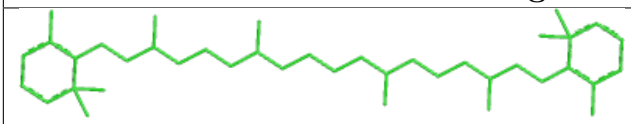


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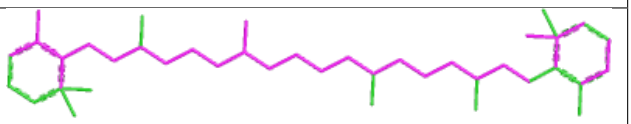


Rings

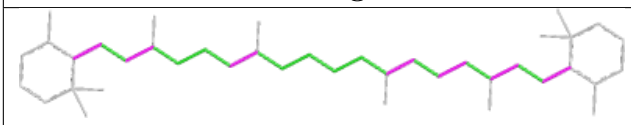
Ligand BCR t 101



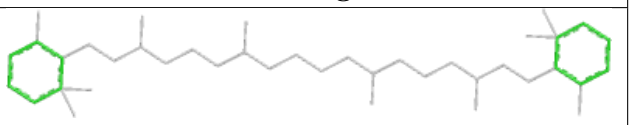
Bond lengths



Bond angles

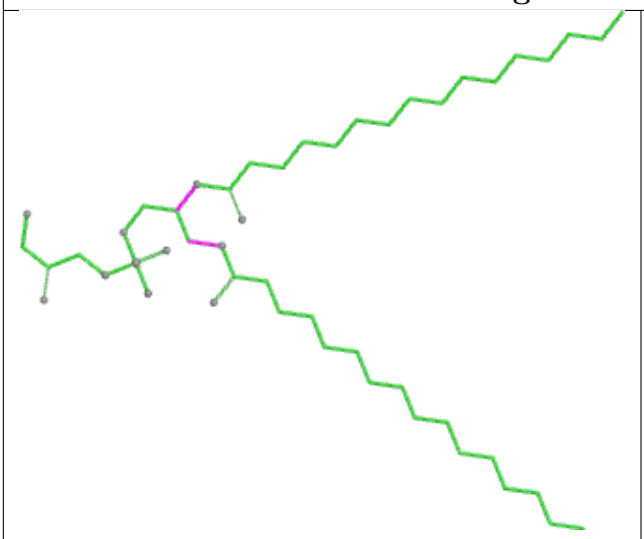


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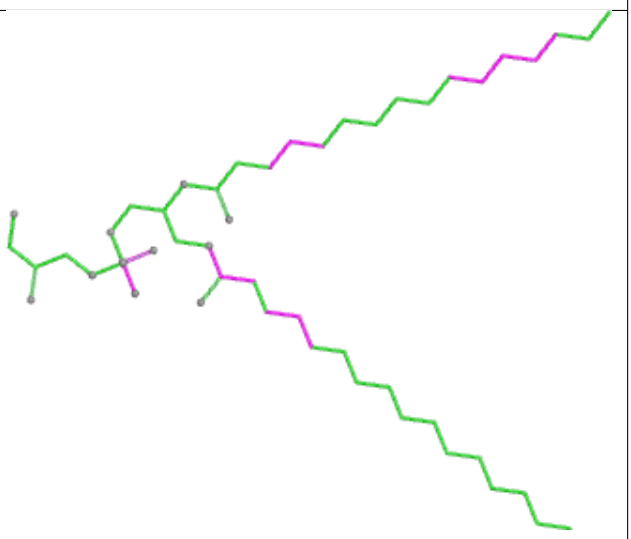


Rings

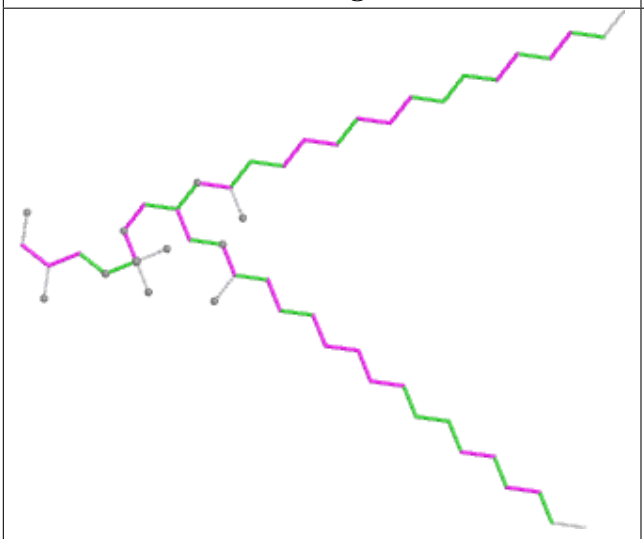
Ligand LHG Y 2630



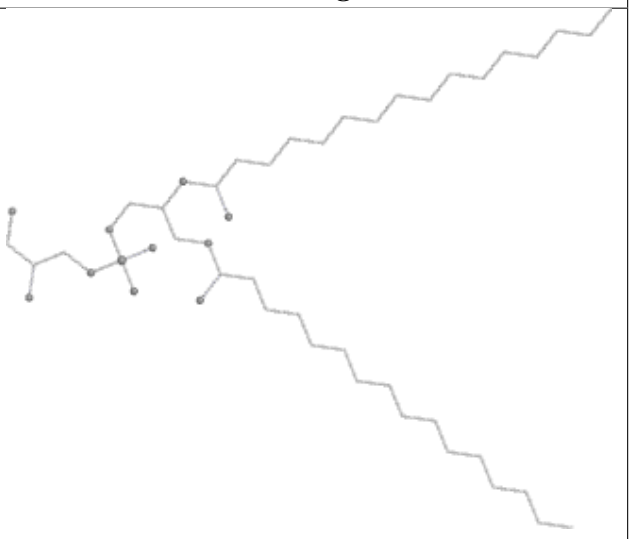
Bond lengths



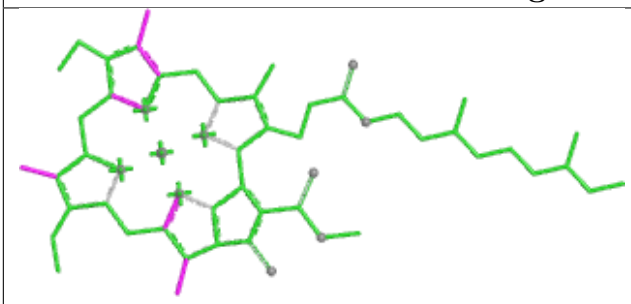
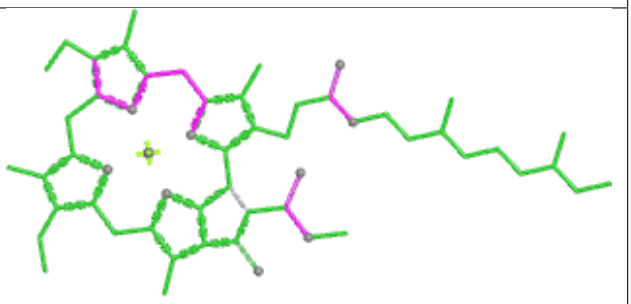
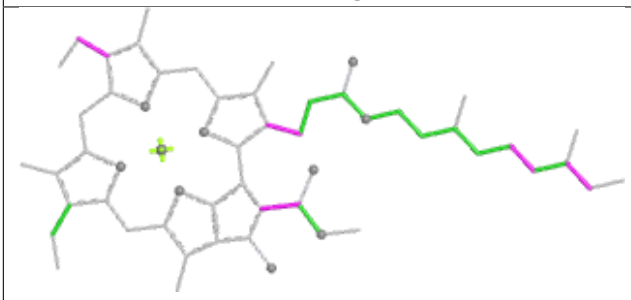
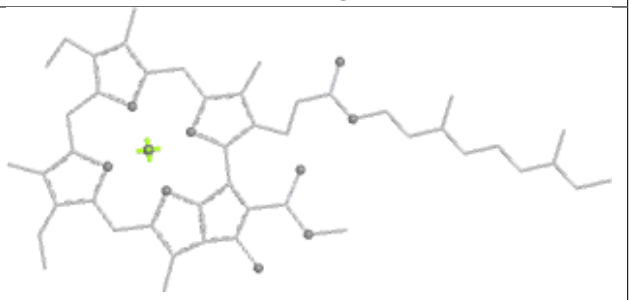
Bond angles

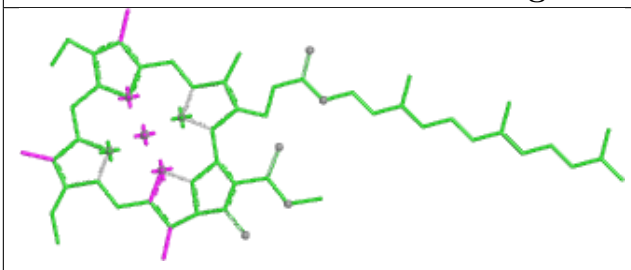
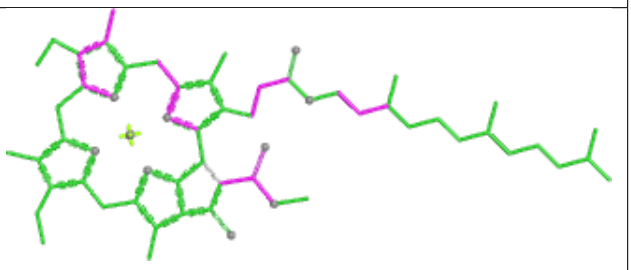
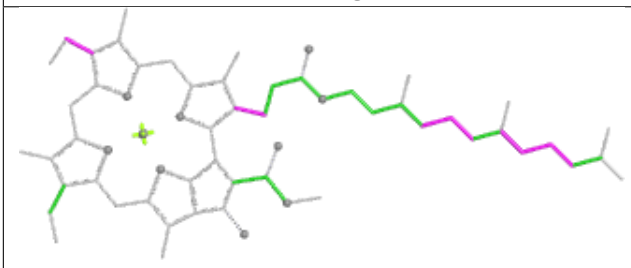
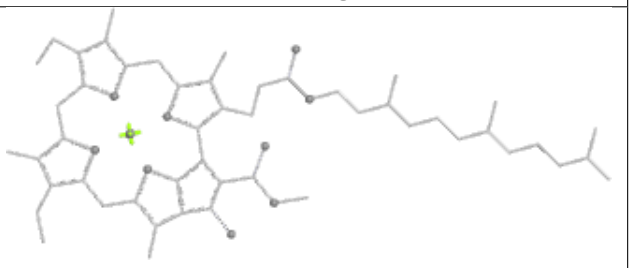


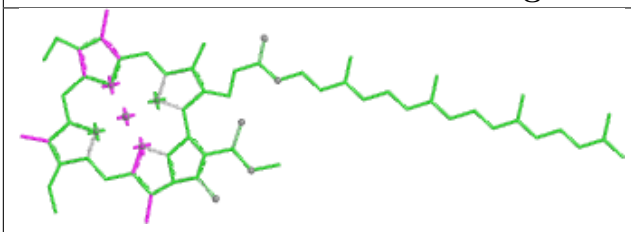
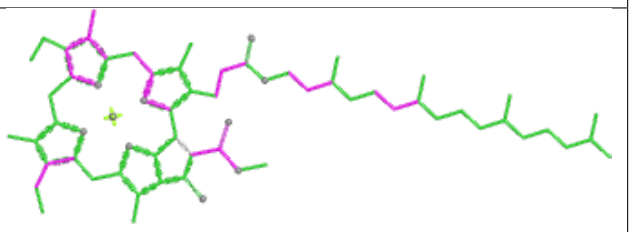
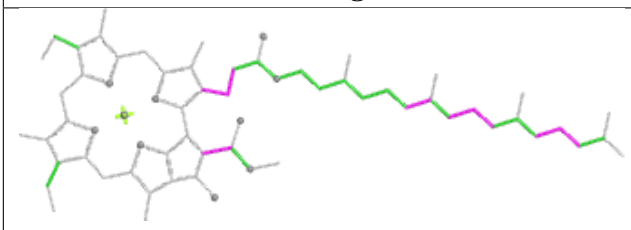
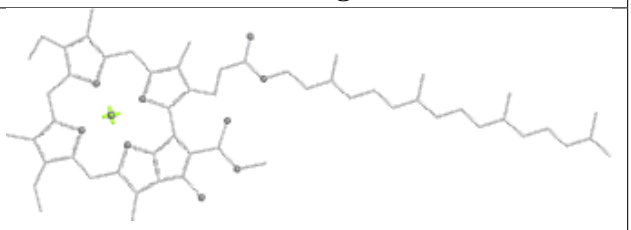
Torsions

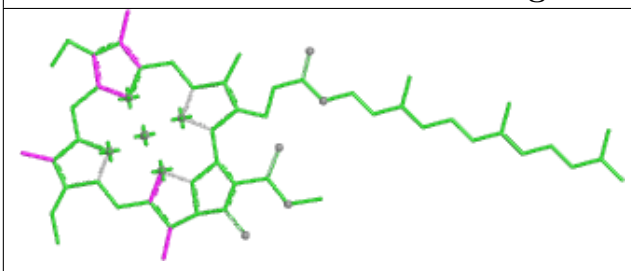
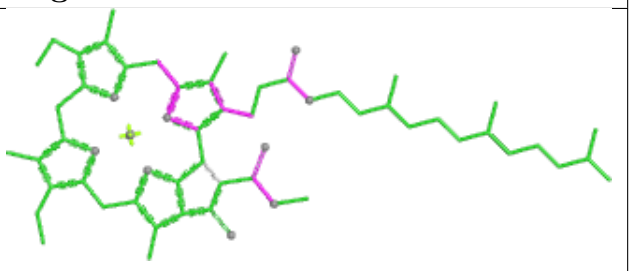
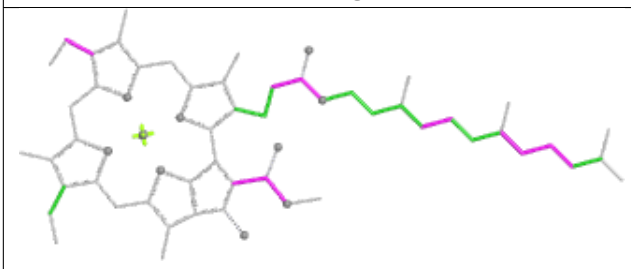
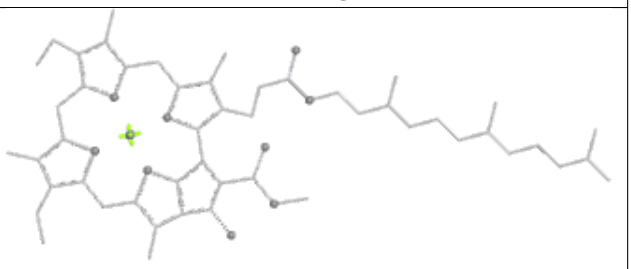


Rings

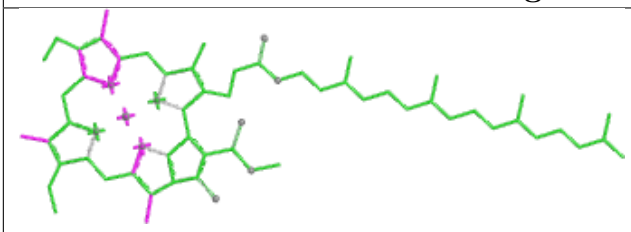
Ligand CLA 5 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

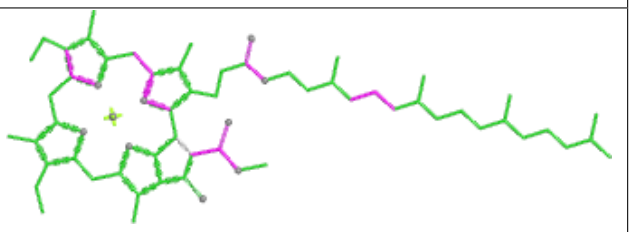
Ligand CLA Y 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

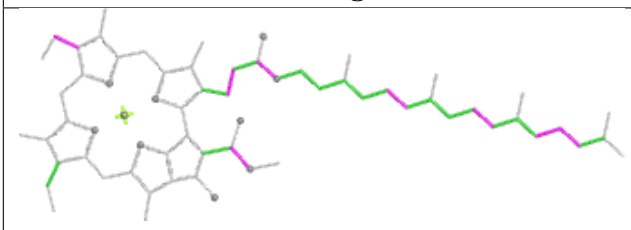
Ligand CLA C 503



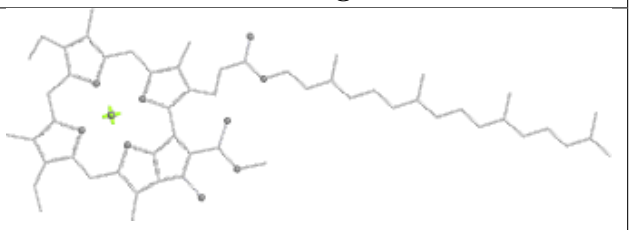
Bond lengths



Bond angles

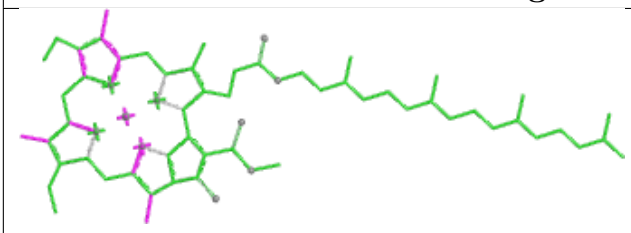


Torsions

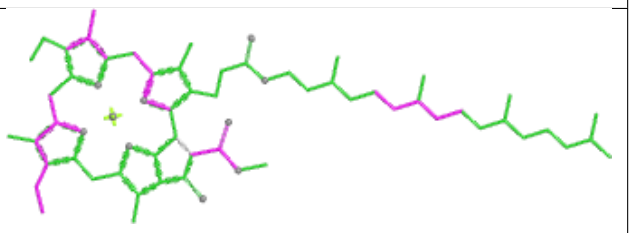


Rings

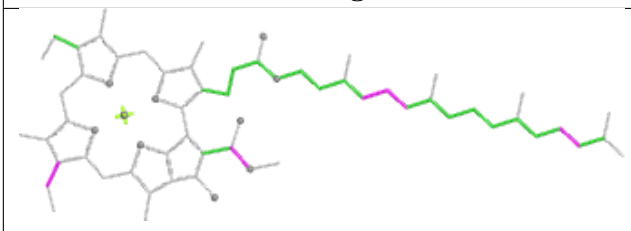
Ligand CLA a 405



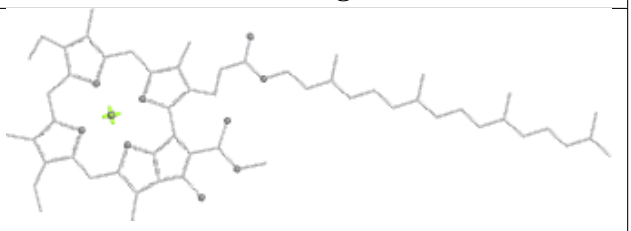
Bond lengths



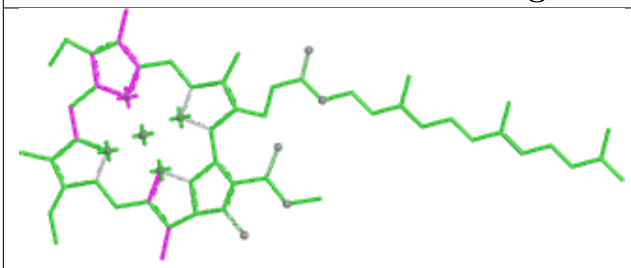
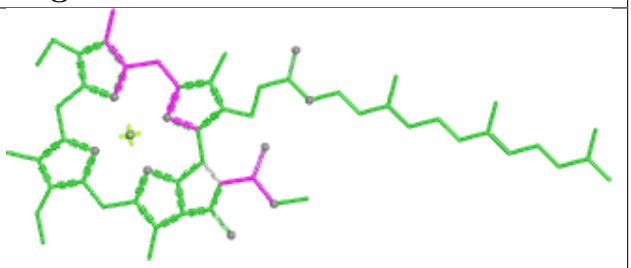
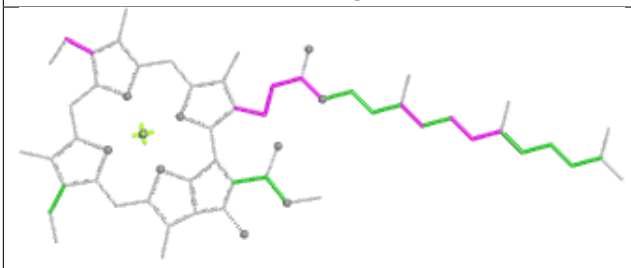
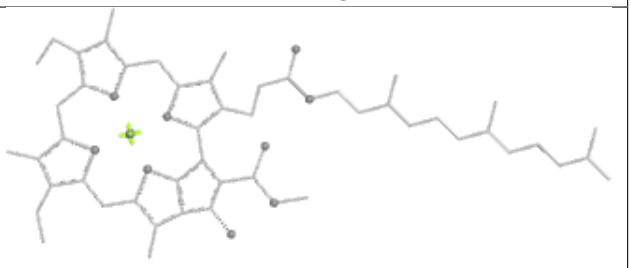
Bond angles

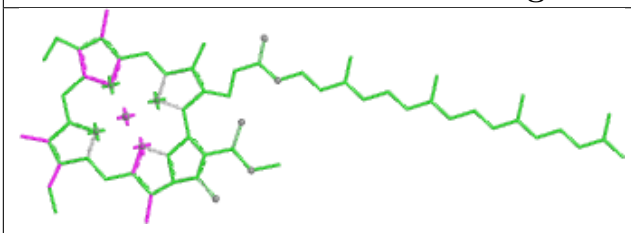
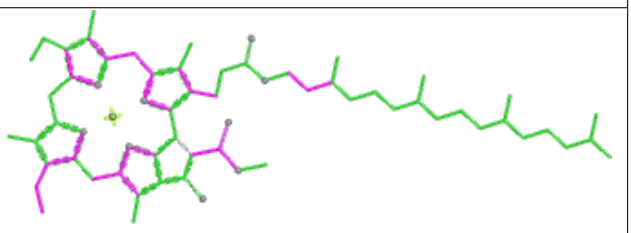
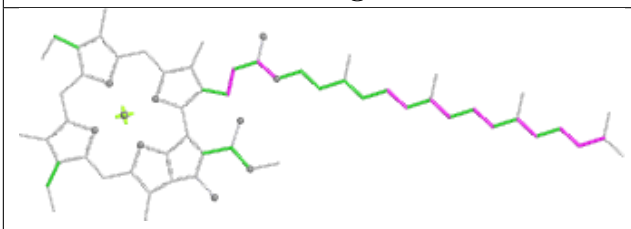
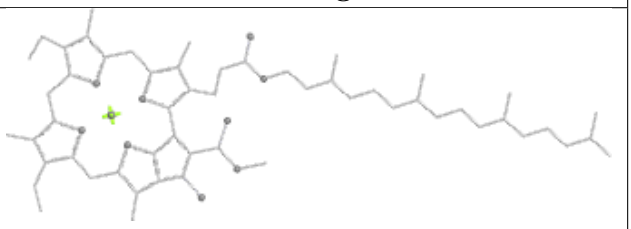


Torsions

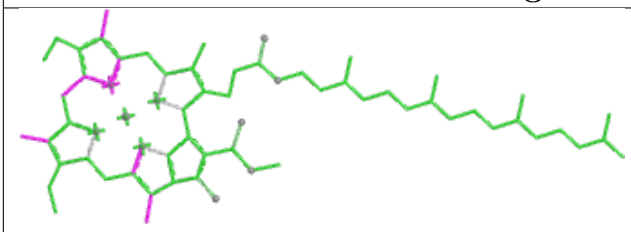


Rings

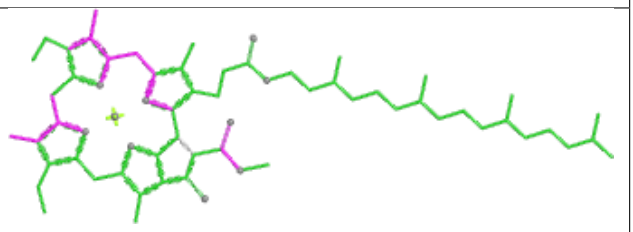
Ligand CLA g 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA n 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

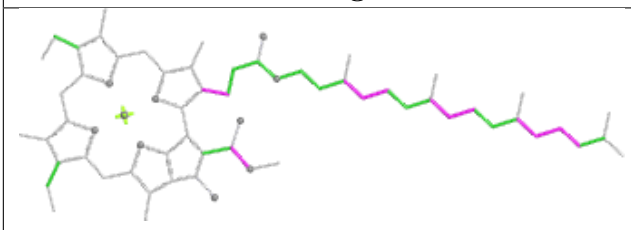
Ligand CLA B 612



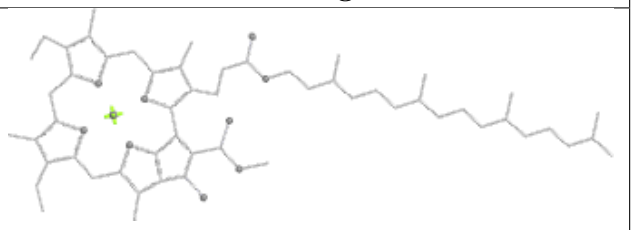
Bond lengths



Bond angles

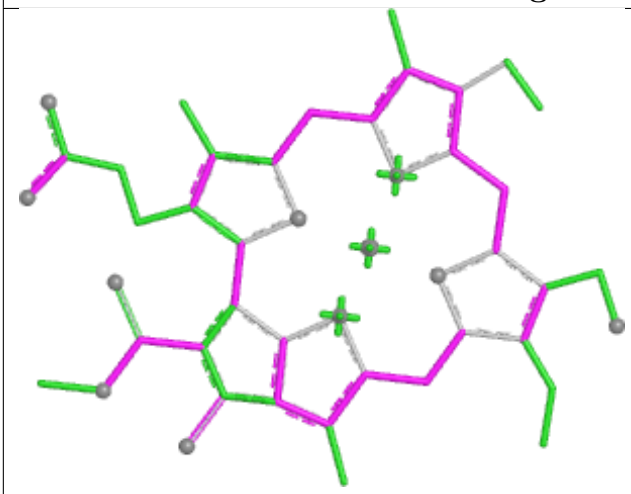


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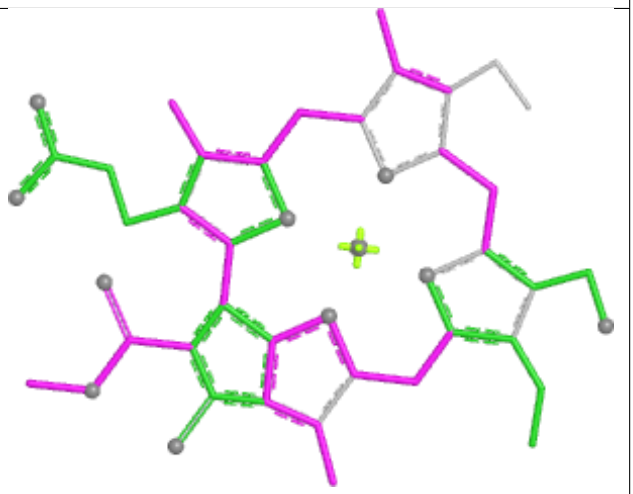


Rings

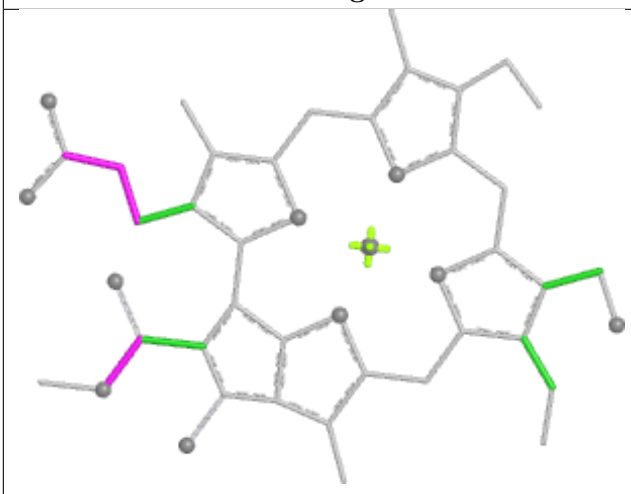
Ligand CHL s 601



Bond lengths



Bond angles

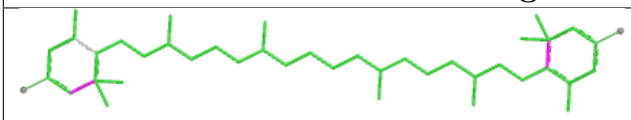


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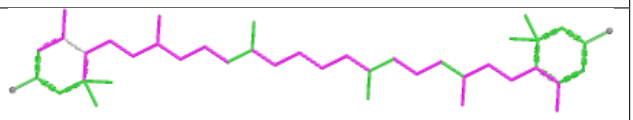


Rings

Ligand LUT 5 1621



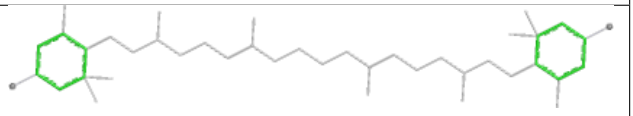
Bond lengths



Bond angles

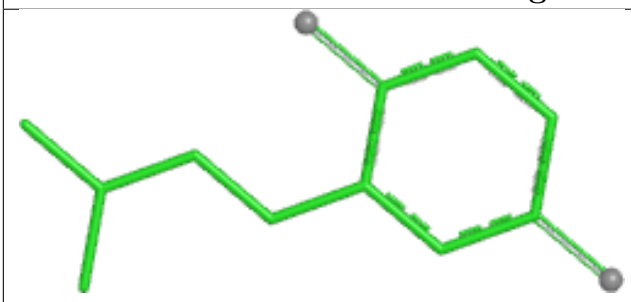


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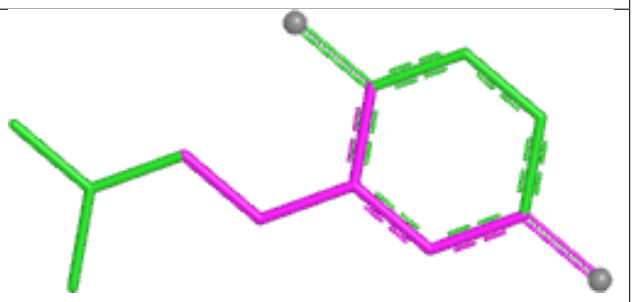


Rings

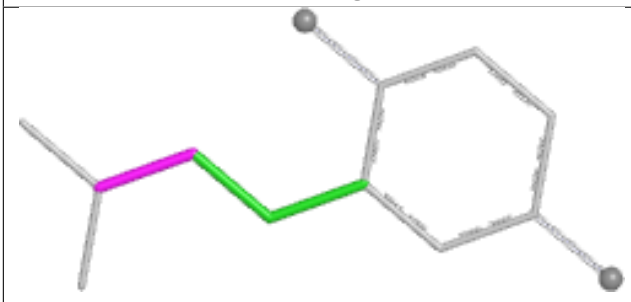
Ligand PL9 A 414



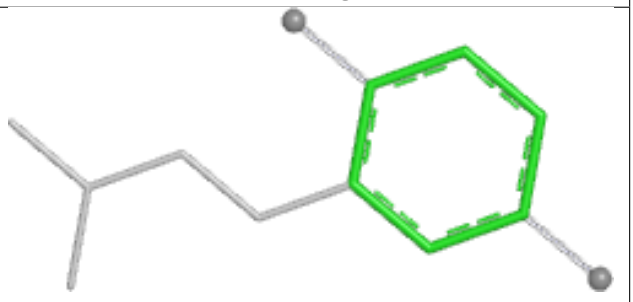
Bond lengths



Bond angles

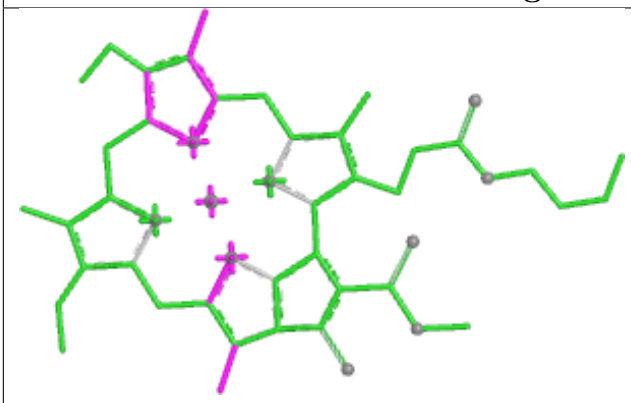


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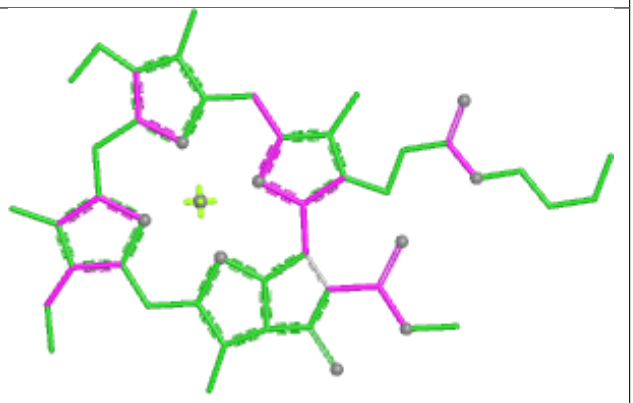


Rings

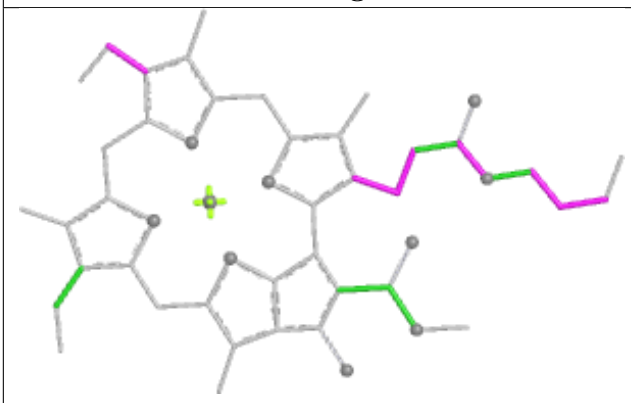
Ligand CLA R 611



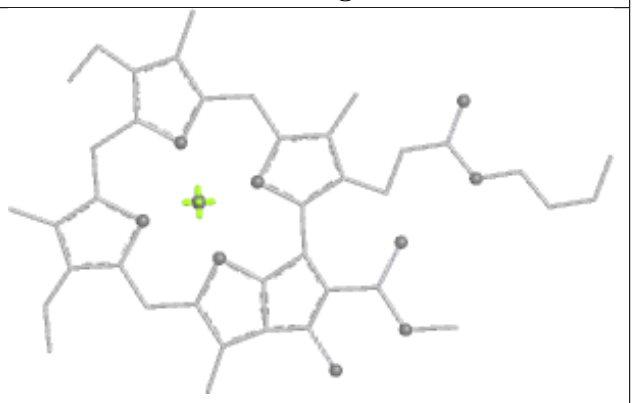
Bond lengths



Bond angles

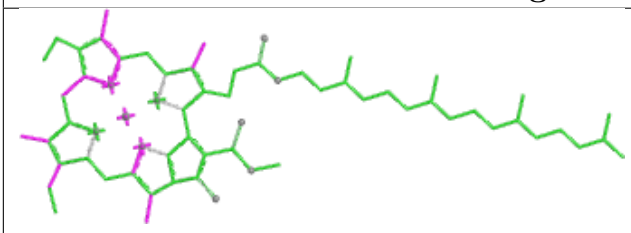


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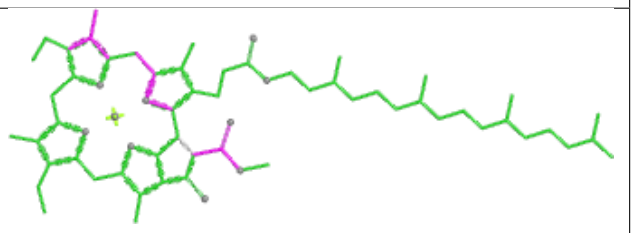


Rings

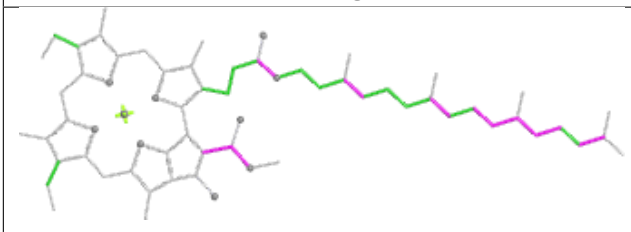
Ligand CLA c 504



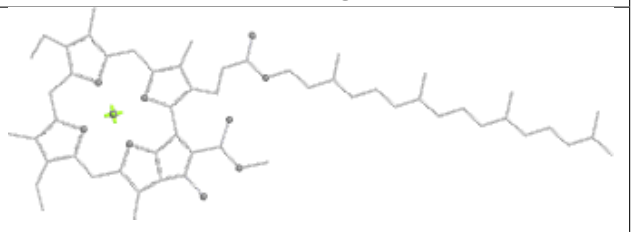
Bond lengths



Bond angles

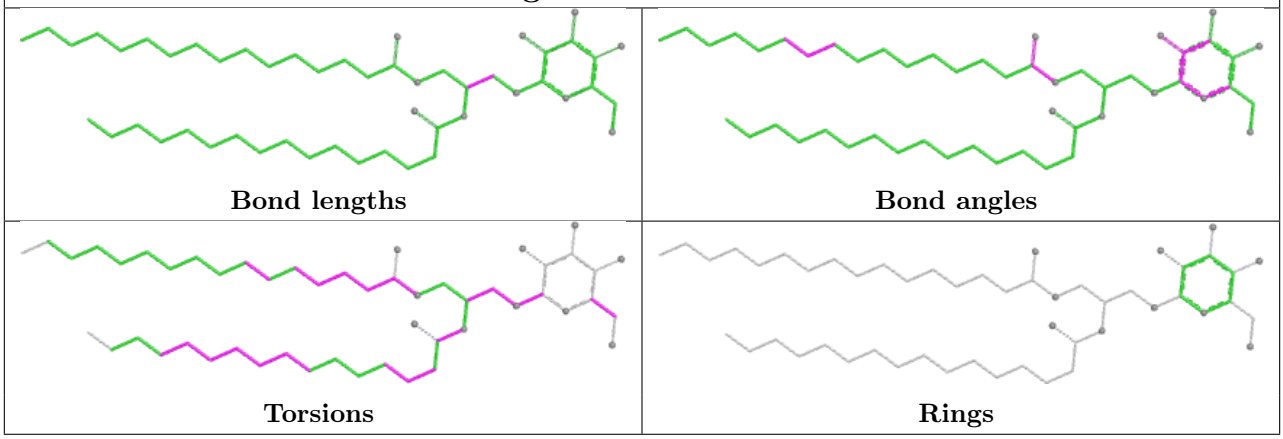


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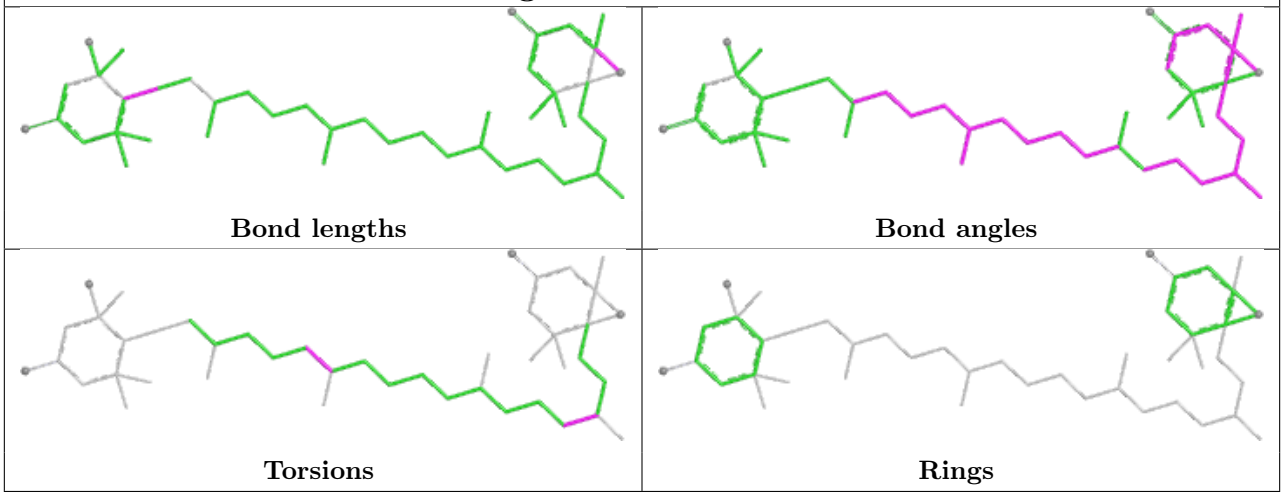


Rings

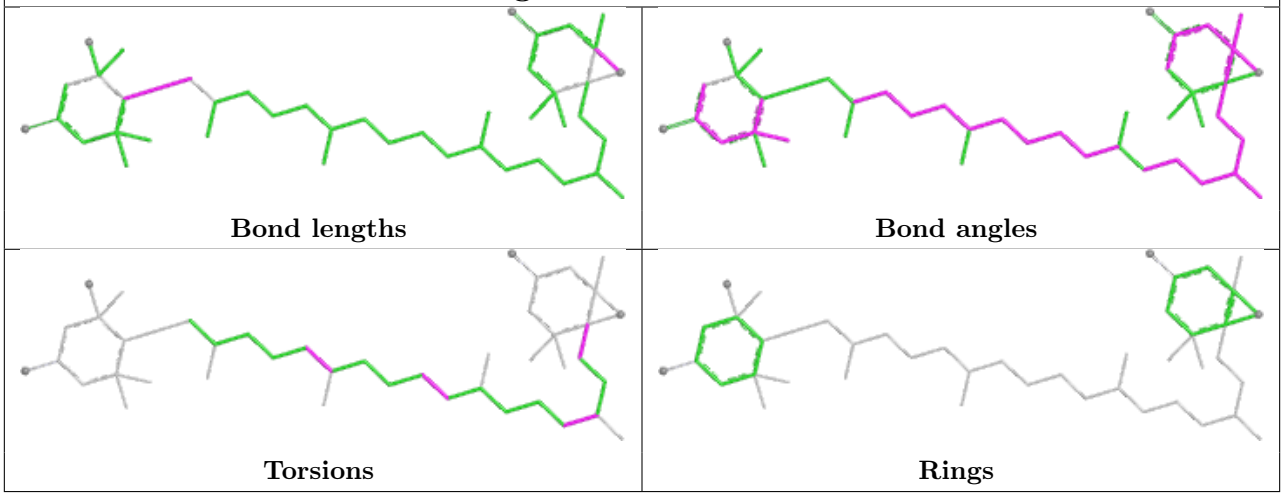
Ligand LMG Z 101



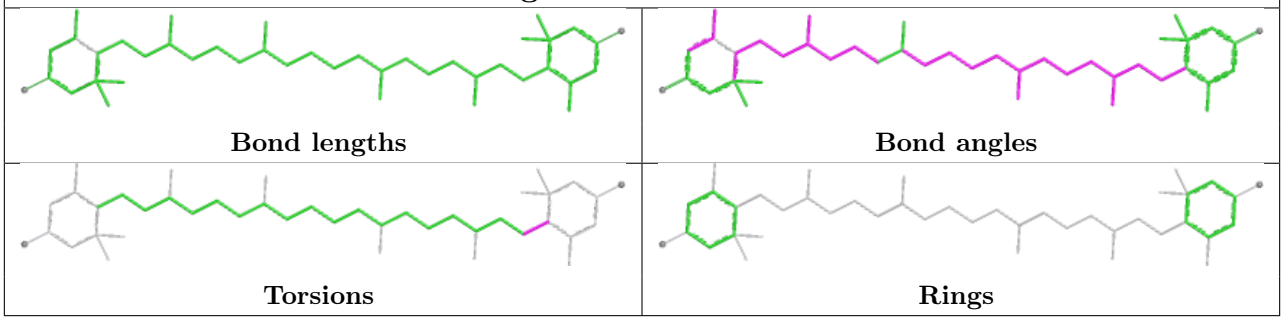
Ligand NEX 7 1623



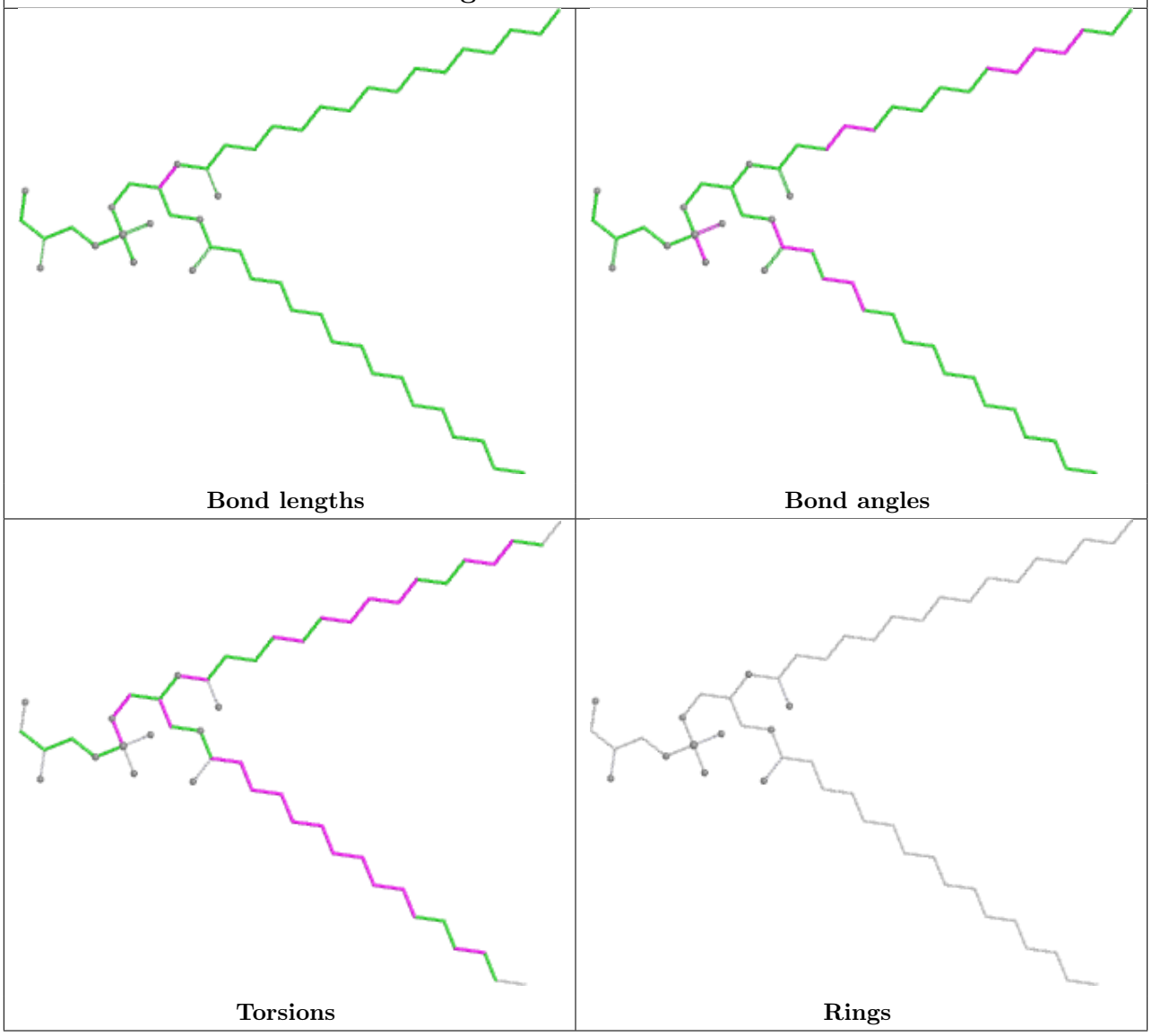
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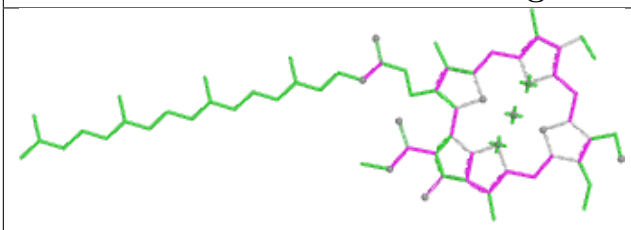
Ligand LUT 2 1620



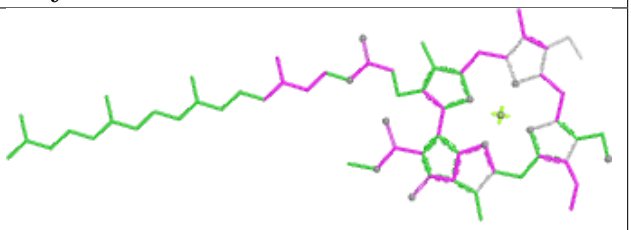
Ligand LHG G 2630



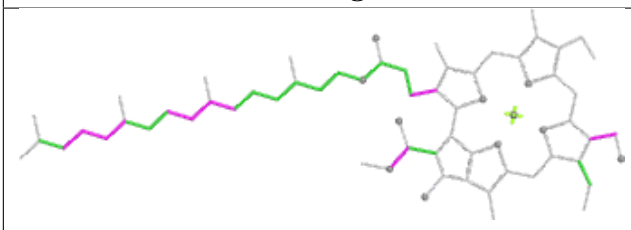
Ligand CHL y 608



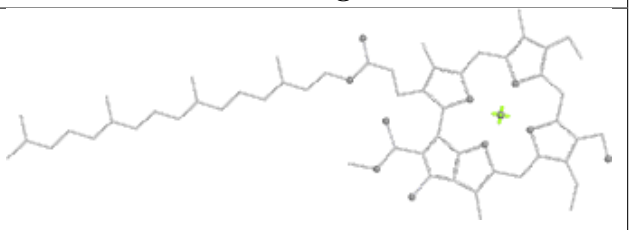
Bond lengths



Bond angles

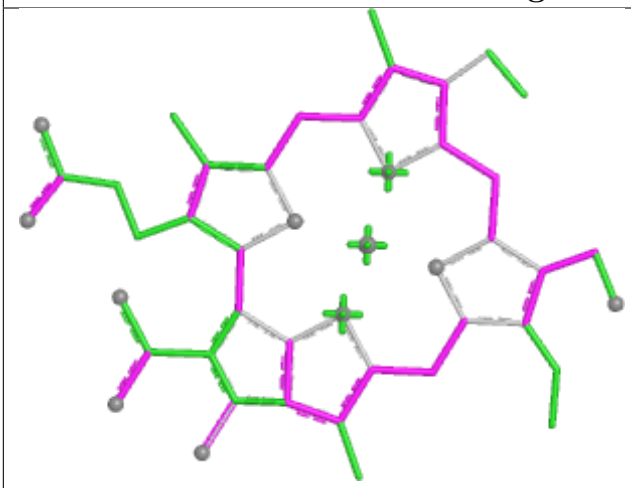


Torsions

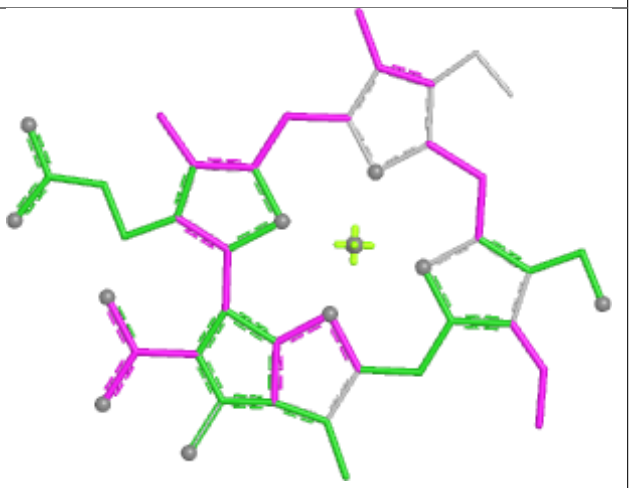


Rings

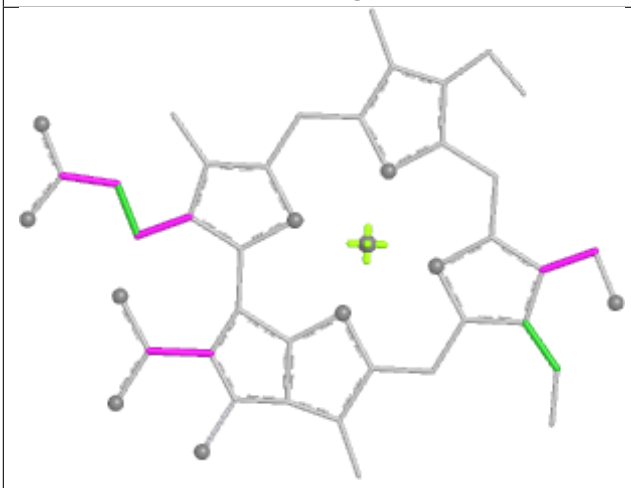
Ligand CHL 8 601



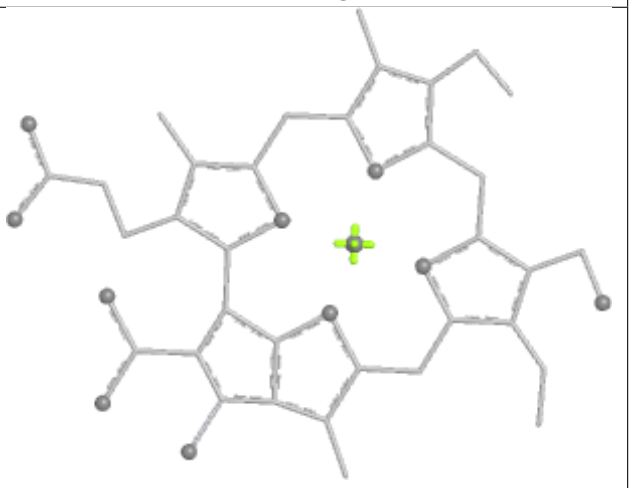
Bond lengths



Bond angles

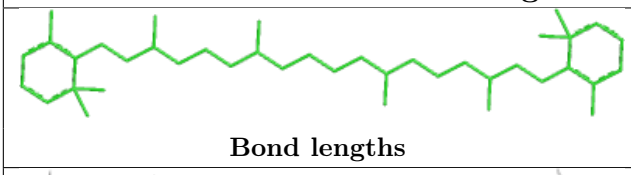


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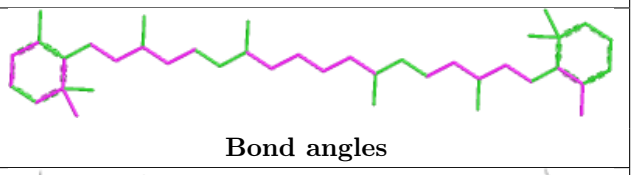


Rings

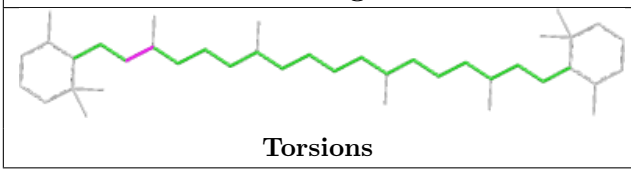
Ligand BCR H 101



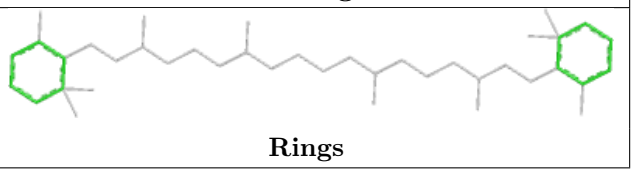
Bond lengths



Bond angles



Torsions

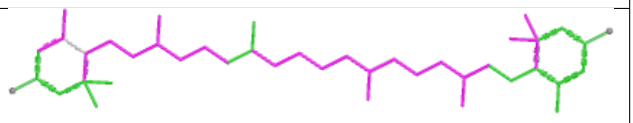


Rings

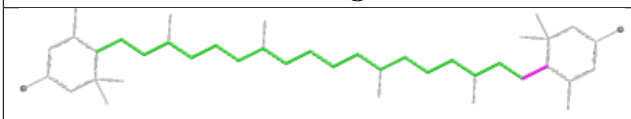
Ligand LUT S 1621



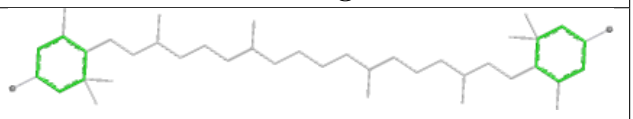
Bond lengths



Bond angles

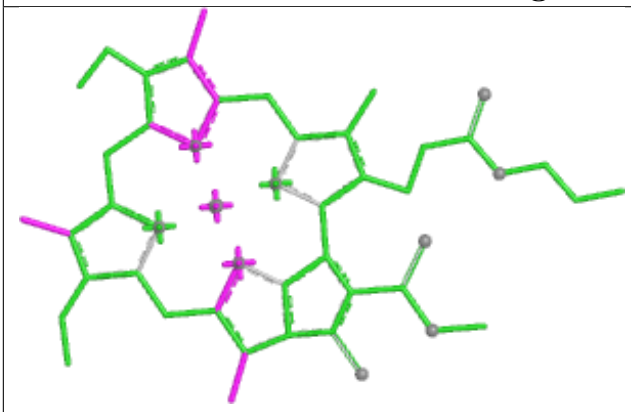


Torsions

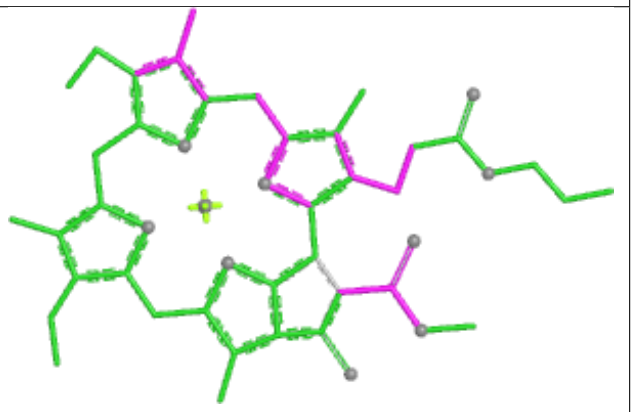


Rings

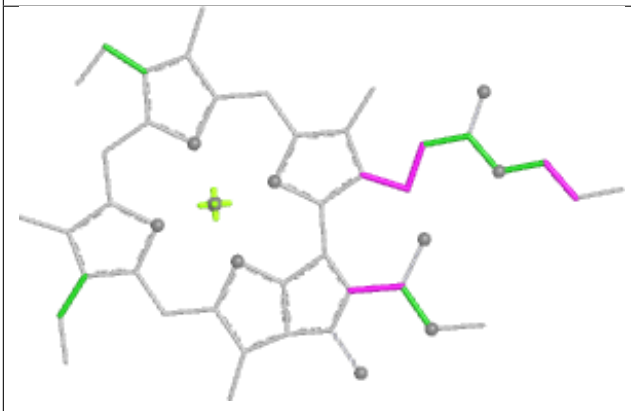
Ligand CLA r 604



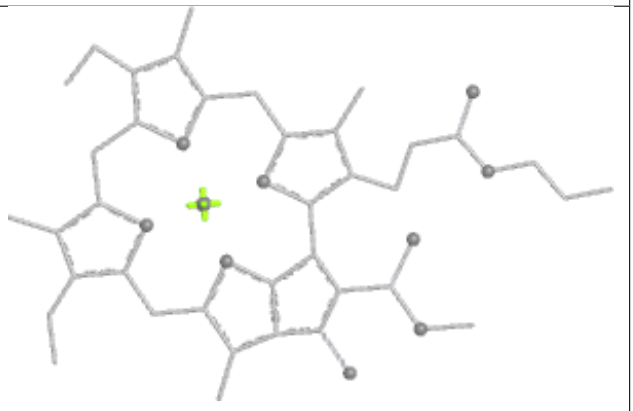
Bond lengths



Bond angles

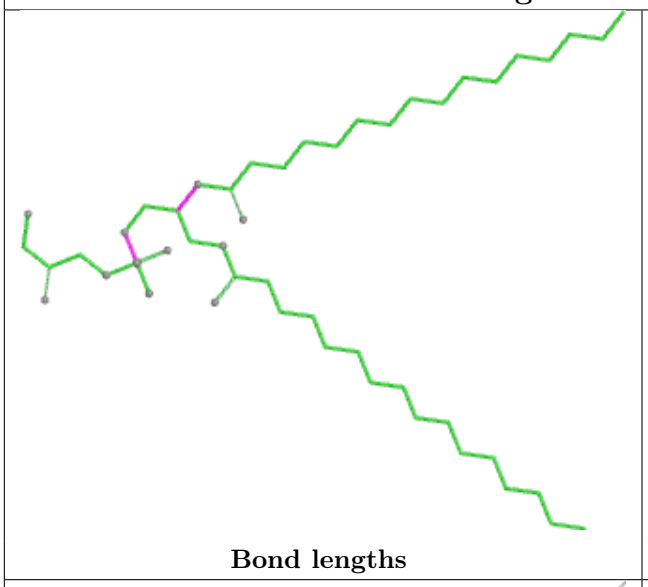


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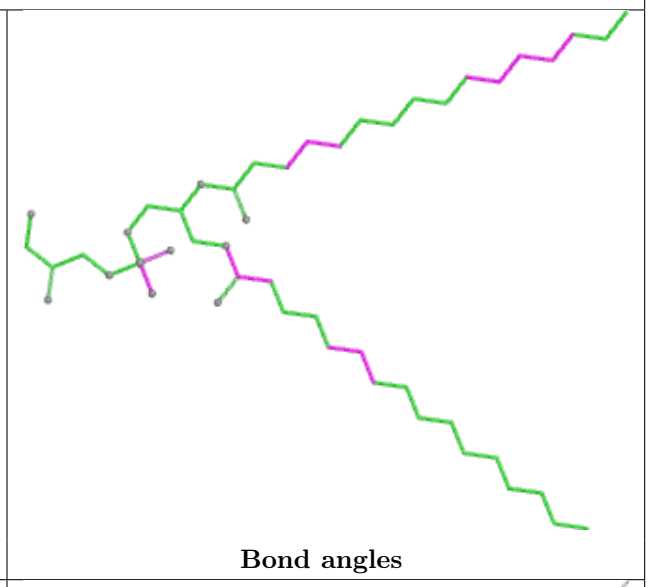


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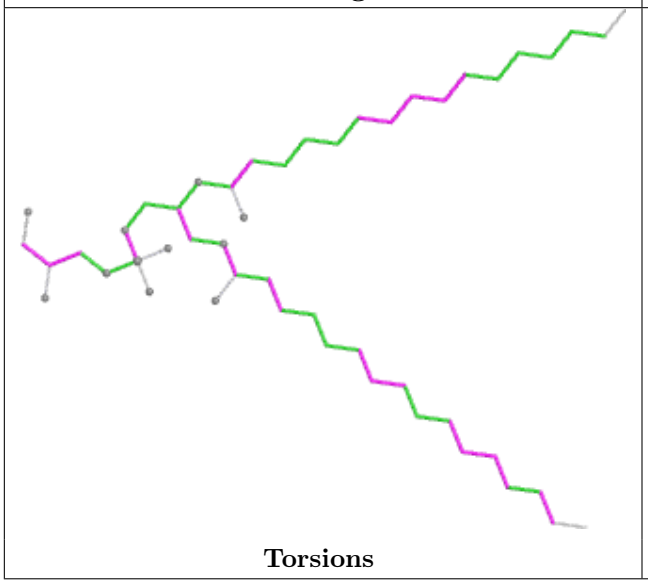
Ligand LHG B 2631



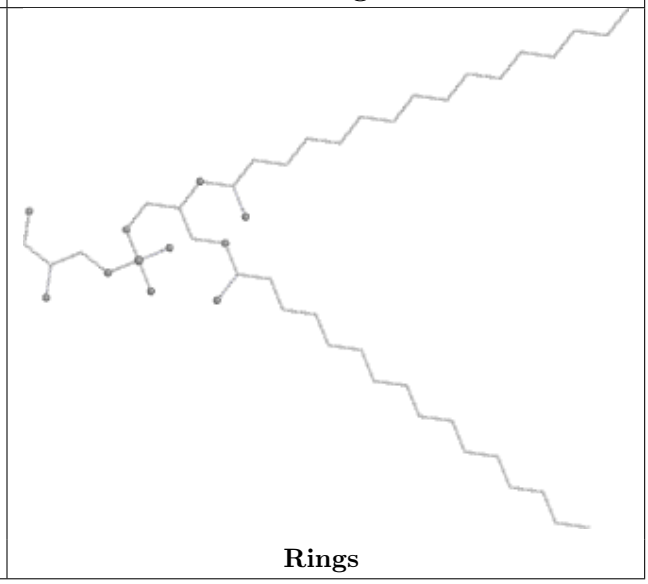
Bond lengths



Bond angles

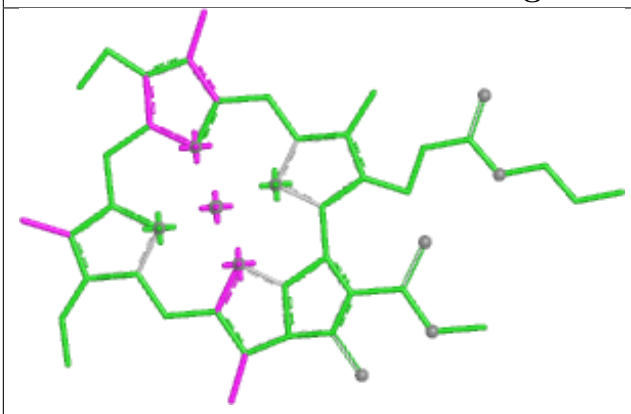


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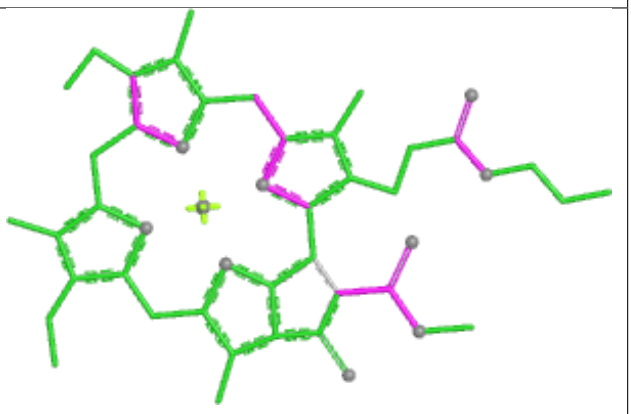


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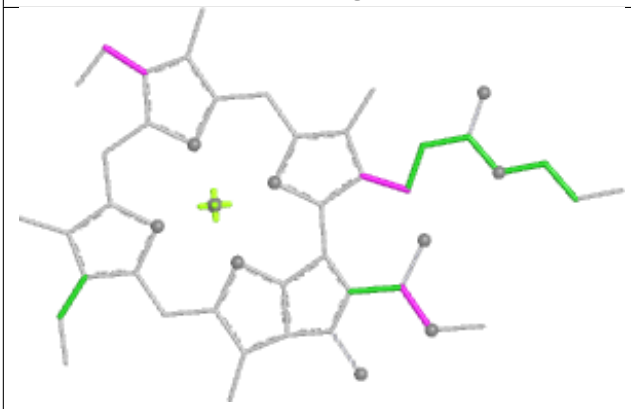
Ligand CLA Y 614



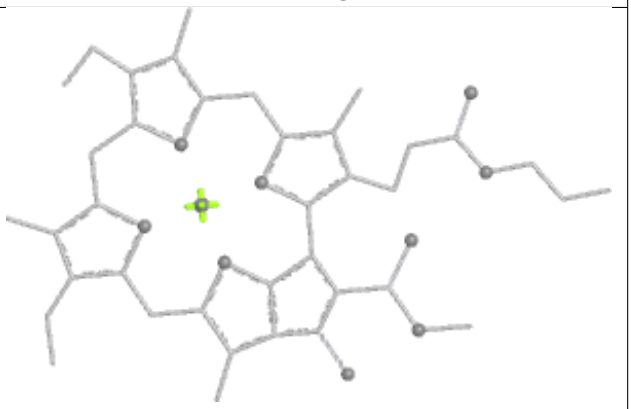
Bond lengths



Bond angles

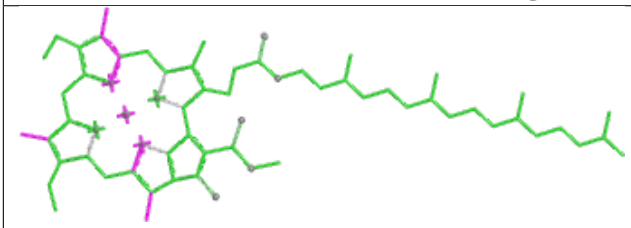


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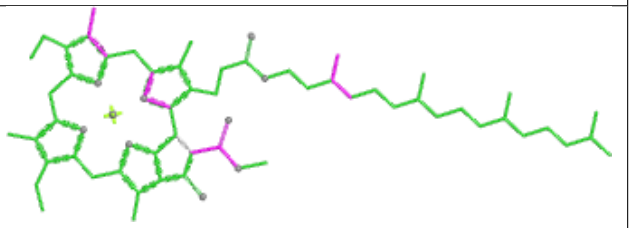


Rings

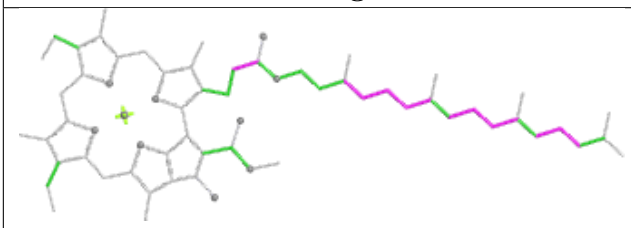
Ligand CLA B 614



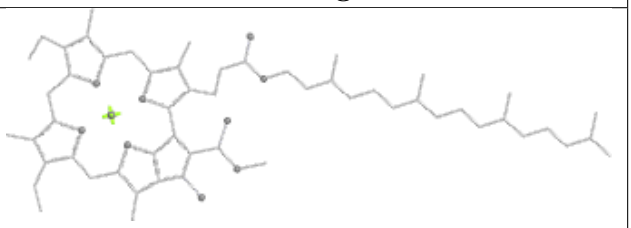
Bond lengths



Bond angles

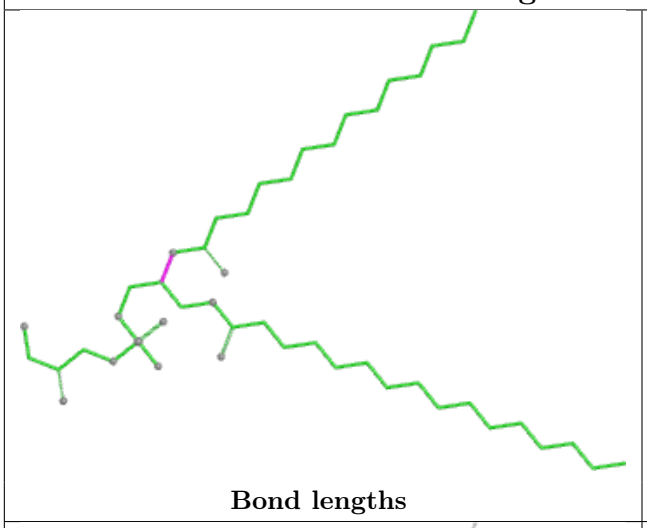


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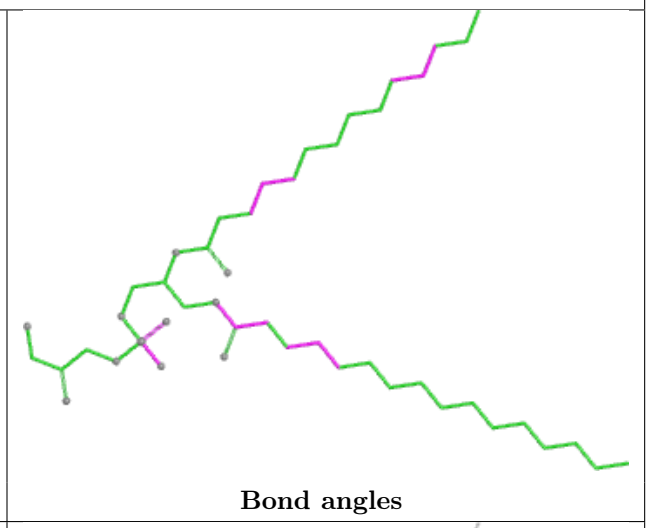


Rings

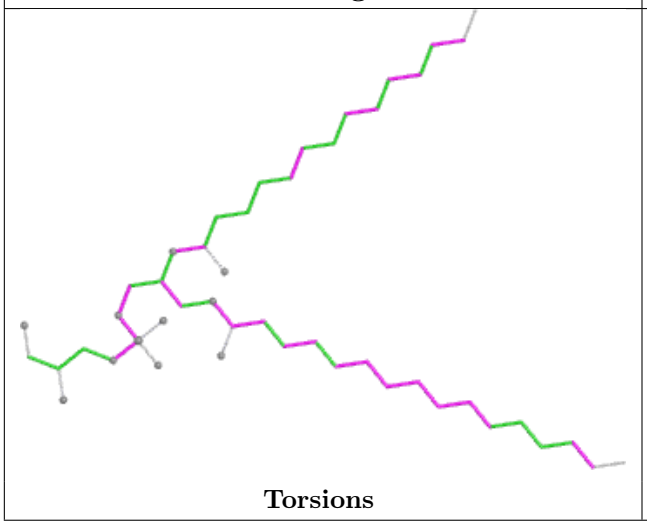
Ligand LHG 7 2630



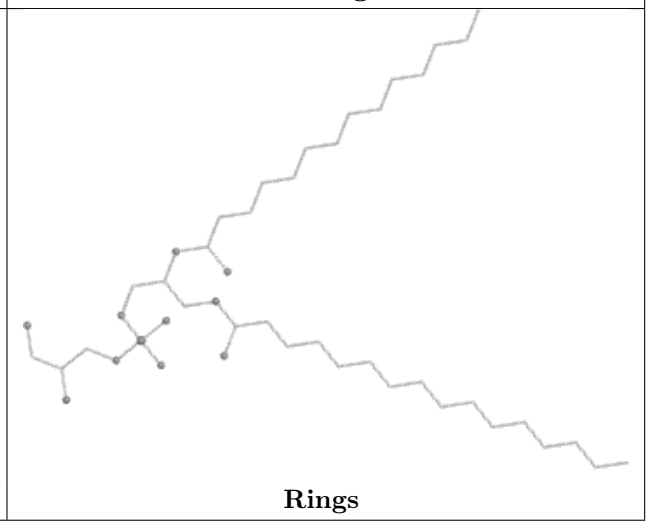
Bond lengths



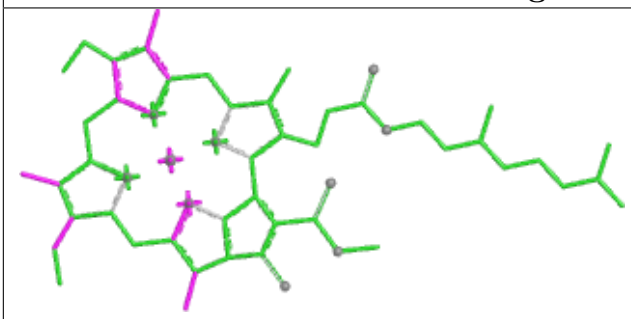
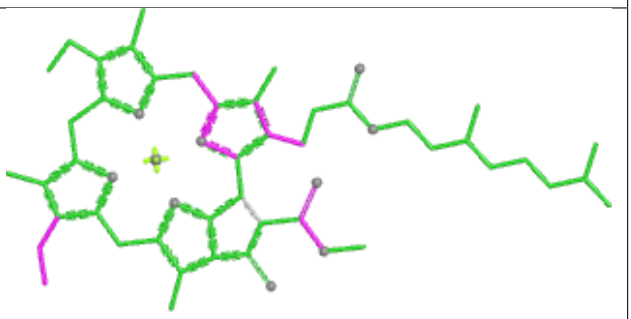
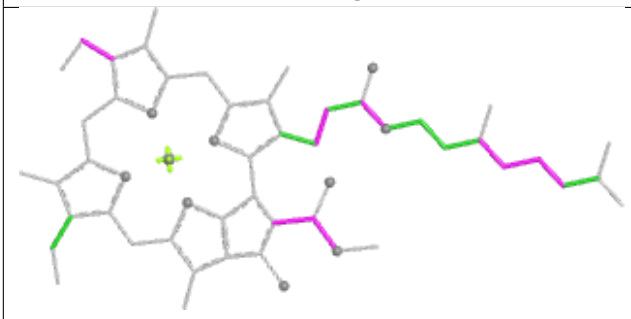
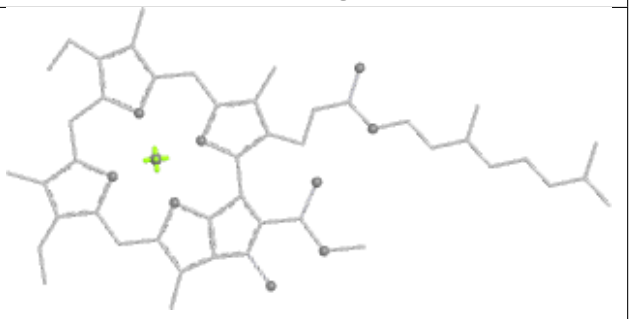
Bond angles

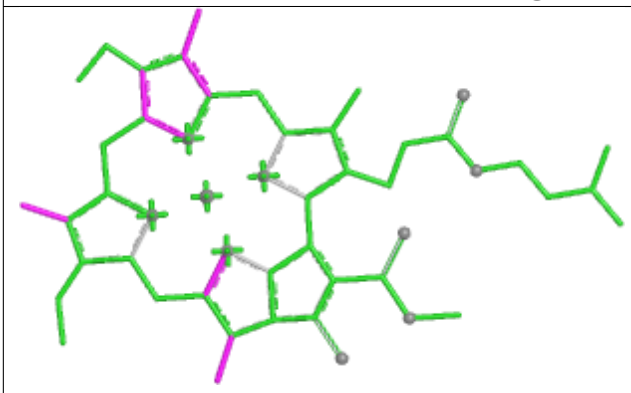
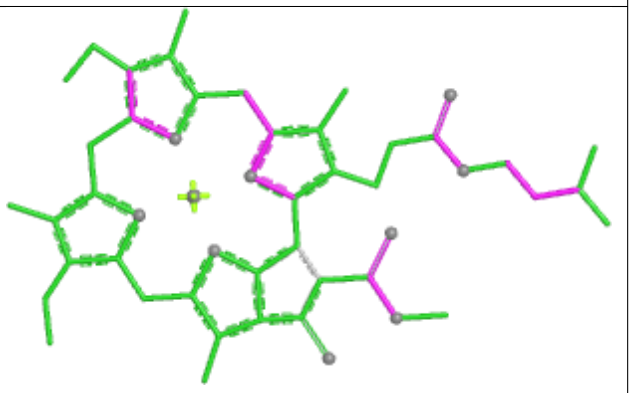
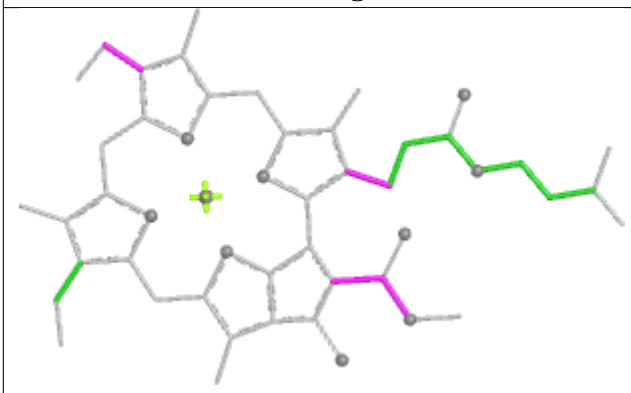
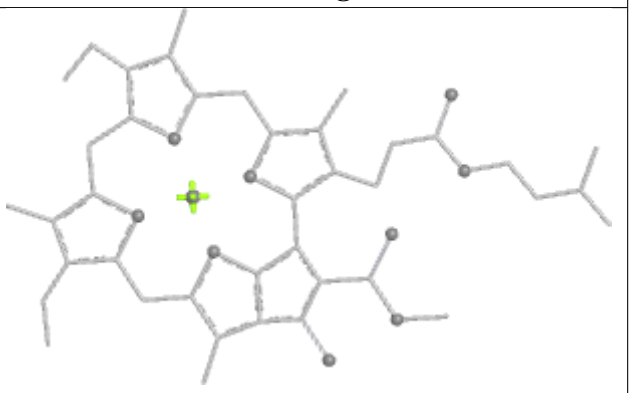


Torsions

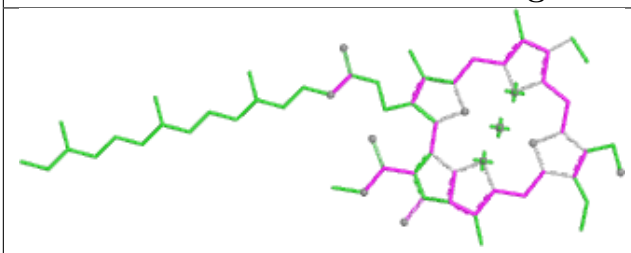


Rings

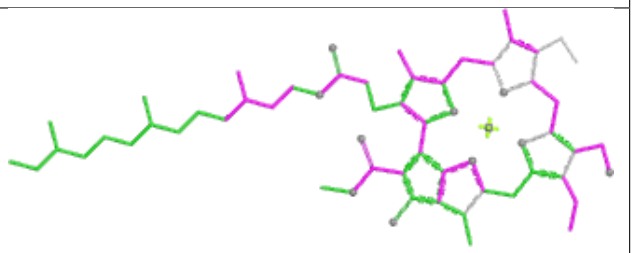
Ligand CLA 1 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

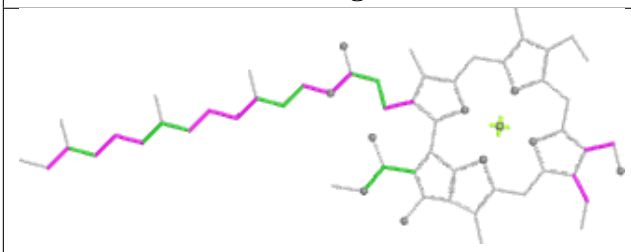
Ligand CHL 5 609



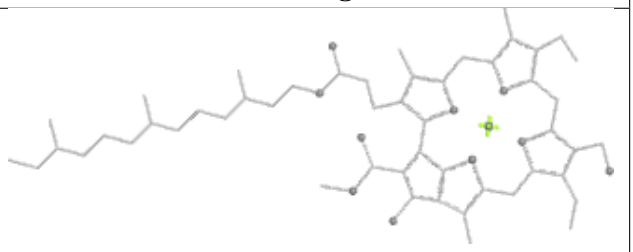
Bond lengths



Bond angles

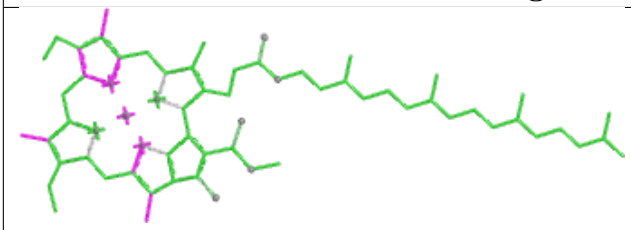


Torsions

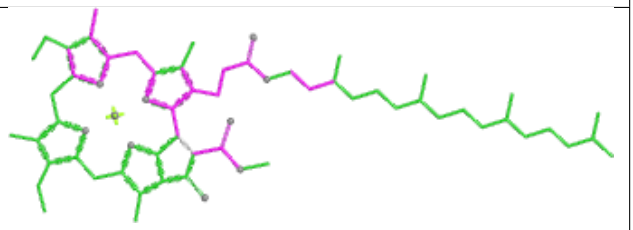


Rings

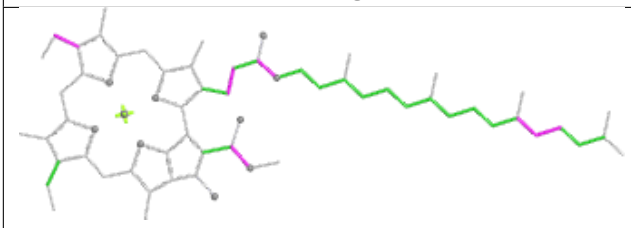
Ligand CLA b 611



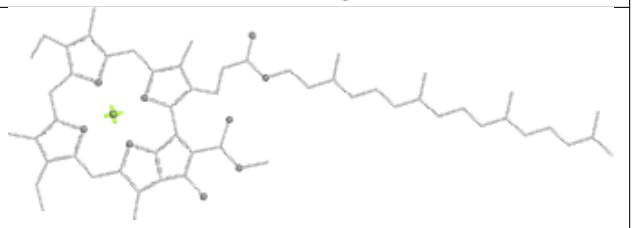
Bond lengths



Bond angles

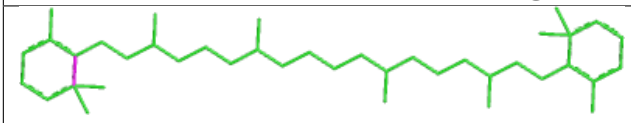


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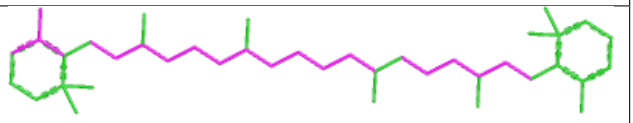


Rings

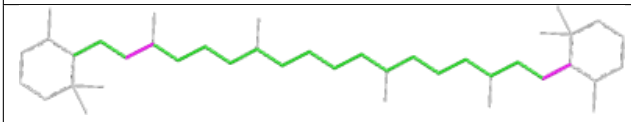
Ligand BCR c 517



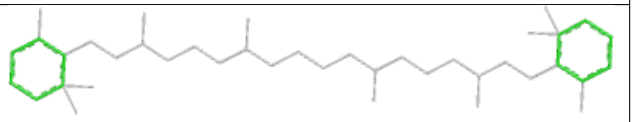
Bond lengths



Bond angles

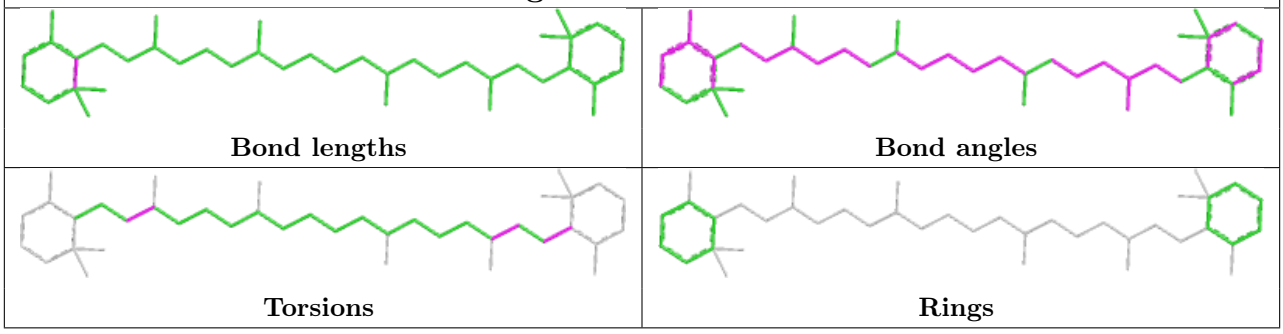


Torsions

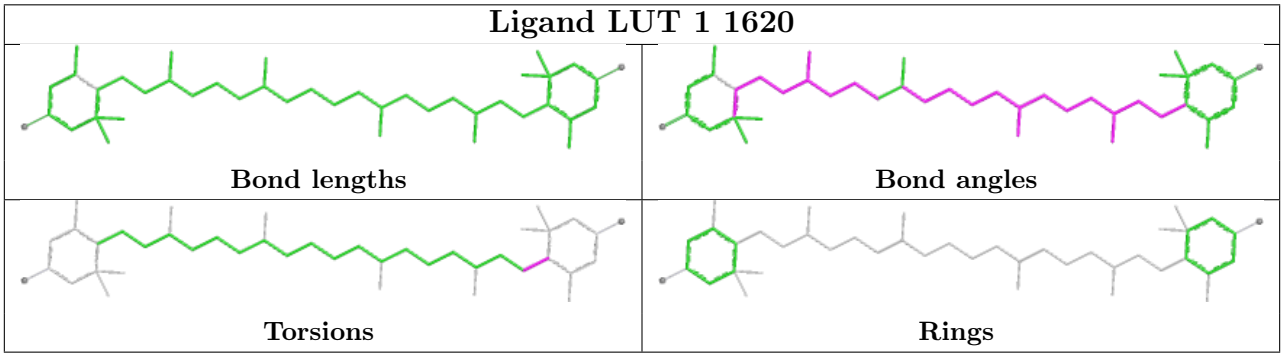


Rings

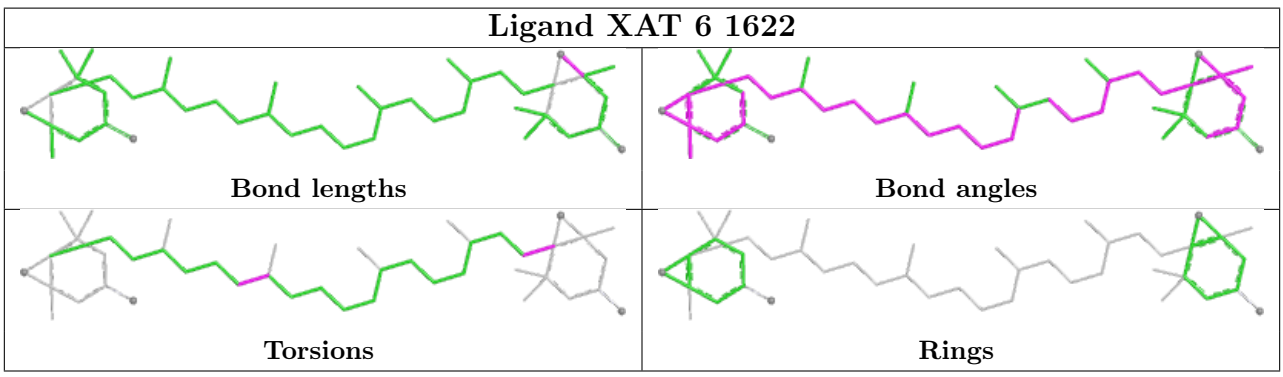
Ligand BCR b 620



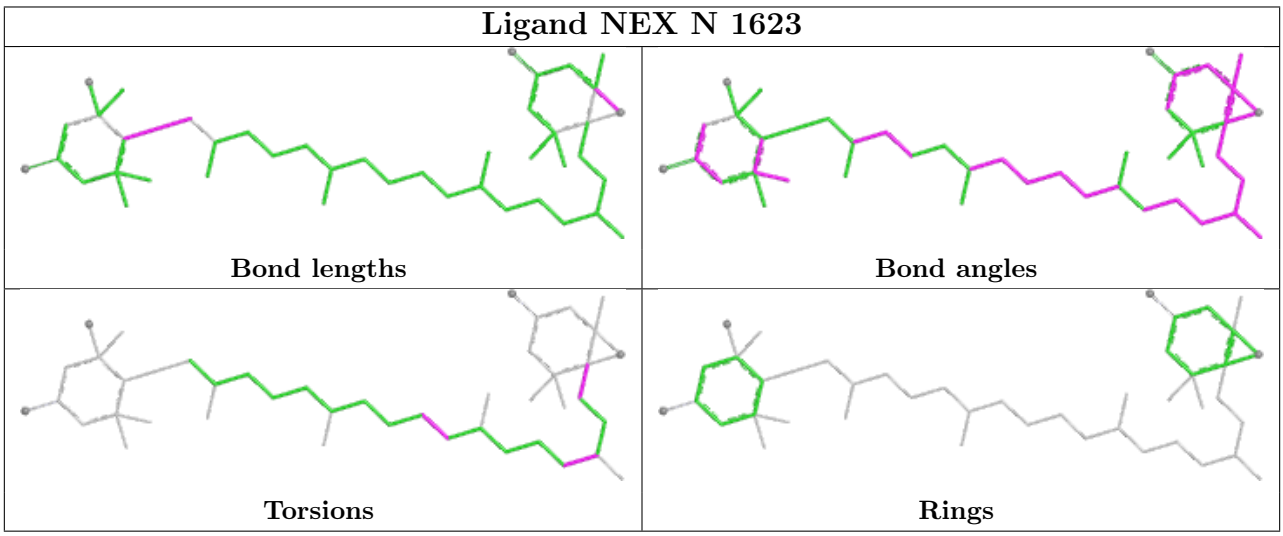
Ligand LUT 1 1620



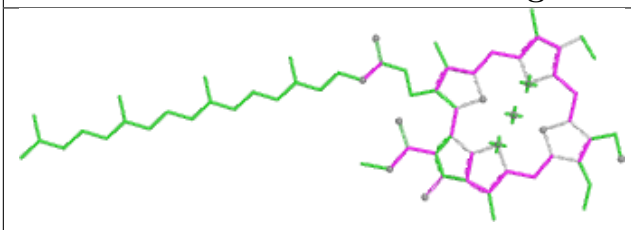
Ligand XAT 6 1622



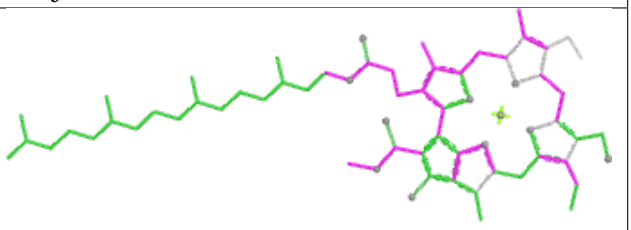
Ligand NEX N 1623



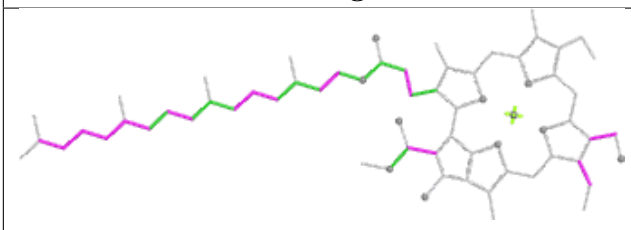
Ligand CHL y 607



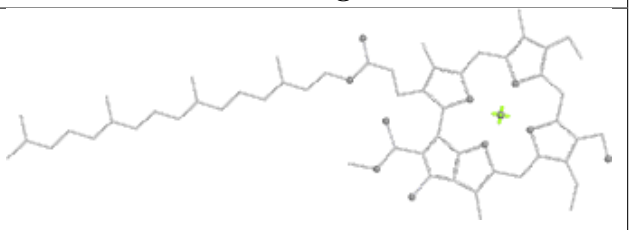
Bond lengths



Bond angles

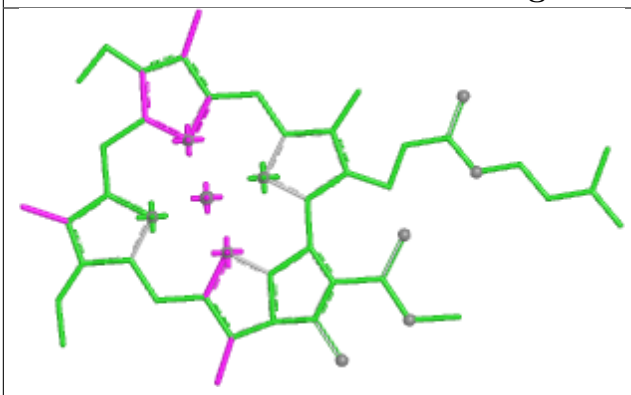


Torsions

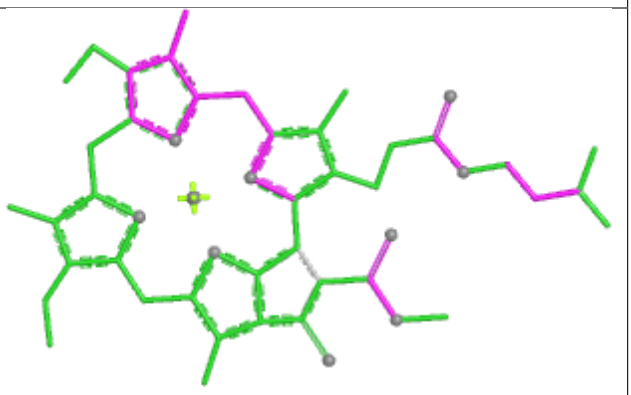


Rings

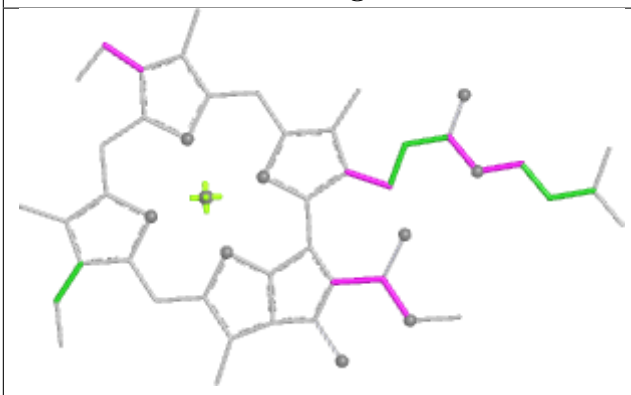
Ligand CLA 1 604



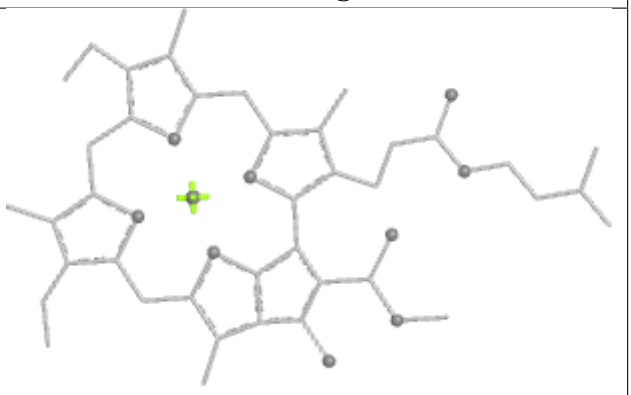
Bond lengths



Bond angles

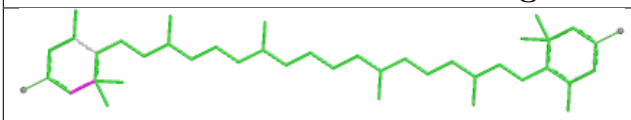


Torsions

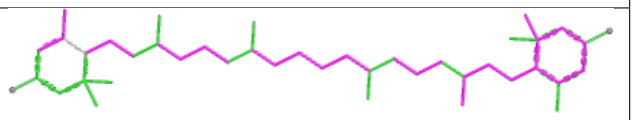


Rings

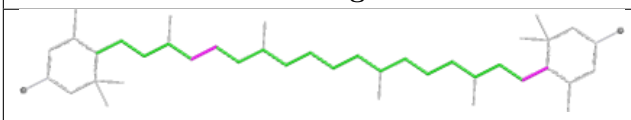
Ligand LUT 7 1621



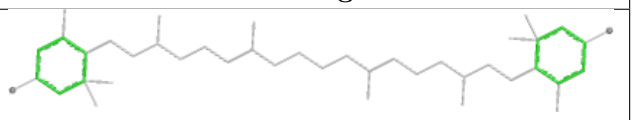
Bond lengths



Bond angles

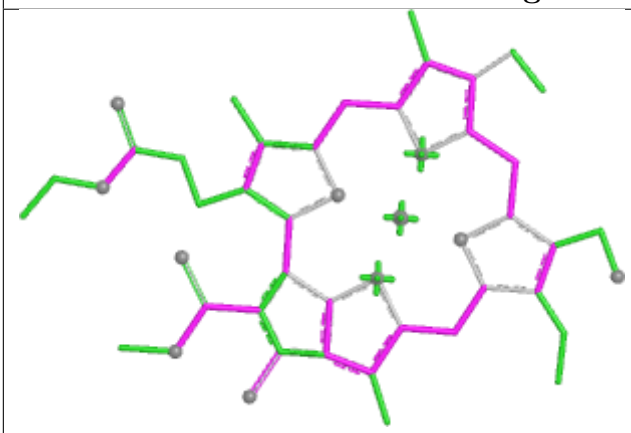


Torsions

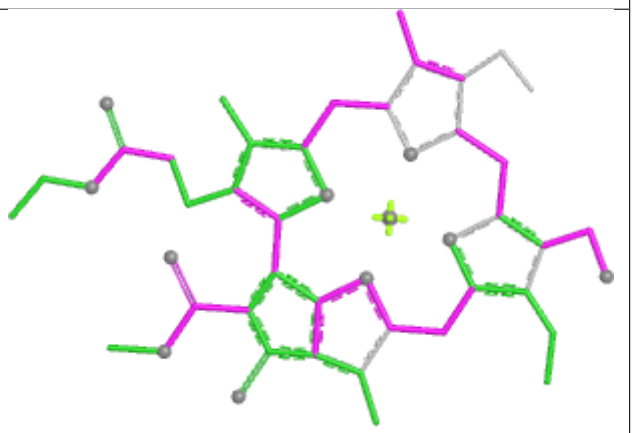


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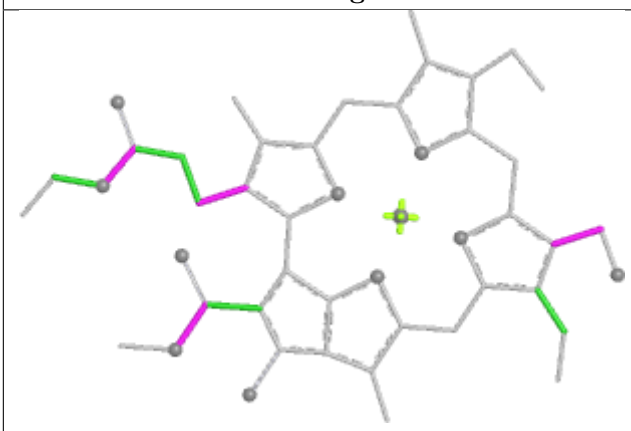
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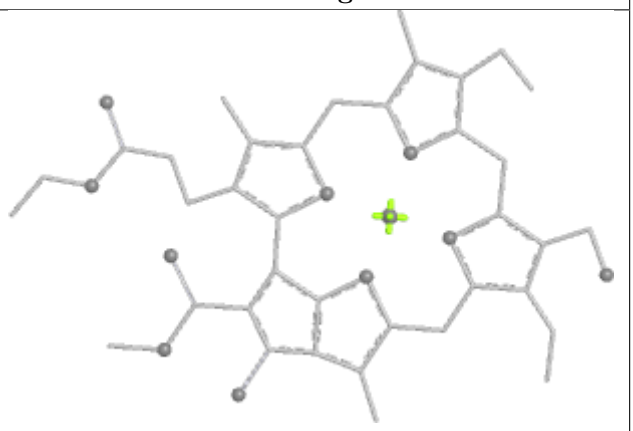
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Bond angles

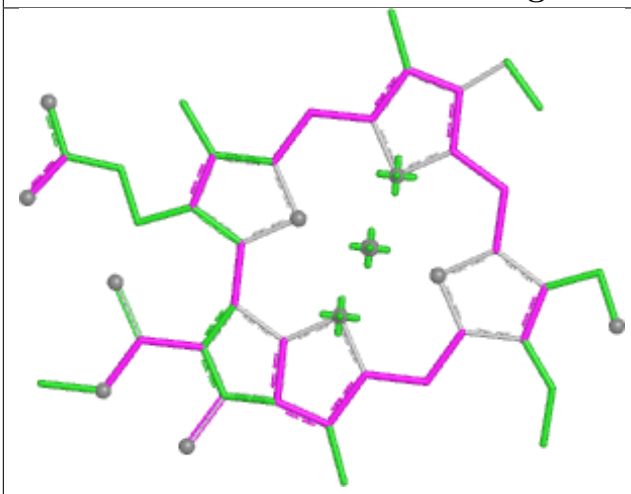


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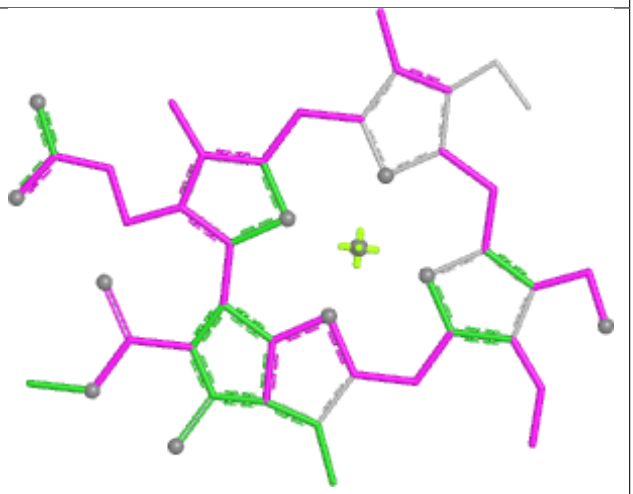


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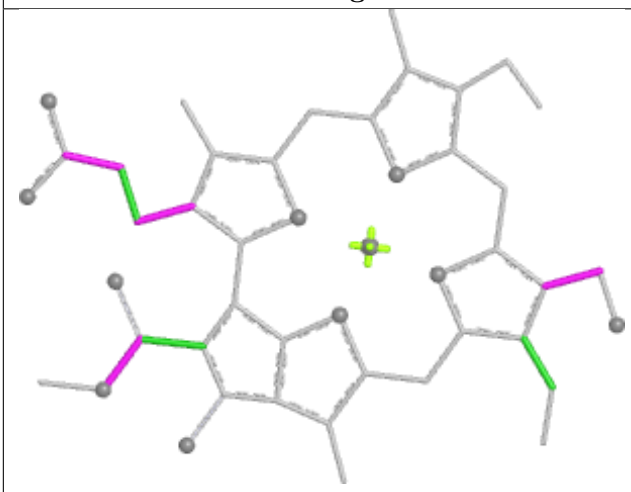
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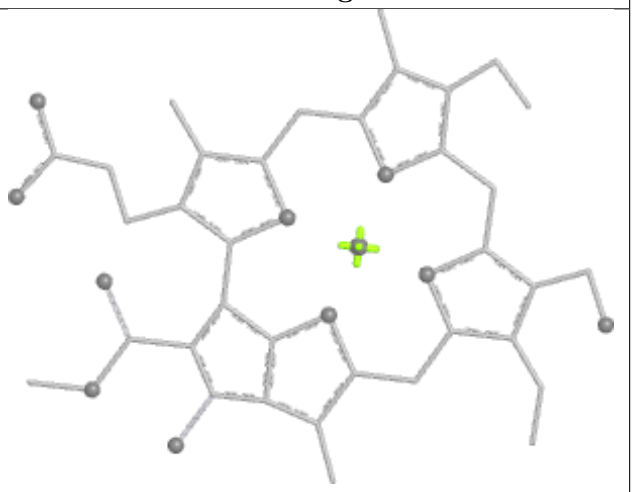
Bond lengths



Bond angles

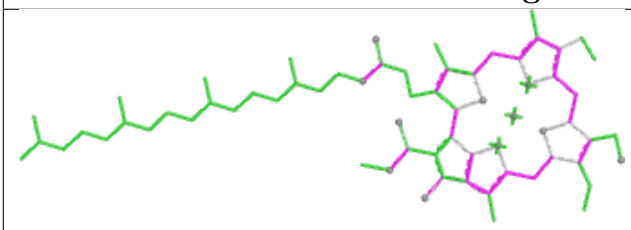


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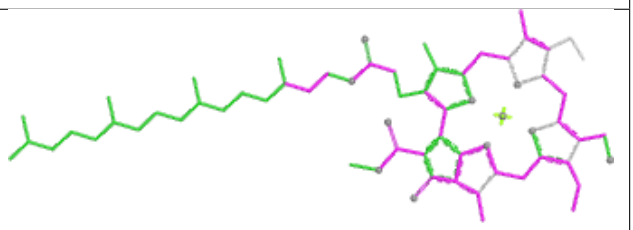


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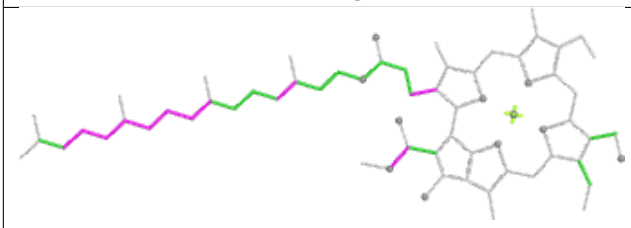
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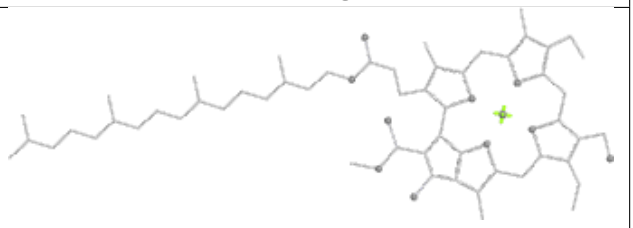
Bond lengths



Bond angles

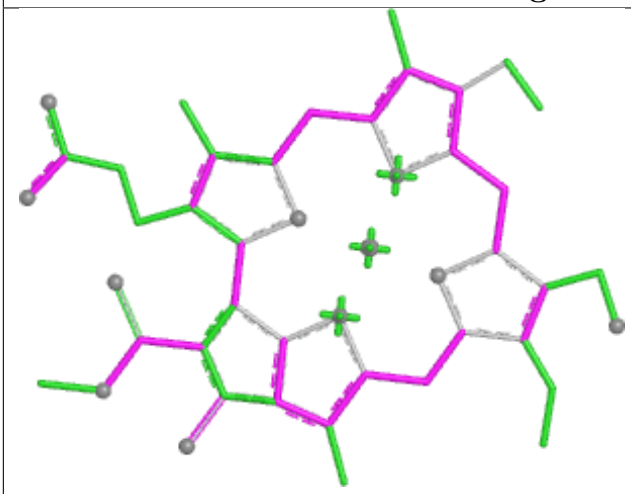


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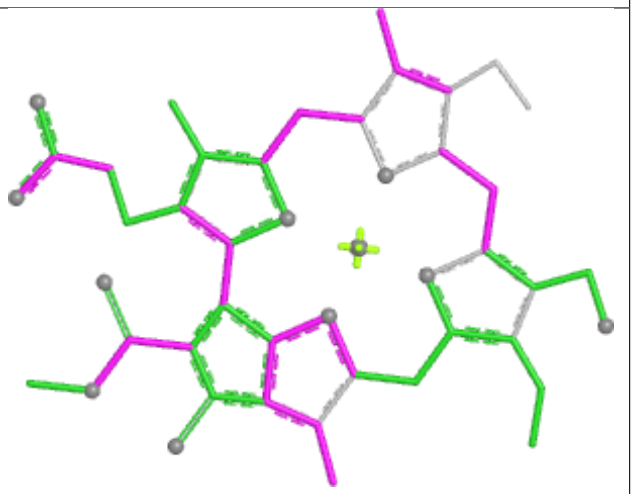


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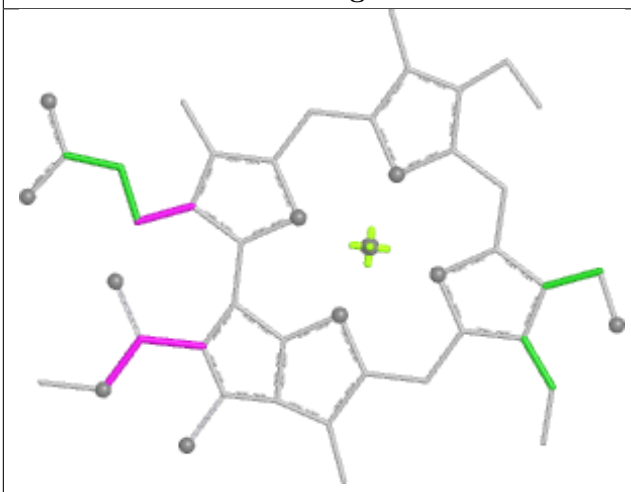
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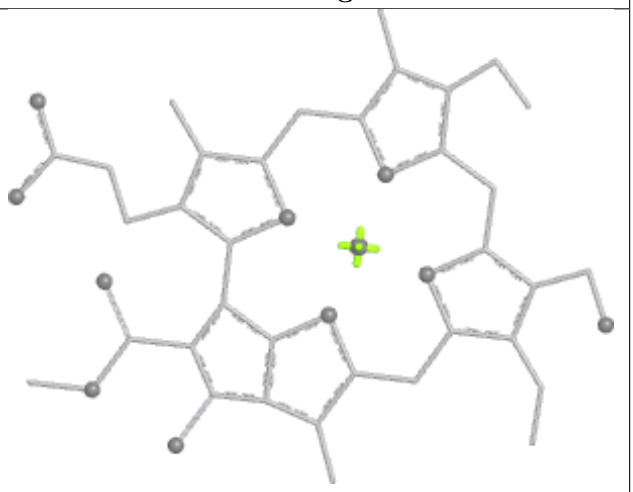
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Bond angles

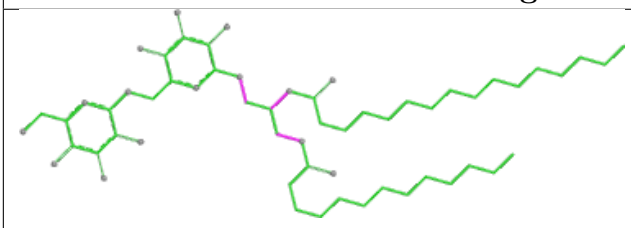


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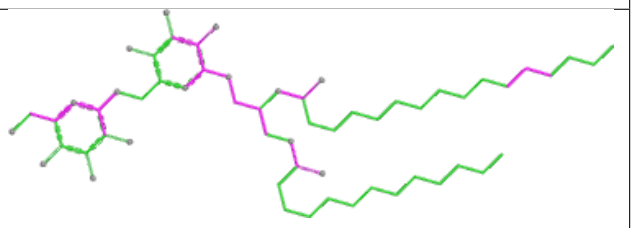


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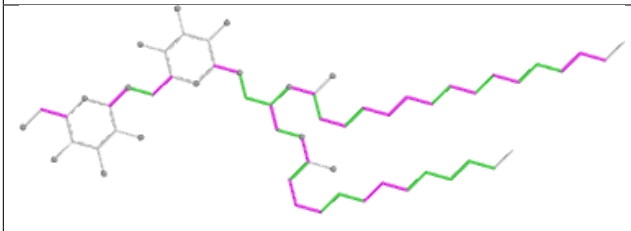
Ligand DGD B 626



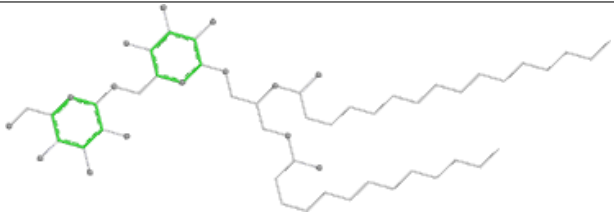
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Bond angles

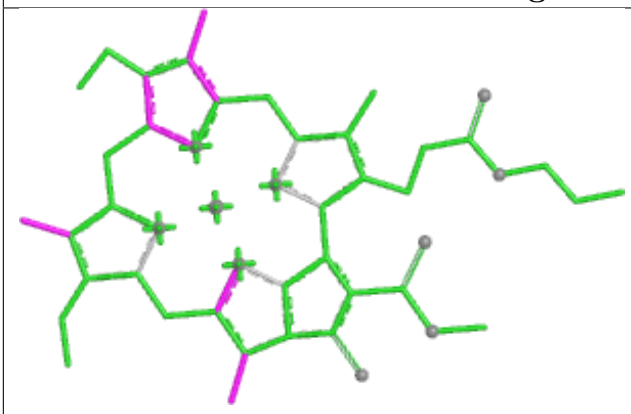


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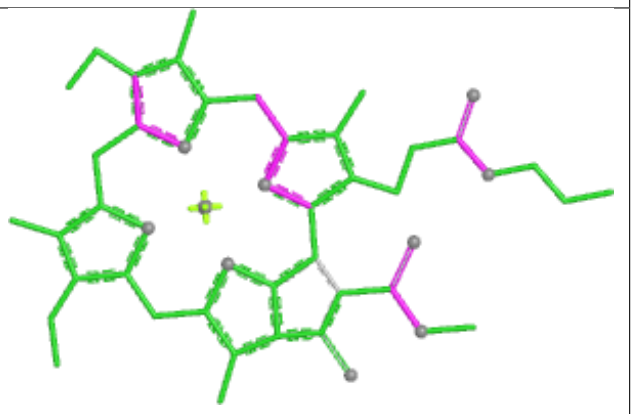


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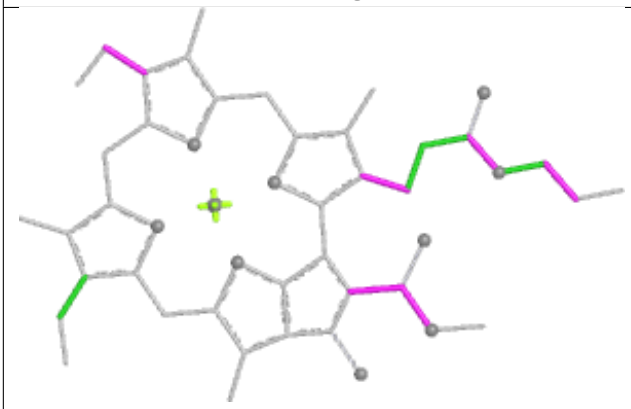
Ligand CLA 3 614



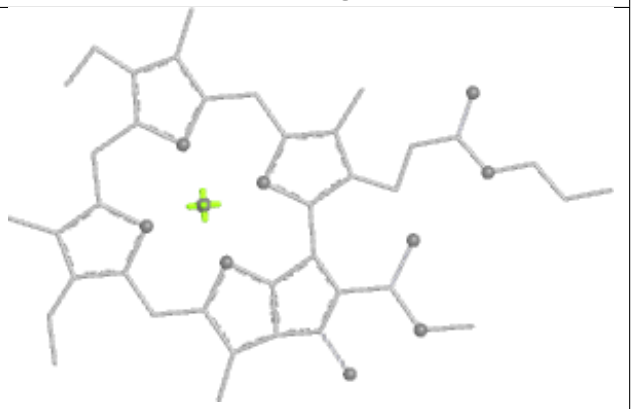
Bond lengths



Bond angles

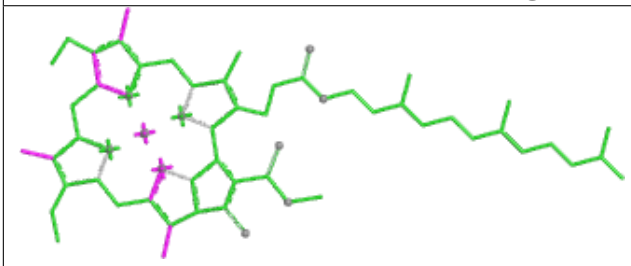


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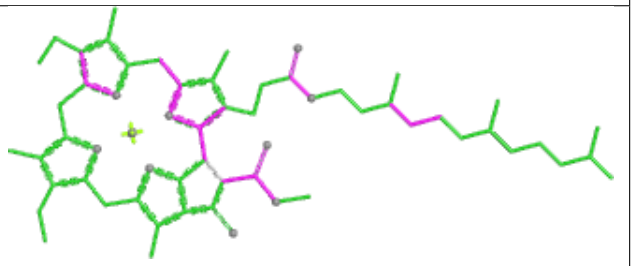


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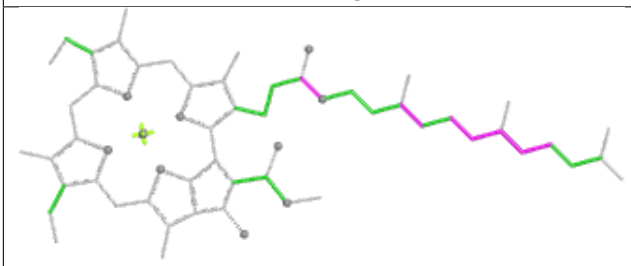
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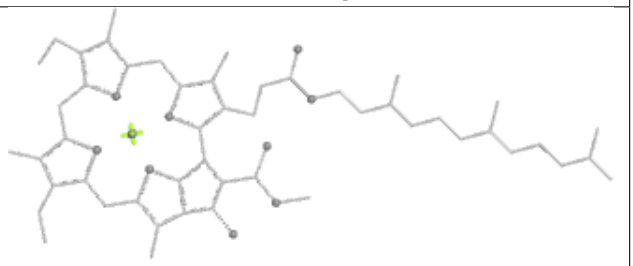
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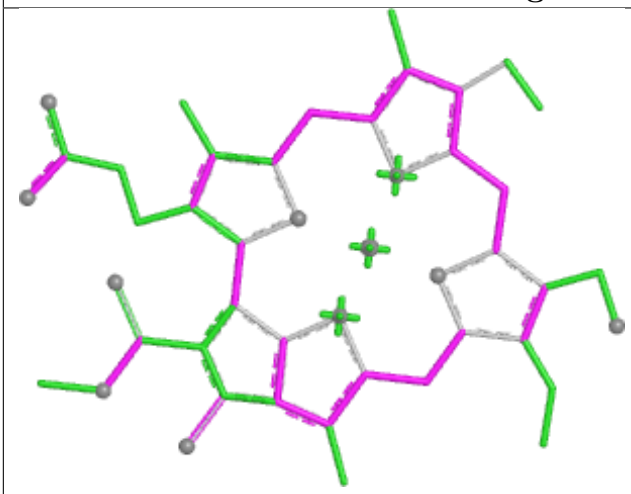


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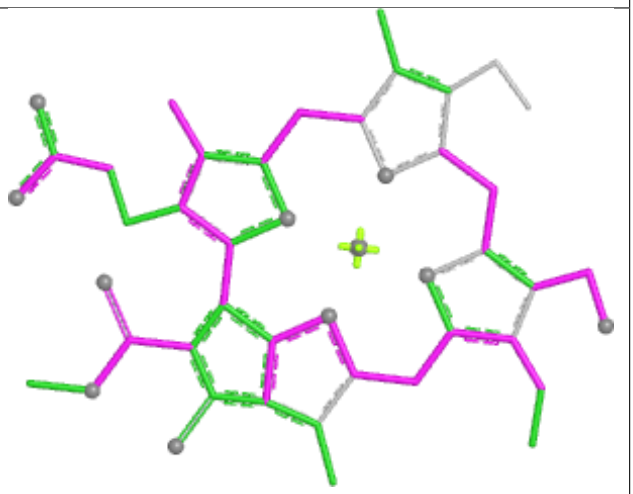


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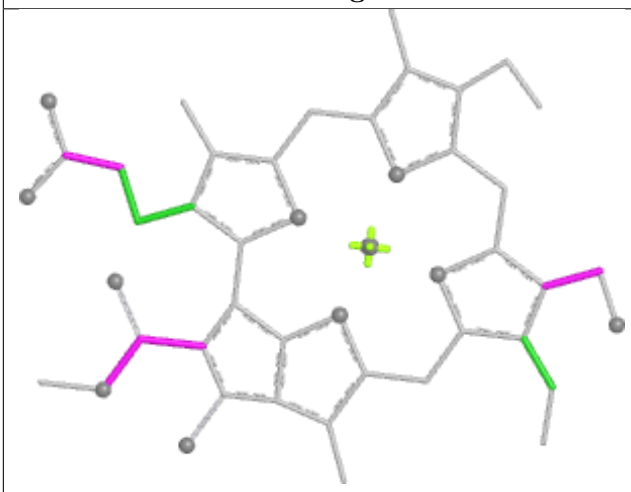
Ligand CHL S 606



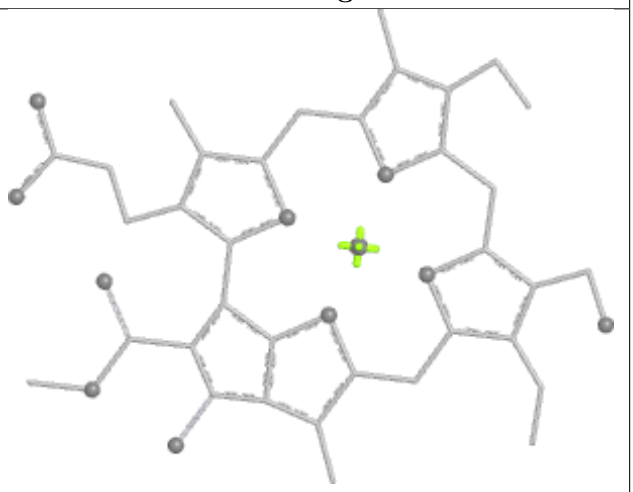
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Bond angles

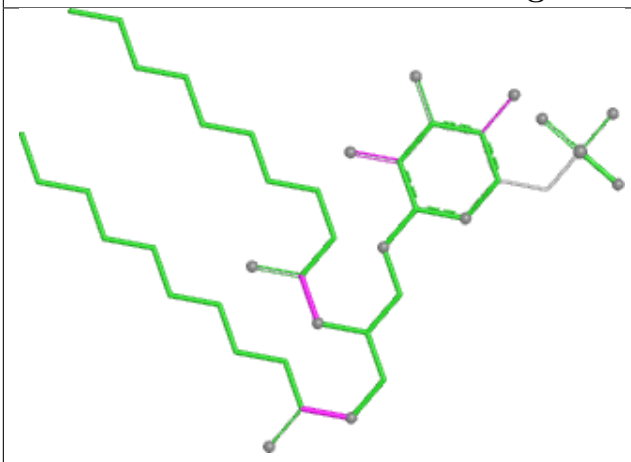


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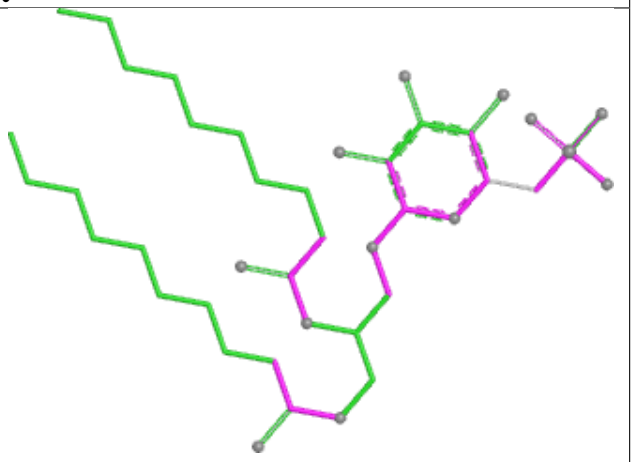


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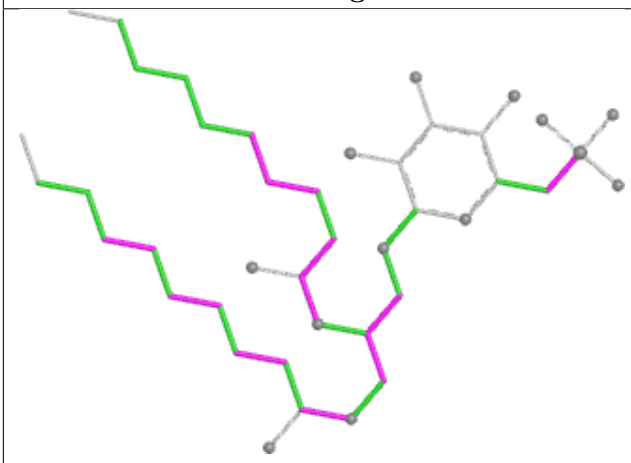
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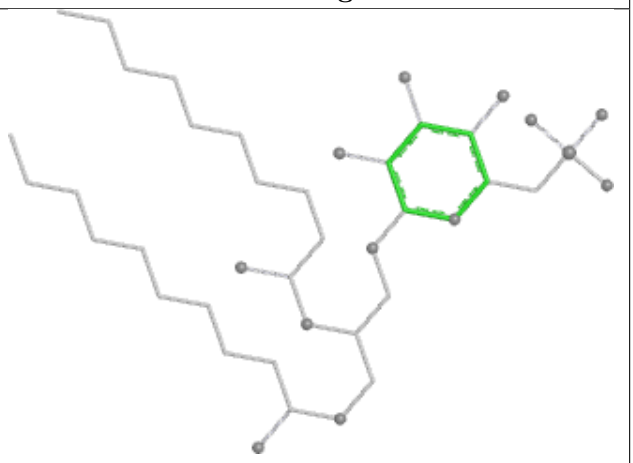
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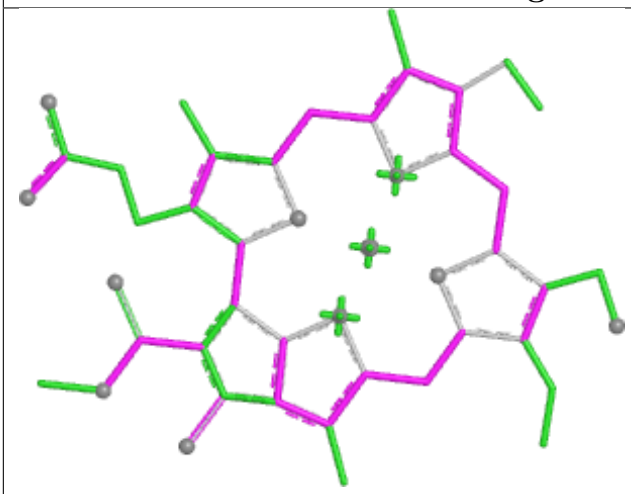


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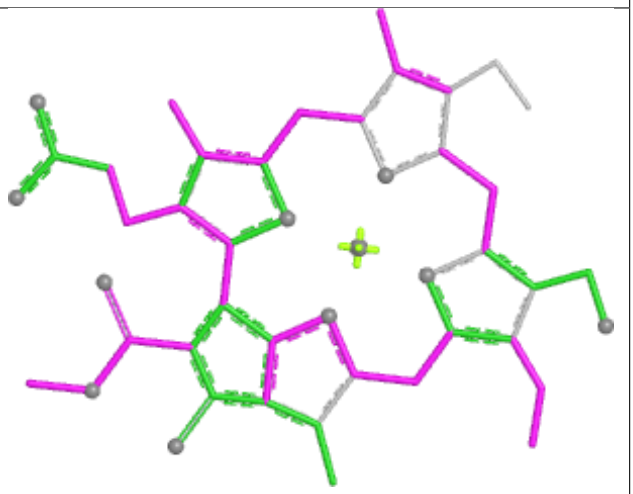


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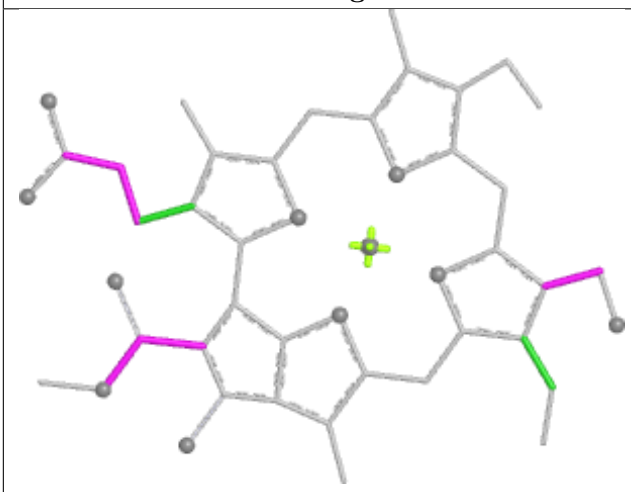
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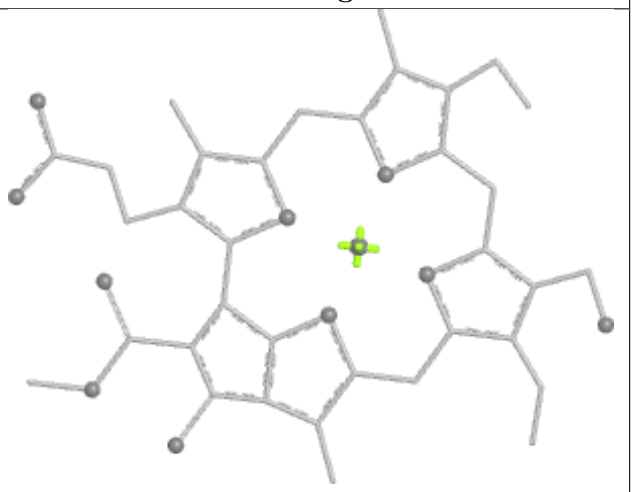
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Bond angles

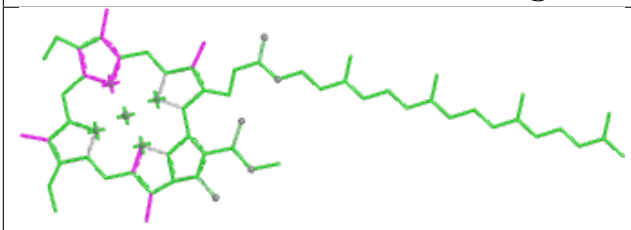


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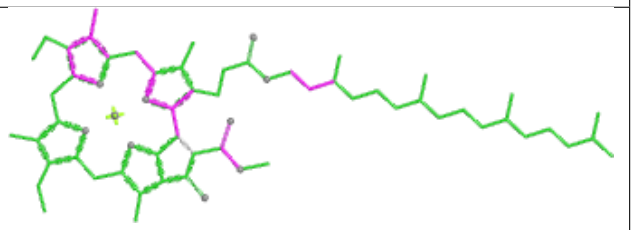


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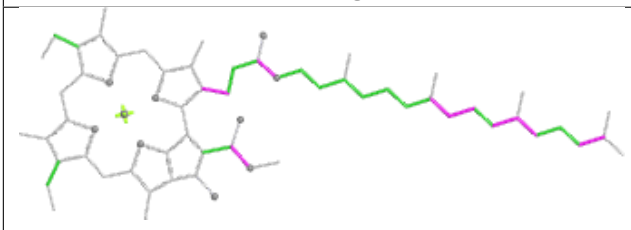
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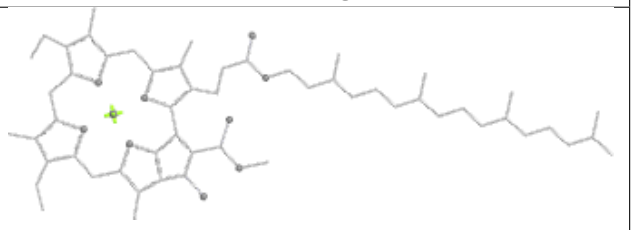
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Bond angles

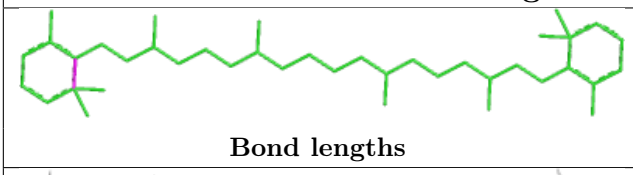


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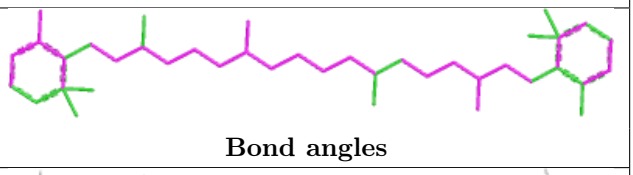


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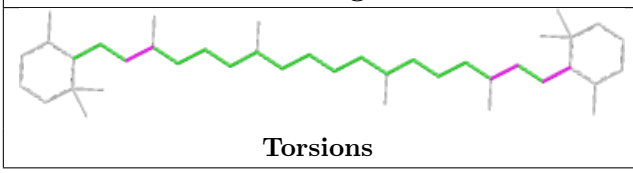
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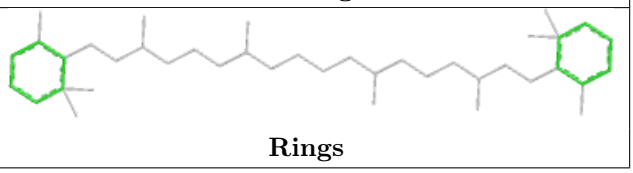
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Bond angles

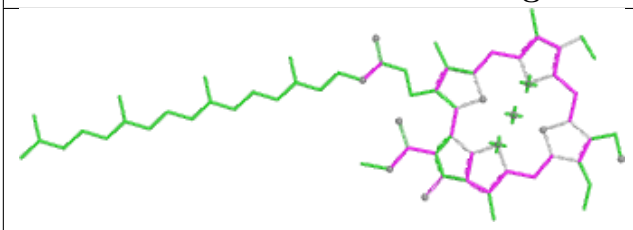


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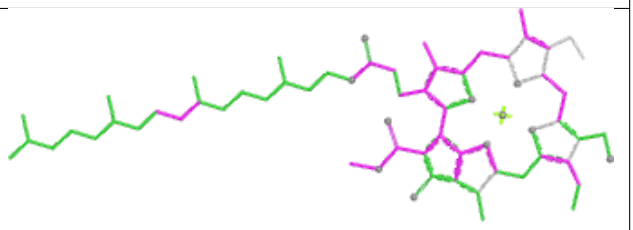


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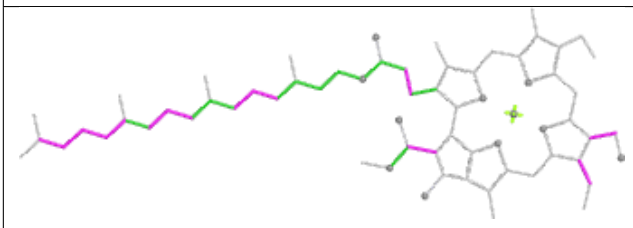
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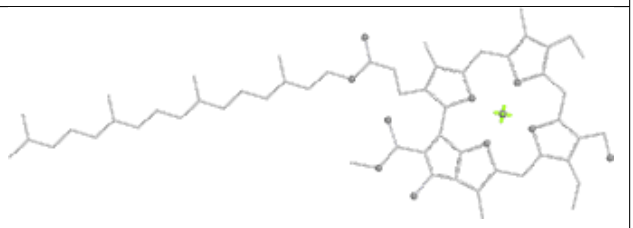
Bond lengths



Bond angles

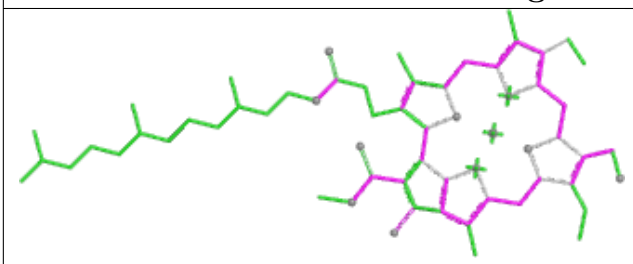


Torsions

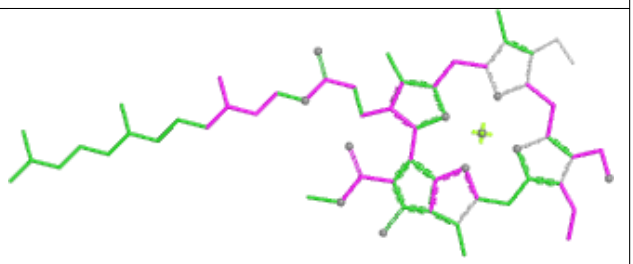


Rings

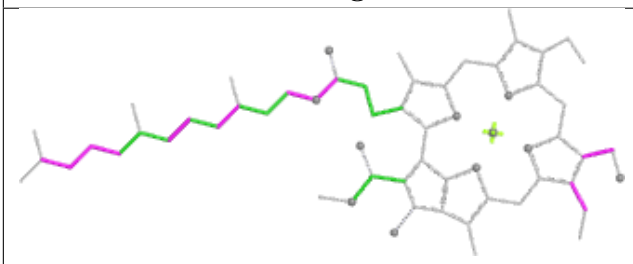
Ligand CHL 6 609



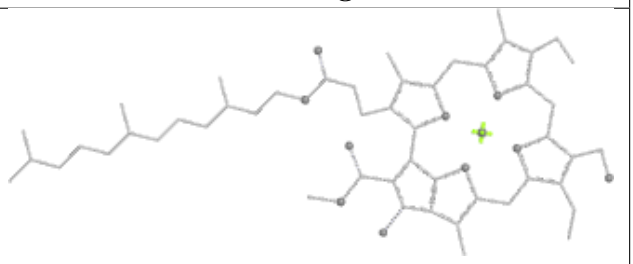
Bond lengths



Bond angles

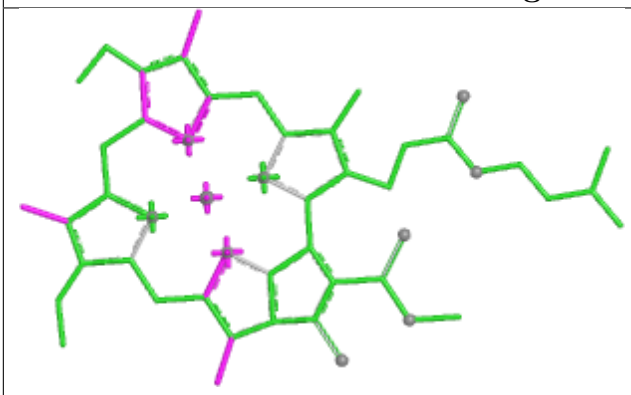


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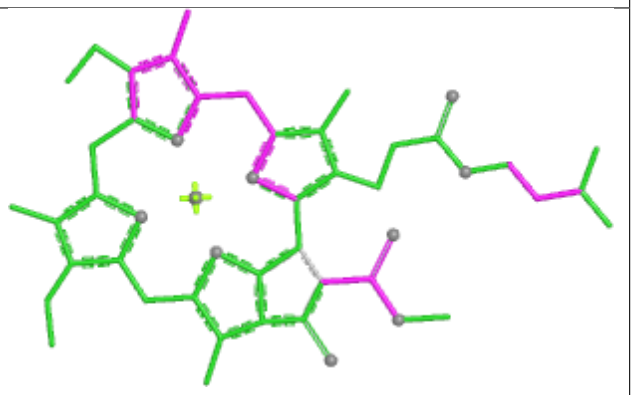


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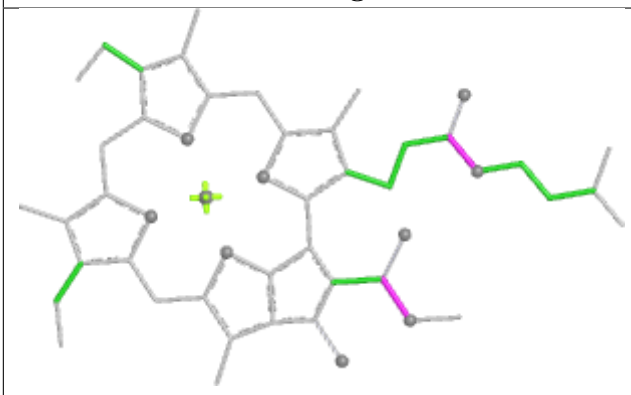
Ligand CLA N 604



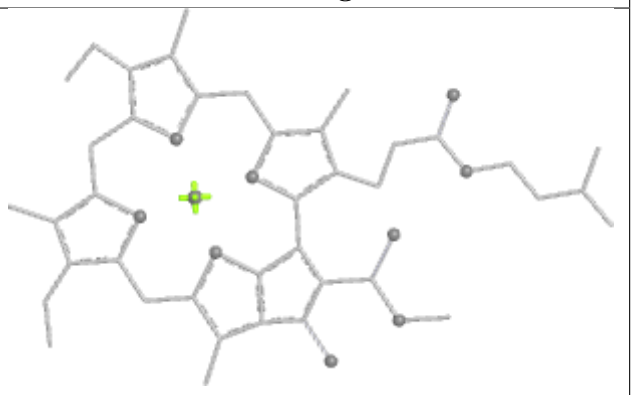
Bond lengths



Bond angles

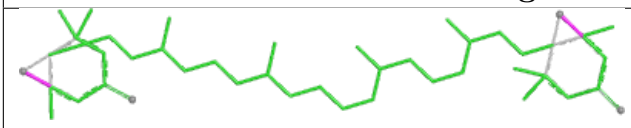


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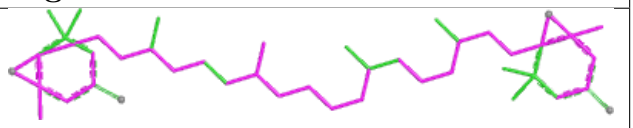


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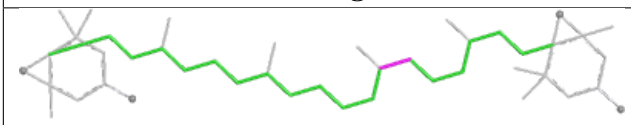
Ligand XAT g 1622



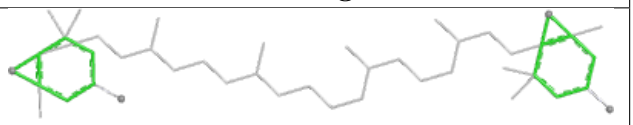
Bond lengths



Bond angles

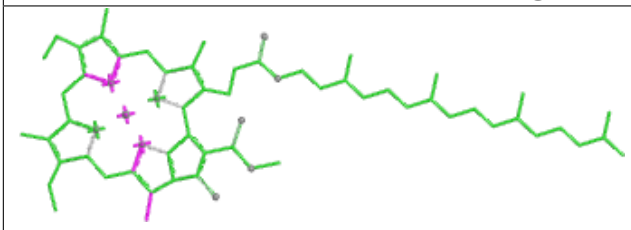


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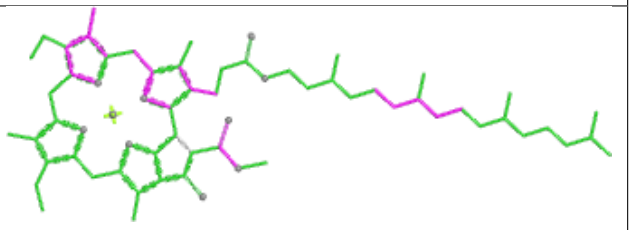


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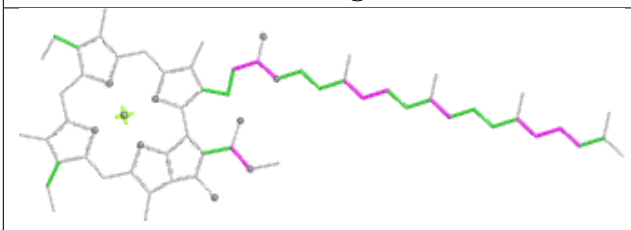
Ligand CLA c 510



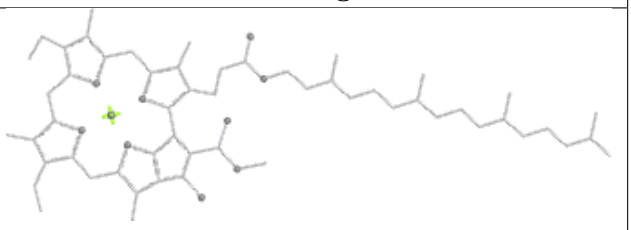
Bond lengths



Bond angles

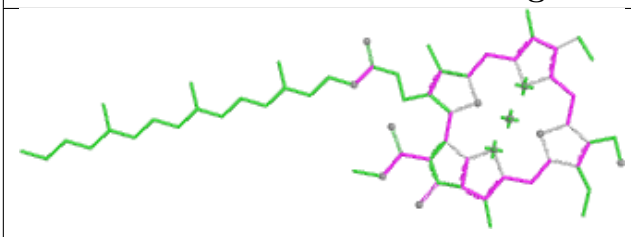


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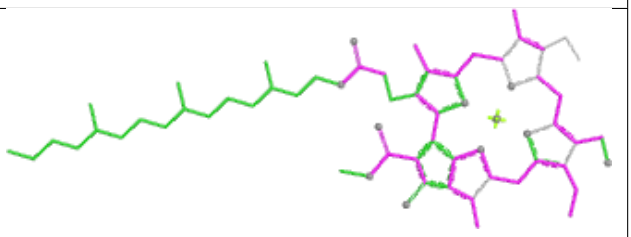


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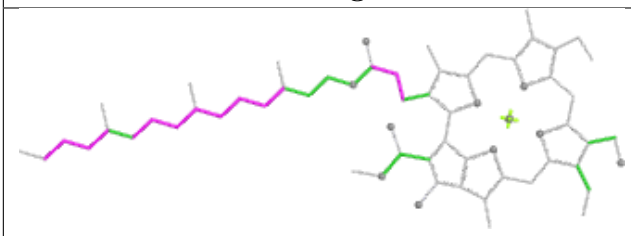
Ligand CHL 7 601



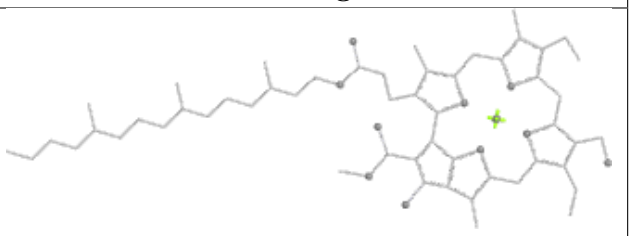
Bond lengths



Bond angles

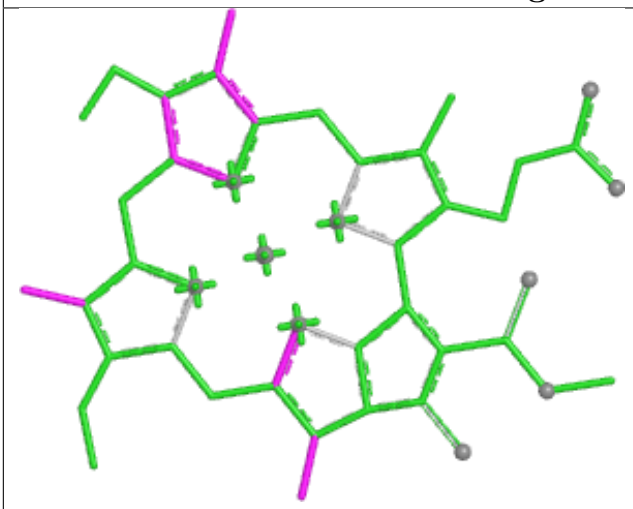


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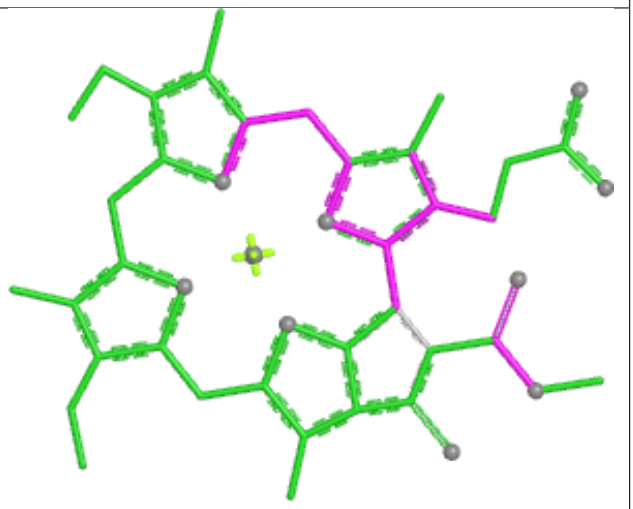


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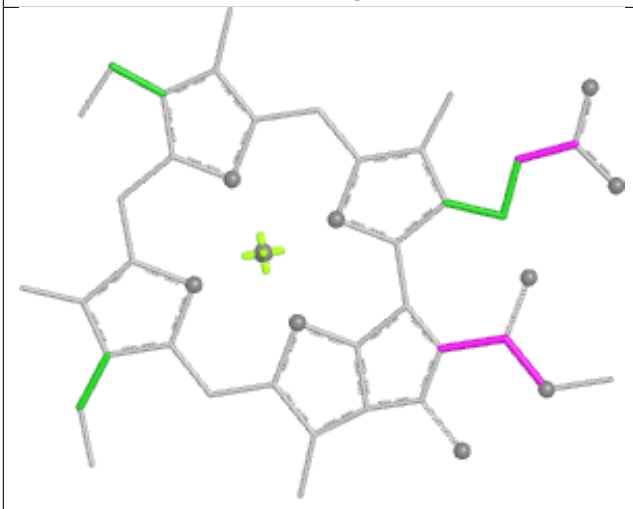
Ligand CLA 2 612



Bond lengths



Bond angles

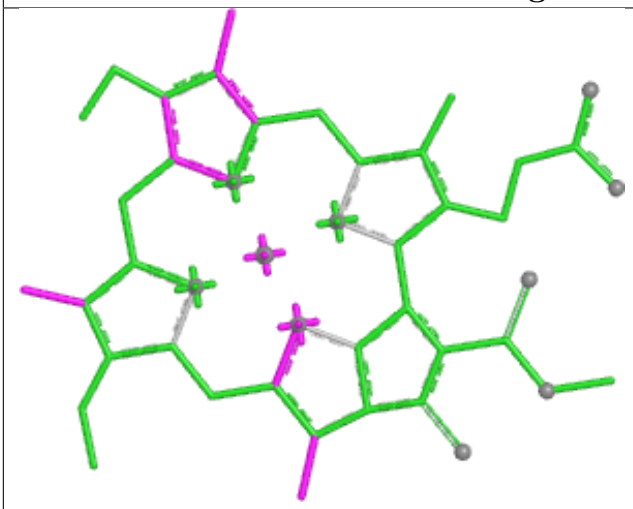


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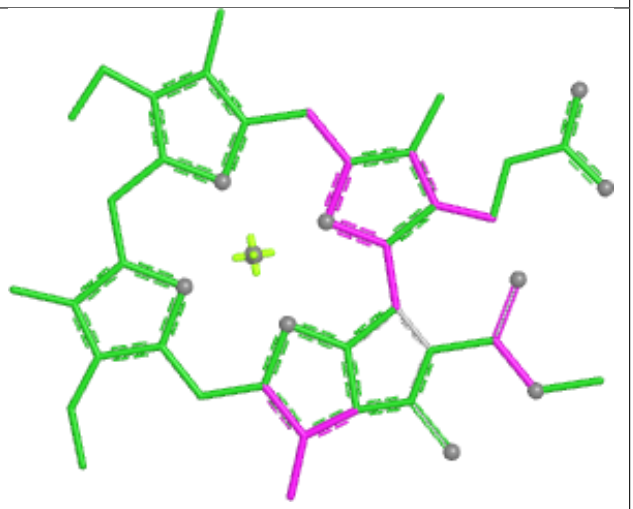


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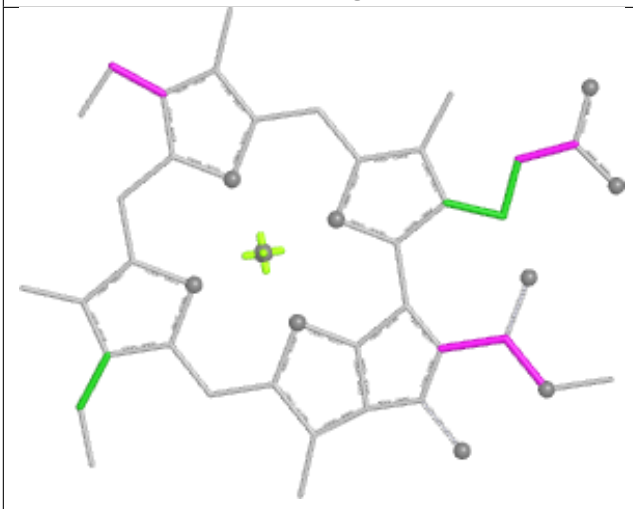
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Bond lengths



Bond angles

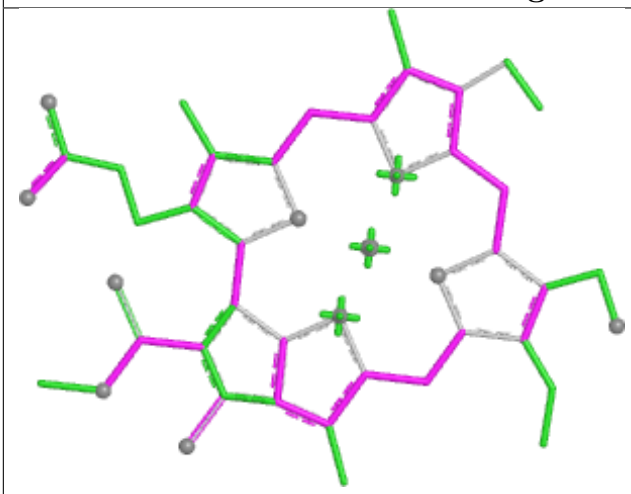


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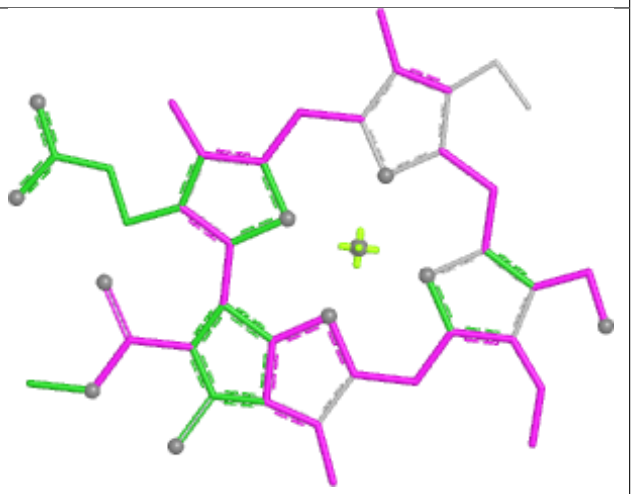


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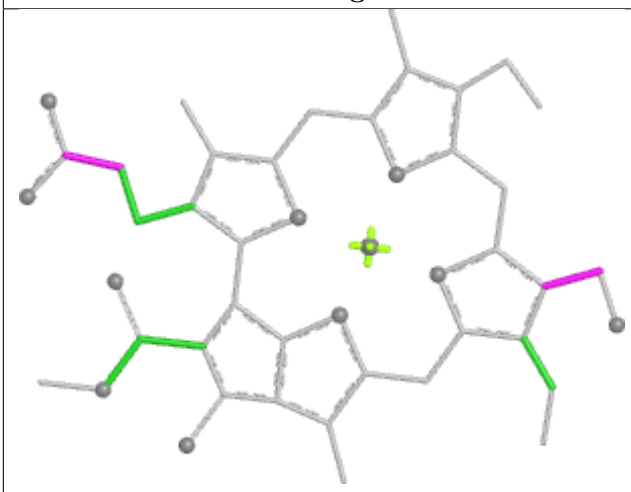
Ligand CHL 5 601



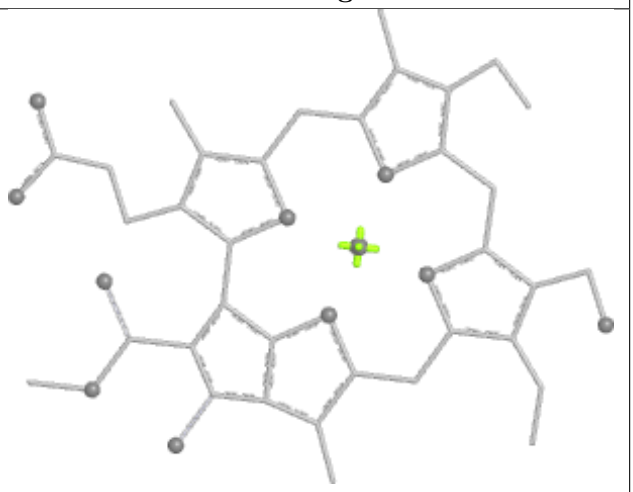
Bond lengths



Bond angles

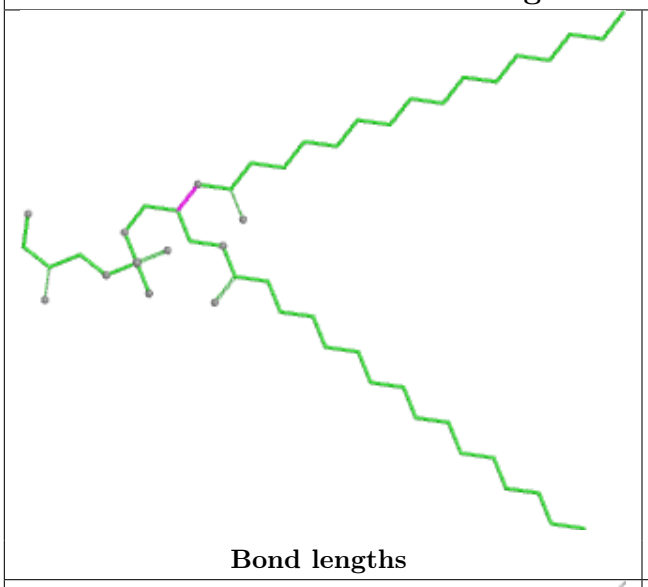


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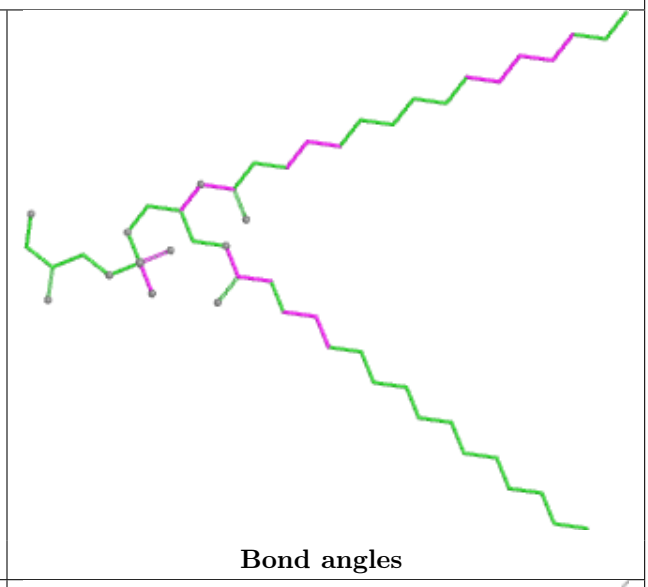


Rings

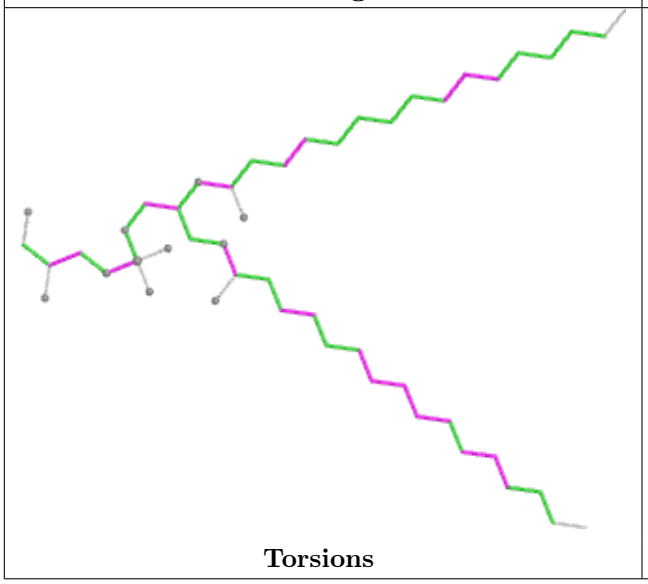
Ligand LHG C 522



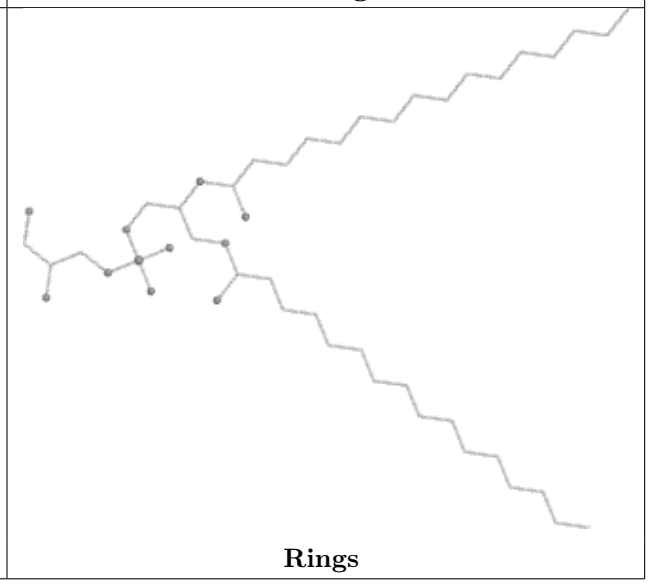
Bond lengths



Bond angles

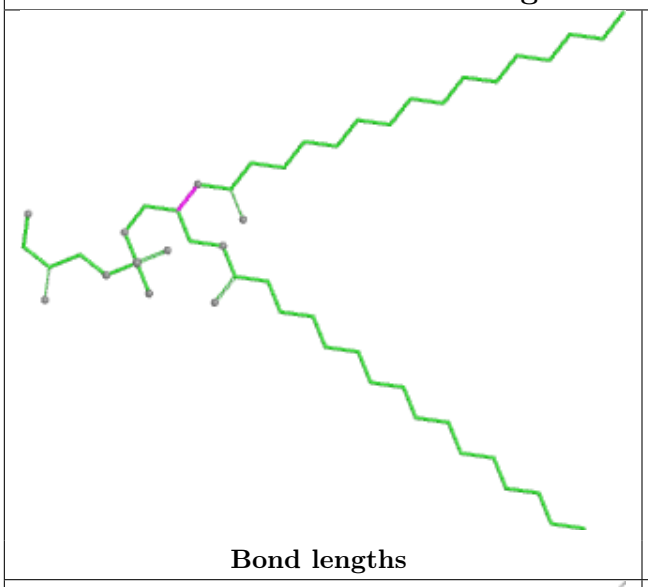


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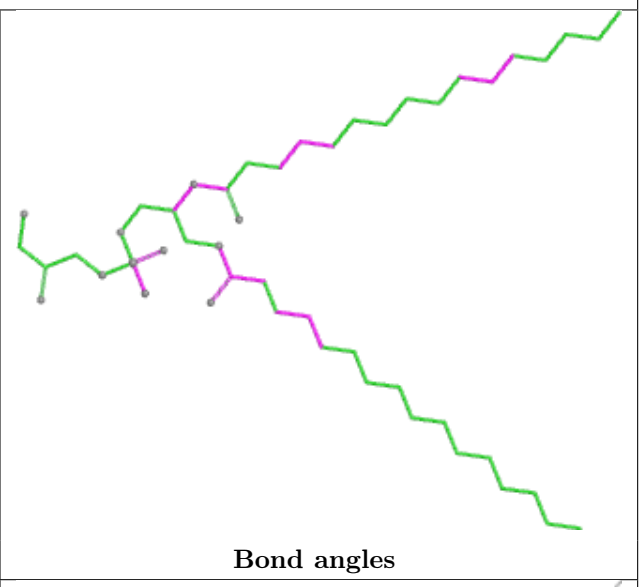


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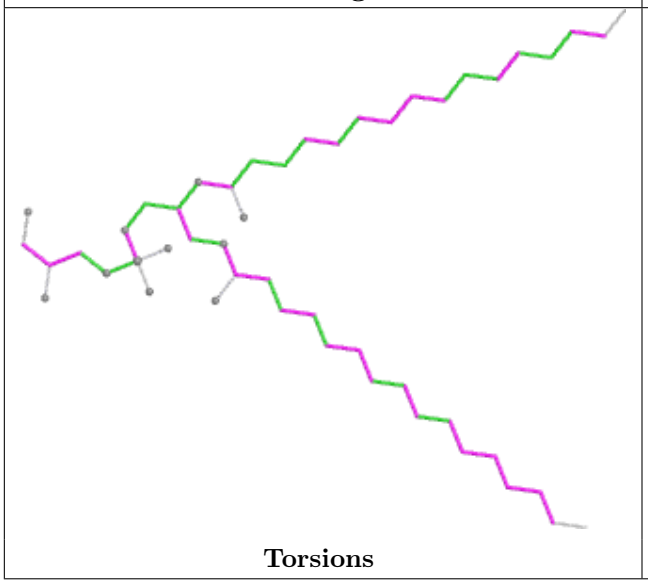
Ligand LHG s 2630



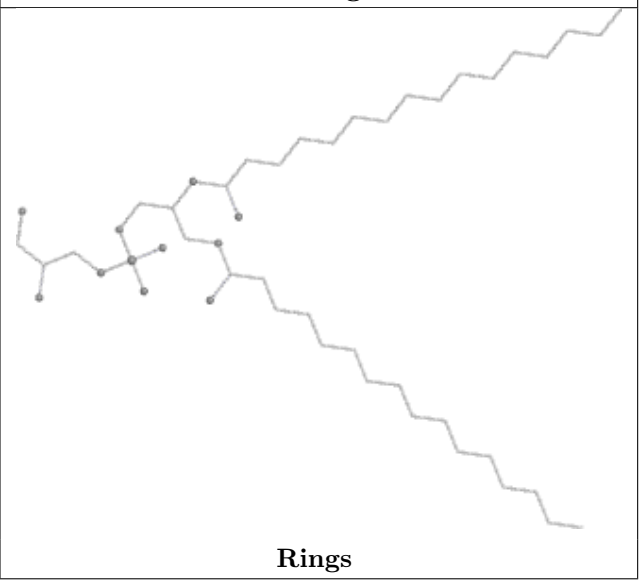
Bond lengths



Bond angles

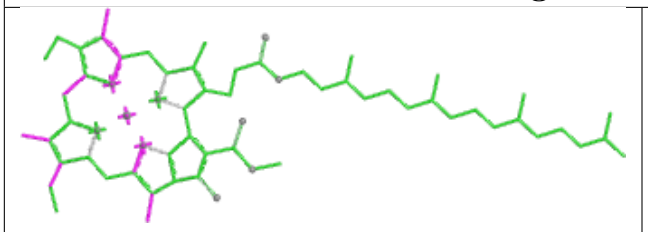


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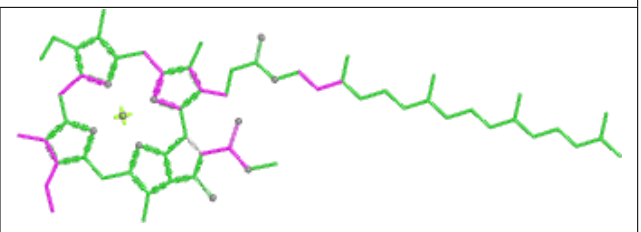


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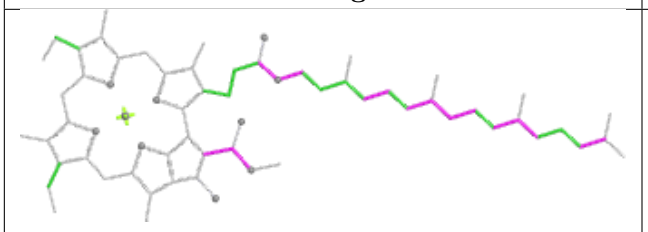
Ligand CLA c 502



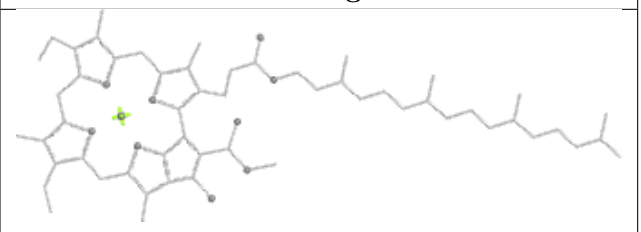
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Bond angles

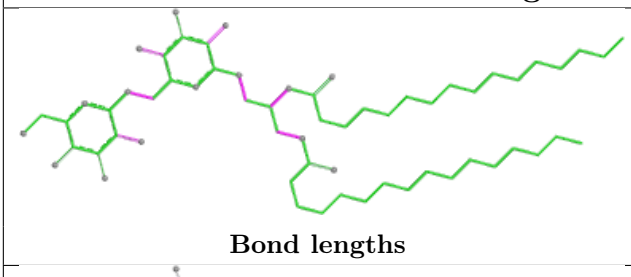


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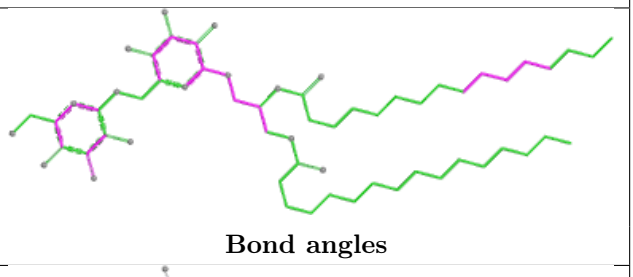


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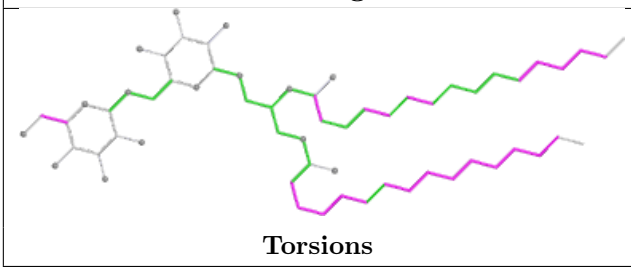
Ligand DGD h 102



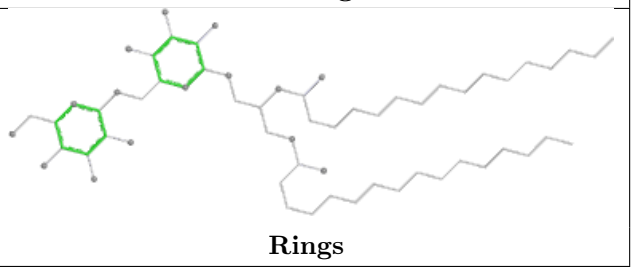
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Bond angles

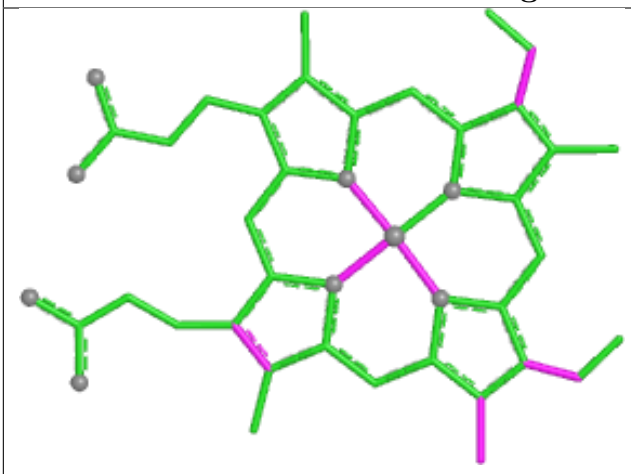


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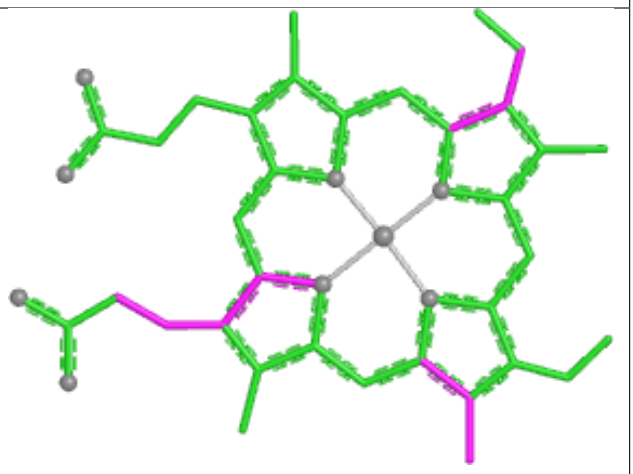


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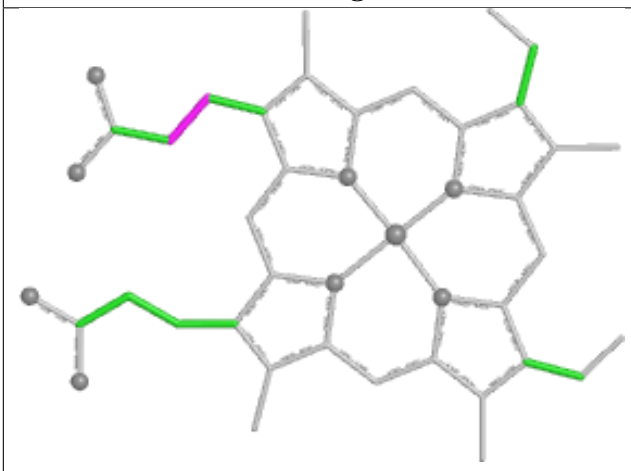
Ligand HEM F 101



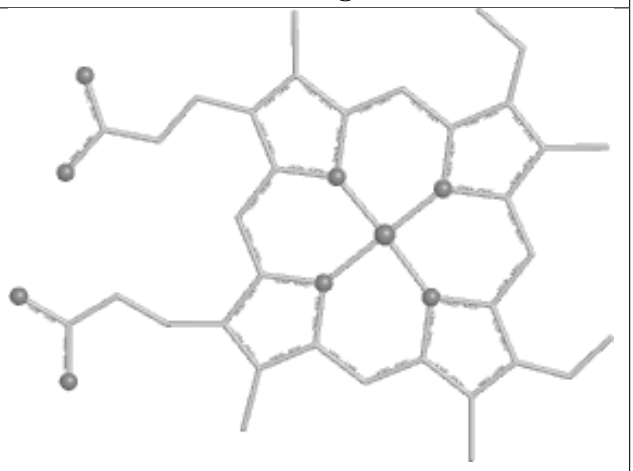
Bond lengths



Bond angles

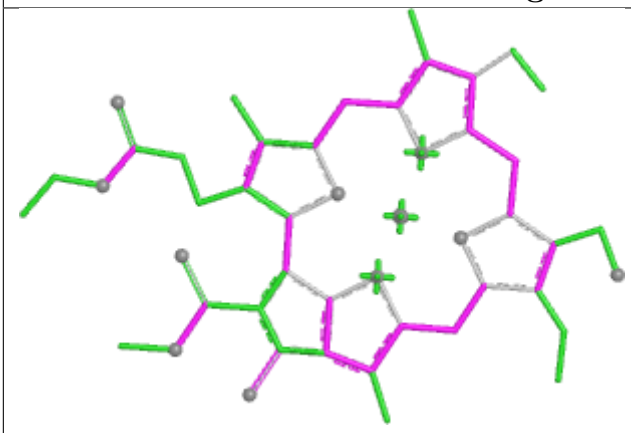


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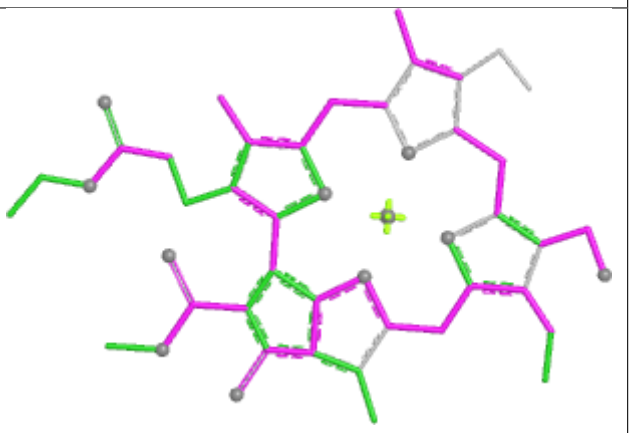


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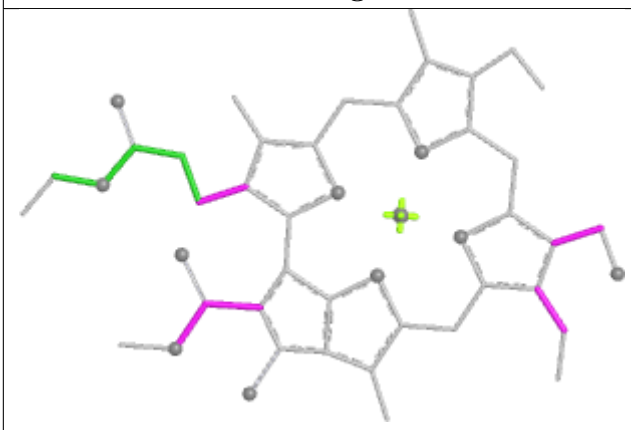
Ligand CHL n 605



Bond lengths



Bond angles

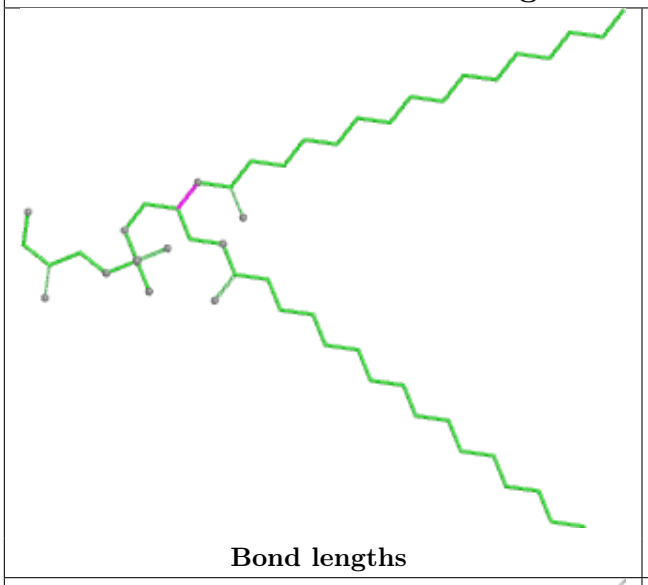


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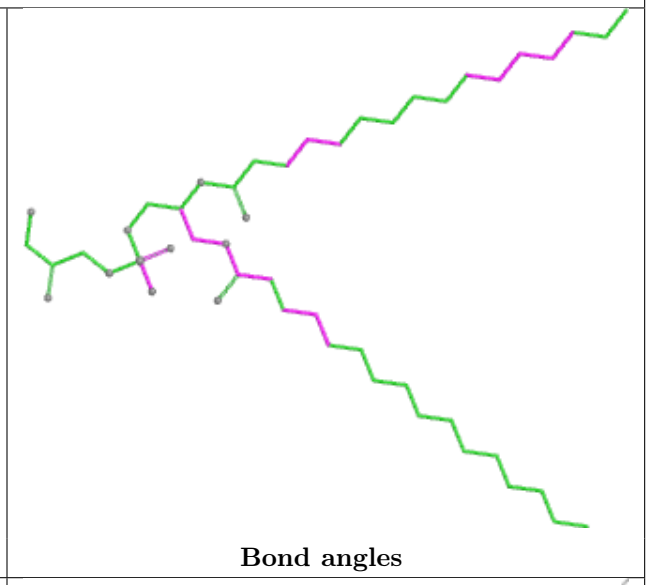


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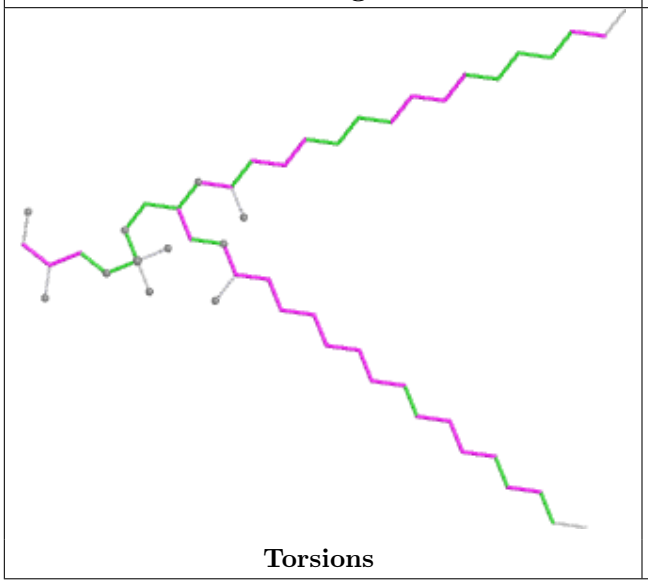
Ligand LHG c 2630



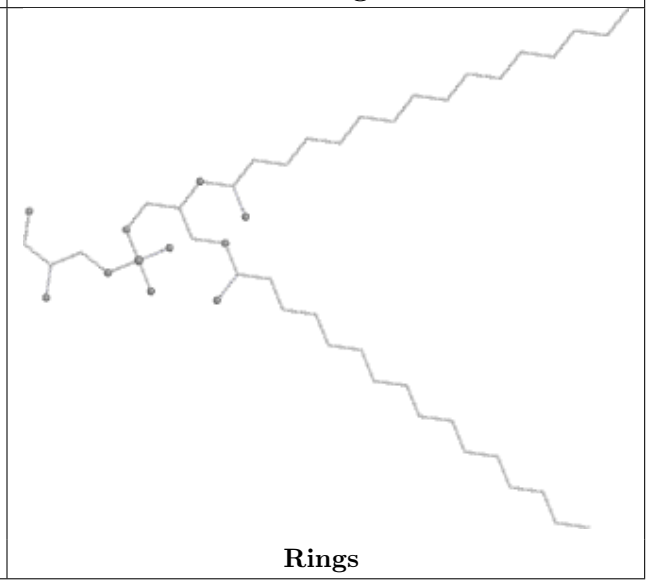
Bond lengths



Bond angles

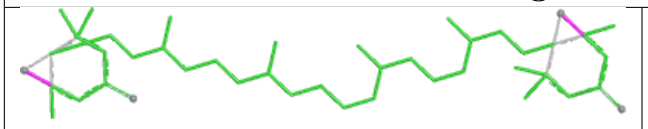


Torsions

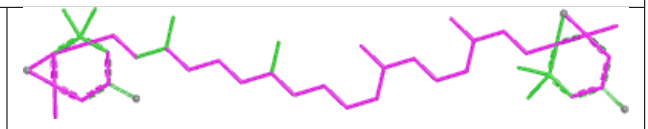


Rings

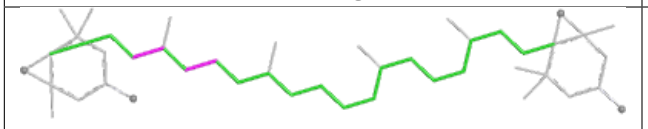
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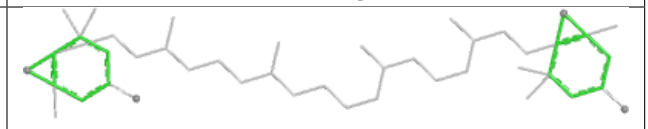
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Bond angles

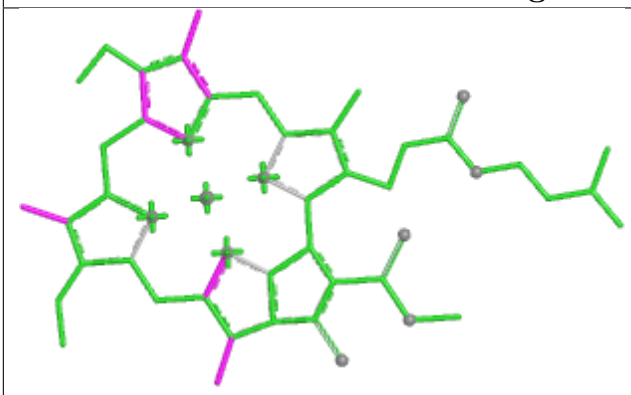


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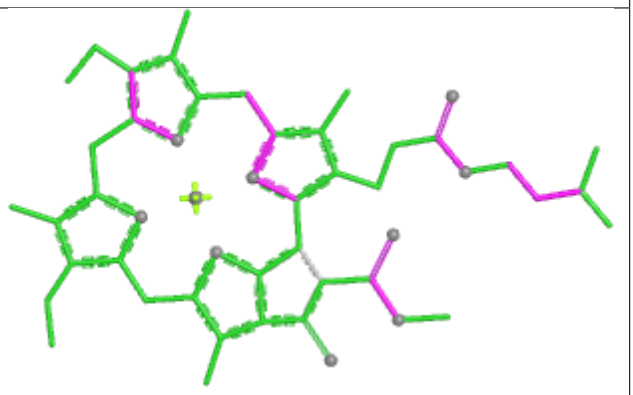


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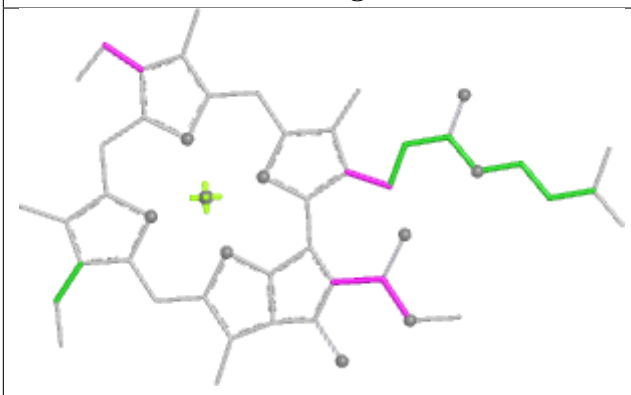
Ligand CLA 2 610



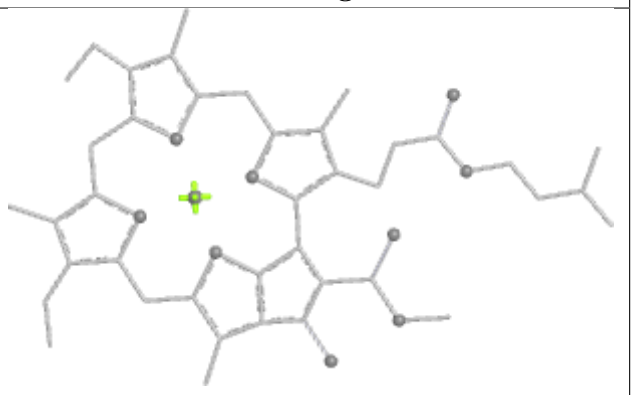
Bond lengths



Bond angles

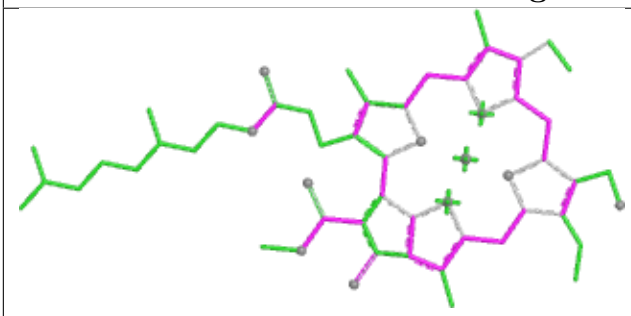


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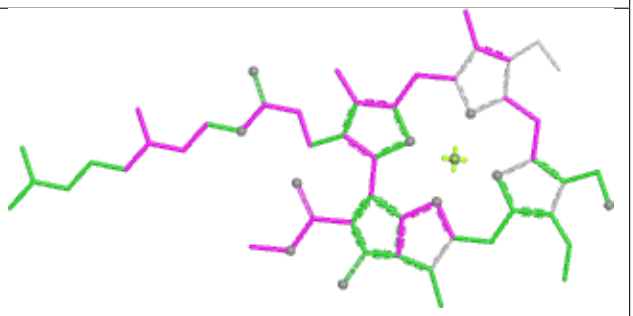


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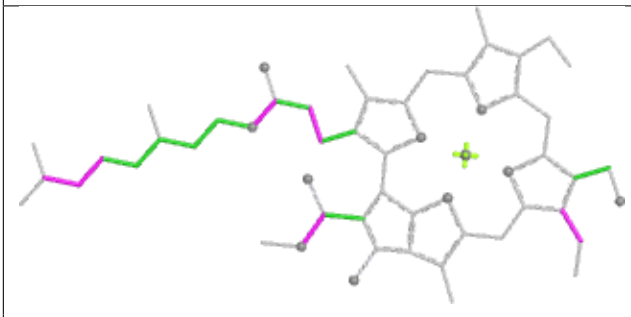
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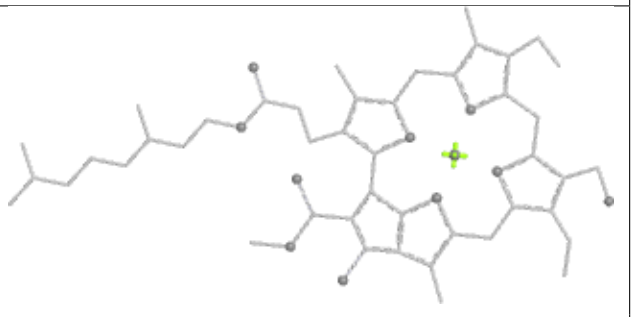
Bond lengths



Bond angles

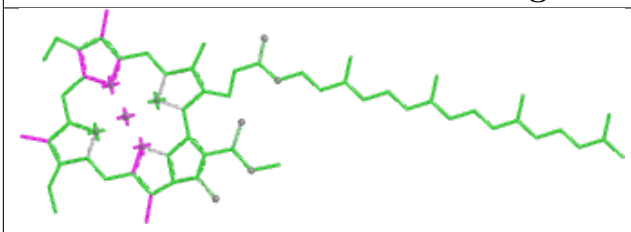


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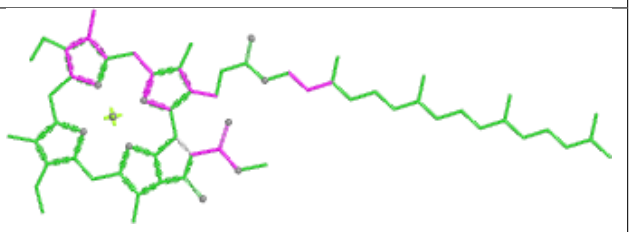


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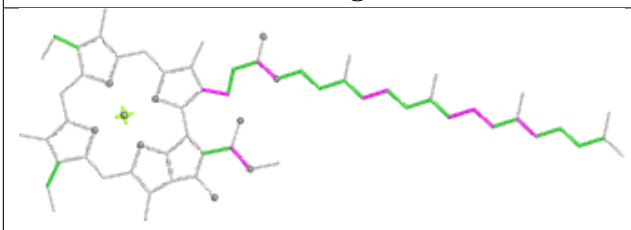
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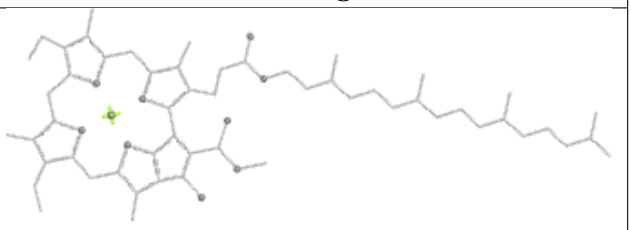
Bond lengths



Bond angles

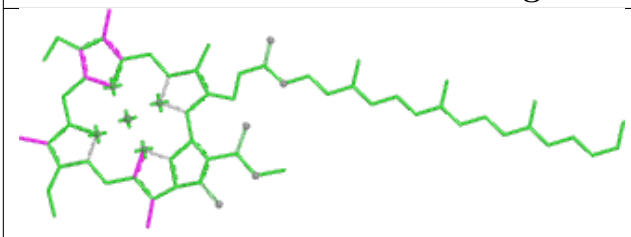


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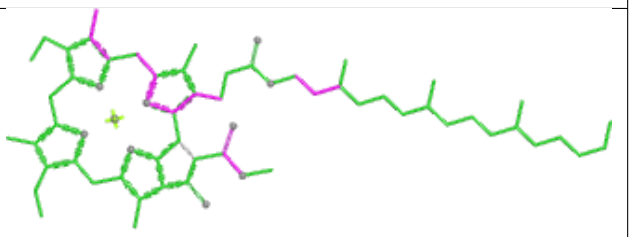


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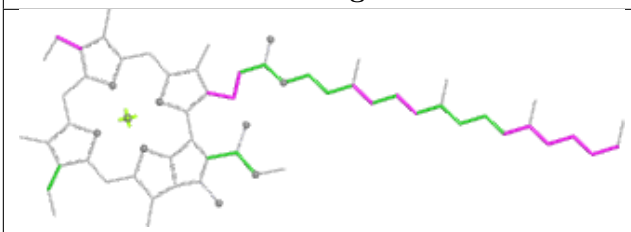
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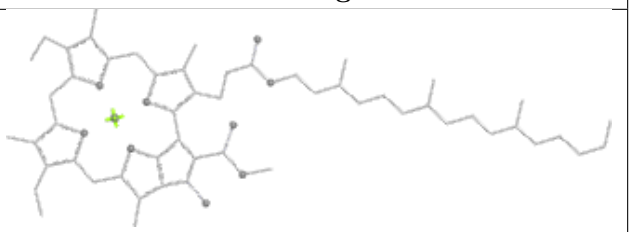
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Bond angles

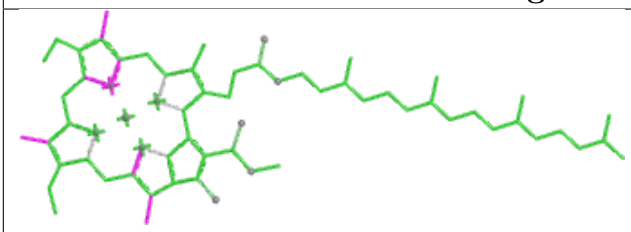


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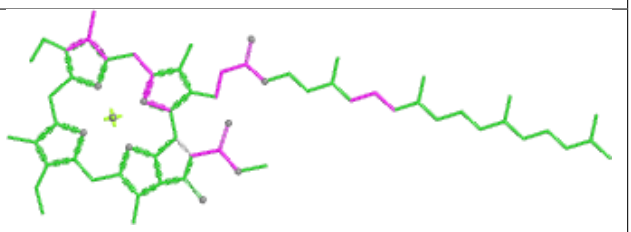


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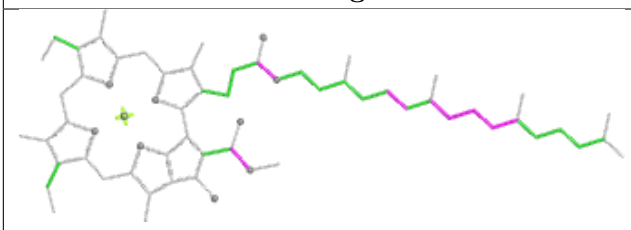
Ligand CLA d 403



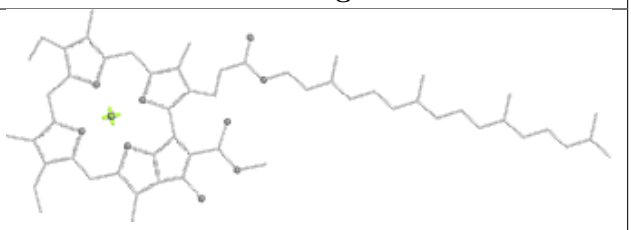
Bond lengths



Bond angles

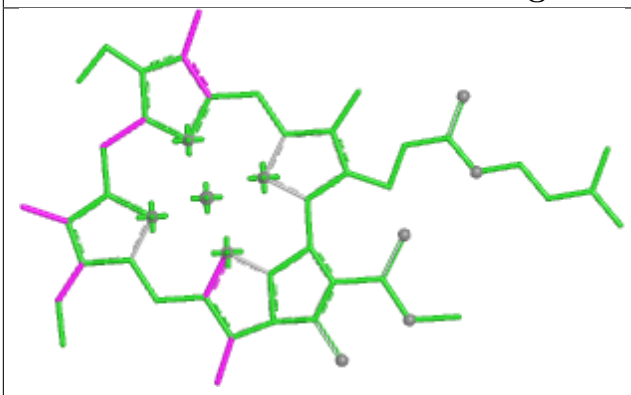


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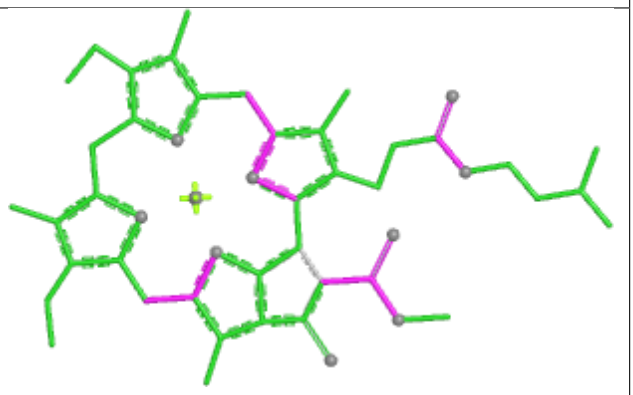


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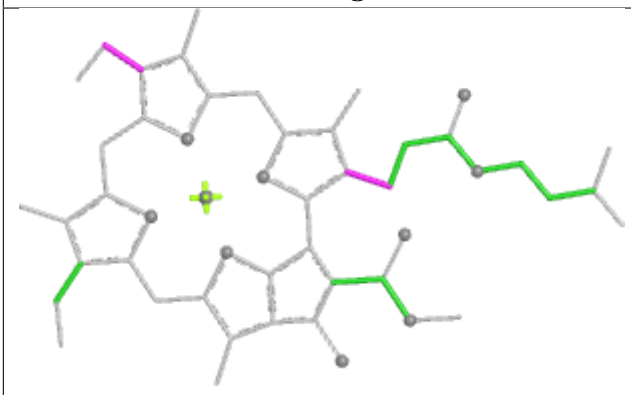
Ligand CLA a 407



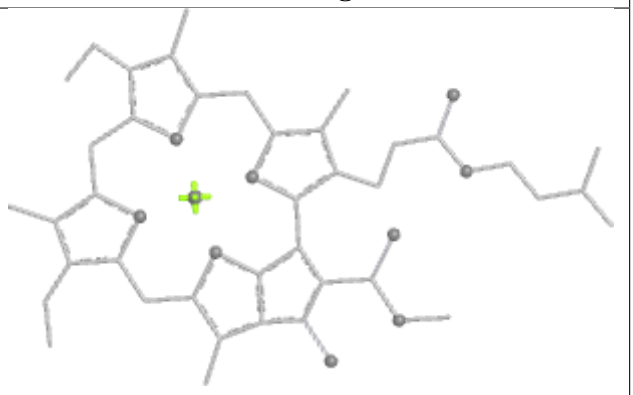
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Bond angles

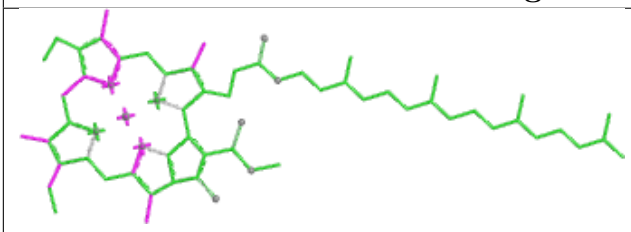


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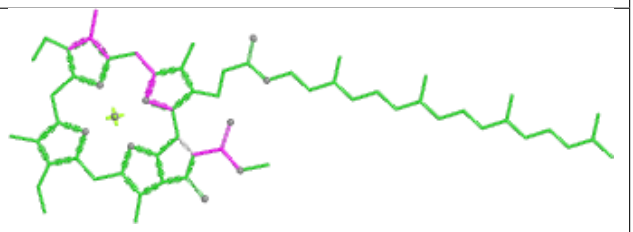


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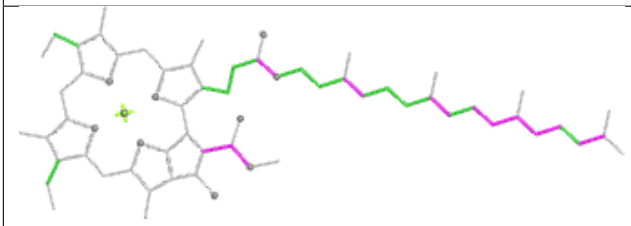
Ligand CLA C 504



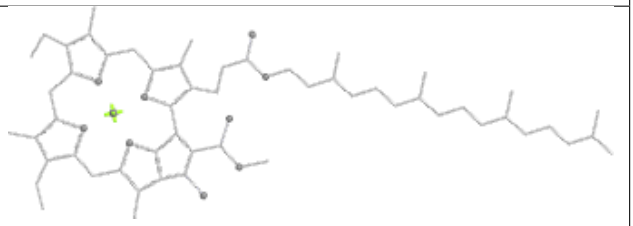
Bond lengths



Bond angles

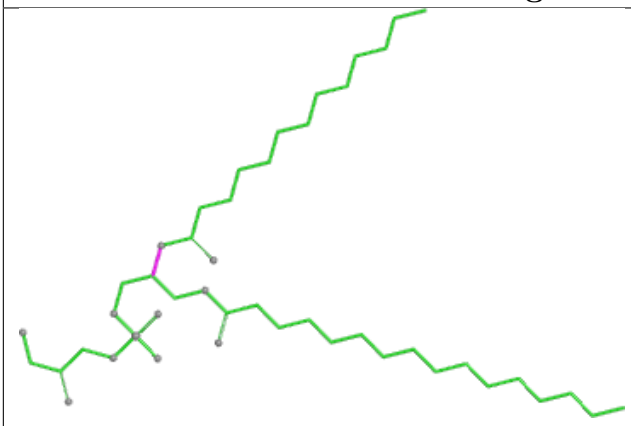


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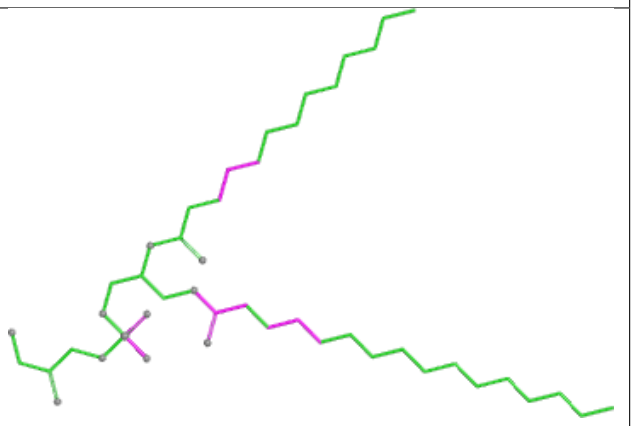


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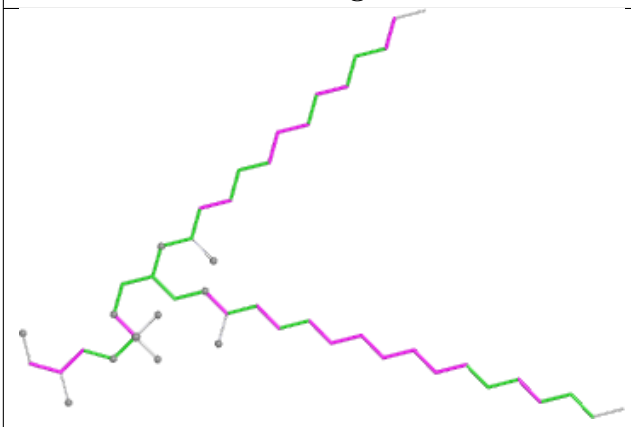
Ligand LHG d 408



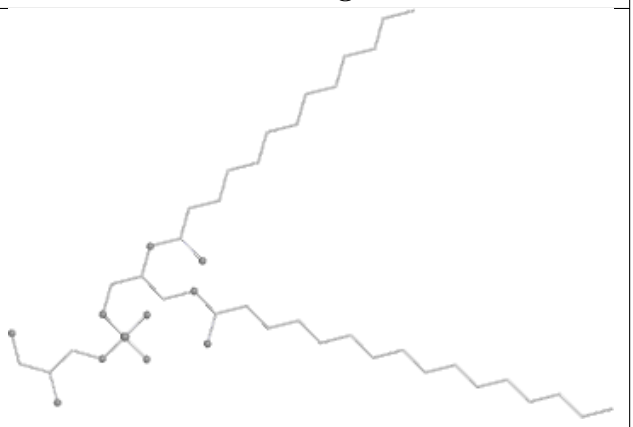
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Bond angles

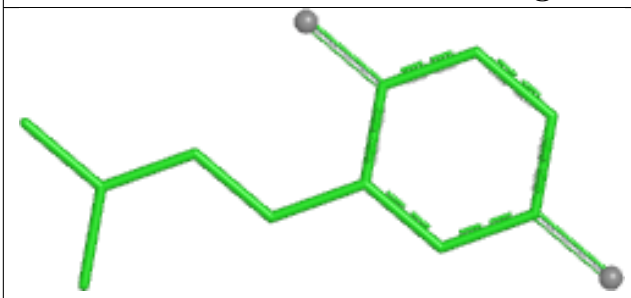


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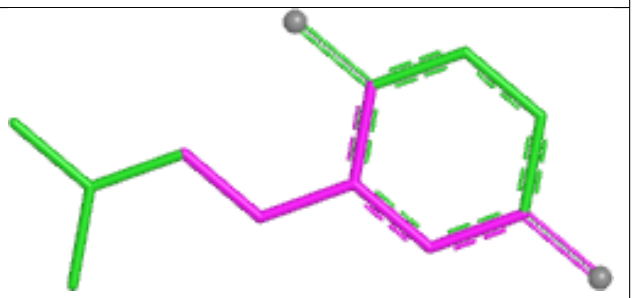


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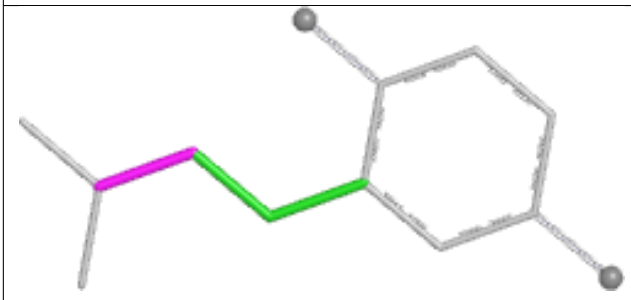
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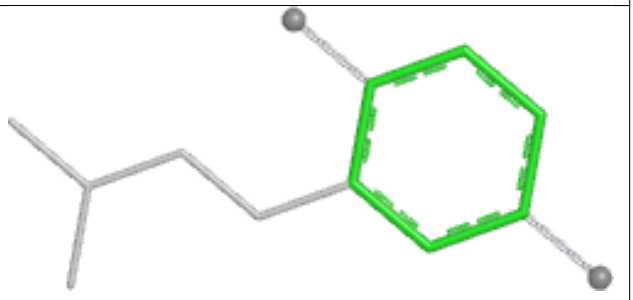
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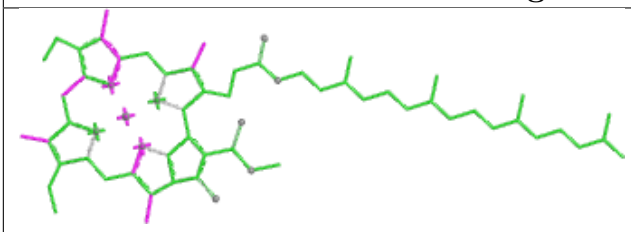


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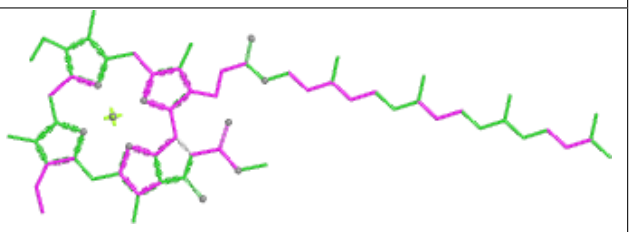


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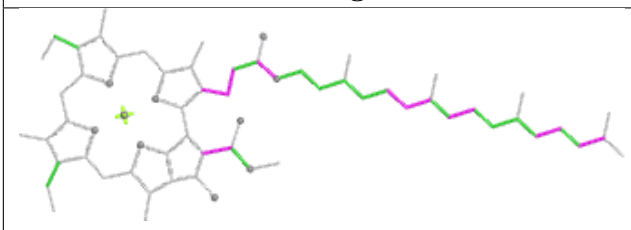
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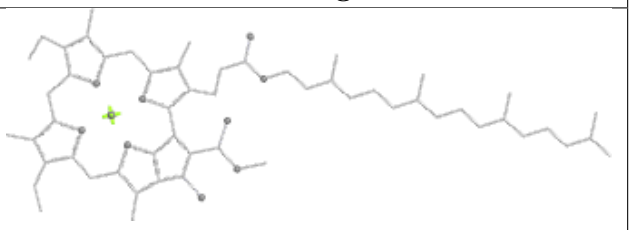
Bond lengths



Bond angles

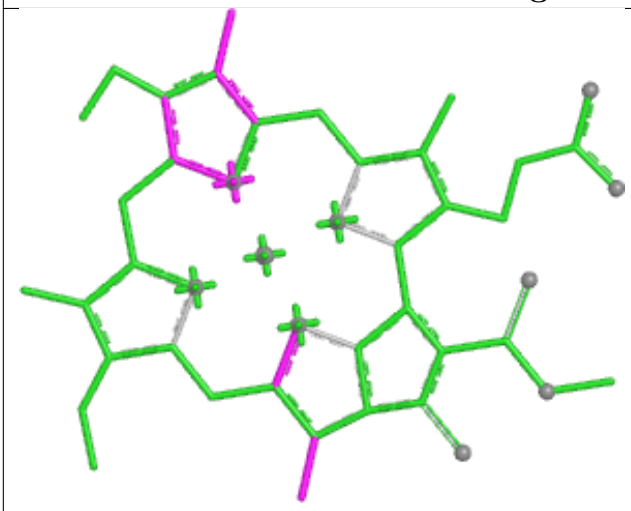


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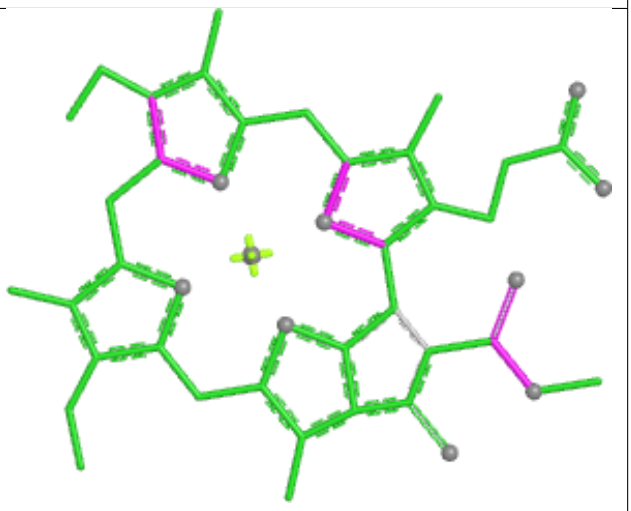


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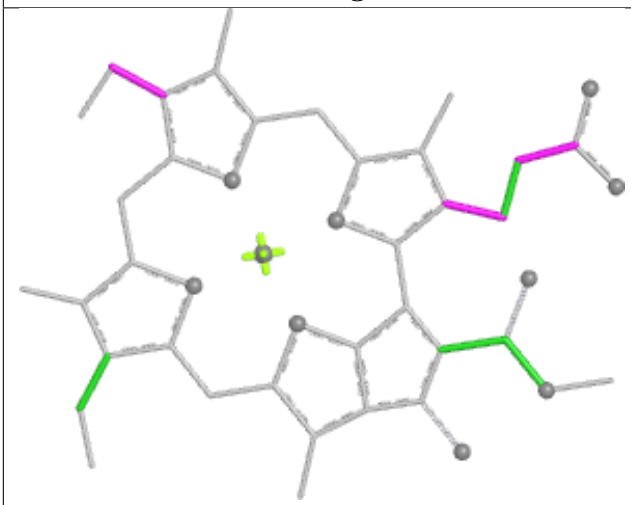
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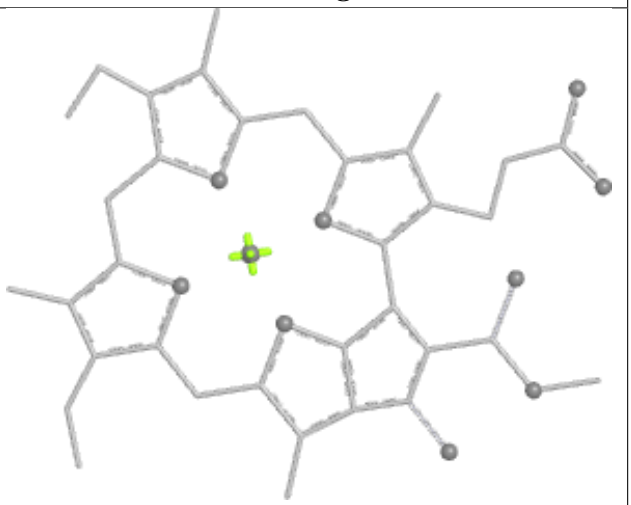
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Bond angles

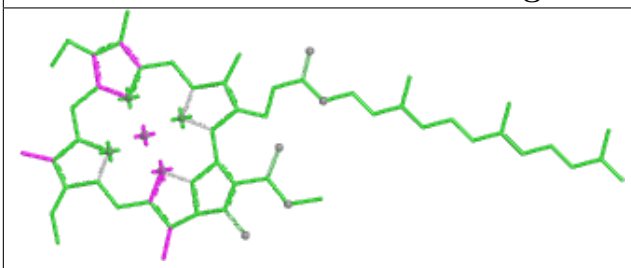


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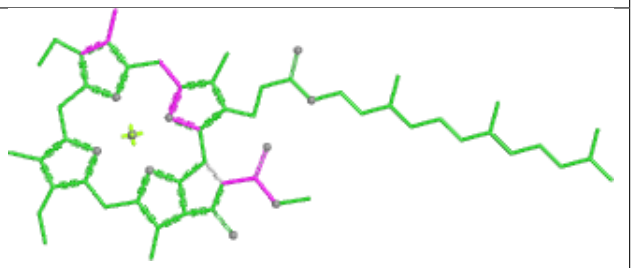


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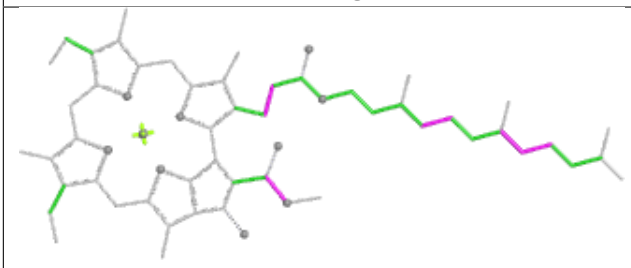
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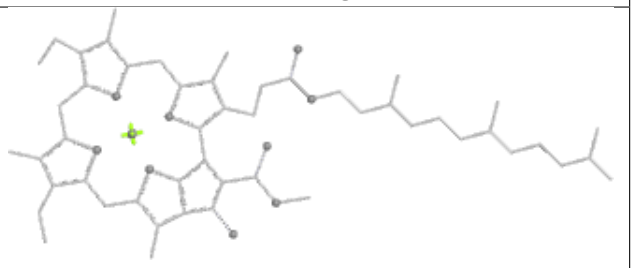
Bond lengths



Bond angles

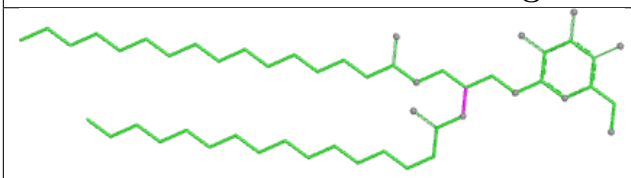


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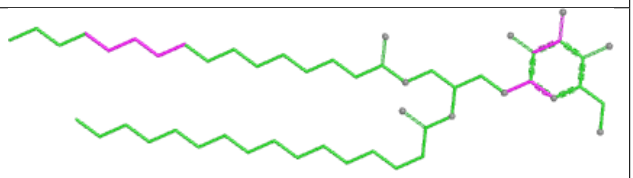


Rings

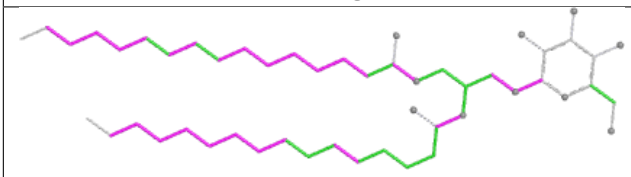
Ligand LMG b 622



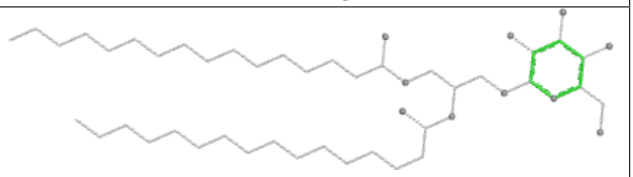
Bond lengths



Bond angles

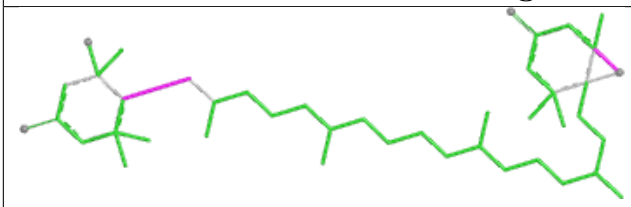


Torsions

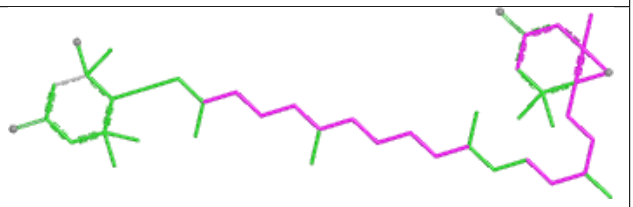


Rings

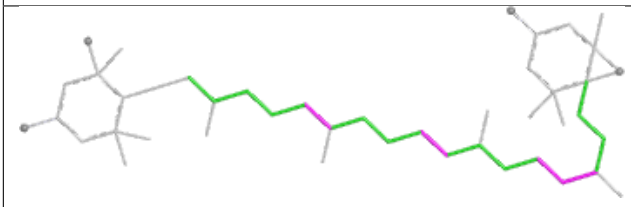
Ligand NEX 5 1623



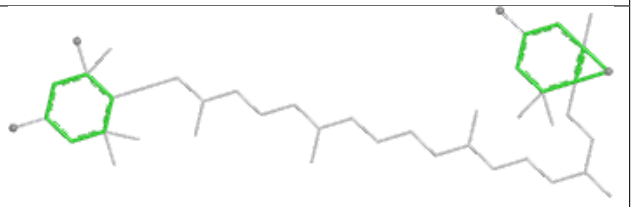
Bond lengths



Bond angles

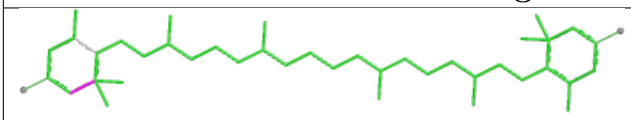


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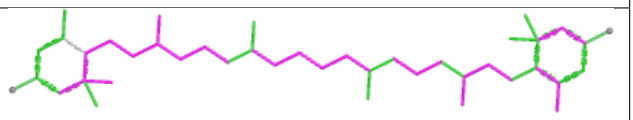


Rings

Ligand LUT G 1621



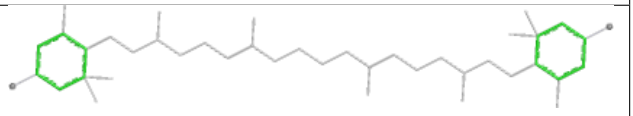
Bond lengths



Bond angles

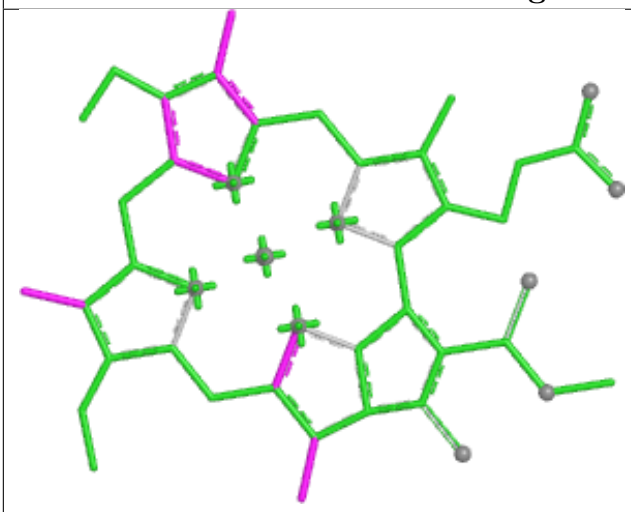


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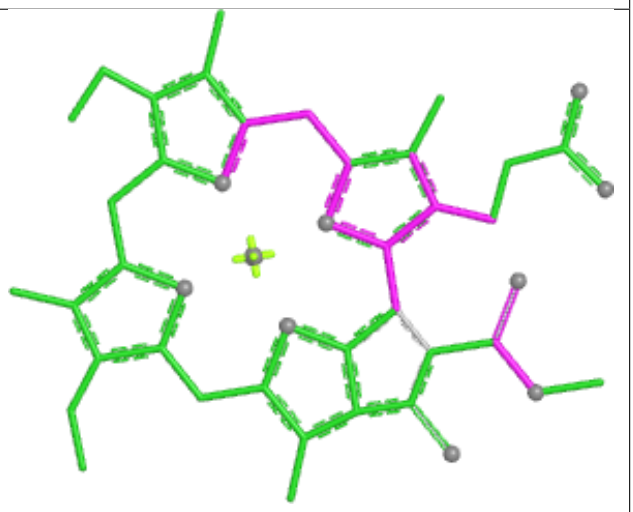


Rings

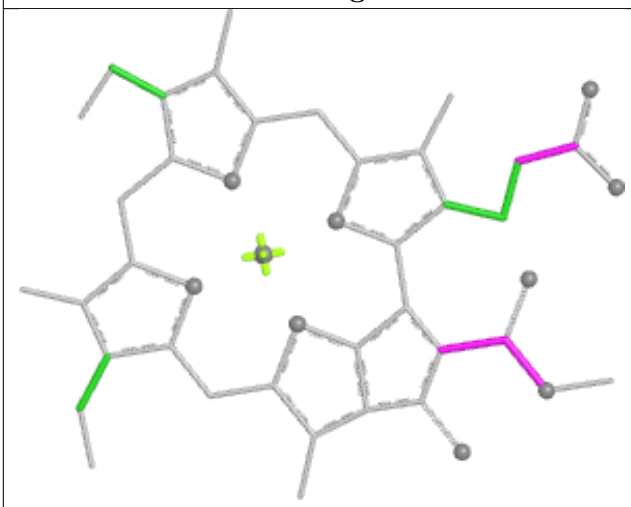
Ligand CLA 6 612



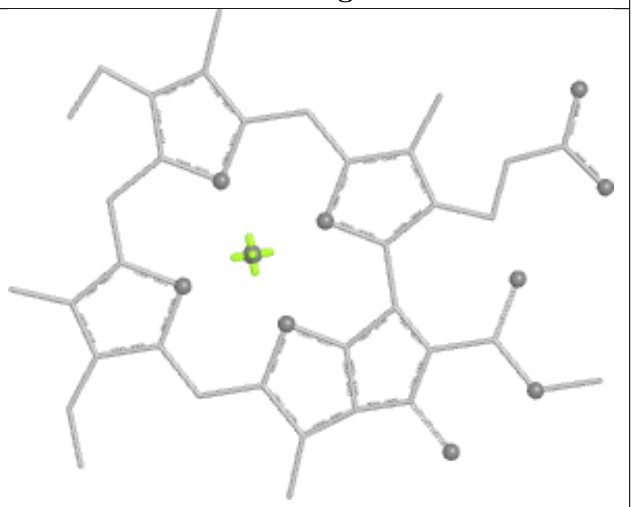
Bond lengths



Bond angles

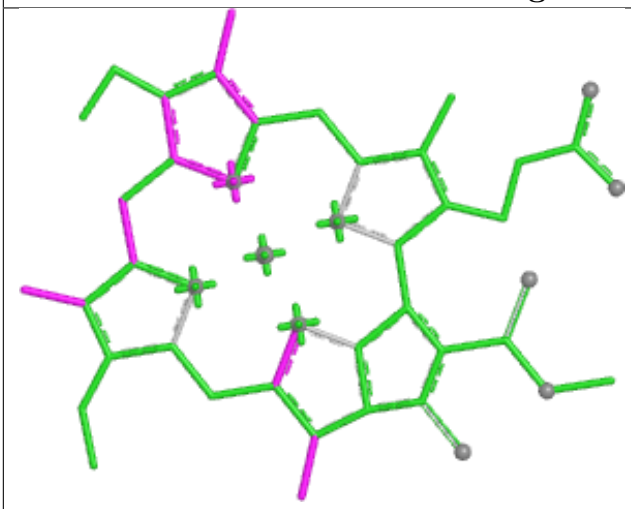


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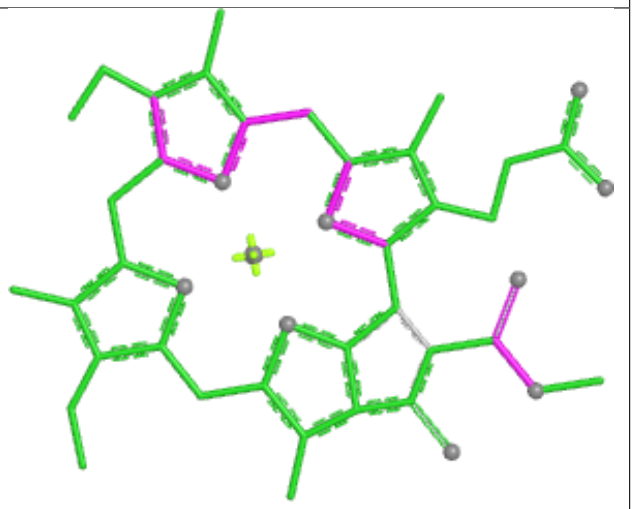


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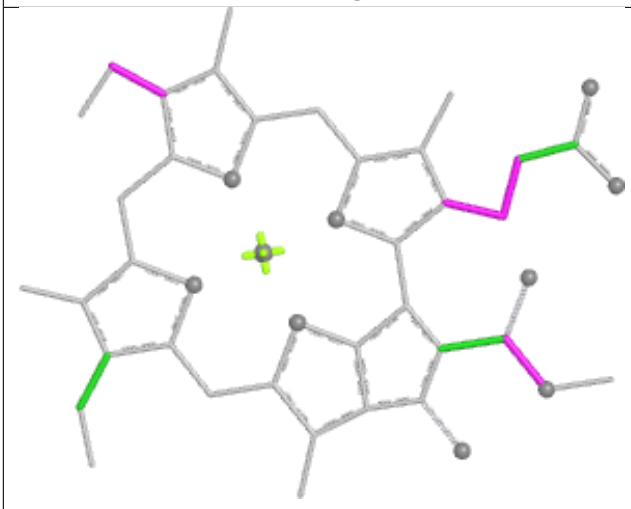
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Bond lengths



Bond angles

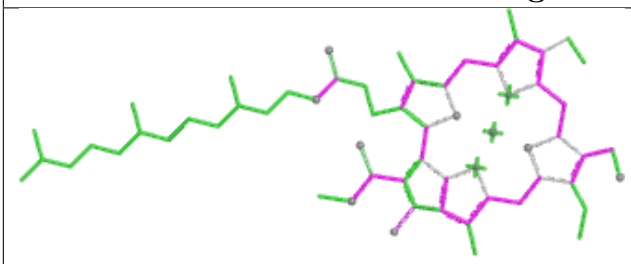


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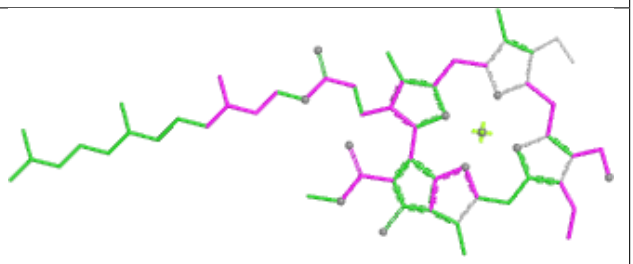


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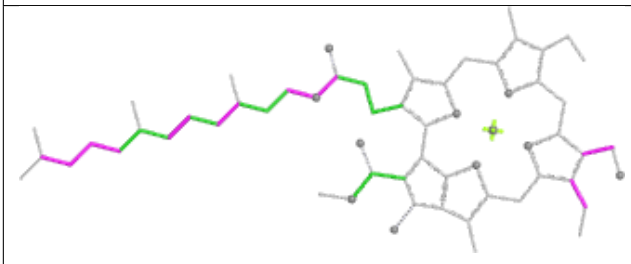
Ligand CHL 2 609



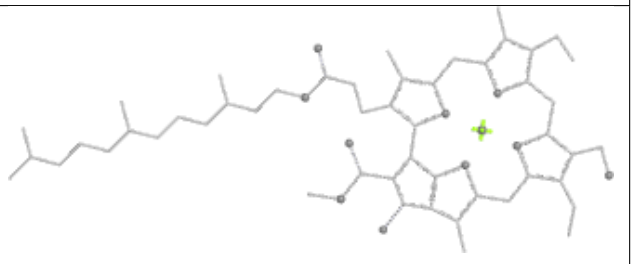
Bond lengths



Bond angles

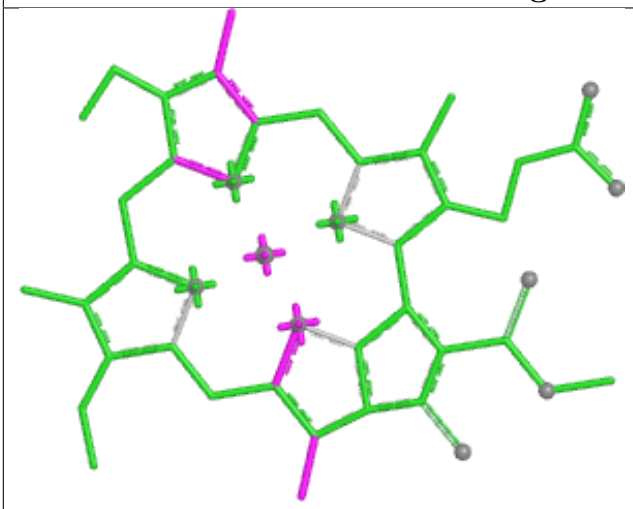


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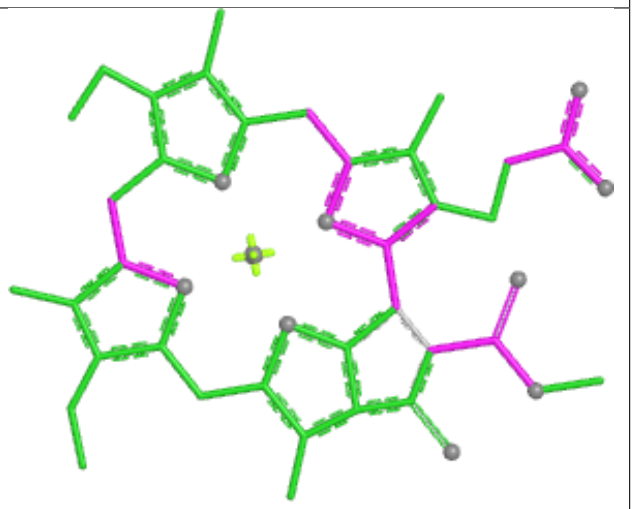


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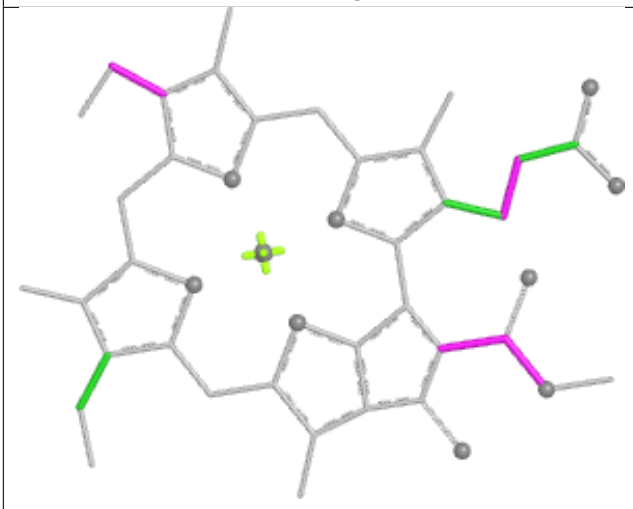
Ligand CLA s 603



Bond lengths



Bond angles

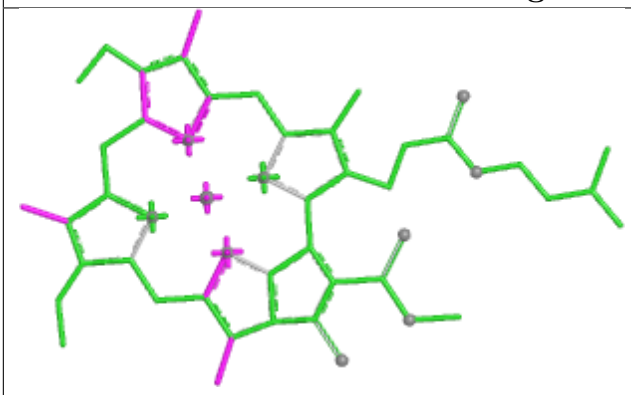


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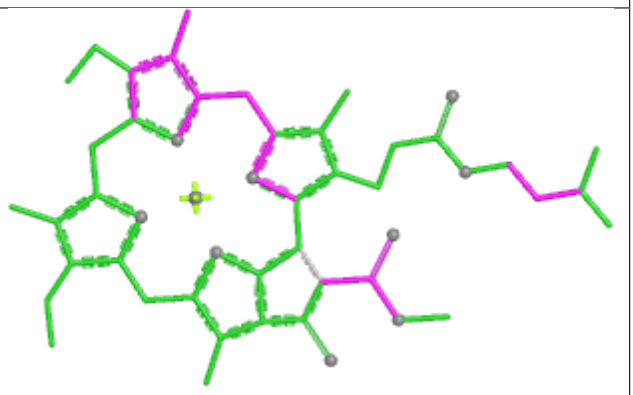


Rings

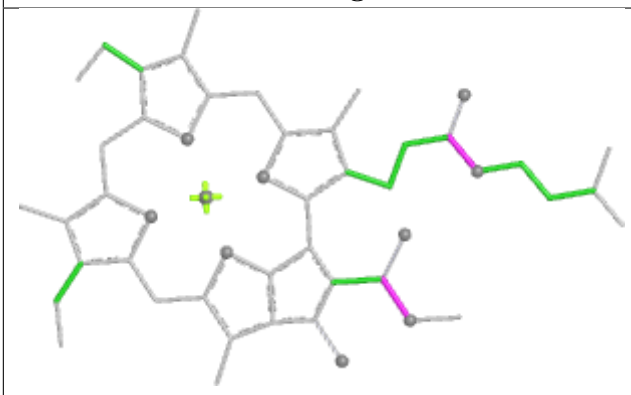
Ligand CLA n 604



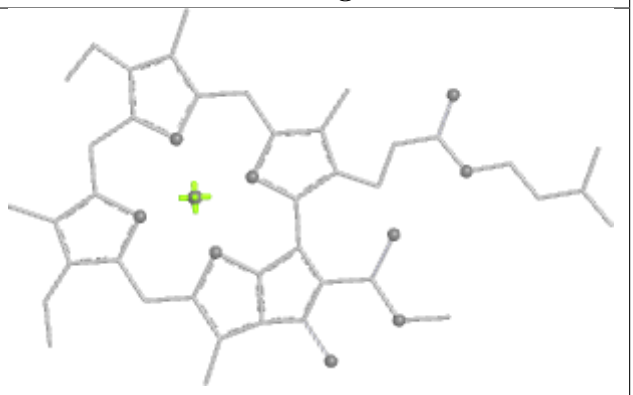
Bond lengths



Bond angles



Torsions

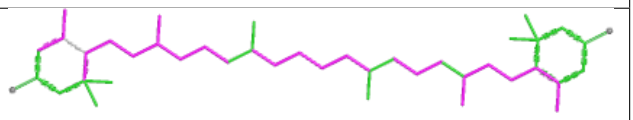


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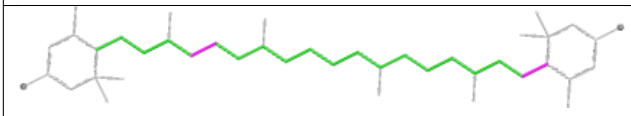
Ligand LUT 1 1621



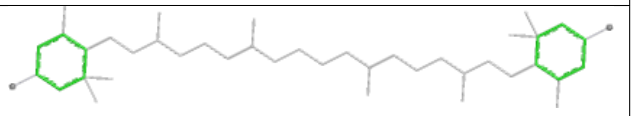
Bond lengths



Bond angles

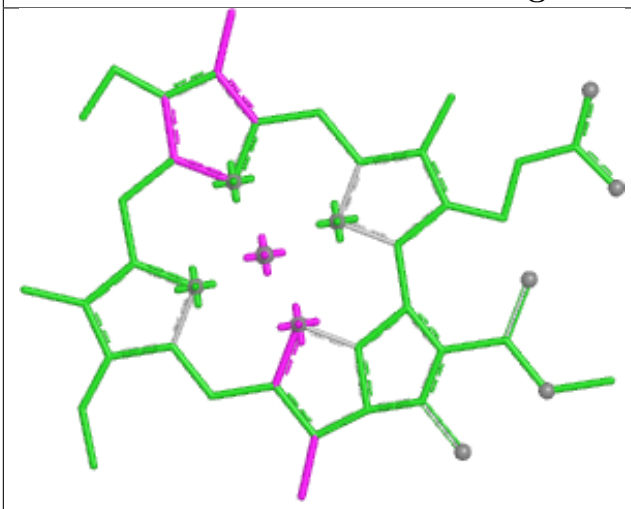


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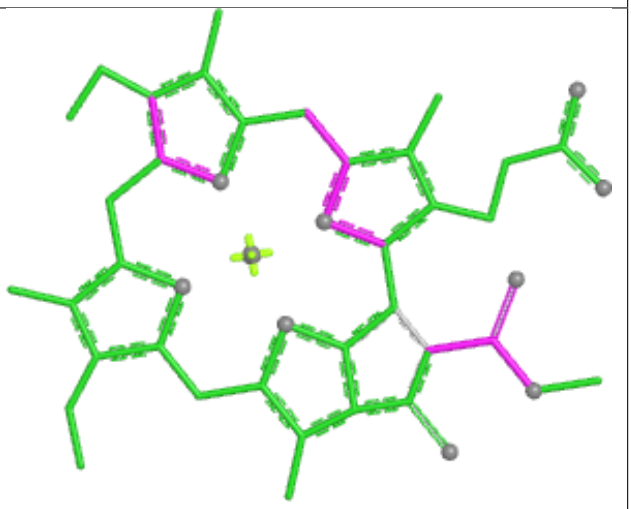


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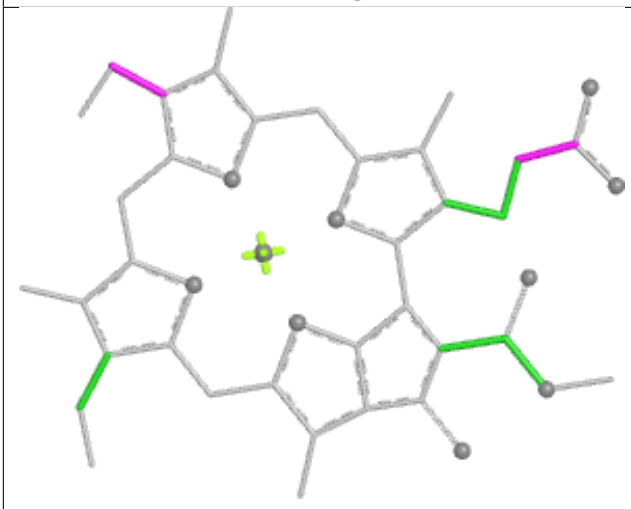
Ligand CLA 6 611



Bond lengths



Bond angles

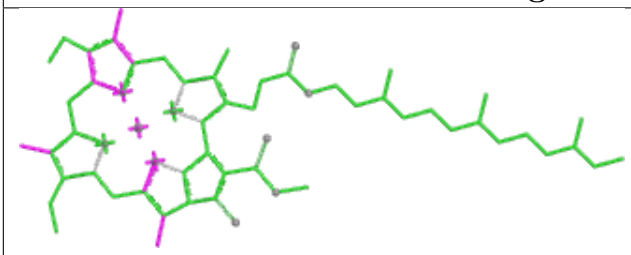


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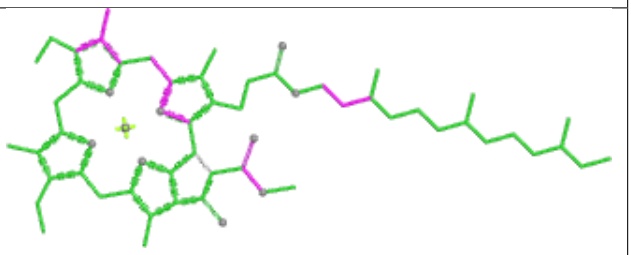


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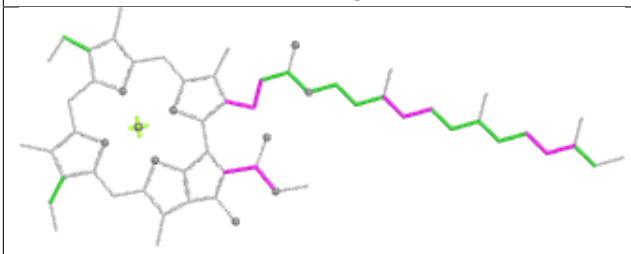
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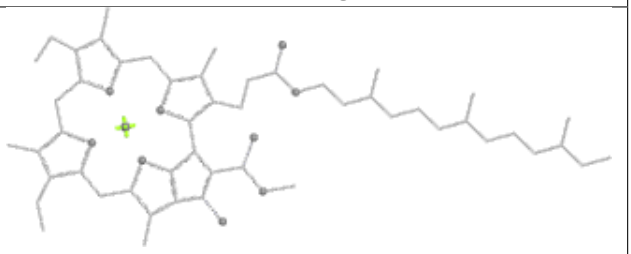
Bond lengths



Bond angles

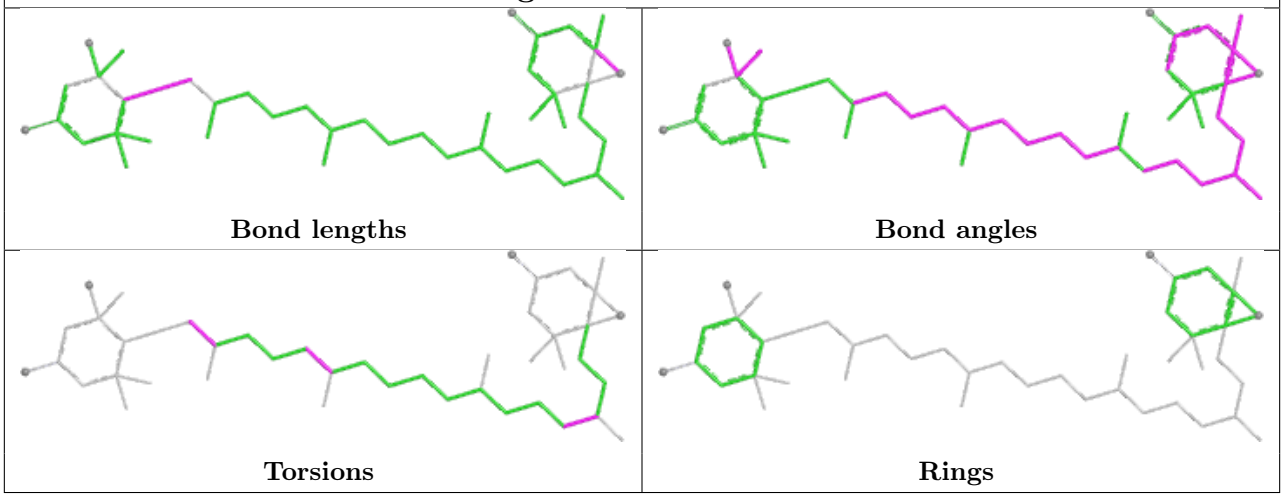


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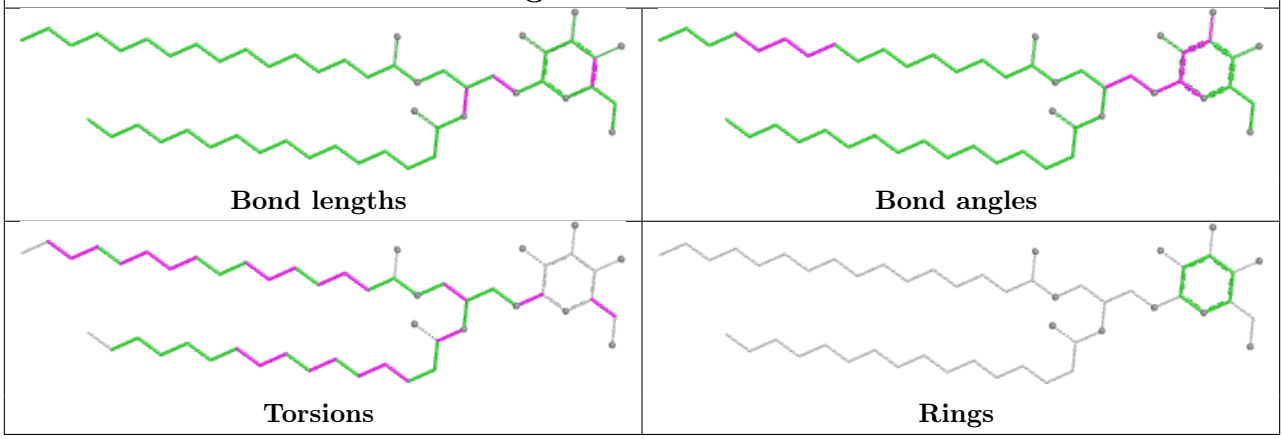


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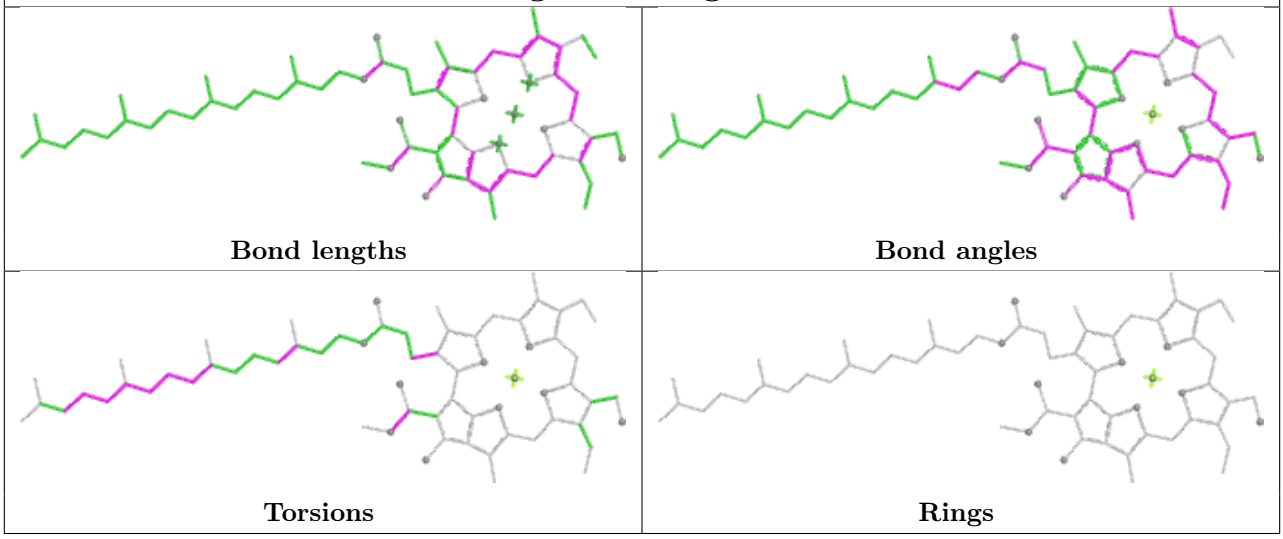
Ligand NEX S 1623



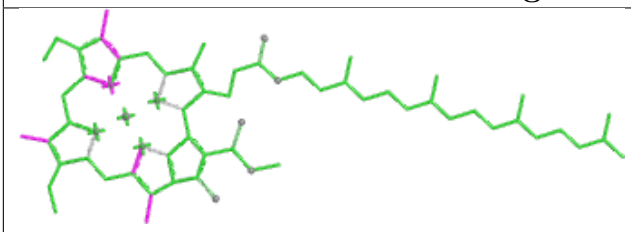
Ligand LMG c 521



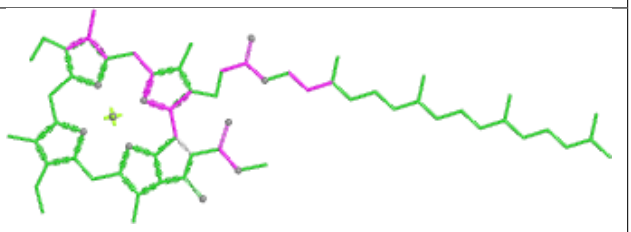
Ligand CHL g 608



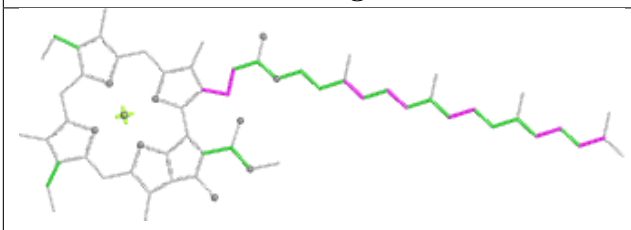
Ligand CLA N 610



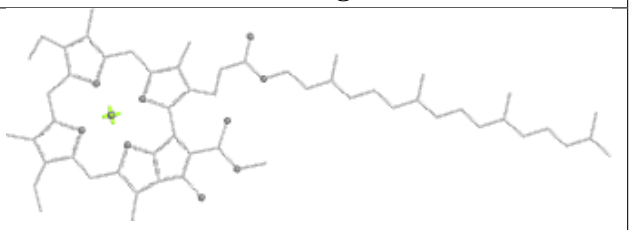
Bond lengths



Bond angles

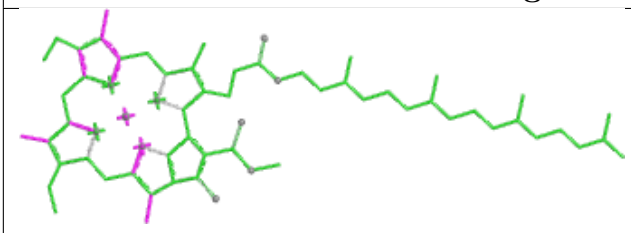


Torsions

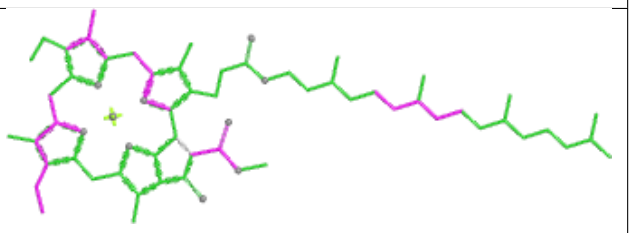


Rings

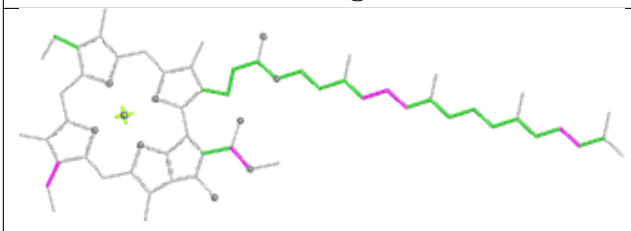
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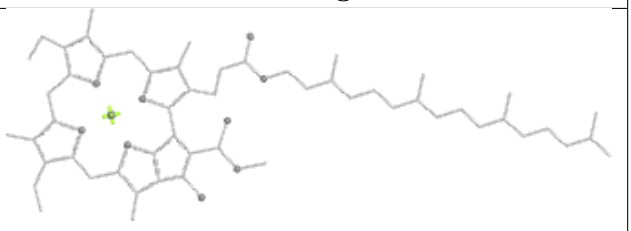
Bond lengths



Bond angles

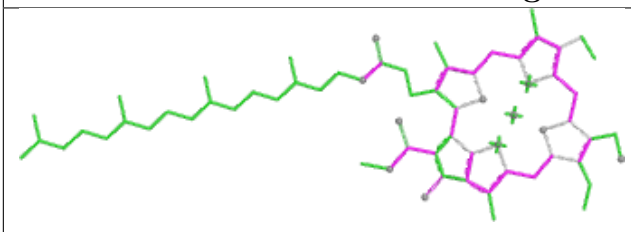


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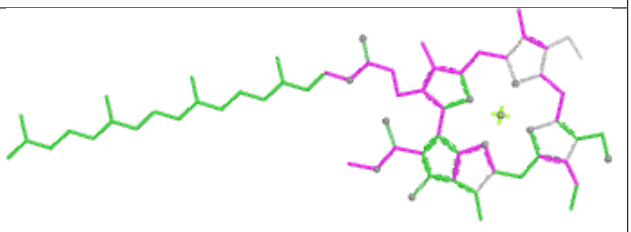


Rings

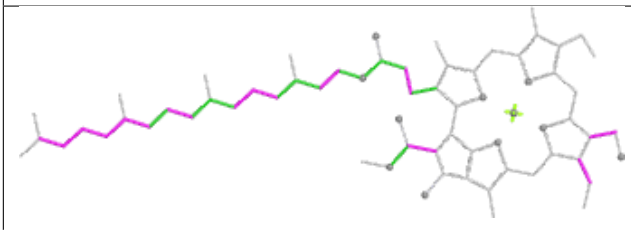
Ligand CHL Y 607



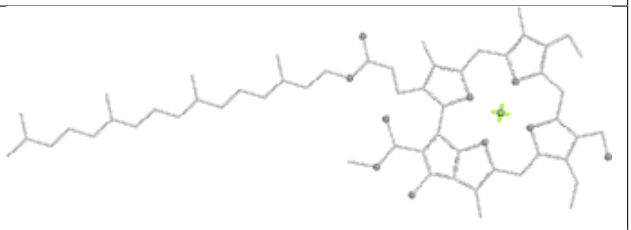
Bond lengths



Bond angles

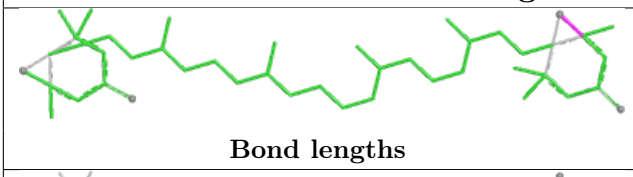


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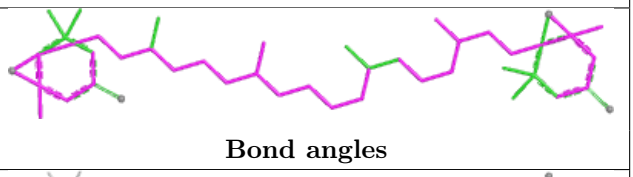


Rings

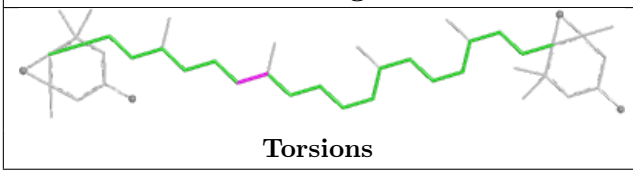
Ligand XAT 3 1622



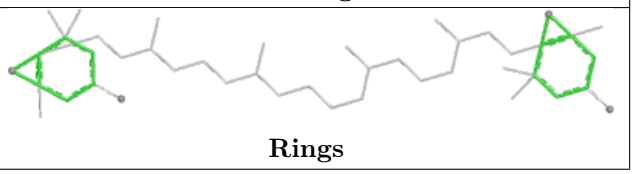
Bond lengths



Bond angles

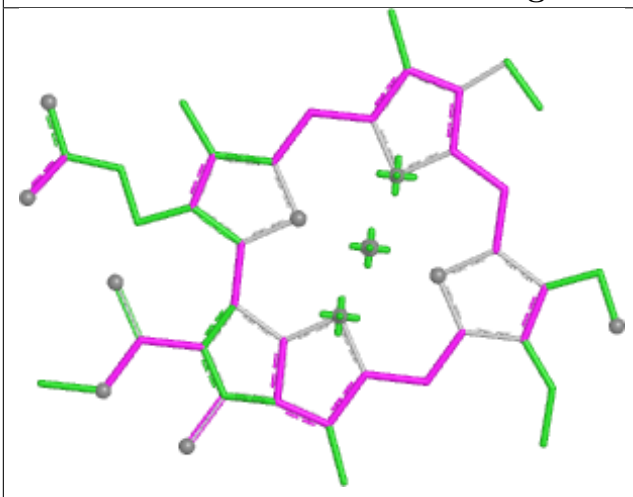


Torsions

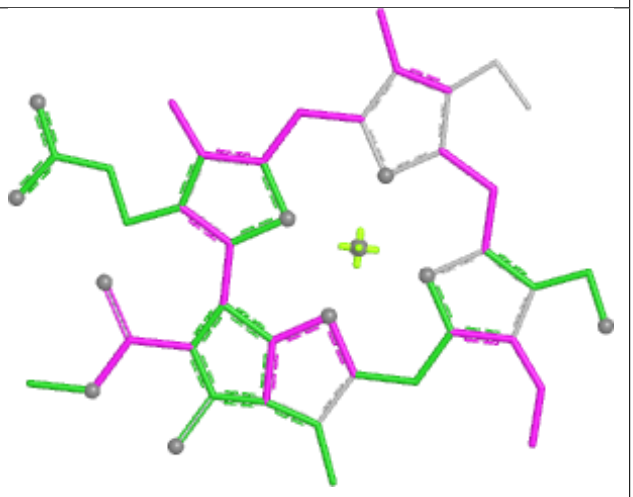


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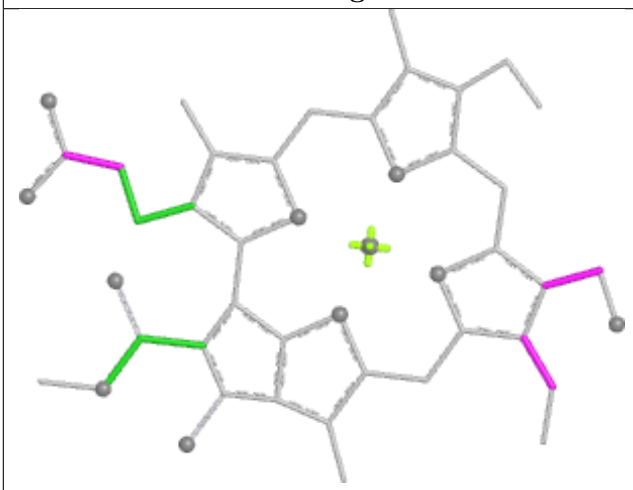
Ligand CHL 8 609



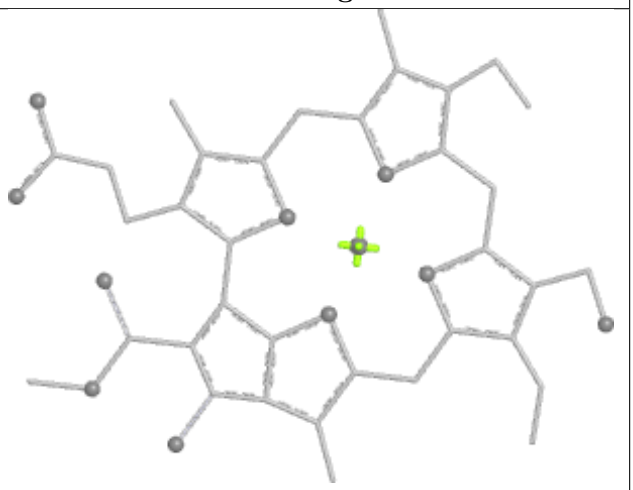
Bond lengths



Bond angles

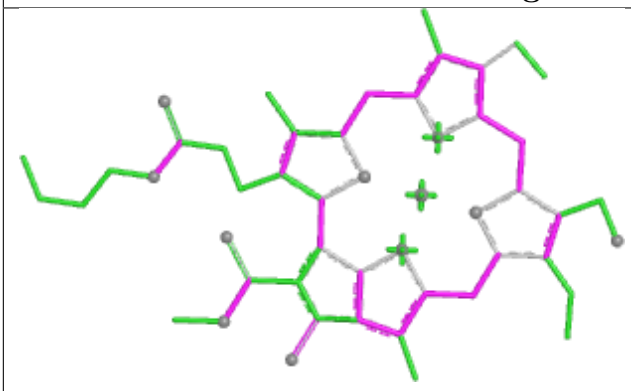


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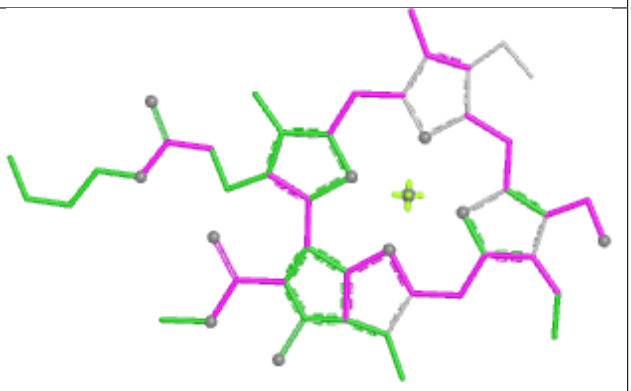


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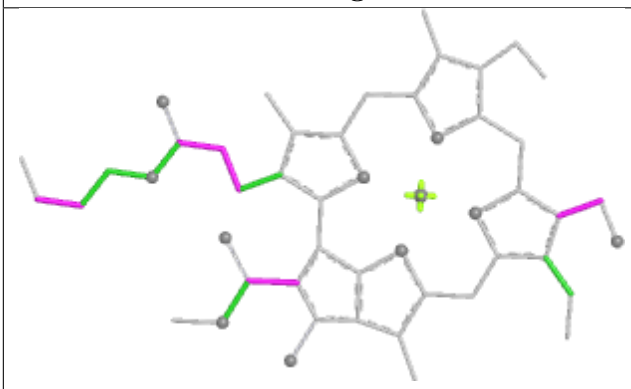
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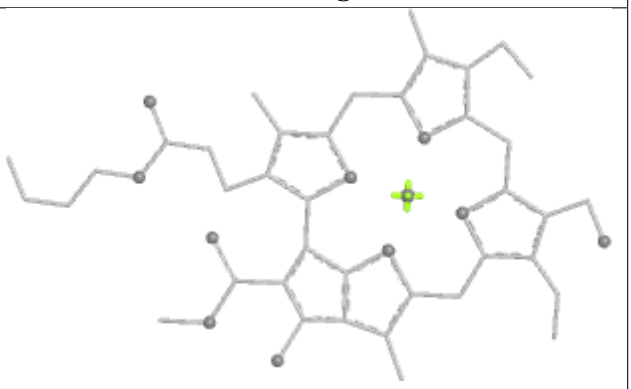
Bond lengths



Bond angles

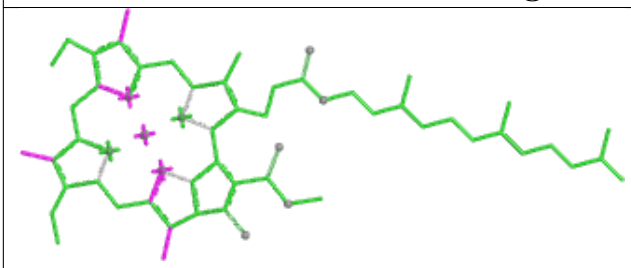


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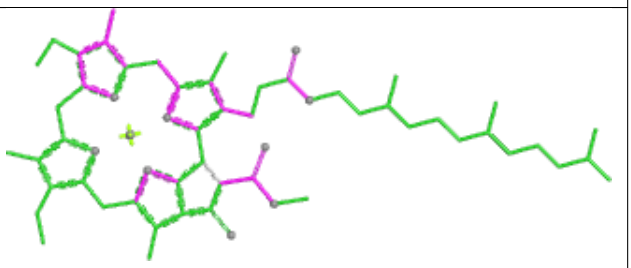


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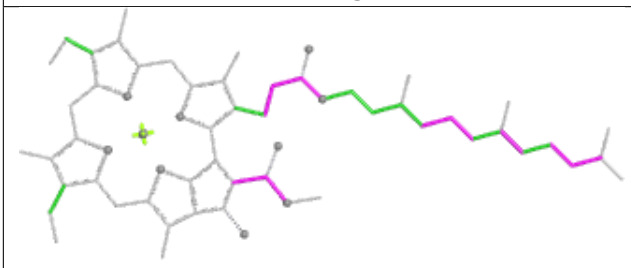
Ligand CLA R 603



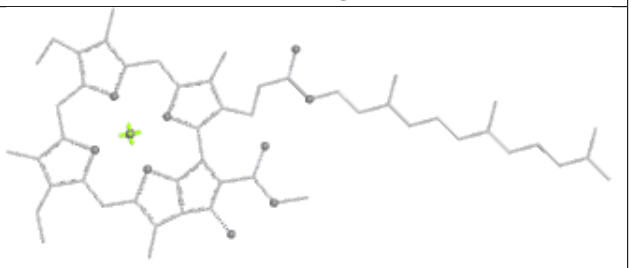
Bond lengths



Bond angles

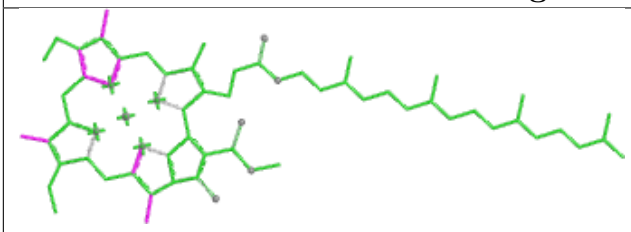


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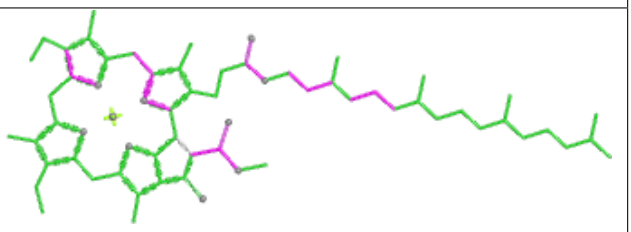


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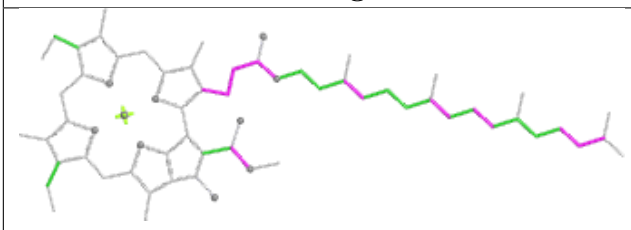
Ligand CLA c 501



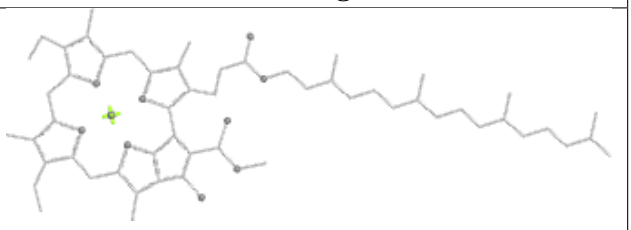
Bond lengths



Bond angles



Torsions

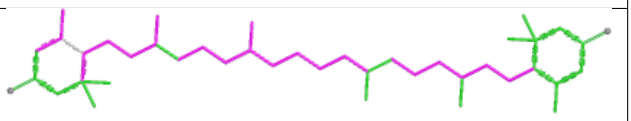


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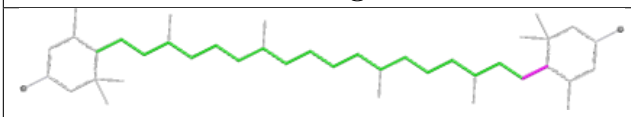
Ligand LUT S 1620



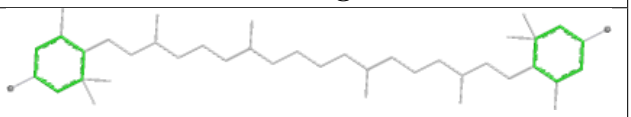
Bond lengths



Bond angles

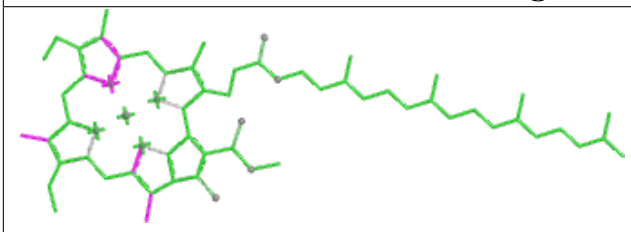


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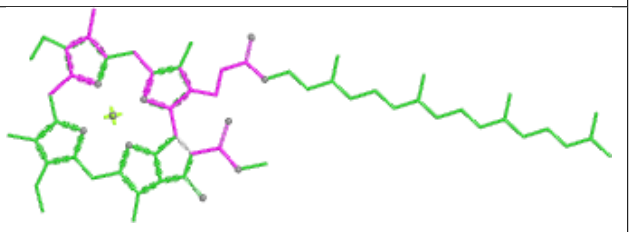


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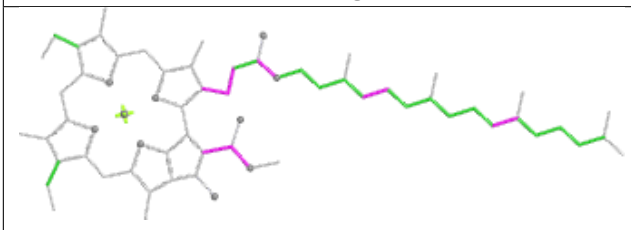
Ligand CLA c 513



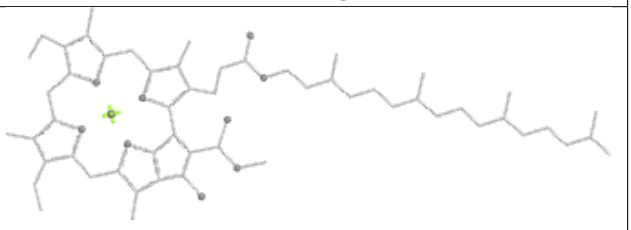
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Bond angles

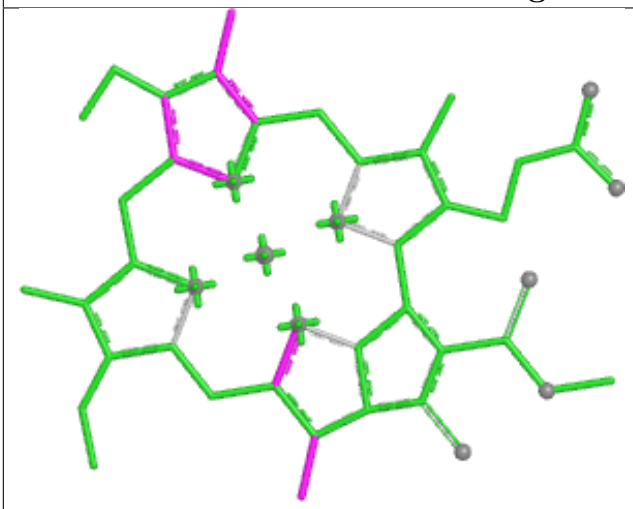


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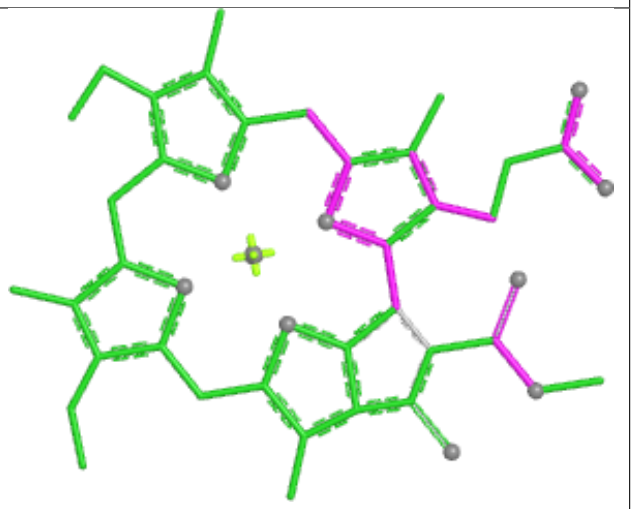


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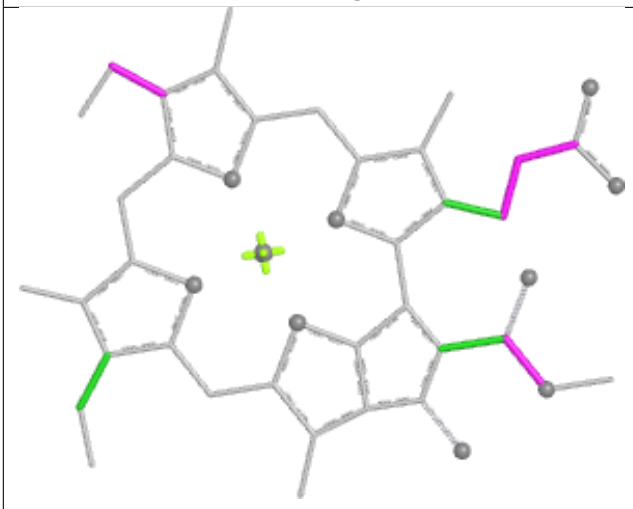
Ligand CLA 8 612



Bond lengths



Bond angles

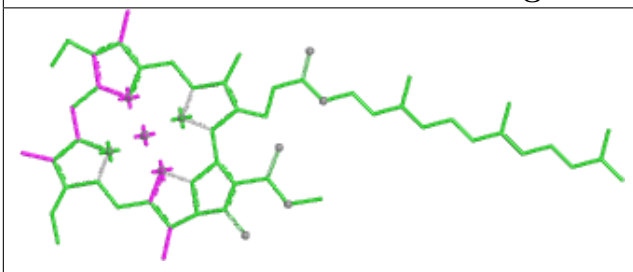


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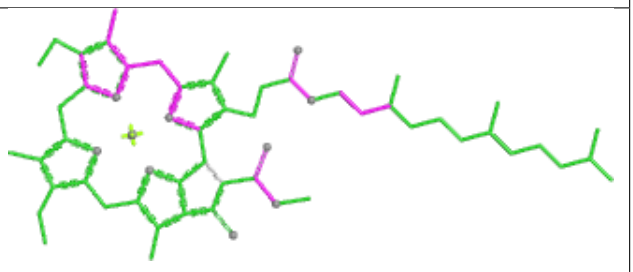


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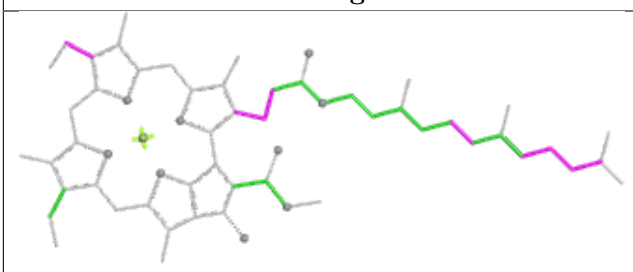
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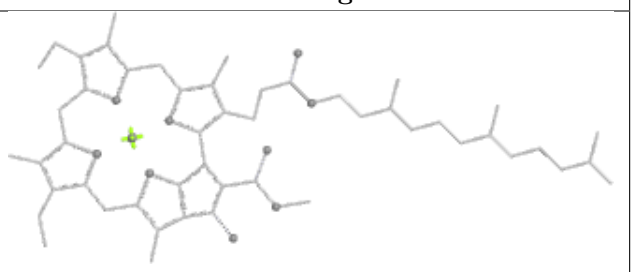
Bond lengths



Bond angles

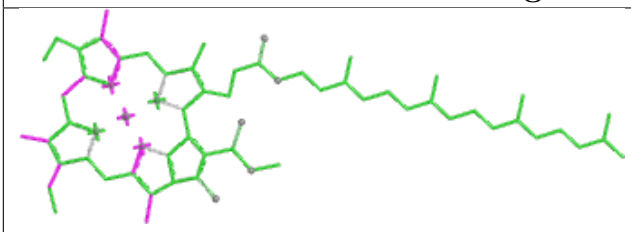


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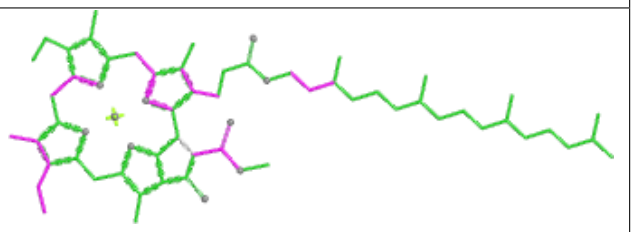


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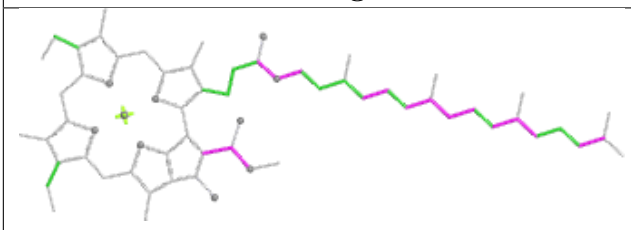
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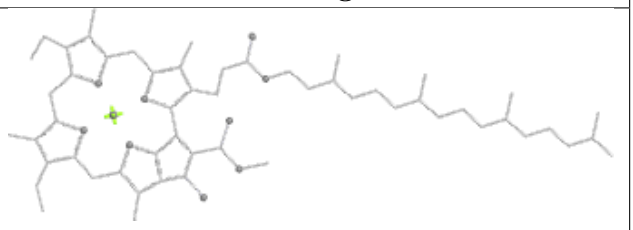
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Bond angles

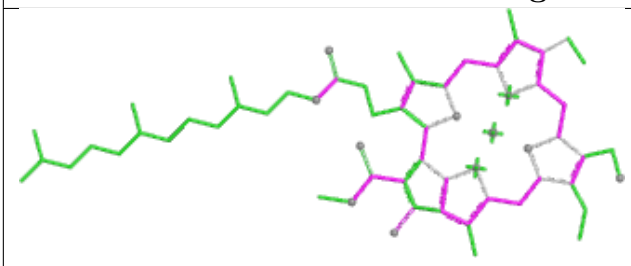


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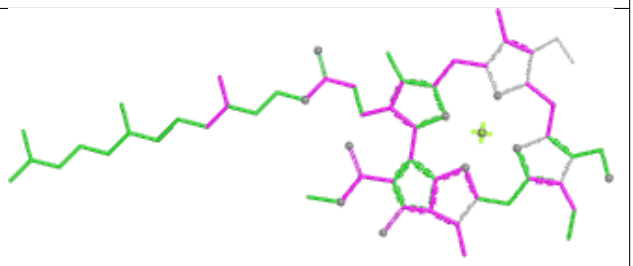


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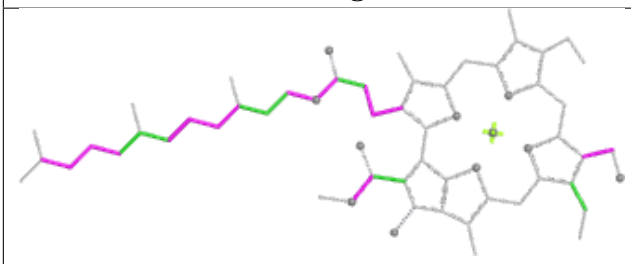
Ligand CHL r 608



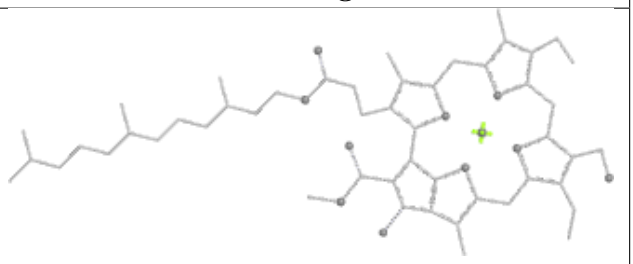
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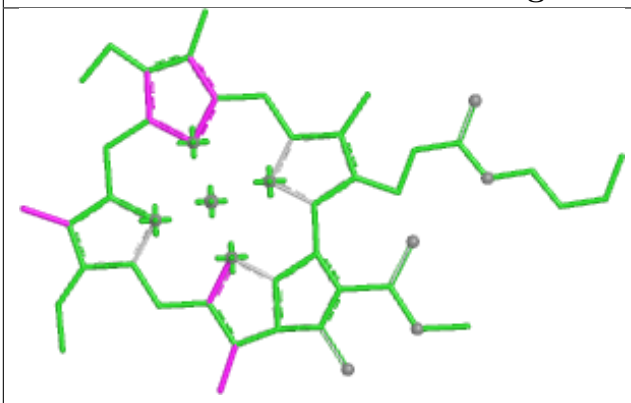


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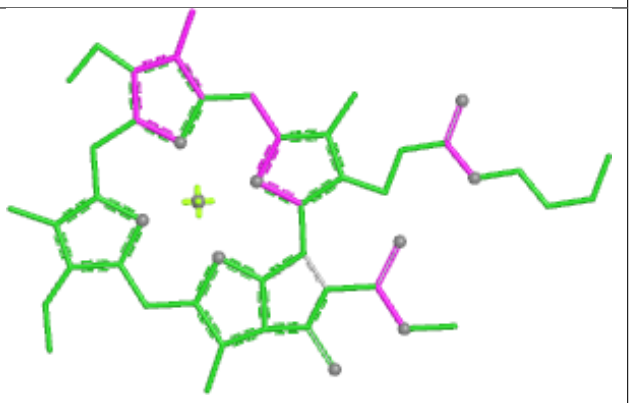


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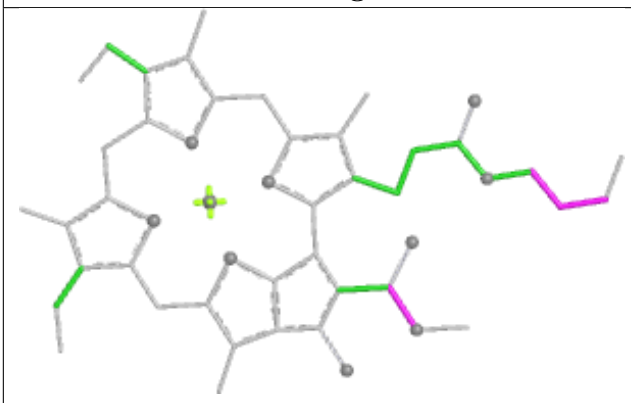
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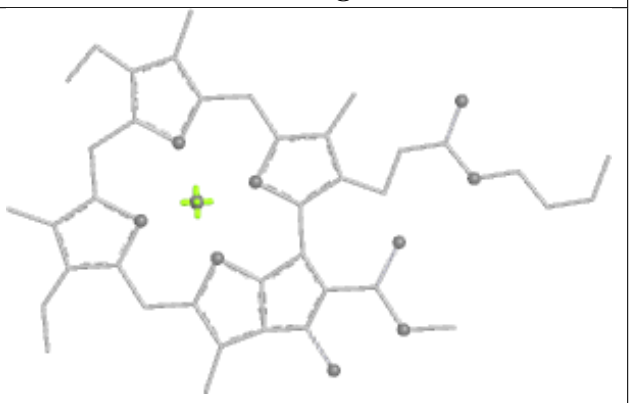
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Bond angles

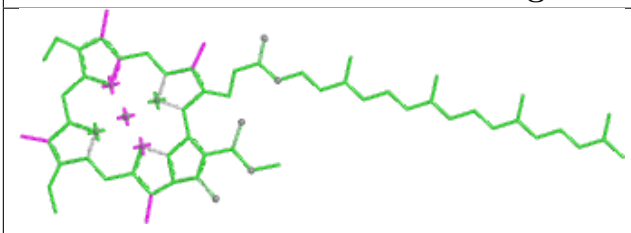


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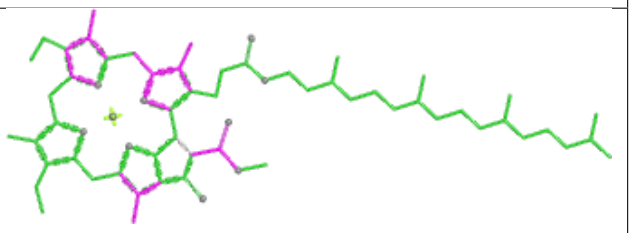


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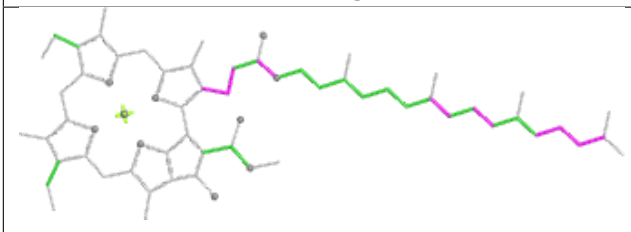
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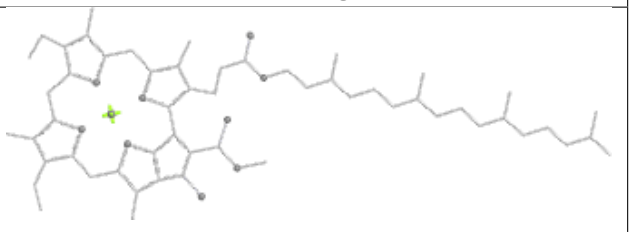
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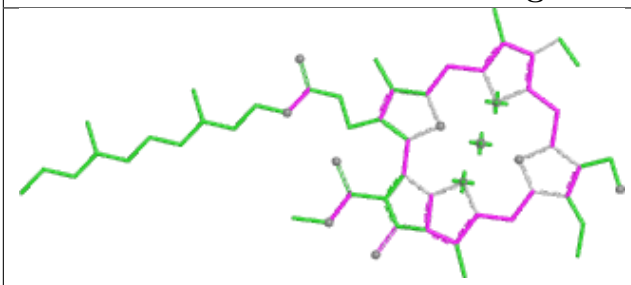


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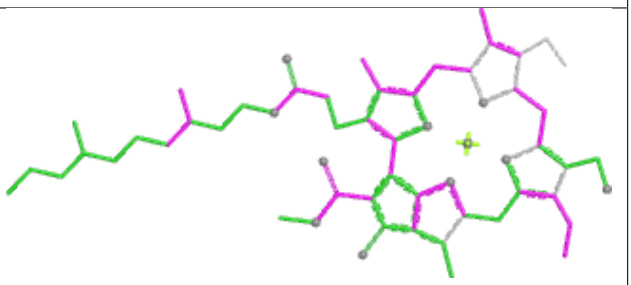


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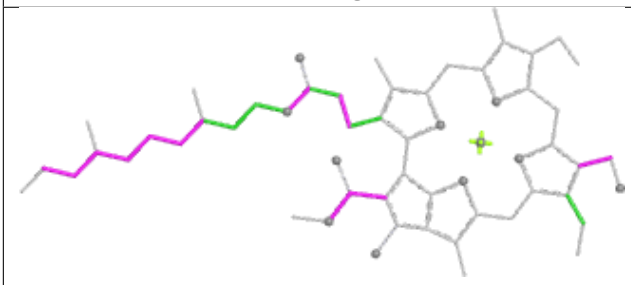
Ligand CHL S 607



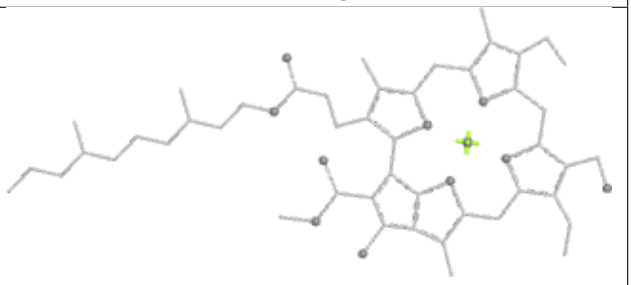
Bond lengths



Bond angles

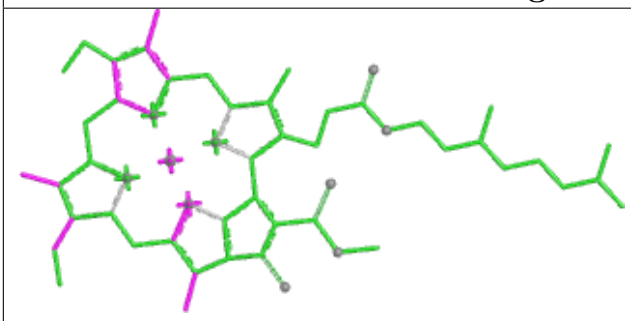


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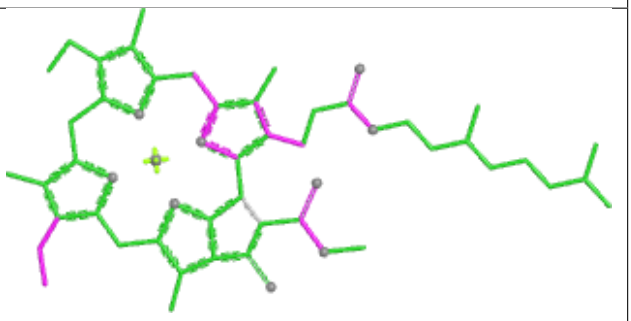


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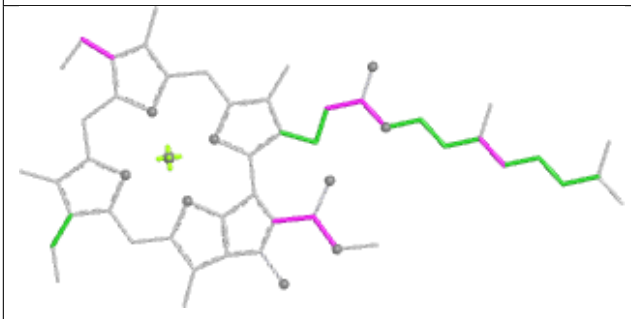
Ligand CLA 2 603



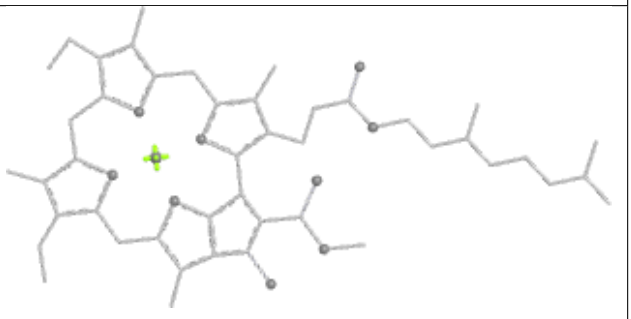
Bond lengths



Bond angles

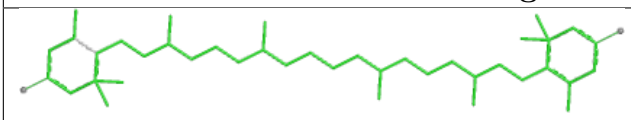


Torsions

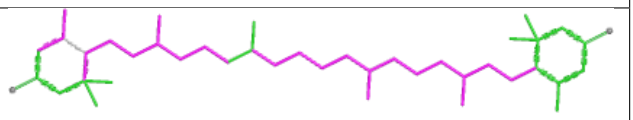


Rings

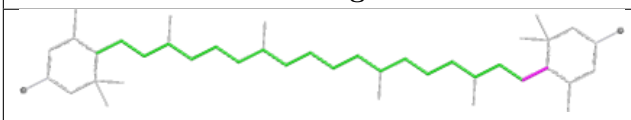
Ligand LUT 6 1620



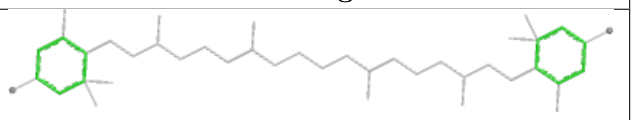
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Bond angles

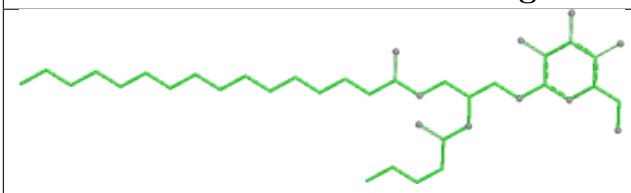


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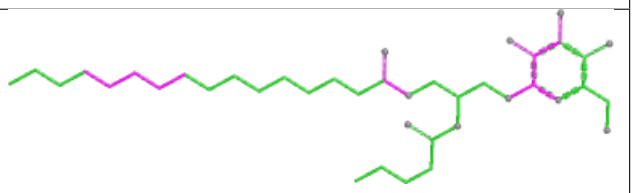


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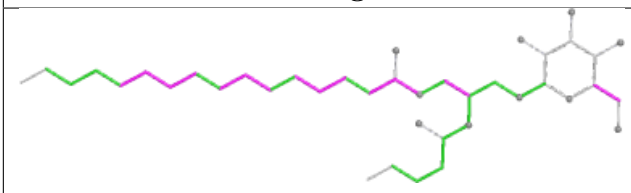
Ligand LMG A 415



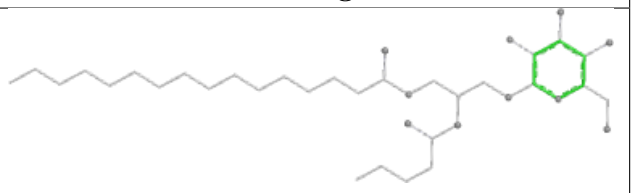
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Bond angles

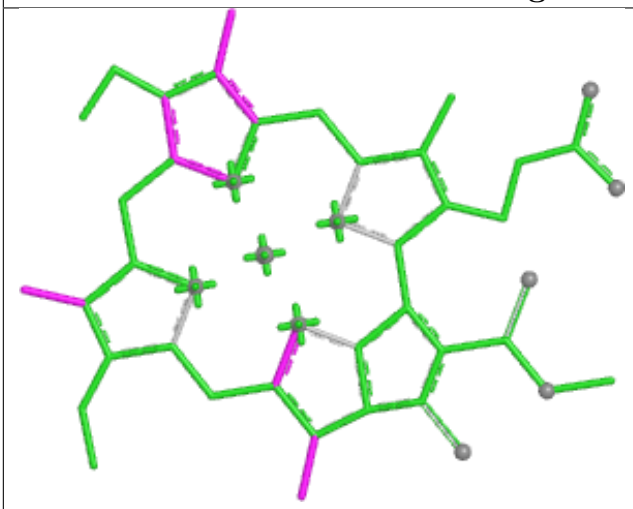


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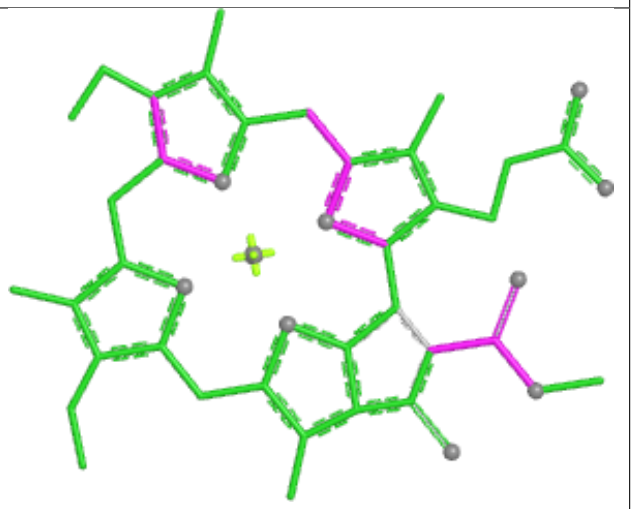


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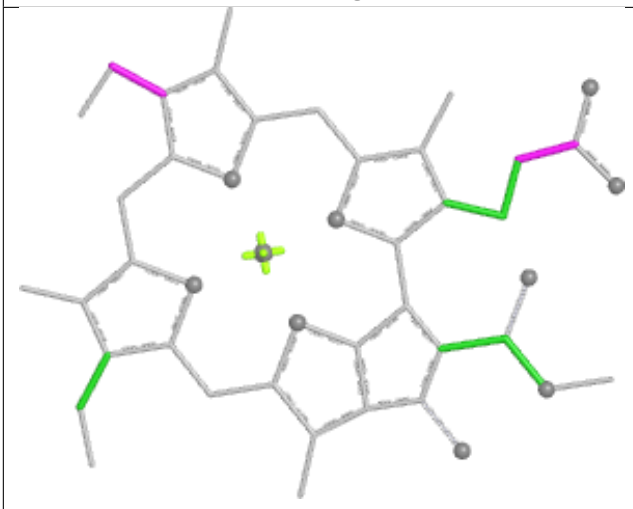
Ligand CLA 2 611



Bond lengths



Bond angles

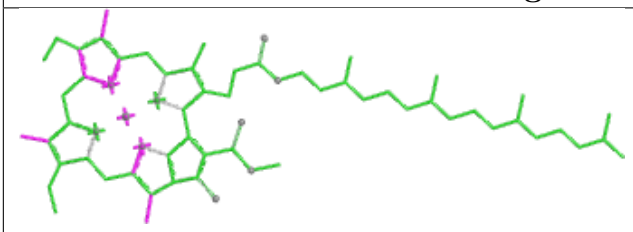


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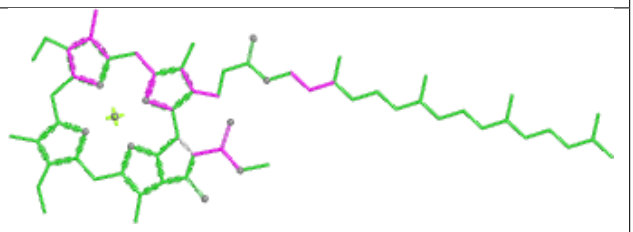


Rings

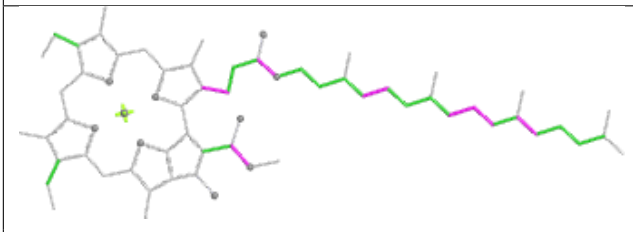
Ligand CLA C 512



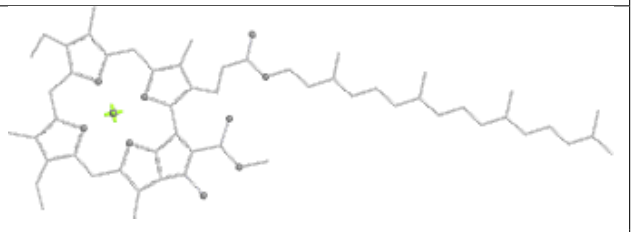
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Bond angles

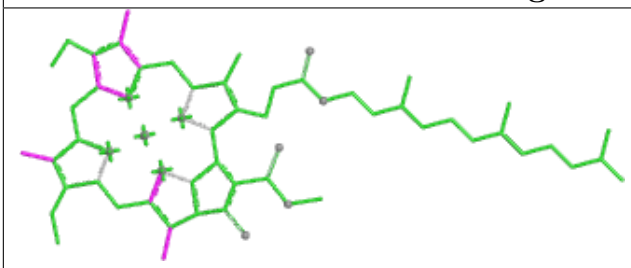


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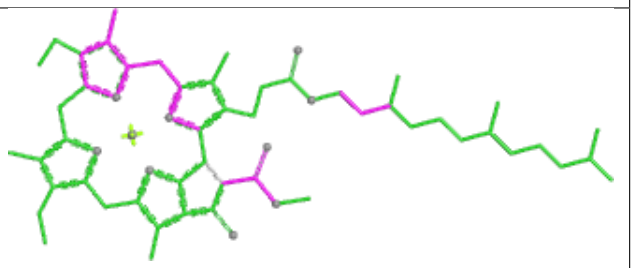


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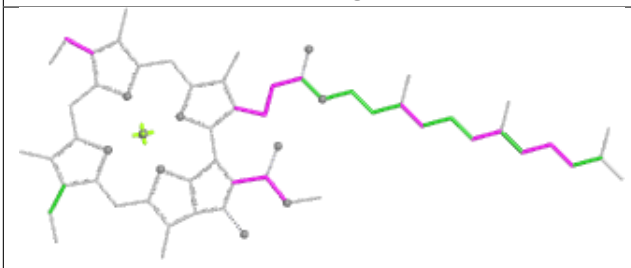
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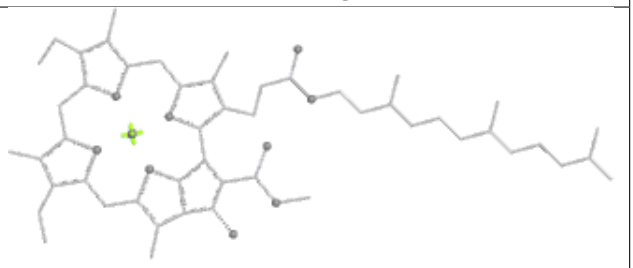
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Bond angles

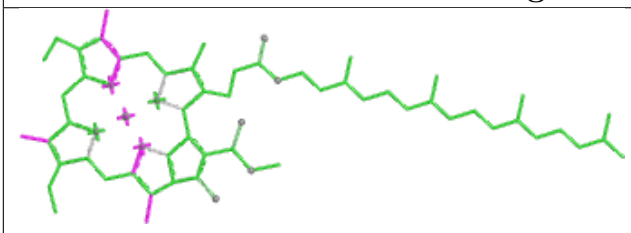


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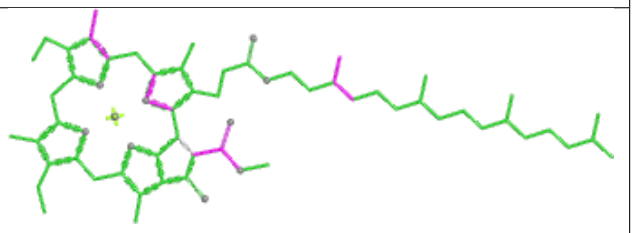


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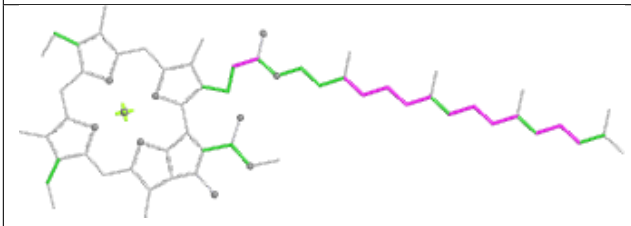
Ligand CLA b 614



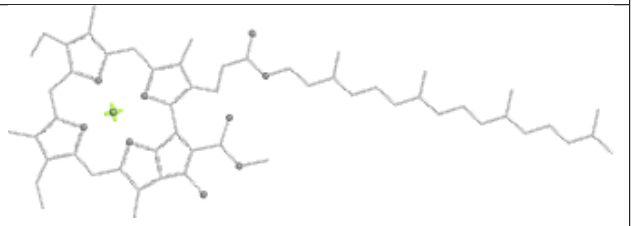
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Bond angles

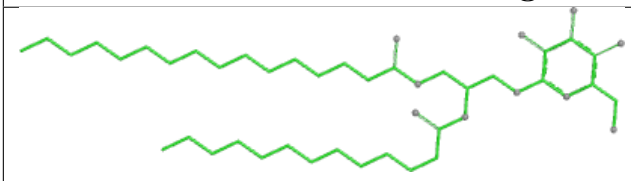


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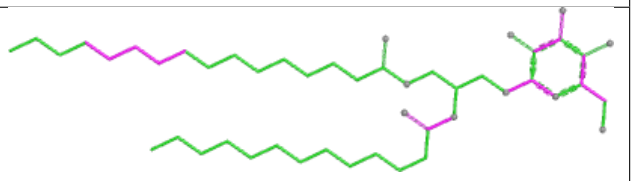


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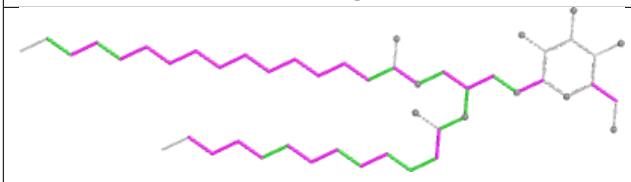
Ligand LMG A 413



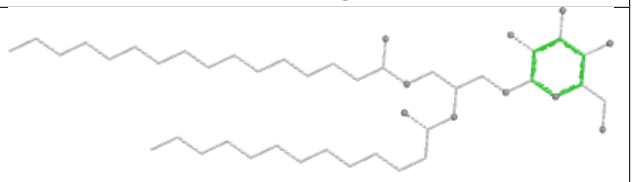
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Bond angles

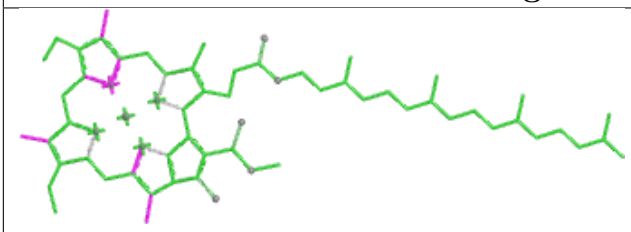


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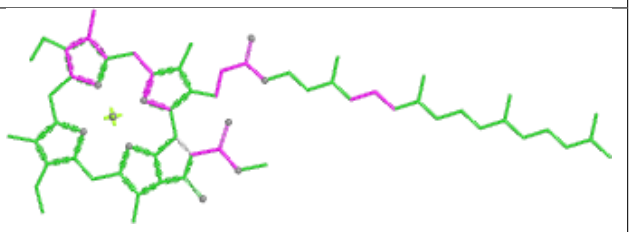


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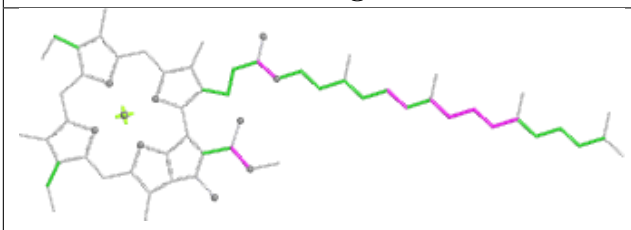
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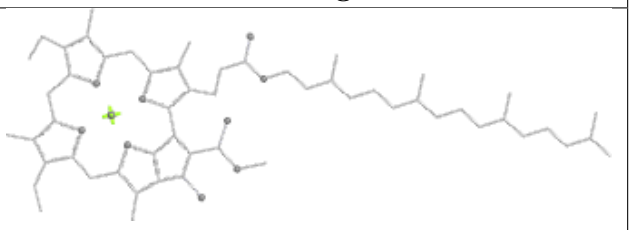
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Bond angles

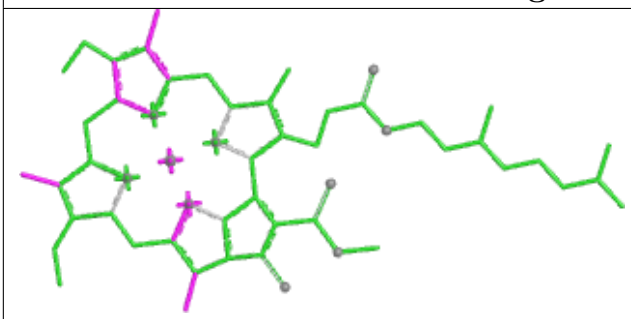


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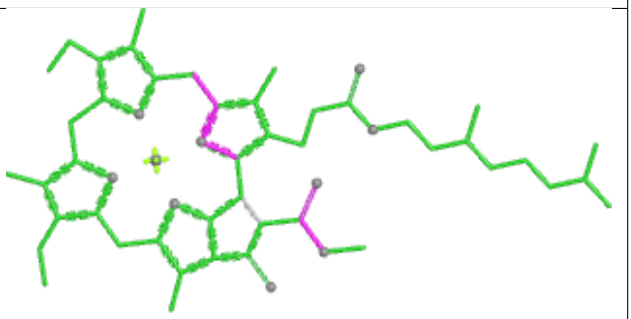


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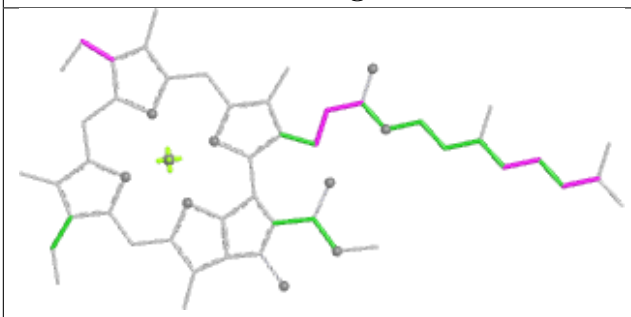
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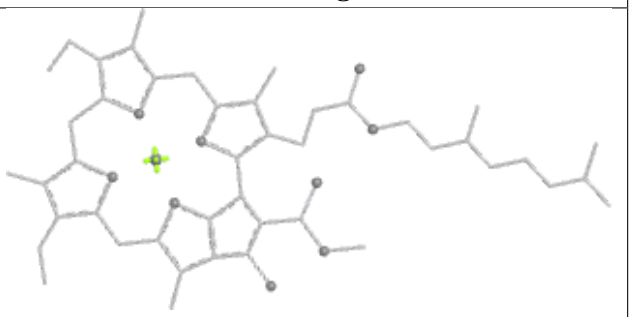
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Bond angles

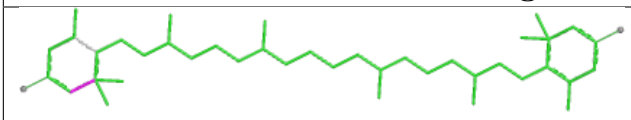


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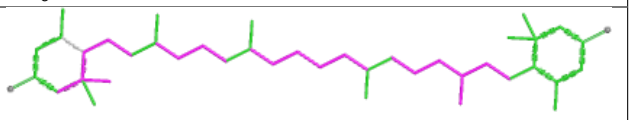


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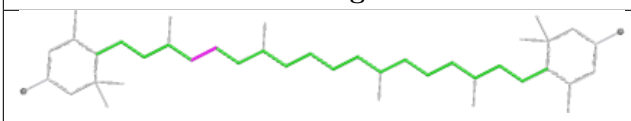
Ligand LUT y 1621



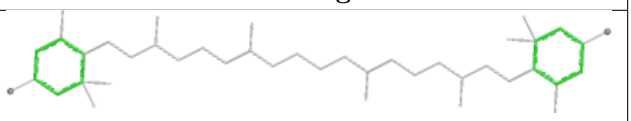
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Bond angles

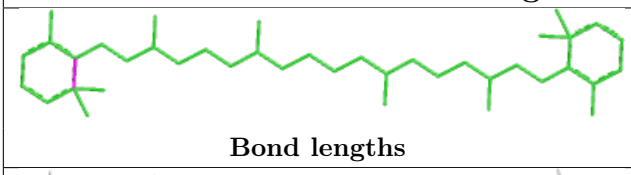


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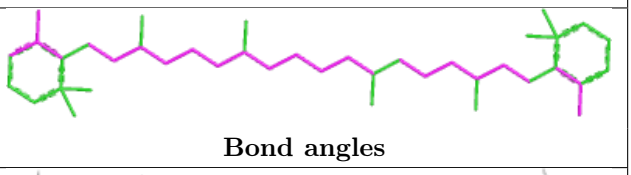


Rings

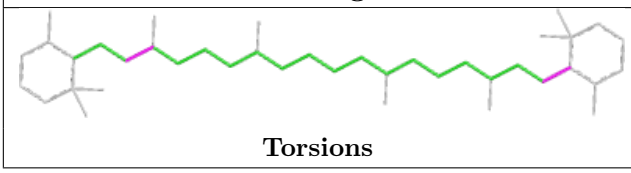
Ligand BCR C 517



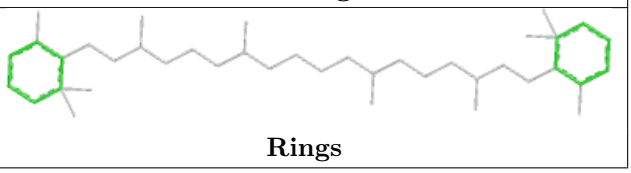
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Bond angles

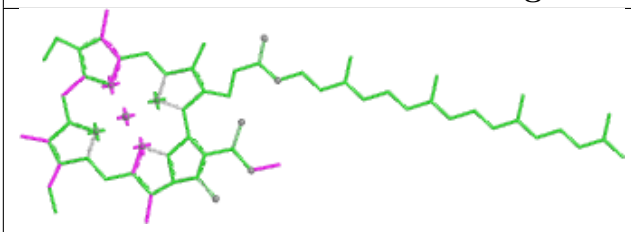


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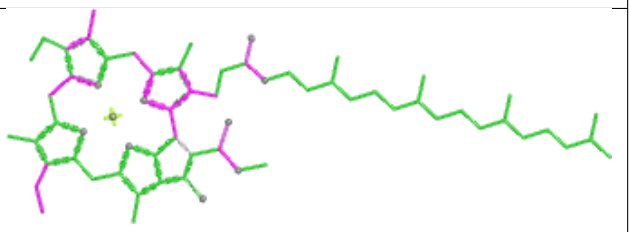


Rings

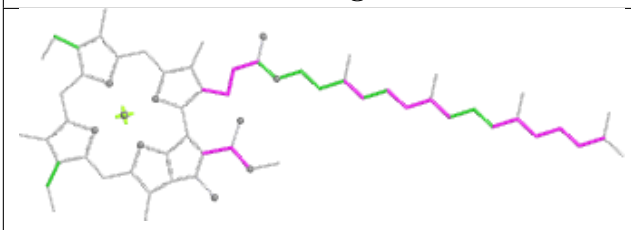
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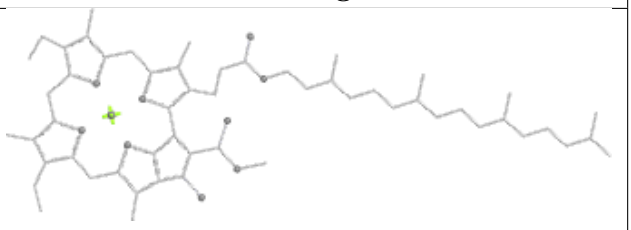
Bond lengths



Bond angles

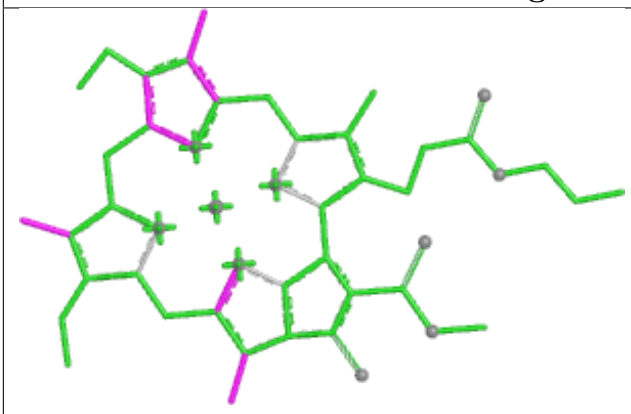


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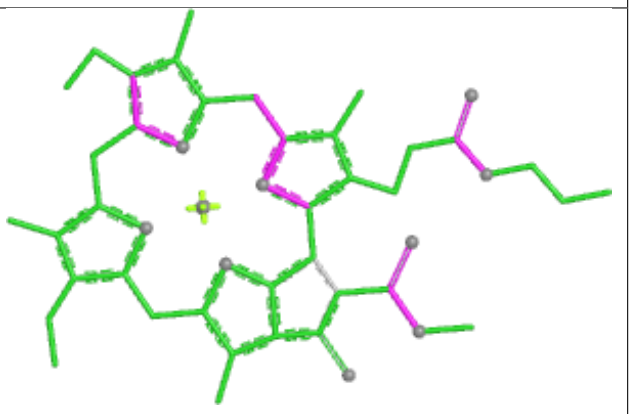


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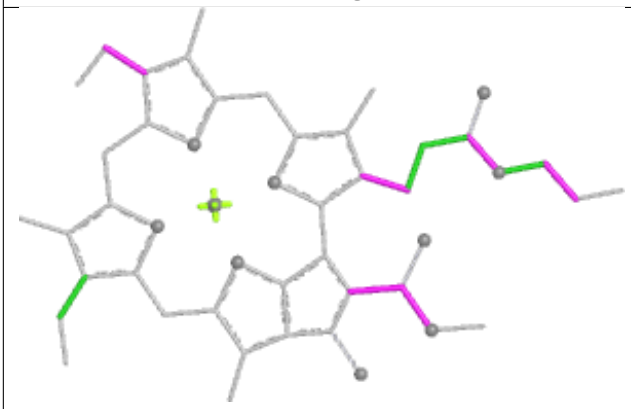
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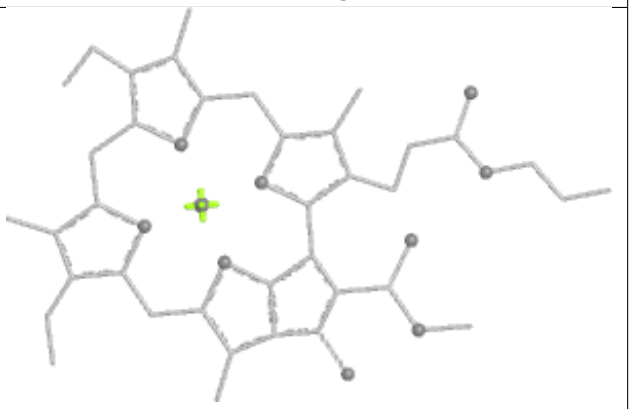
Bond lengths



Bond angles

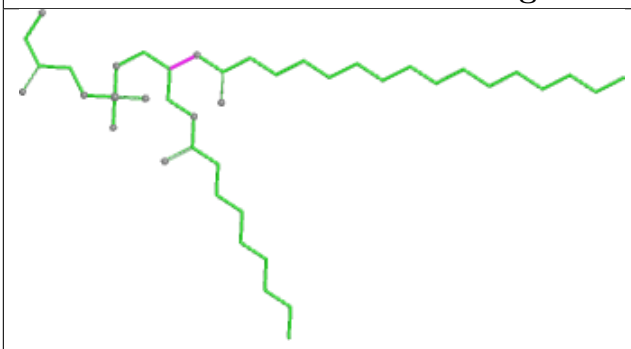


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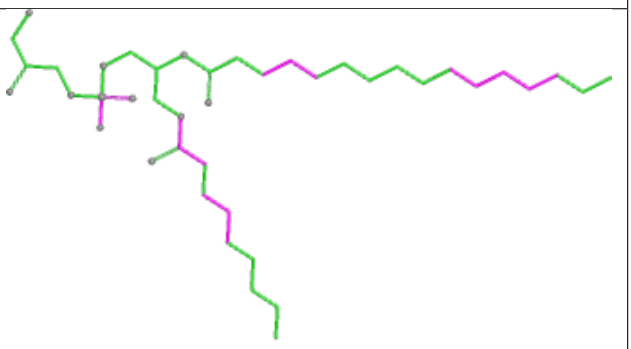


Rings

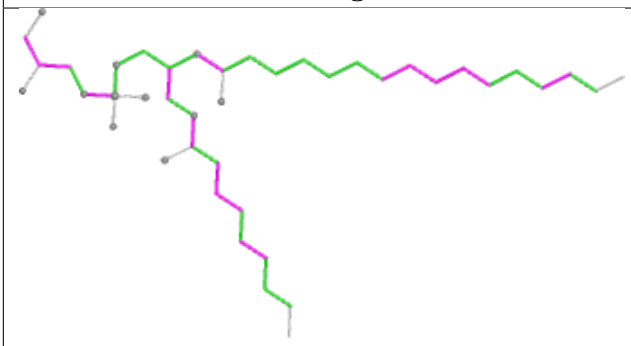
Ligand LHG r 2630



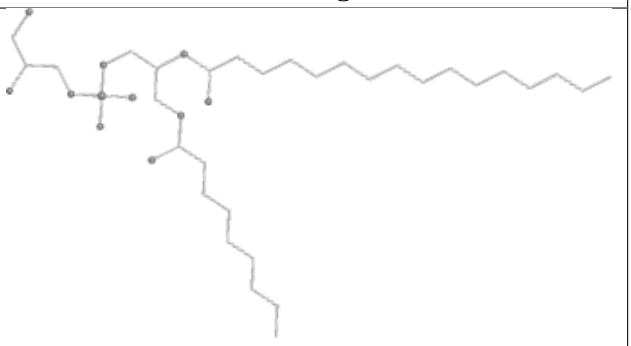
Bond lengths



Bond angles

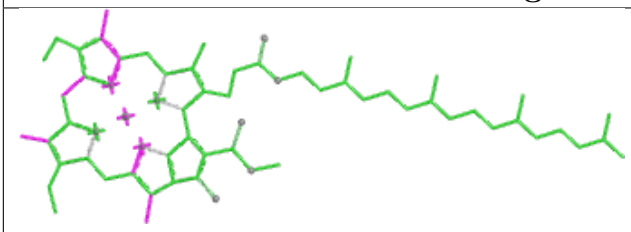


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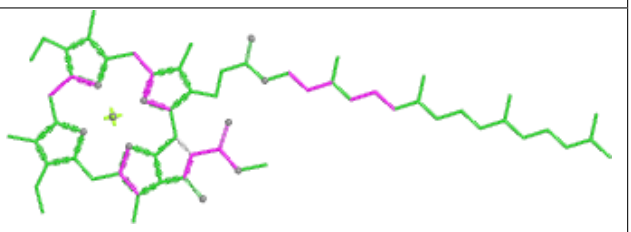


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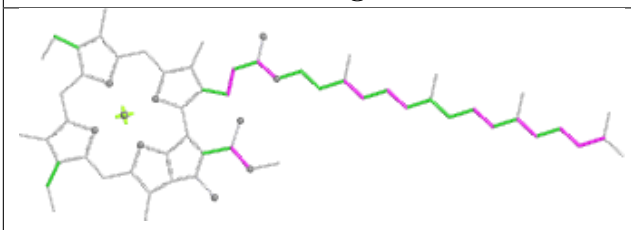
Ligand CLA C 505



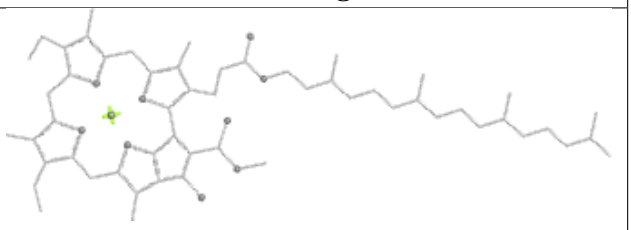
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Bond angles

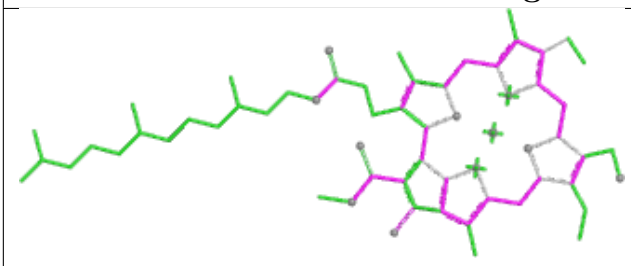


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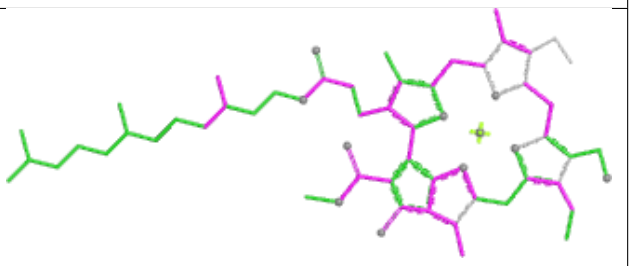


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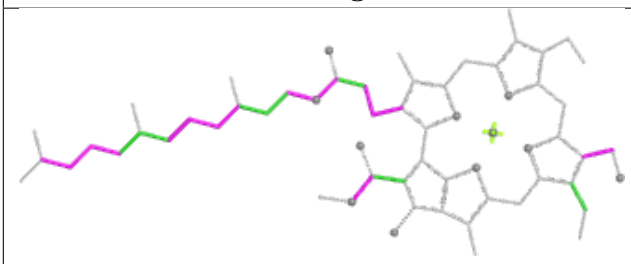
Ligand CHL R 608



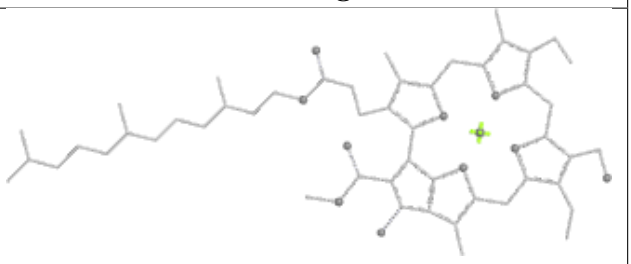
Bond lengths



Bond angles

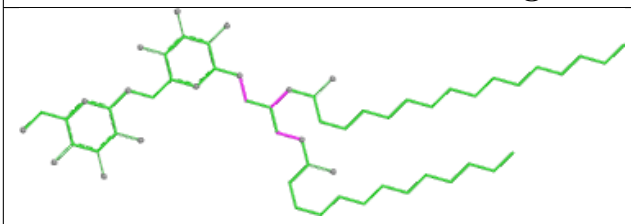


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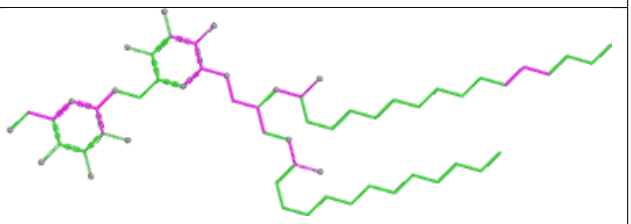


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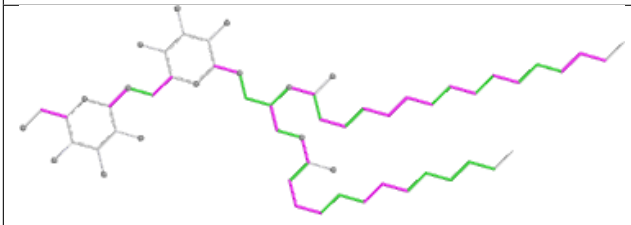
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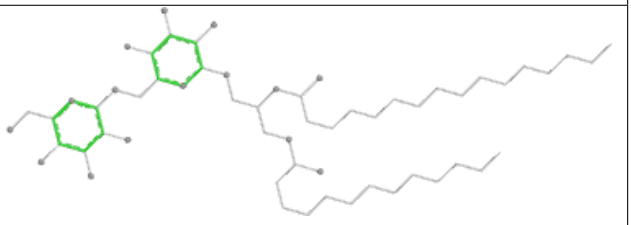
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Bond angles

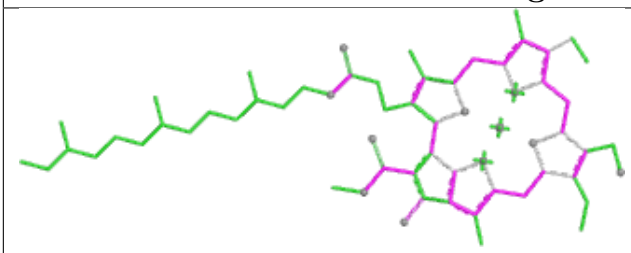


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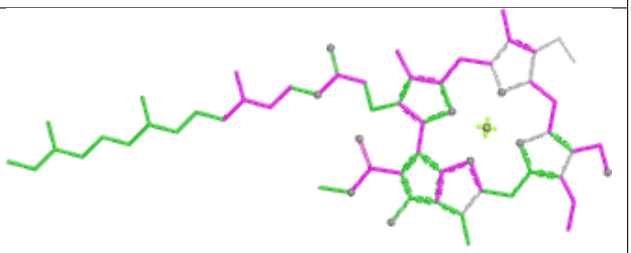


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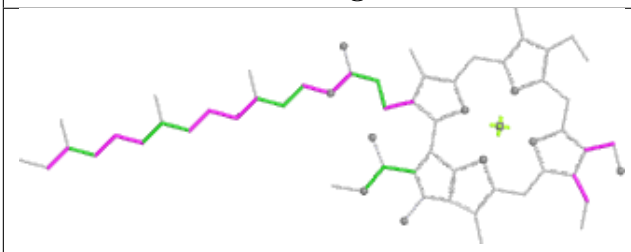
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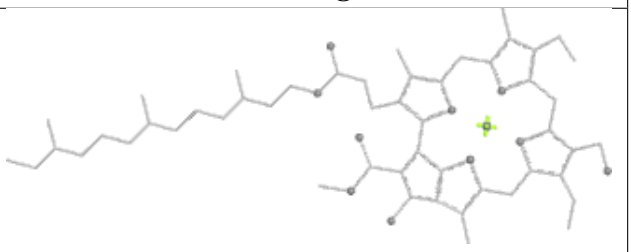
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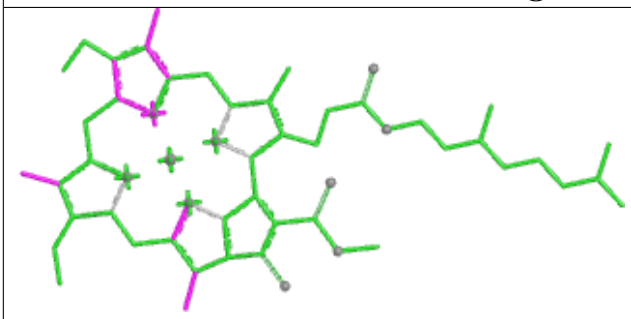


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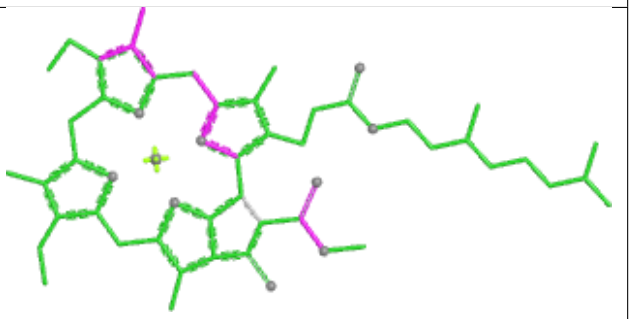


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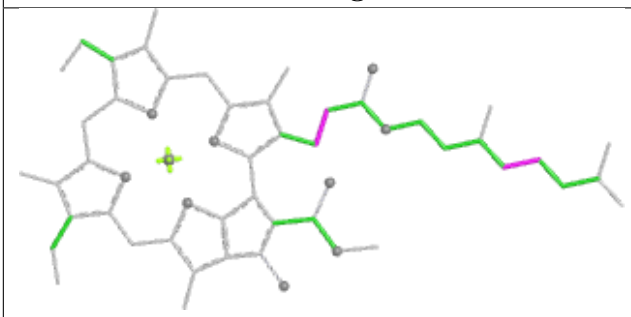
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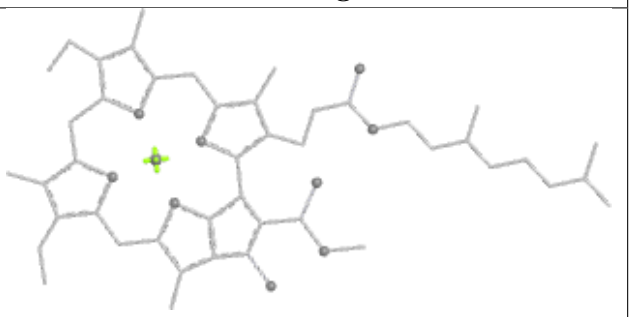
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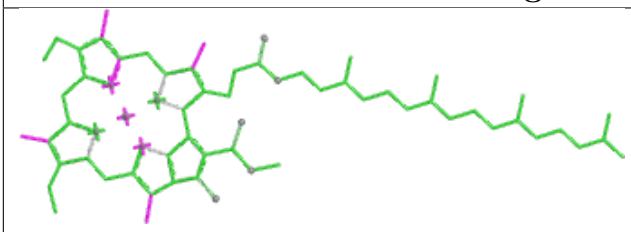


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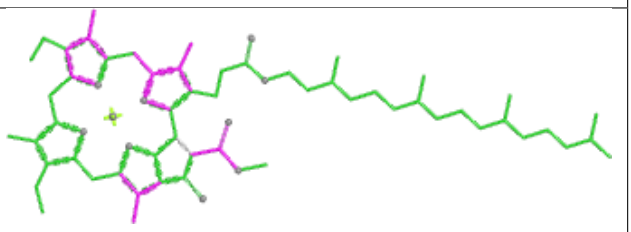


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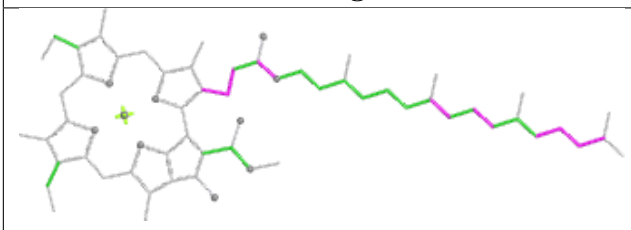
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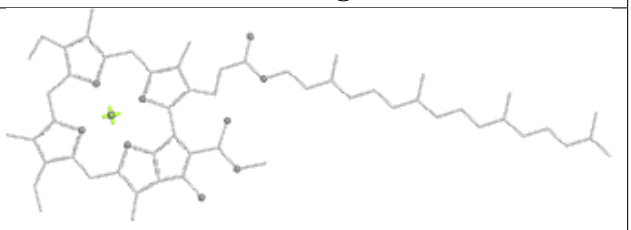
Bond lengths



Bond angles



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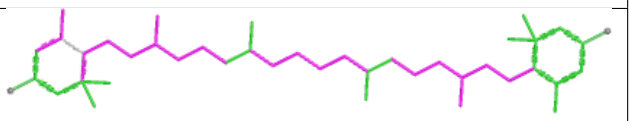


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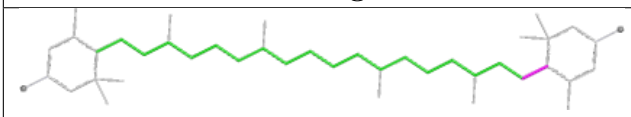
Ligand LUT Y 1620



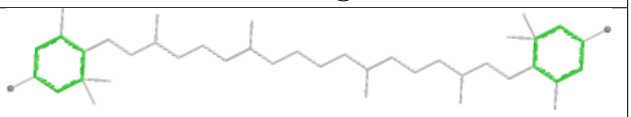
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Bond angles

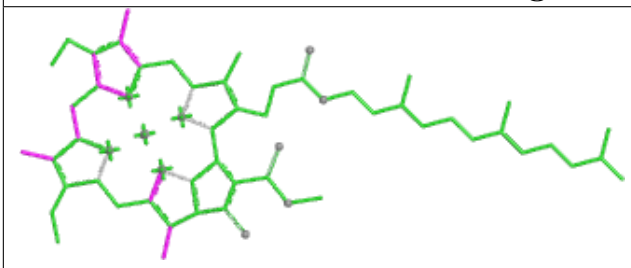


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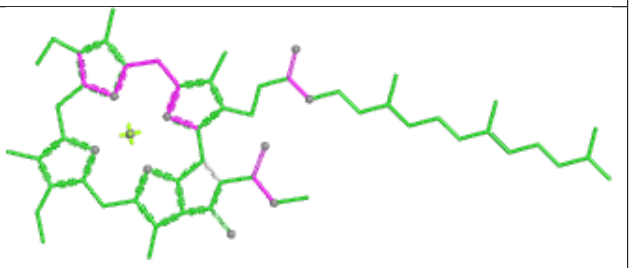


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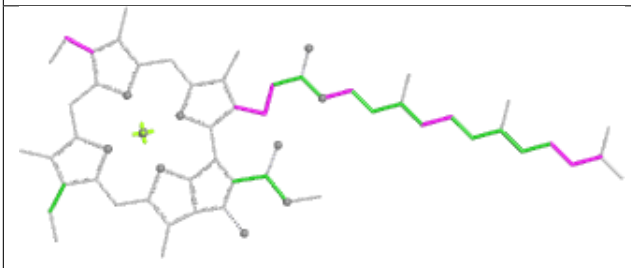
Ligand CLA 7 610



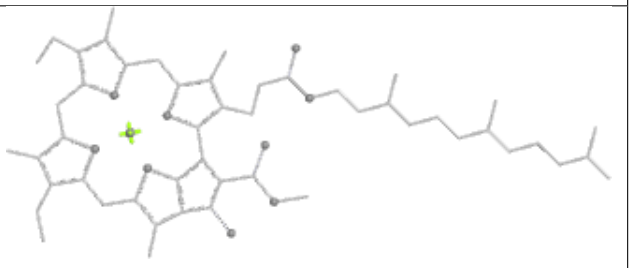
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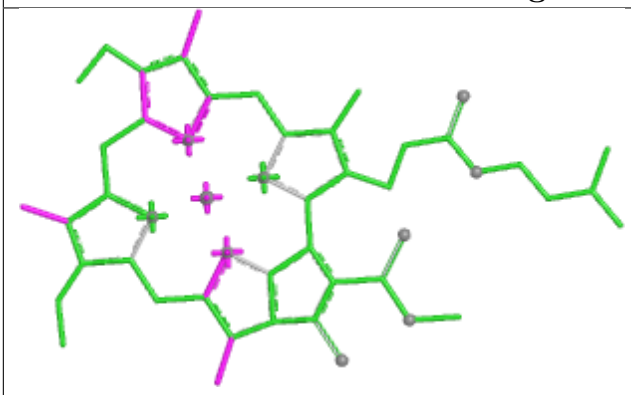


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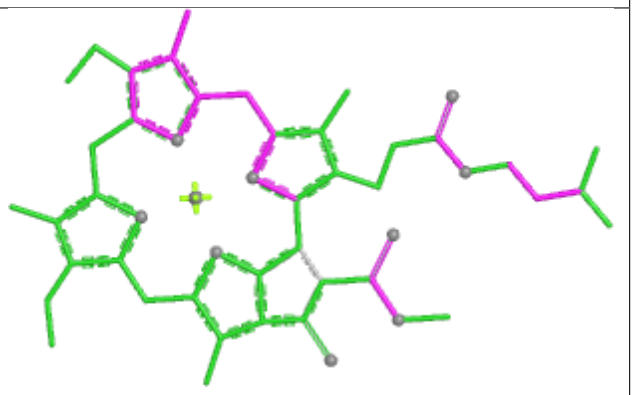


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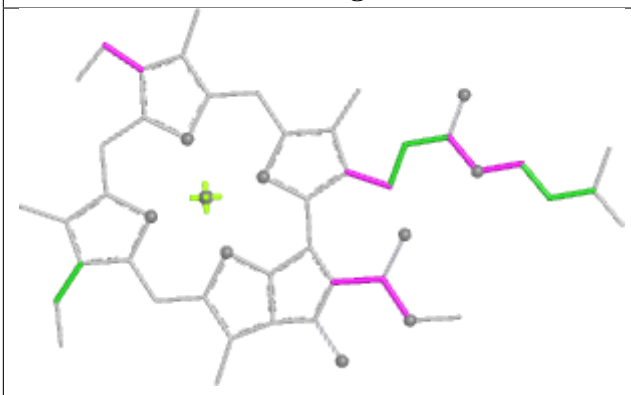
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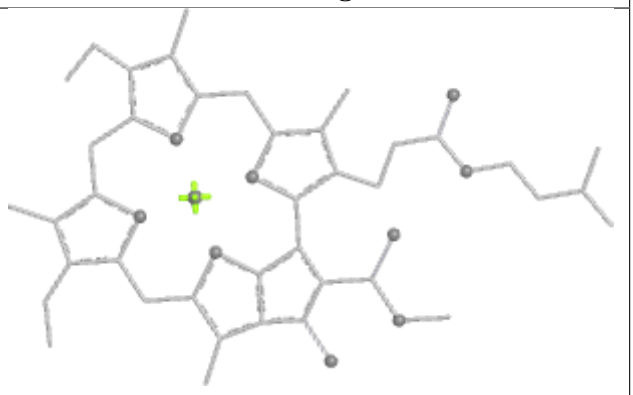
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Bond angles

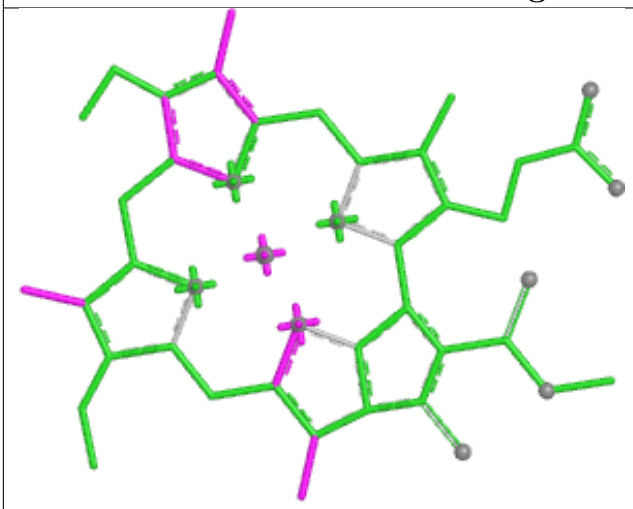


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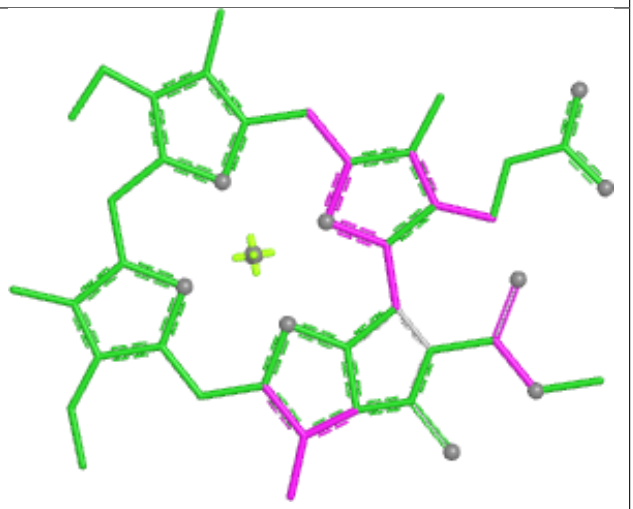


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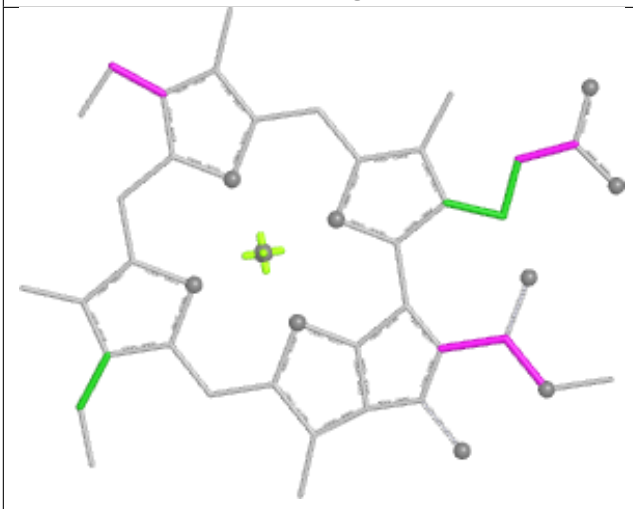
Ligand CLA 7 612



Bond lengths



Bond angles

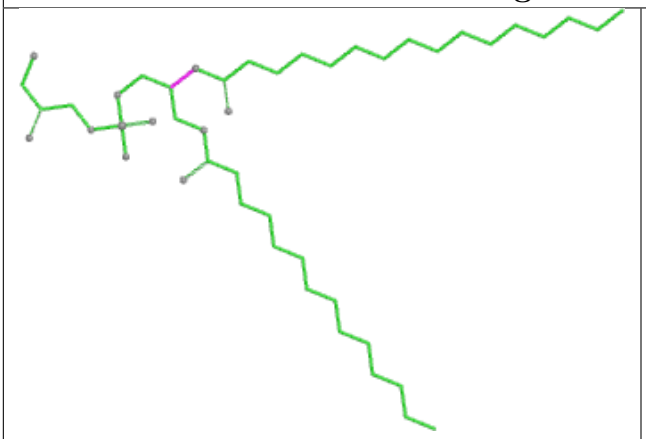


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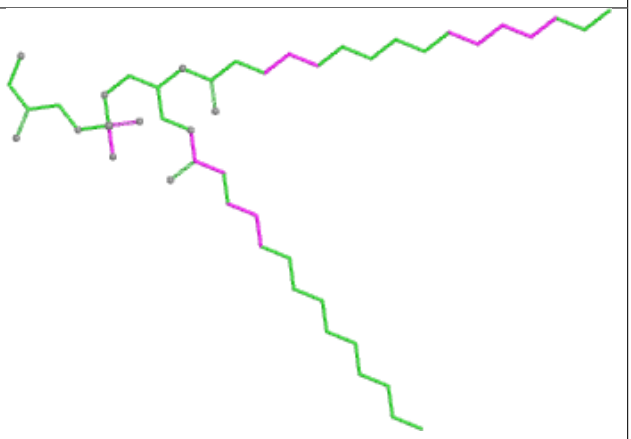


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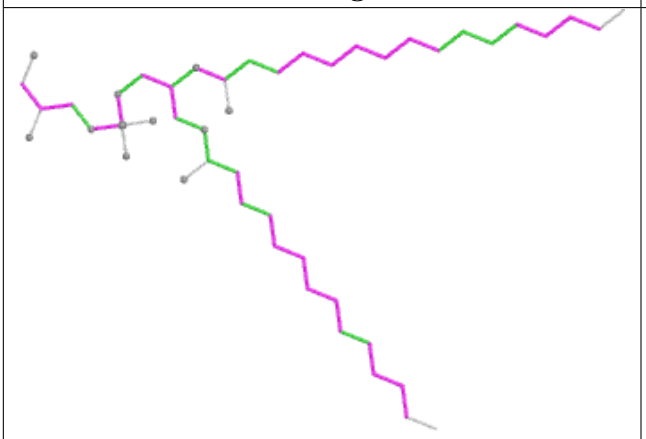
Ligand LHG B 2630



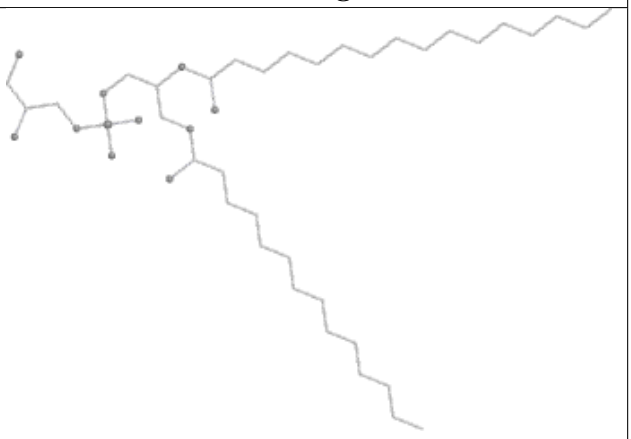
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Bond angles

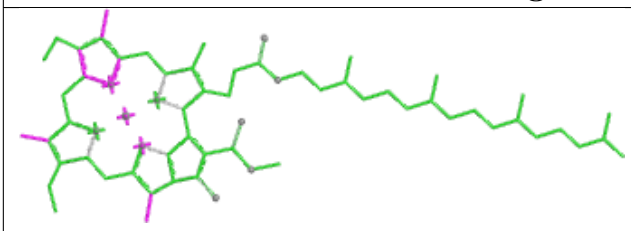


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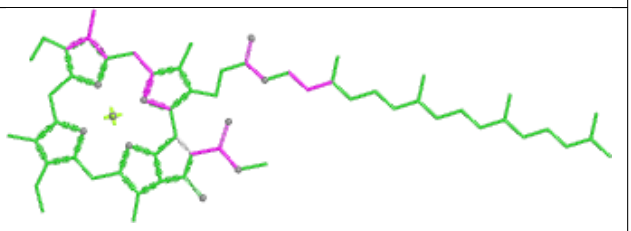


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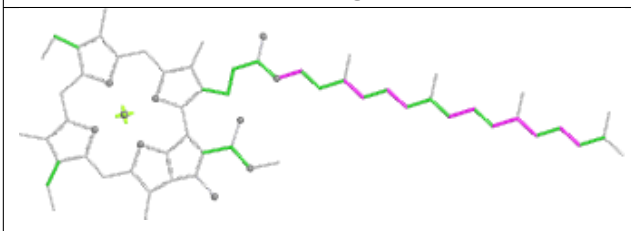
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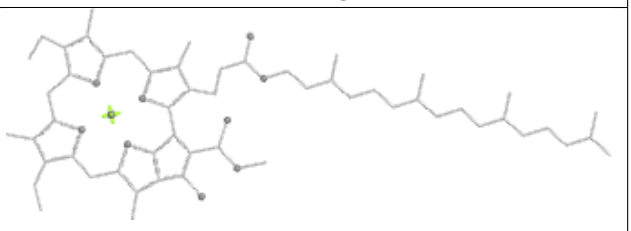
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Bond angles

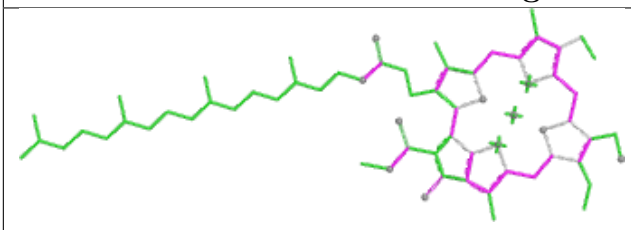


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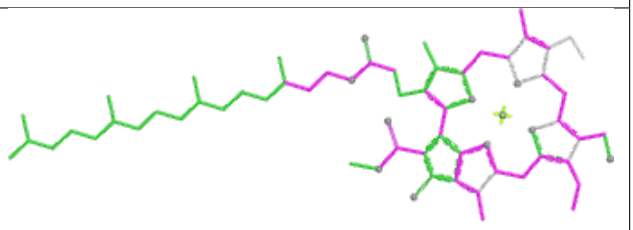


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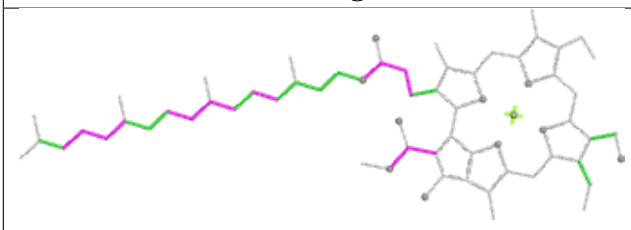
Ligand CHL N 601



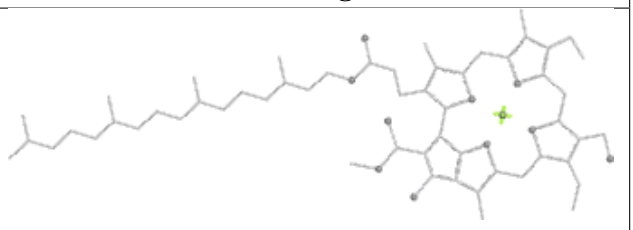
Bond lengths



Bond angles



Torsions

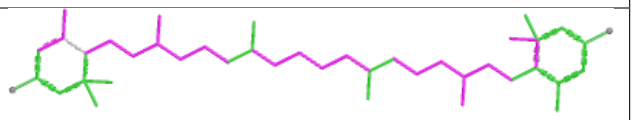


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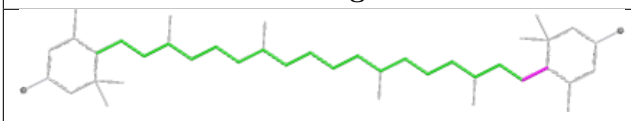
Ligand LUT N 1620



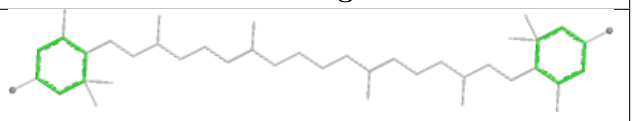
Bond lengths



Bond angles

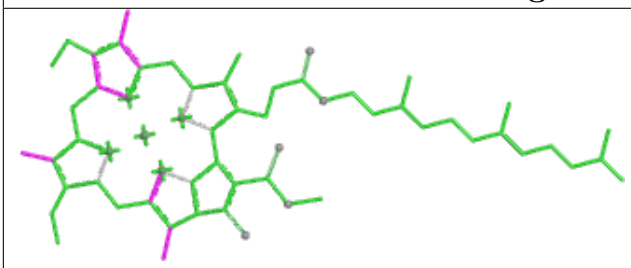


Torsions

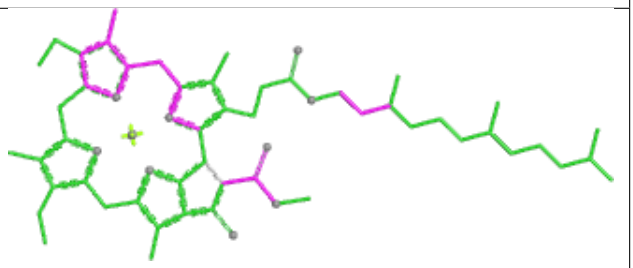


Rings

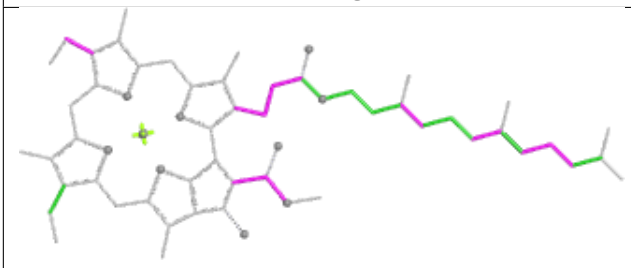
Ligand CLA 7 602



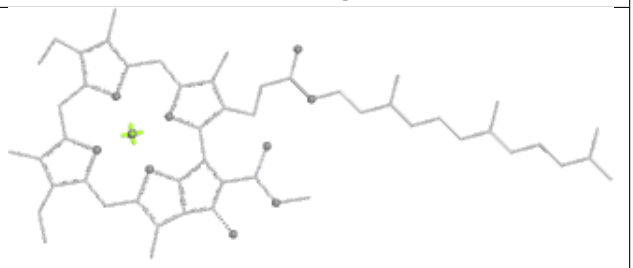
Bond lengths



Bond angles

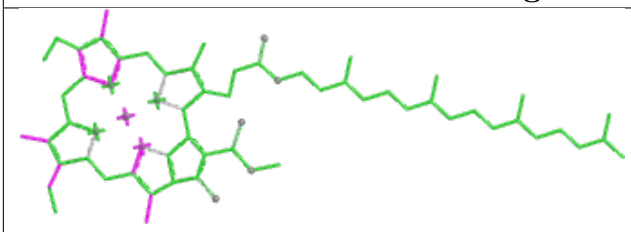


Torsions

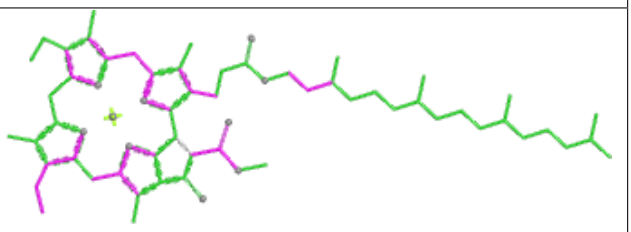


Rings

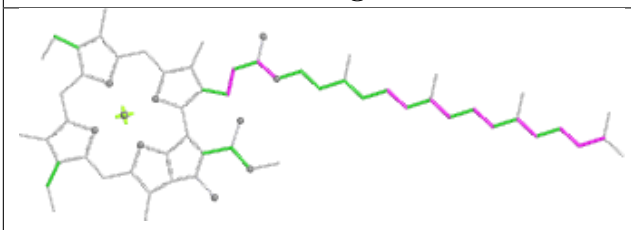
Ligand CLA N 603



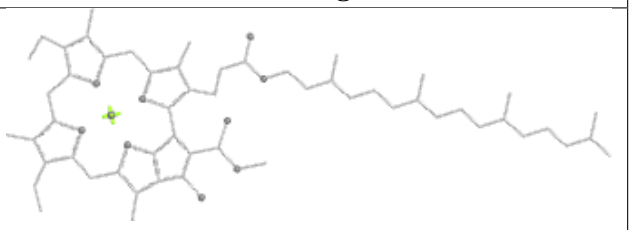
Bond lengths



Bond angles

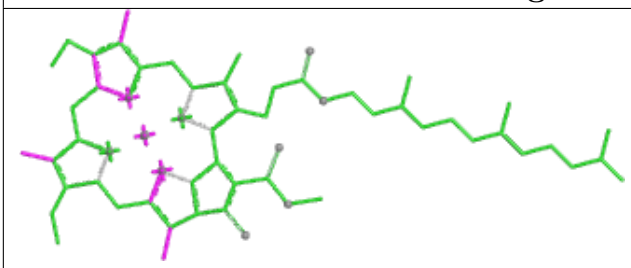


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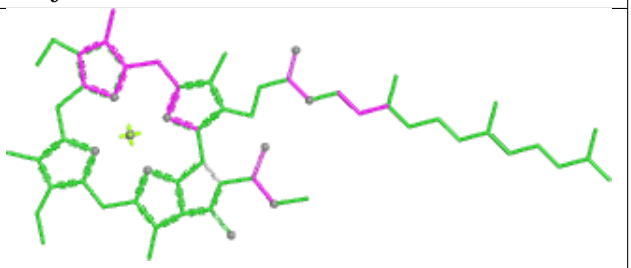


Rings

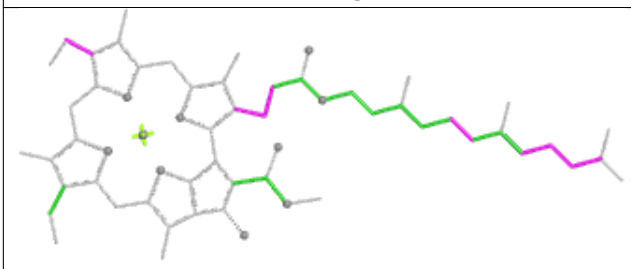
Ligand CLA y 610



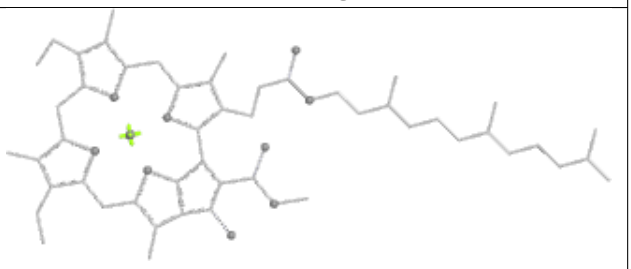
Bond lengths



Bond angles

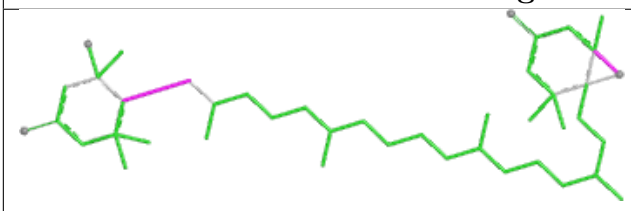


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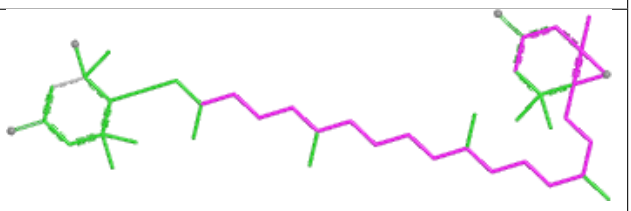


Rings

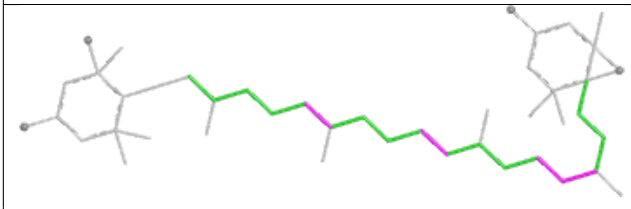
Ligand NEX 1 1623



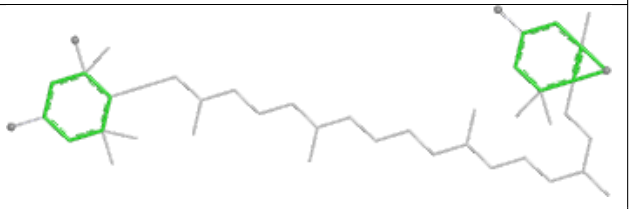
Bond lengths



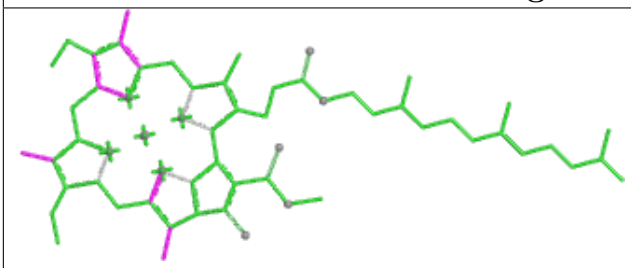
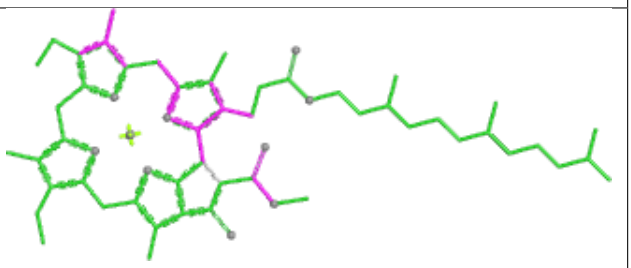
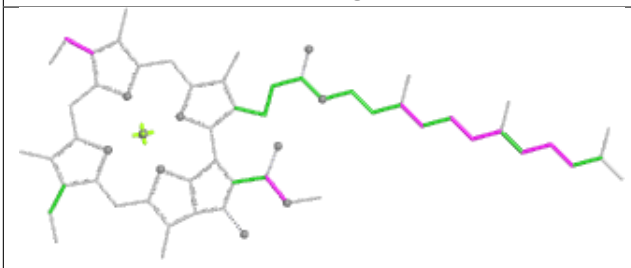
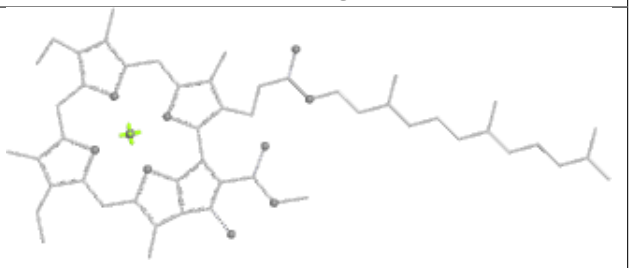
Bond angles

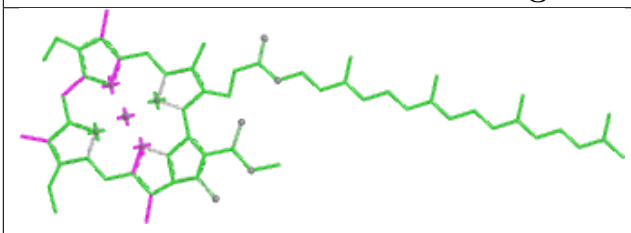
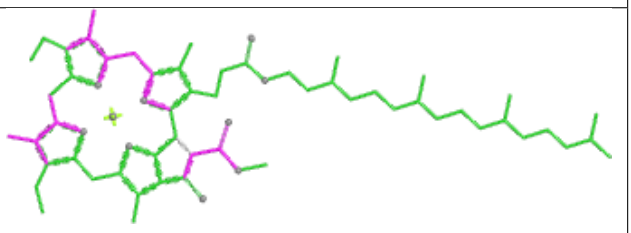
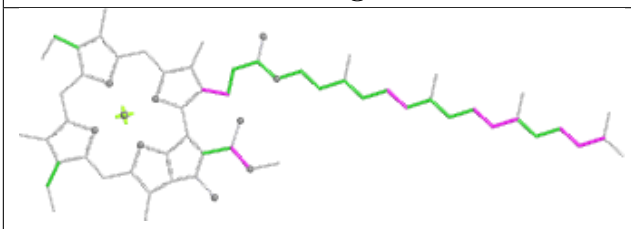
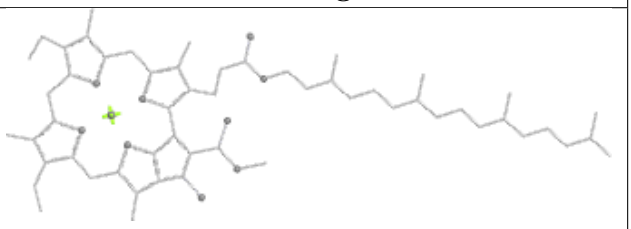


Torsions

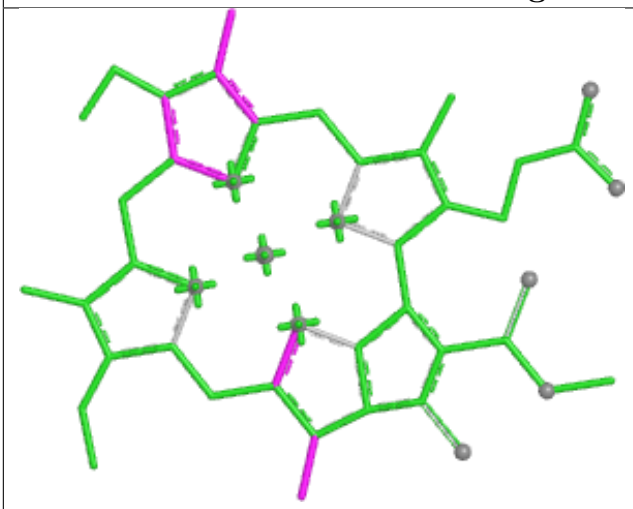


Rings

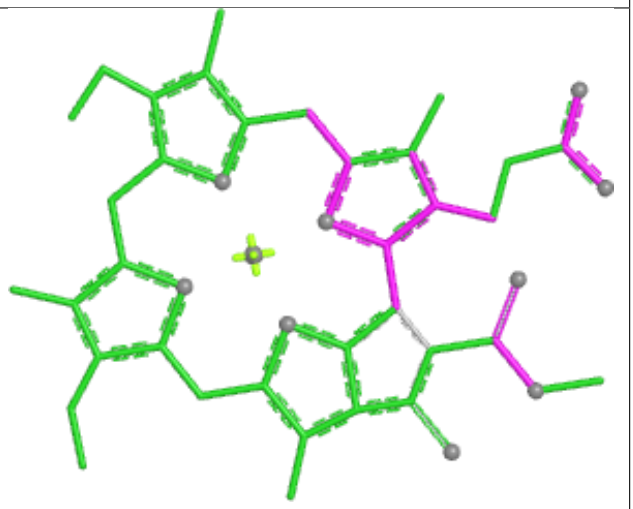
Ligand CLA n 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

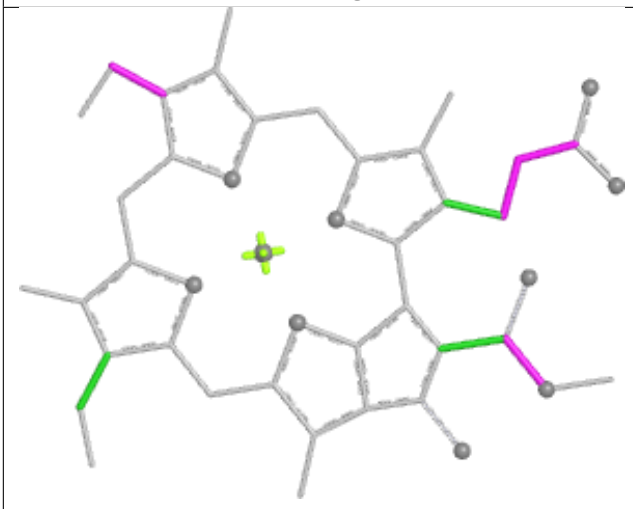
Ligand CLA 4 612



Bond lengths



Bond angles

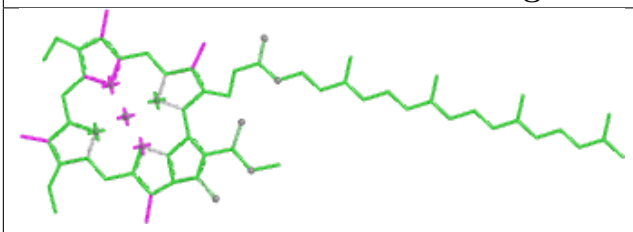


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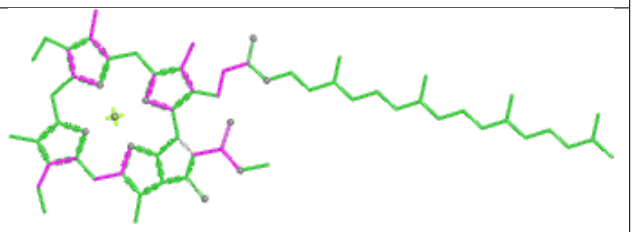


Rings

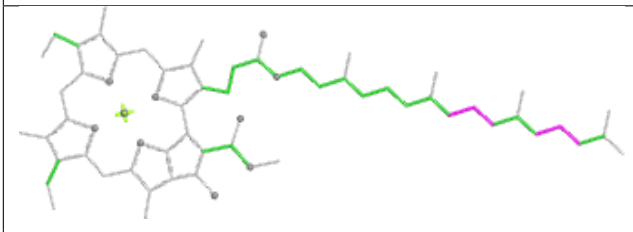
Ligand CLA D 402



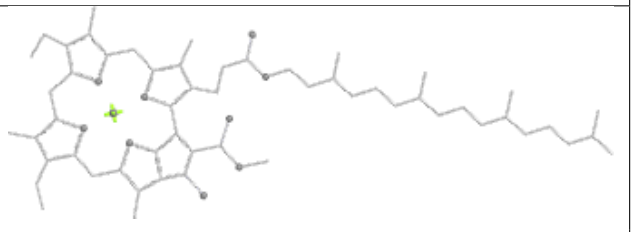
Bond lengths



Bond angles

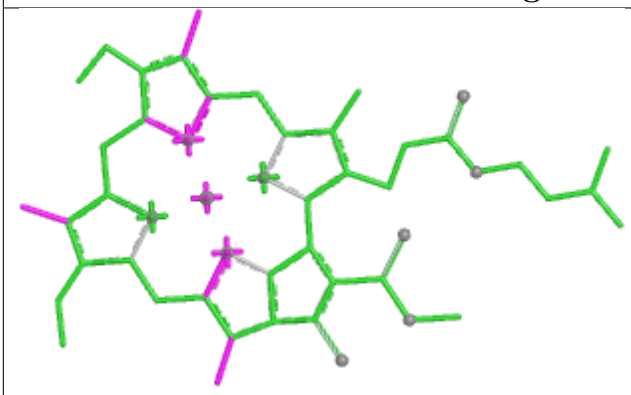


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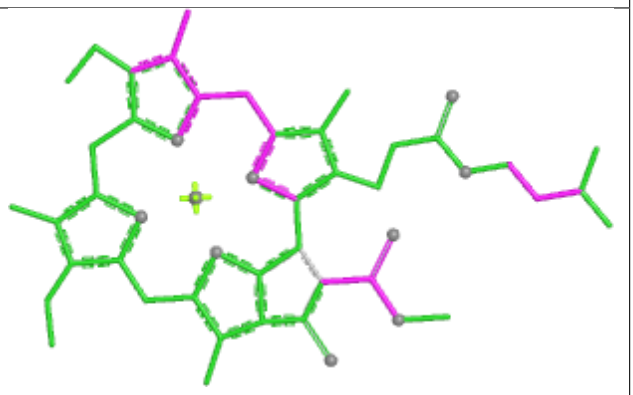


Rings

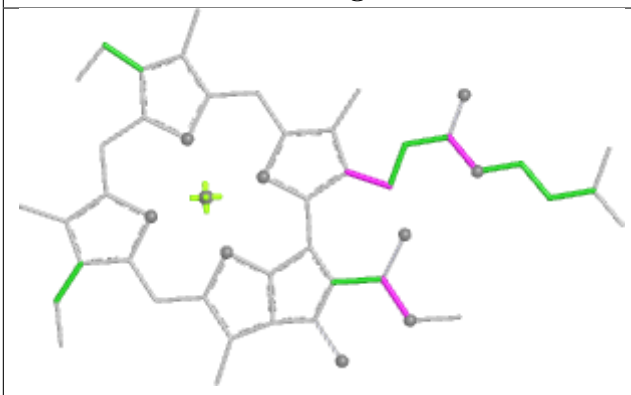
Ligand CLA G 604



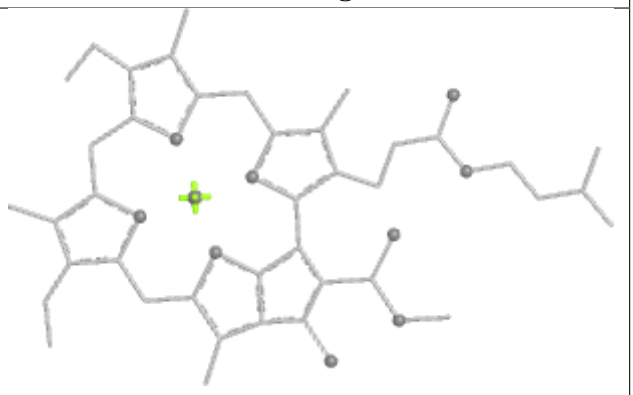
Bond lengths



Bond angles

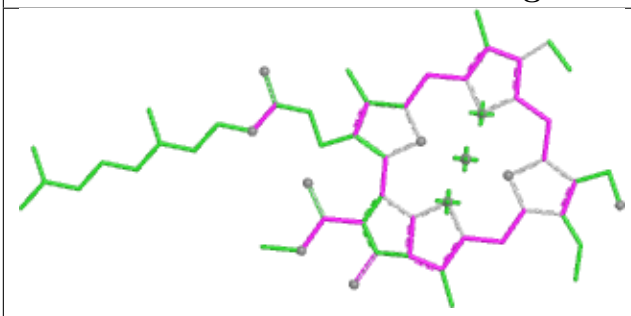


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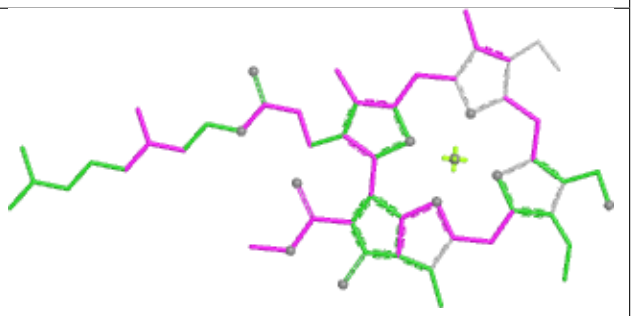


Rings

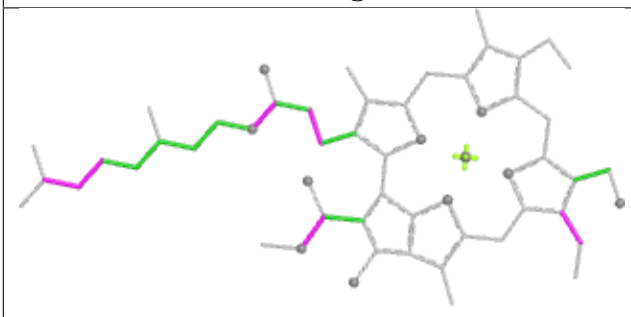
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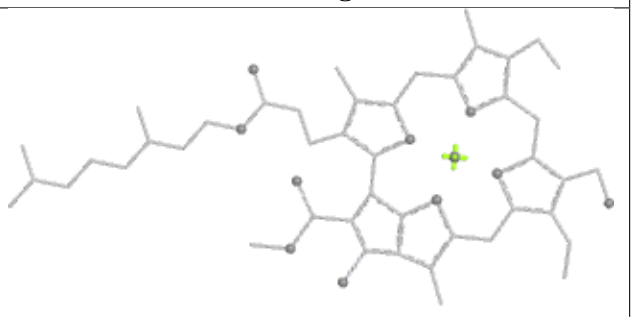
Bond lengths



Bond angles

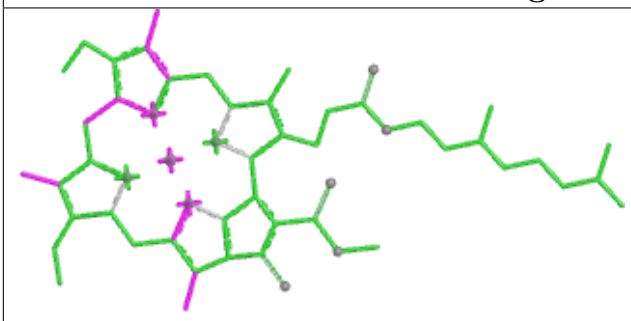


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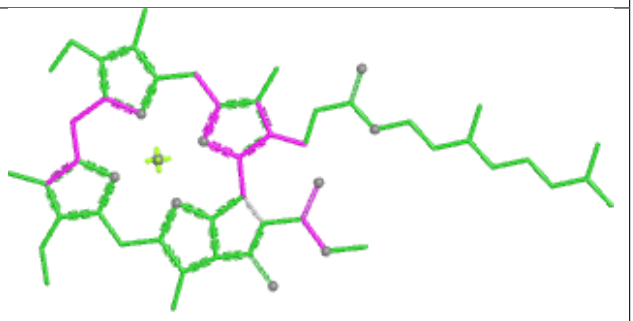


Rings

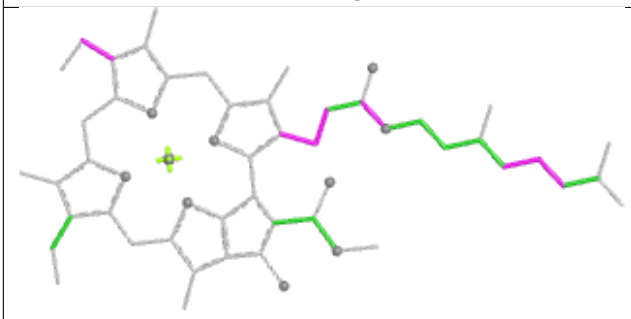
Ligand CLA 3 611



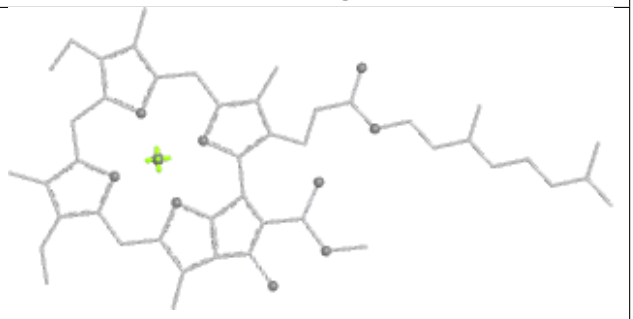
Bond lengths



Bond angles

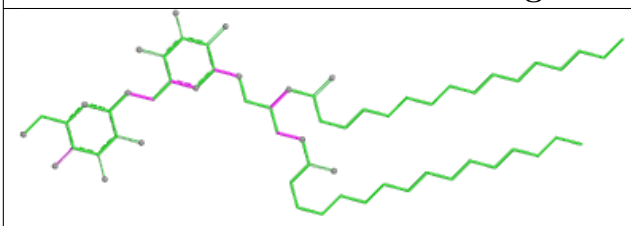


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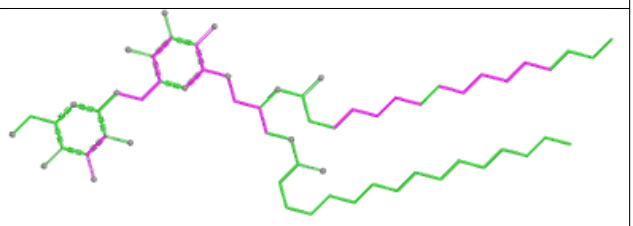


Rings

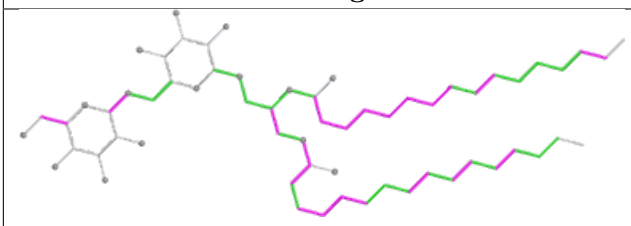
Ligand DGD c 519



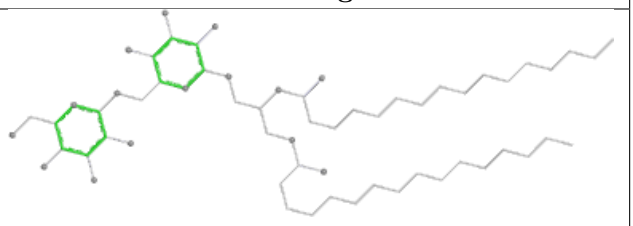
Bond lengths



Bond angles

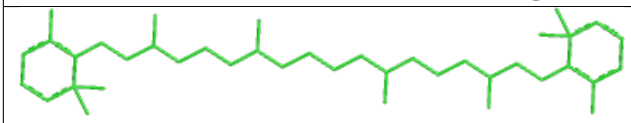


Torsions

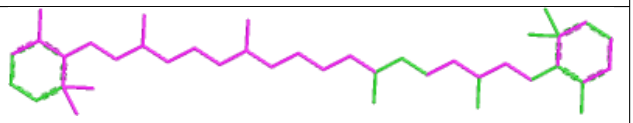


Rings

Ligand BCR c 516



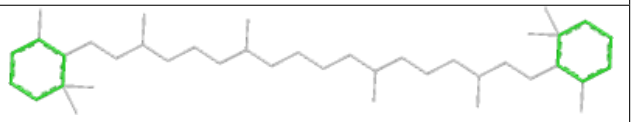
Bond lengths



Bond angles

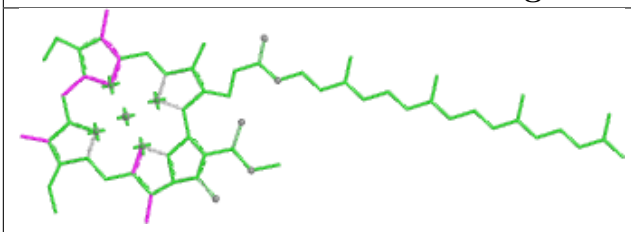


Torsions

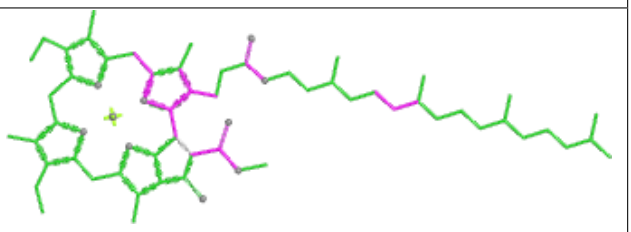


Rings

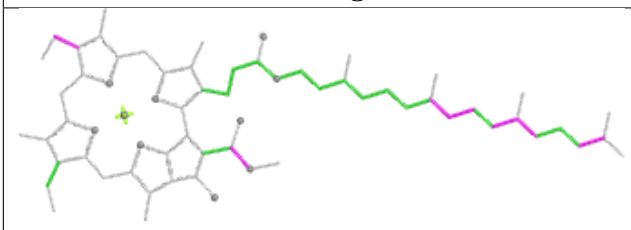
Ligand CLA B 616



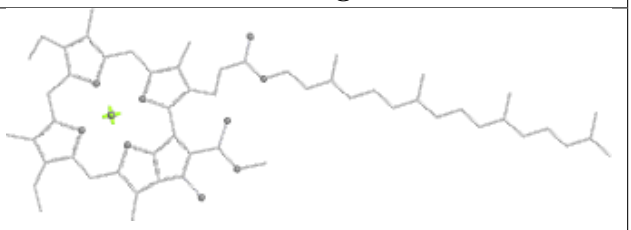
Bond lengths



Bond angles

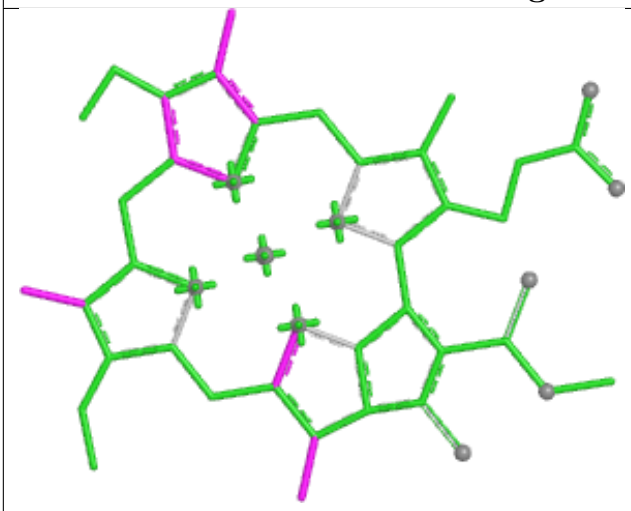


Torsions

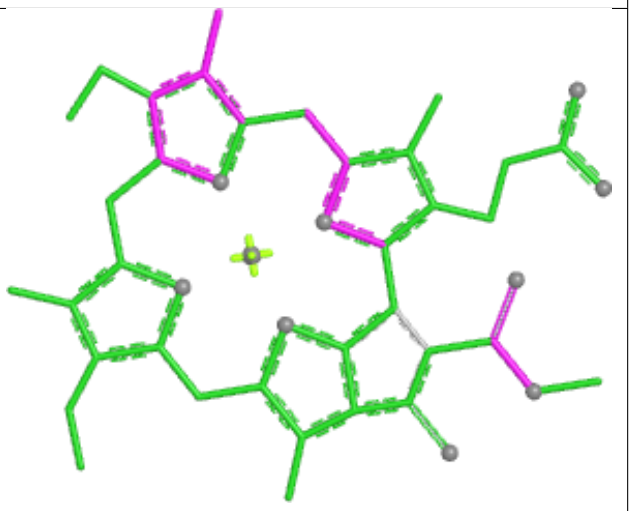


Rings

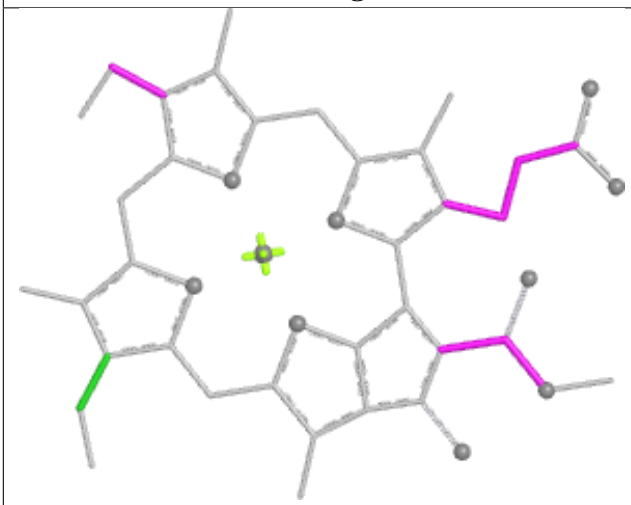
Ligand CLA 7 604



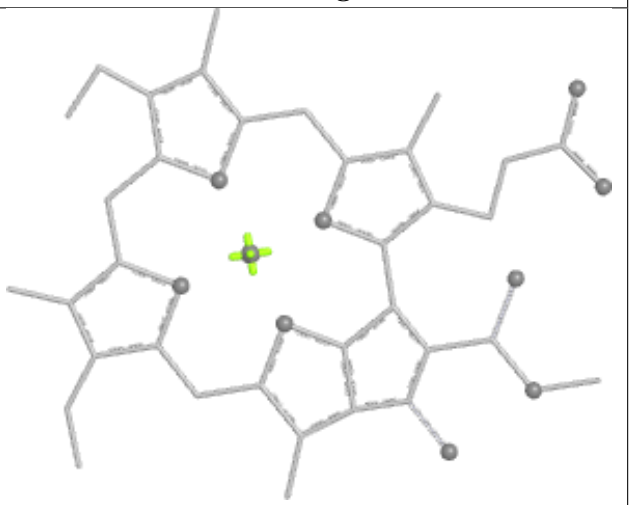
Bond lengths



Bond angles

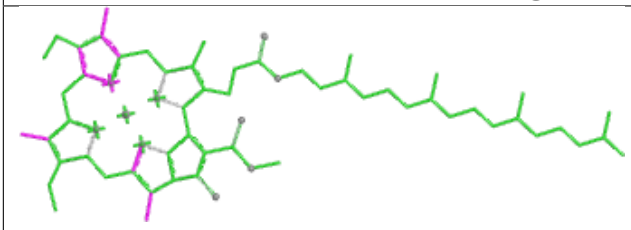


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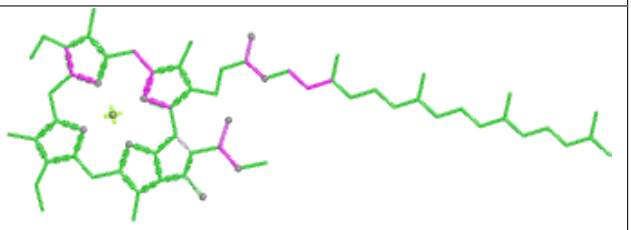


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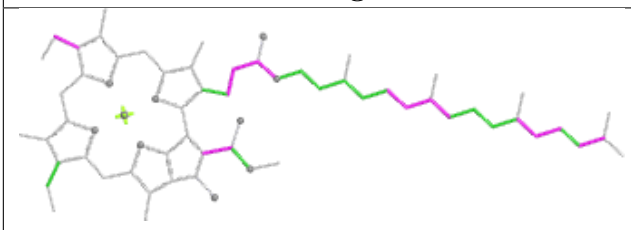
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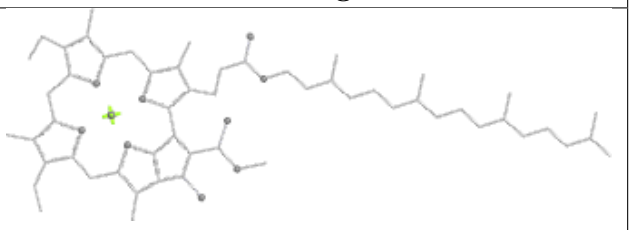
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Bond angles

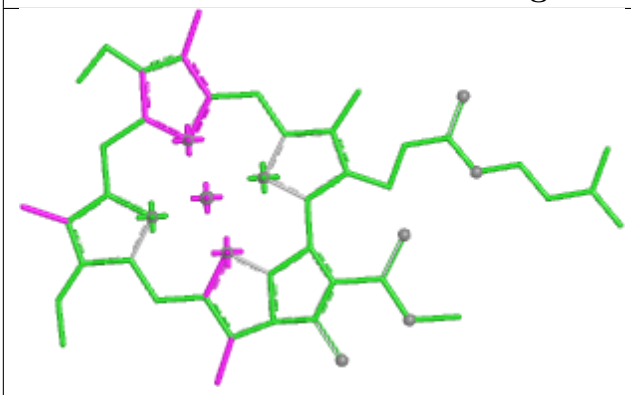


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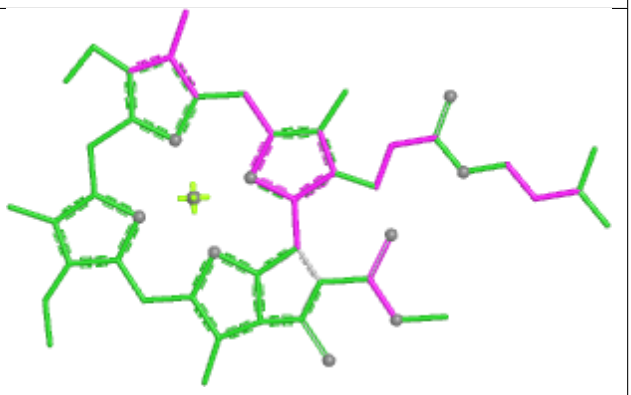


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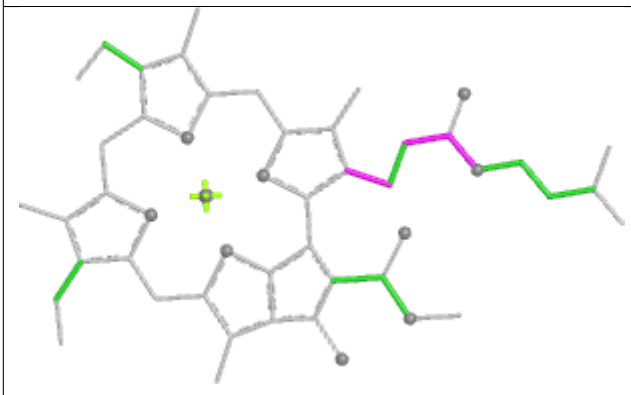
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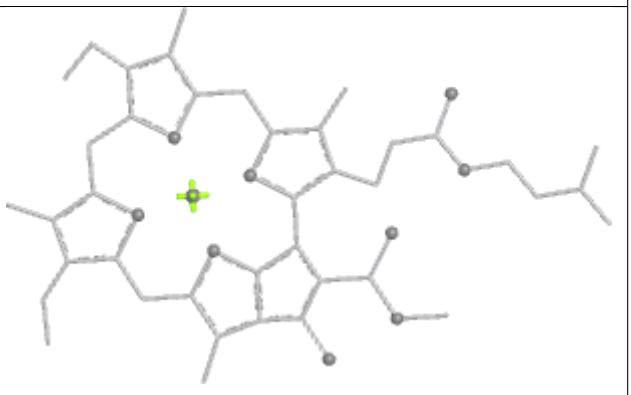
Bond lengths



Bond angles

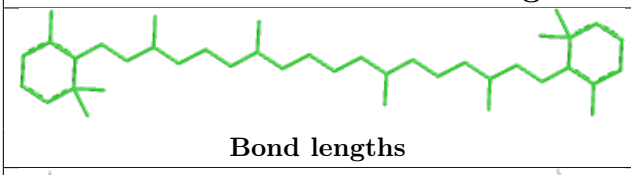


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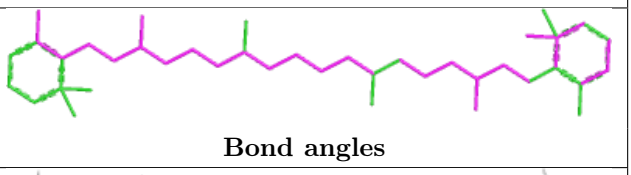


Rings

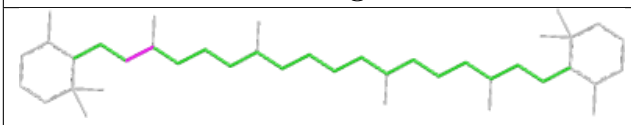
Ligand BCR B 619



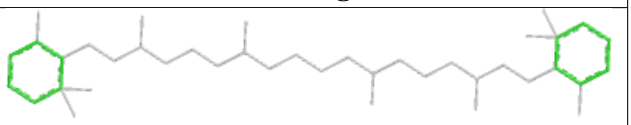
Bond lengths



Bond angles

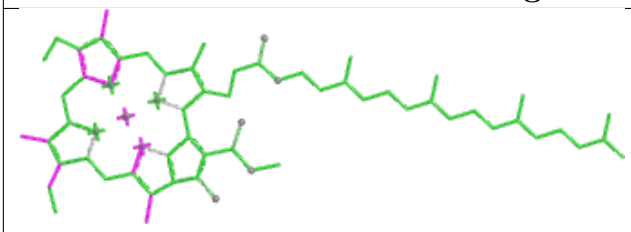


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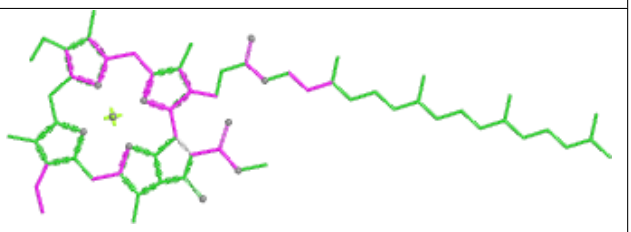


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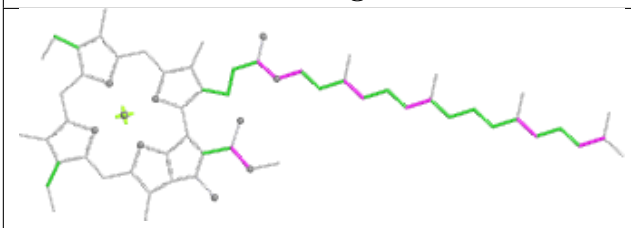
Ligand CLA Y 603



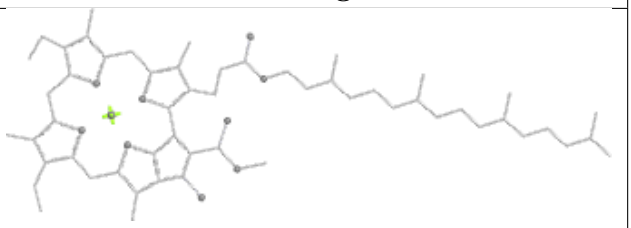
Bond lengths



Bond angles

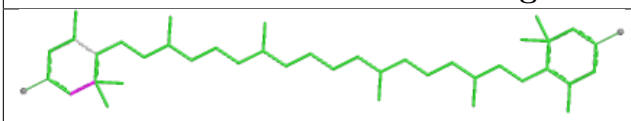


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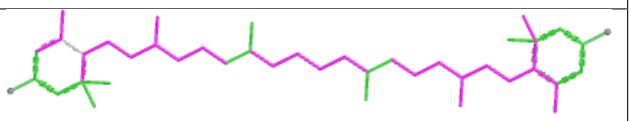


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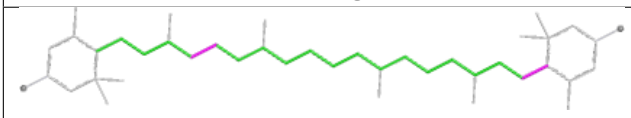
Ligand LUT 6 1621



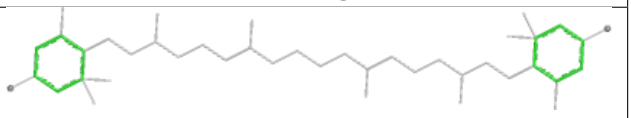
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Bond angles

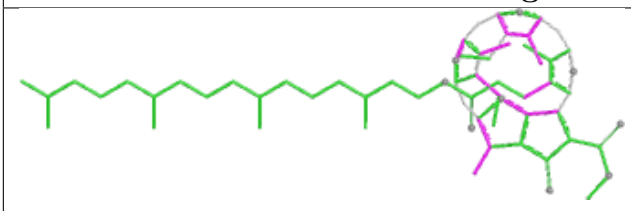


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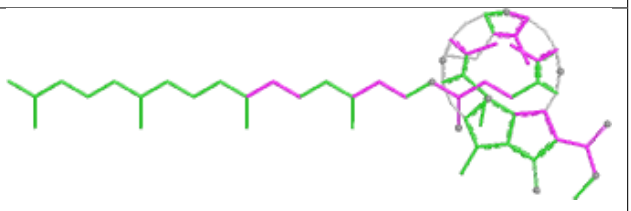


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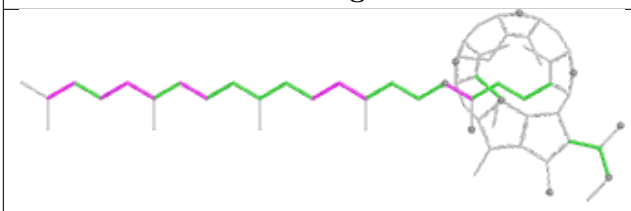
Ligand PHO A 408



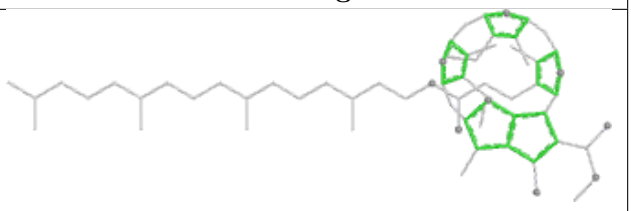
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Bond angles

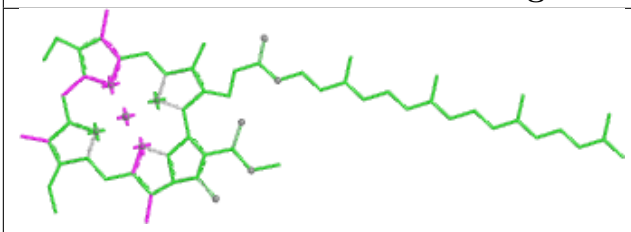


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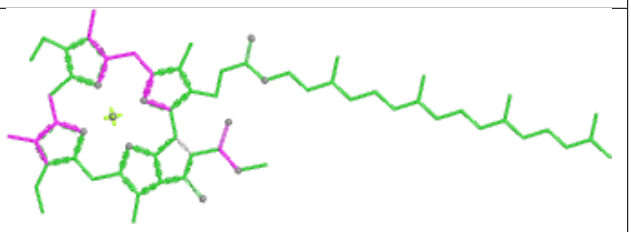


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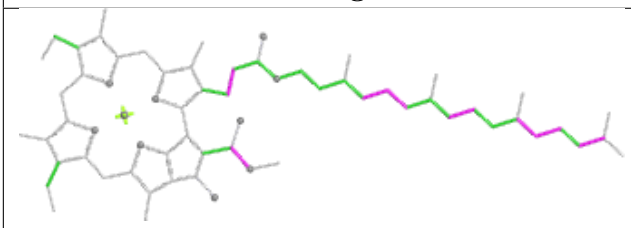
Ligand CLA b 608



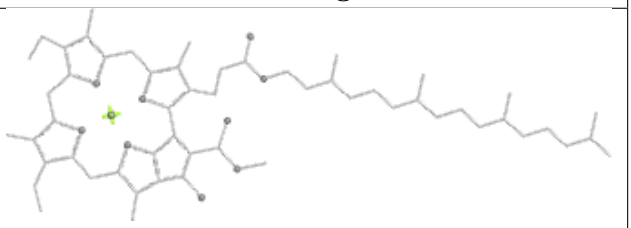
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Bond angles

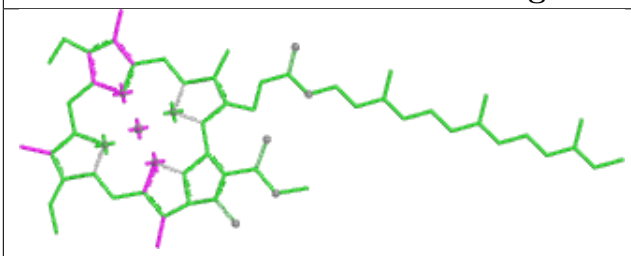


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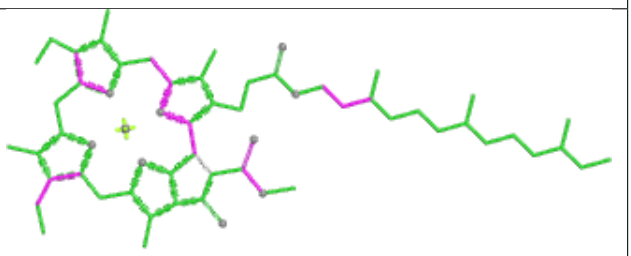


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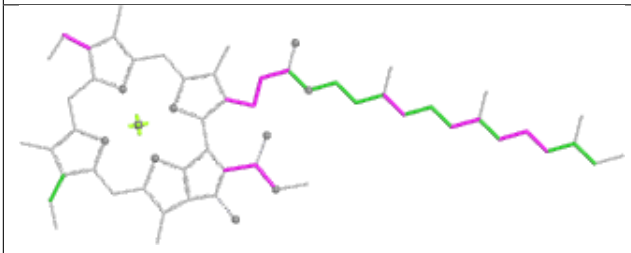
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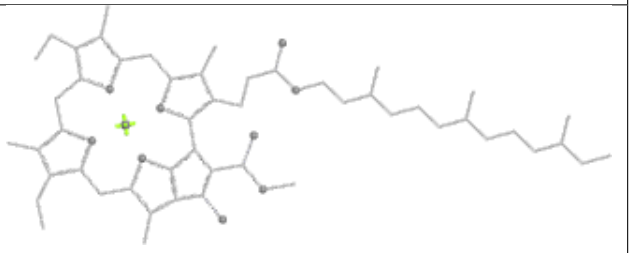
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Bond angles

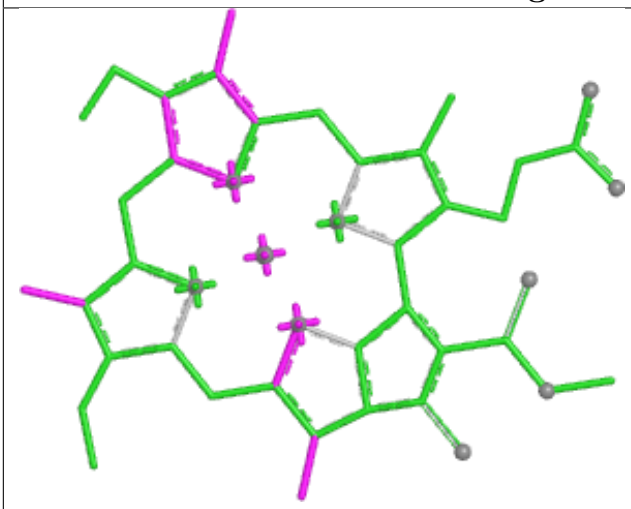


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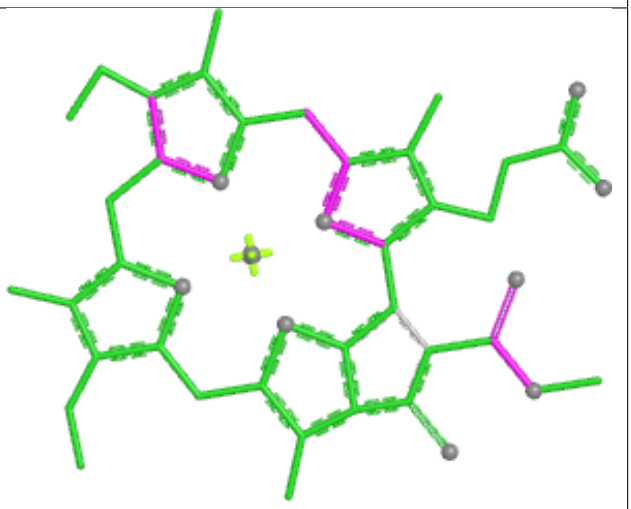


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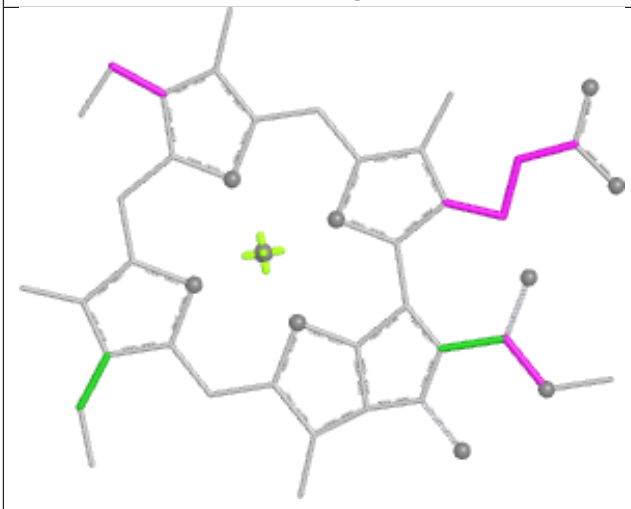
Ligand CLA 1 611



Bond lengths



Bond angles

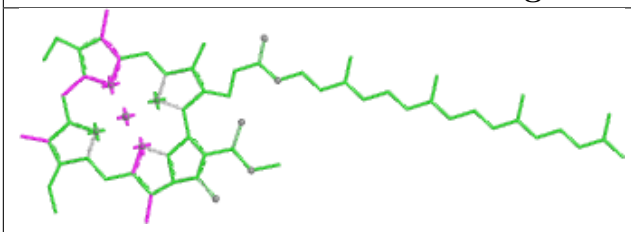


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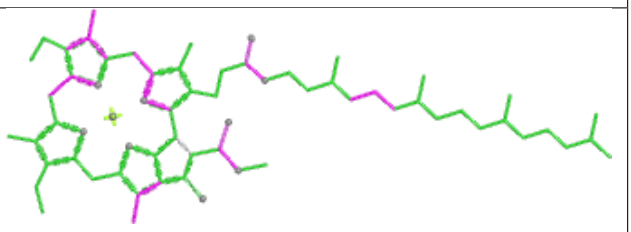


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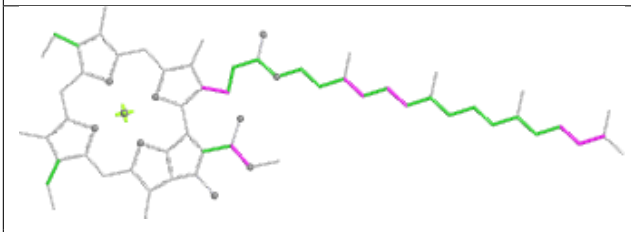
Ligand CLA B 610



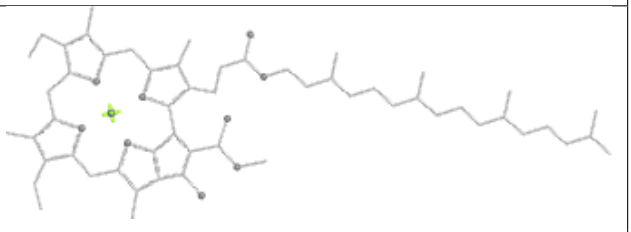
Bond lengths



Bond angles

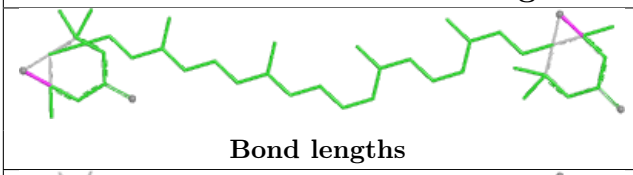


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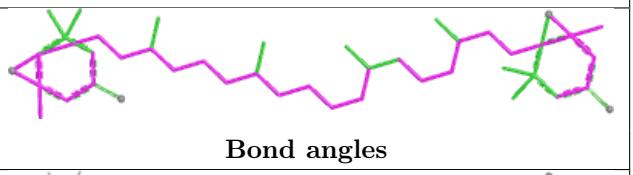


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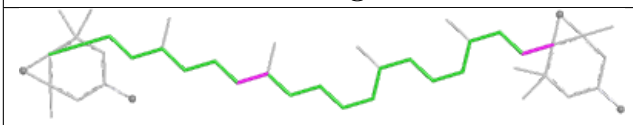
Ligand XAT 2 1622



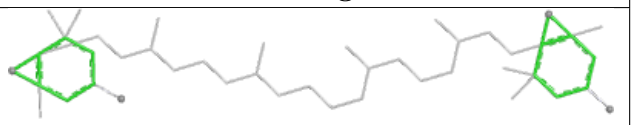
Bond lengths



Bond angles

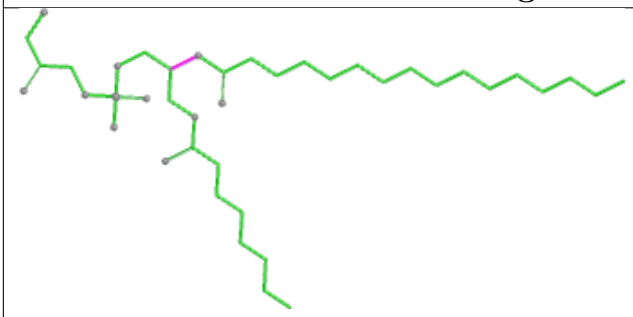


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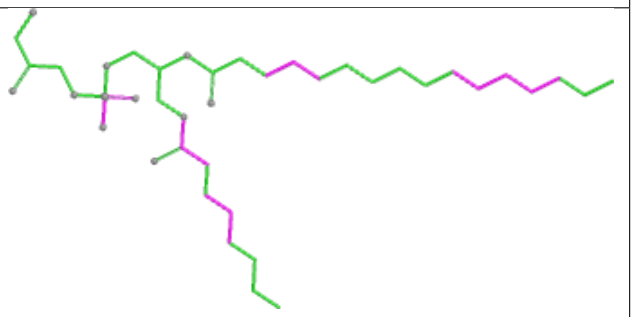


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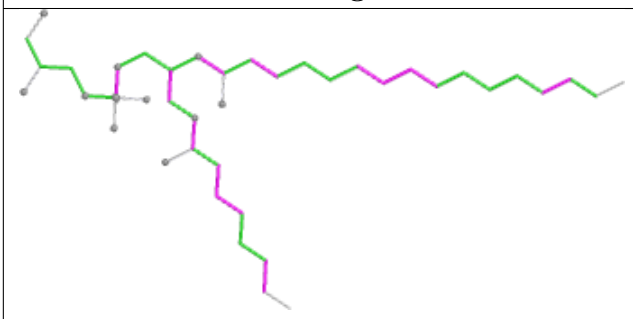
Ligand LHG 1 2630



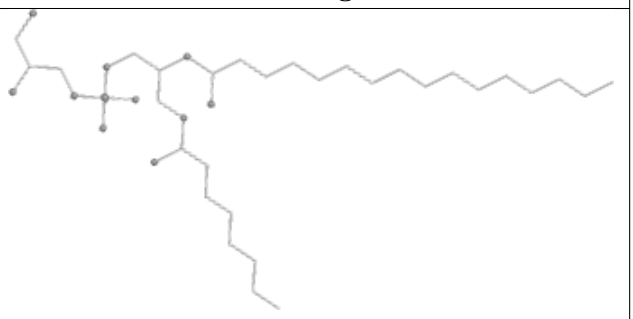
Bond lengths



Bond angles

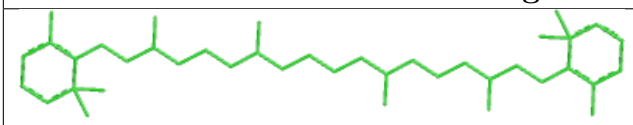


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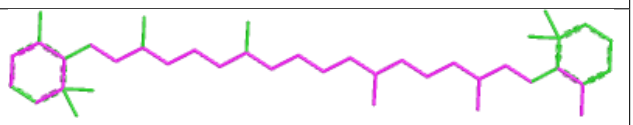


Rings

Ligand BCR C 515



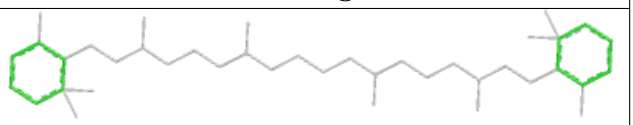
Bond lengths



Bond angles

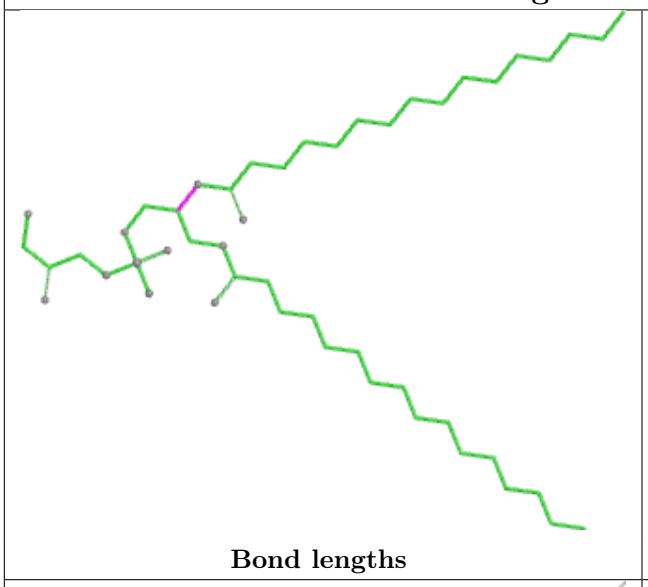


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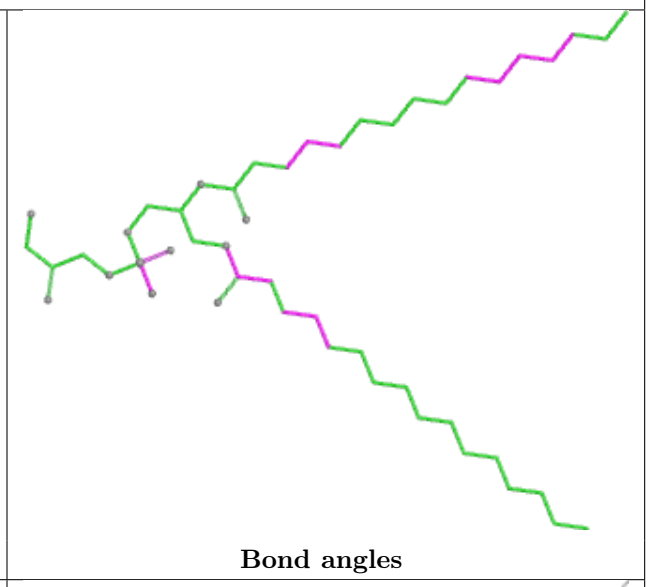


Rings

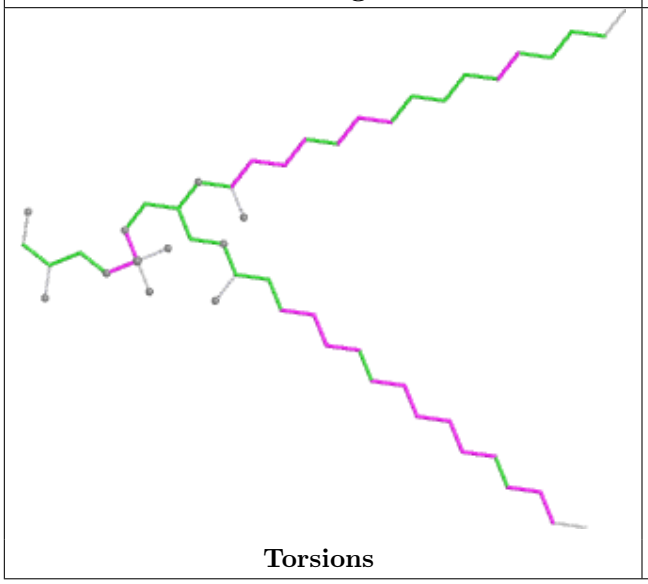
Ligand LHG l 101



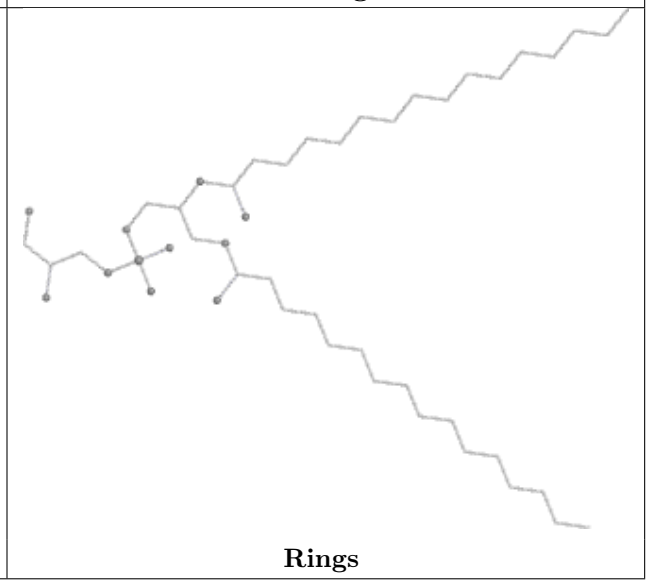
Bond lengths



Bond angles

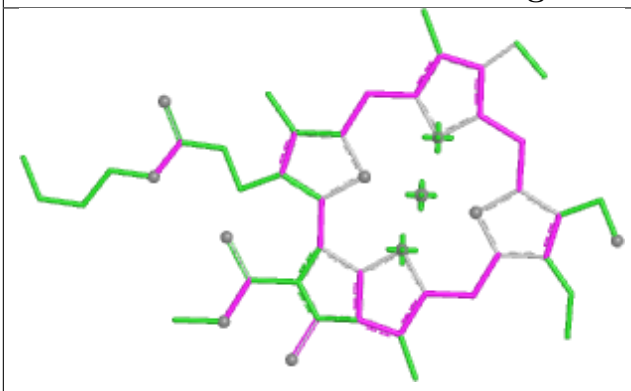


Torsions

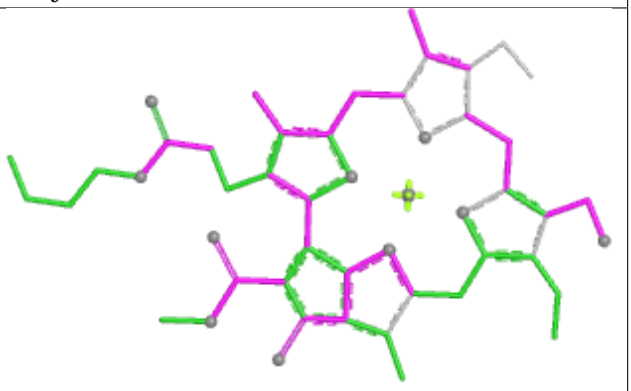


Rings

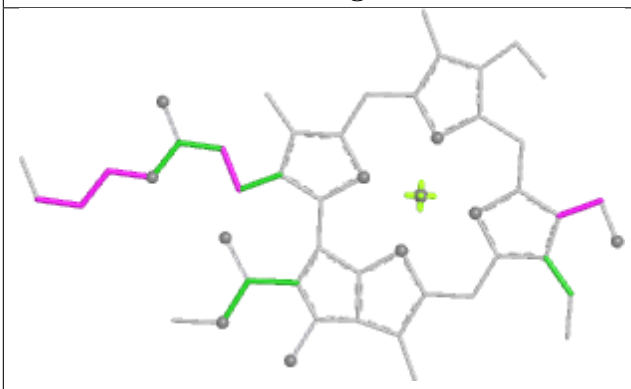
Ligand CHL y 606



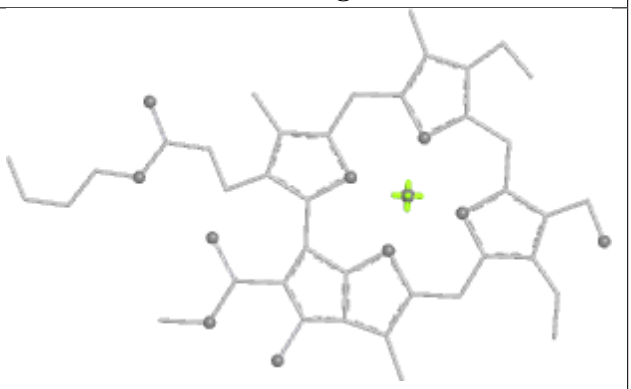
Bond lengths



Bond angles

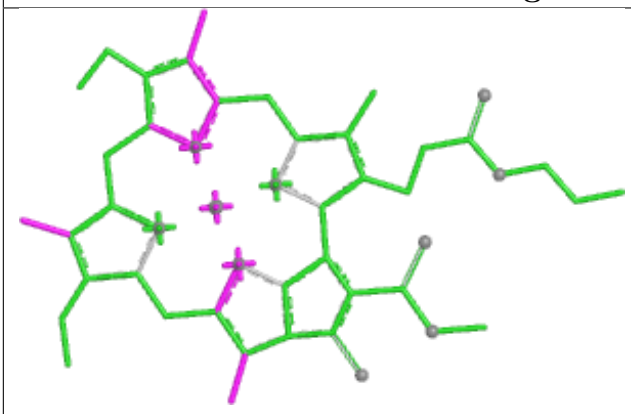


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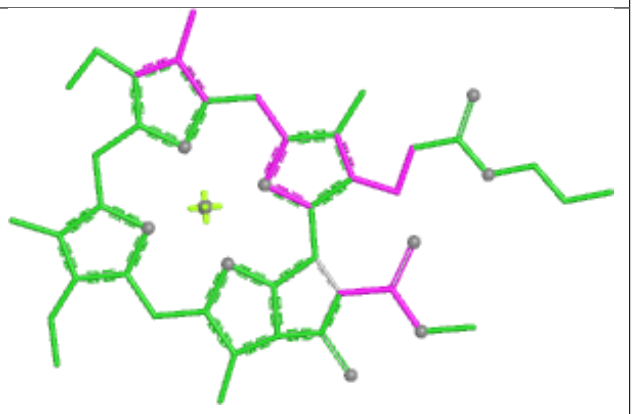


Rings

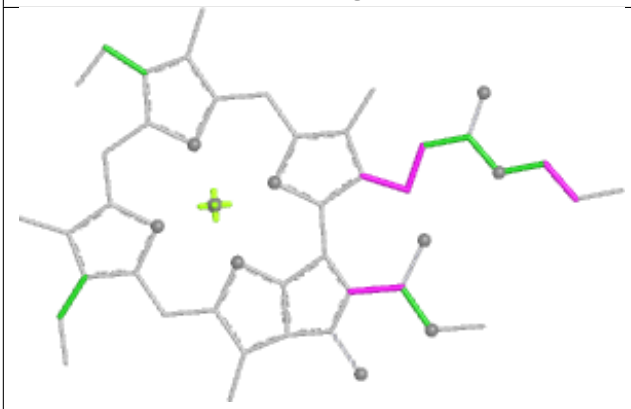
Ligand CLA R 604



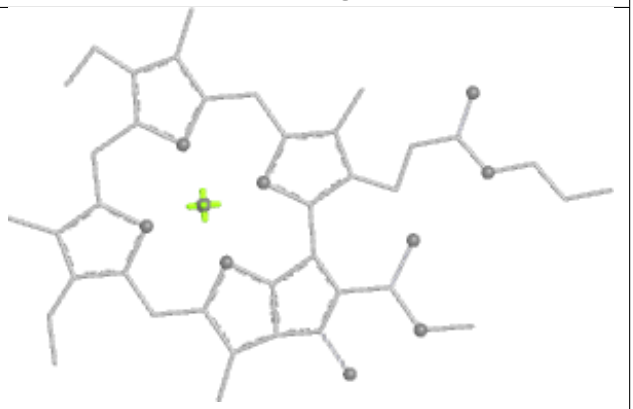
Bond lengths



Bond angles

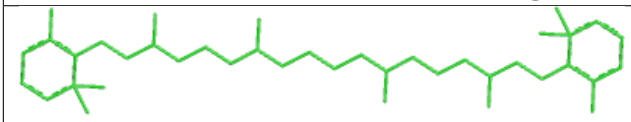


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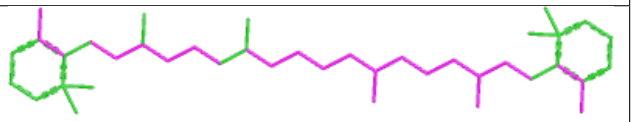


Rings

Ligand BCR a 411



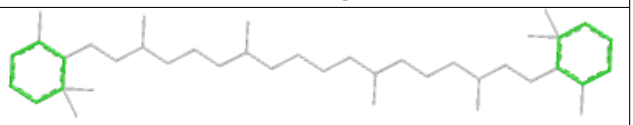
Bond lengths



Bond angles



Torsions

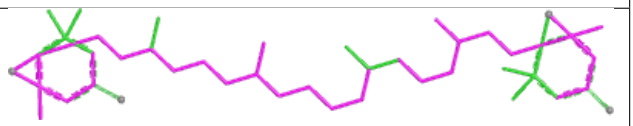


Rings

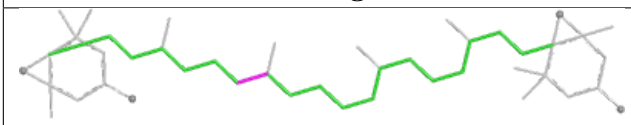
Ligand XAT 7 1622



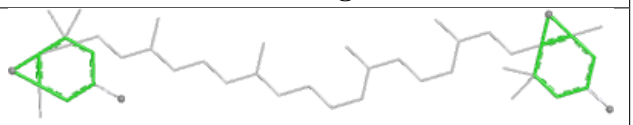
Bond lengths



Bond angles

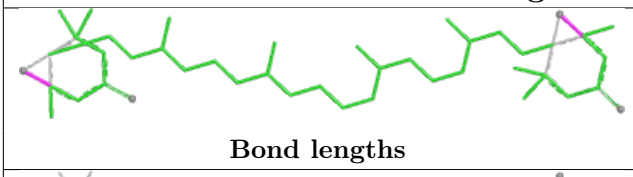


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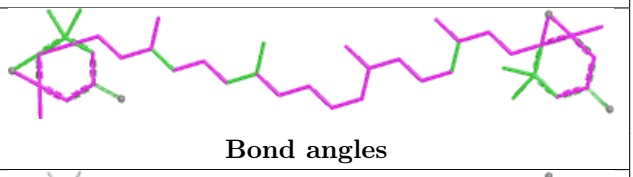


Rings

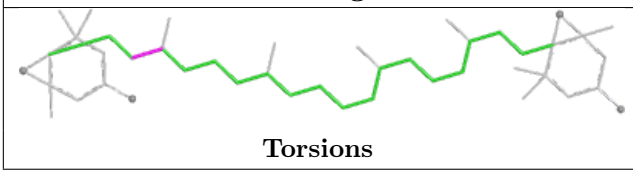
Ligand XAT 4 622



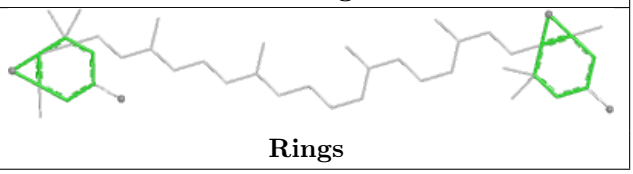
Bond lengths



Bond angles

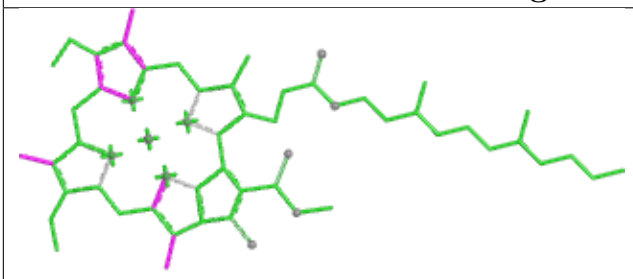


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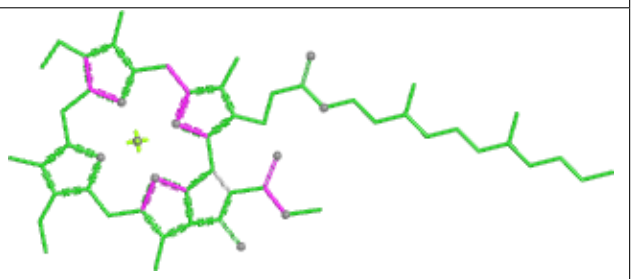


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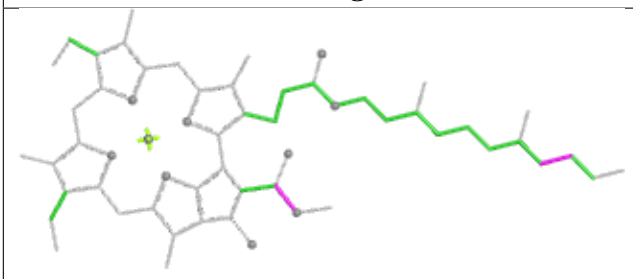
Ligand CLA r 609



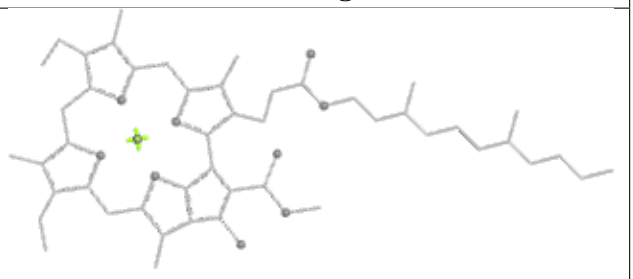
Bond lengths



Bond angles

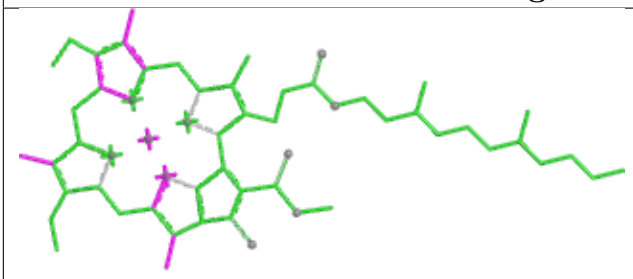


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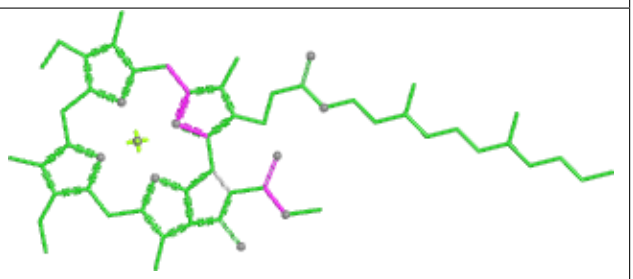


Rings

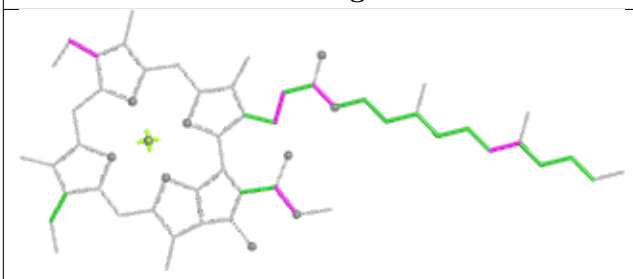
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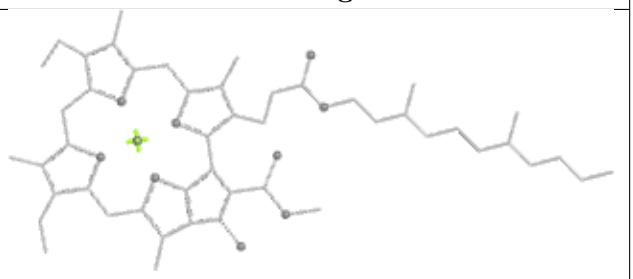
Bond lengths



Bond angles

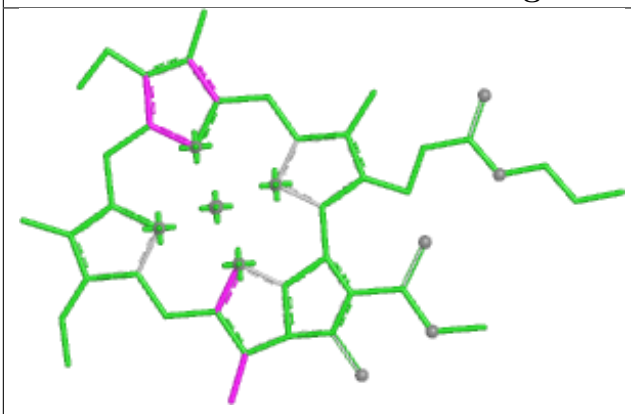


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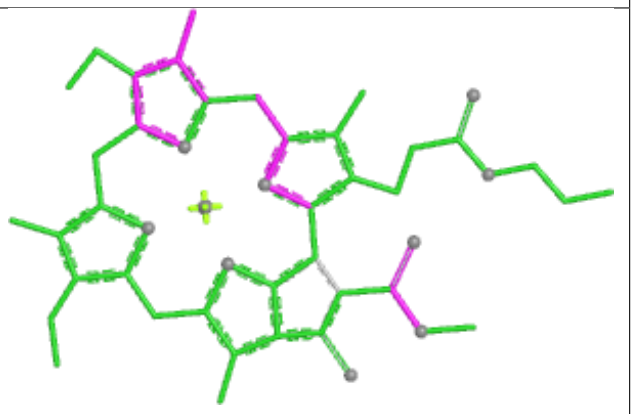


Rings

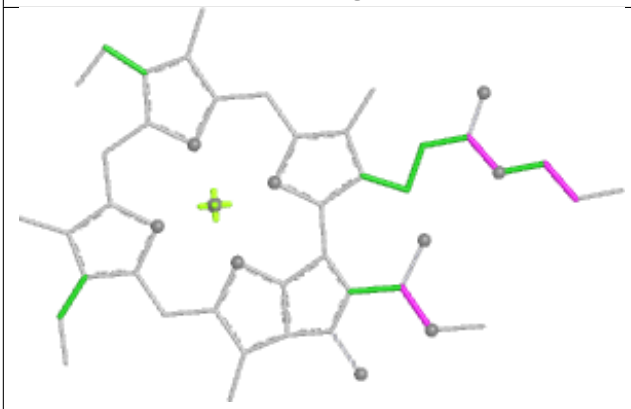
Ligand CLA N 614



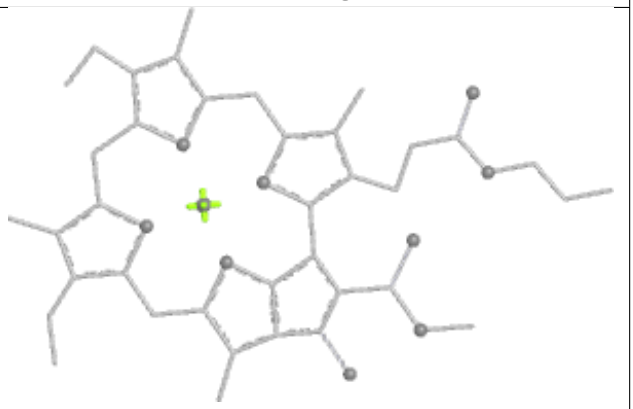
Bond lengths



Bond angles

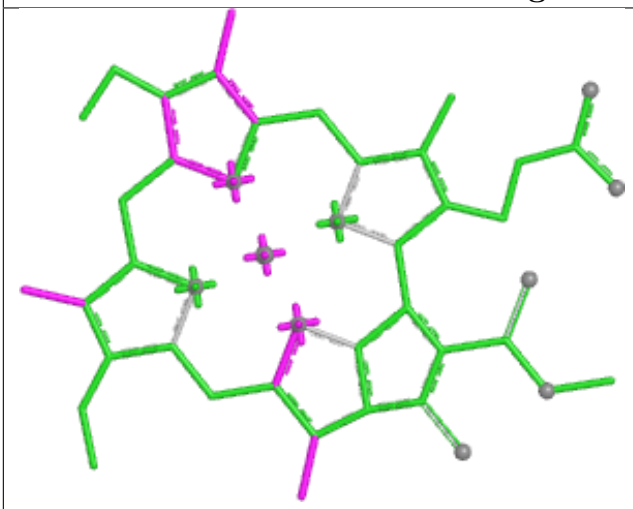


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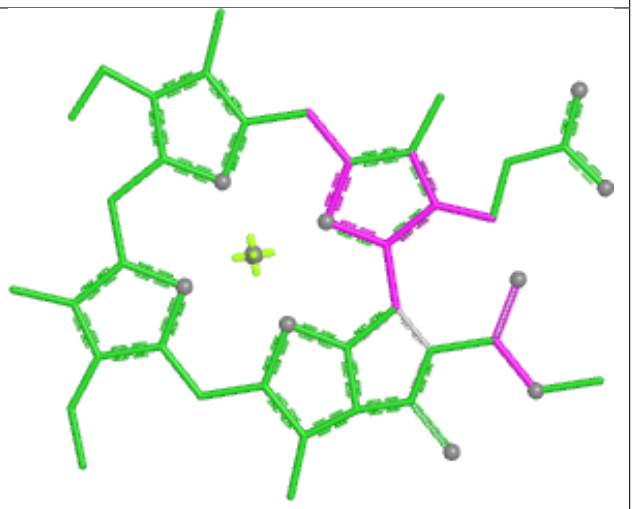


Rings

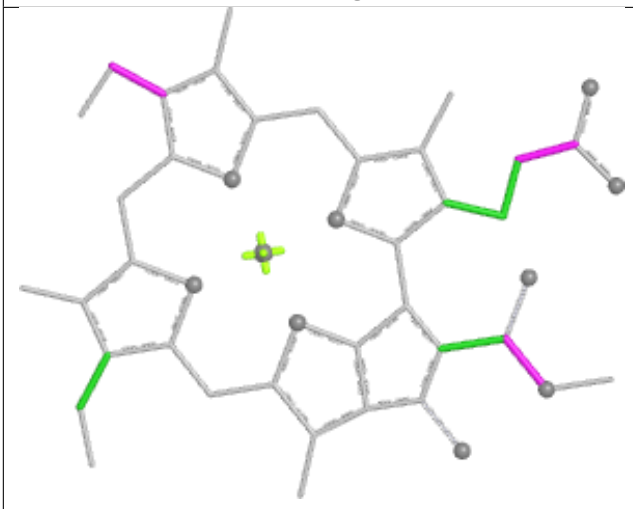
Ligand CLA 8 603



Bond lengths



Bond angles

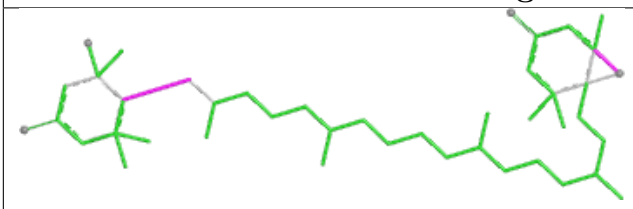


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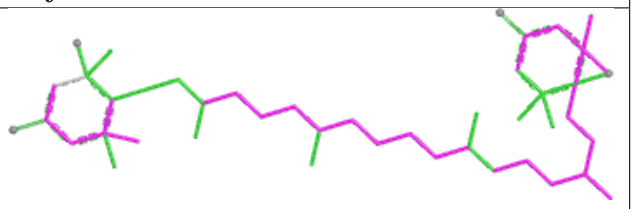


Rings

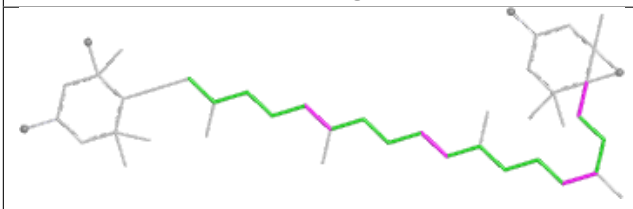
Ligand NEX y 1623



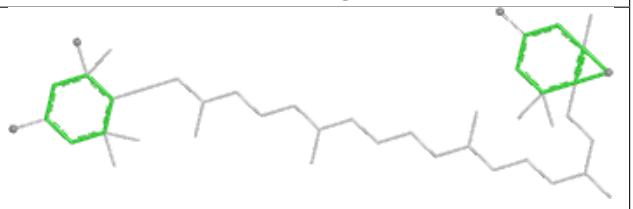
Bond lengths



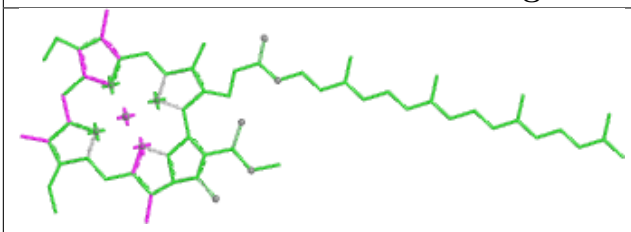
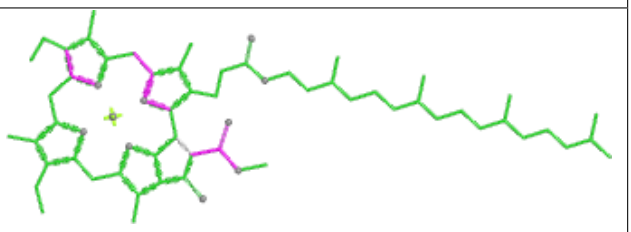
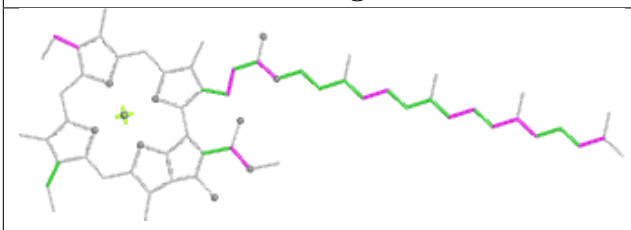
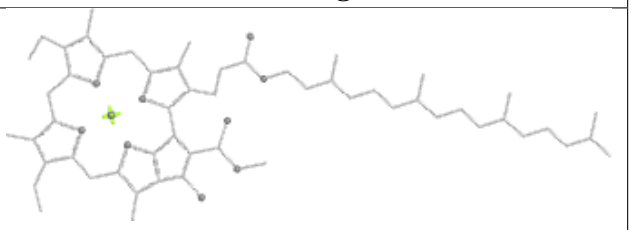
Bond angles

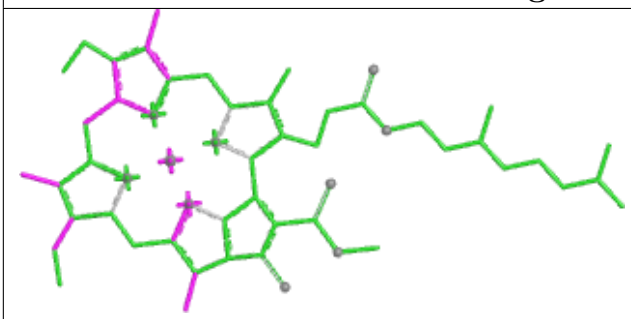
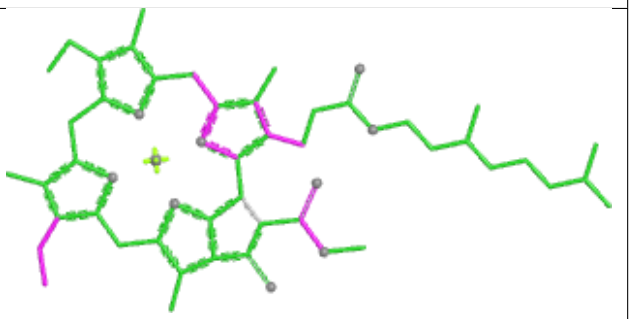
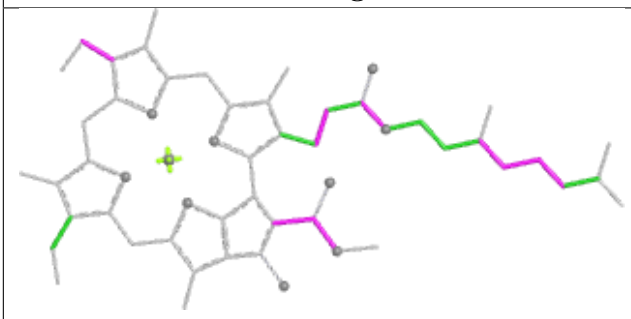
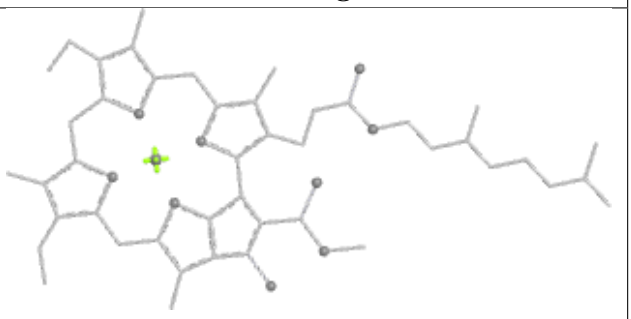


Torsions

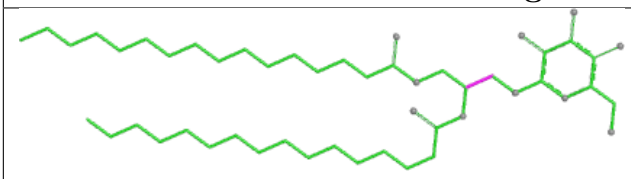


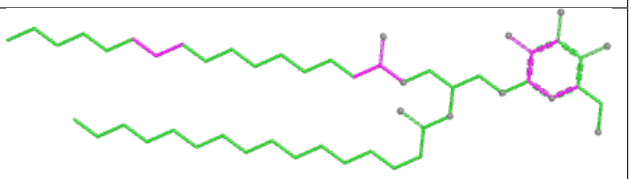
Rings

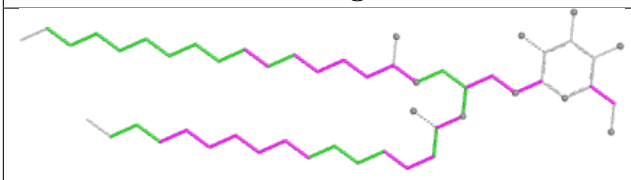
Ligand CLA G 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

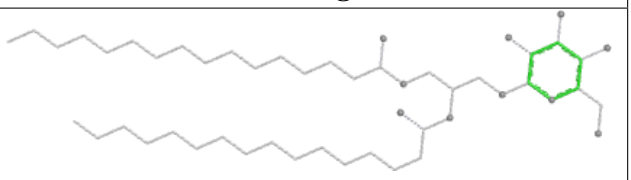
Ligand CLA 5 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG z 101

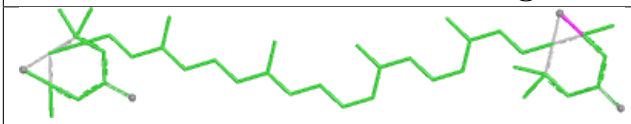

Bond lengths

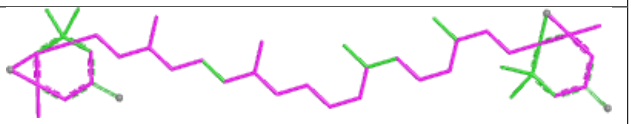

Bond angles

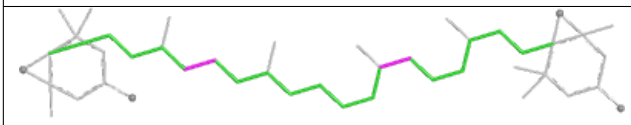

Torsions

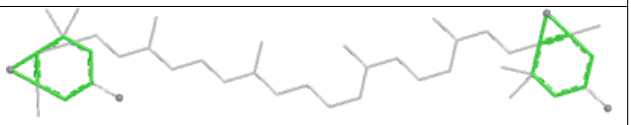

Rings

Ligand XAT n 1622

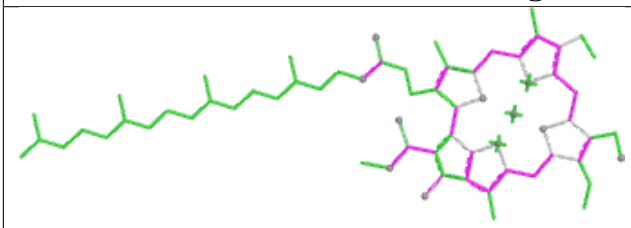

Bond lengths

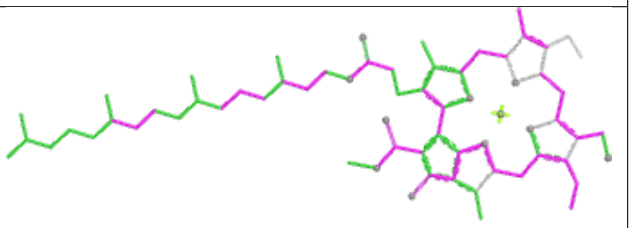

Bond angles

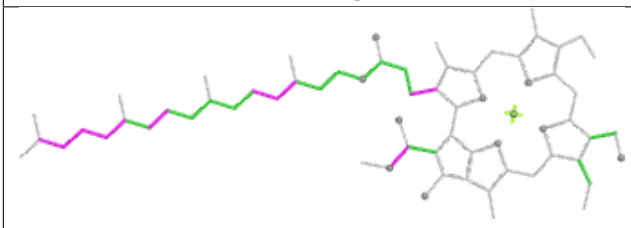

Torsions

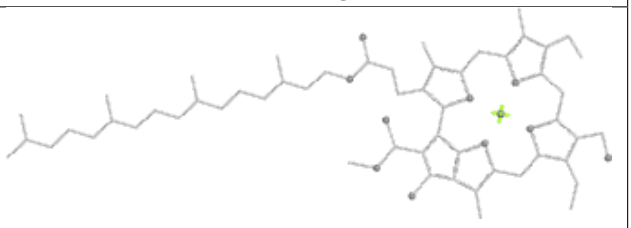

Rings

Ligand CHL n 608

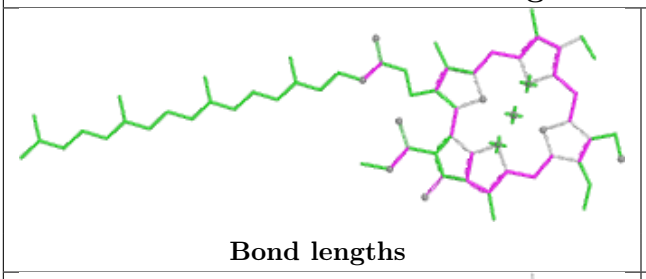

Bond lengths


Bond angles

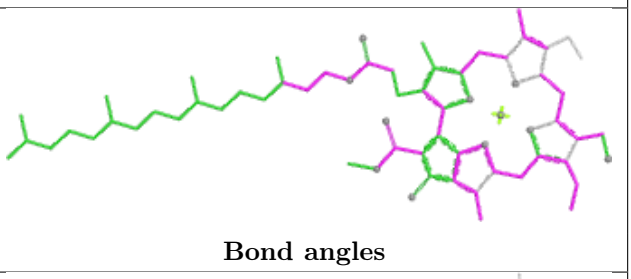

Torsions


Rings

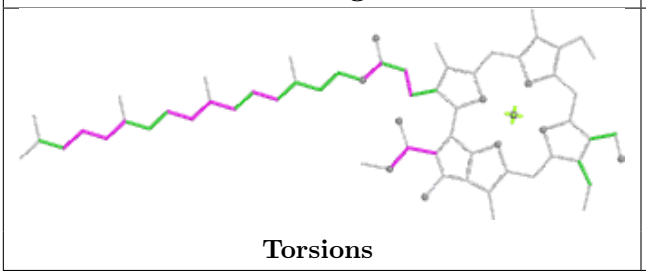
Ligand CHL n 601



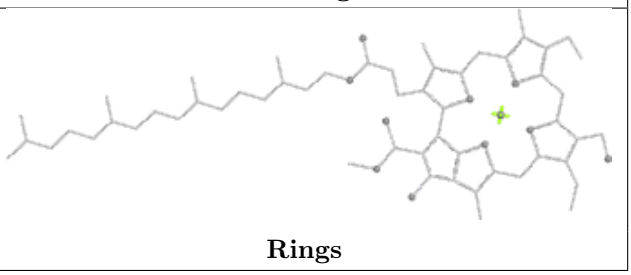
Bond lengths



Bond angles

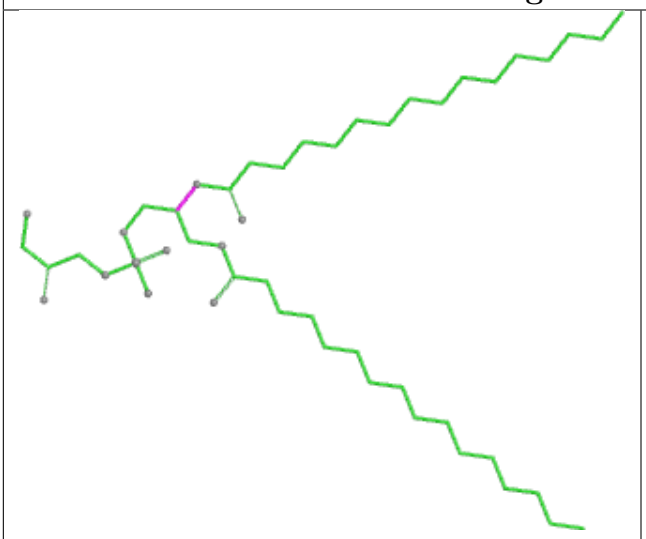


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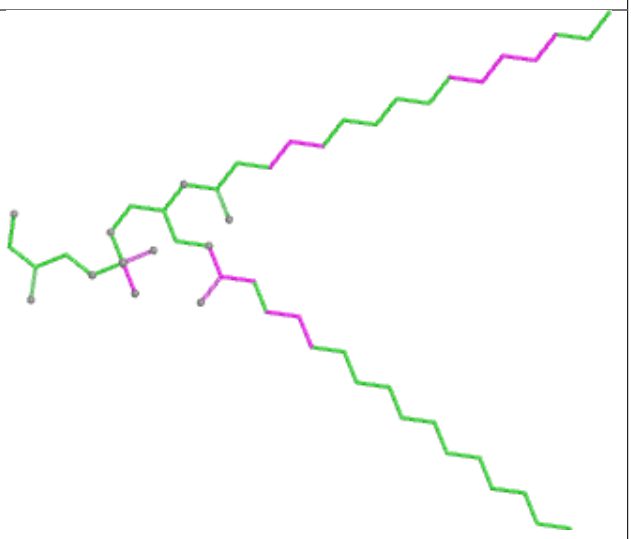


Rings

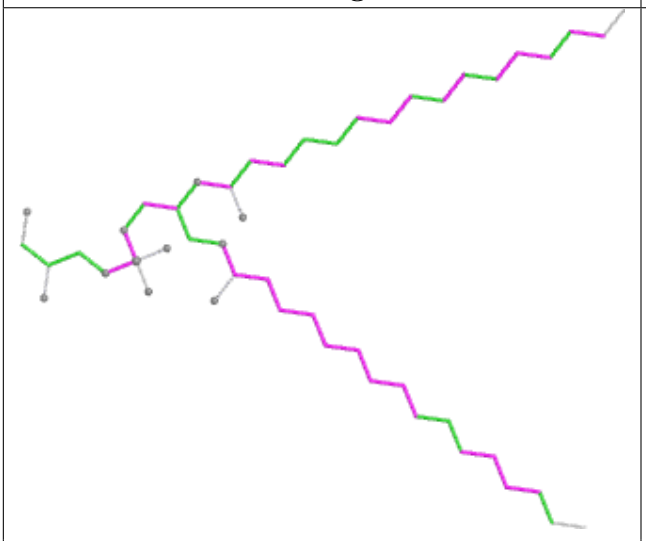
Ligand LHG d 409



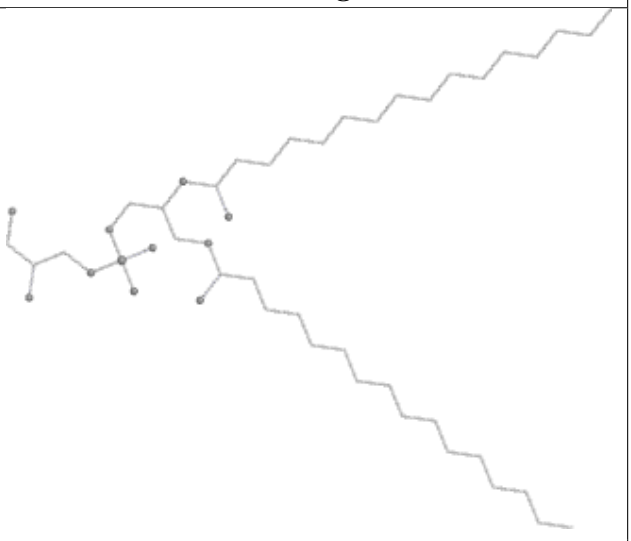
Bond lengths



Bond angles

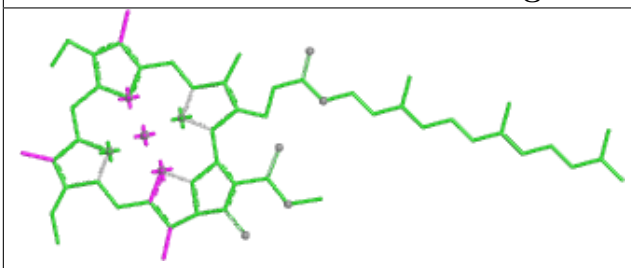


Torsions

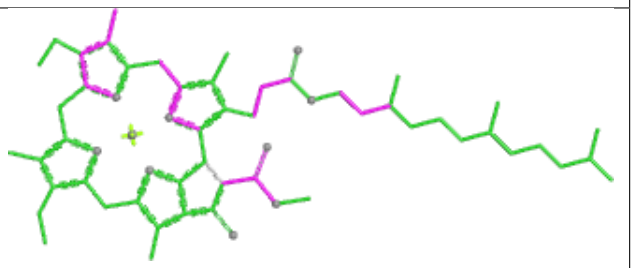


Rings

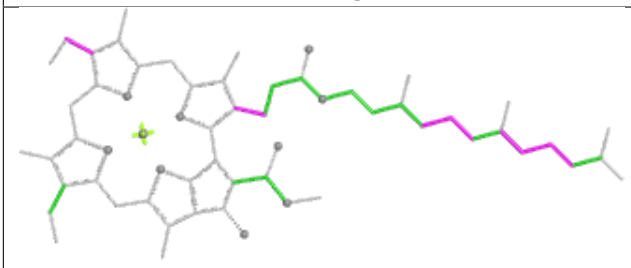
Ligand CLA A 410



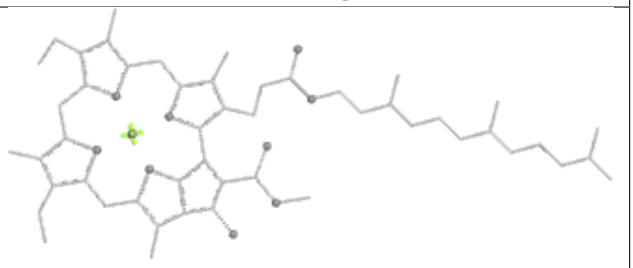
Bond lengths



Bond angles

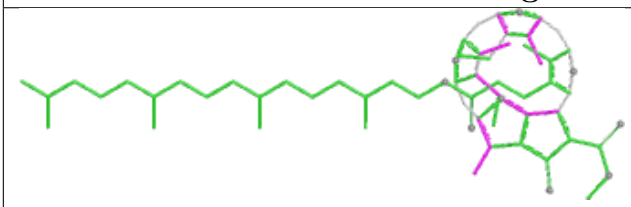


Torsions

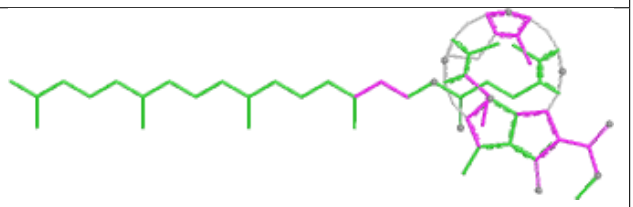


Rings

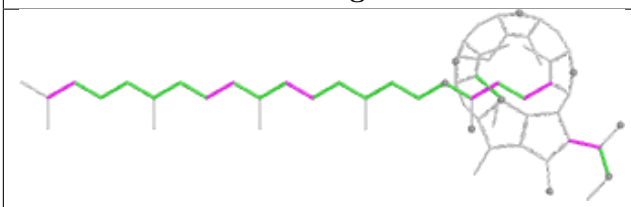
Ligand PHO A 409



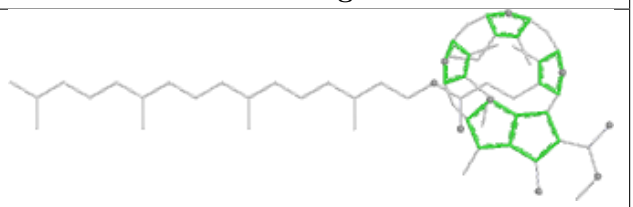
Bond lengths



Bond angles

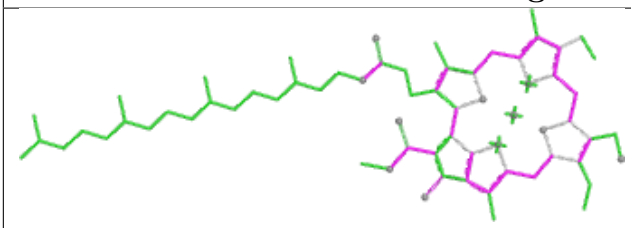


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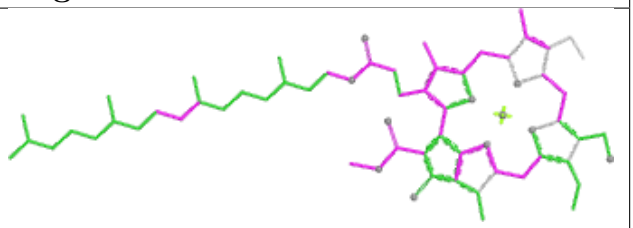


Rings

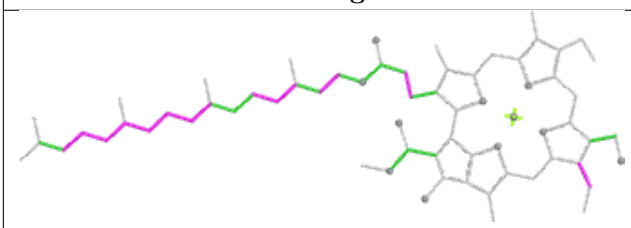
Ligand CHL g 607



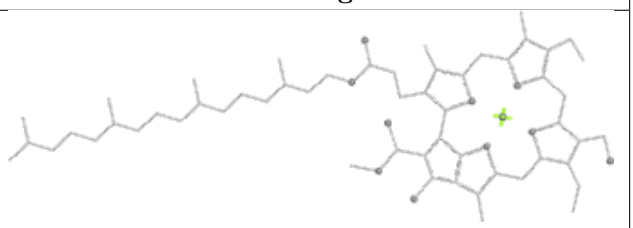
Bond lengths



Bond angles

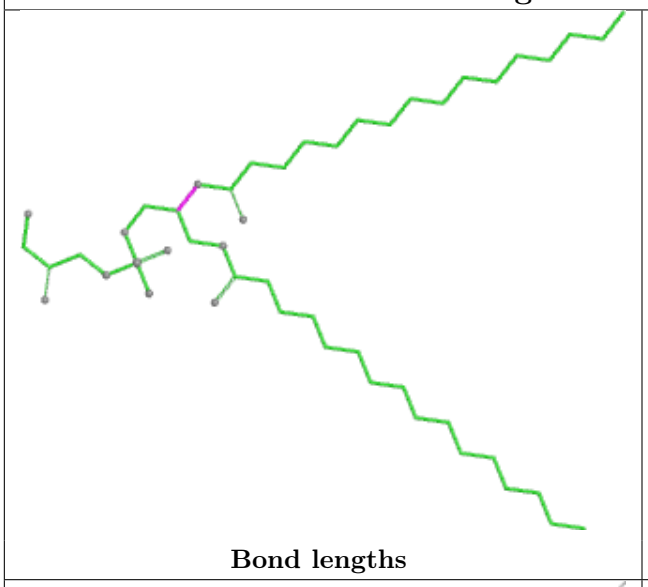


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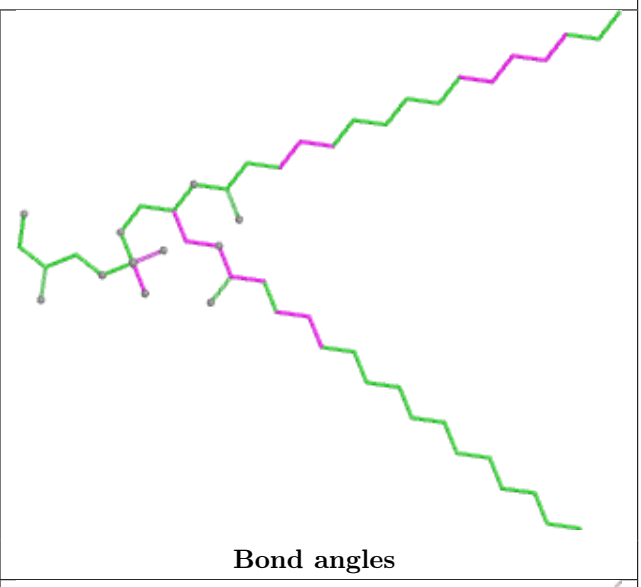


Rings

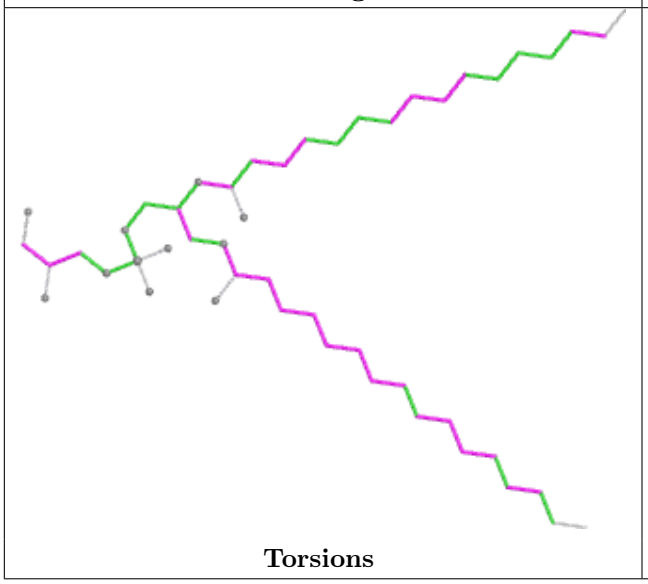
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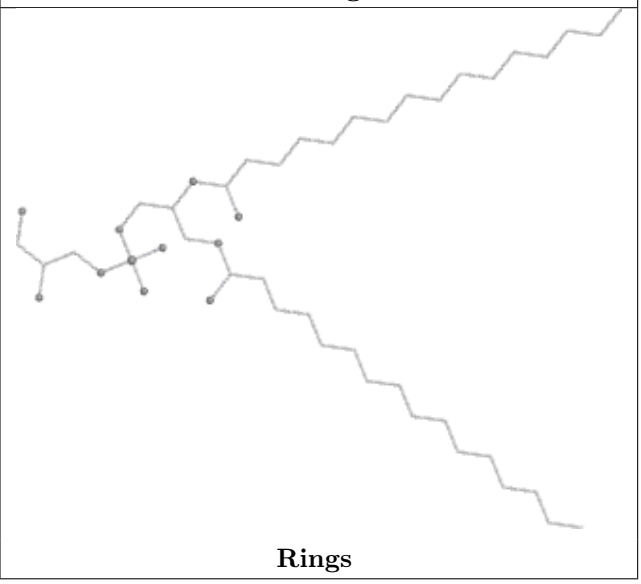
Bond lengths



Bond angles

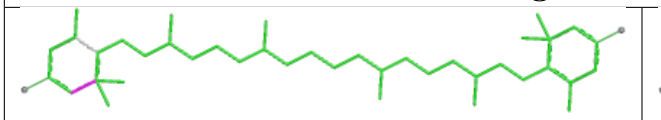


Torsions



Rings

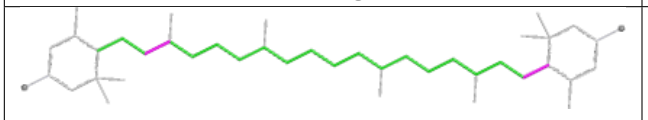
Ligand LUT r 620



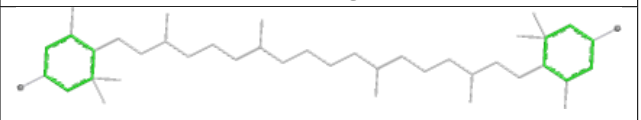
Bond lengths



Bond angles

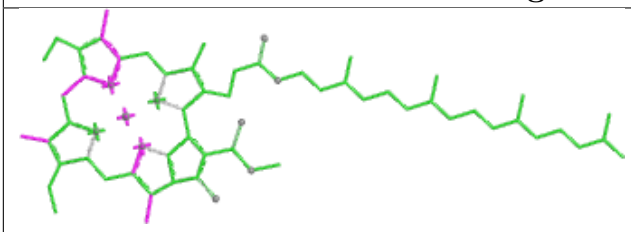


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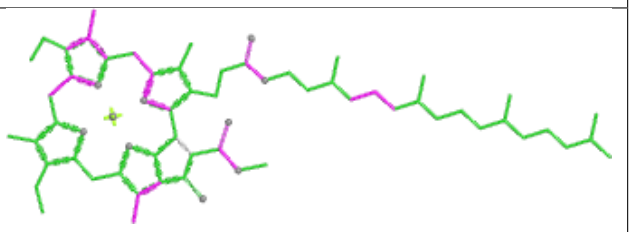


Rings

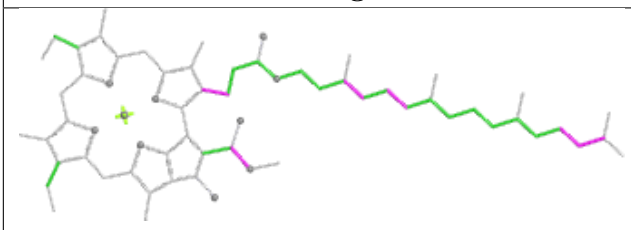
Ligand CLA b 610



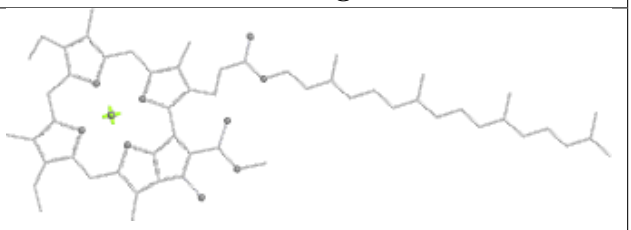
Bond lengths



Bond angles



Torsions

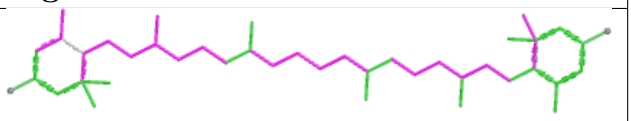


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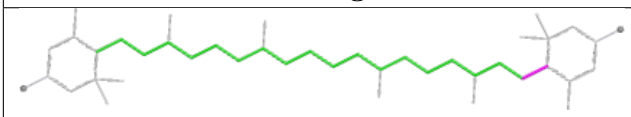
Ligand LUT g 1620



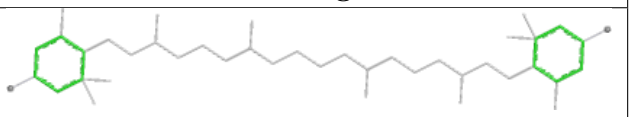
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Bond angles

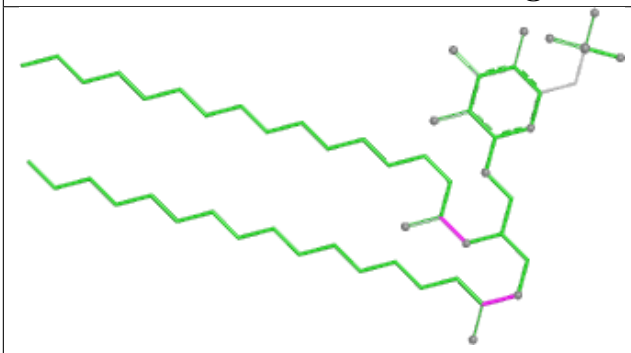


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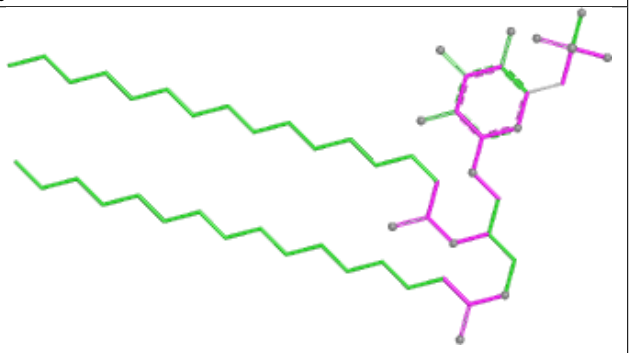


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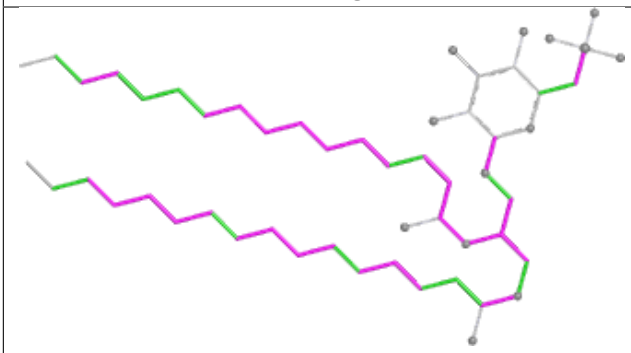
Ligand SQD B 621



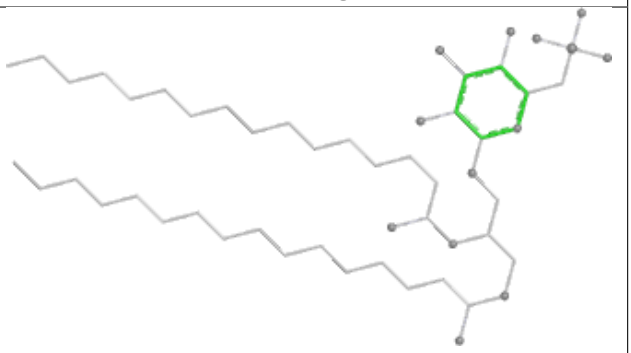
Bond lengths



Bond angles

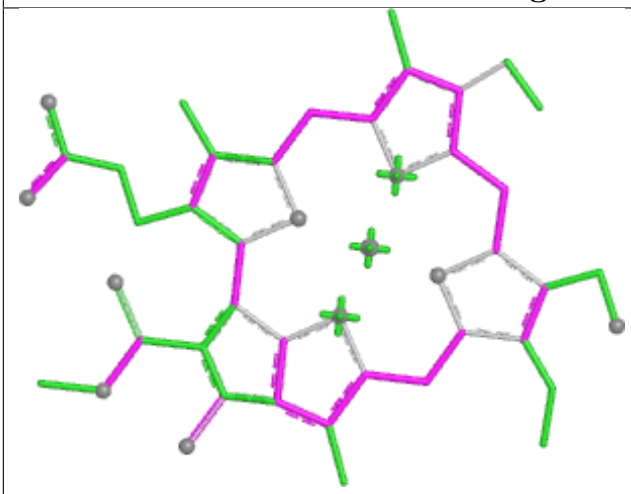


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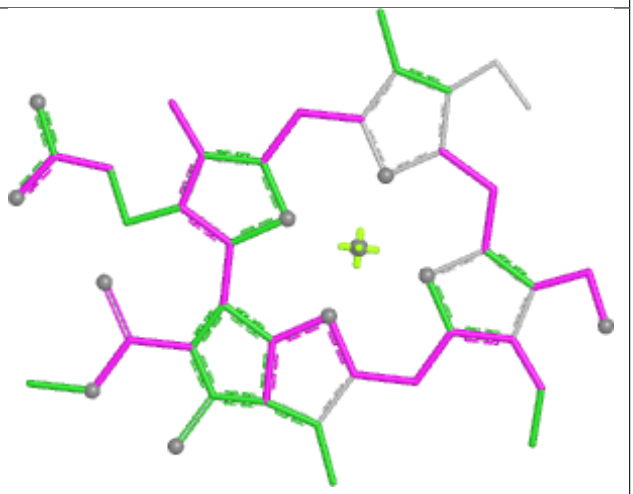


Rings

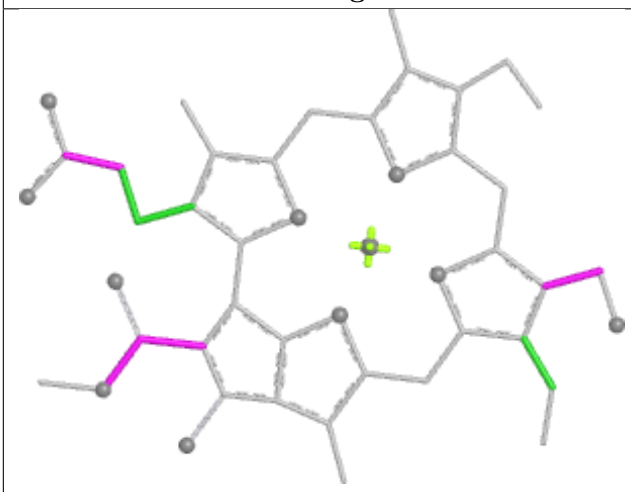
Ligand CHL s 606



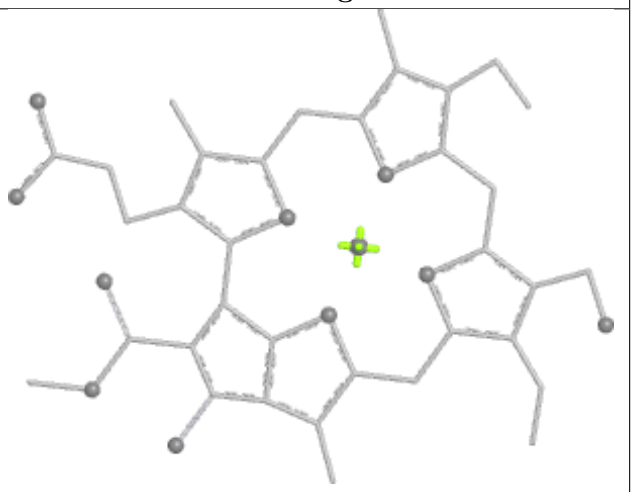
Bond lengths



Bond angles



Torsions

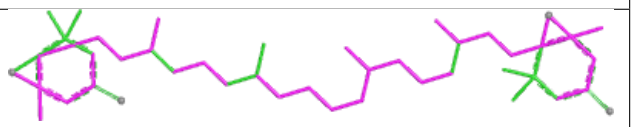


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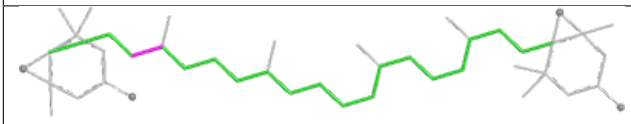
Ligand XAT 8 622



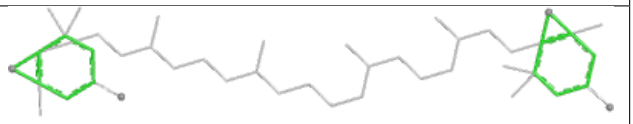
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Bond angles

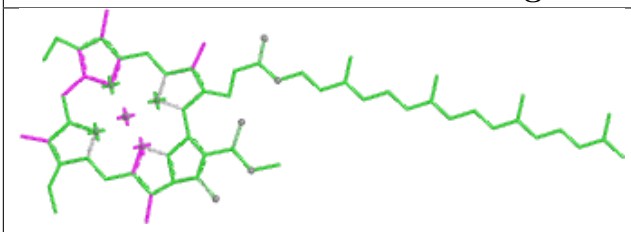


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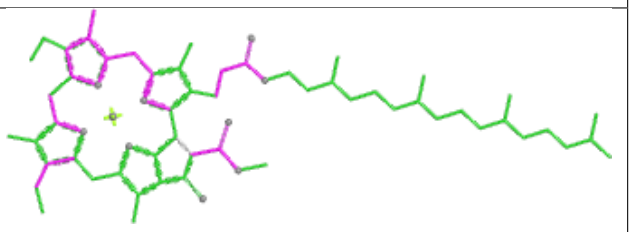


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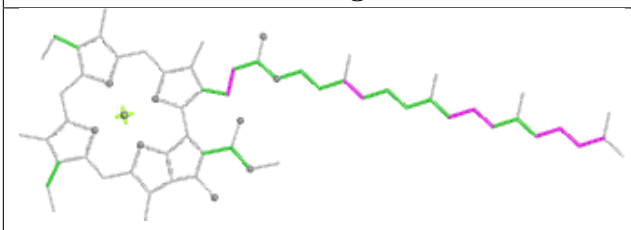
Ligand CLA B 607



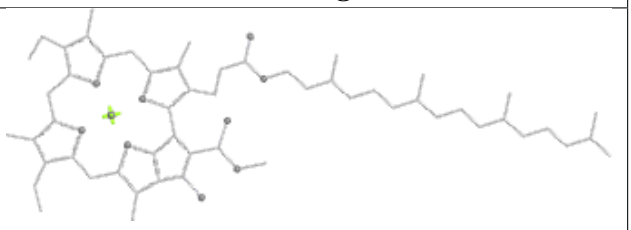
Bond lengths



Bond angles



Torsions



Rings

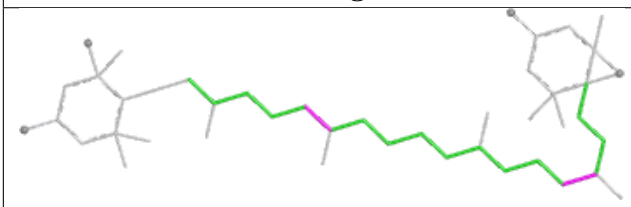
Ligand NEX 3 1623



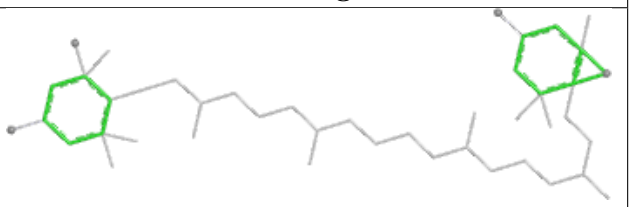
Bond lengths



Bond angles

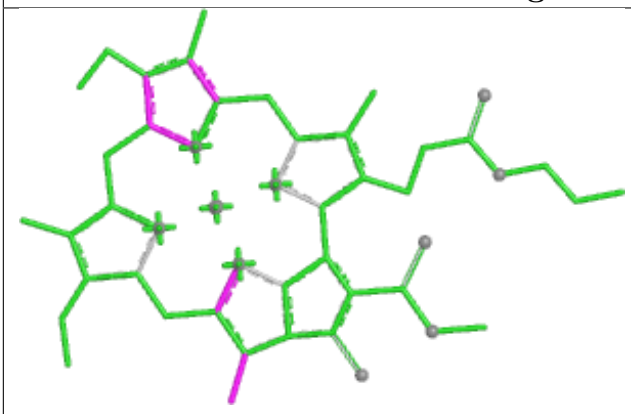


Torsions

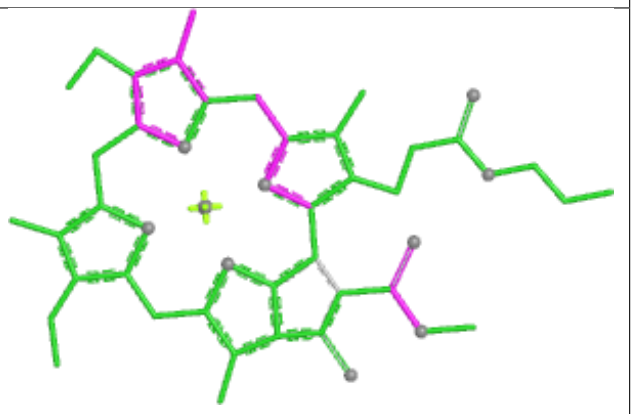


Rings

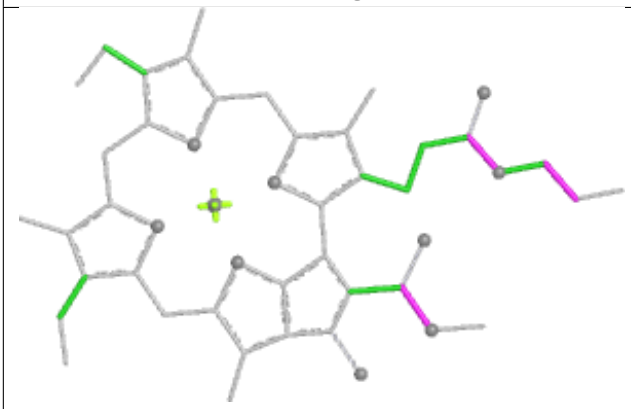
Ligand CLA n 614



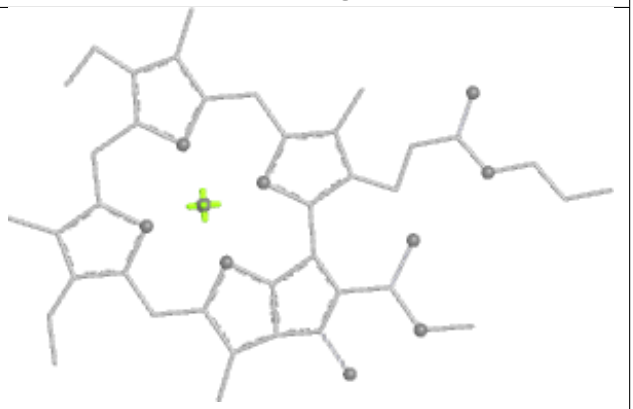
Bond lengths



Bond angles

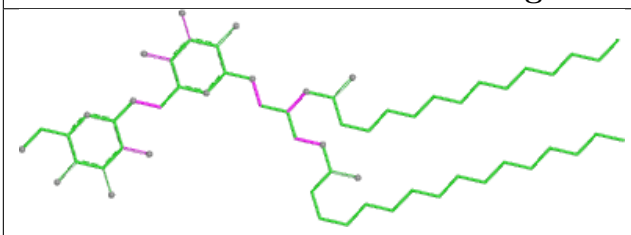


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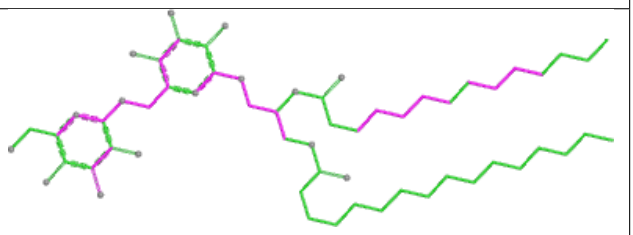


Rings

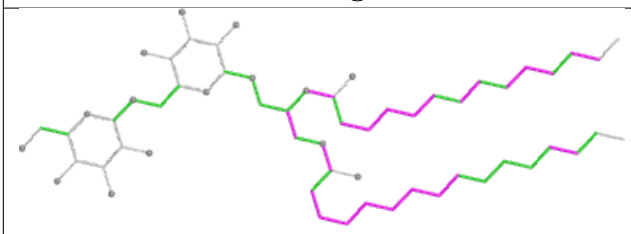
Ligand DGD c 520



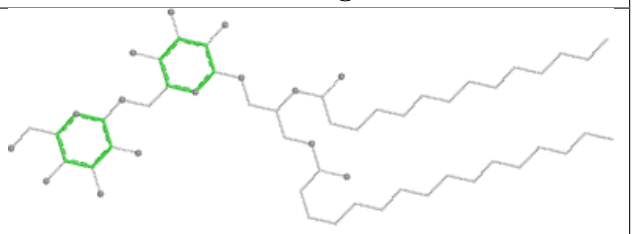
Bond lengths



Bond angles

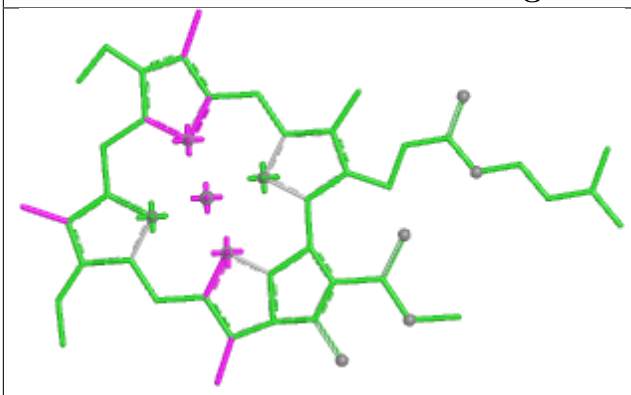


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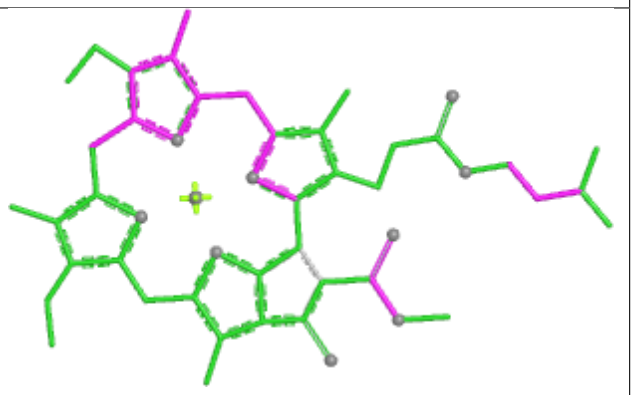


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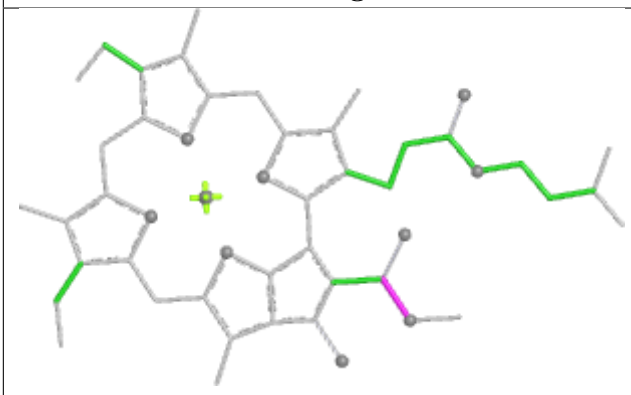
Ligand CLA Y 604



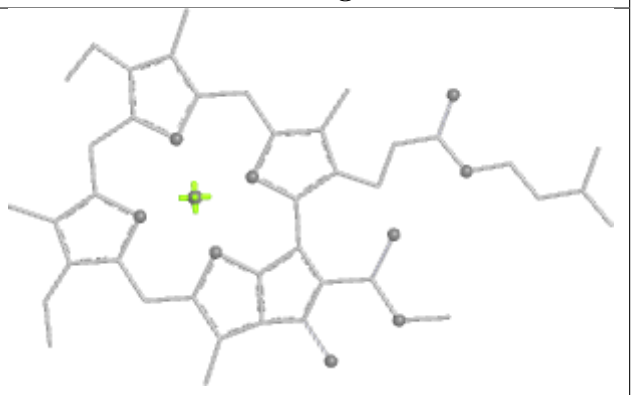
Bond lengths



Bond angles

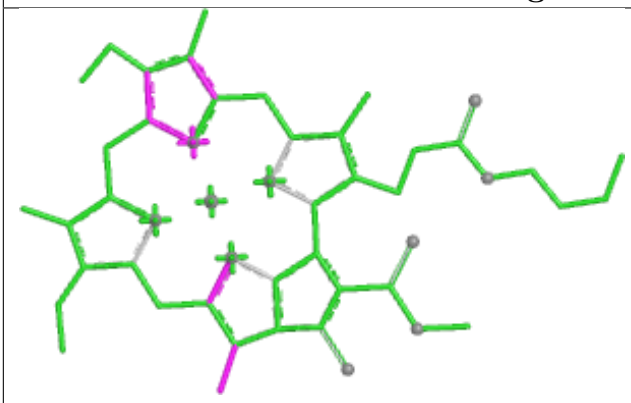


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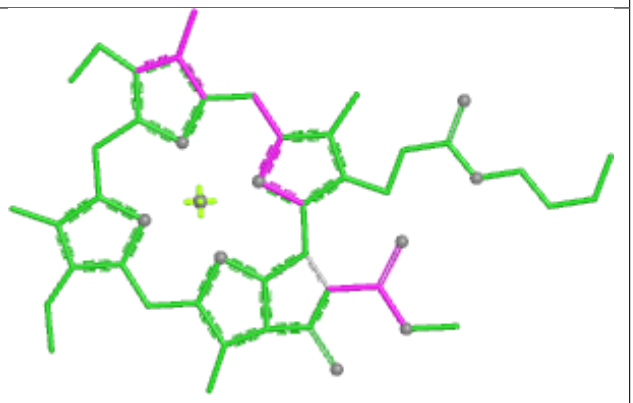


Rings

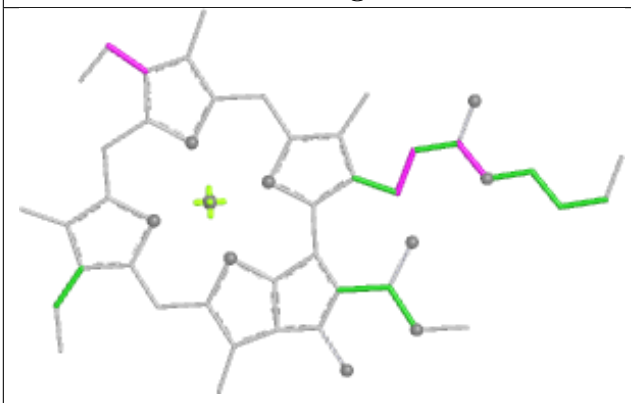
Ligand CLA S 614



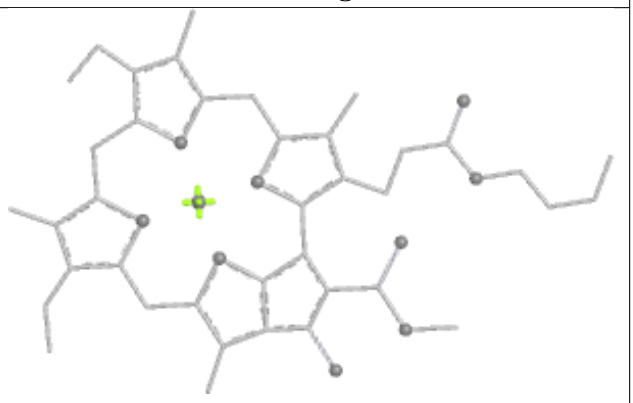
Bond lengths



Bond angles

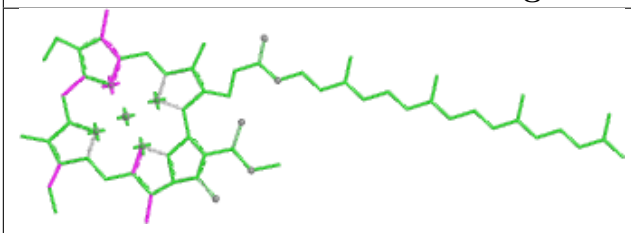


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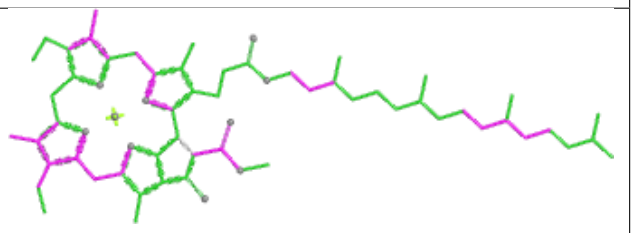


Rings

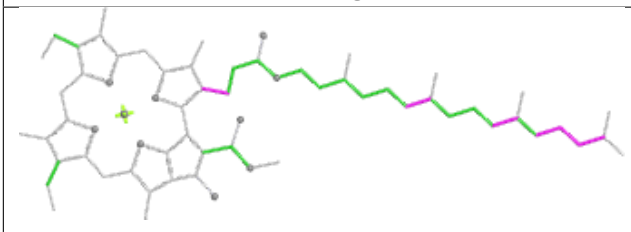
Ligand CLA A 406



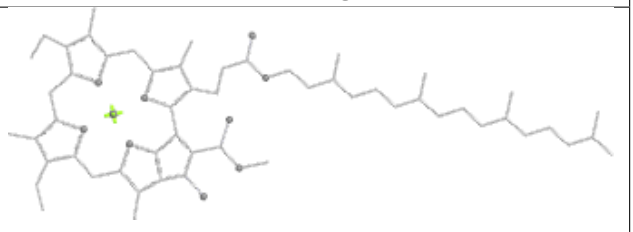
Bond lengths



Bond angles

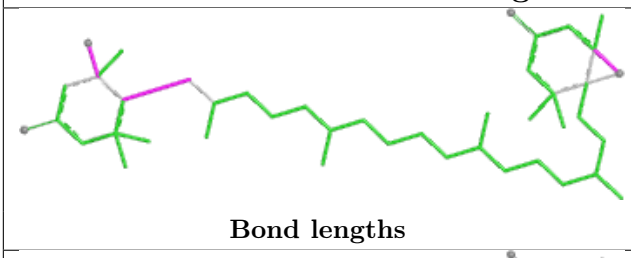


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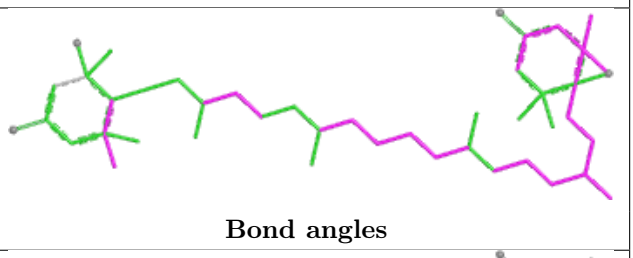


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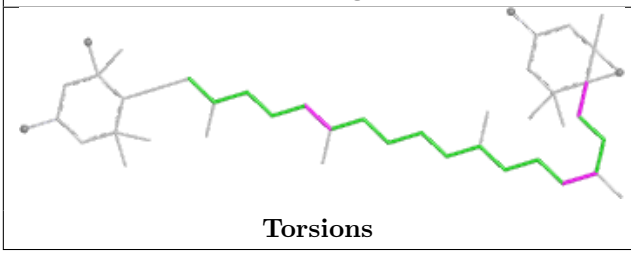
Ligand NEX G 1623



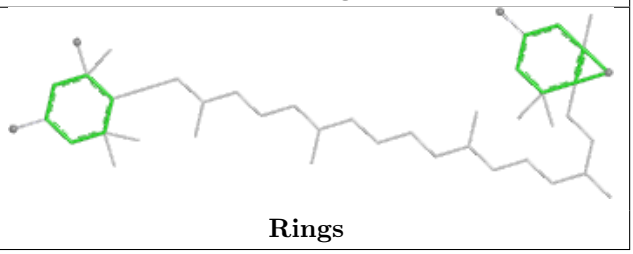
Bond lengths



Bond angles

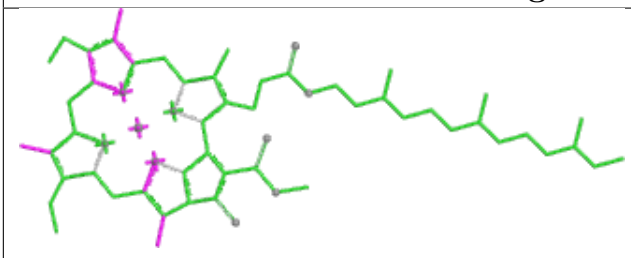


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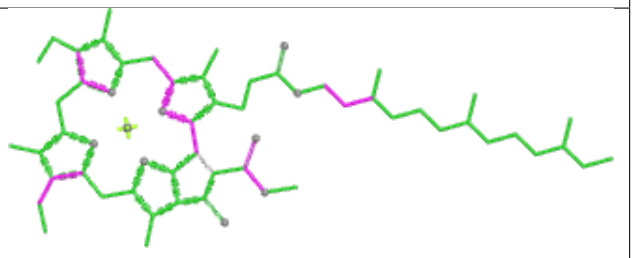


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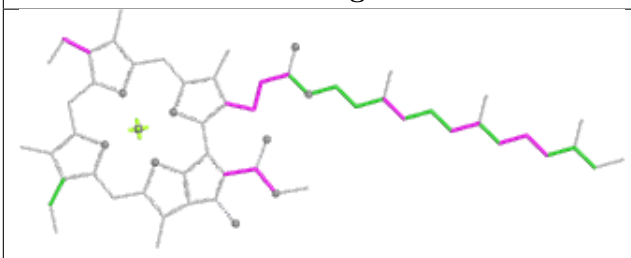
Ligand CLA 1 602



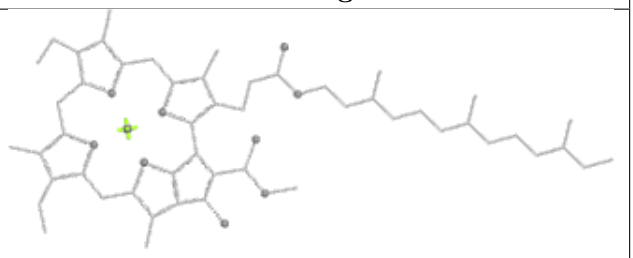
Bond lengths



Bond angles

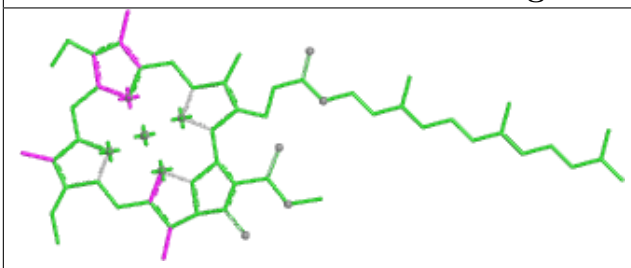


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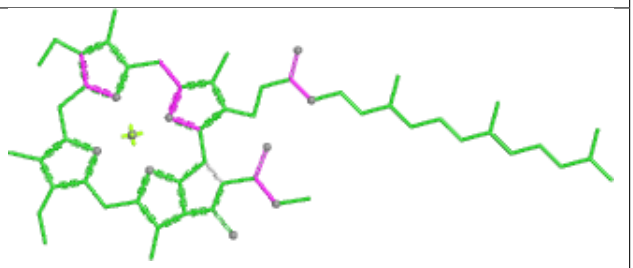


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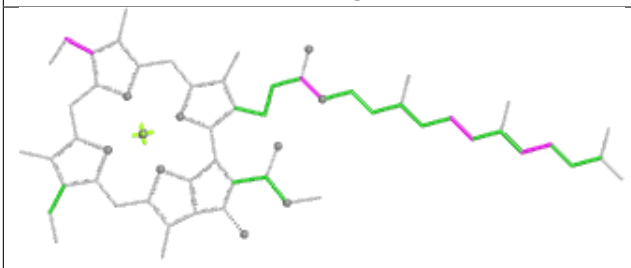
Ligand CLA n 611



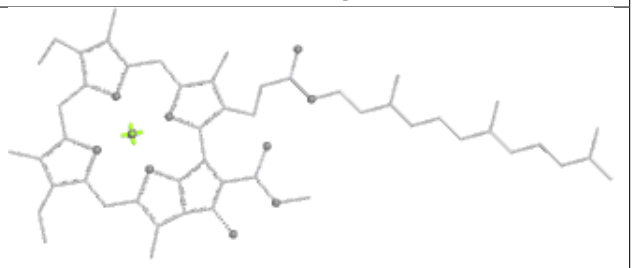
Bond lengths



Bond angles

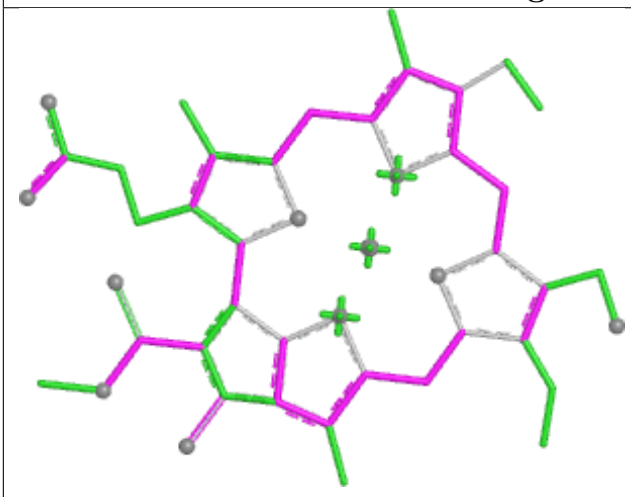


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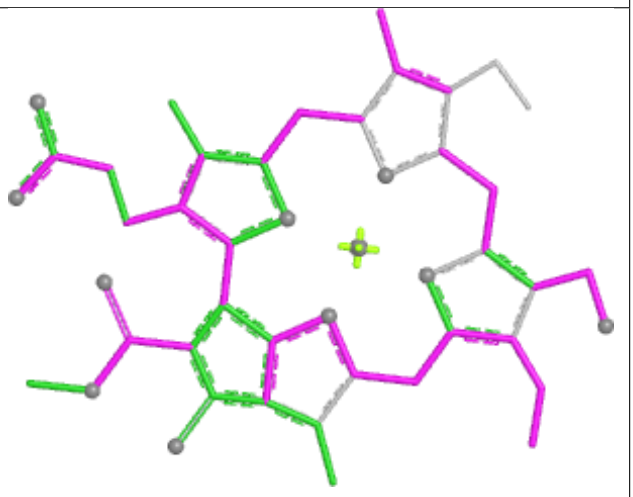


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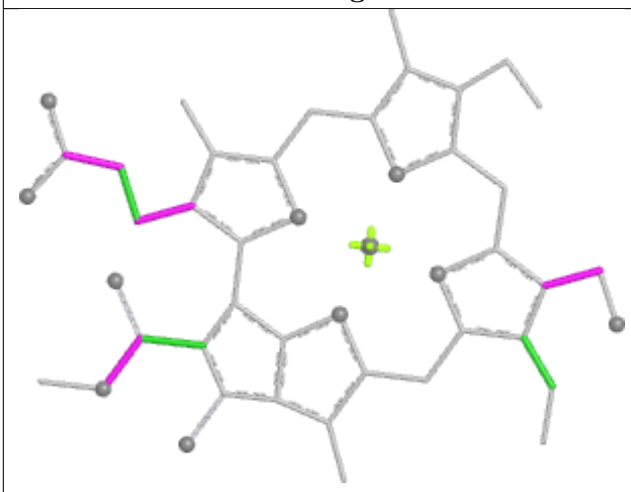
Ligand CHL 5 605



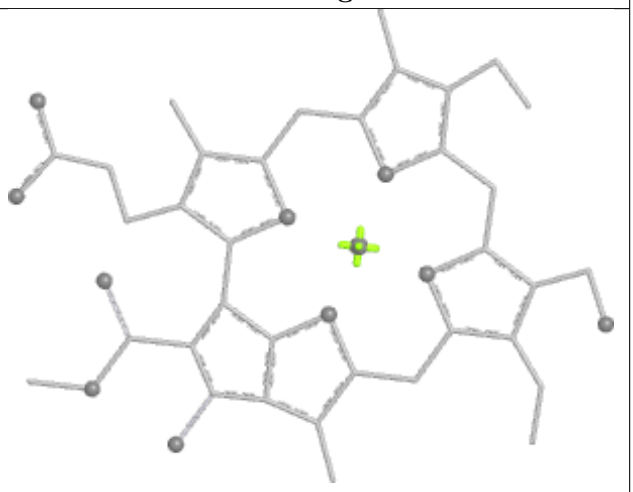
Bond lengths



Bond angles

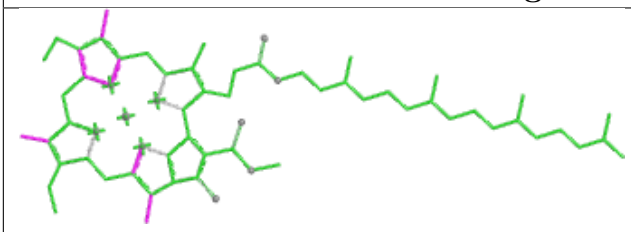


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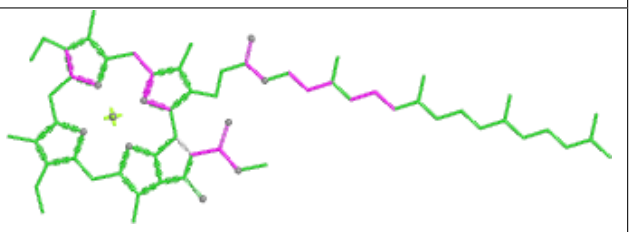


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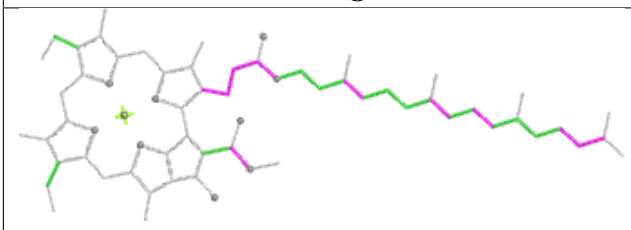
Ligand CLA C 501



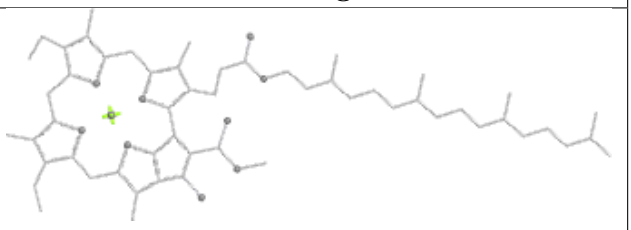
Bond lengths



Bond angles

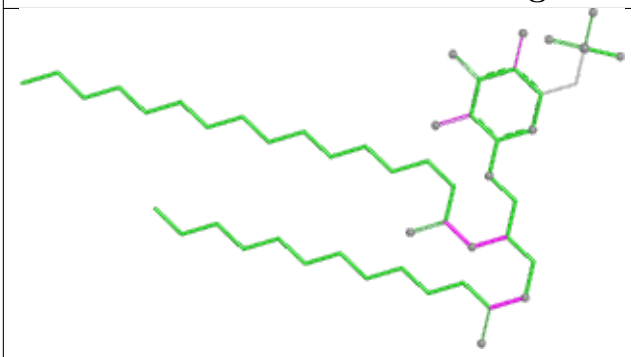


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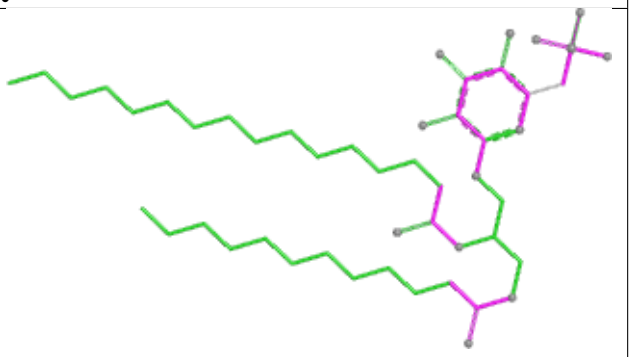


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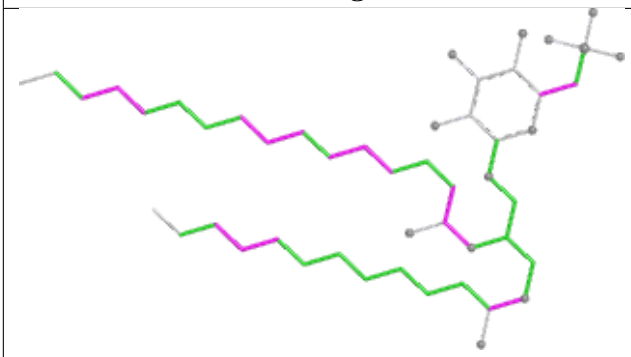
Ligand SQD a 412



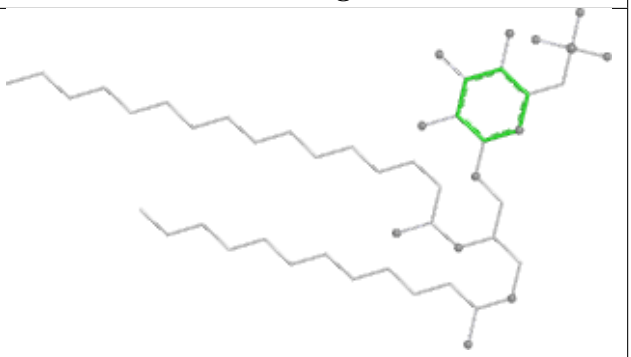
Bond lengths



Bond angles

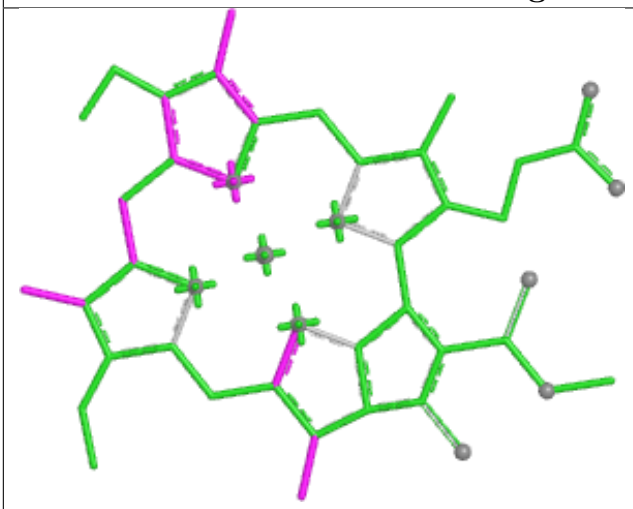


Torsions

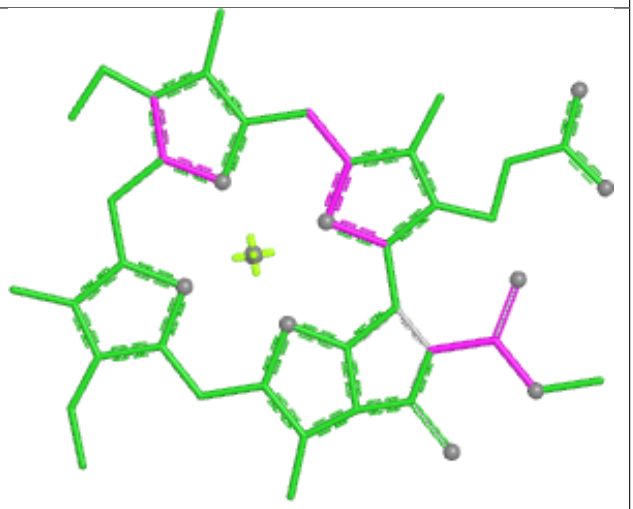


Rings

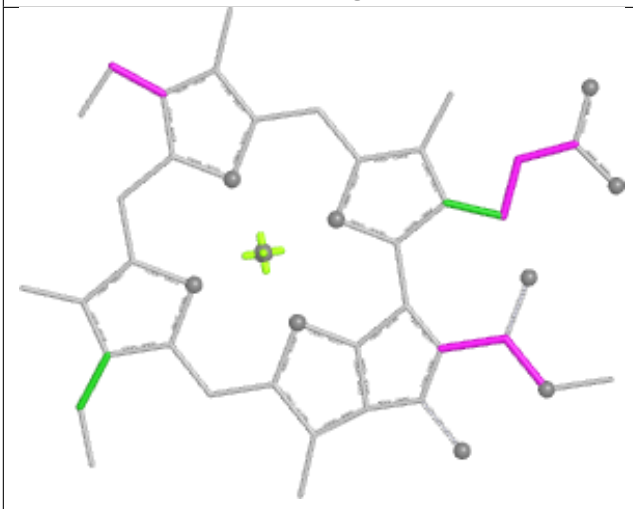
Ligand CLA 4 602



Bond lengths



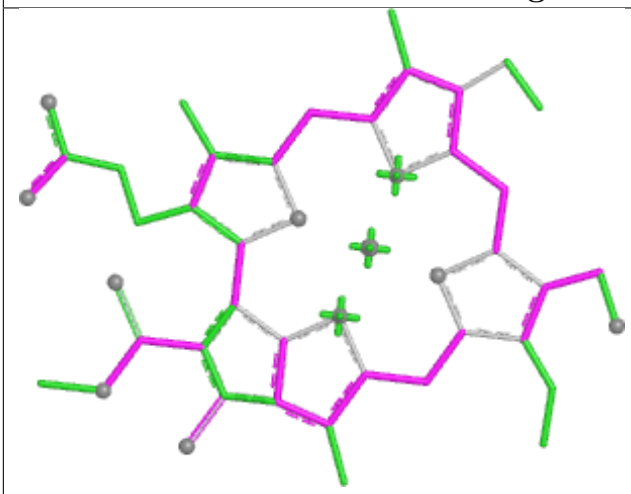
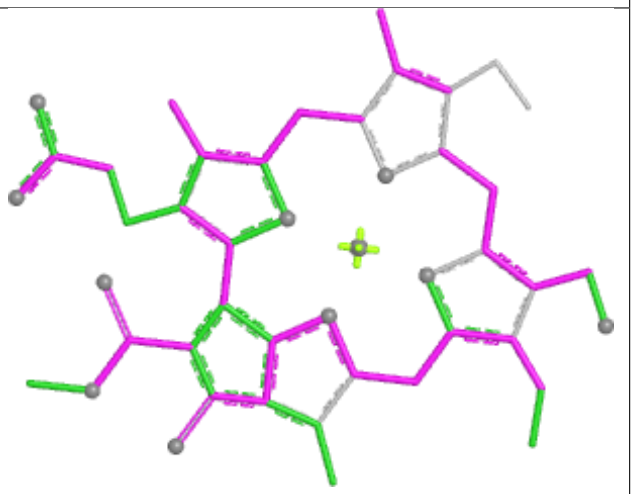
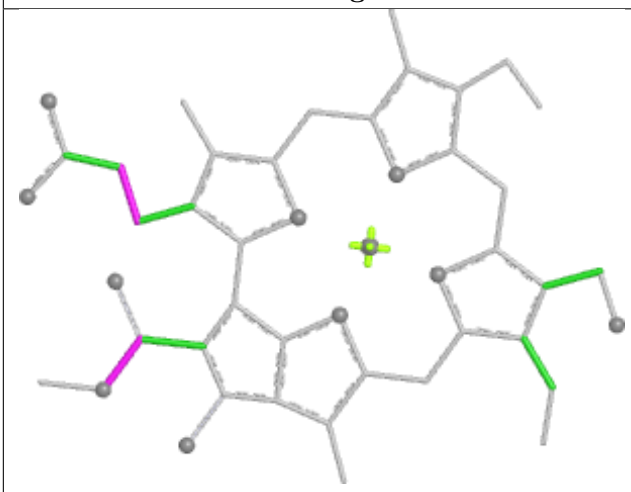
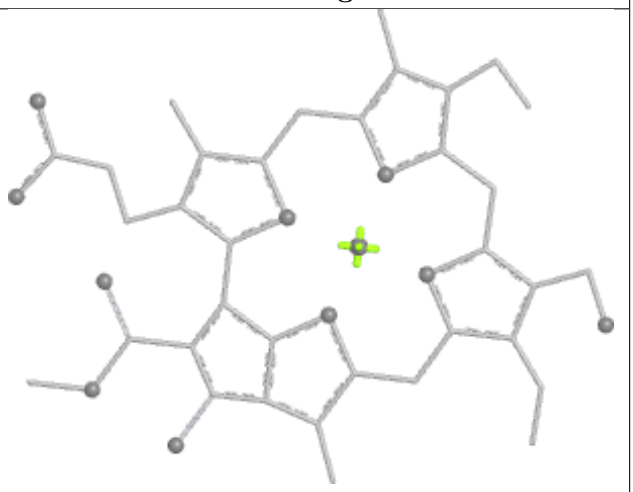
Bond angles

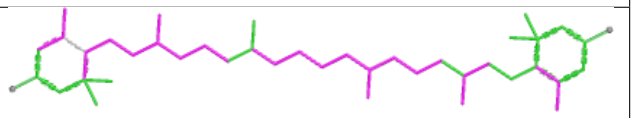
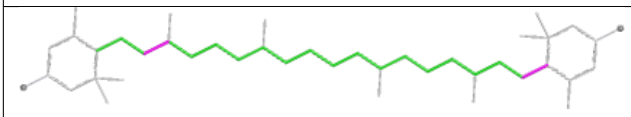
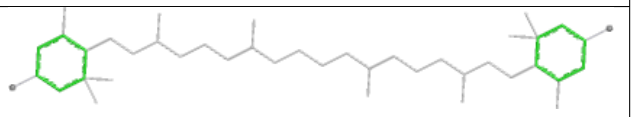


Torsions

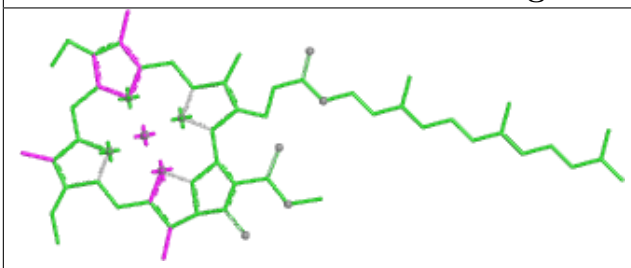


Rings

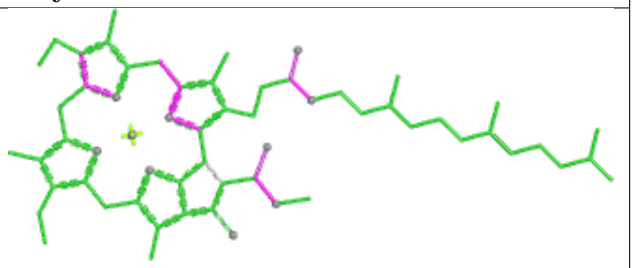
Ligand CHL 7 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT R 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

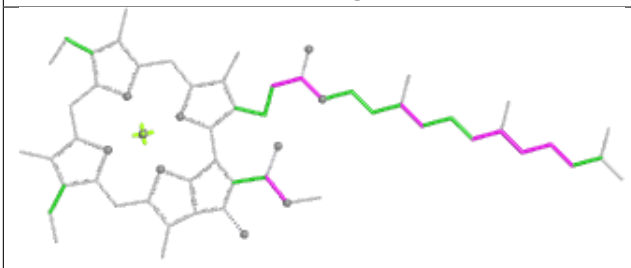
Ligand CLA y 612



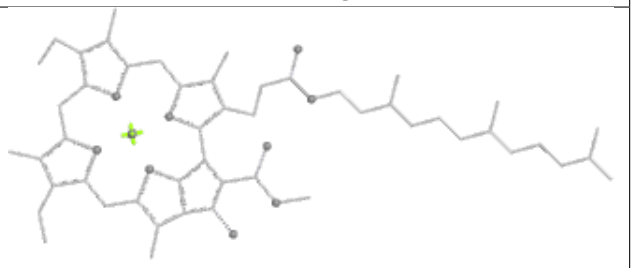
Bond lengths



Bond angles

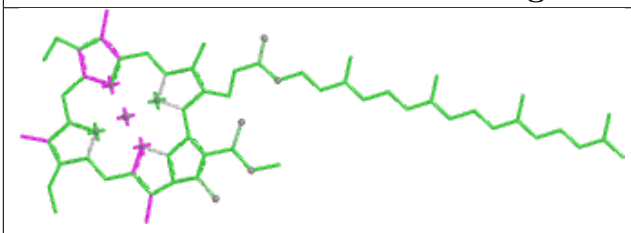


Torsions

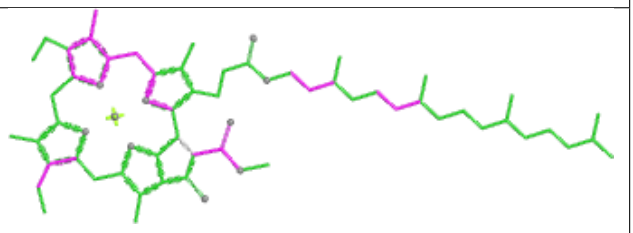


Rings

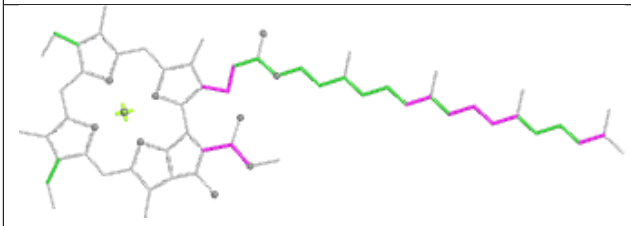
Ligand CLA n 602



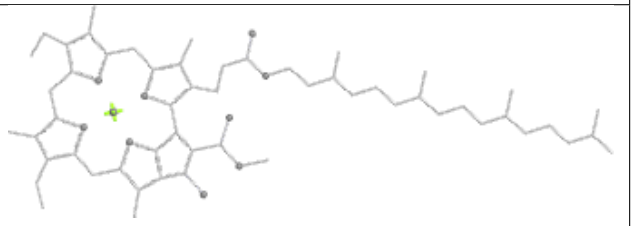
Bond lengths



Bond angles



Torsions

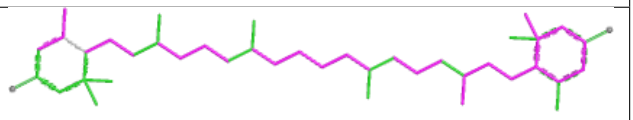


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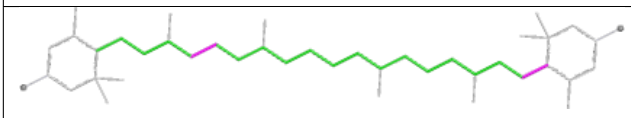
Ligand LUT 3 1621



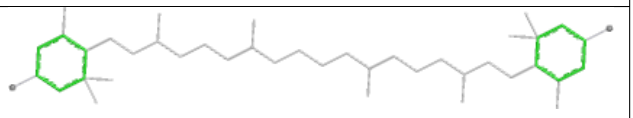
Bond lengths



Bond angles

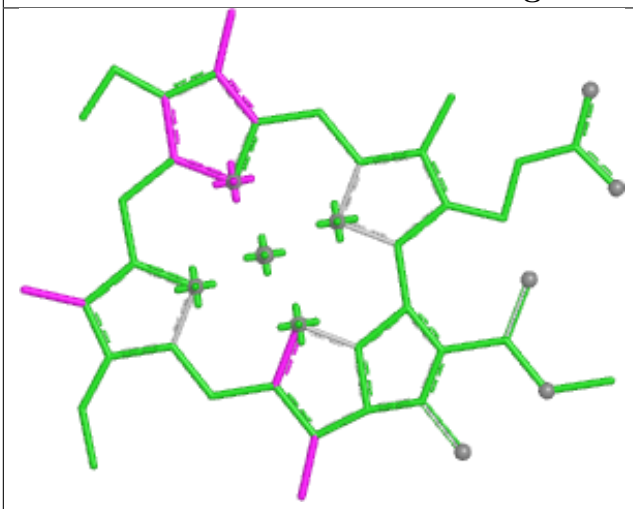


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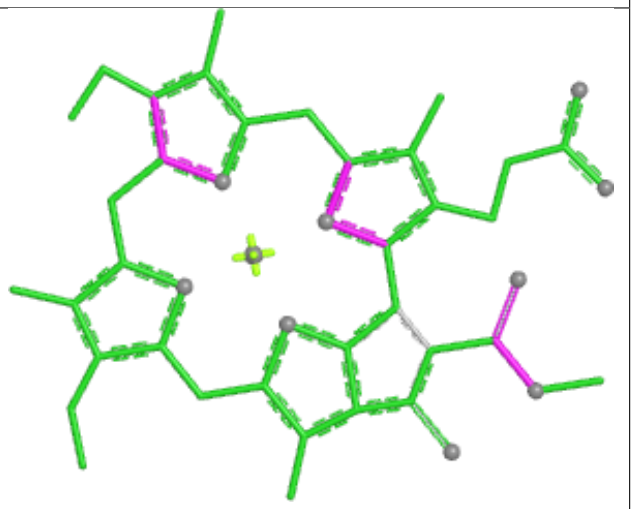


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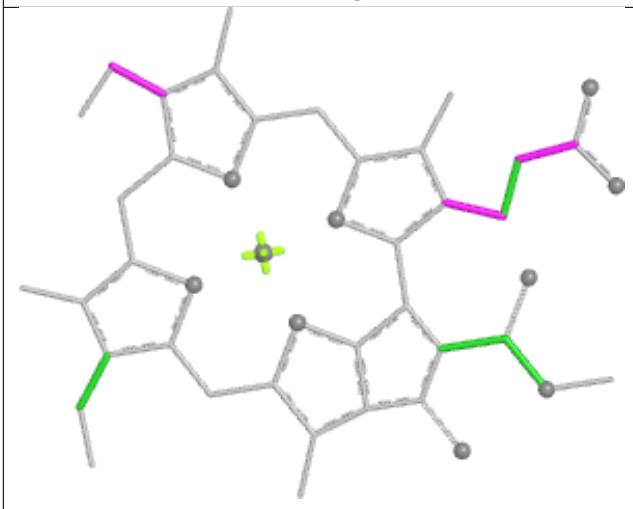
Ligand CLA R 616



Bond lengths



Bond angles

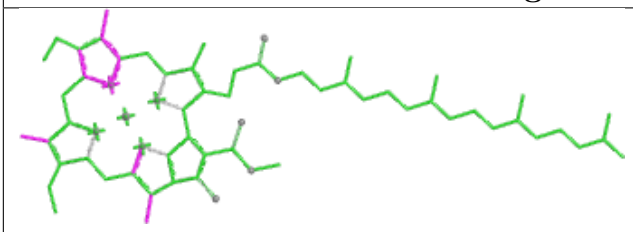


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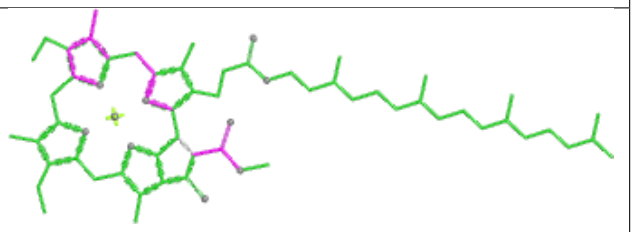


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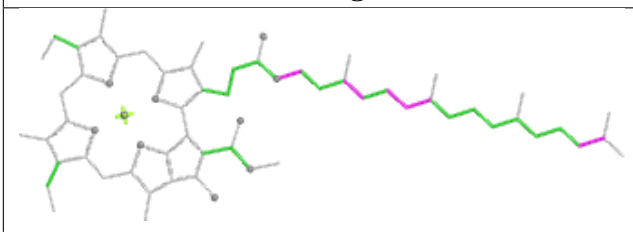
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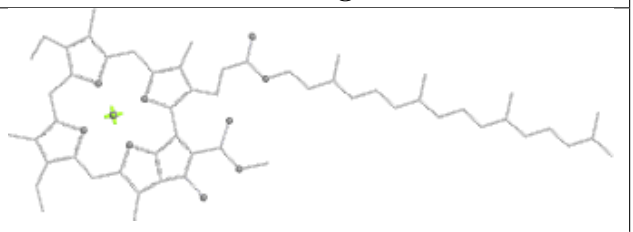
Bond lengths



Bond angles

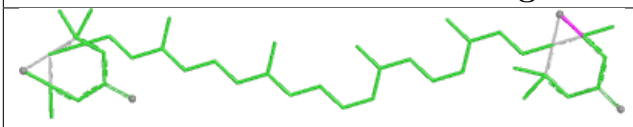


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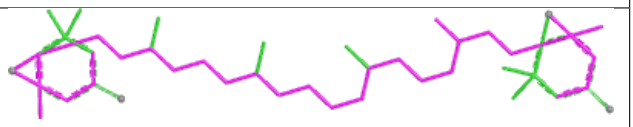


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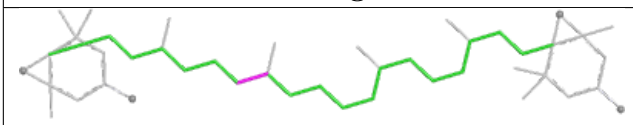
Ligand XAT 1 1622



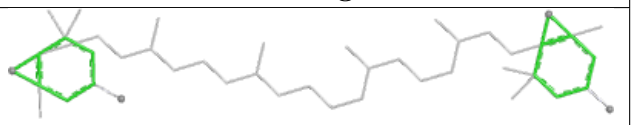
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Bond angles

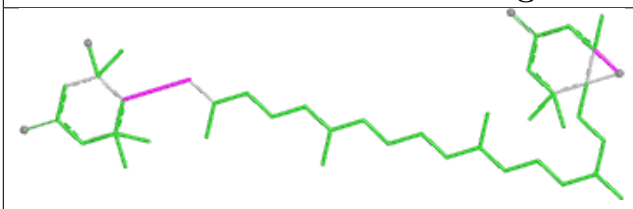


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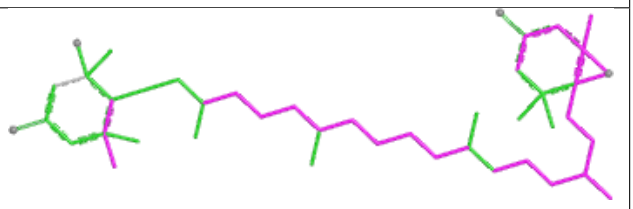


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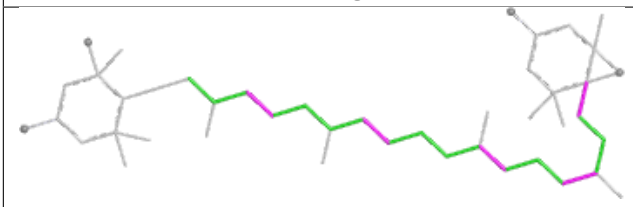
Ligand NEX 6 1623



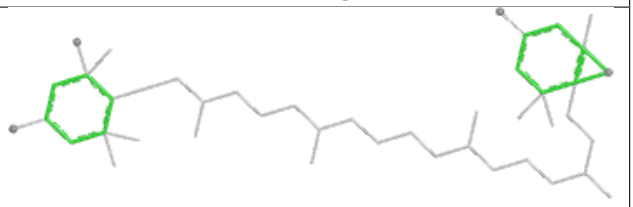
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Bond angles

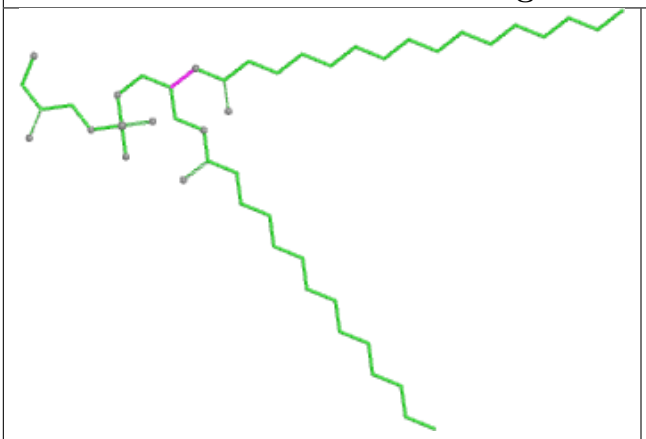


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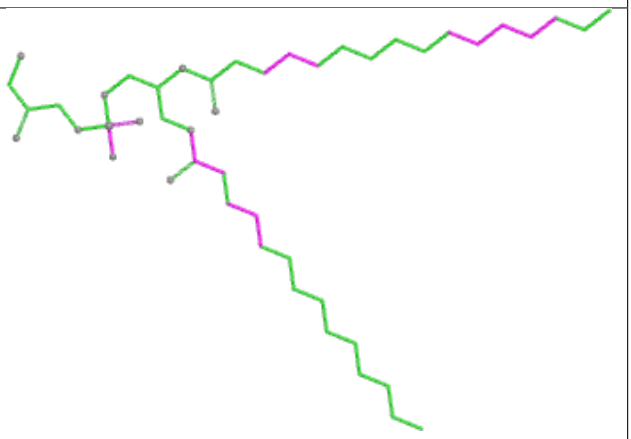


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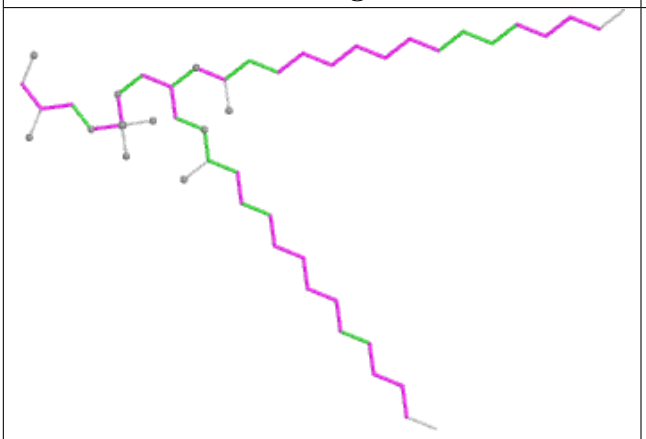
Ligand LHG b 2630



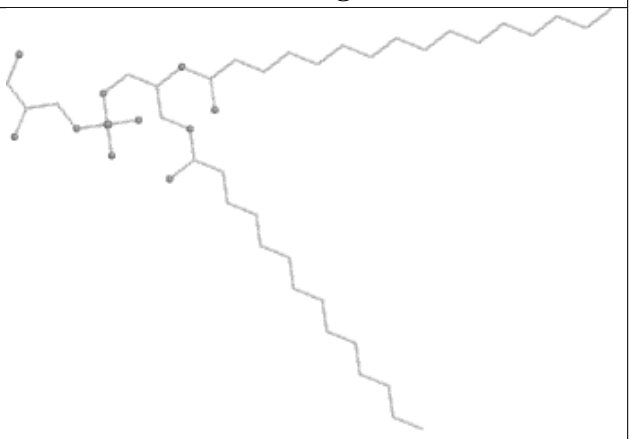
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Bond angles

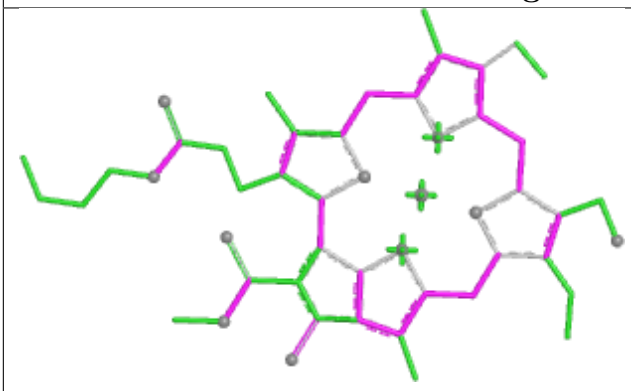


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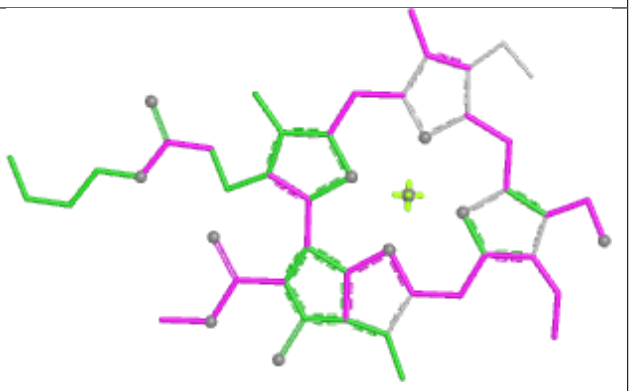


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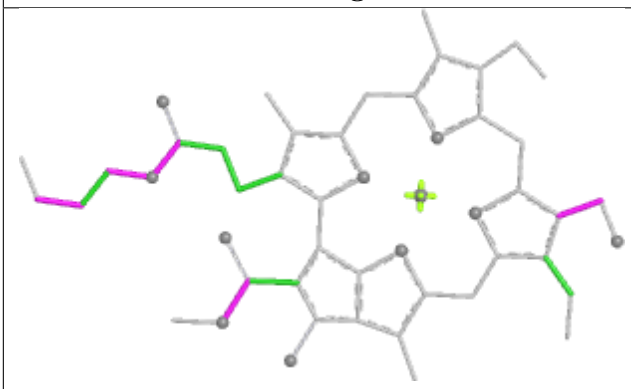
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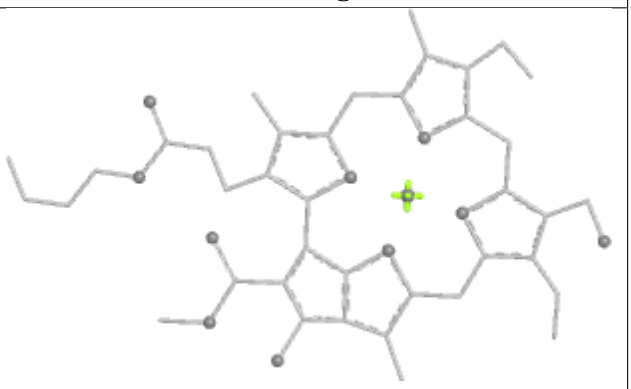
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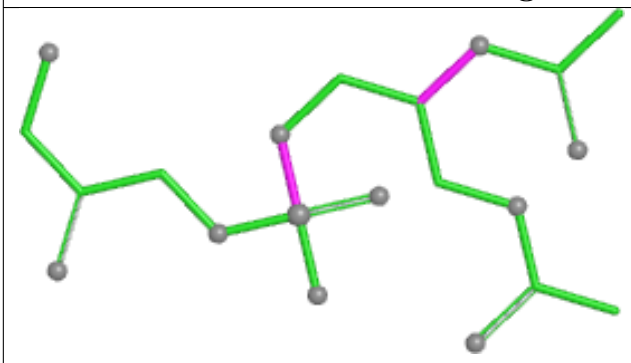


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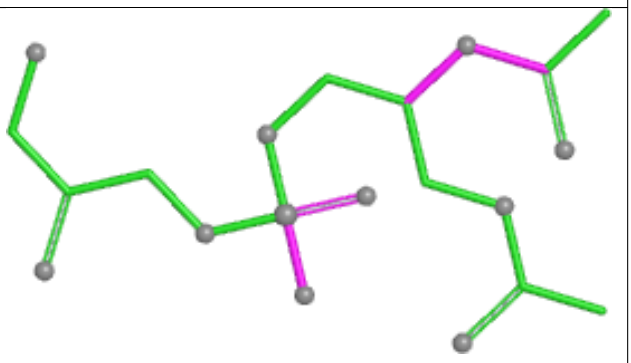


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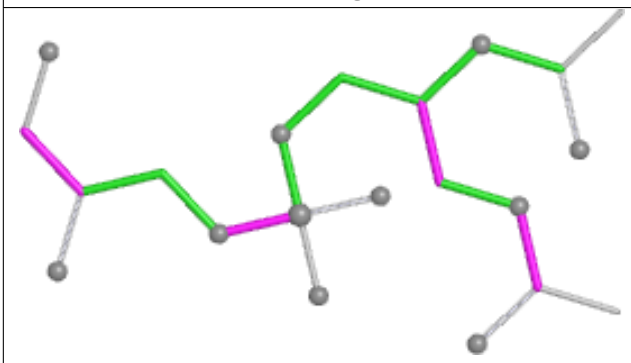
Ligand LHG 8 2630



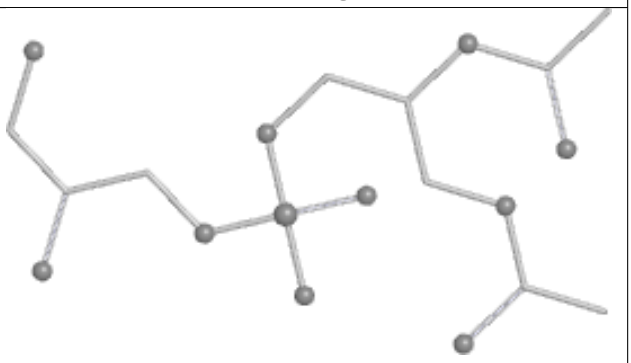
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Bond angles

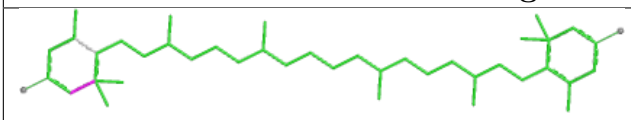


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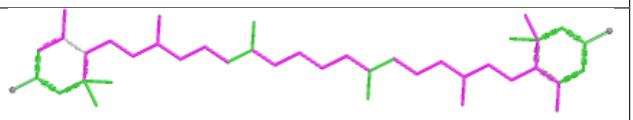


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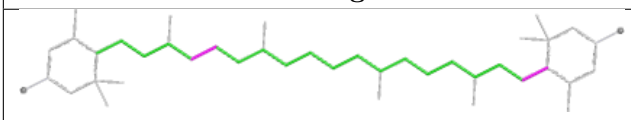
Ligand LUT 2 1621



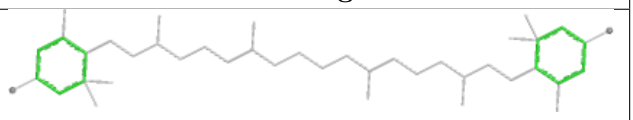
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Bond angles

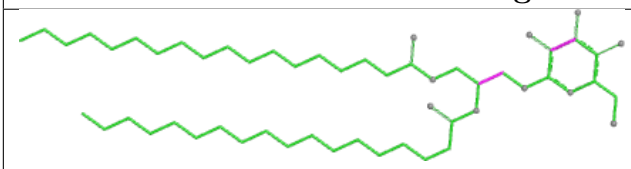


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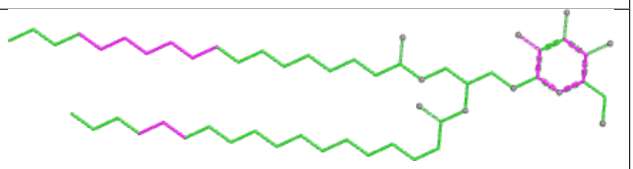


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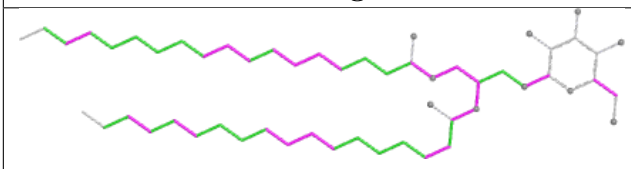
Ligand LMG b 2633



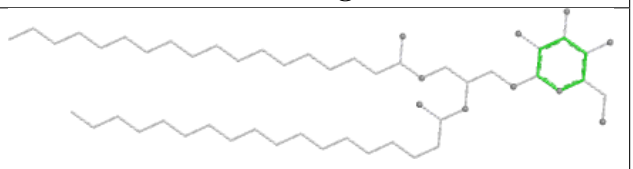
Bond lengths



Bond angles

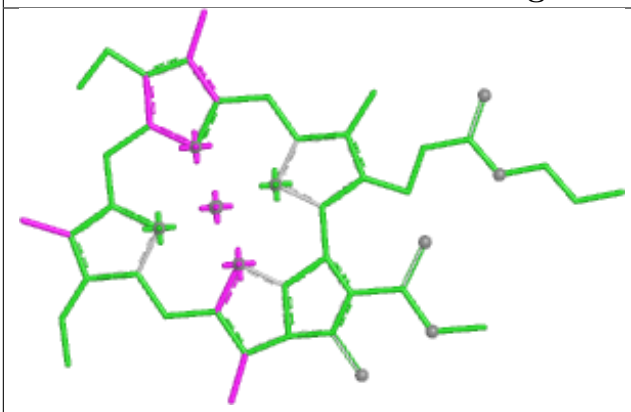


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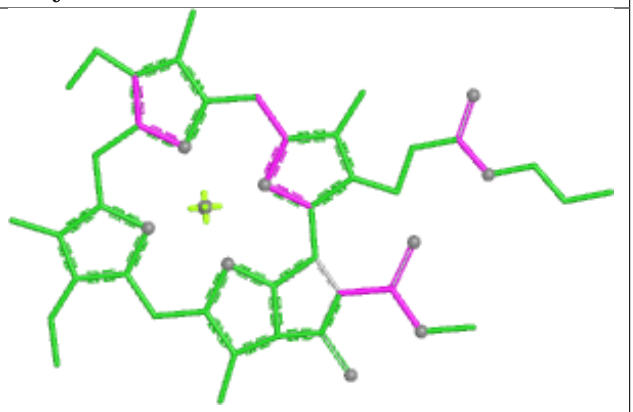


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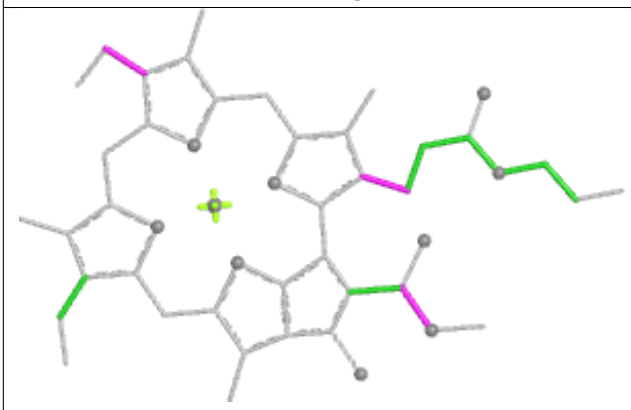
Ligand CLA y 614



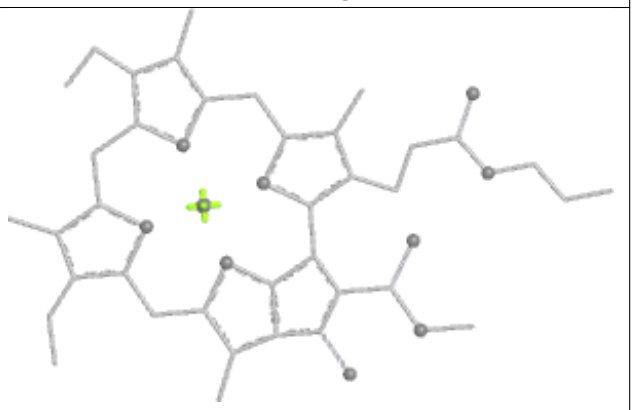
Bond lengths



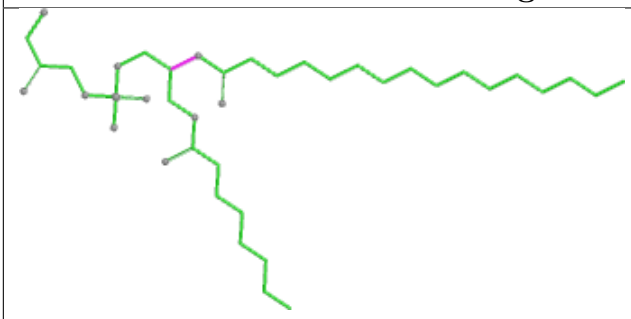
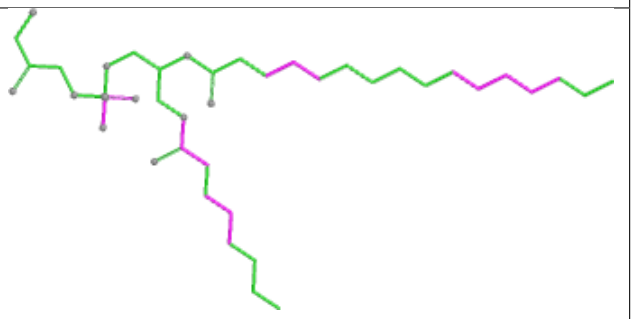
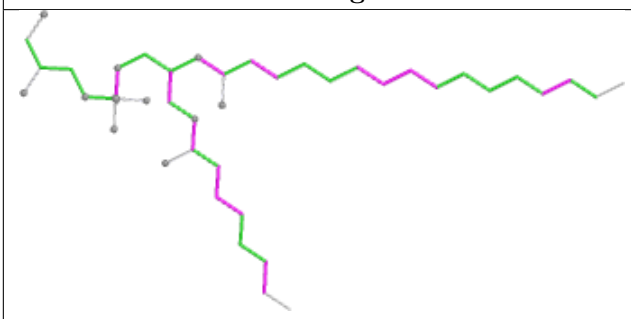
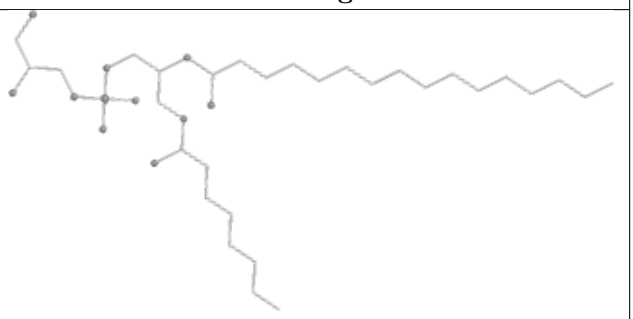
Bond angles

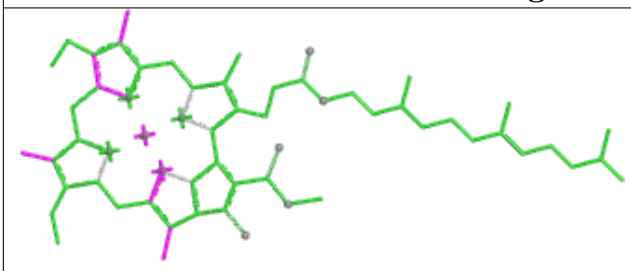
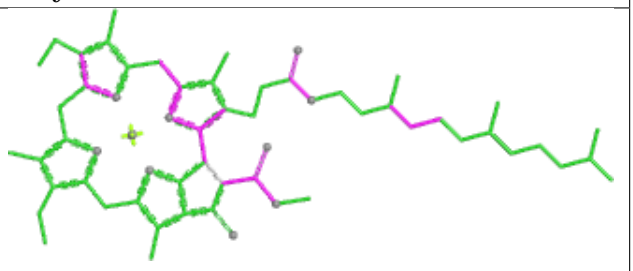
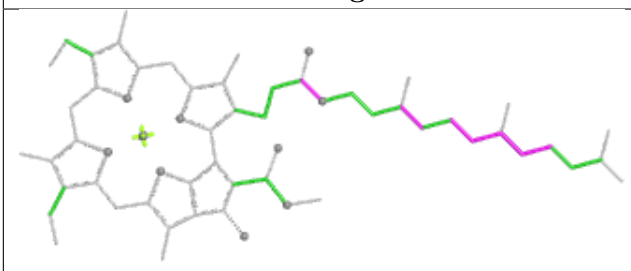
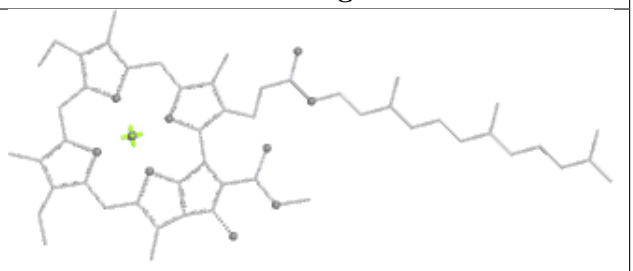


Torsions

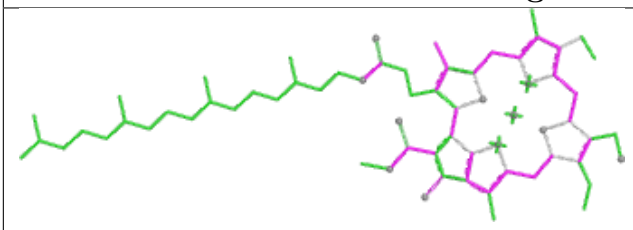


Rings

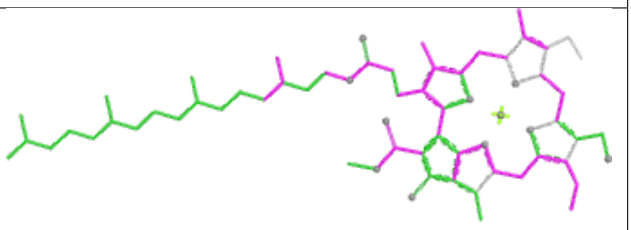
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 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA y 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

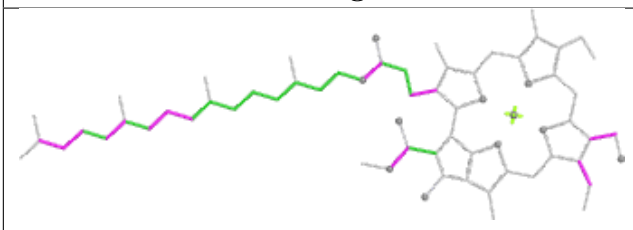
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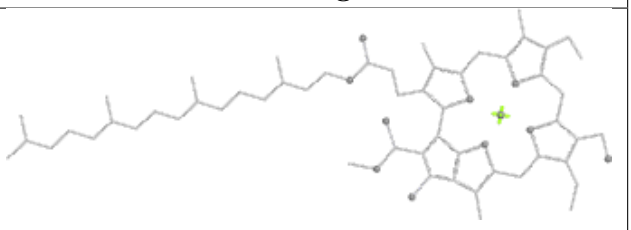
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Bond angles

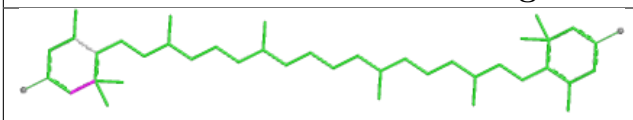


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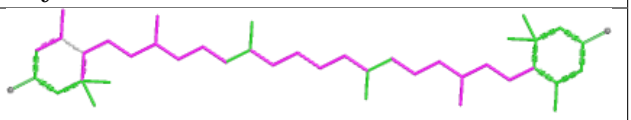


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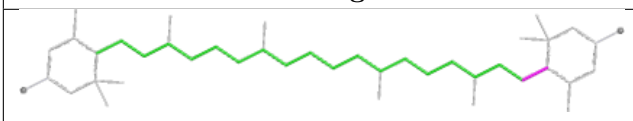
Ligand LUT y 1620



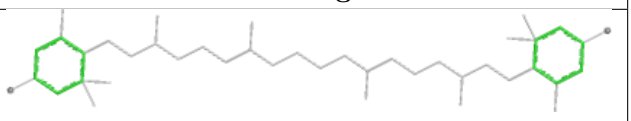
Bond lengths



Bond angles

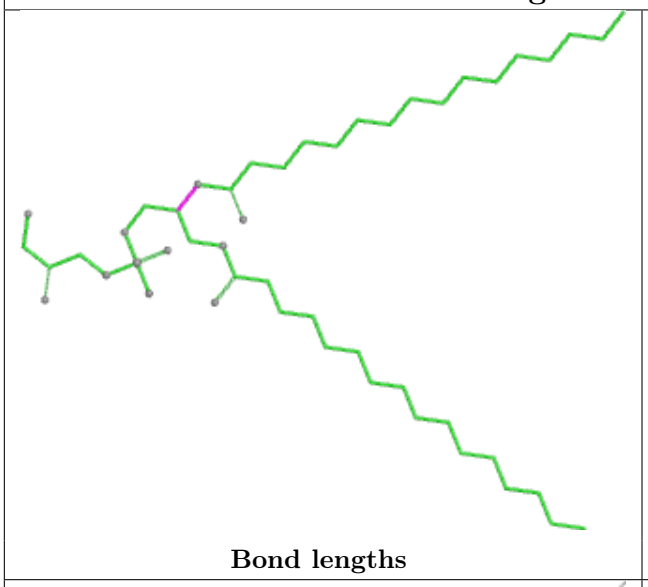


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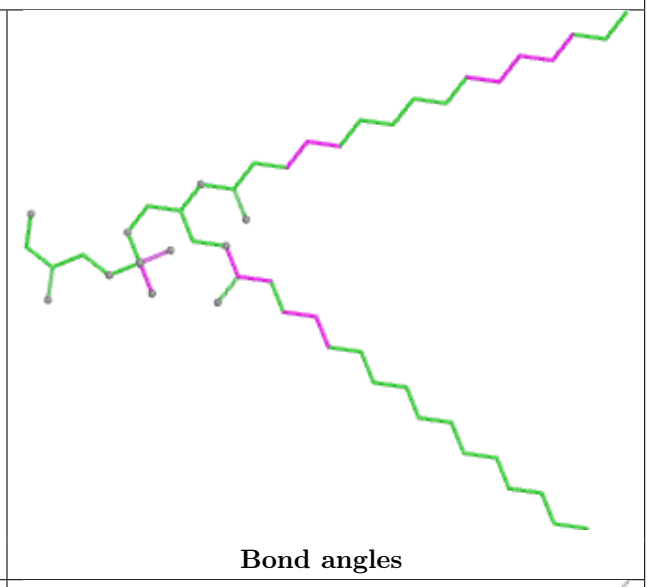


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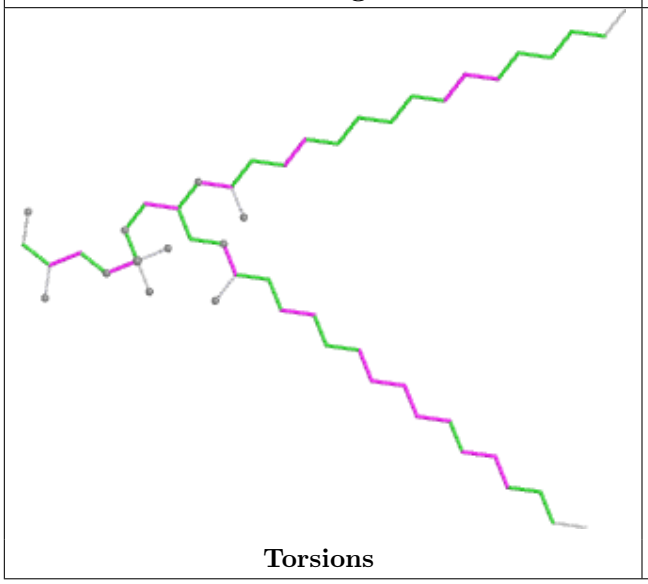
Ligand LHG c 522



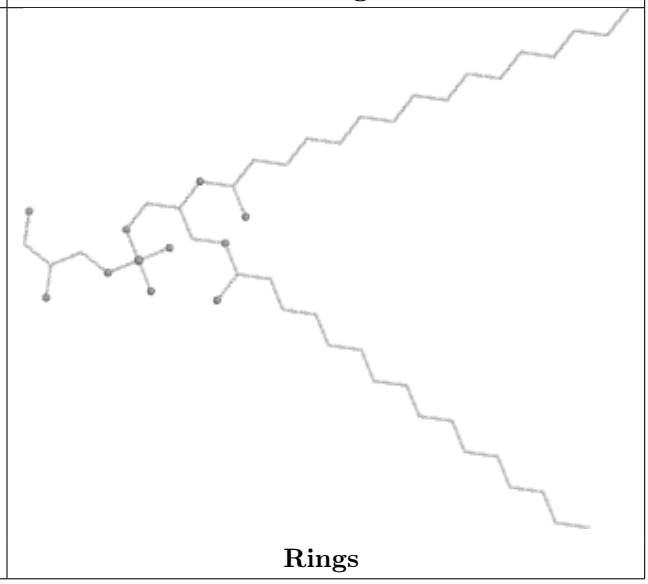
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Bond angles

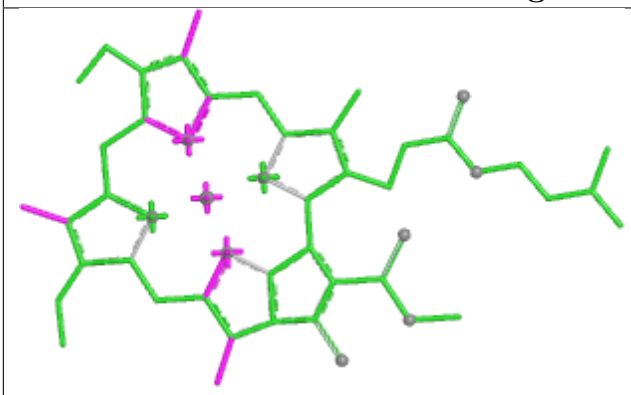


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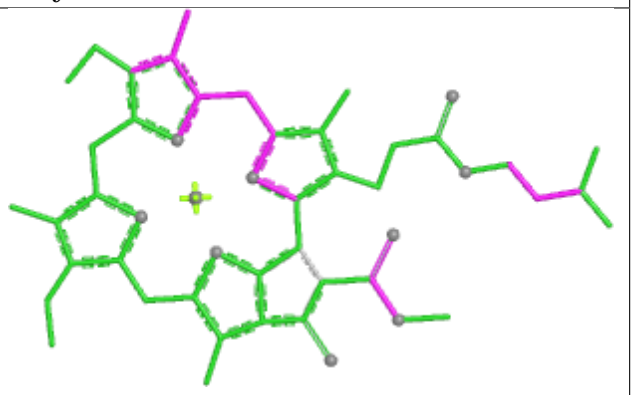


Rings

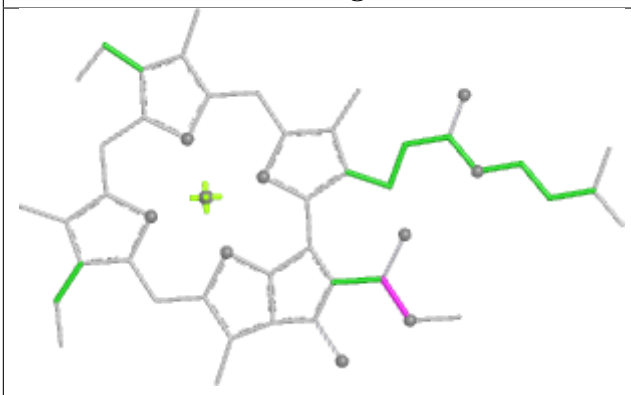
Ligand CLA y 604



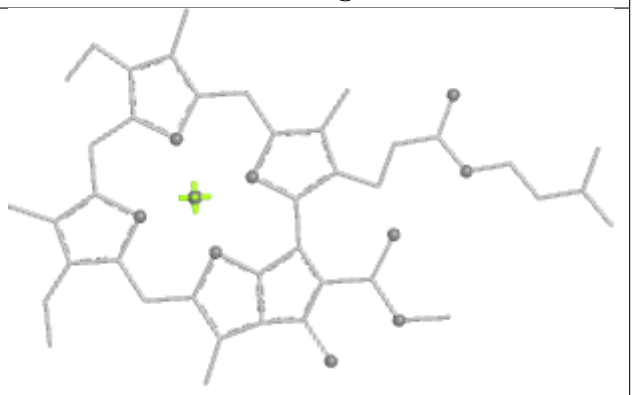
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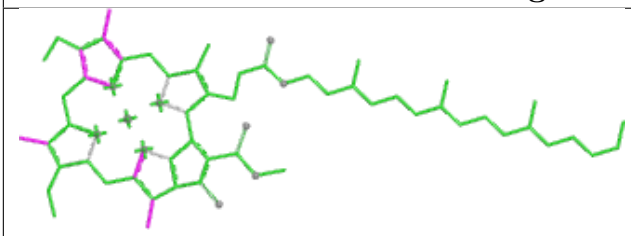


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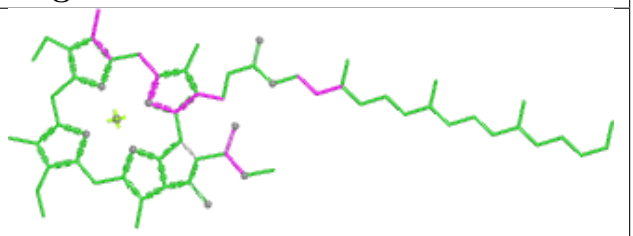


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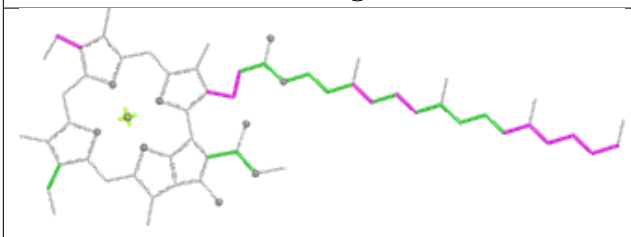
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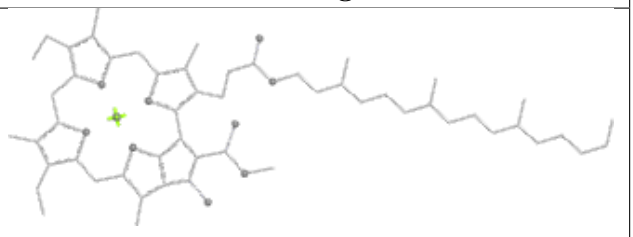
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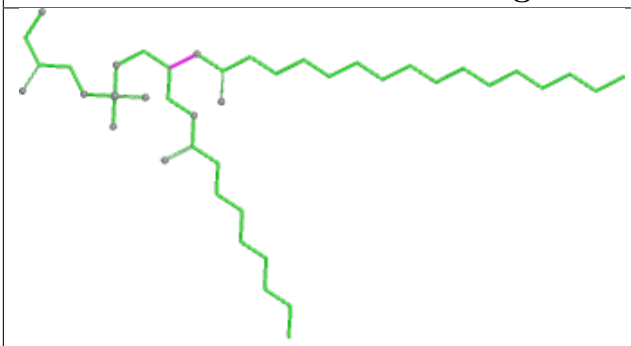


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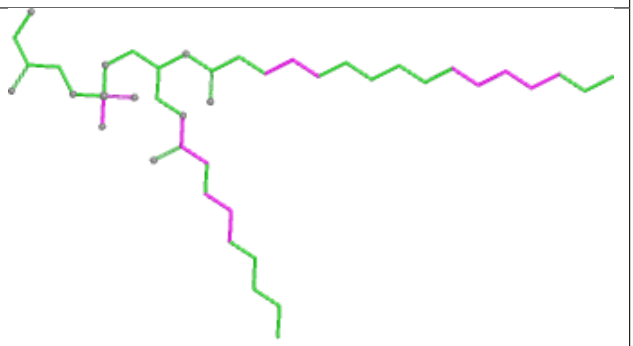


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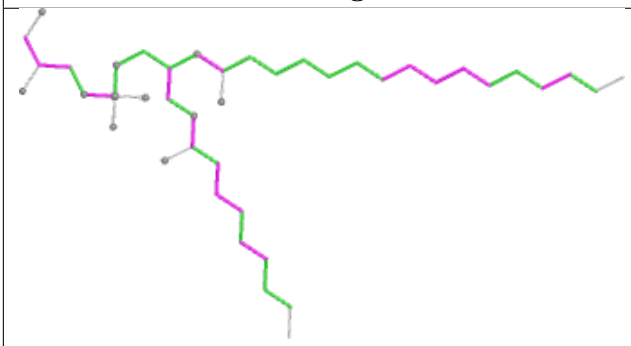
Ligand LHG R 2630



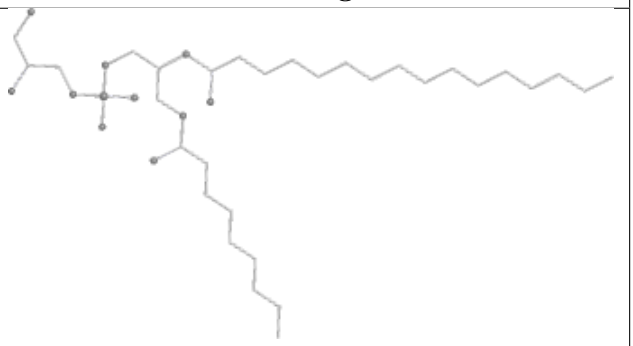
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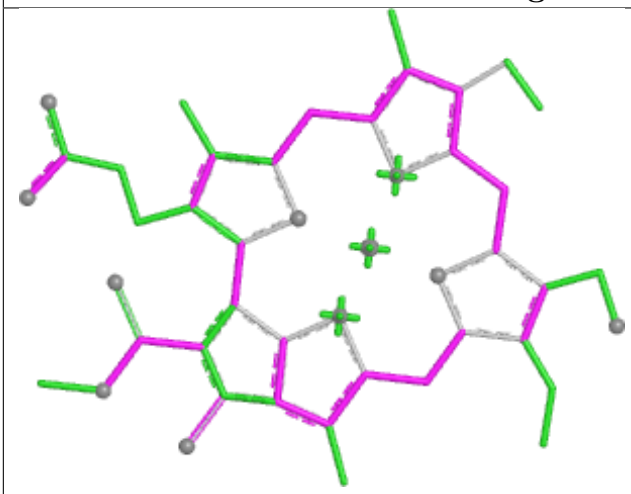


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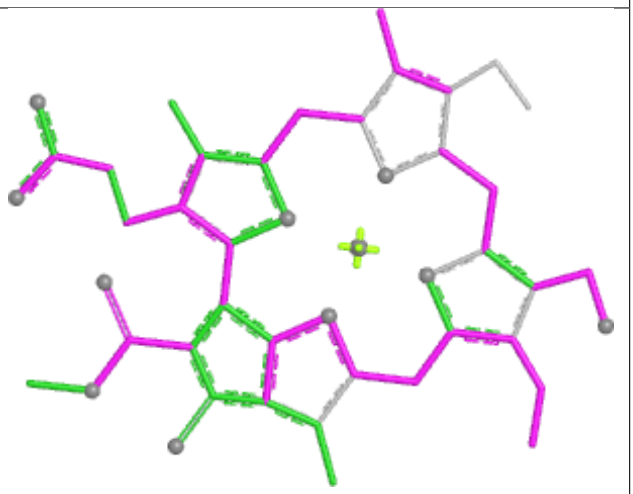


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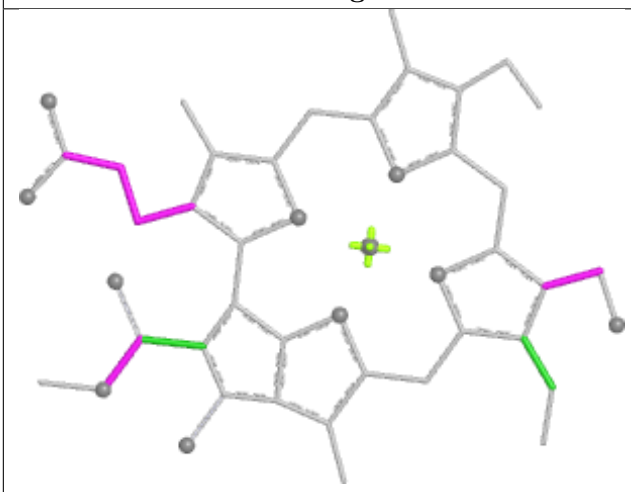
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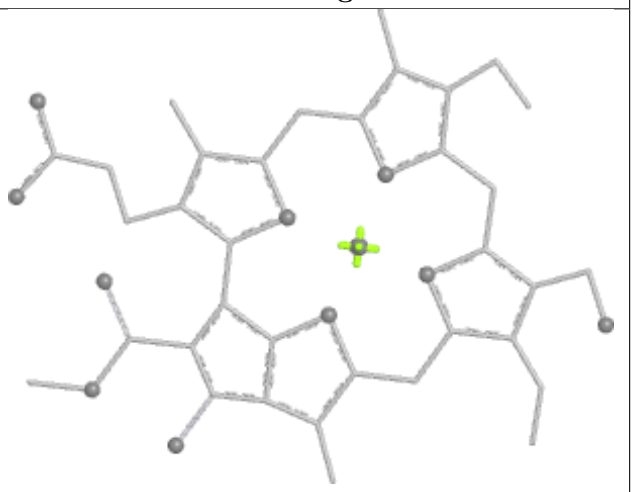
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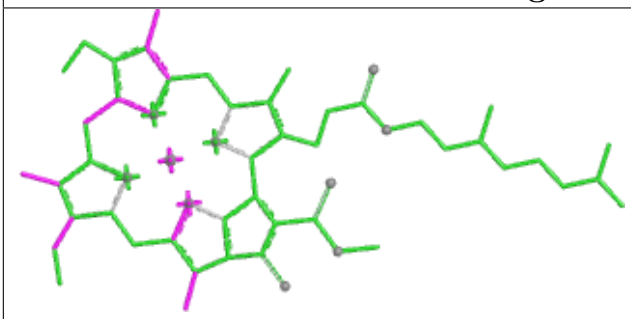


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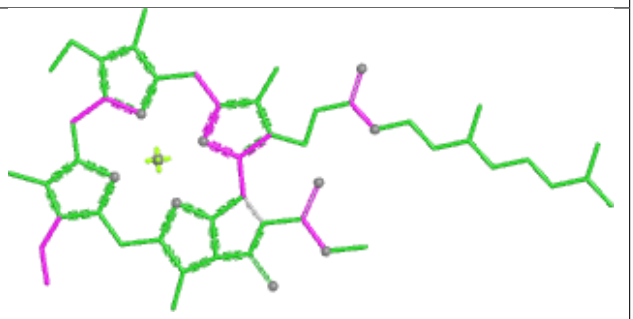


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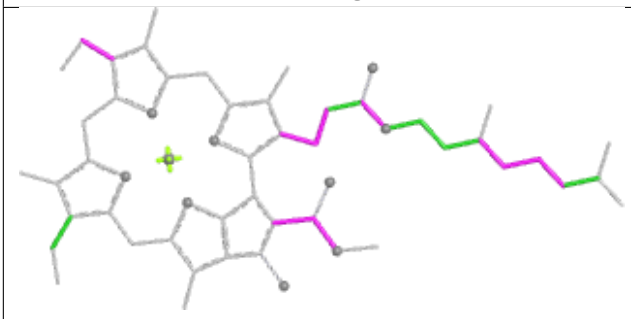
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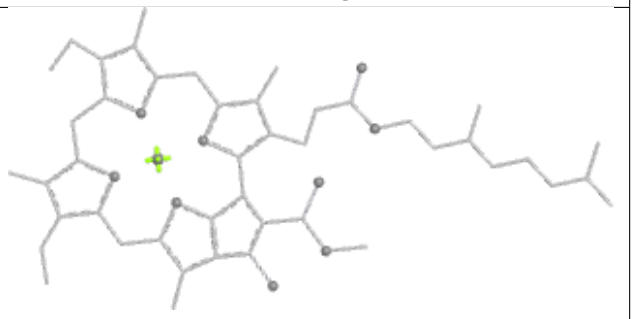
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Bond angles

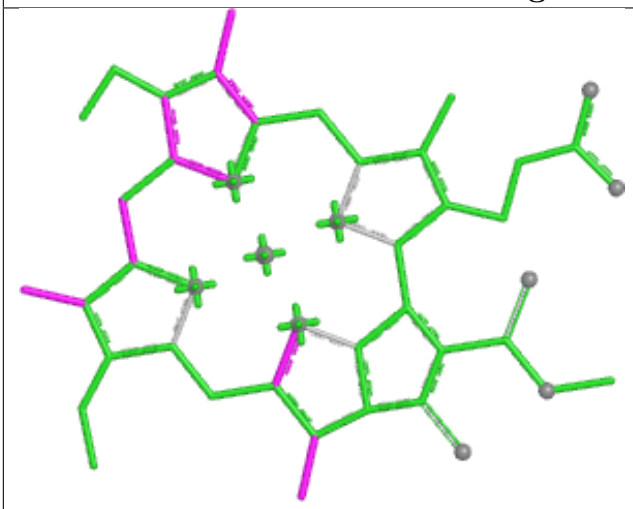


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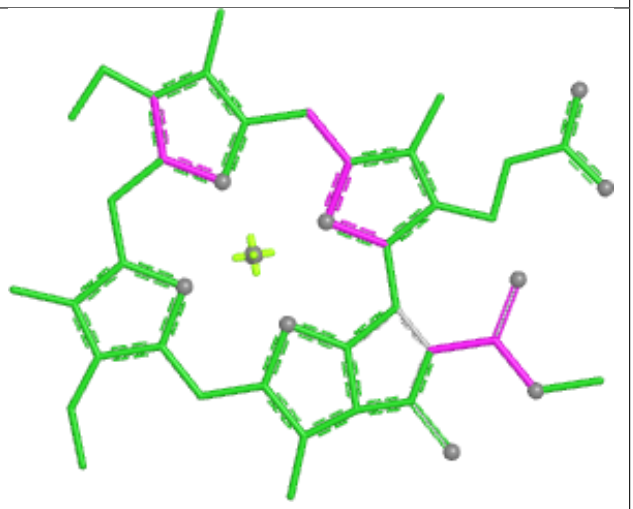


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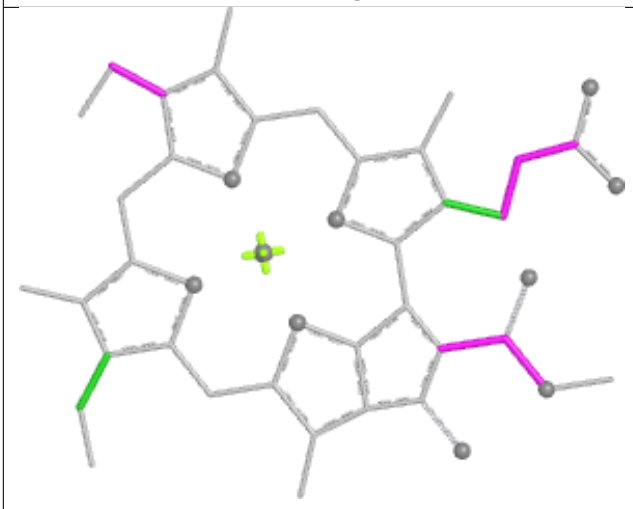
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Bond lengths



Bond angles

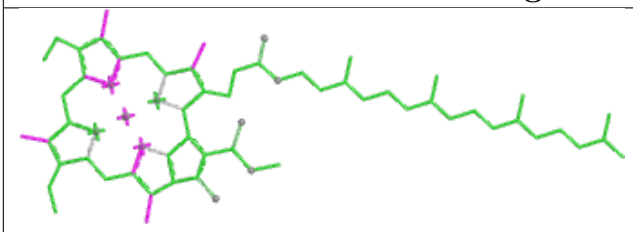


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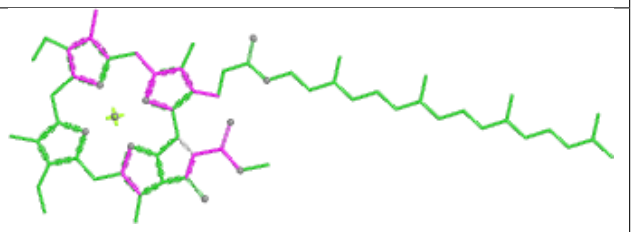


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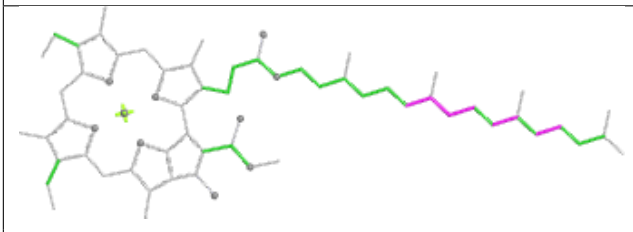
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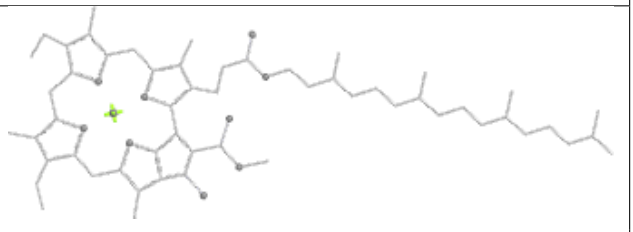
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Bond angles

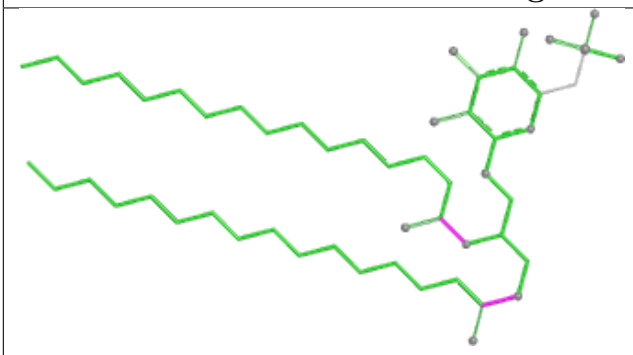


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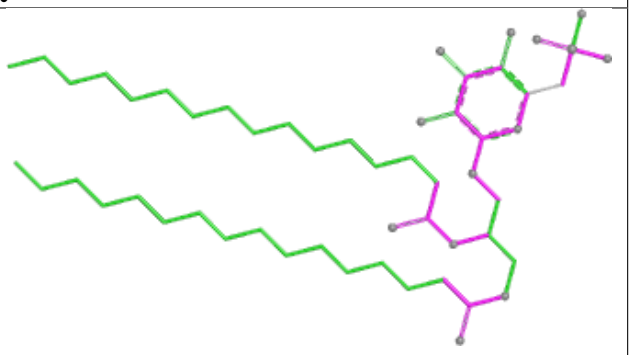


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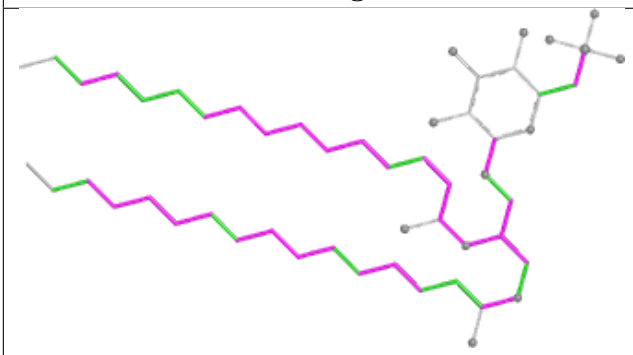
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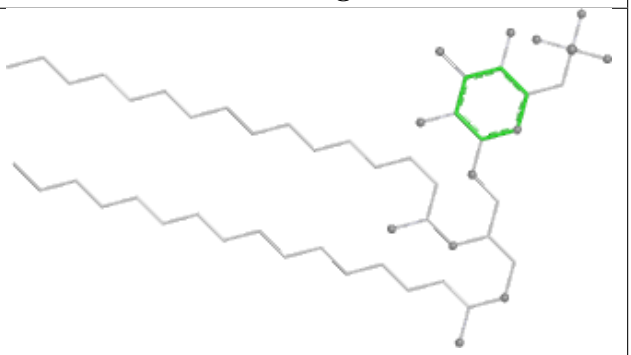
Bond lengths



Bond angles

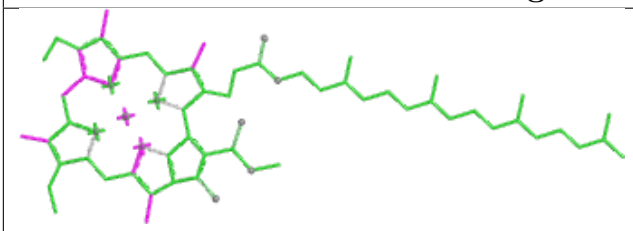


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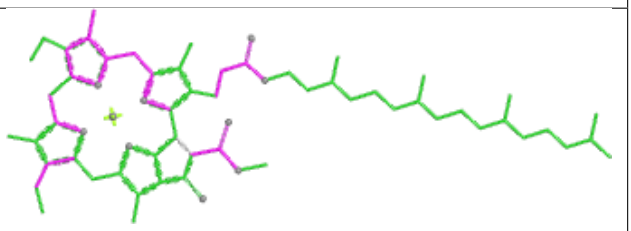


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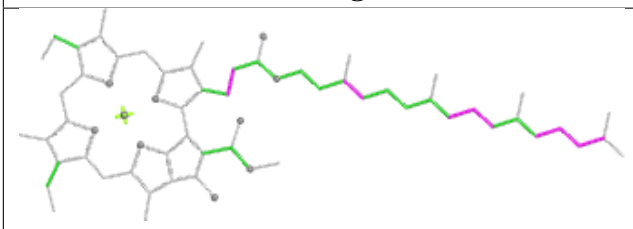
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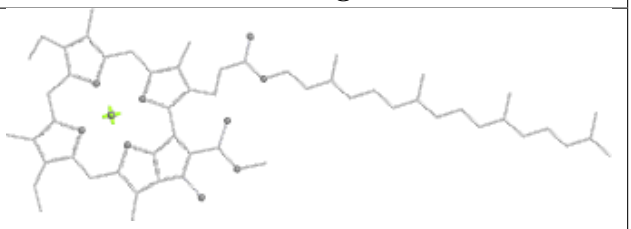
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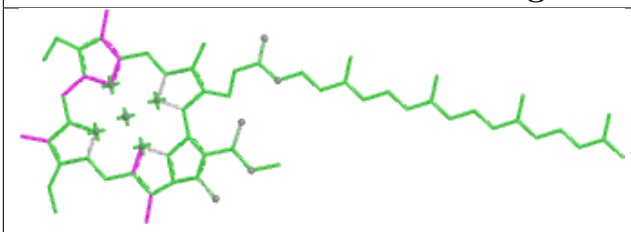
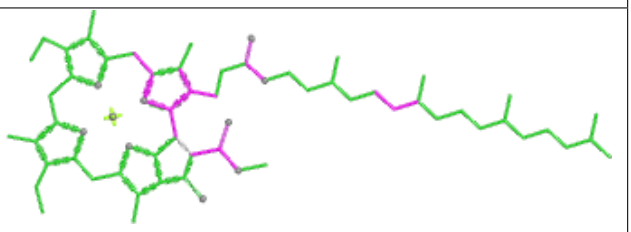
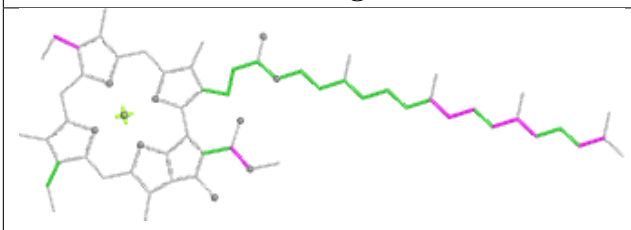
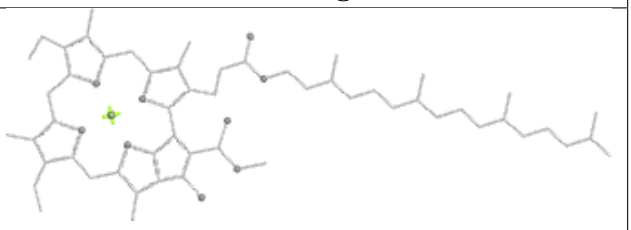
Bond angles

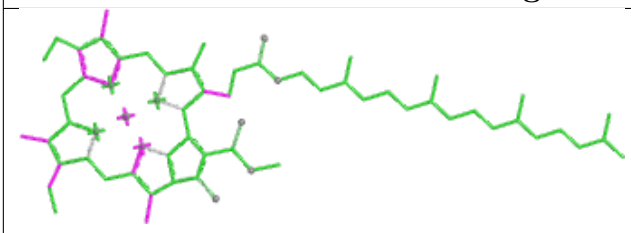
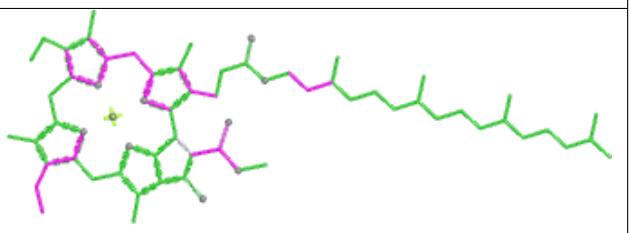
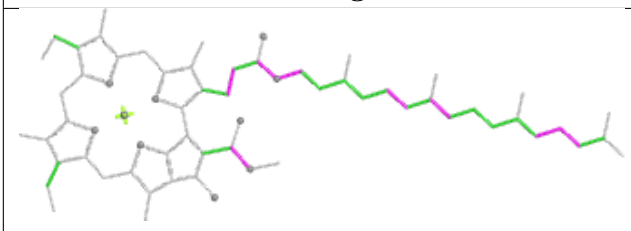
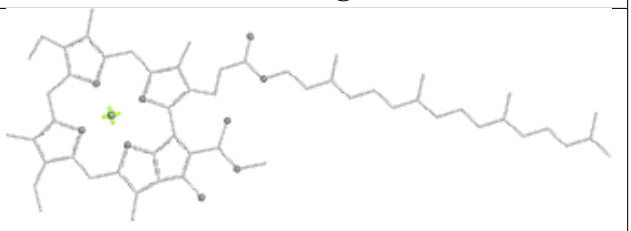


Torsions

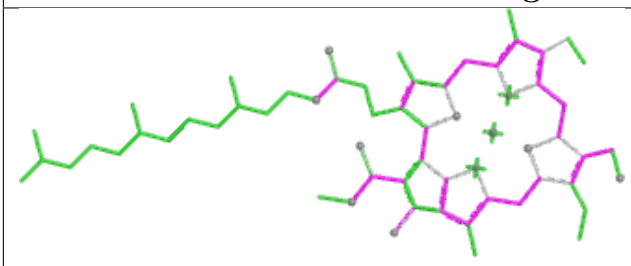


Rings

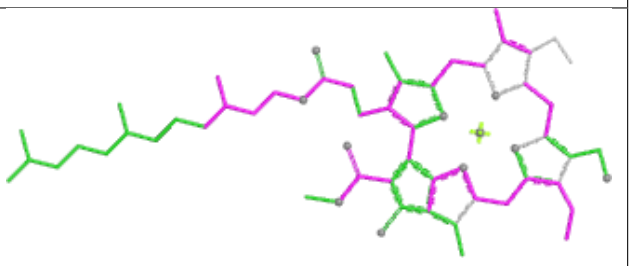
Ligand CLA b 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

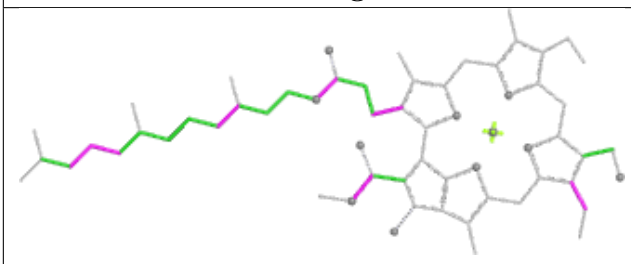
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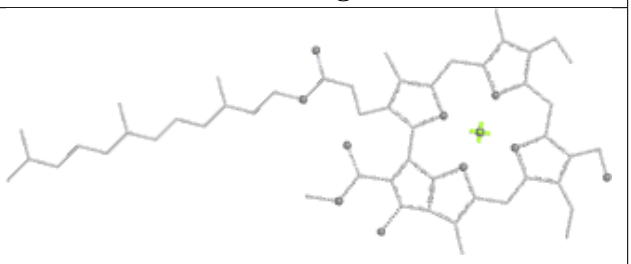
Bond lengths



Bond angles

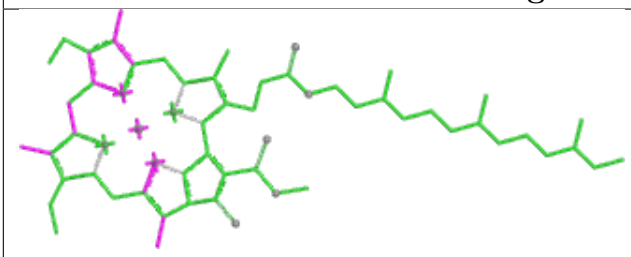


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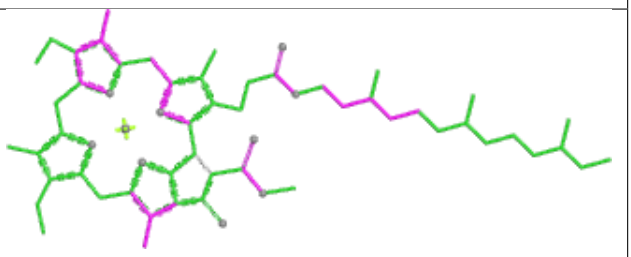


Rings

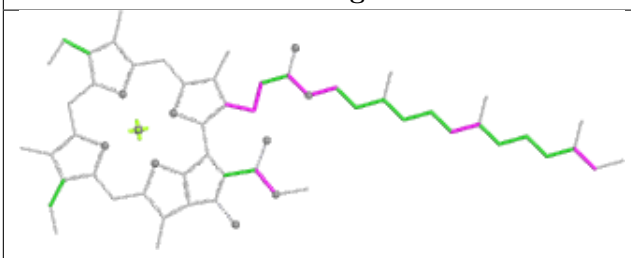
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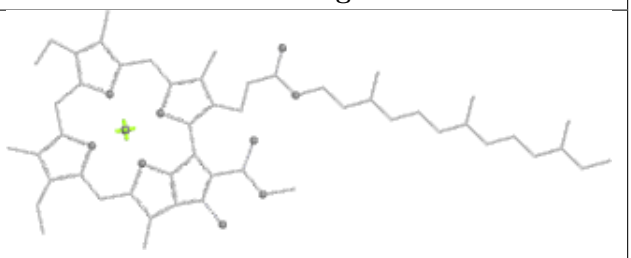
Bond lengths



Bond angles

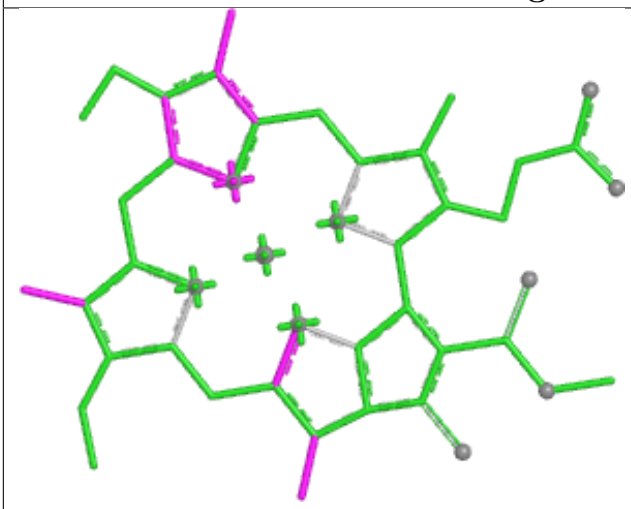


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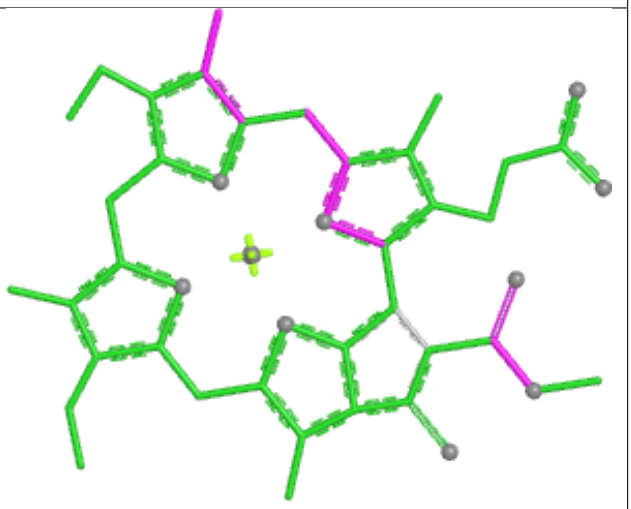


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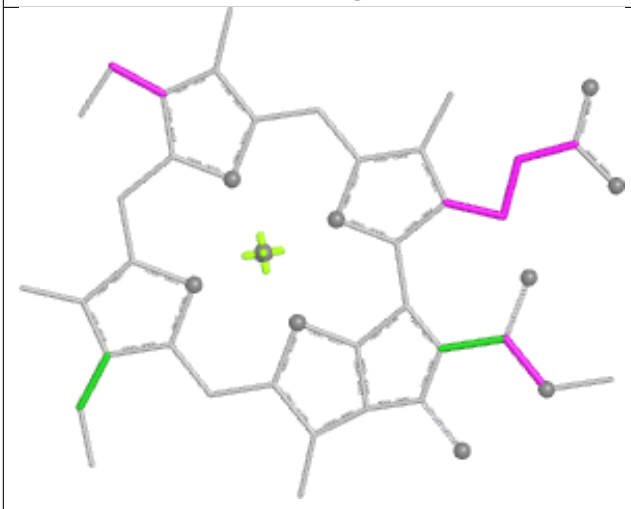
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Bond lengths



Bond angles

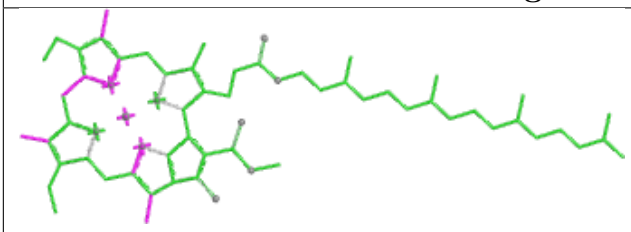


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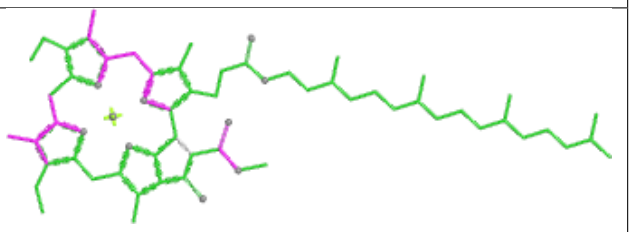


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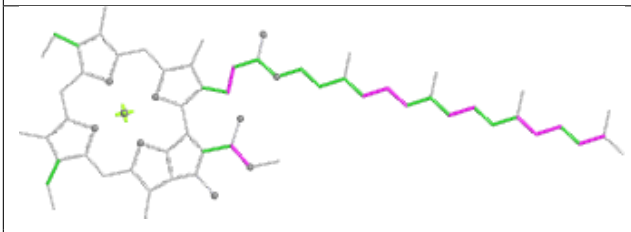
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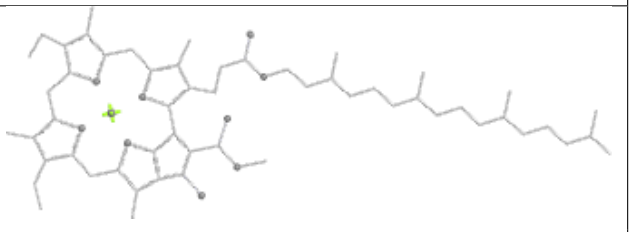
Bond lengths



Bond angles

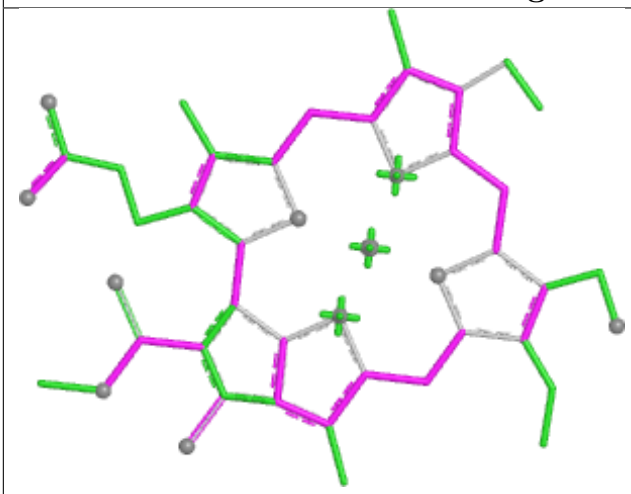


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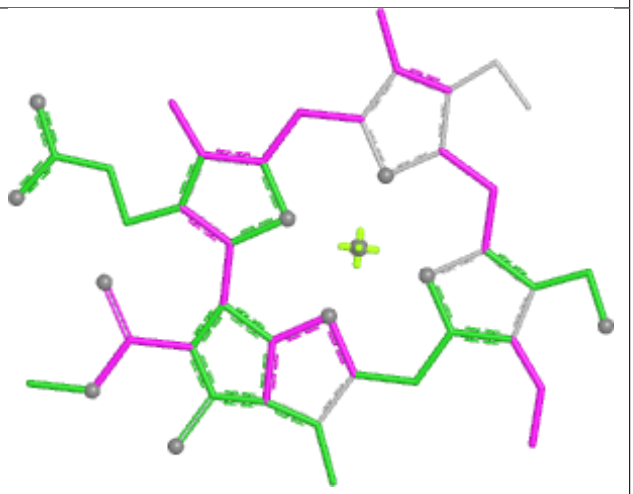


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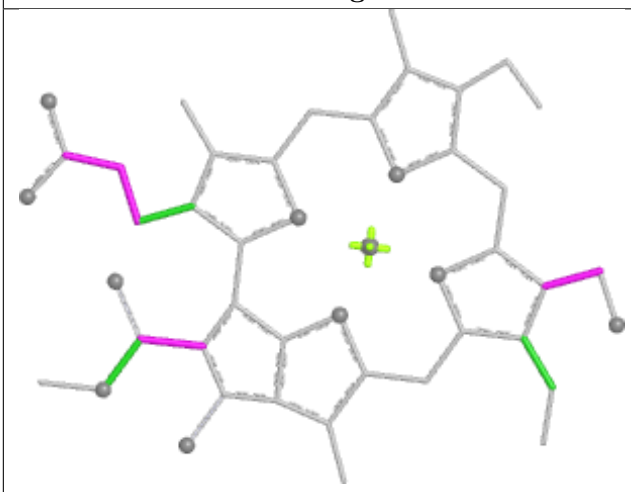
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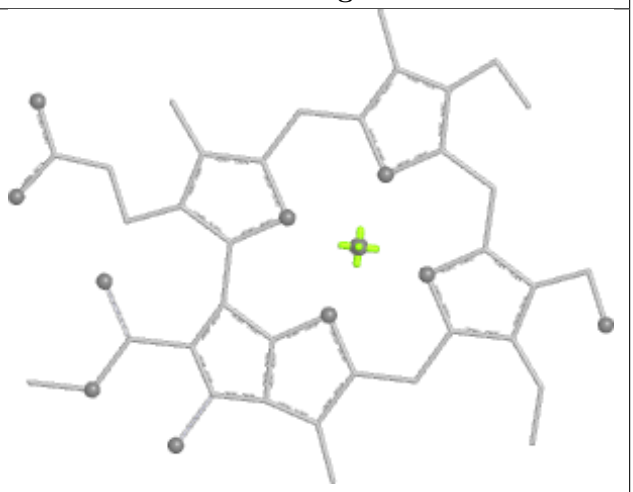
Bond lengths



Bond angles

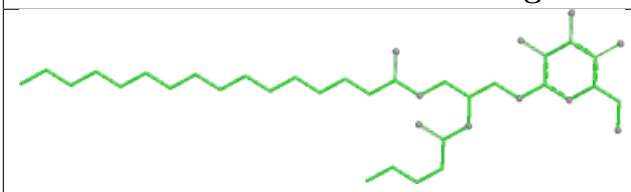


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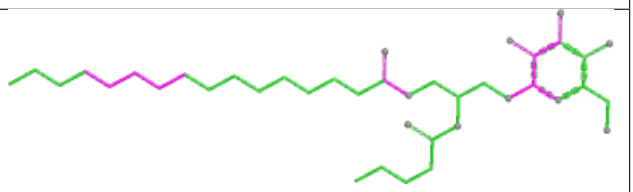


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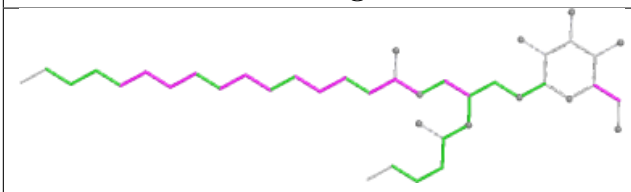
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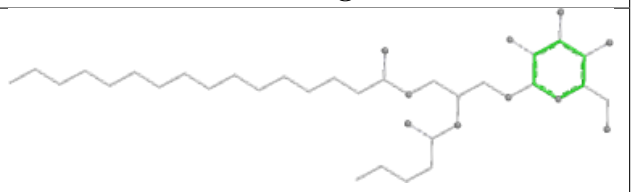
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Bond angles

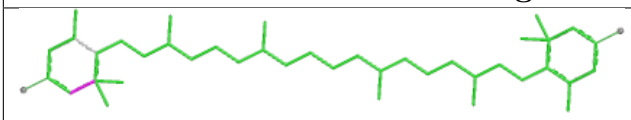


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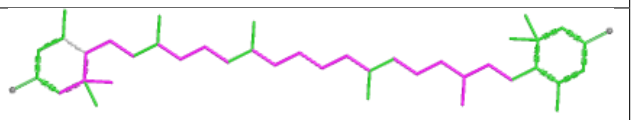


Rings

Ligand LUT Y 1621



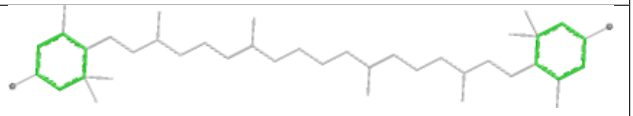
Bond lengths



Bond angles

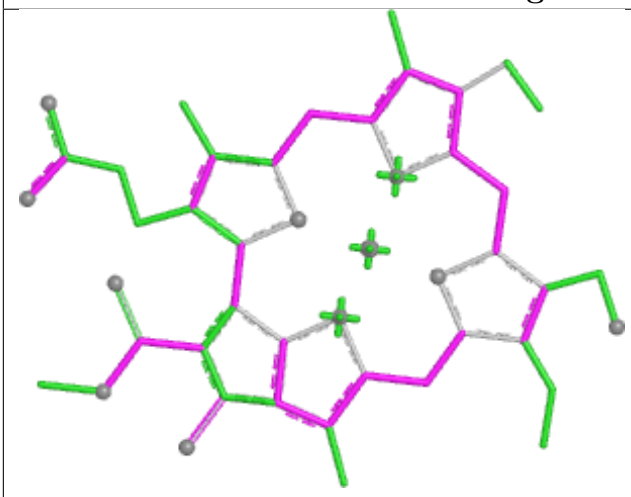


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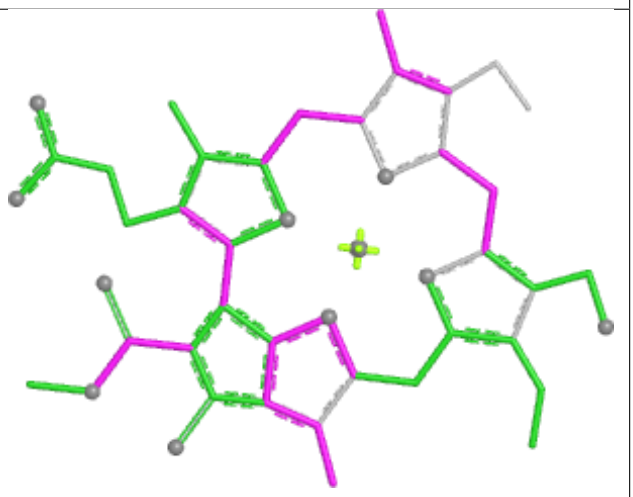


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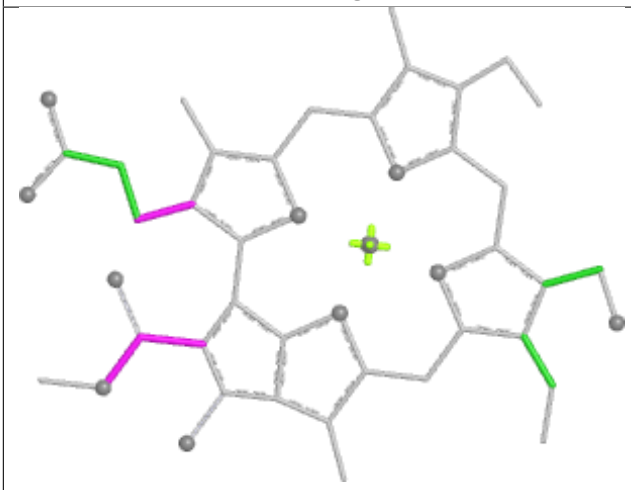
Ligand CHL S 608



Bond lengths



Bond angles

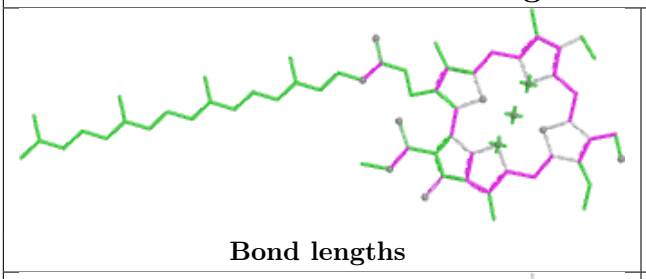


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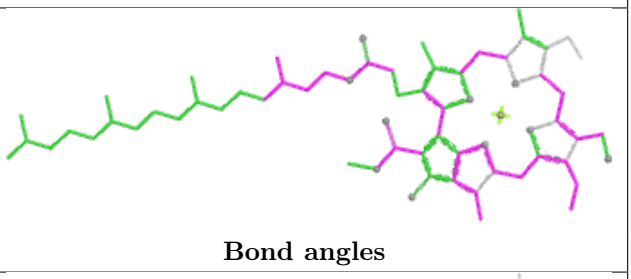


Rings

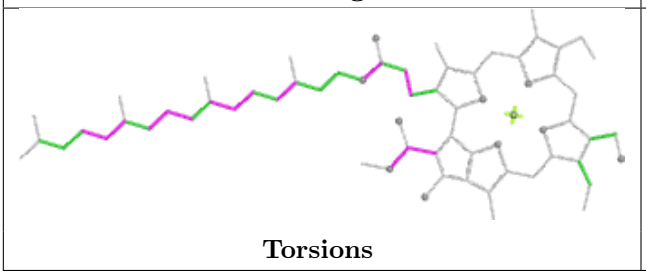
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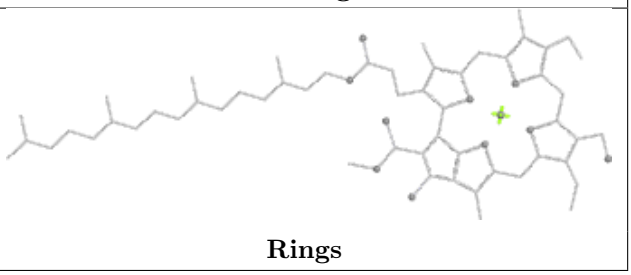
Bond lengths



Bond angles

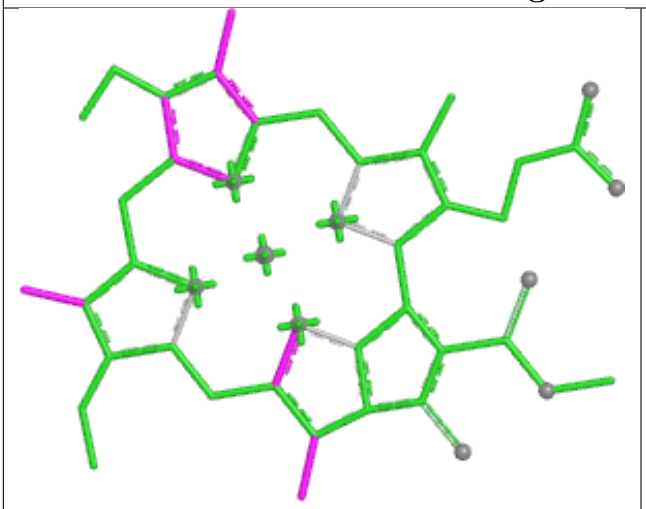


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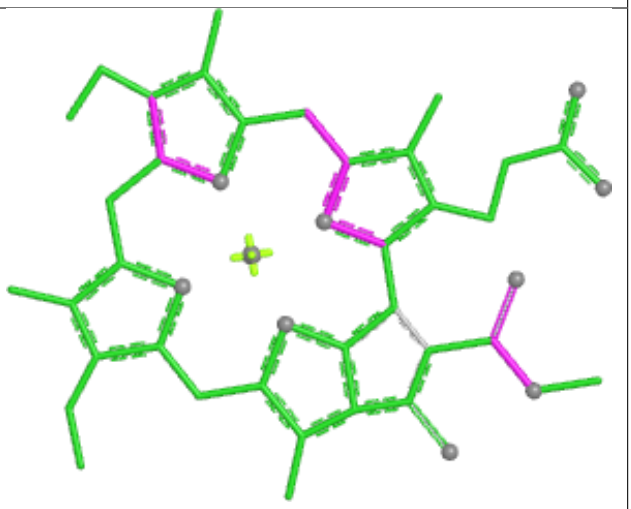


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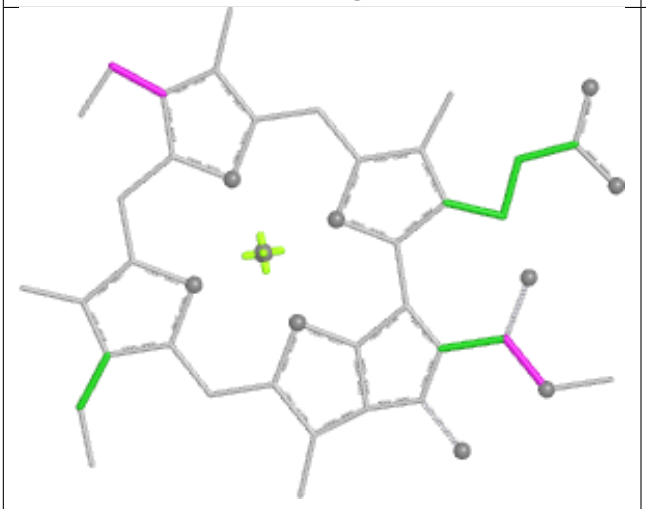
Ligand CLA 5 614



Bond lengths



Bond angles

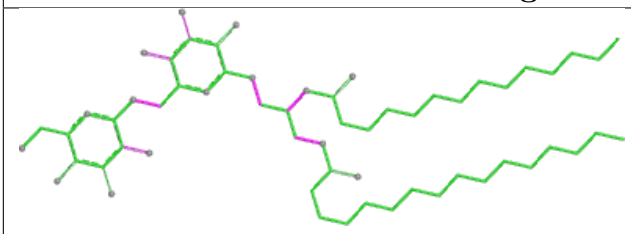


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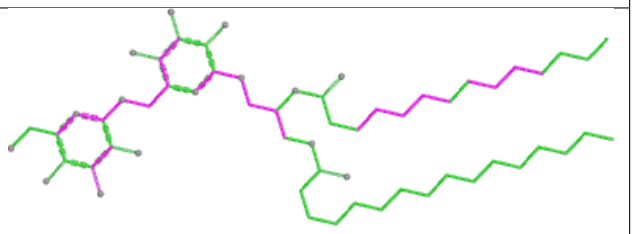


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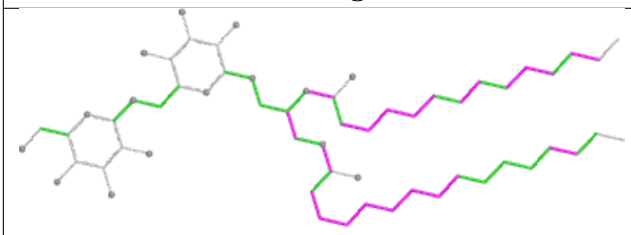
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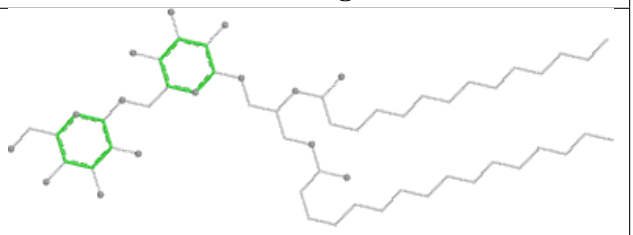
Bond lengths



Bond angles

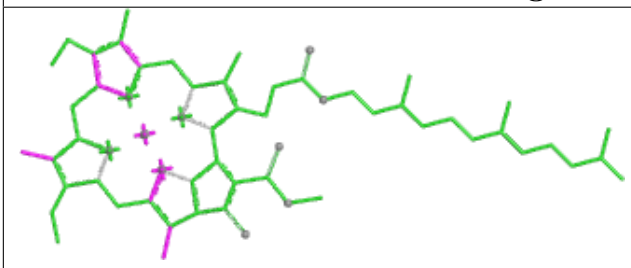


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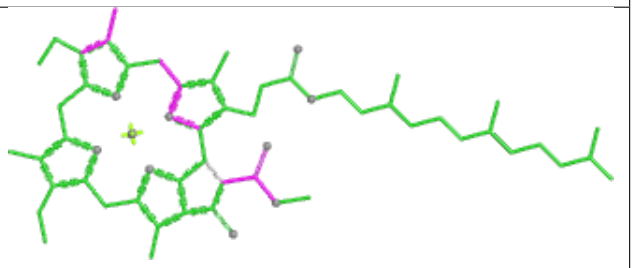


Rings

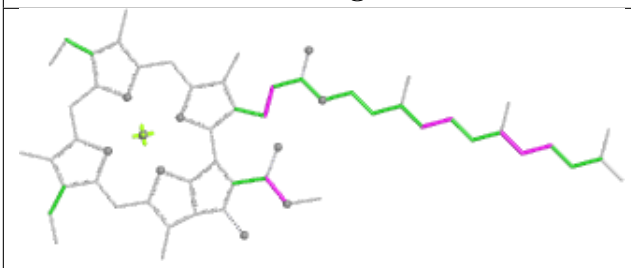
Ligand CLA n 613



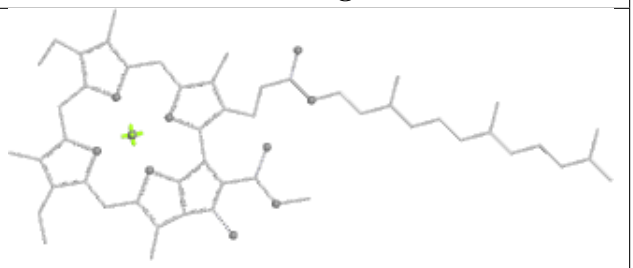
Bond lengths



Bond angles

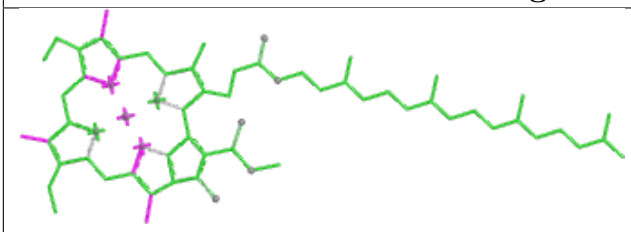


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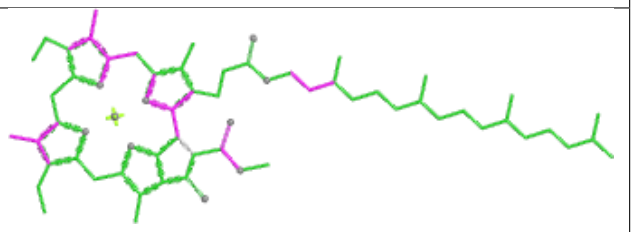


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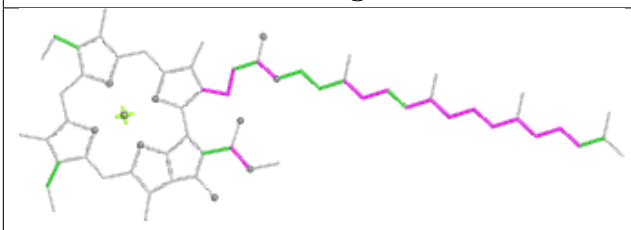
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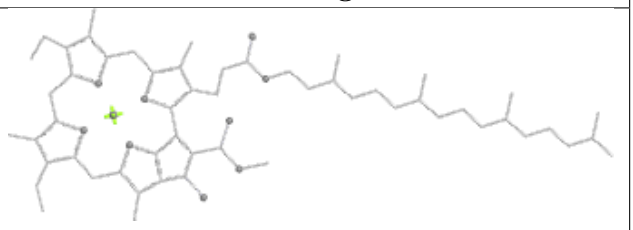
Bond lengths



Bond angles

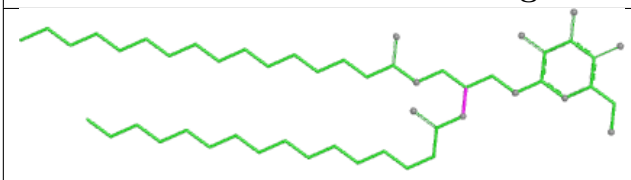


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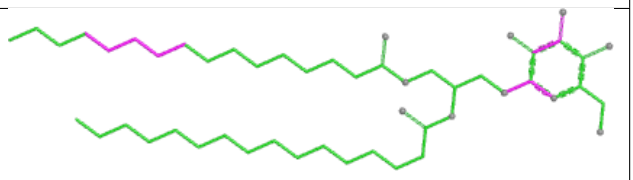


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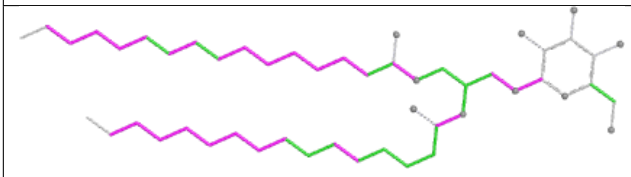
Ligand LMG B 622



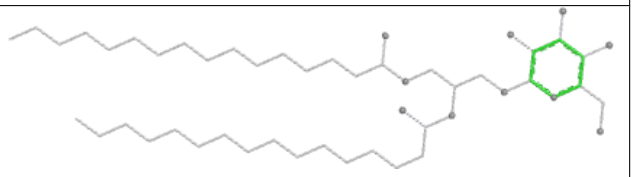
Bond lengths



Bond angles

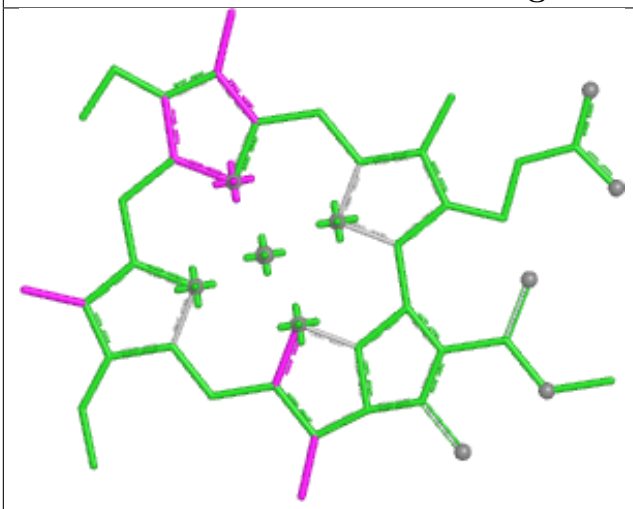


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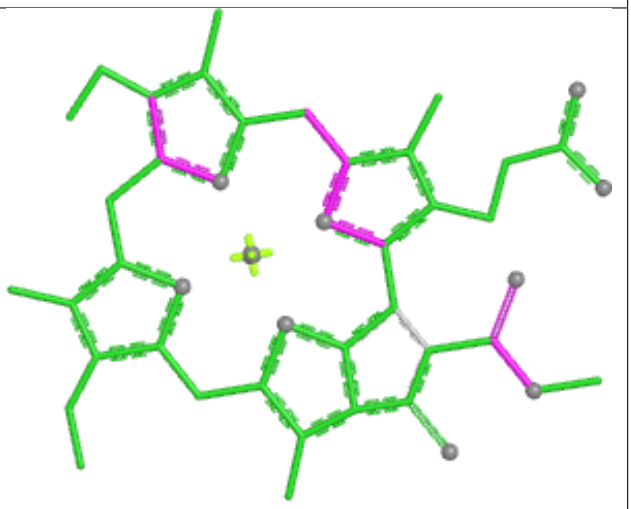


Rings

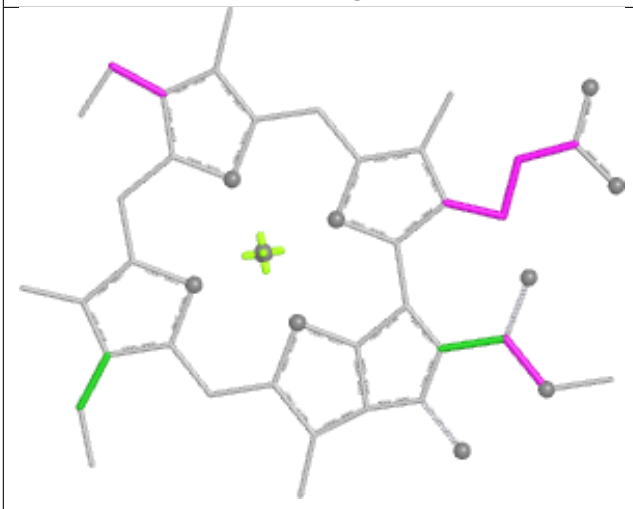
Ligand CLA 8 604



Bond lengths



Bond angles

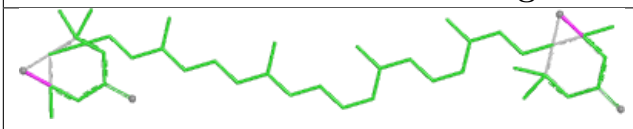


Torsions

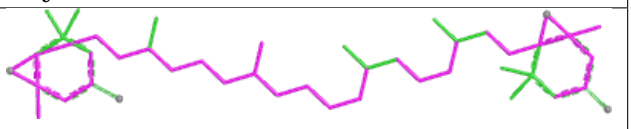


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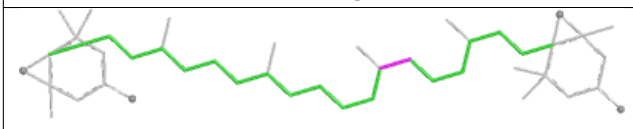
Ligand XAT y 1622



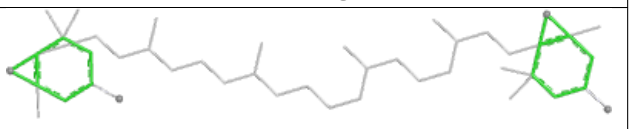
Bond lengths



Bond angles

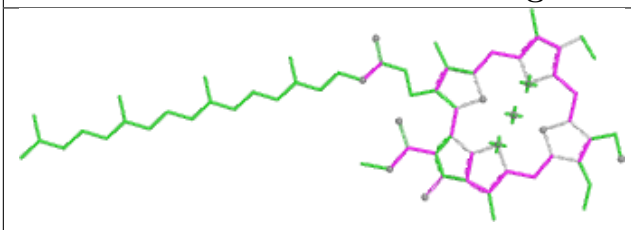


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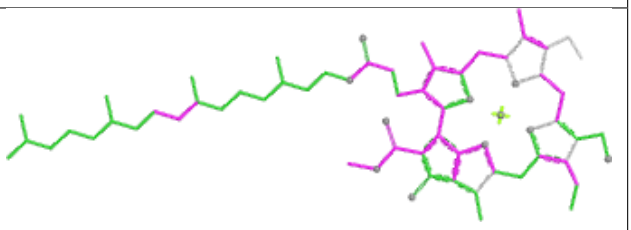


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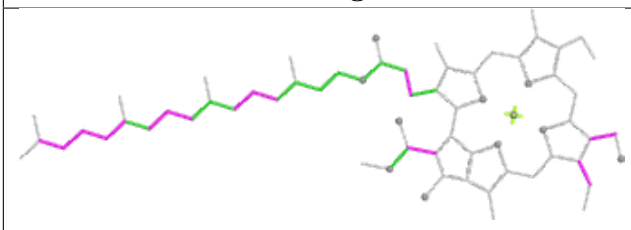
Ligand CHL n 607



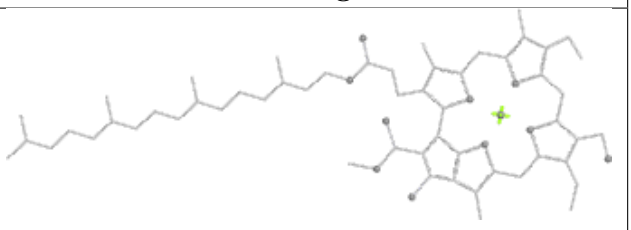
Bond lengths



Bond angles

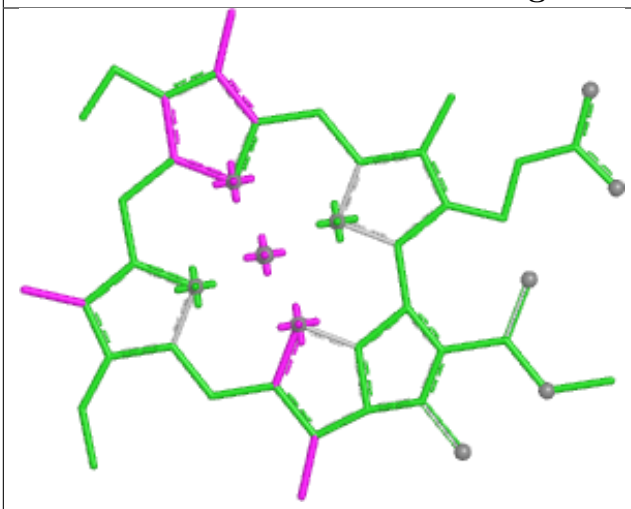


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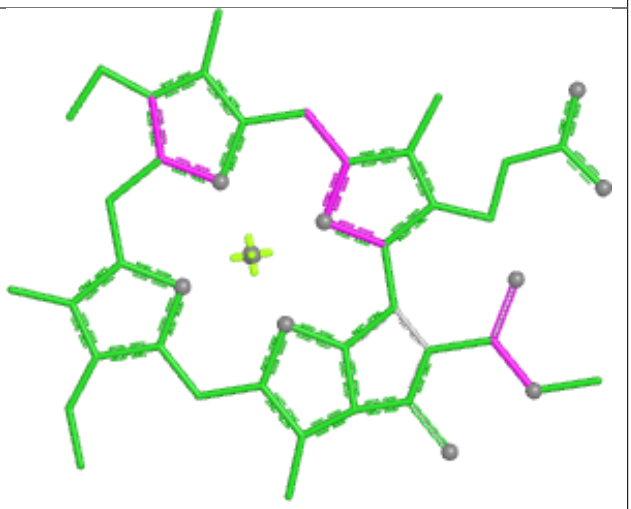


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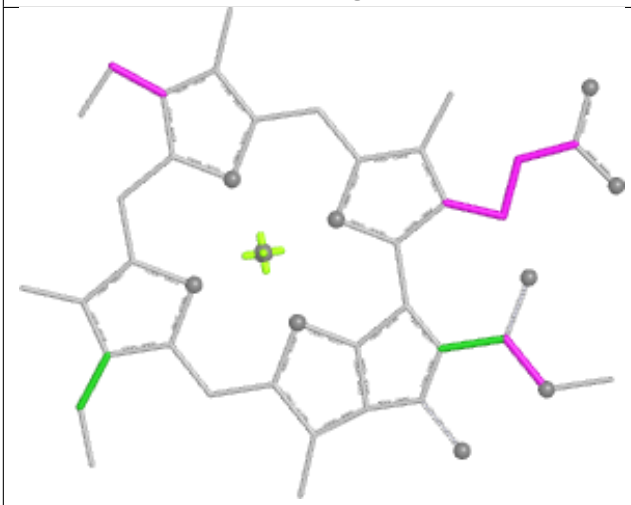
Ligand CLA 5 611



Bond lengths



Bond angles

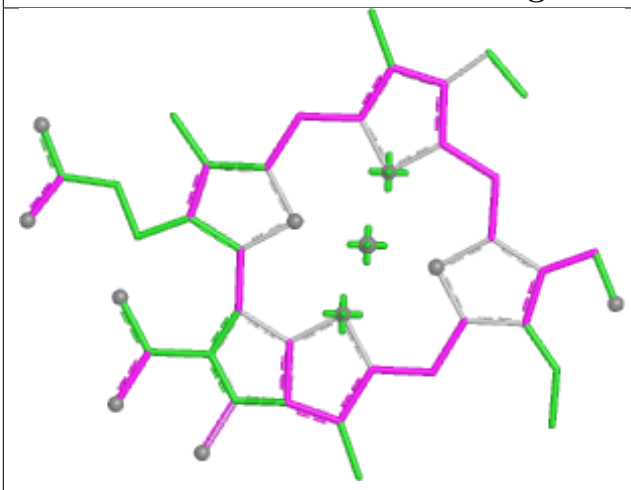


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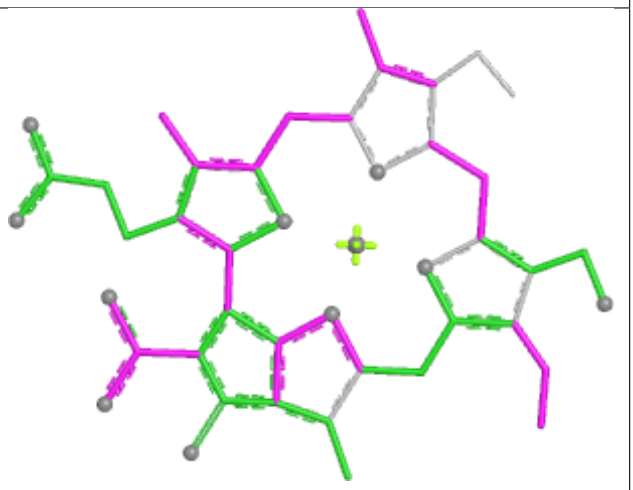


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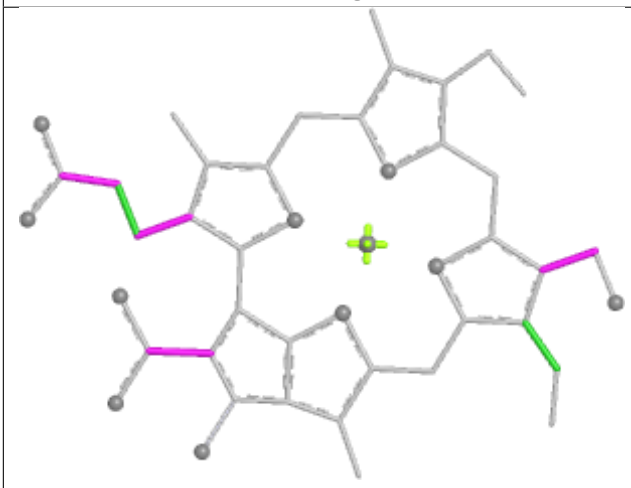
Ligand CHL 4 601



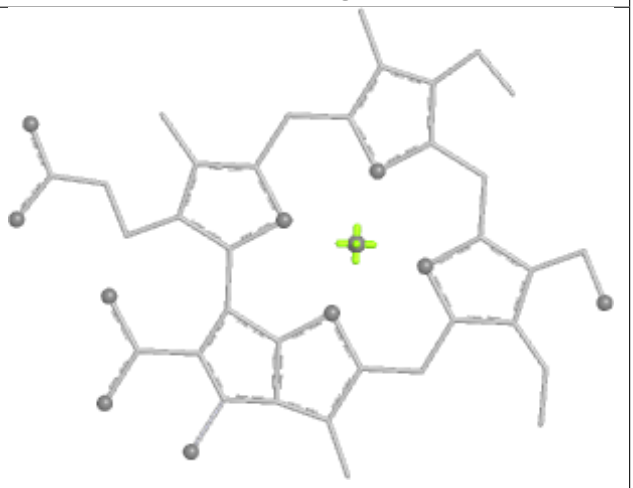
Bond lengths



Bond angles

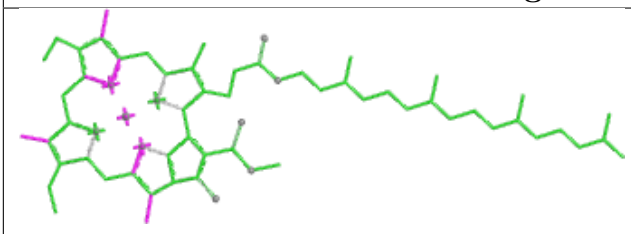


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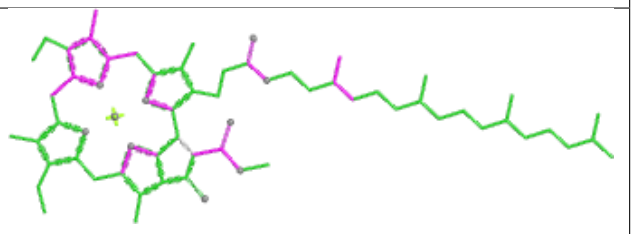


Rings

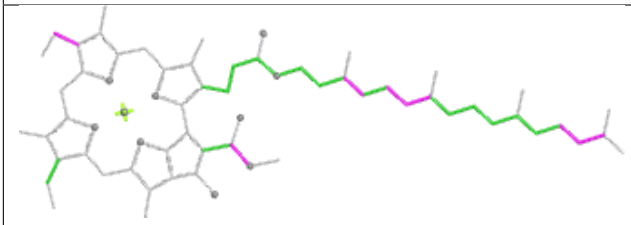
Ligand CLA B 604



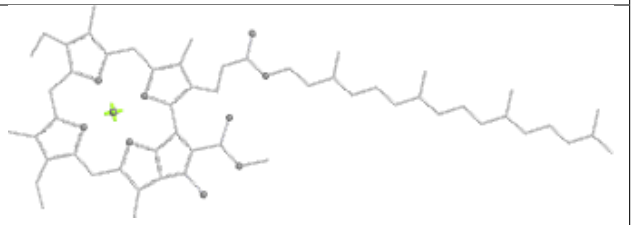
Bond lengths



Bond angles

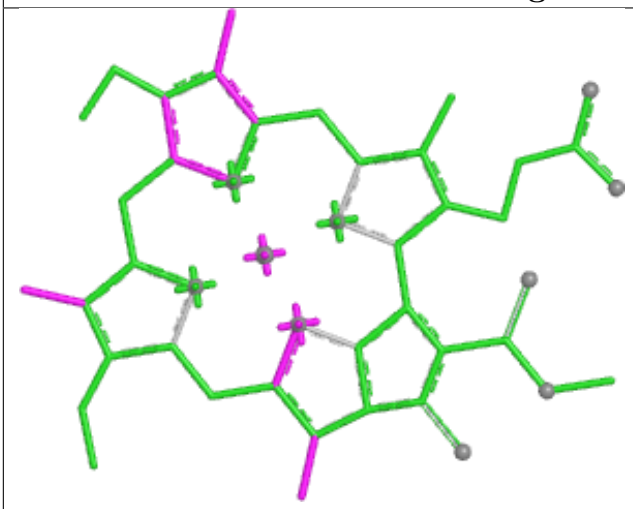


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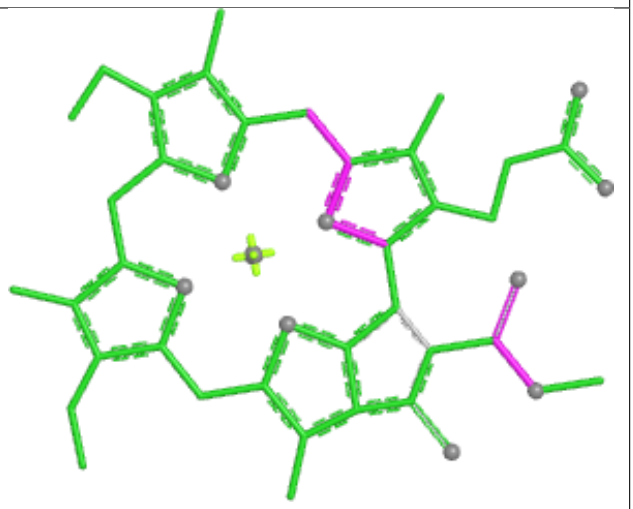


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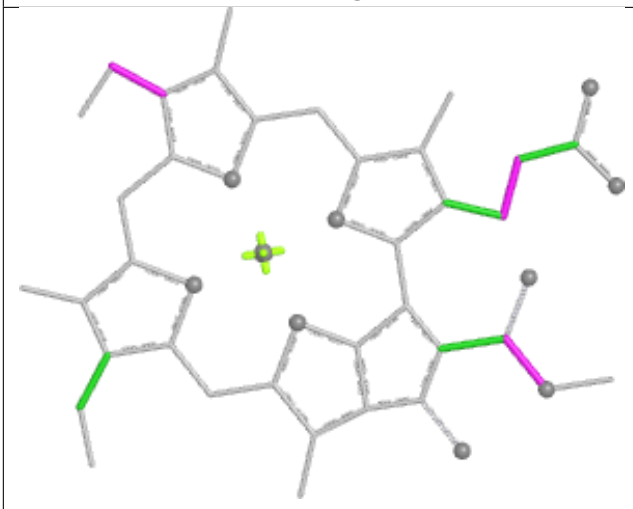
Ligand CLA 6 613



Bond lengths



Bond angles

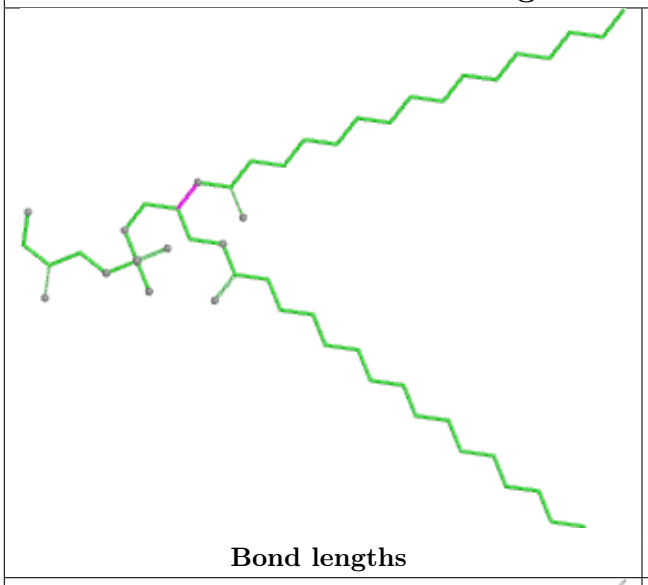


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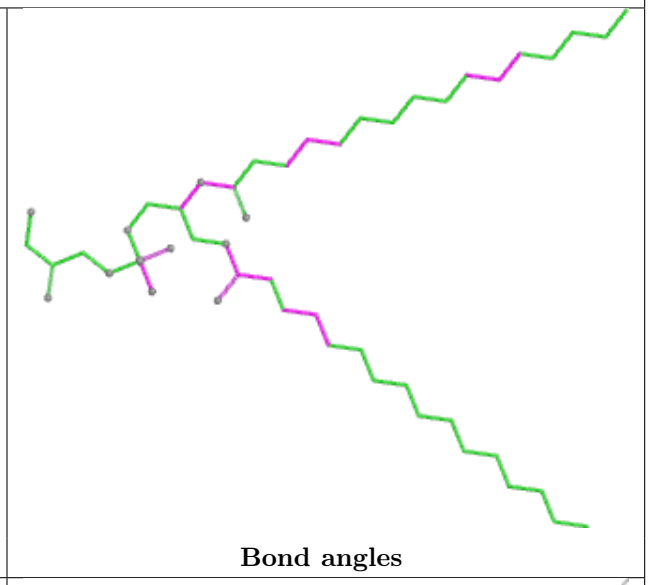


Rings

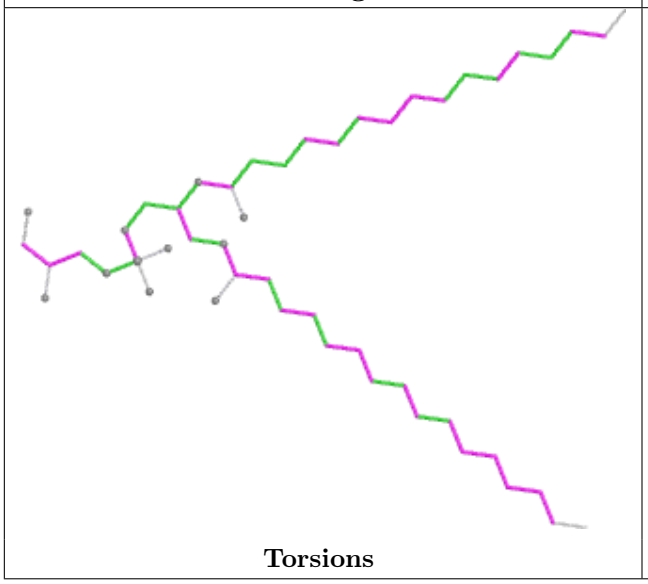
Ligand LHG S 2630



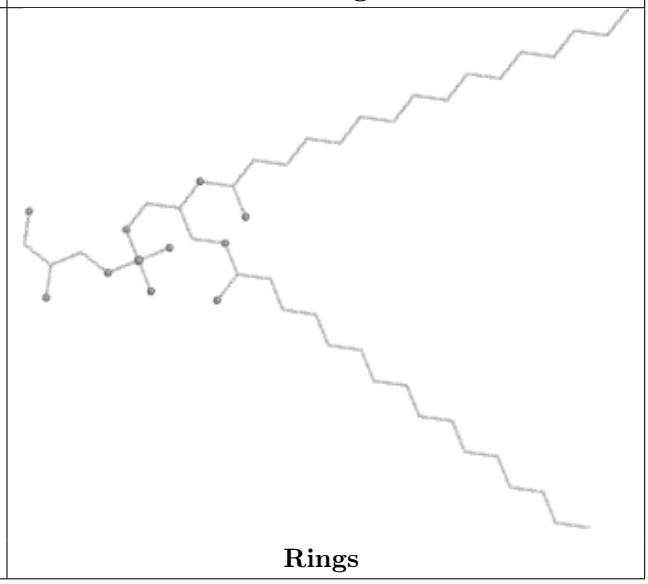
Bond lengths



Bond angles

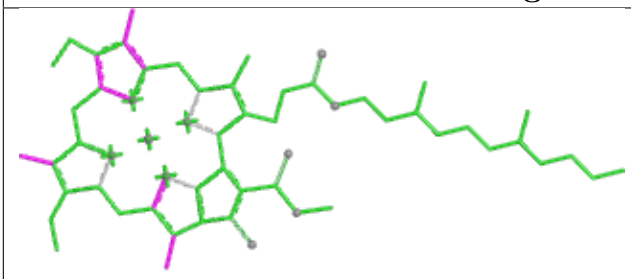


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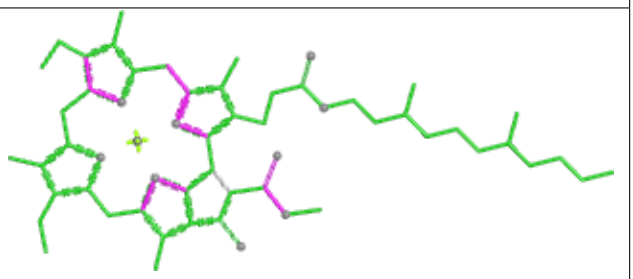


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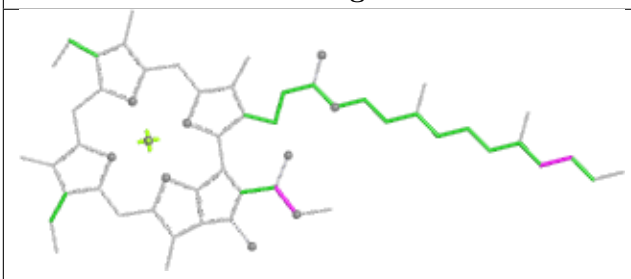
Ligand CLA R 609



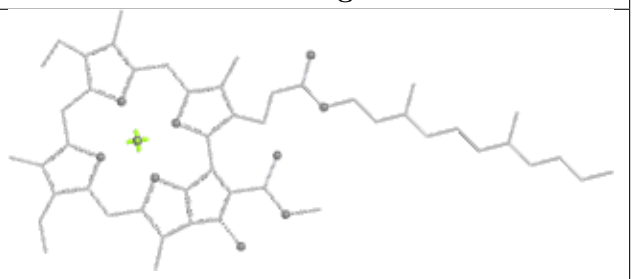
Bond lengths



Bond angles

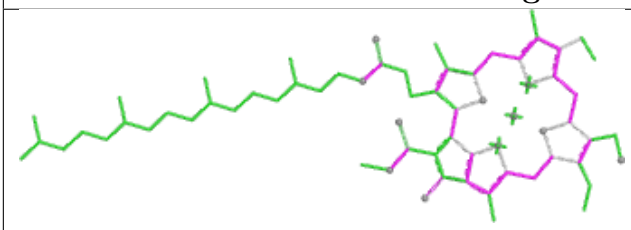


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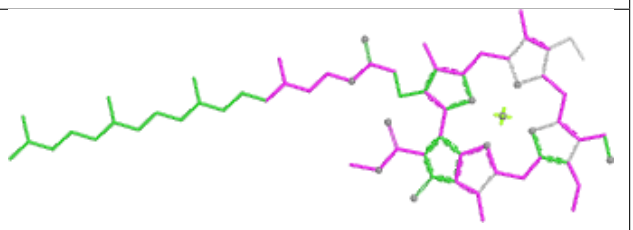


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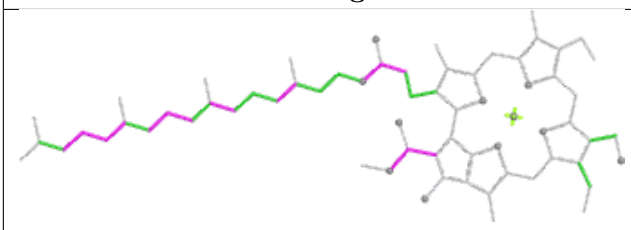
Ligand CHL G 601



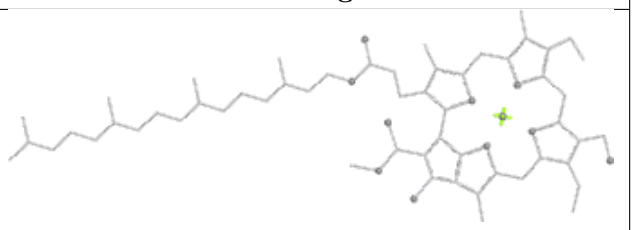
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Bond angles

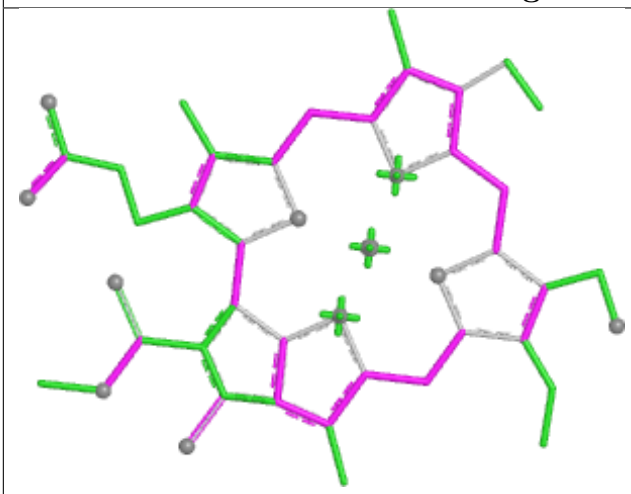


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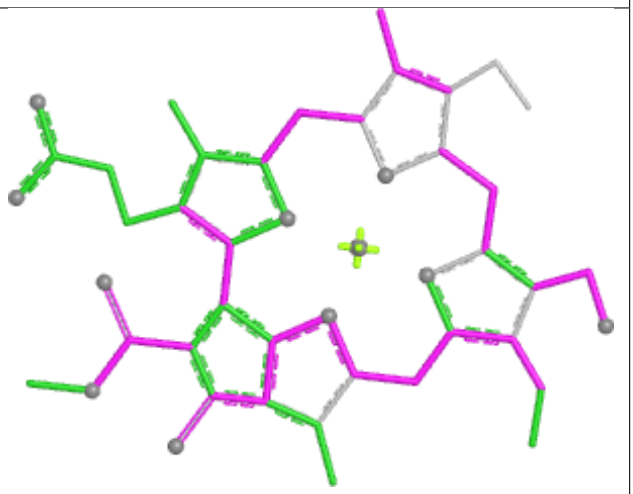


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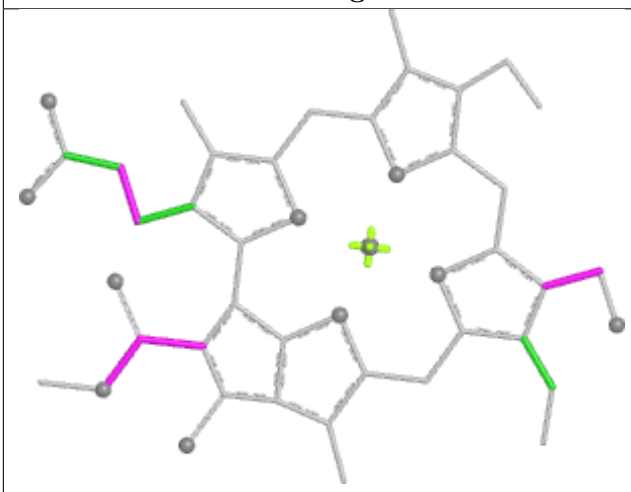
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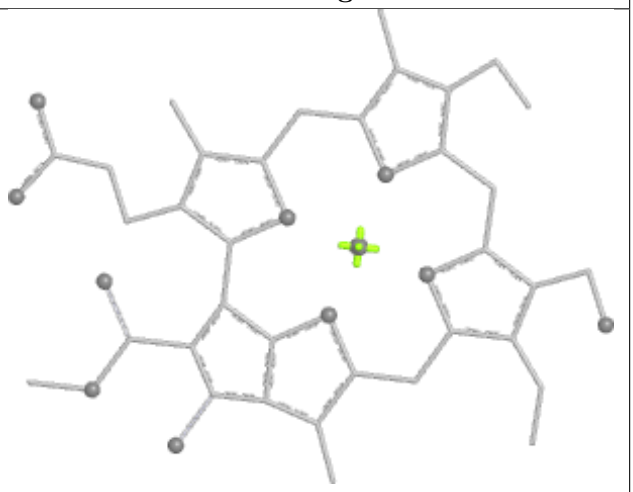
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Bond angles

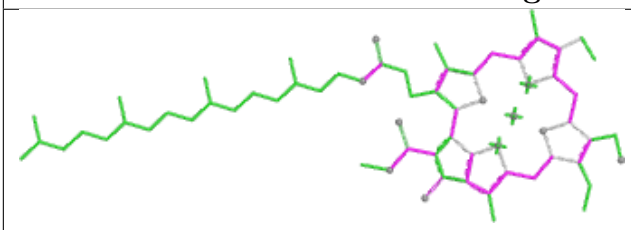


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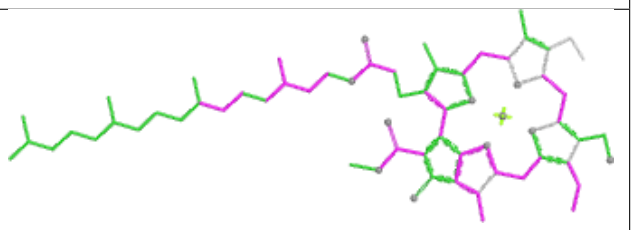


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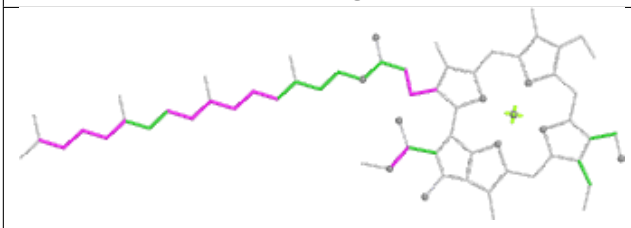
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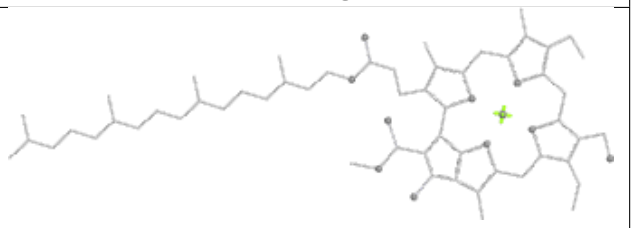
Bond lengths



Bond angles

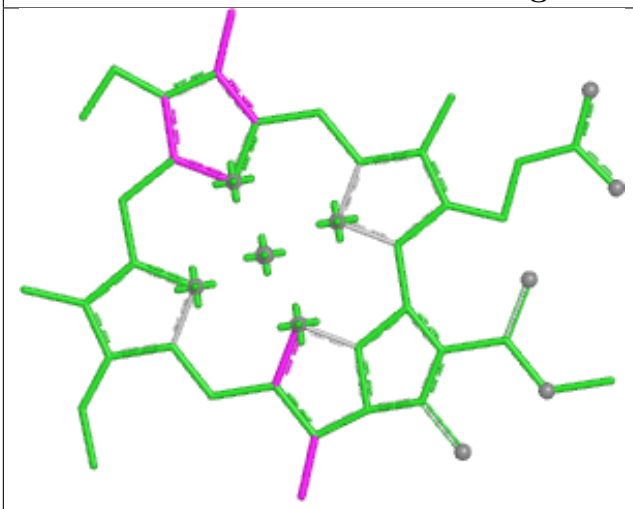


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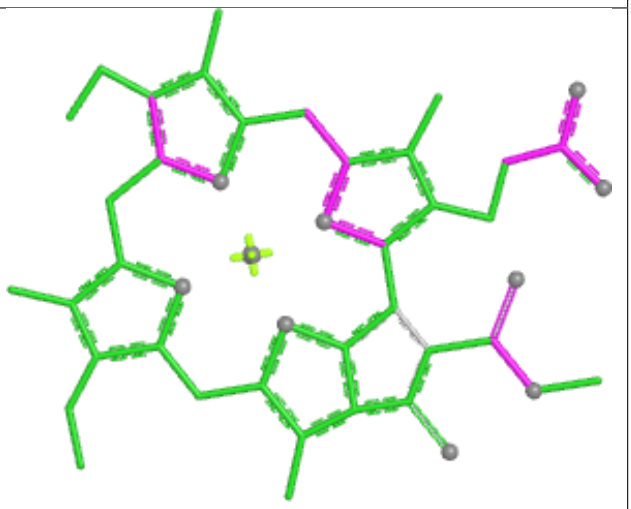


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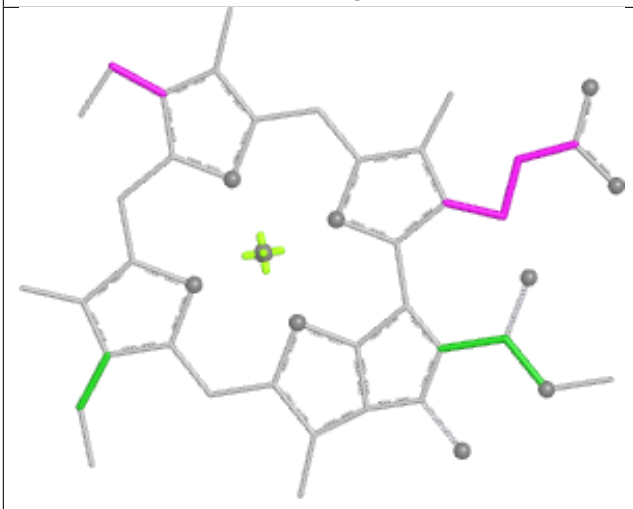
Ligand CLA s 609



Bond lengths



Bond angles

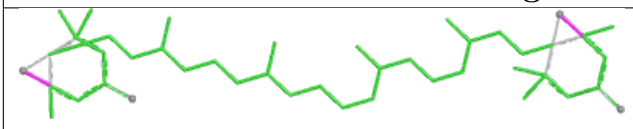


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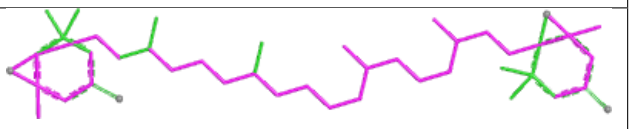


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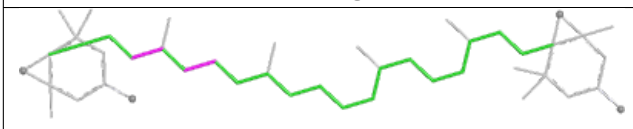
Ligand XAT R 622



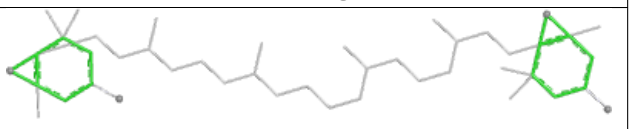
Bond lengths



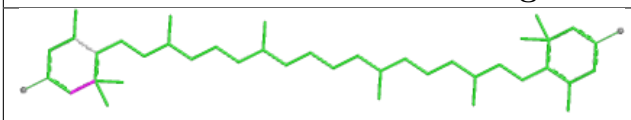
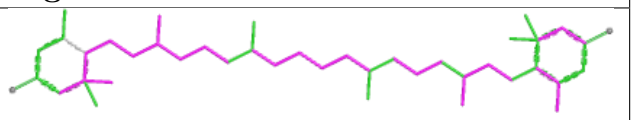
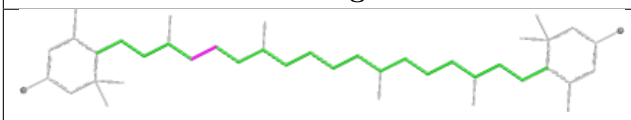
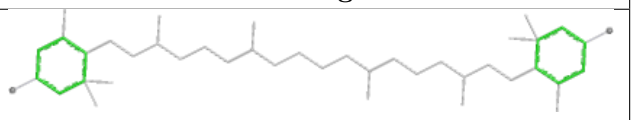
Bond angles

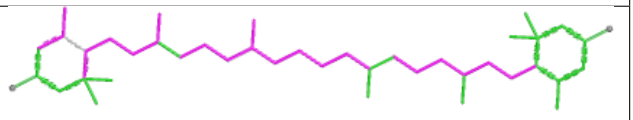
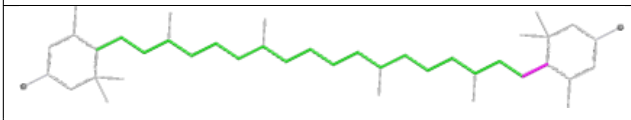
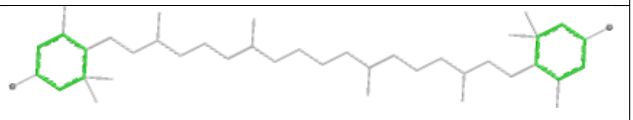


Torsions

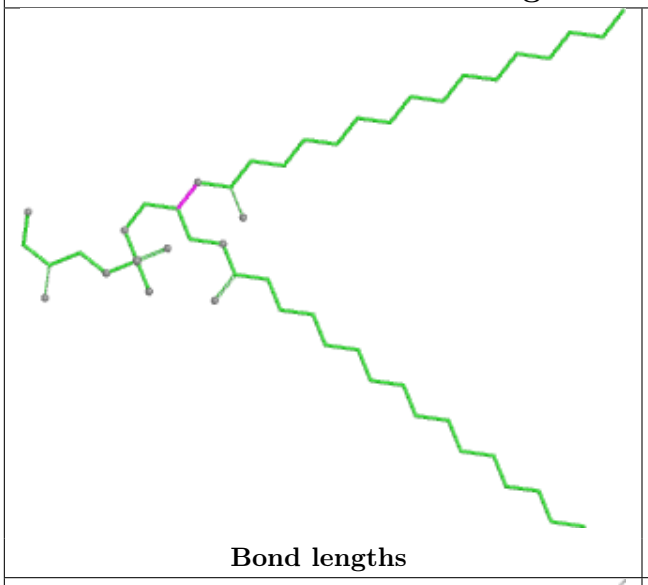


Rings

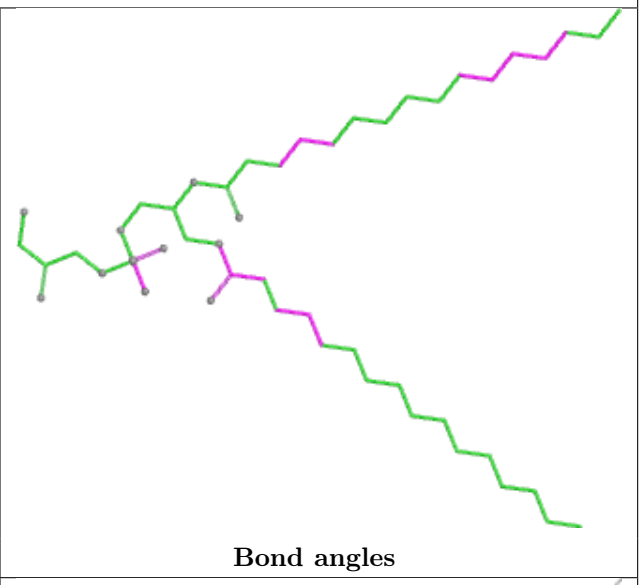
Ligand LUT g 1621	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT s 1620	
 Bond lengths	 Bond angles
 Torsions	 Rings

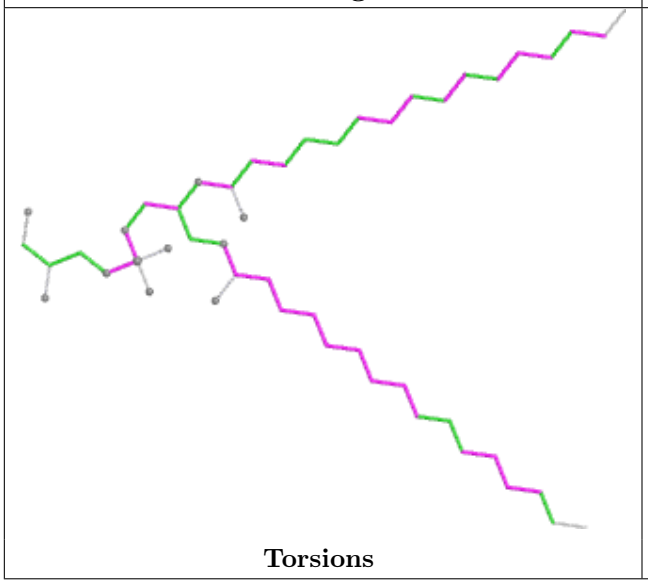
Ligand LHG D 409



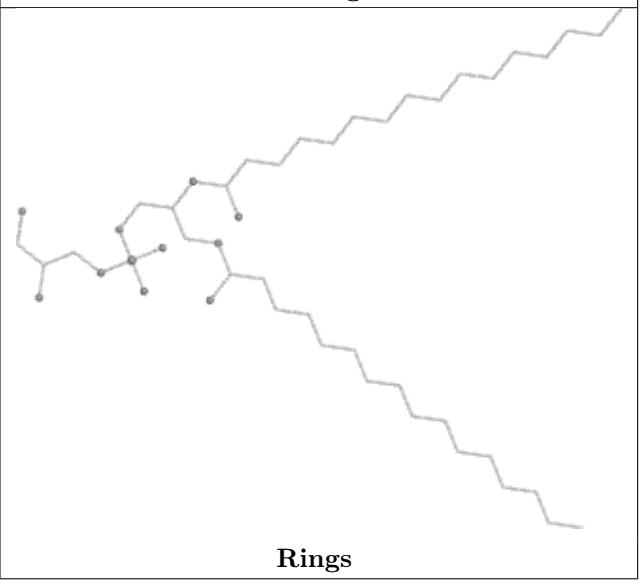
Bond lengths



Bond angles



Torsions

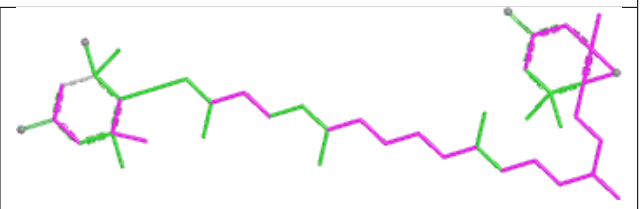


Rings

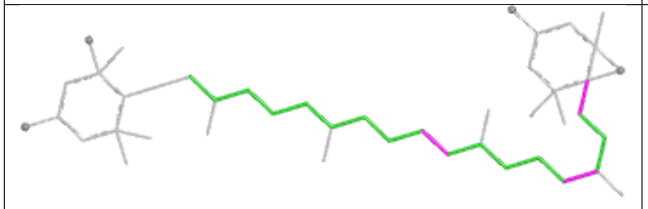
Ligand NEX n 1623



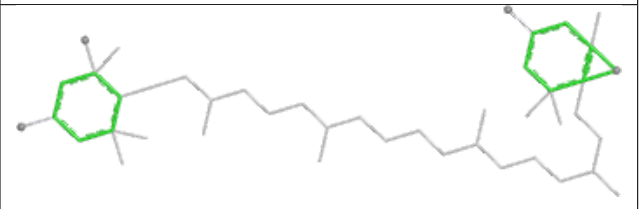
Bond lengths



Bond angles

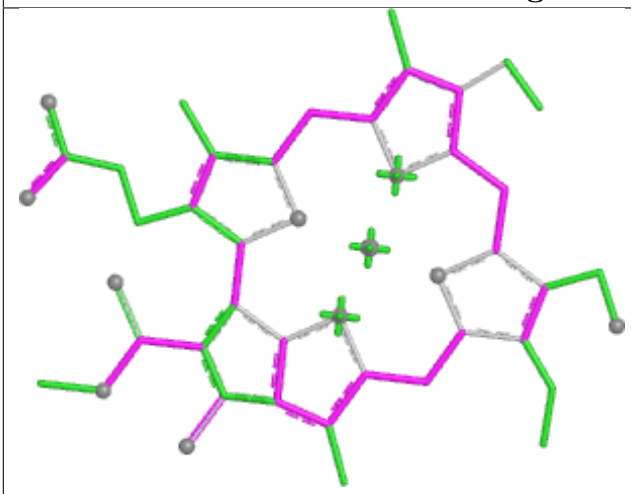


Torsions

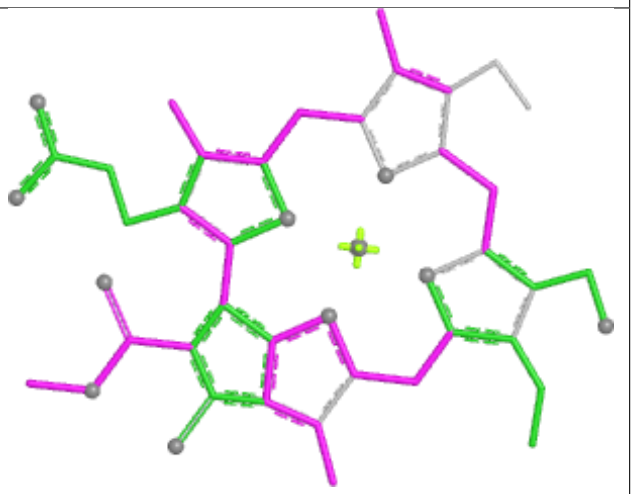


Rings

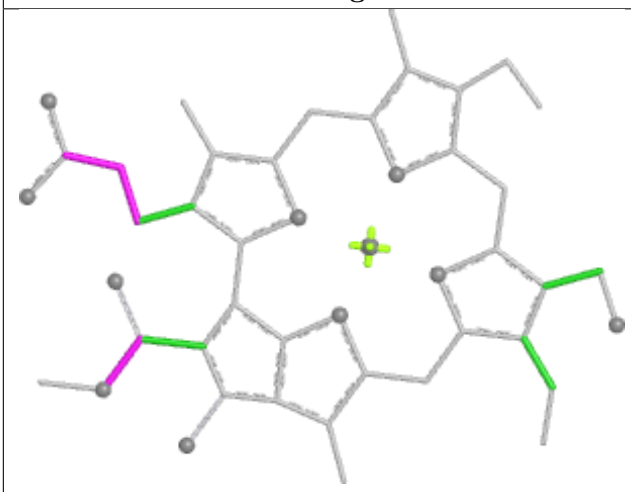
Ligand CHL S 601



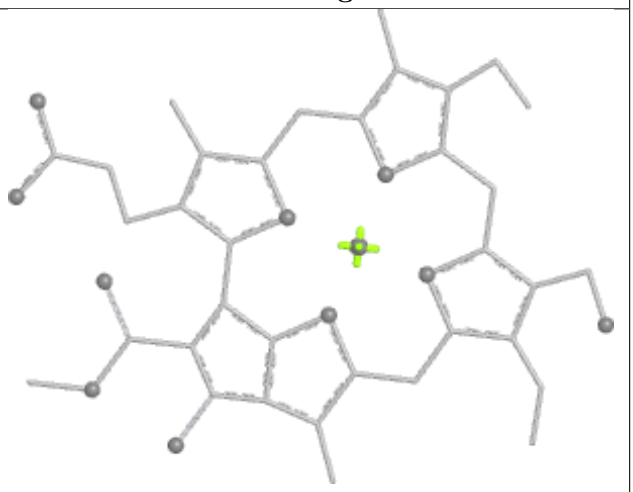
Bond lengths



Bond angles

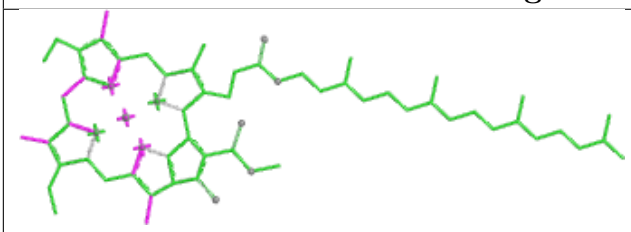


Torsions

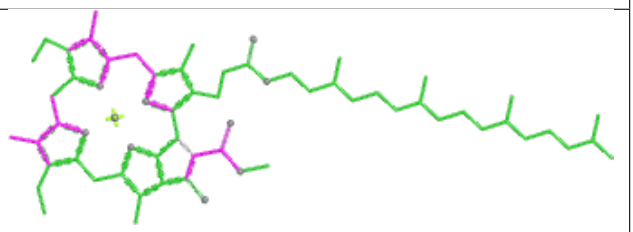


Rings

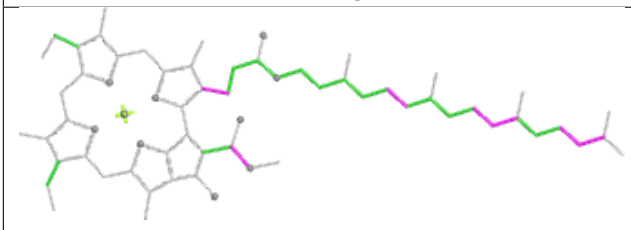
Ligand CLA C 508



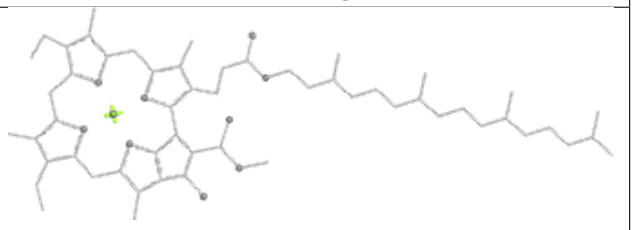
Bond lengths



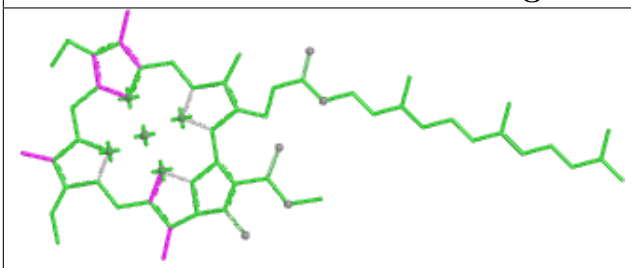
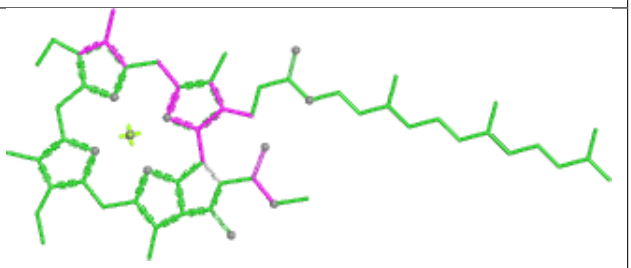
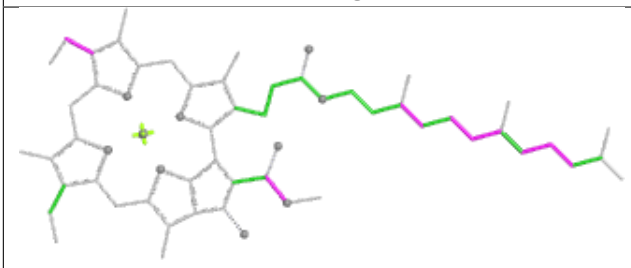
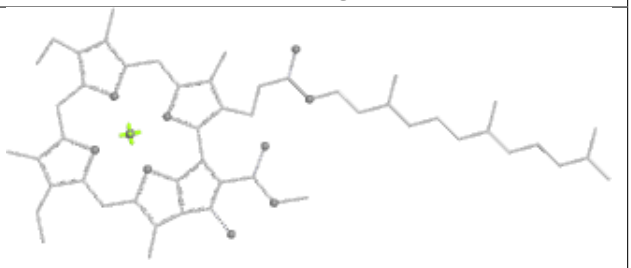
Bond angles

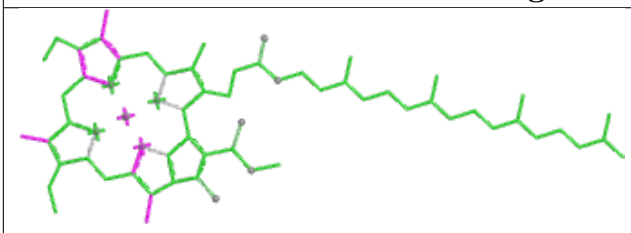
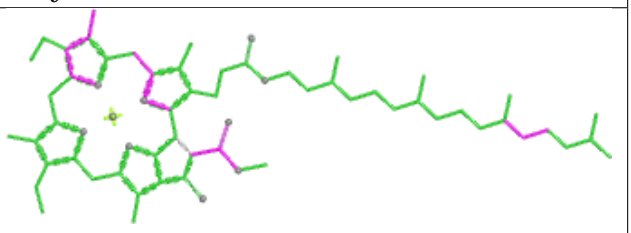
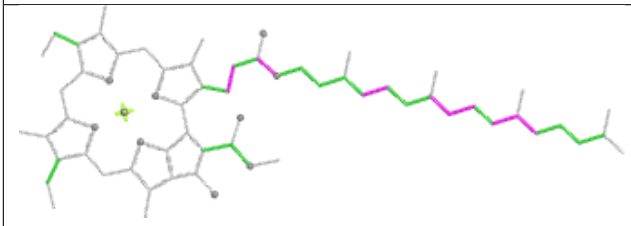
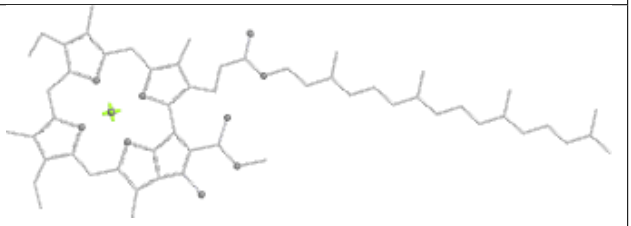


Torsions

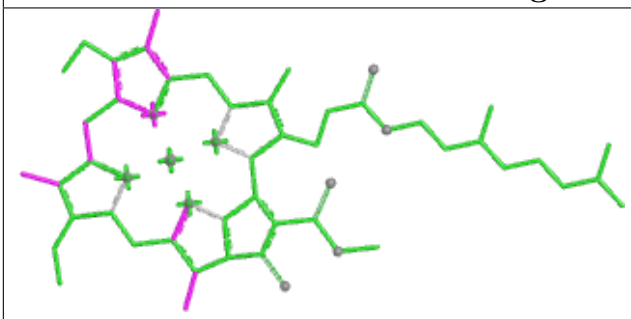


Rings

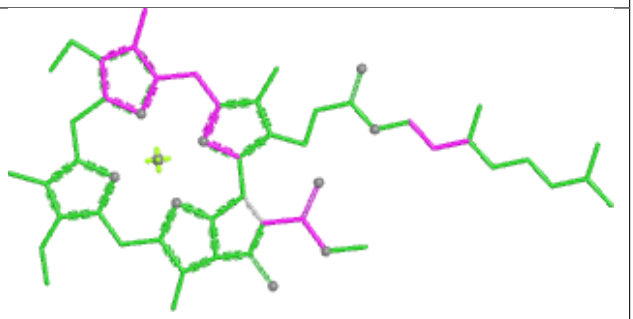
Ligand CLA N 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA y 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

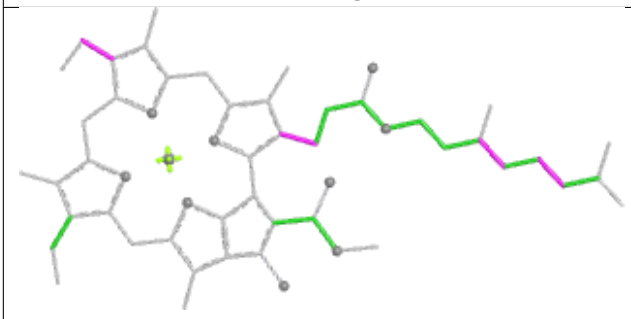
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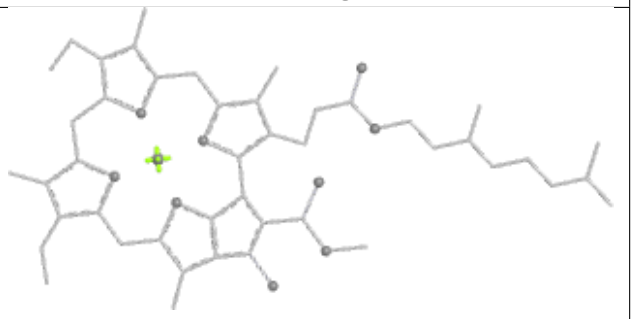
Bond lengths



Bond angles

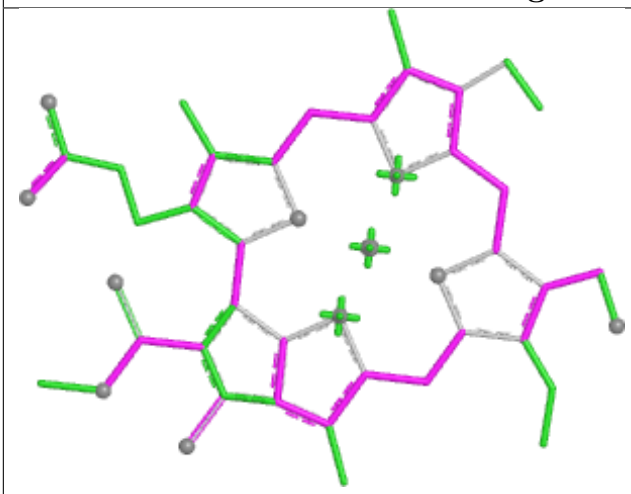


Torsions

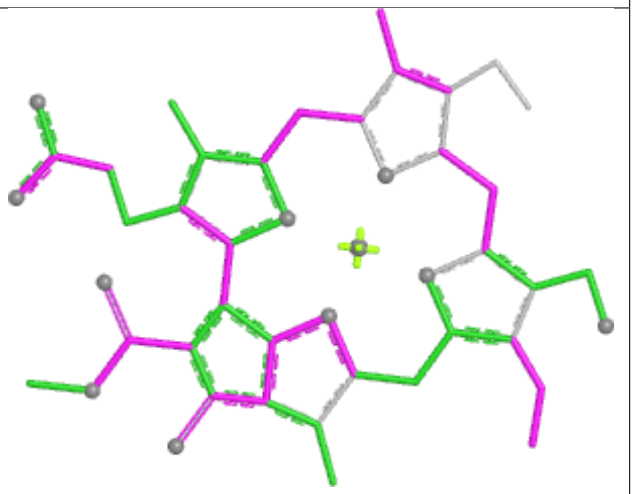


Rings

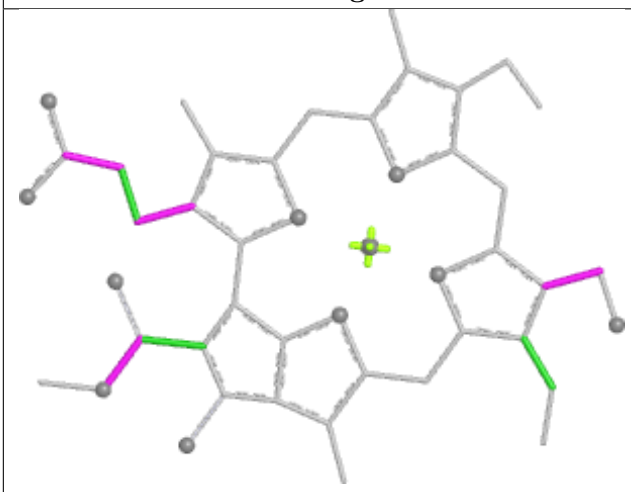
Ligand CHL 2 608



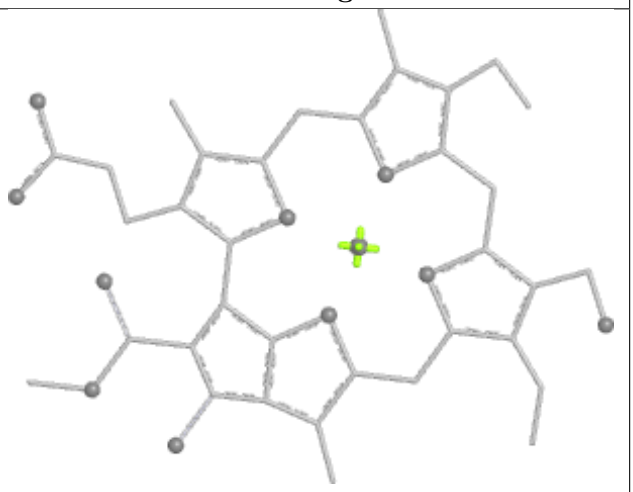
Bond lengths



Bond angles

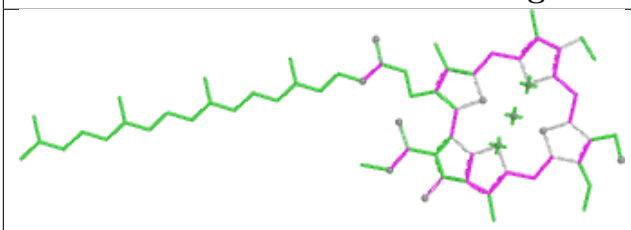


Torsions

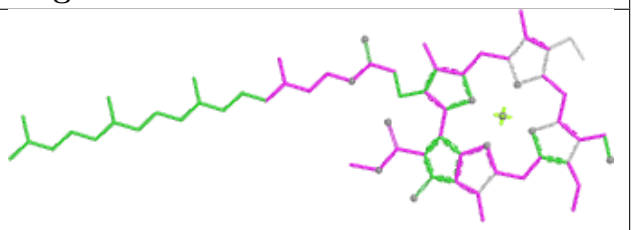


Rings

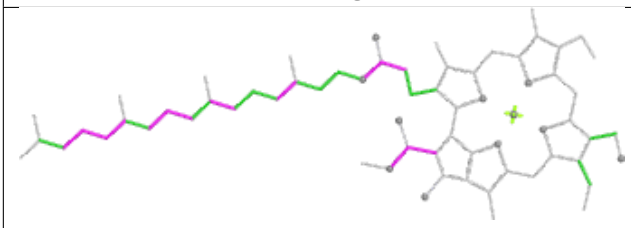
Ligand CHL g 601



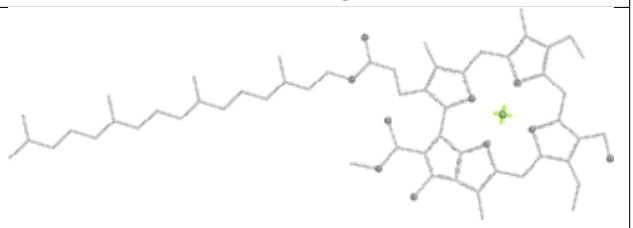
Bond lengths



Bond angles

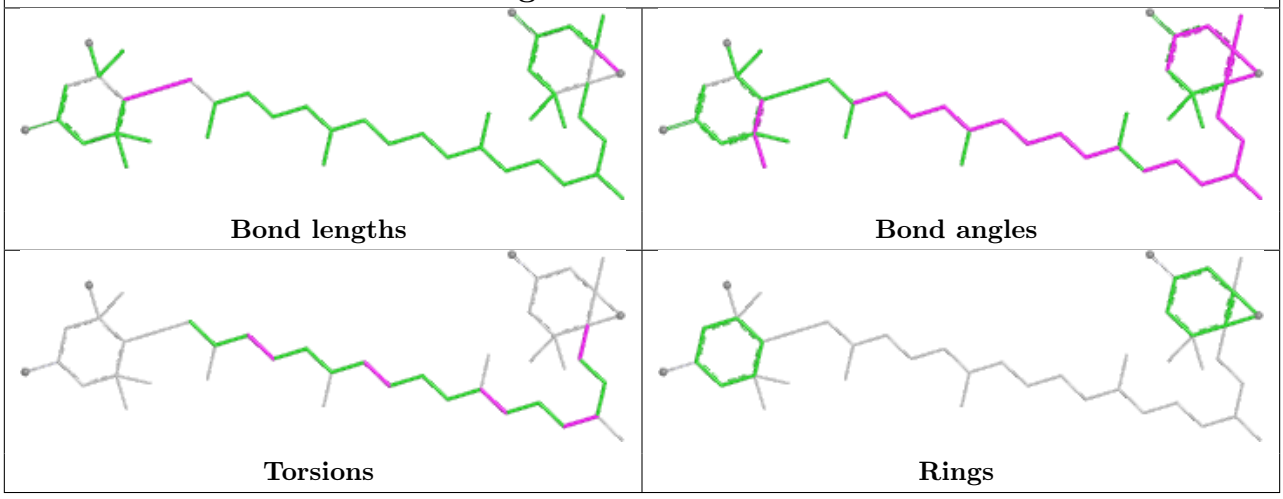


Torsions

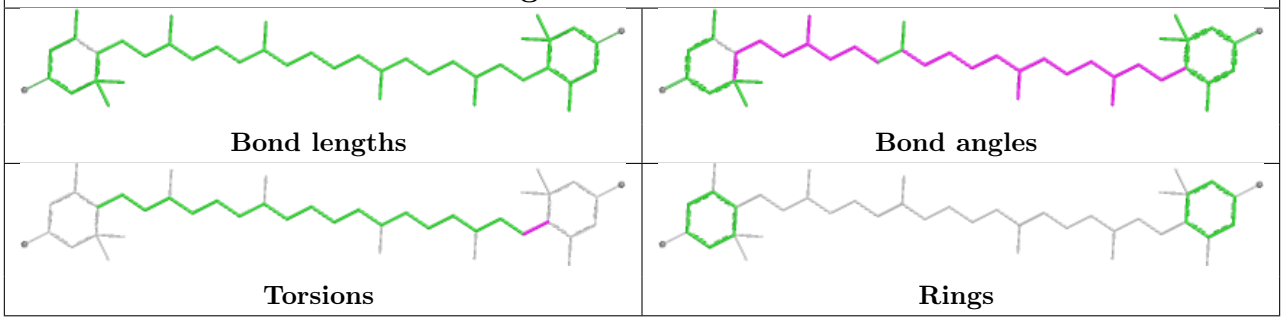


Rings

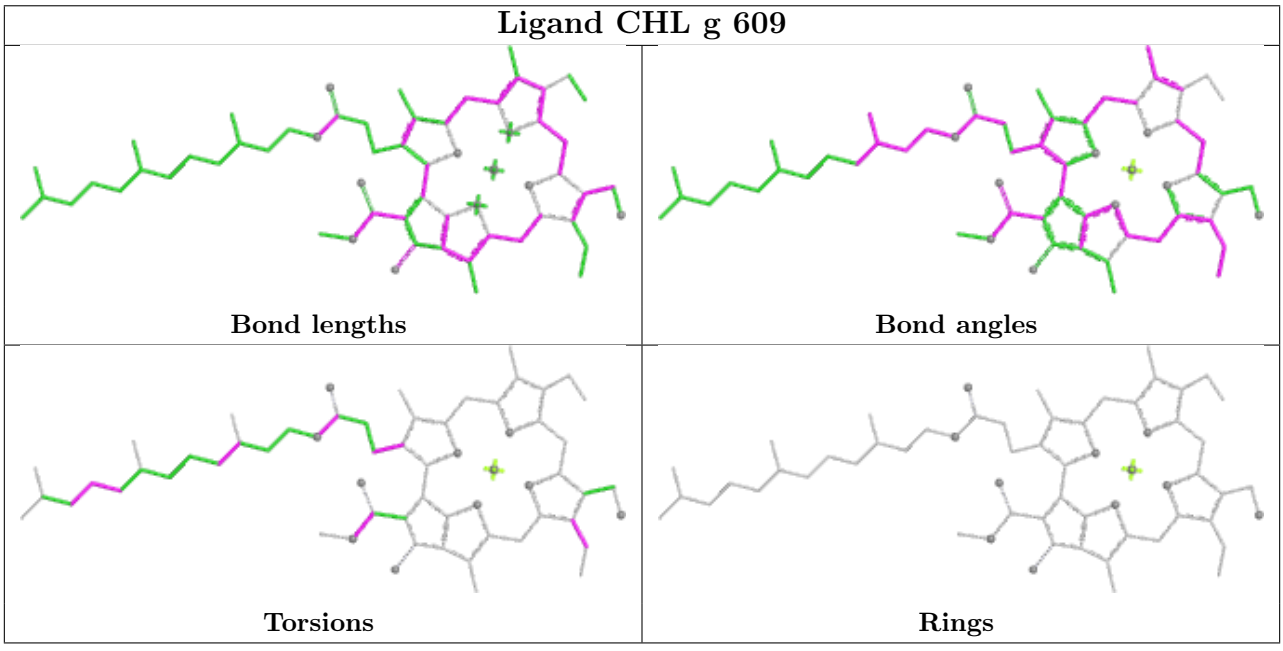
Ligand NEX 2 1623



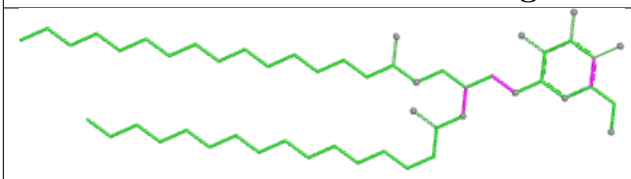
Ligand LUT 5 1620

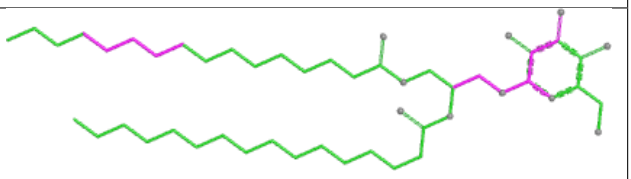


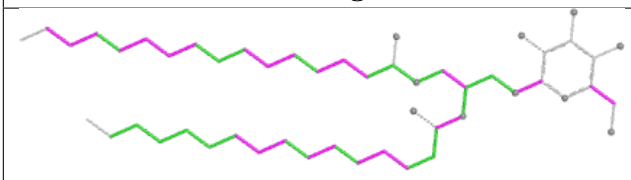
Ligand CHL g 609

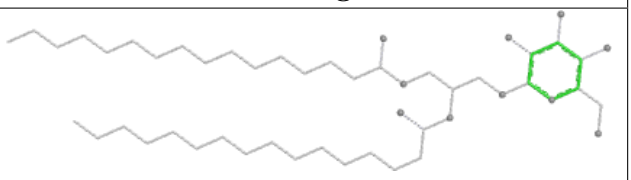


Ligand LMG C 521

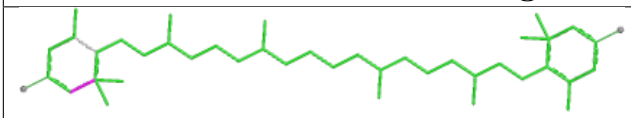

Bond lengths

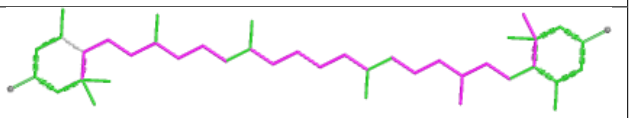

Bond angles

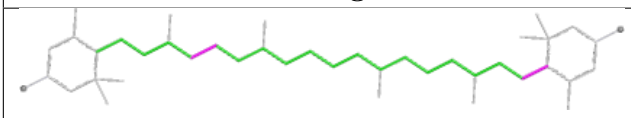

Torsions

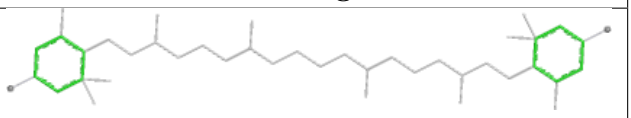

Rings

Ligand LUT n 1621

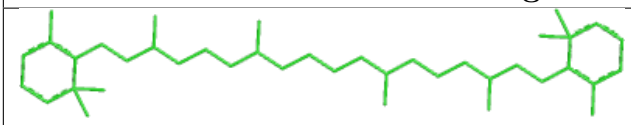

Bond lengths

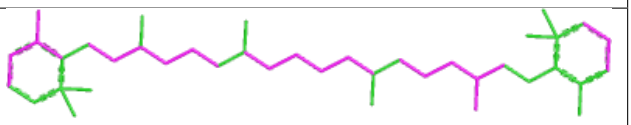

Bond angles

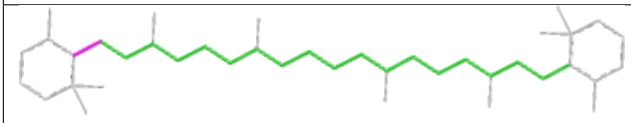

Torsions

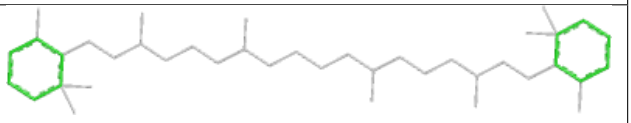

Rings

Ligand BCR B 618

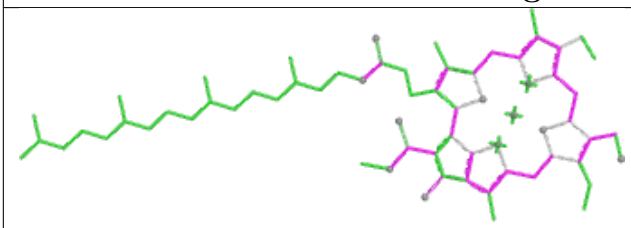

Bond lengths

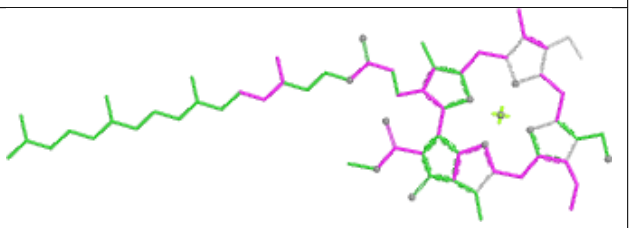

Bond angles

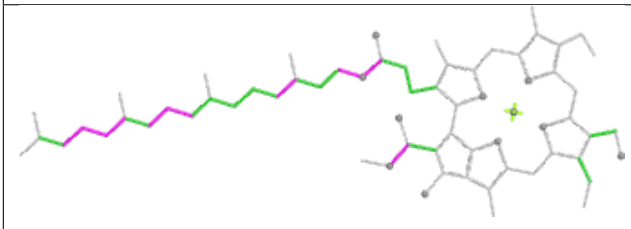

Torsions

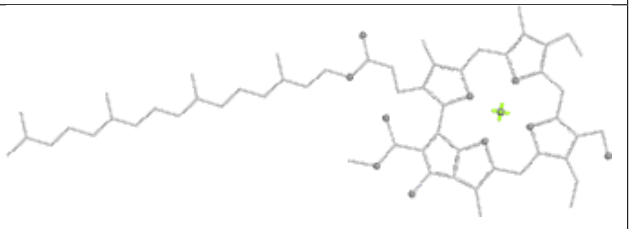

Rings

Ligand CHL Y 609

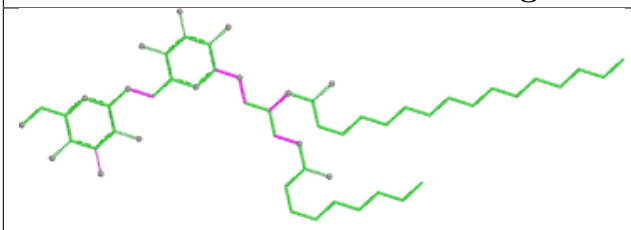

Bond lengths


Bond angles

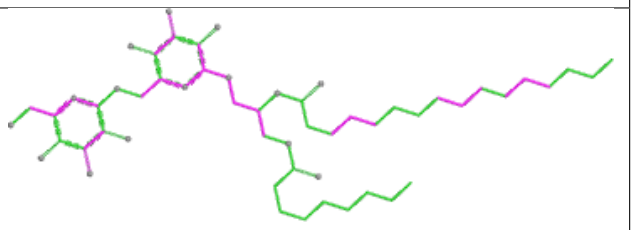

Torsions


Rings

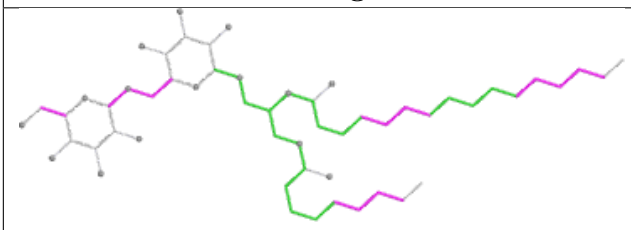
Ligand DGD C 518



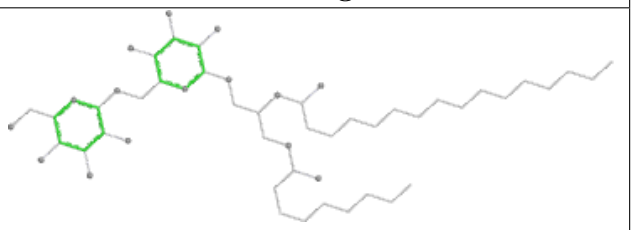
Bond lengths



Bond angles

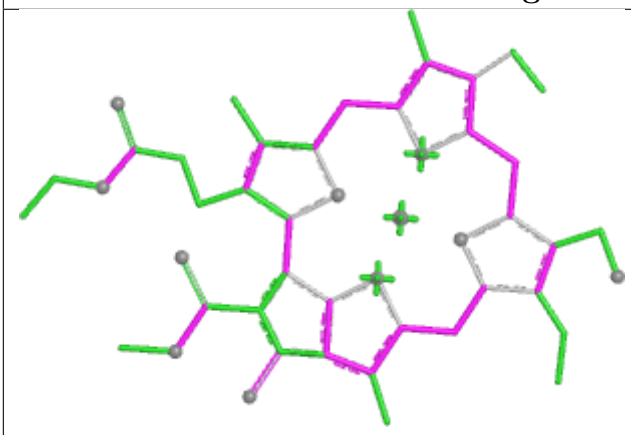


Torsions

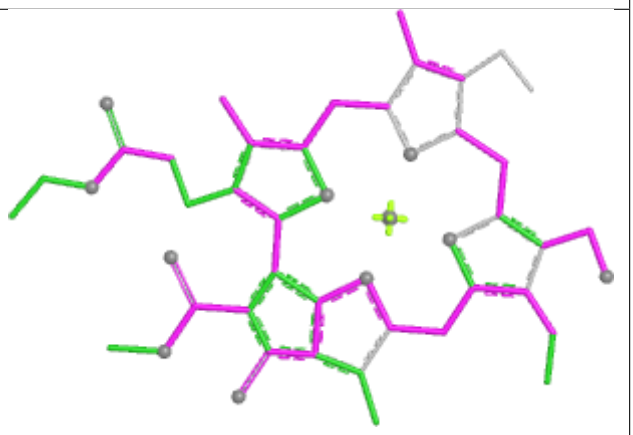


Rings

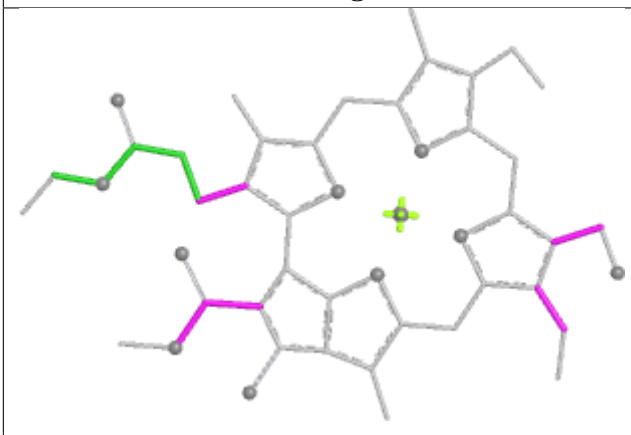
Ligand CHL N 605



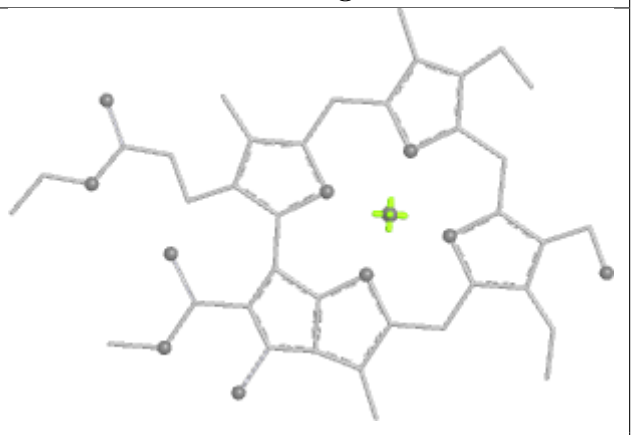
Bond lengths



Bond angles

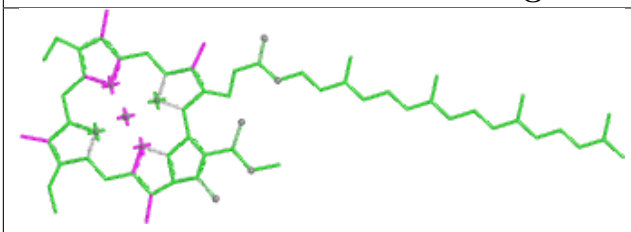


Torsions

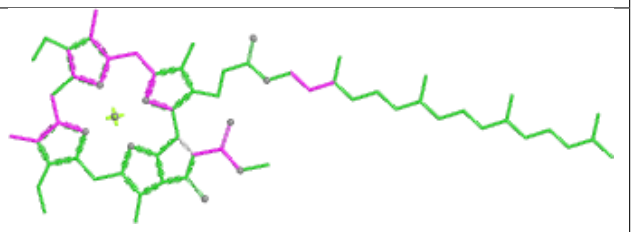


Rings

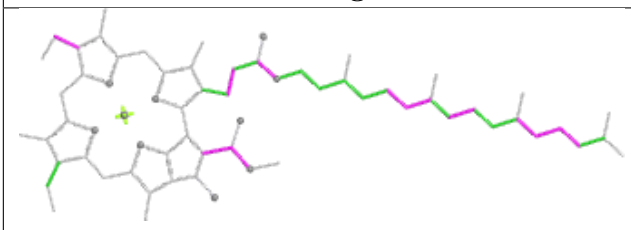
Ligand CLA B 606



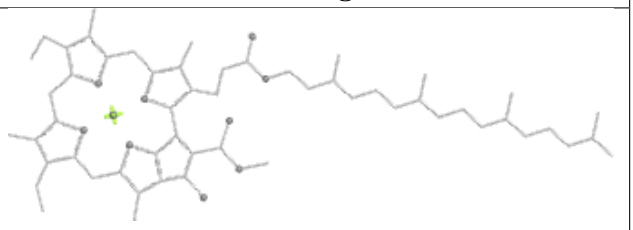
Bond lengths



Bond angles

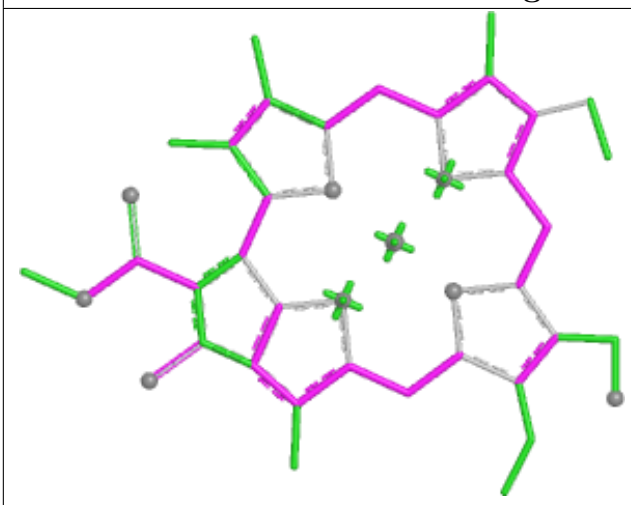


Torsions



Rings

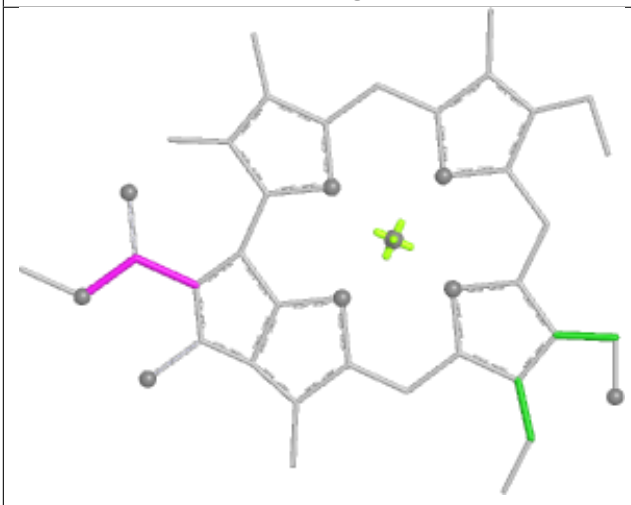
Ligand CHL R 614



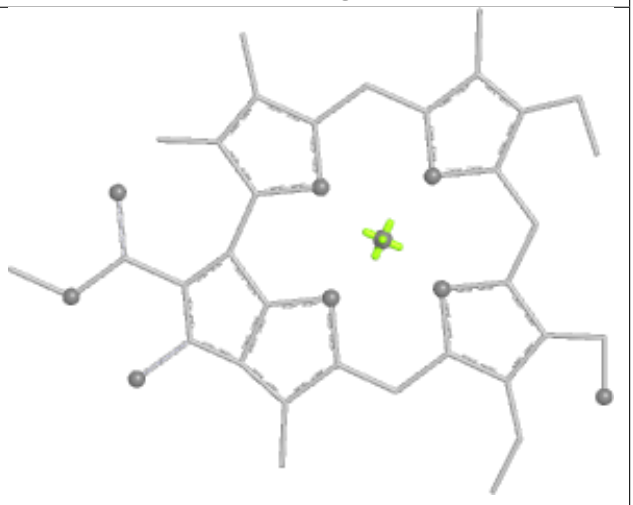
Bond lengths



Bond angles

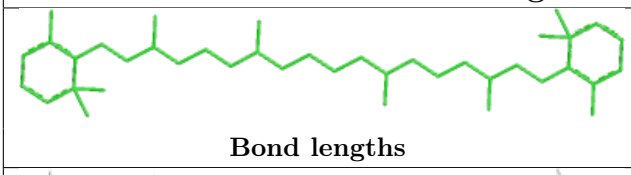


Torsions

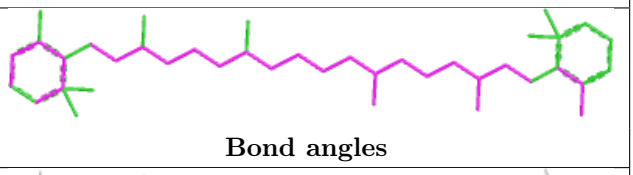


Rings

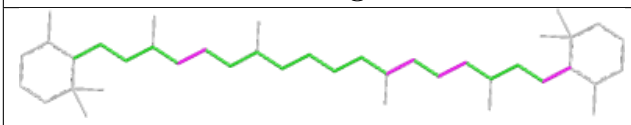
Ligand BCR c 515



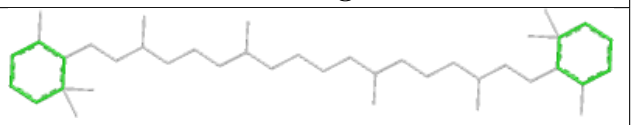
Bond lengths



Bond angles

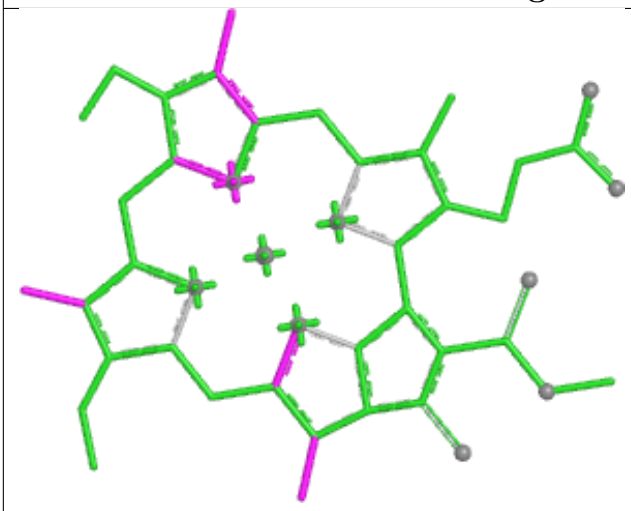


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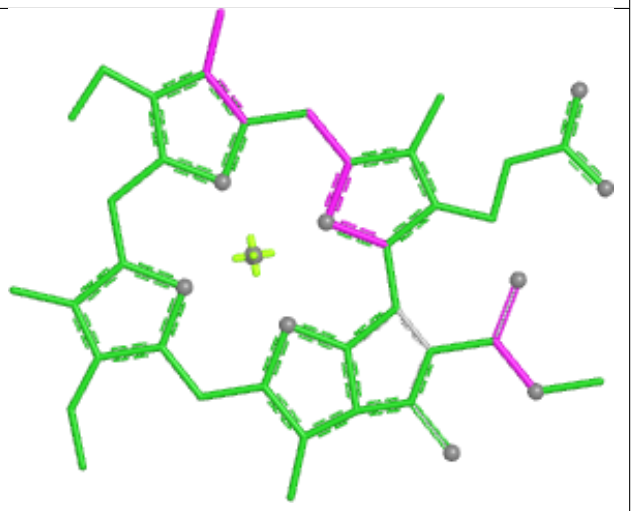


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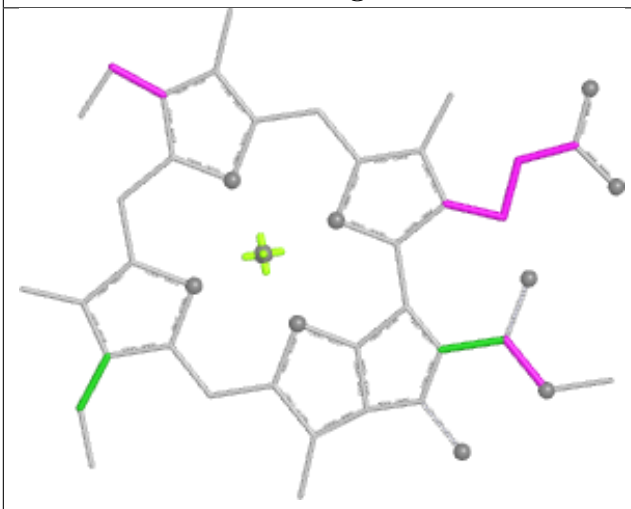
Ligand CLA 2 604



Bond lengths



Bond angles

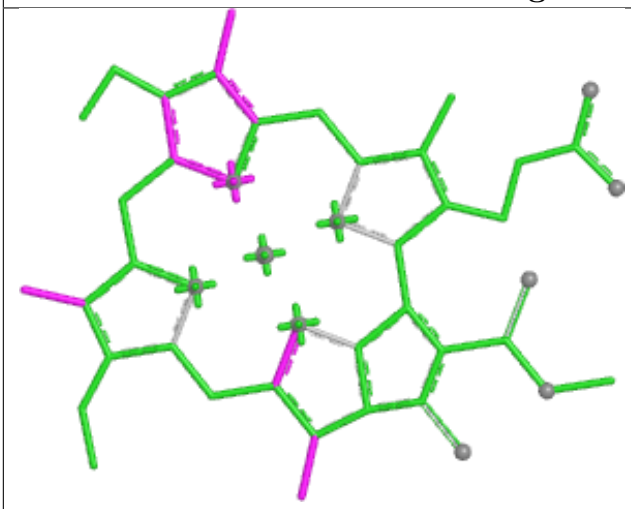


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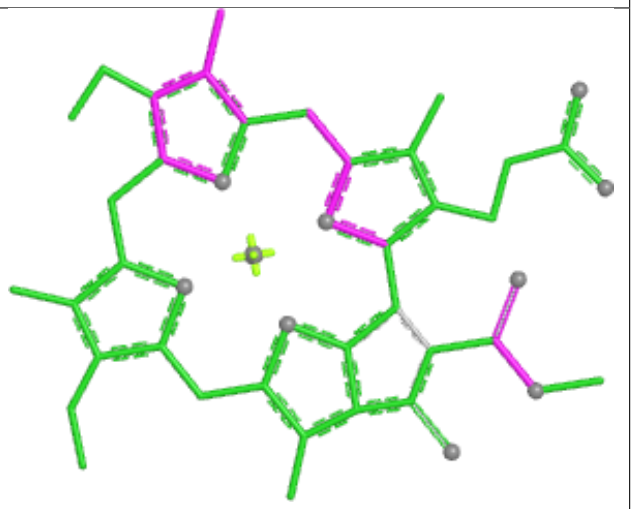


Rings

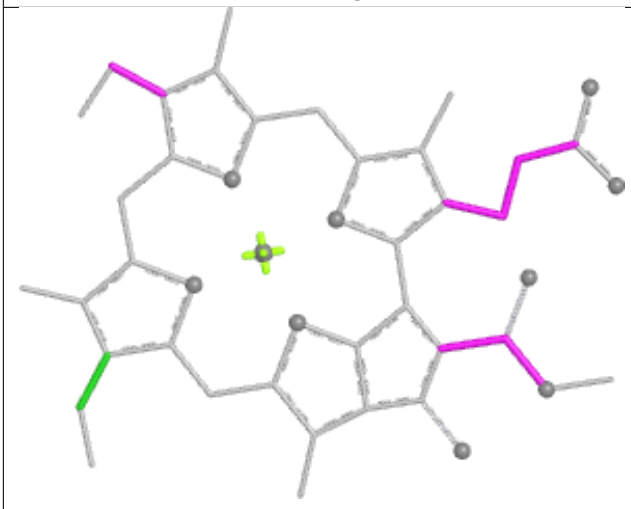
Ligand CLA 3 604



Bond lengths



Bond angles

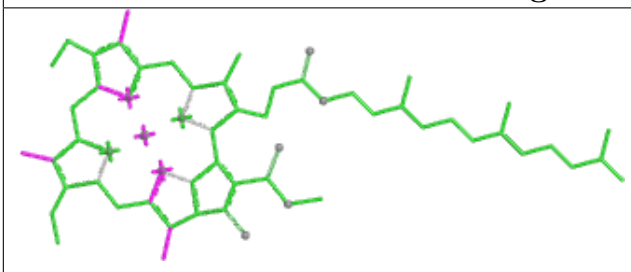


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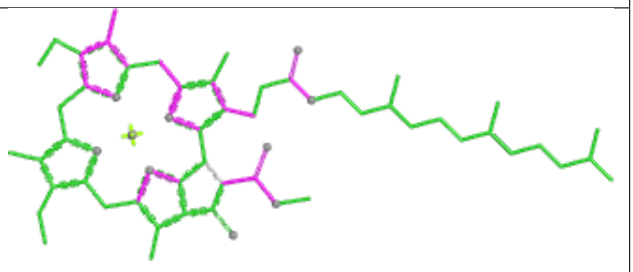


Rings

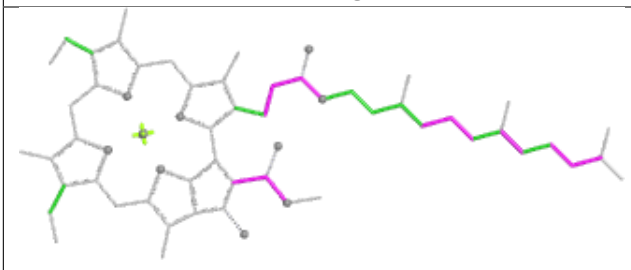
Ligand CLA r 603



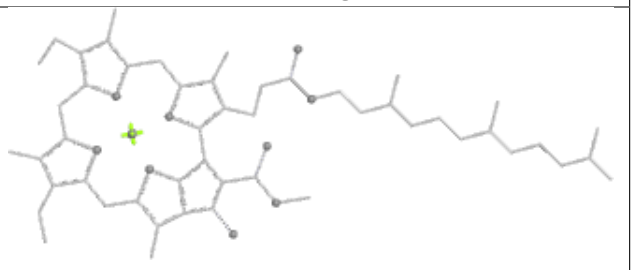
Bond lengths



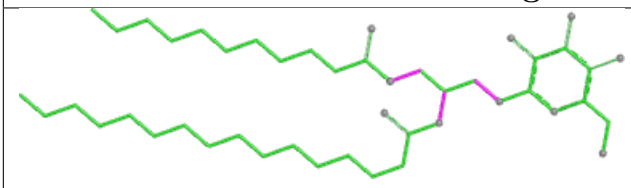
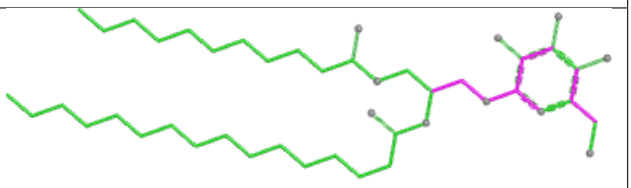
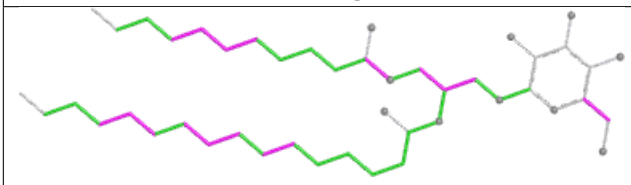
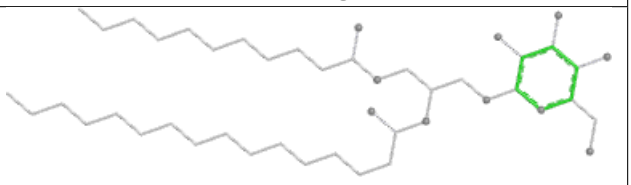
Bond angles

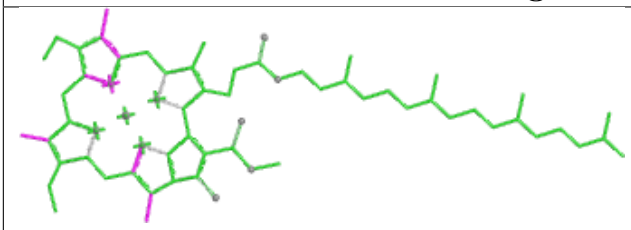
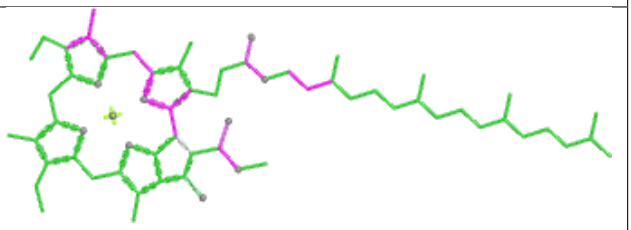
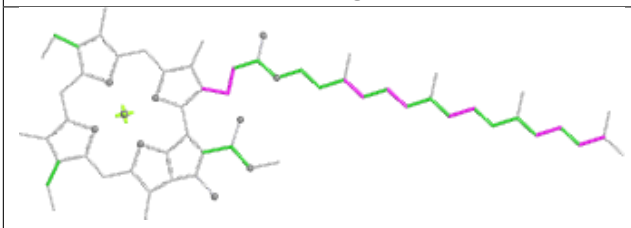
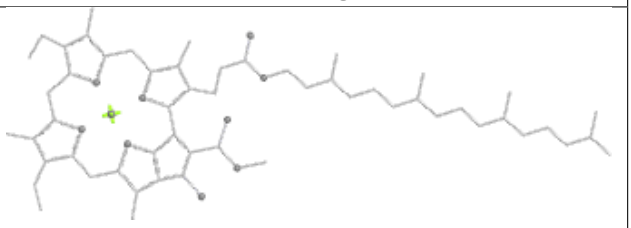


Torsions

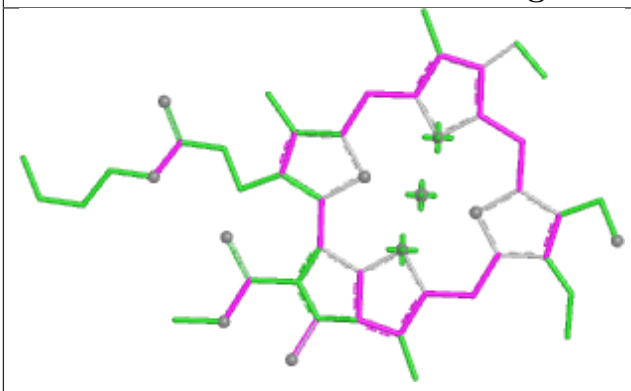


Rings

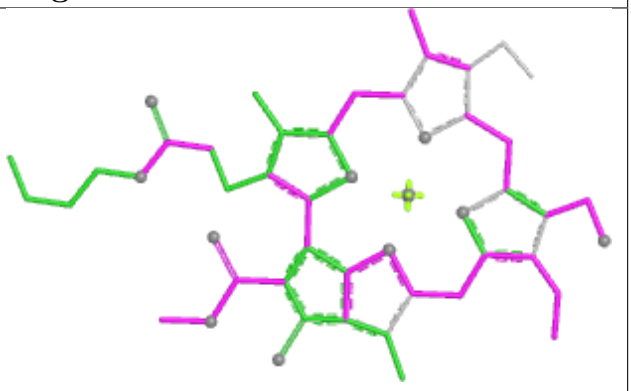
Ligand LMG d 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

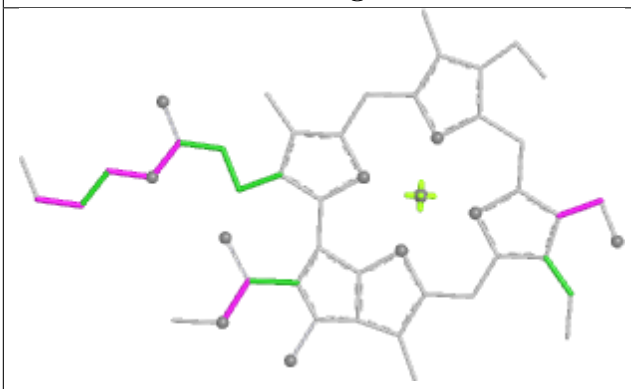
Ligand CHL g 606



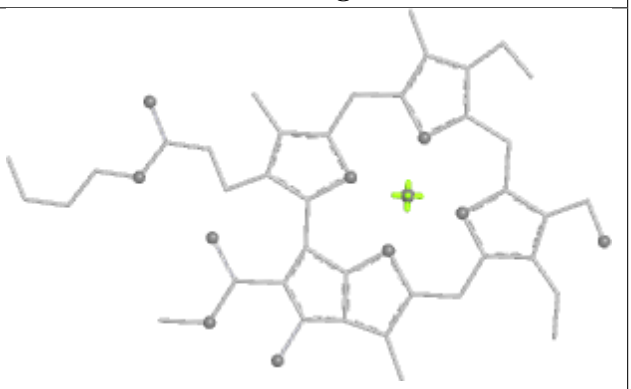
Bond lengths



Bond angles

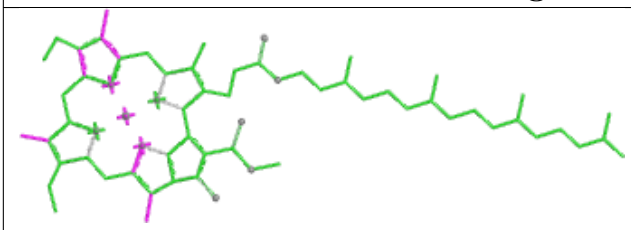


Torsions

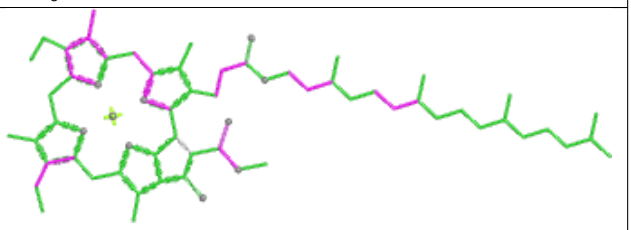


Rings

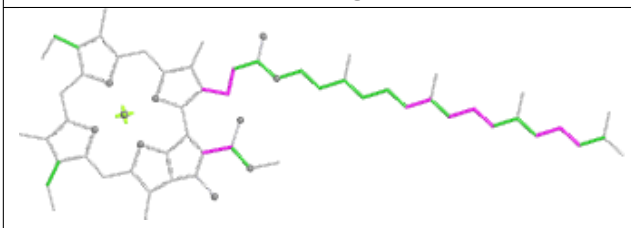
Ligand CLA y 602



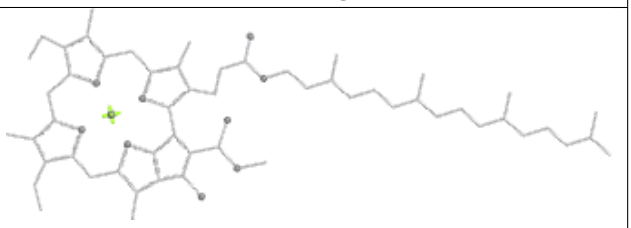
Bond lengths



Bond angles

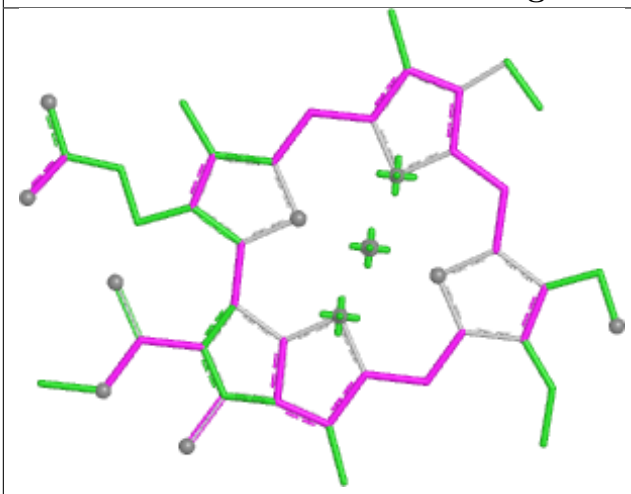


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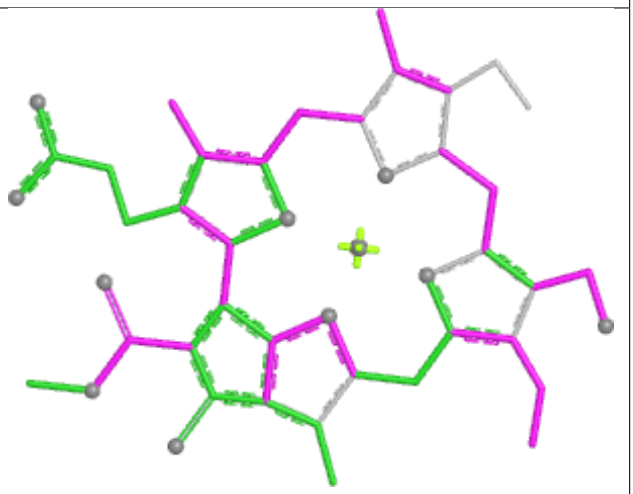


Rings

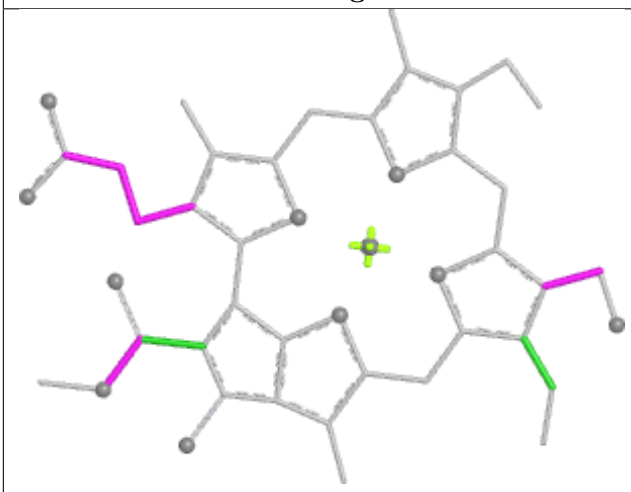
Ligand CHL 3 606



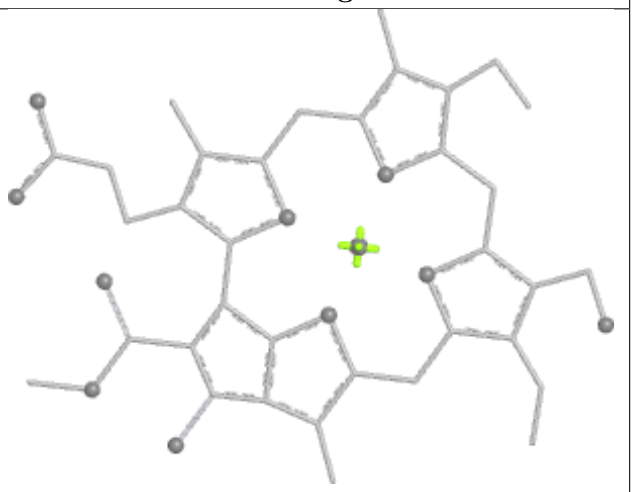
Bond lengths



Bond angles

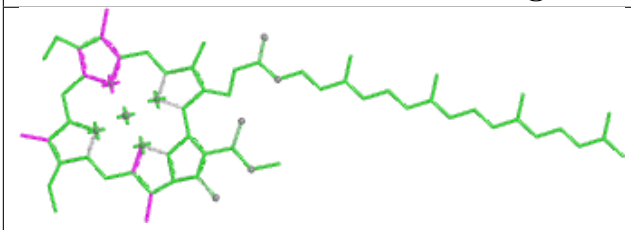


Torsions

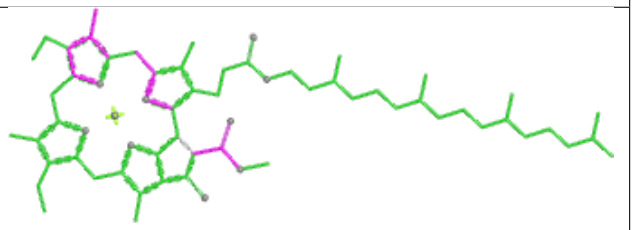


Rings

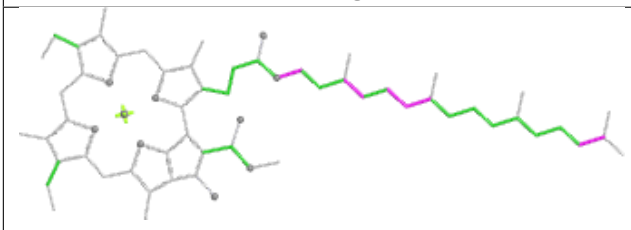
Ligand CLA b 603



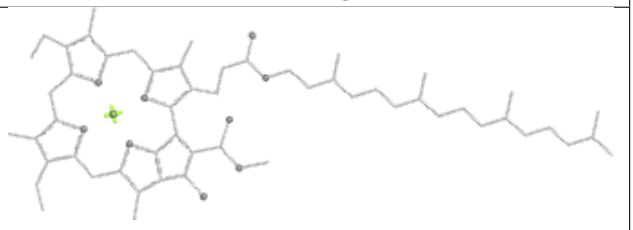
Bond lengths



Bond angles

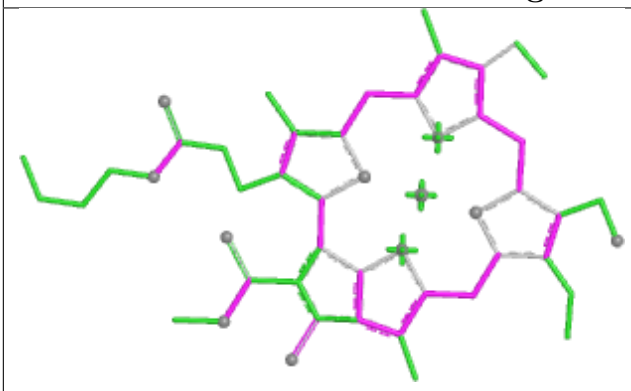


Torsions

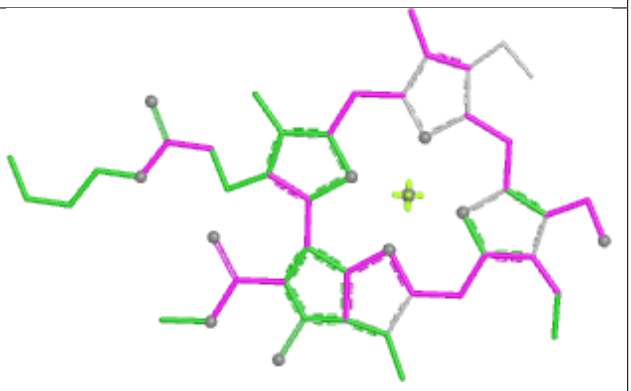


Rings

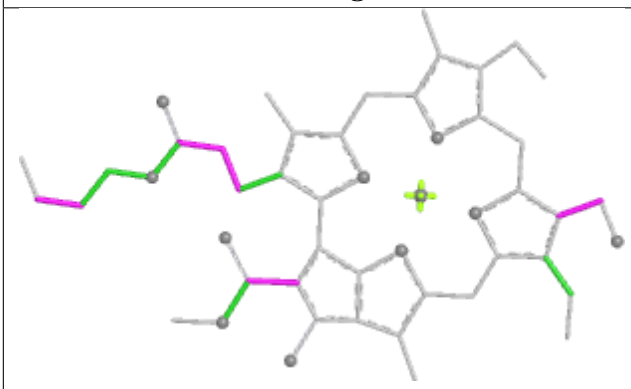
Ligand CHL n 606



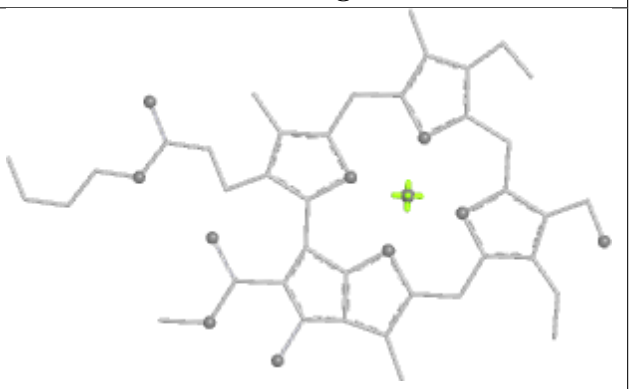
Bond lengths



Bond angles

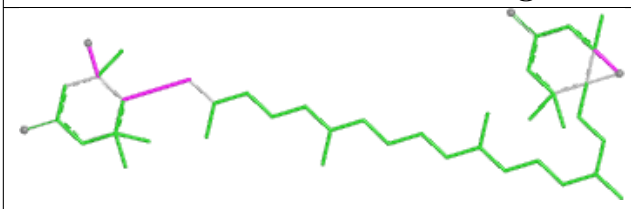


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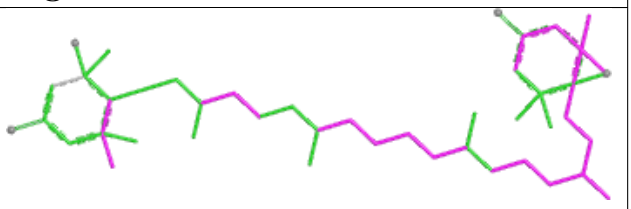


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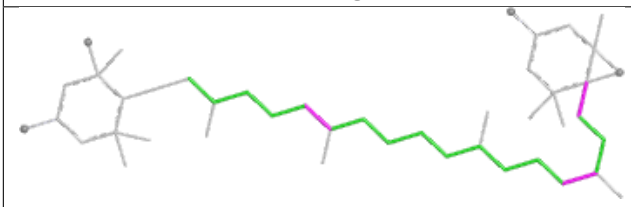
Ligand NEX g 1623



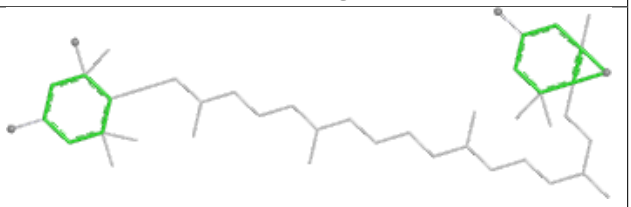
Bond lengths



Bond angles

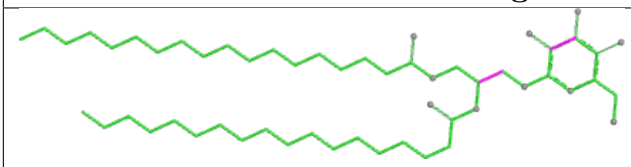


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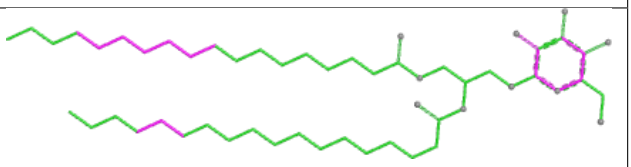


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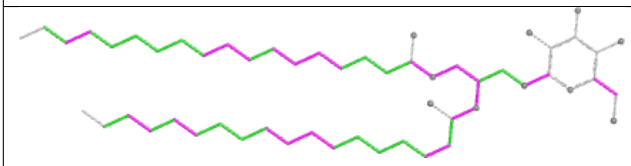
Ligand LMG B 2633



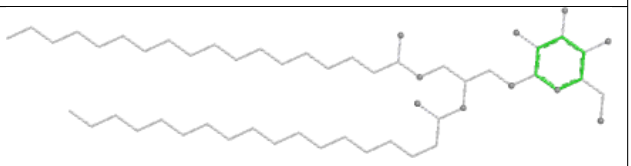
Bond lengths



Bond angles

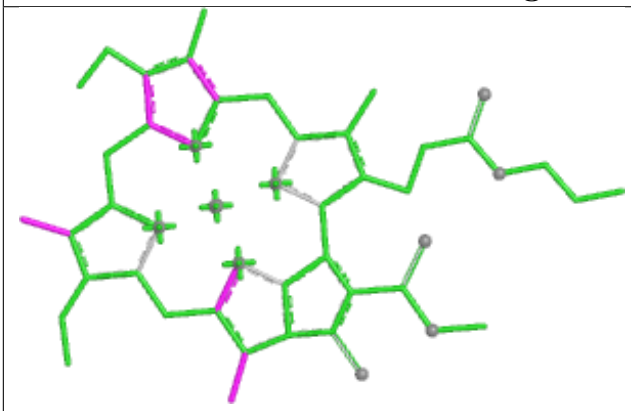


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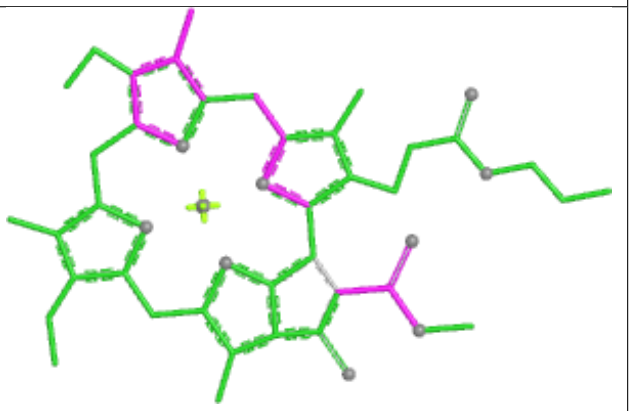


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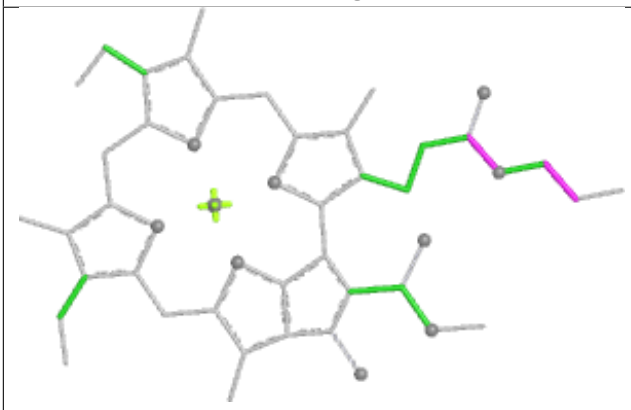
Ligand CLA G 614



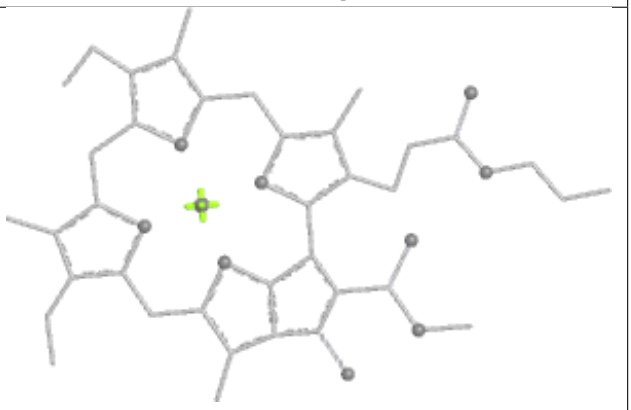
Bond lengths



Bond angles

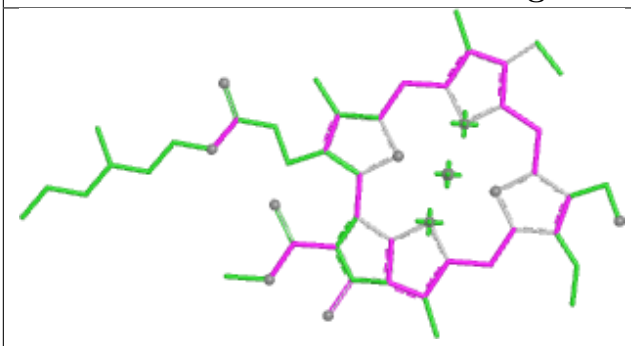


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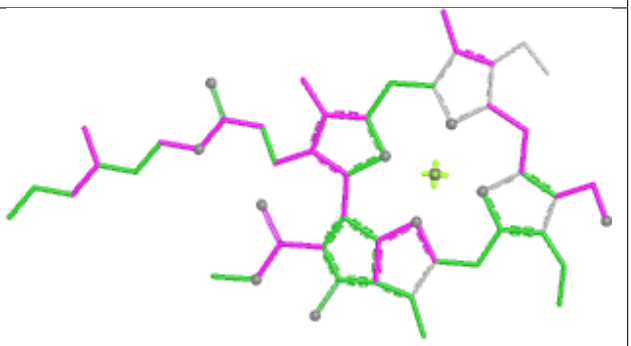


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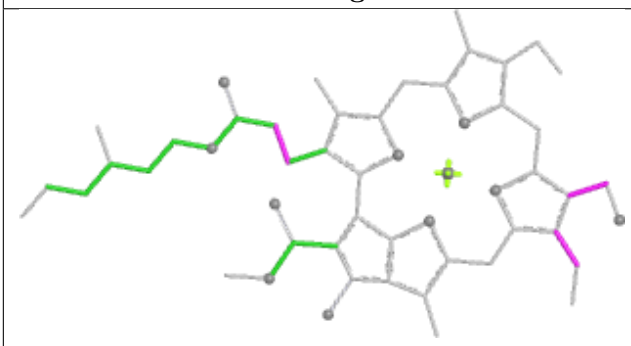
Ligand CHL 3 607



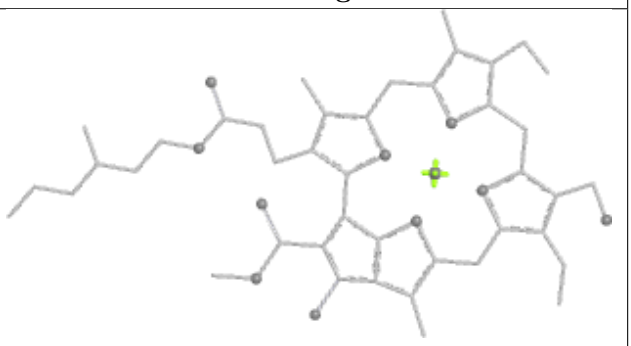
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Bond angles

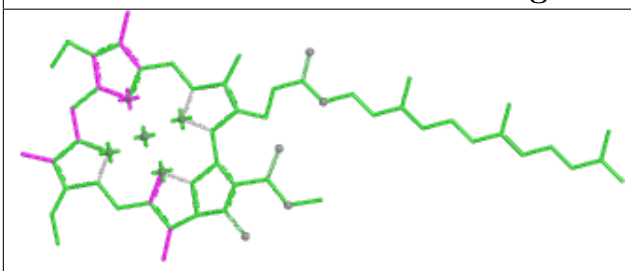


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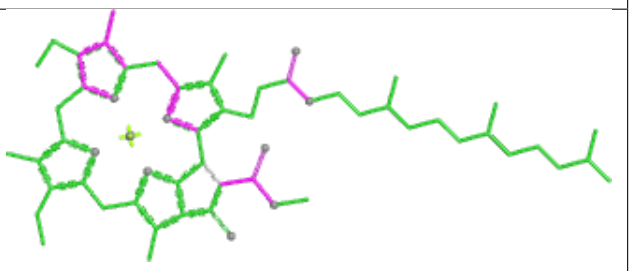


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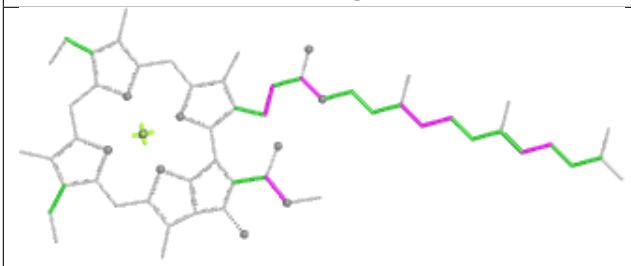
Ligand CLA r 602



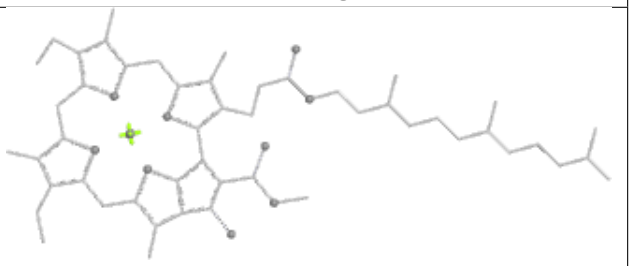
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Bond angles

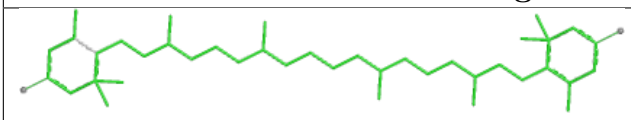


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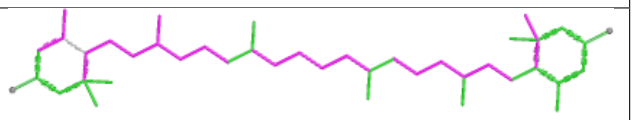


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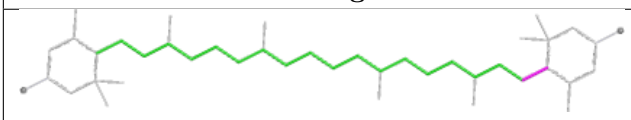
Ligand LUT G 1620



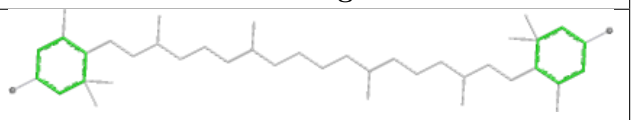
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Bond angles

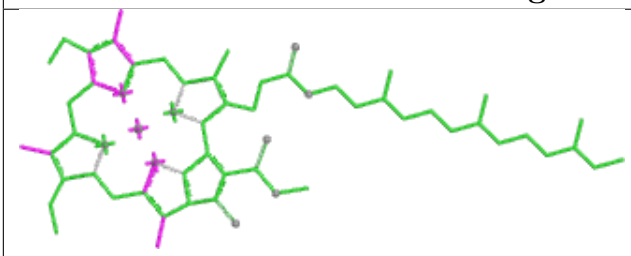


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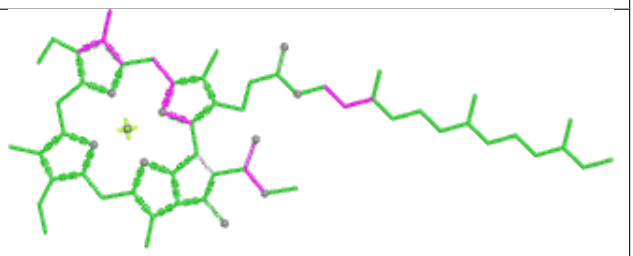


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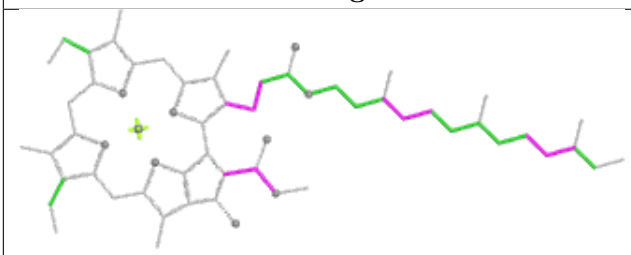
Ligand CLA 2 602



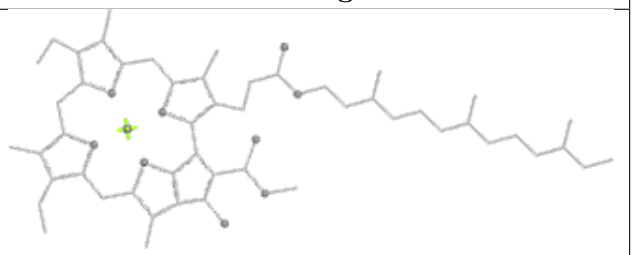
Bond lengths



Bond angles

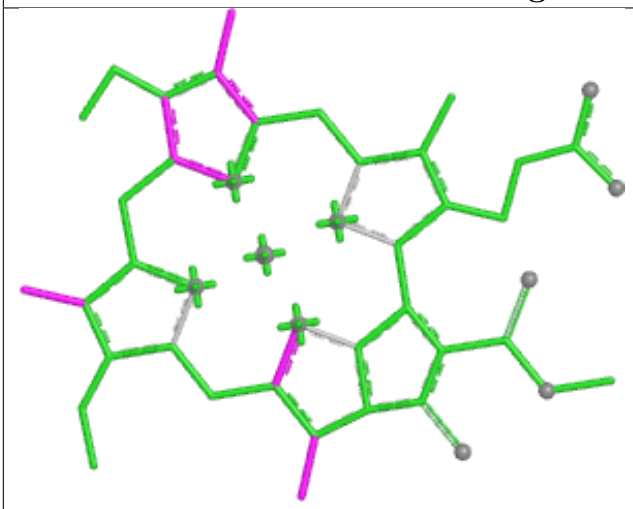


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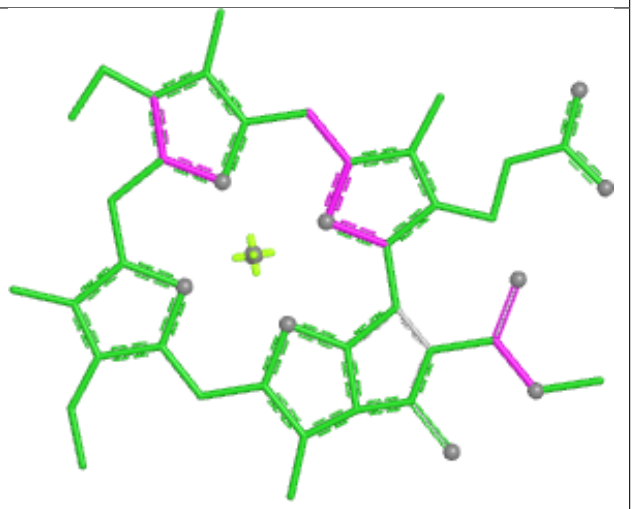


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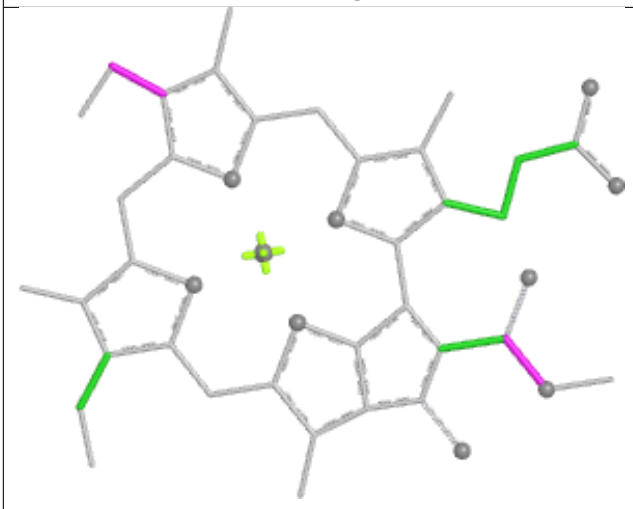
Ligand CLA 1 614



Bond lengths



Bond angles

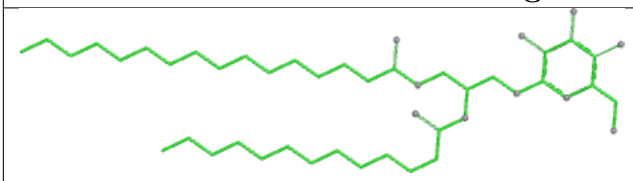


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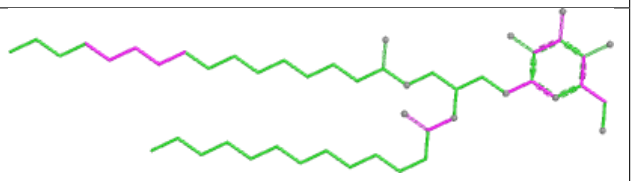


Rings

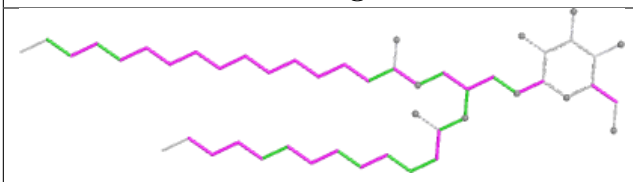
Ligand LMG a 413



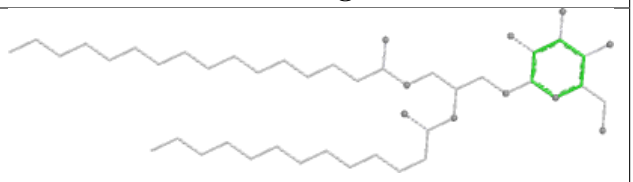
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Bond angles

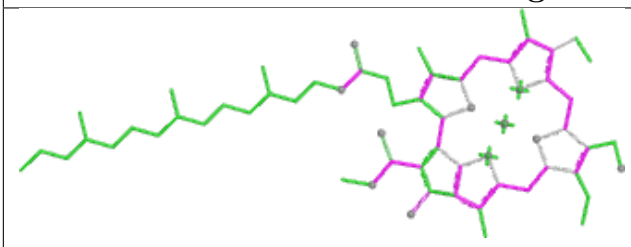


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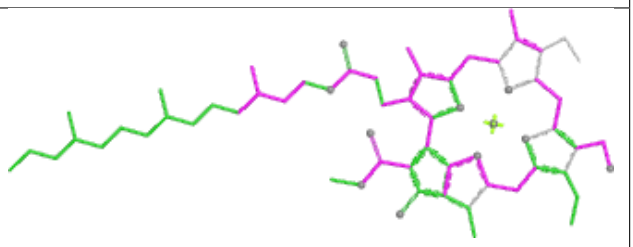


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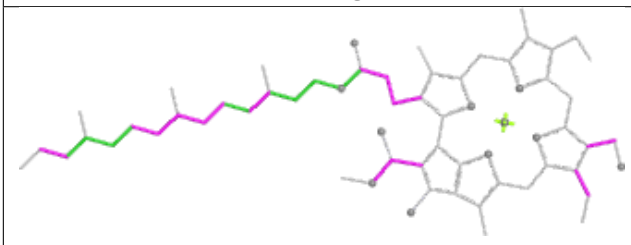
Ligand CHL 1 607



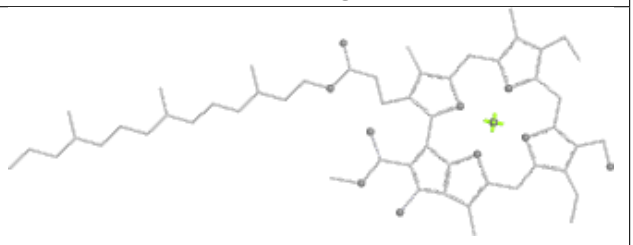
Bond lengths



Bond angles

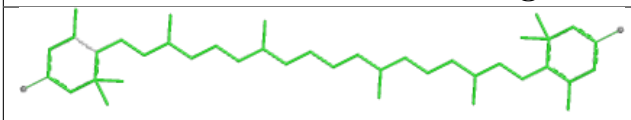


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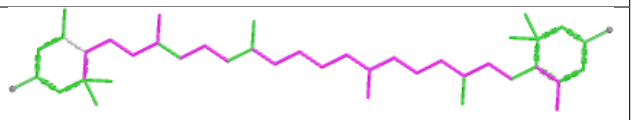


Rings

Ligand LUT 7 1620



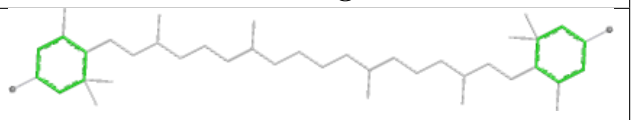
Bond lengths



Bond angles

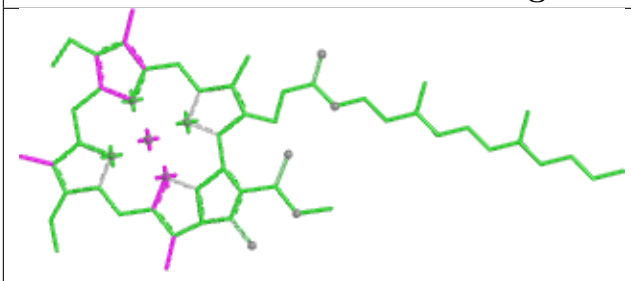


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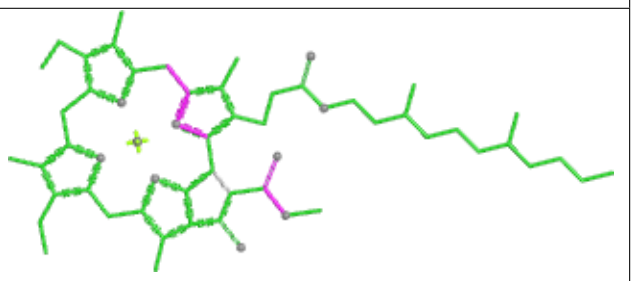


Rings

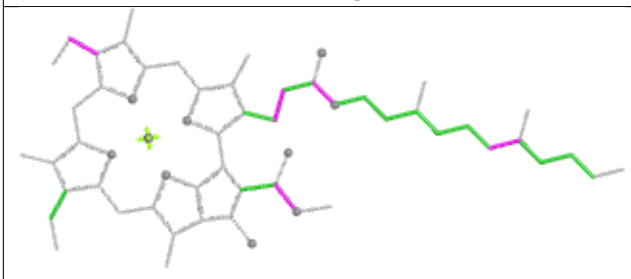
Ligand CLA 3 613



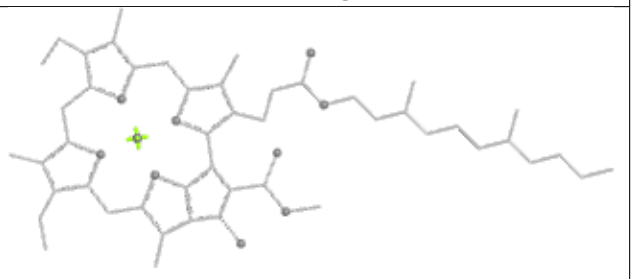
Bond lengths



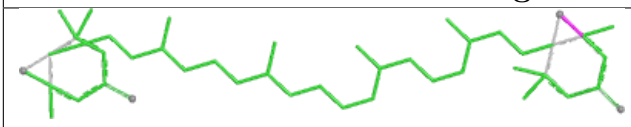
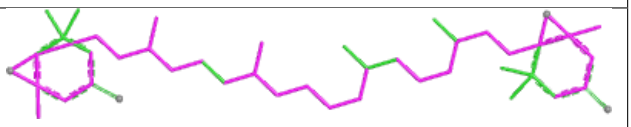
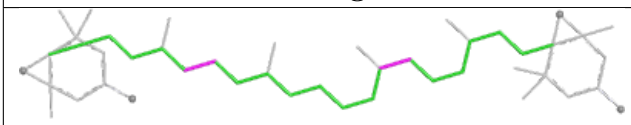
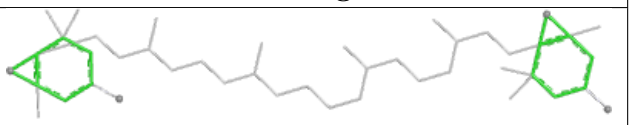
Bond angles

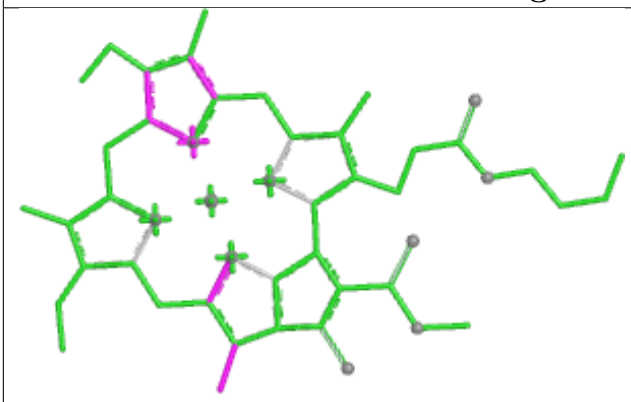
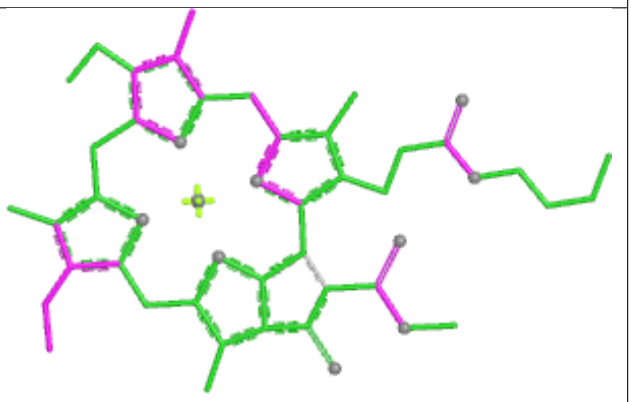
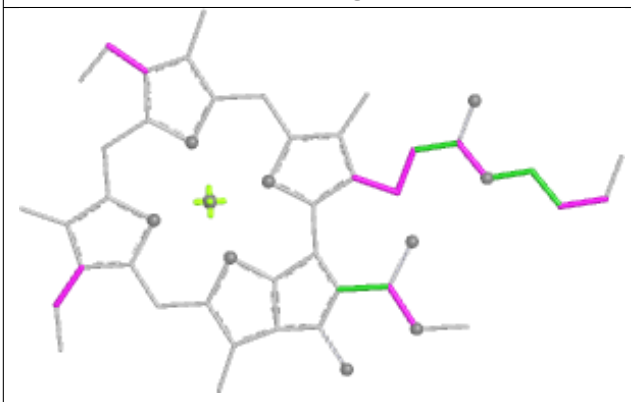
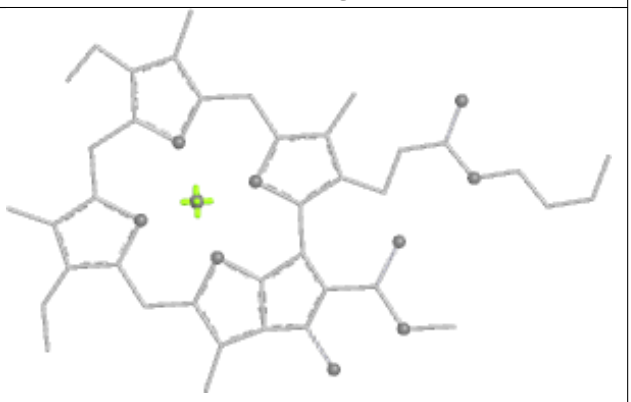


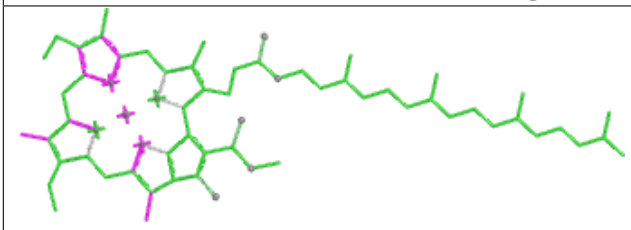
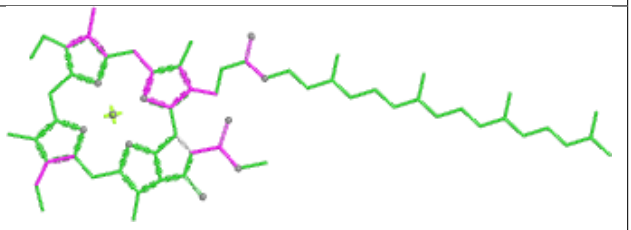
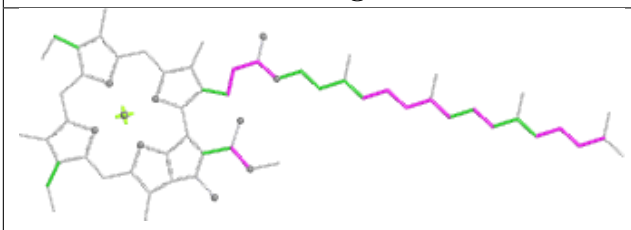
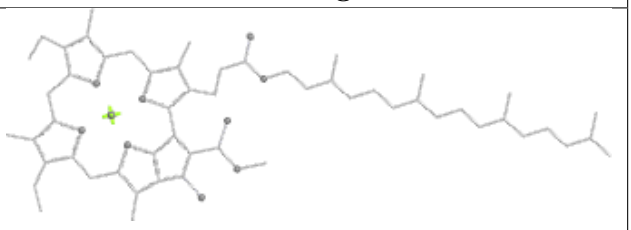
Torsions

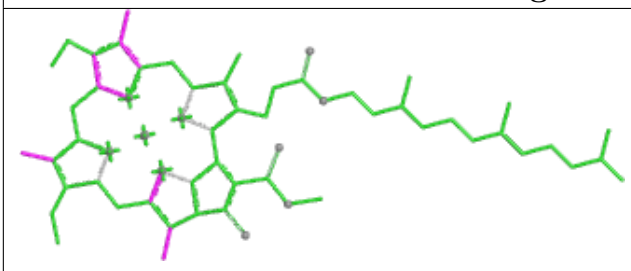
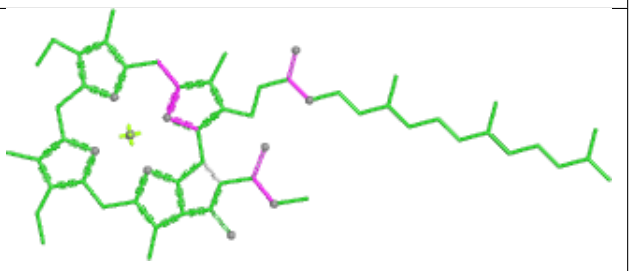
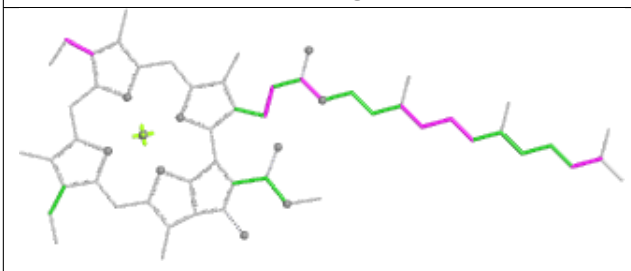
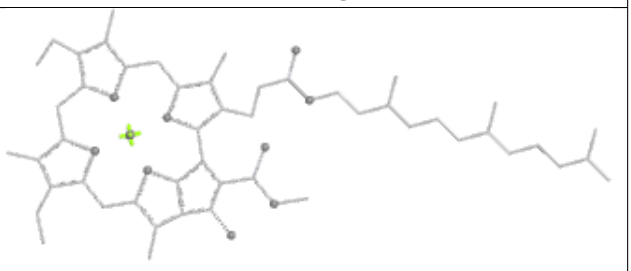


Rings

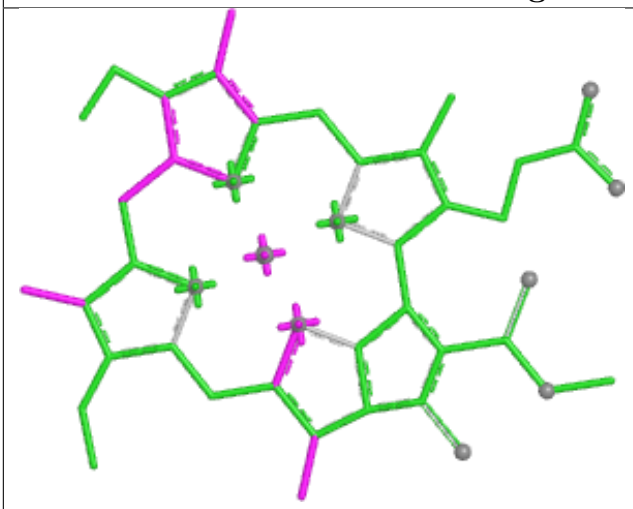
Ligand XAT N 1622	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

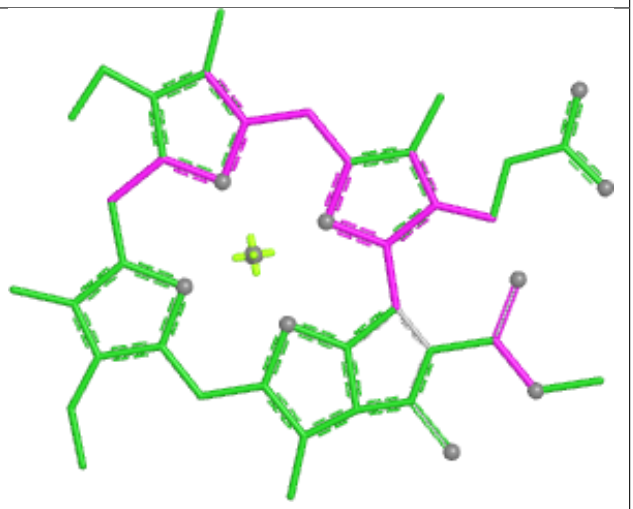
Ligand CLA B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA r 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

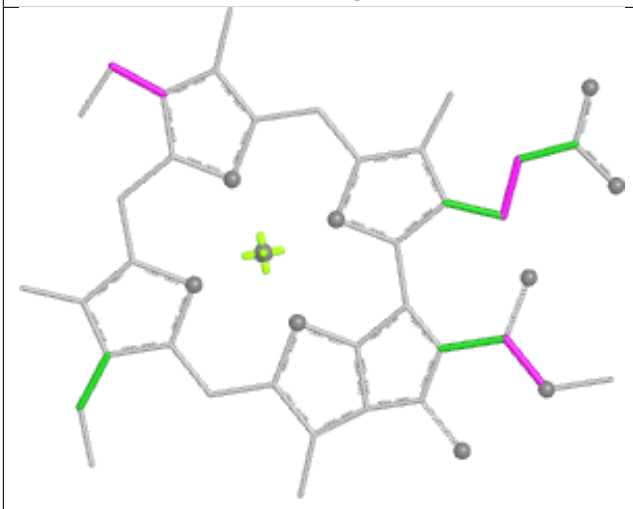
Ligand CLA 1 612



Bond lengths



Bond angles

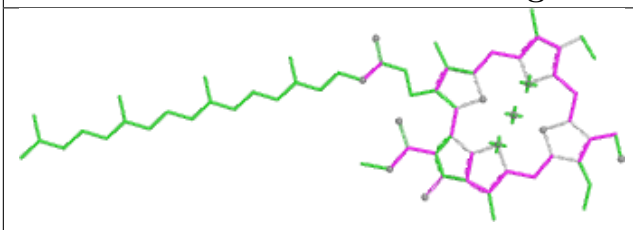


Torsions

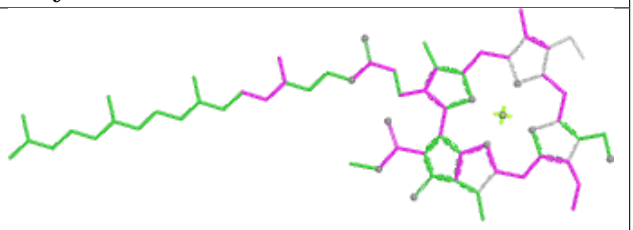


Rings

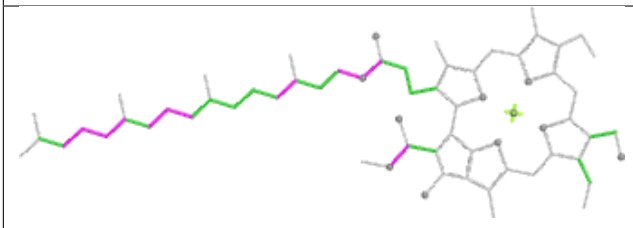
Ligand CHL y 609



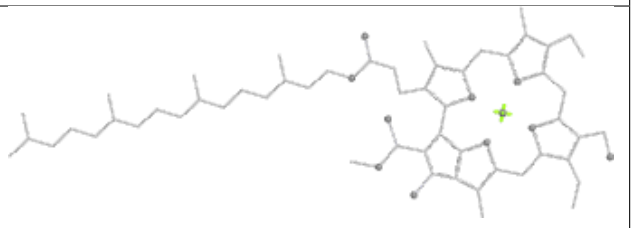
Bond lengths



Bond angles

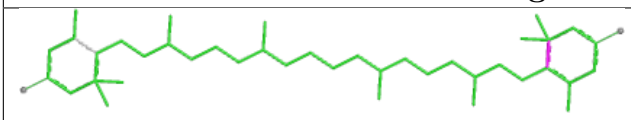


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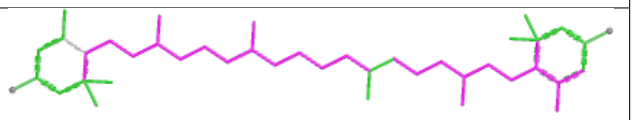


Rings

Ligand LUT 8 620



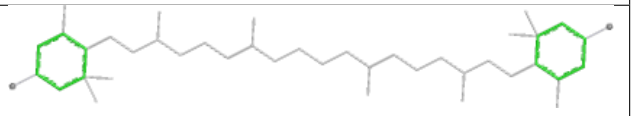
Bond lengths



Bond angles

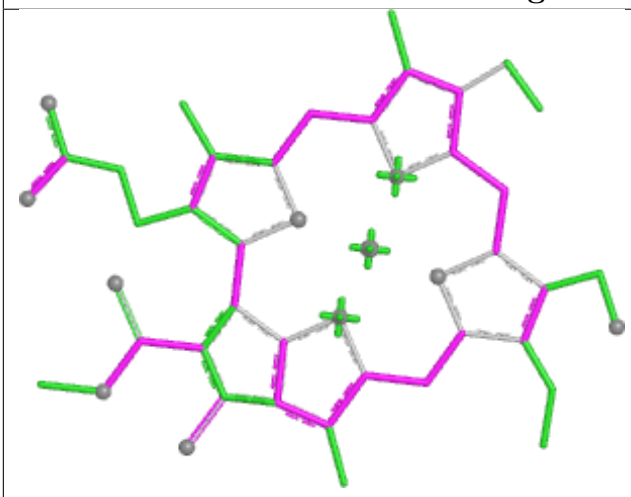


Torsions

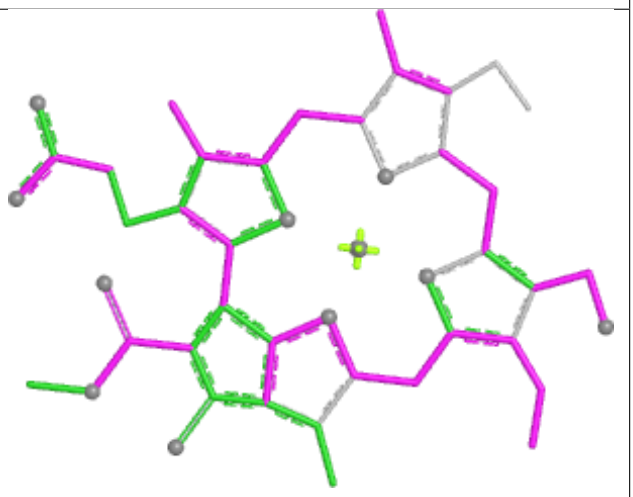


Rings

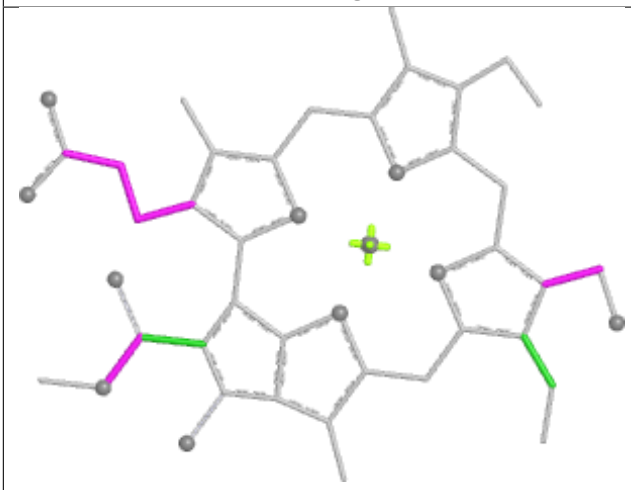
Ligand CHL 4 607



Bond lengths



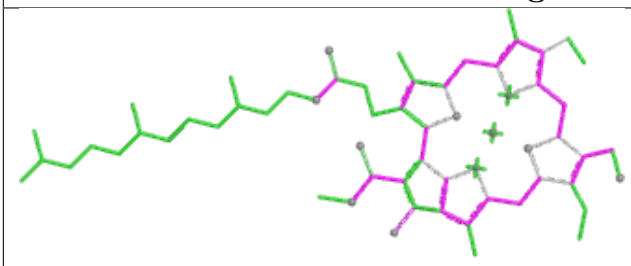
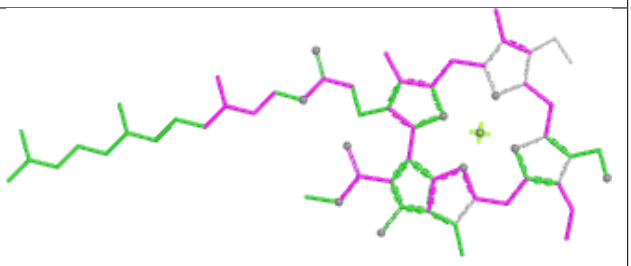
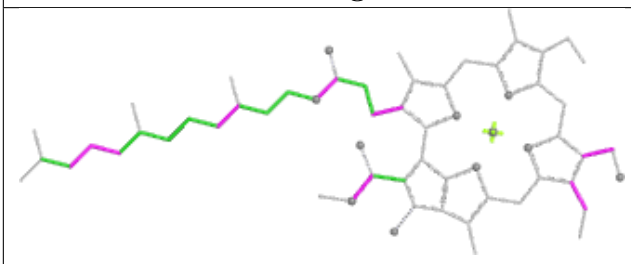
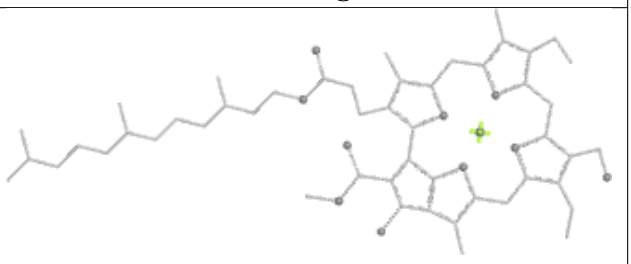
Bond angles

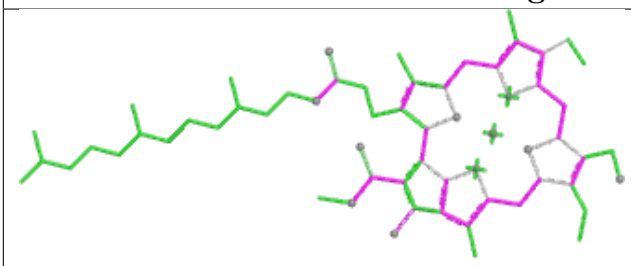
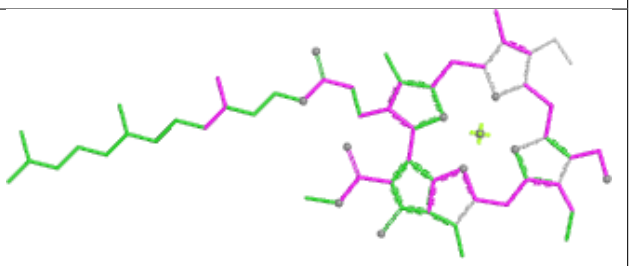
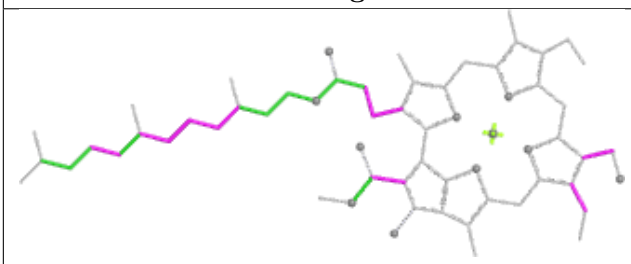
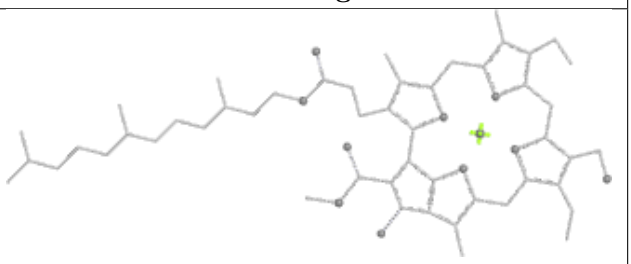


Torsions

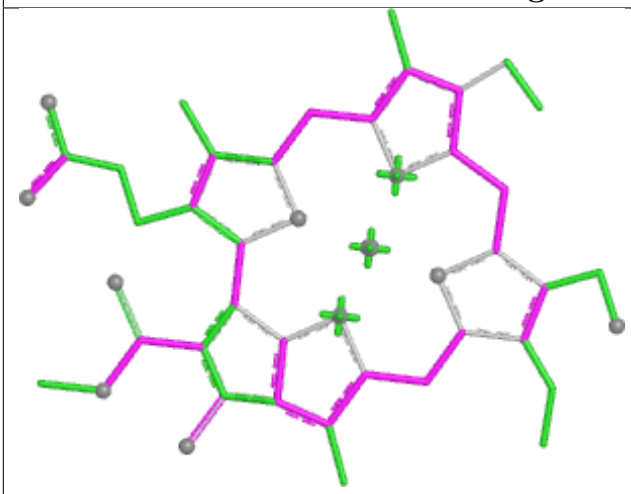


Rings

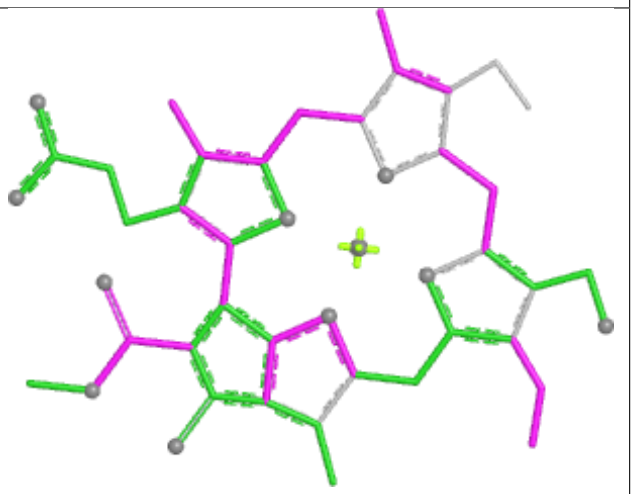
Ligand CHL 3 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 6 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

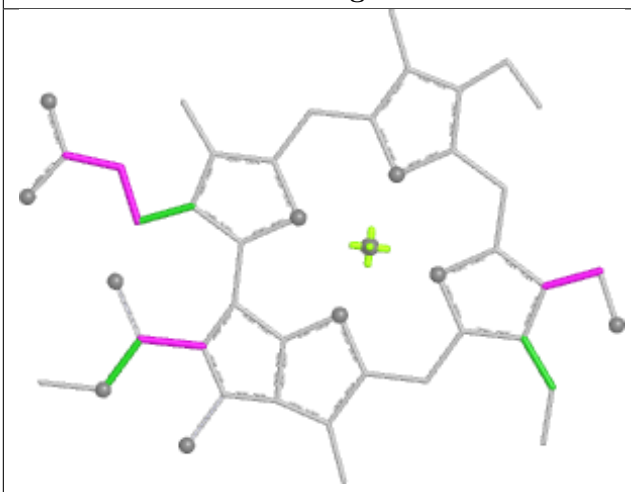
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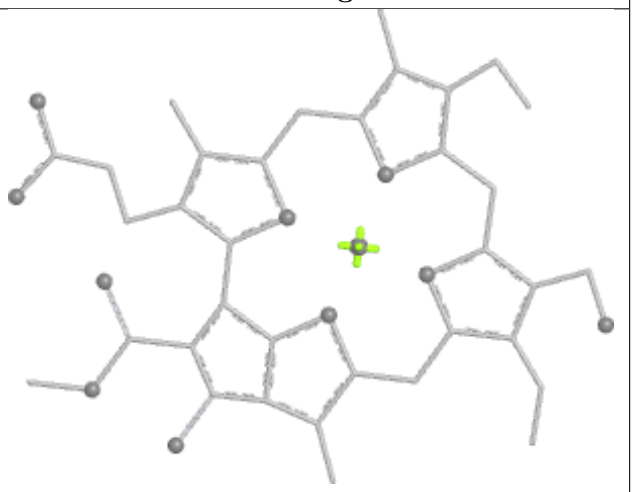
Bond lengths



Bond angles

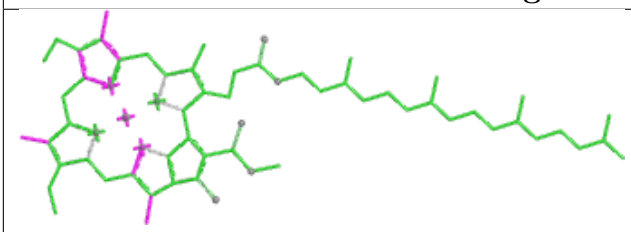


Torsions

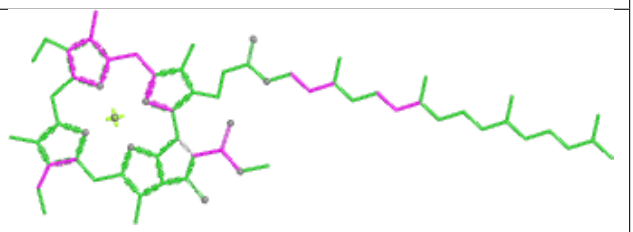


Rings

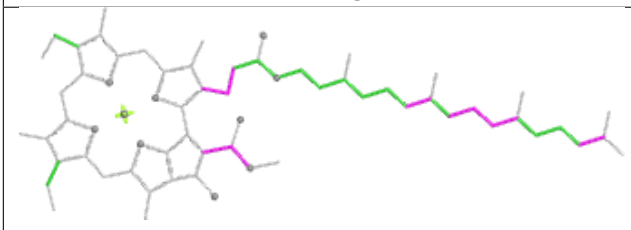
Ligand CLA N 602



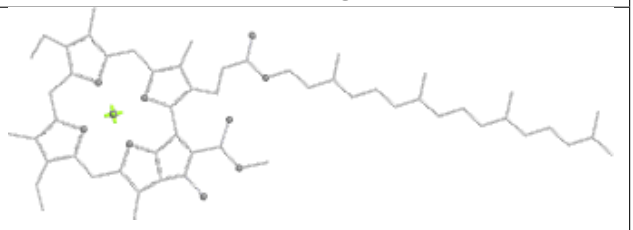
Bond lengths



Bond angles

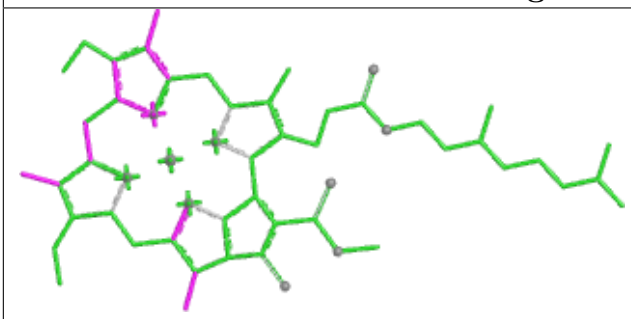


Torsions

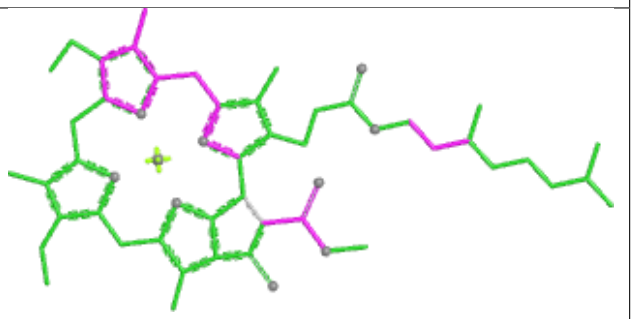


Rings

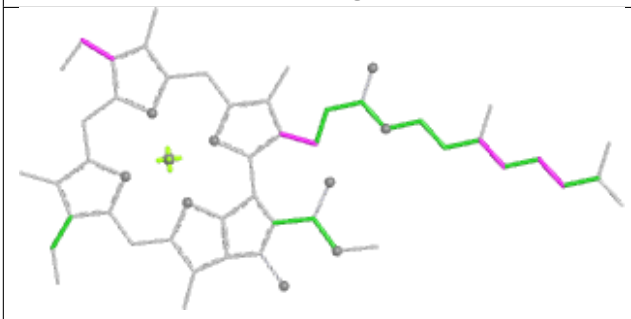
Ligand CLA S 610



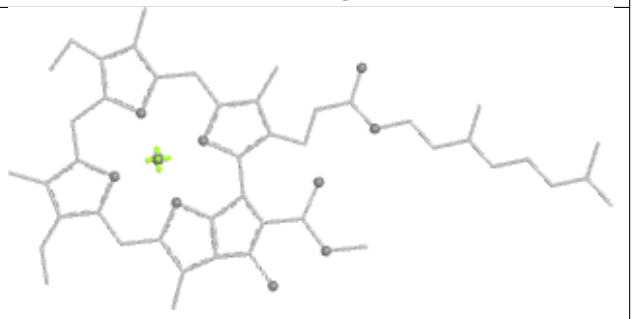
Bond lengths



Bond angles

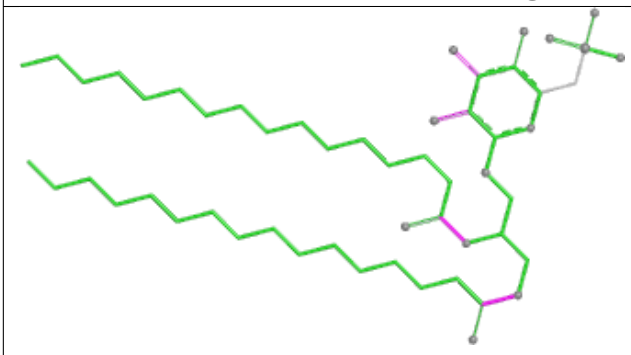


Torsions

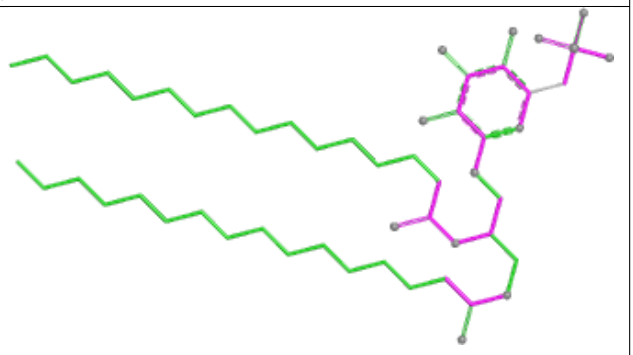


Rings

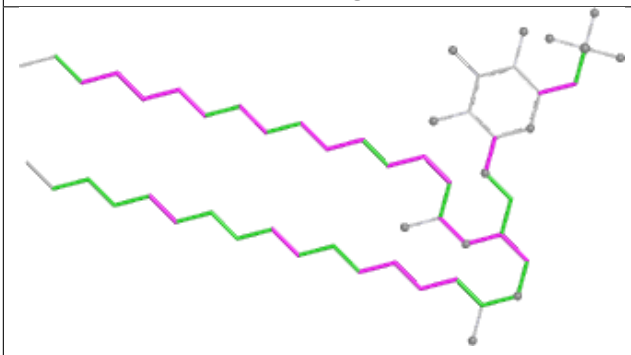
Ligand SQD A 418



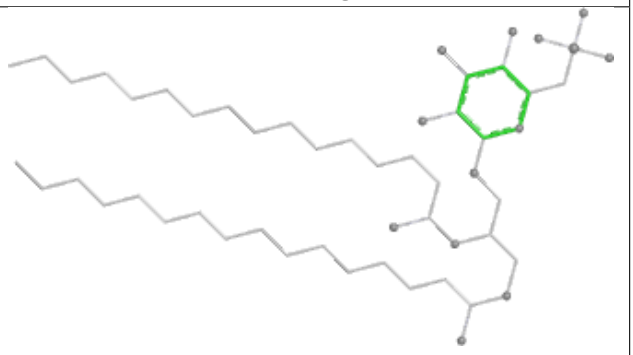
Bond lengths



Bond angles

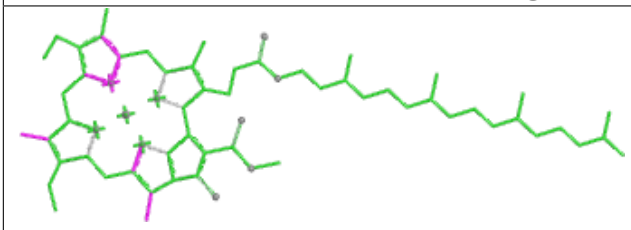


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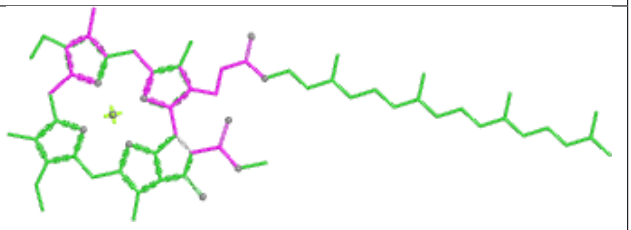


Rings

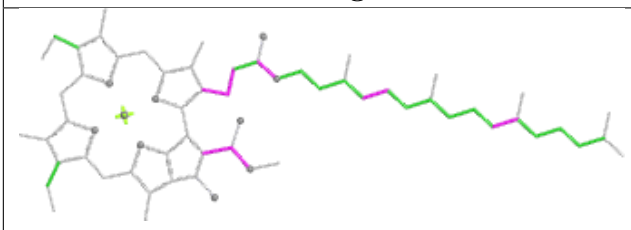
Ligand CLA C 513



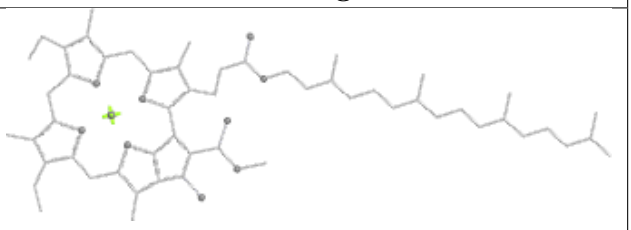
Bond lengths



Bond angles

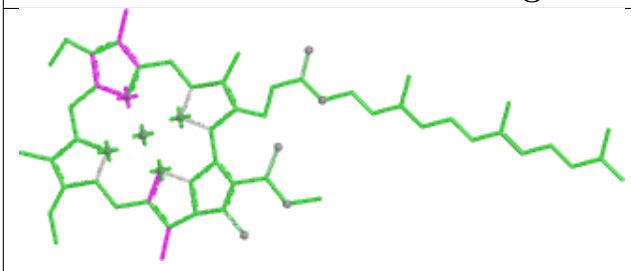


Torsions

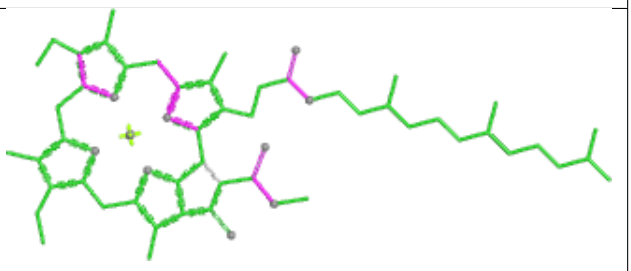


Rings

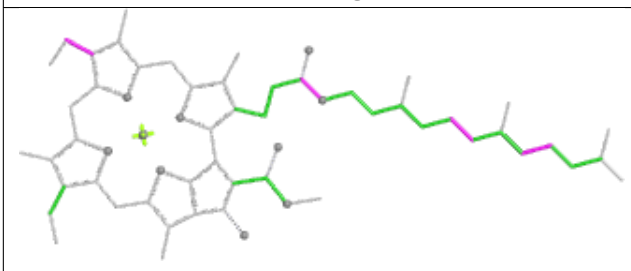
Ligand CLA N 611



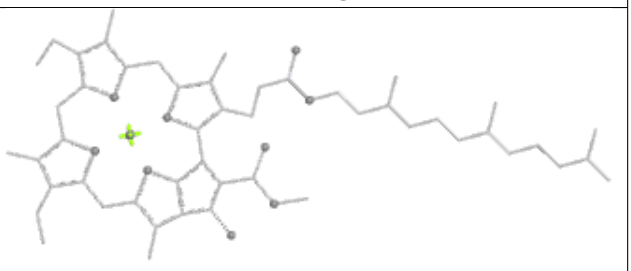
Bond lengths



Bond angles

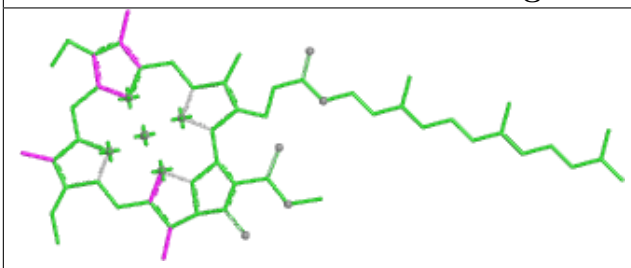


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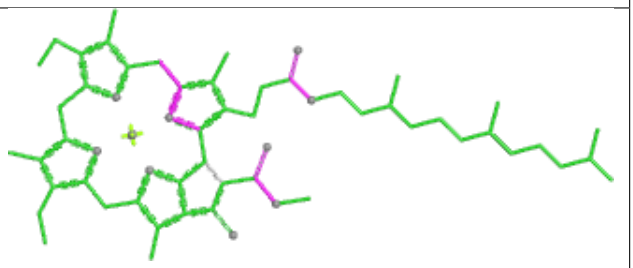


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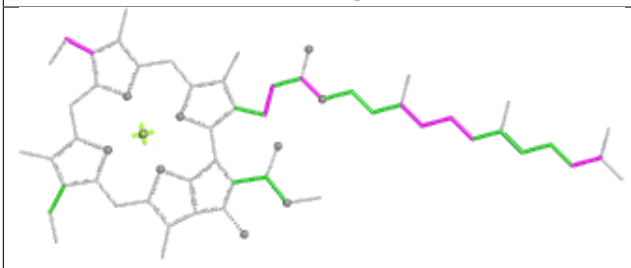
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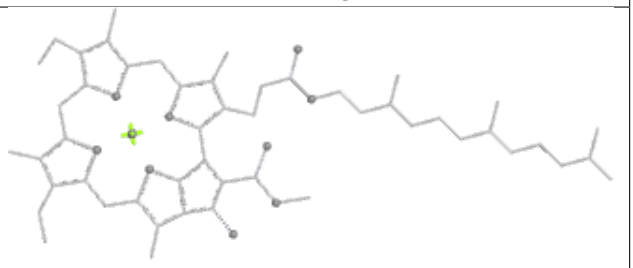
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Bond angles

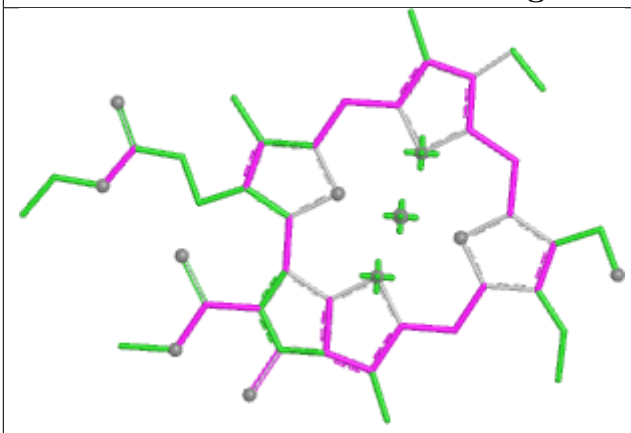


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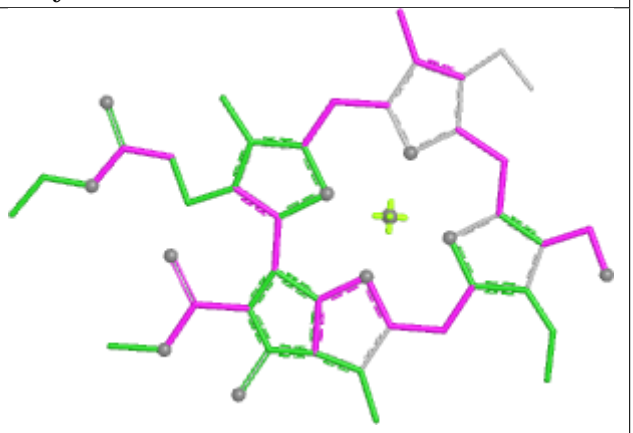


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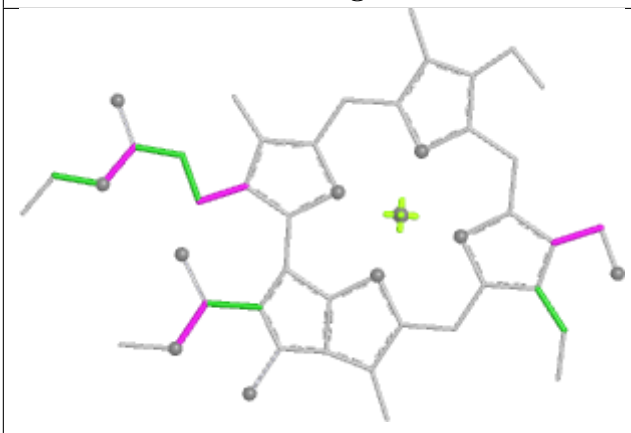
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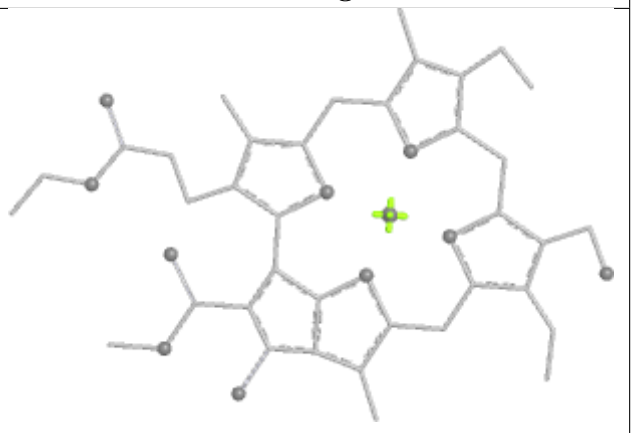
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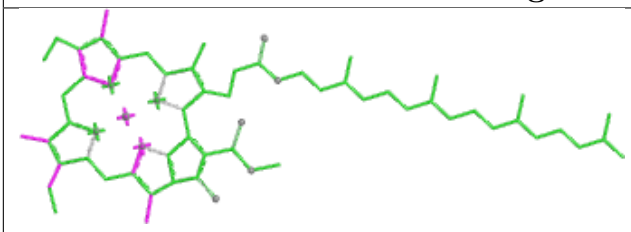


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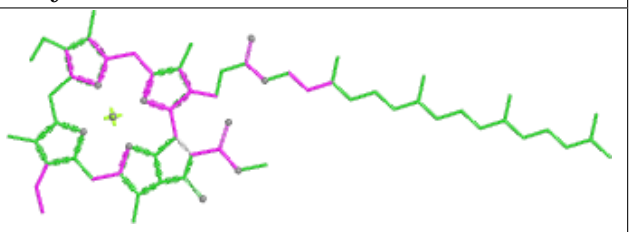


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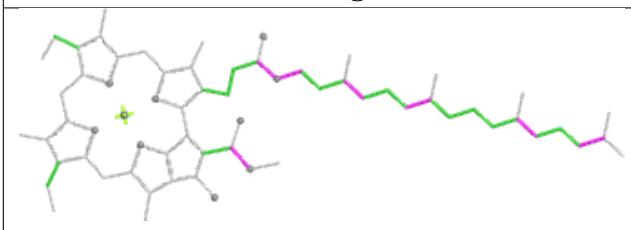
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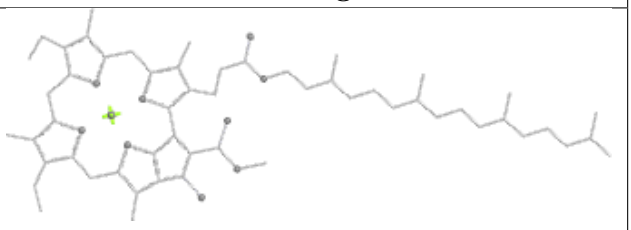
Bond lengths



Bond angles



Torsions

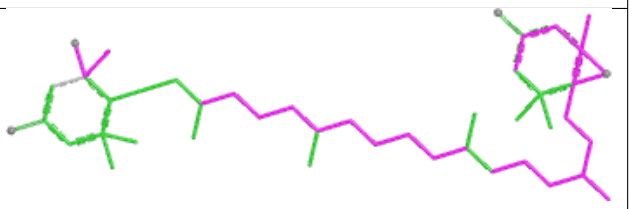


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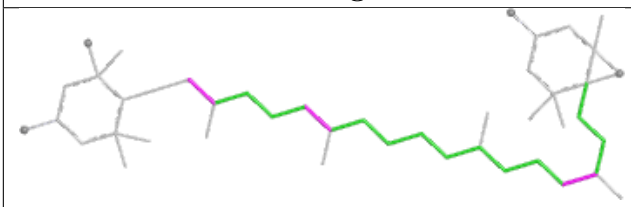
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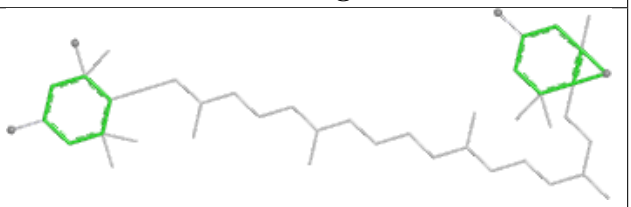
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Bond angles

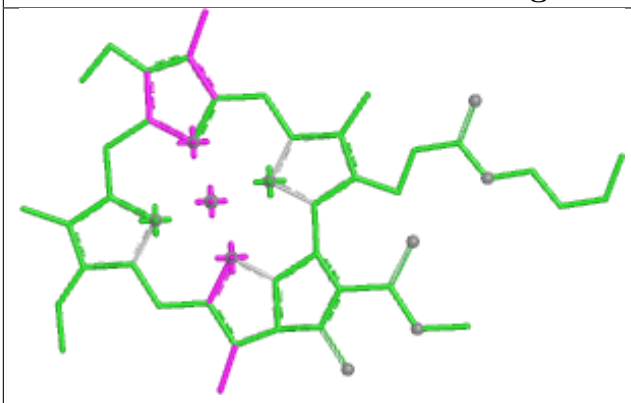


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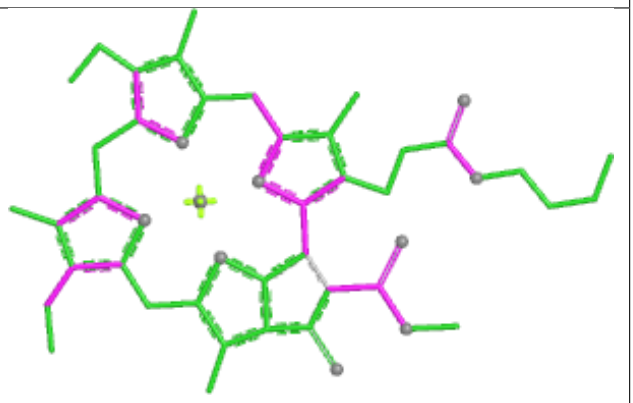


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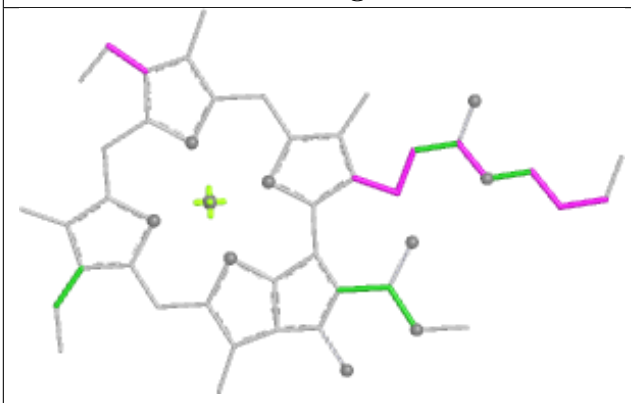
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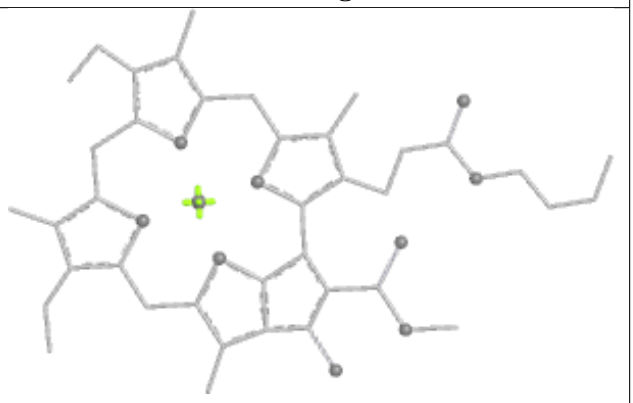
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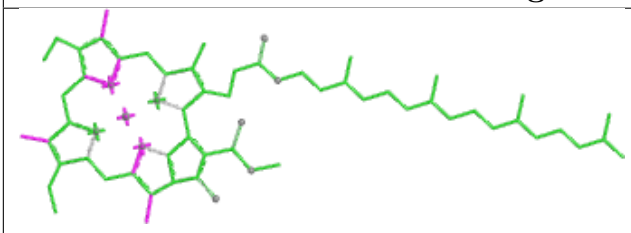


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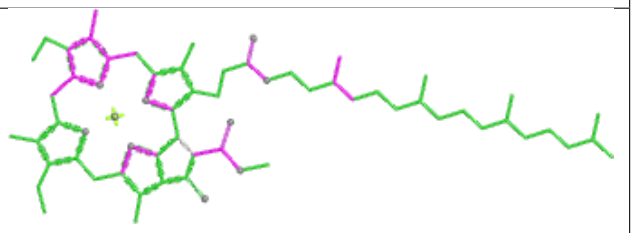


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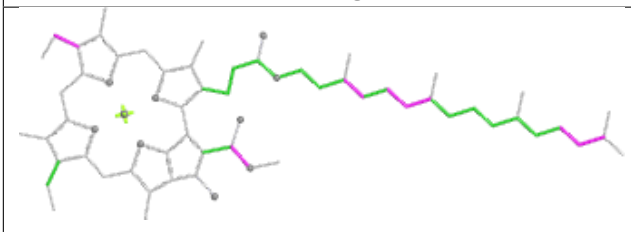
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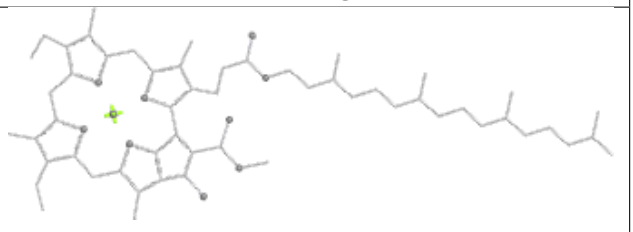
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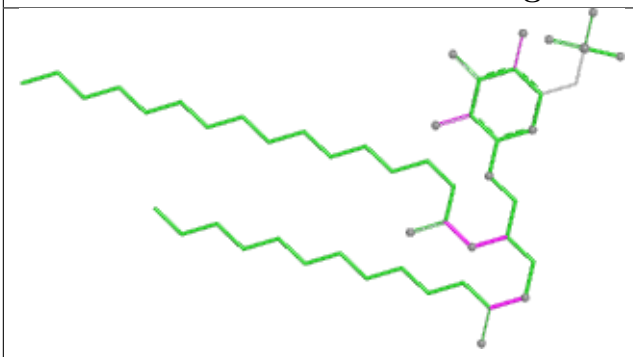


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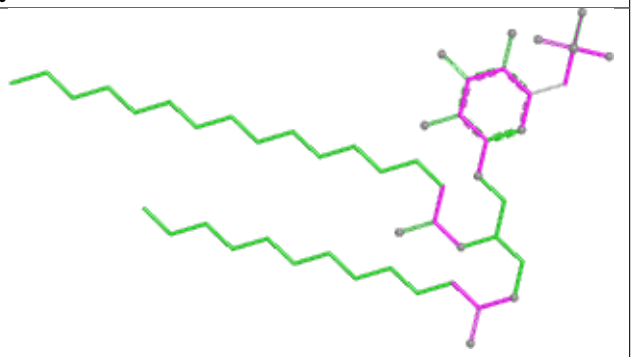


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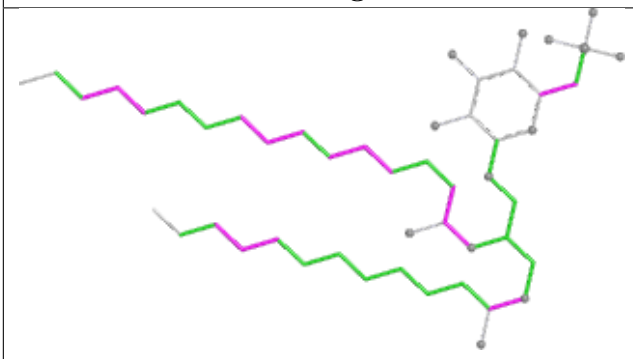
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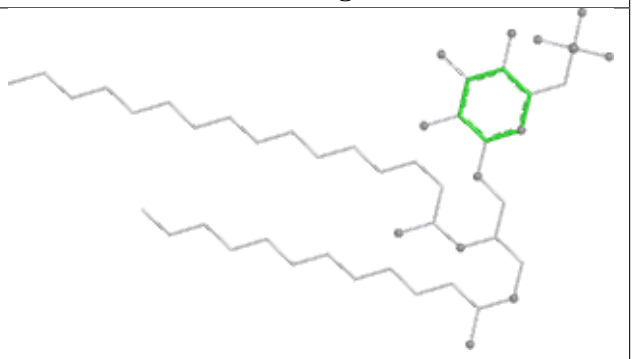
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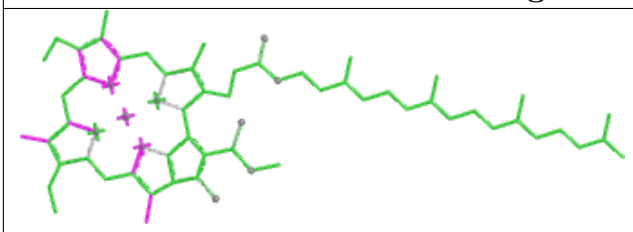


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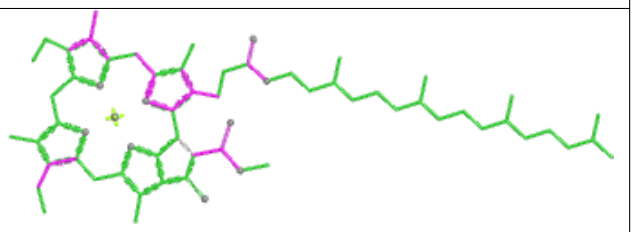


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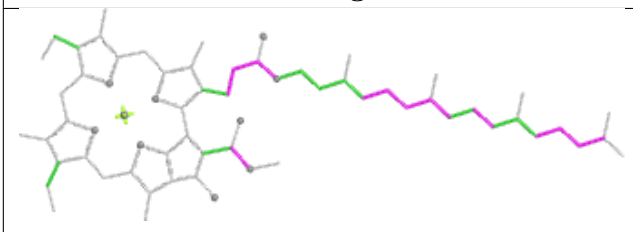
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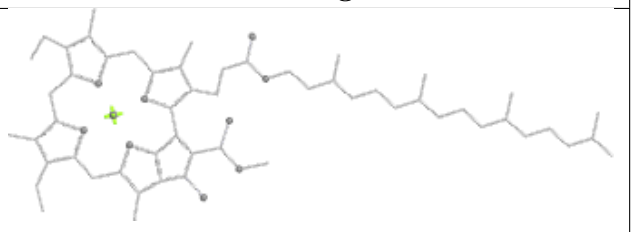
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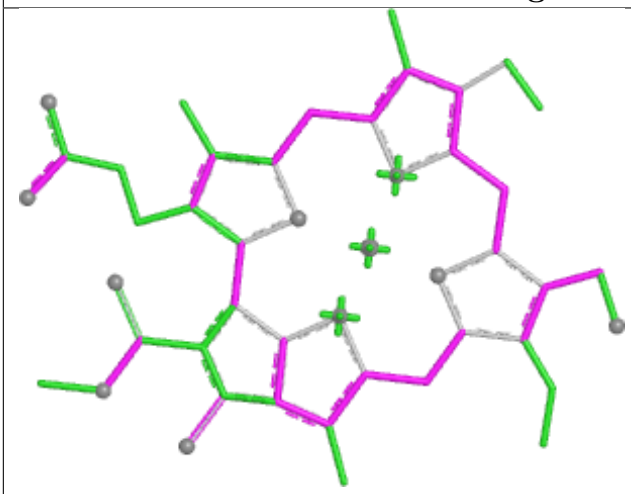


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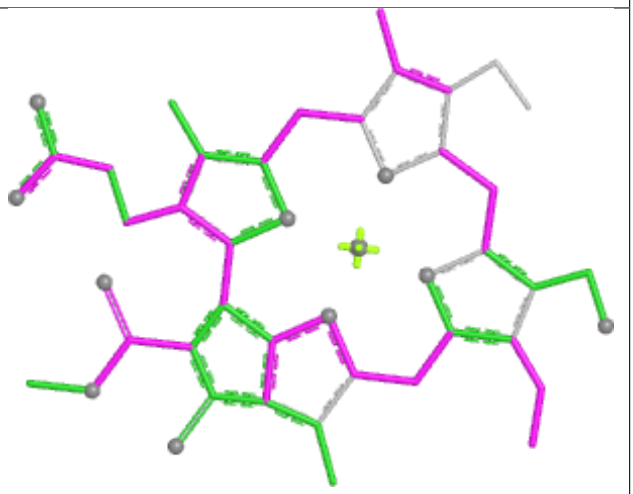


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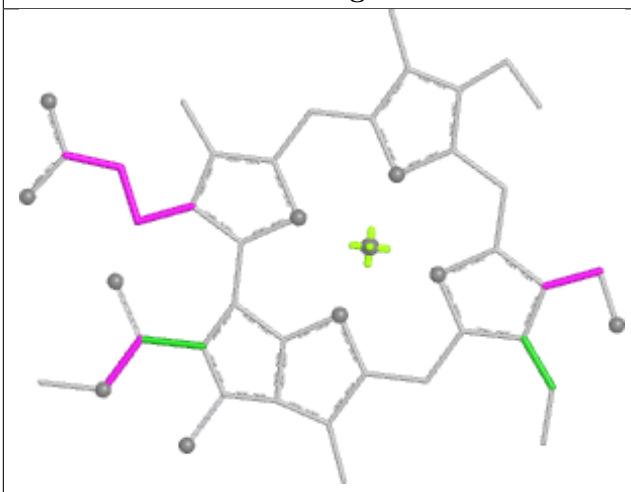
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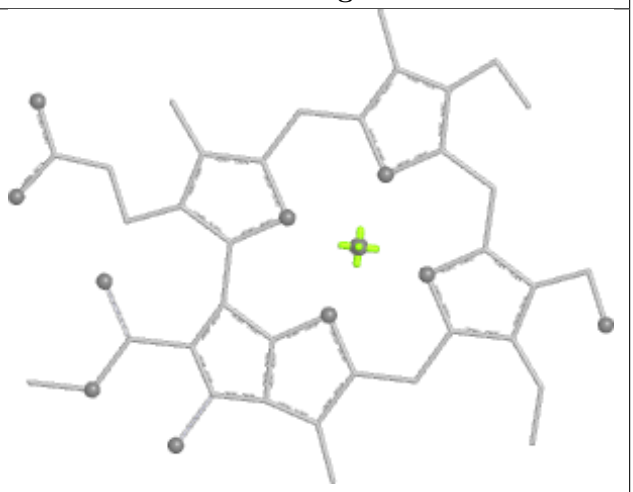
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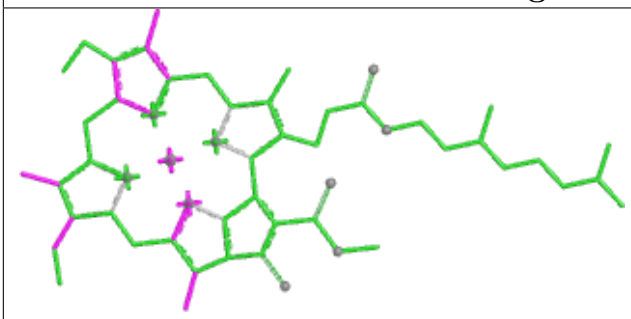


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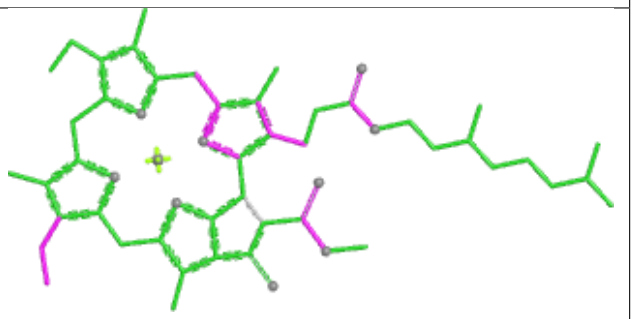


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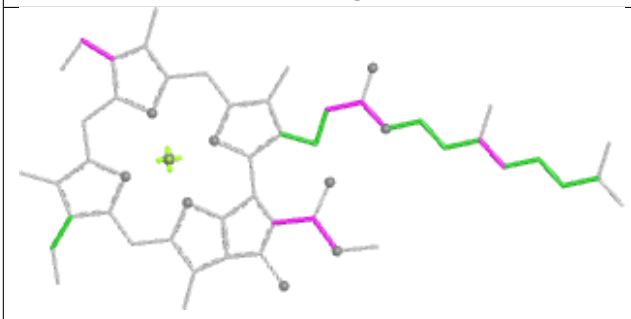
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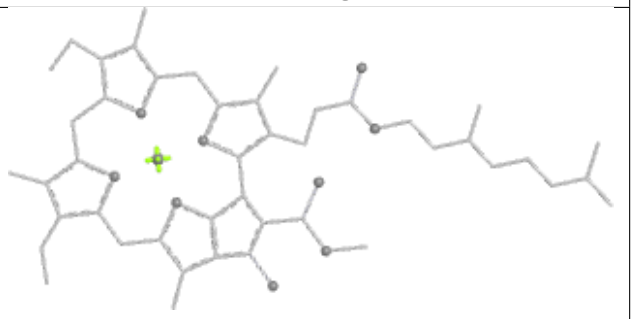
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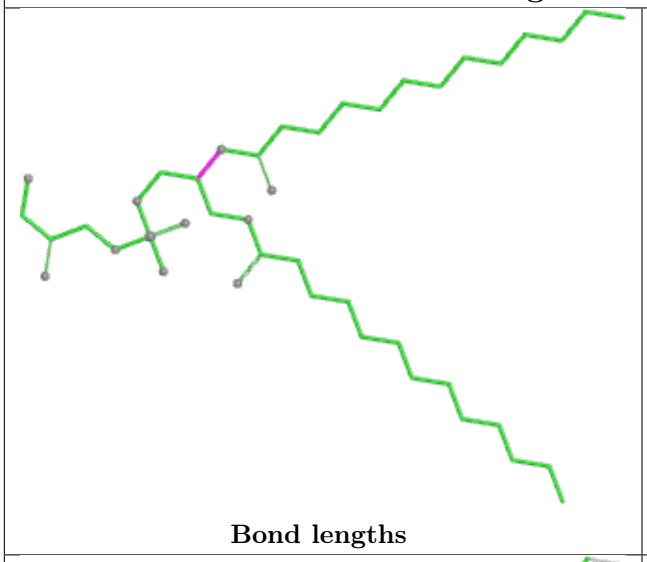


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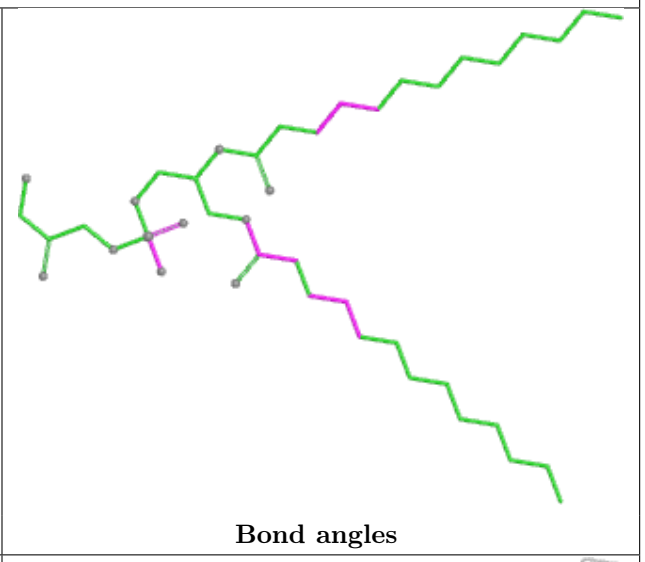


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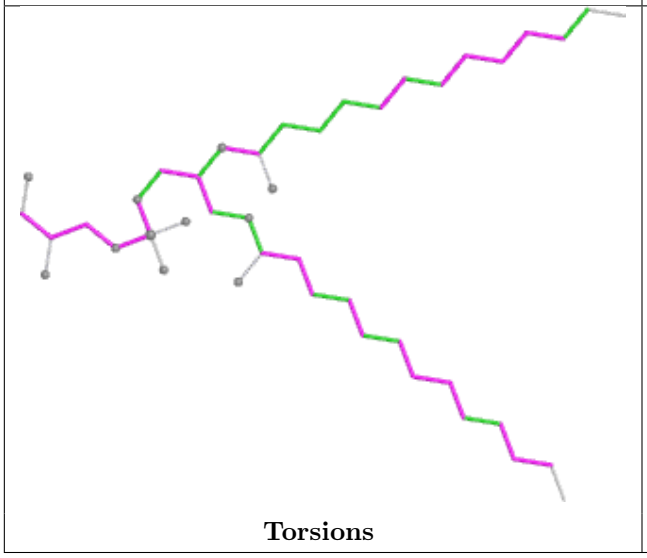
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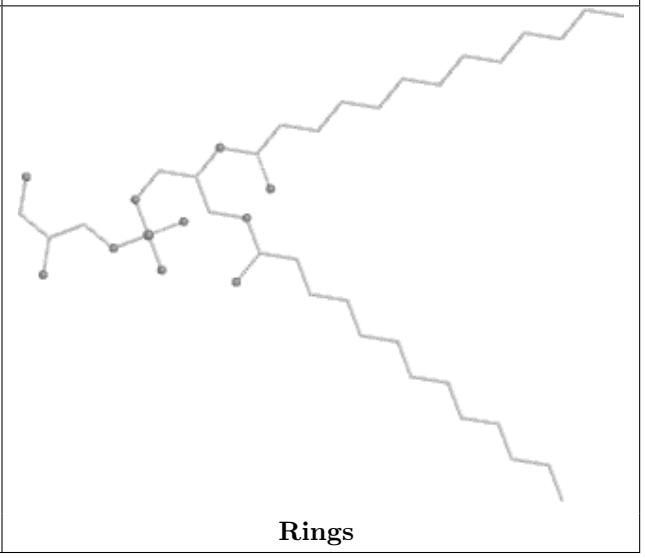
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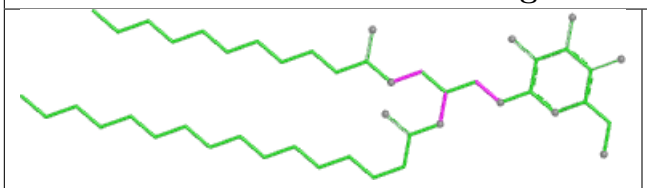


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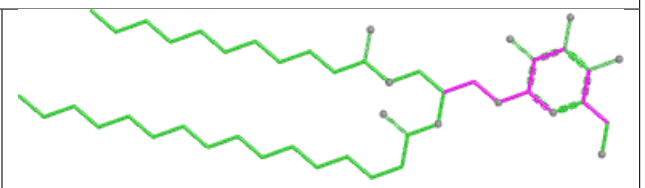


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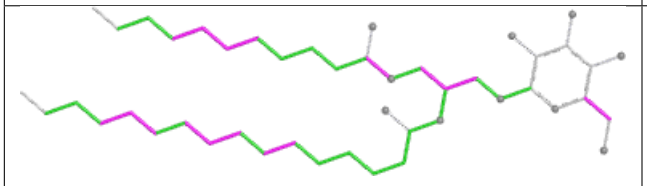
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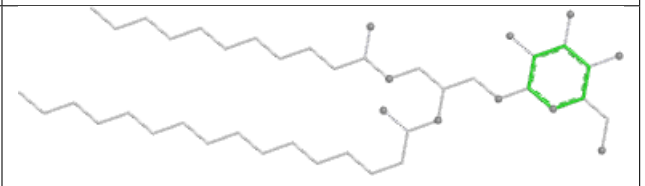
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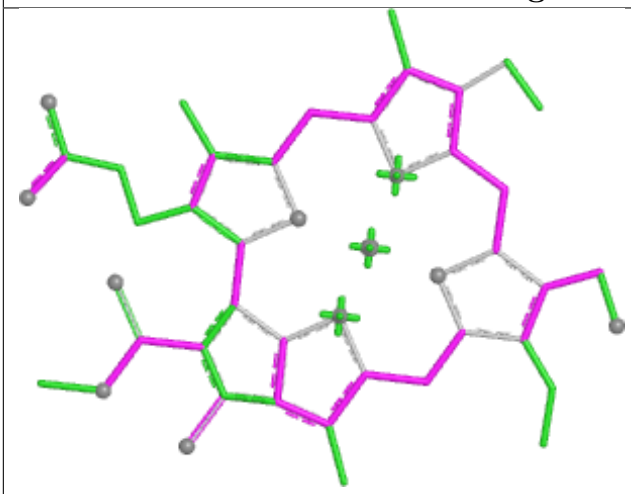


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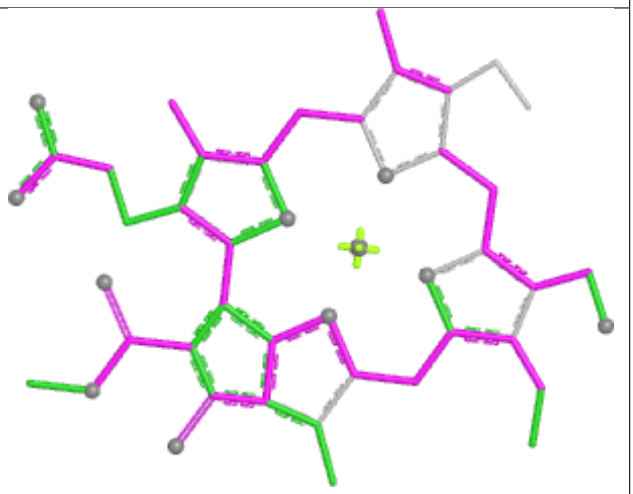


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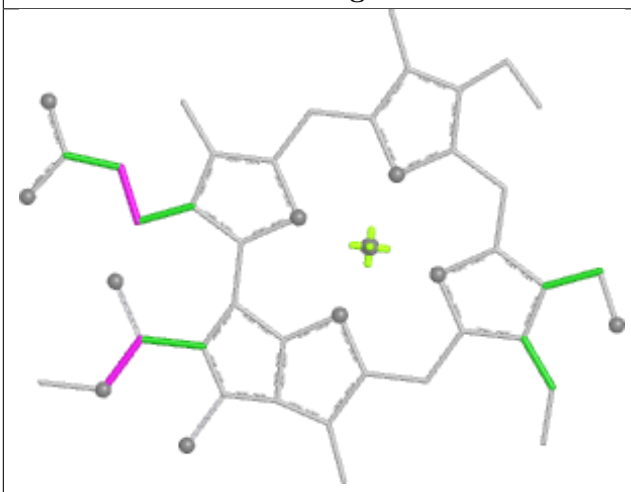
Ligand CHL 3 608



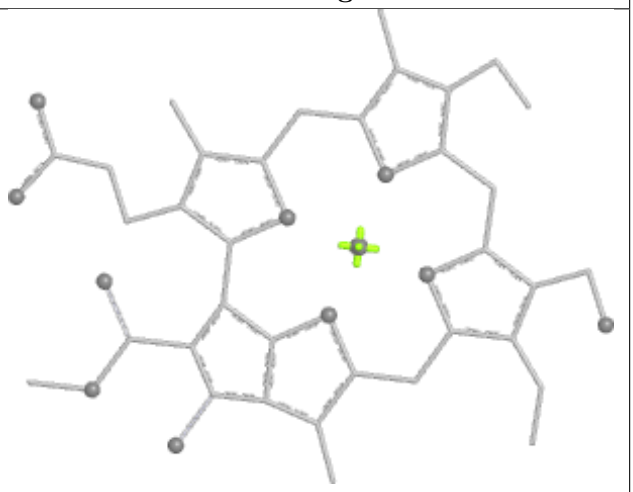
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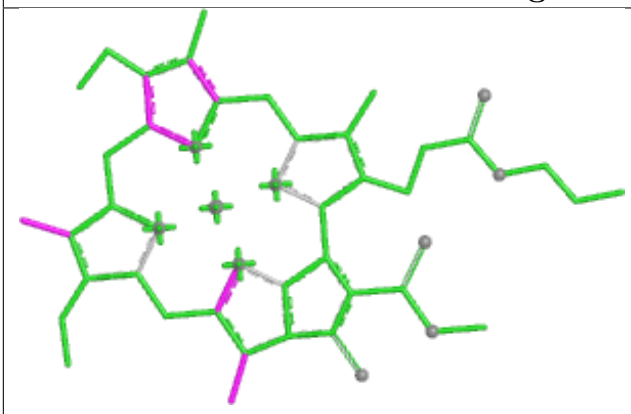


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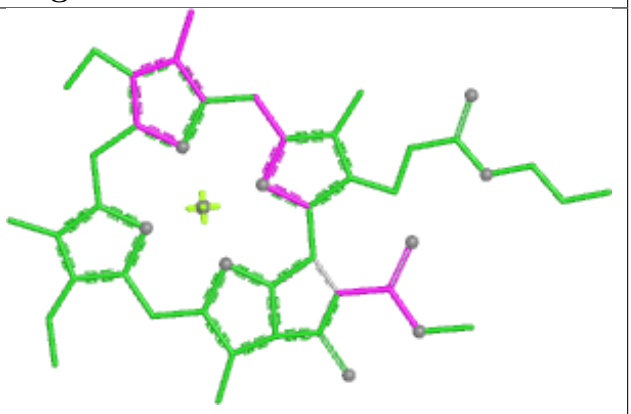


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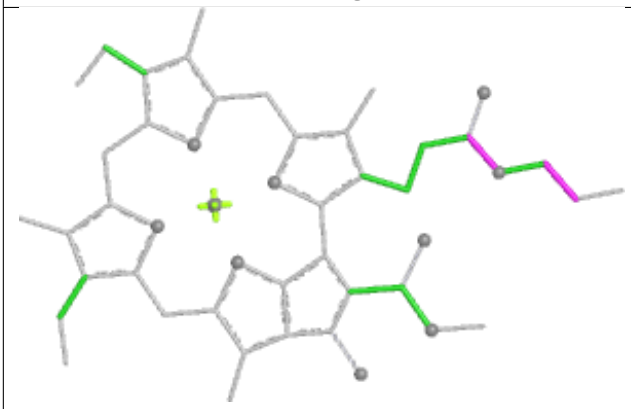
Ligand CLA g 614



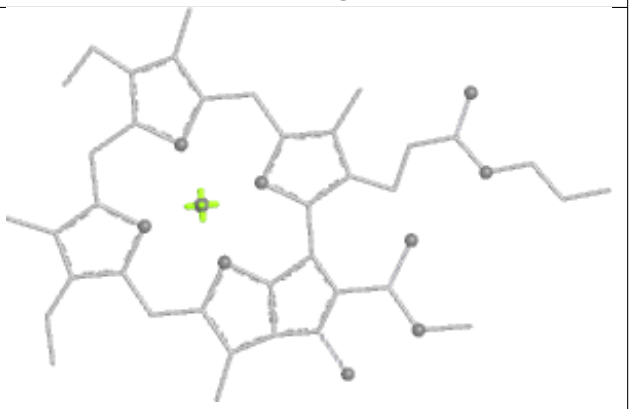
Bond lengths



Bond angles

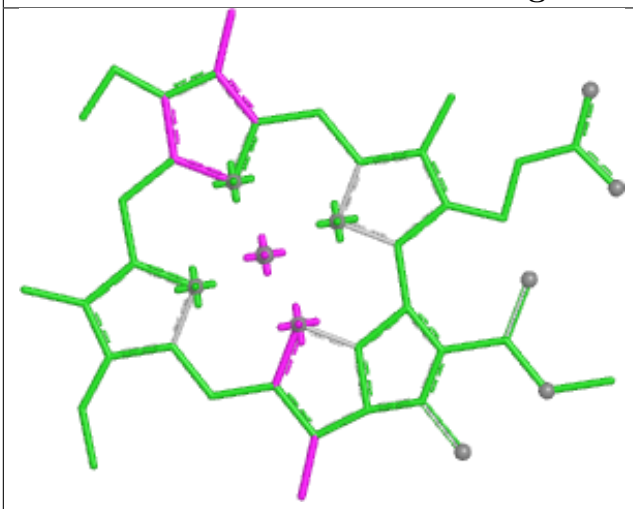


Torsions

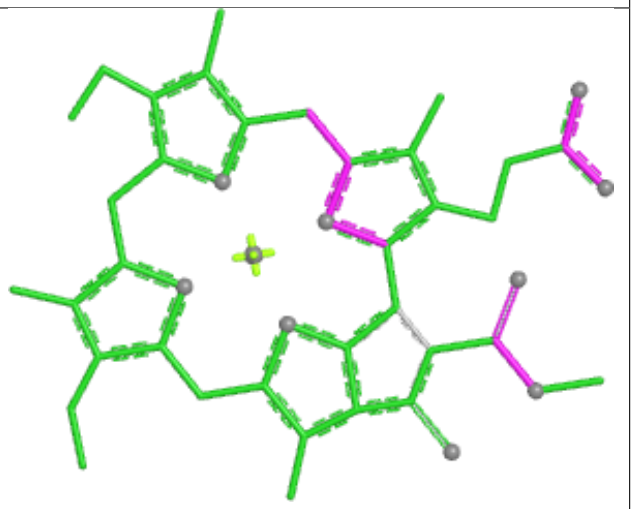


Rings

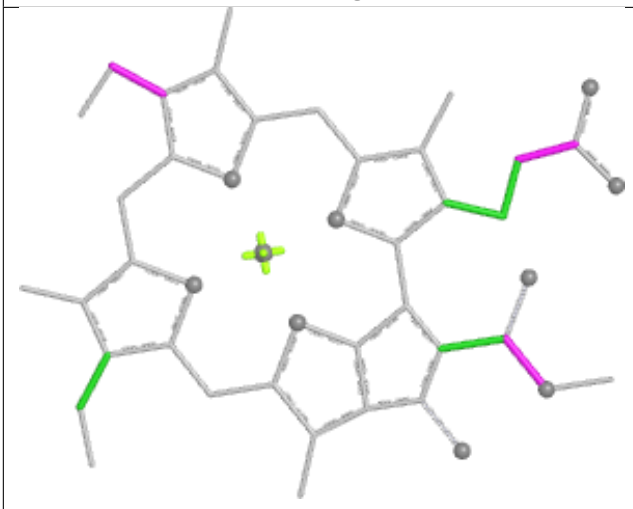
Ligand CLA 8 611



Bond lengths



Bond angles

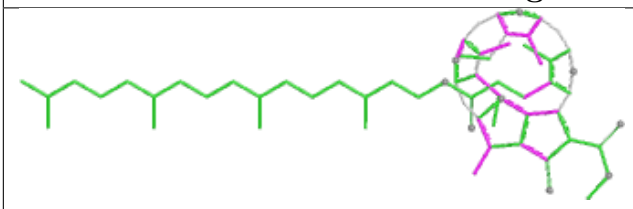


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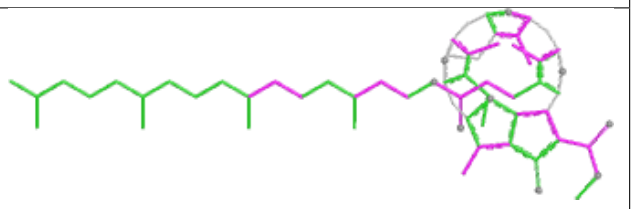


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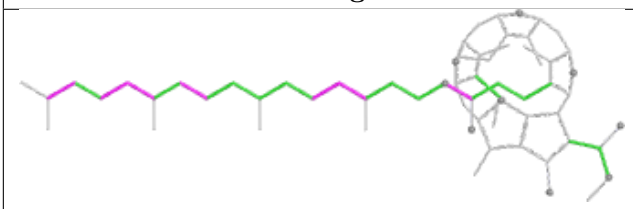
Ligand PHO a 408



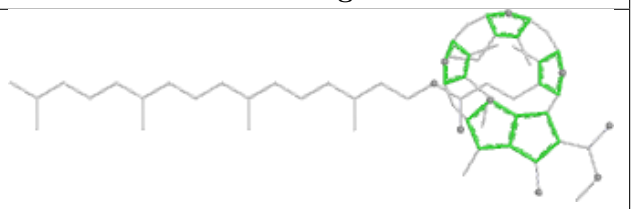
Bond lengths



Bond angles

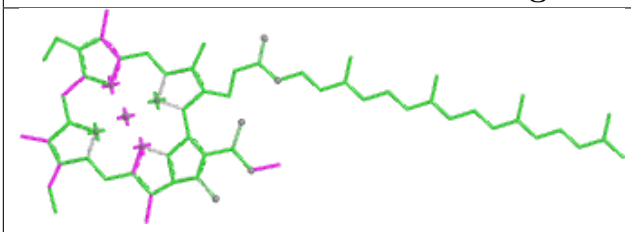


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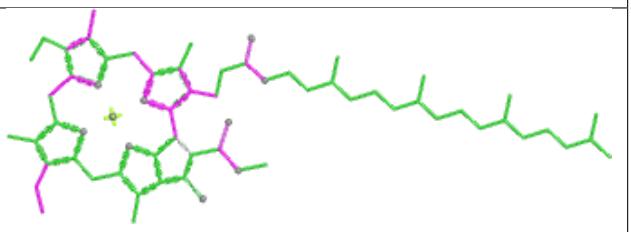


Rings

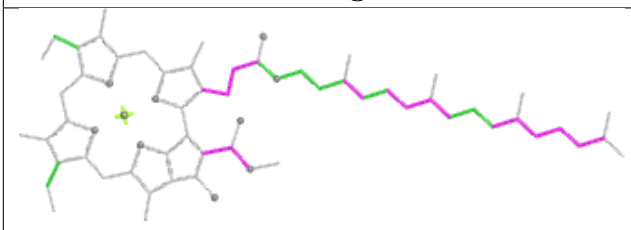
Ligand CLA c 507



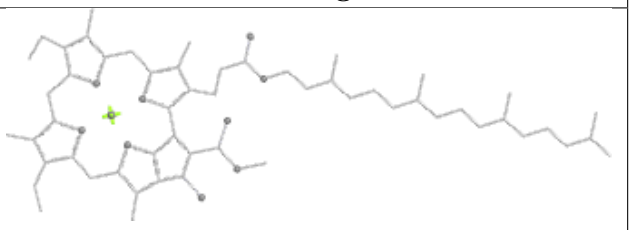
Bond lengths



Bond angles

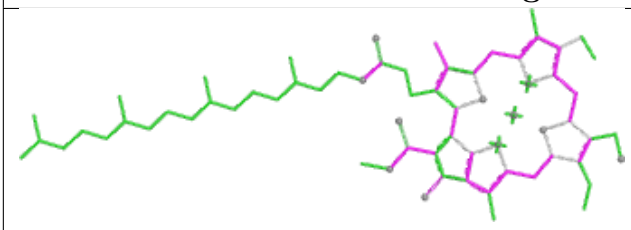


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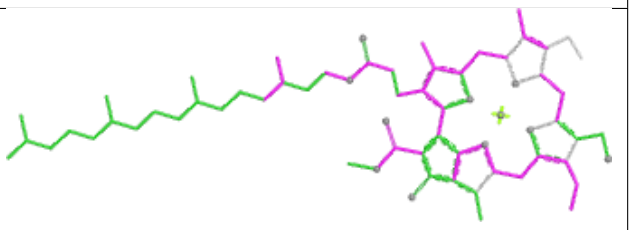


Rings

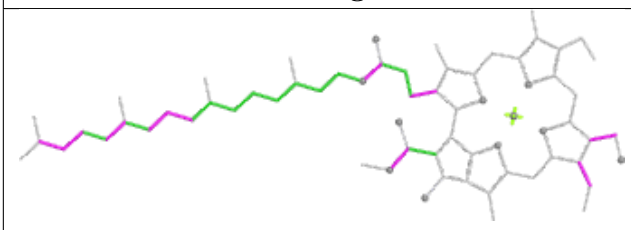
Ligand CHL N 609



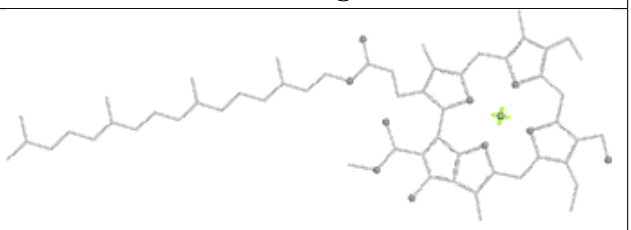
Bond lengths



Bond angles

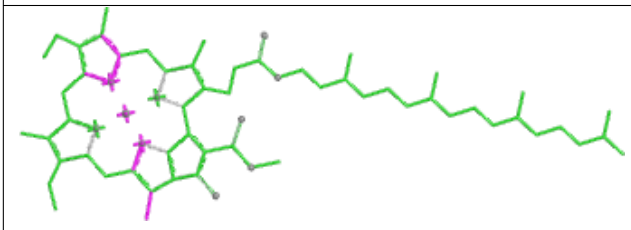


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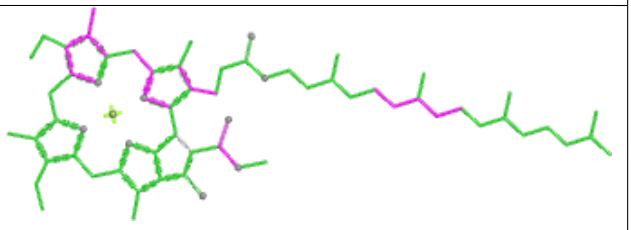


Rings

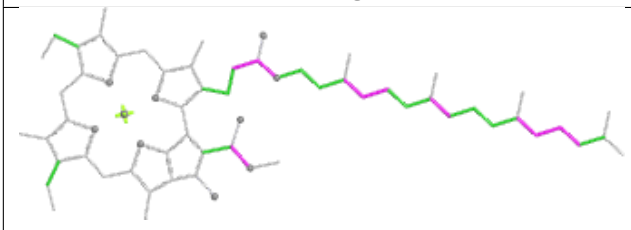
Ligand CLA C 510



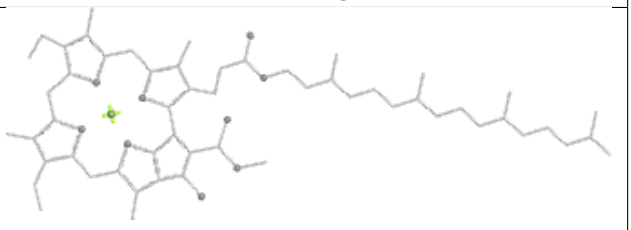
Bond lengths



Bond angles

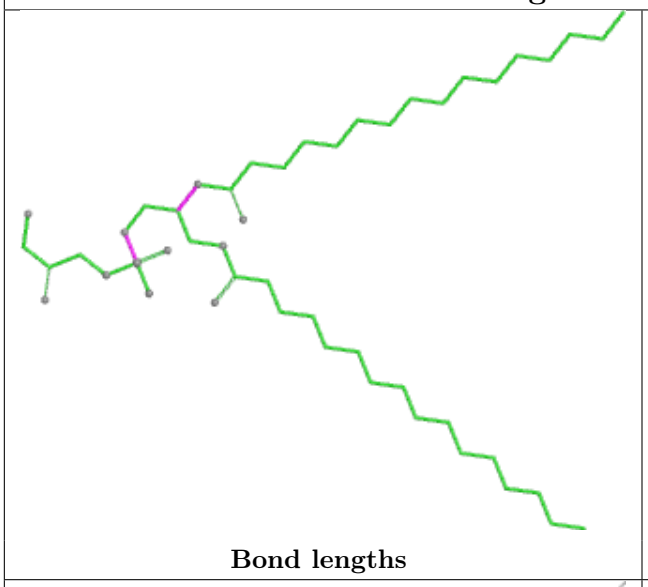


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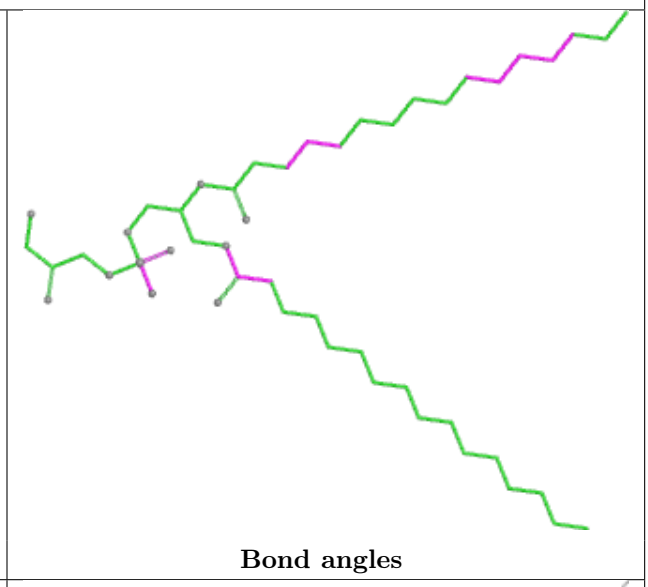


Rings

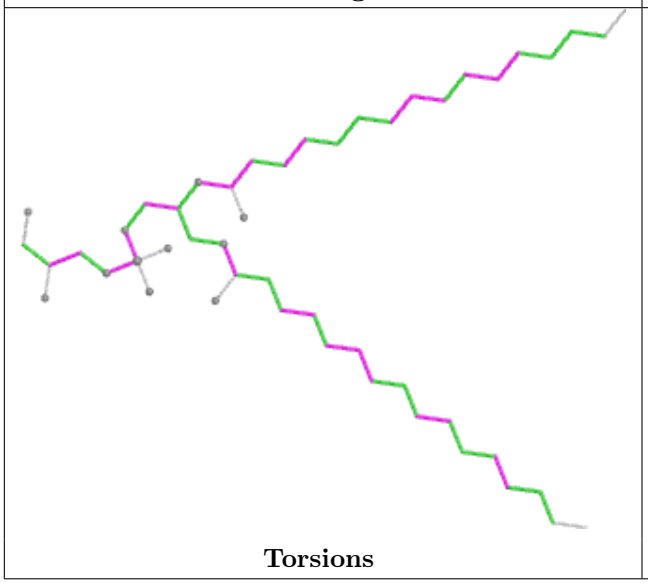
Ligand LHG c 523



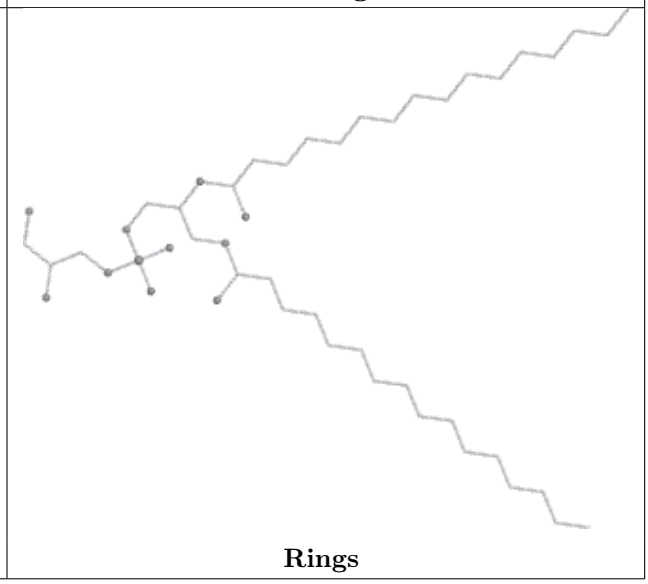
Bond lengths



Bond angles

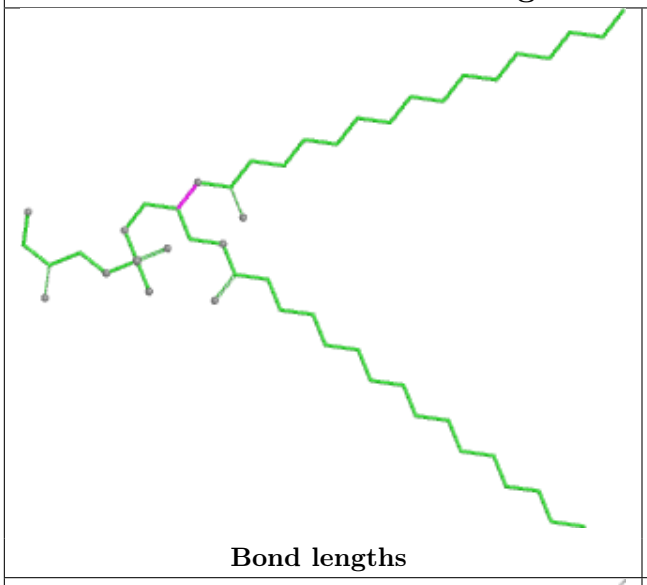


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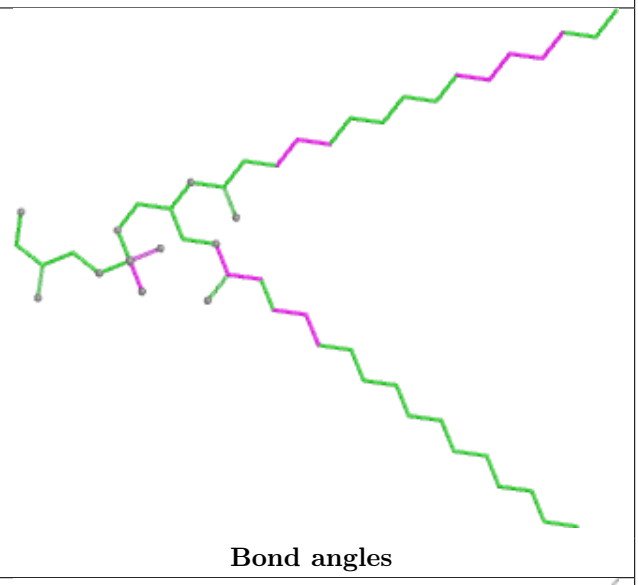


Rings

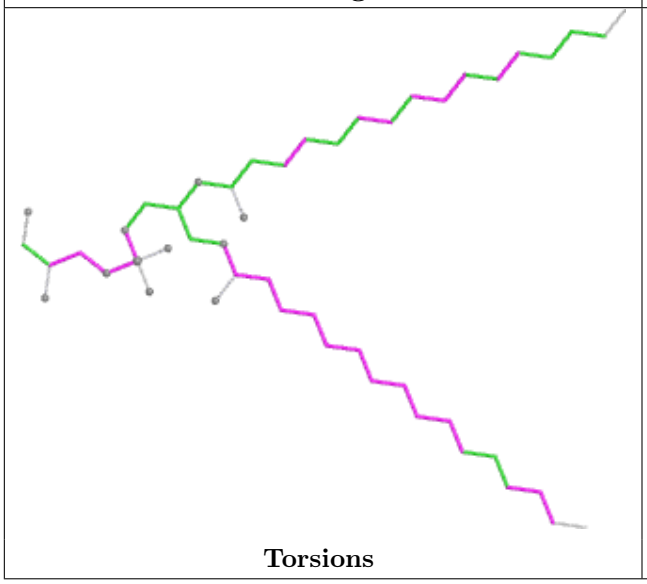
Ligand LHG n 2630



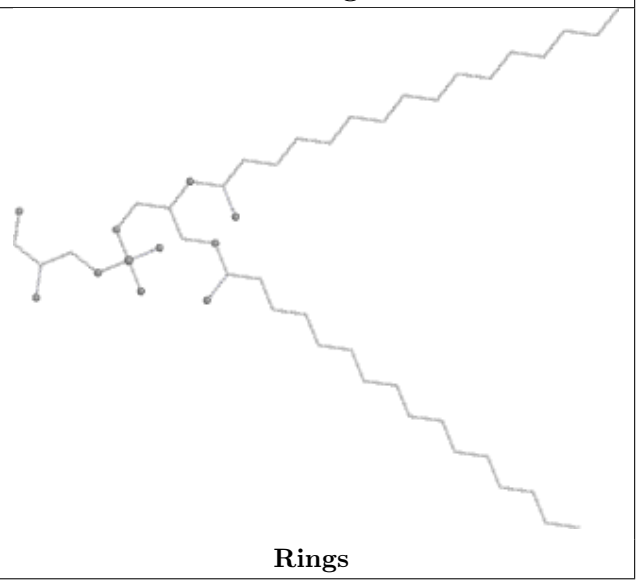
Bond lengths



Bond angles



Torsions

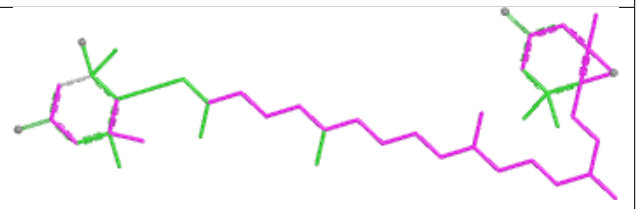


Rings

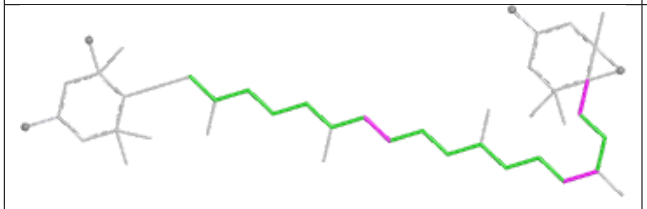
Ligand NEX R 623



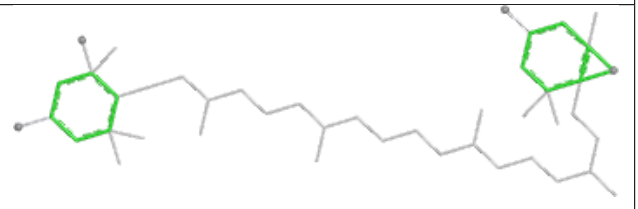
Bond lengths



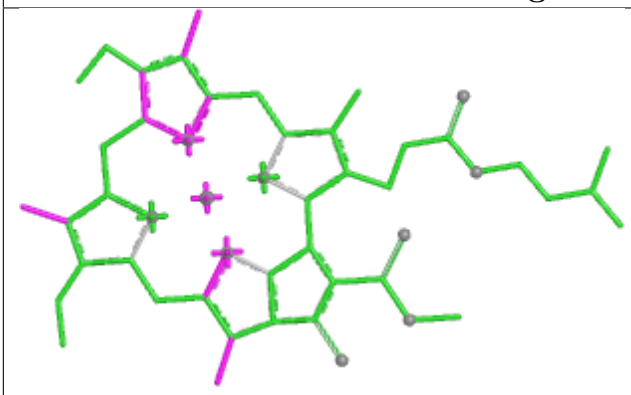
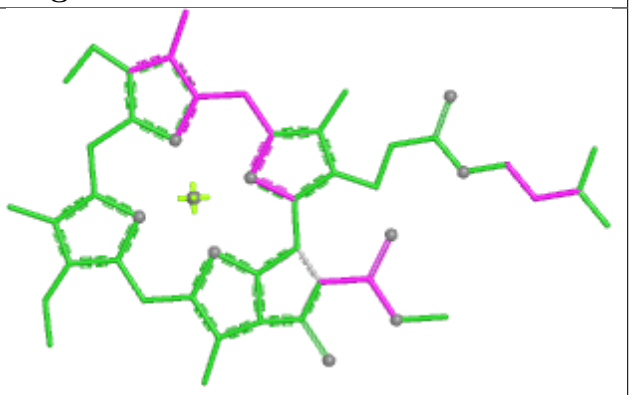
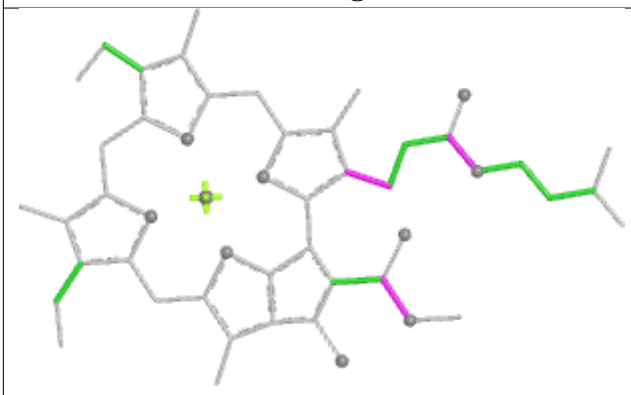
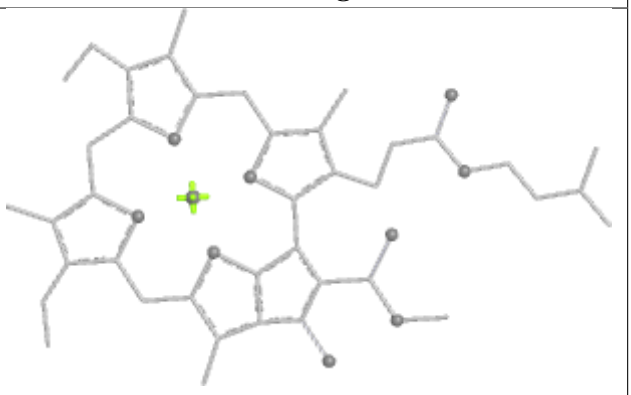
Bond angles

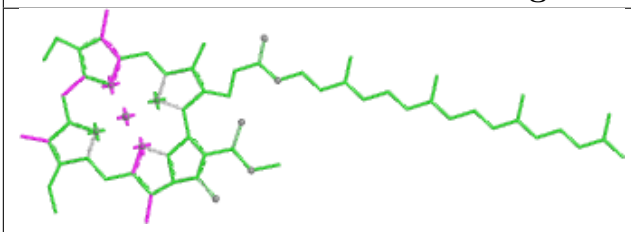
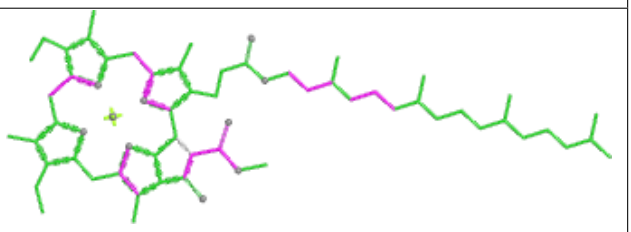
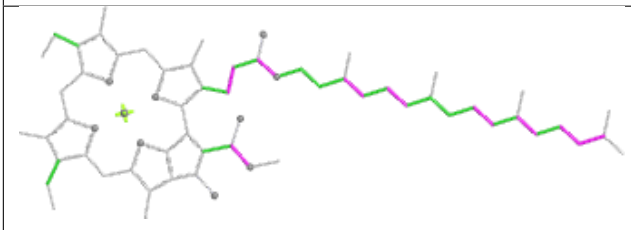
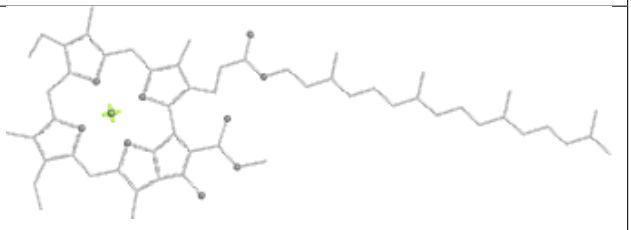


Torsions

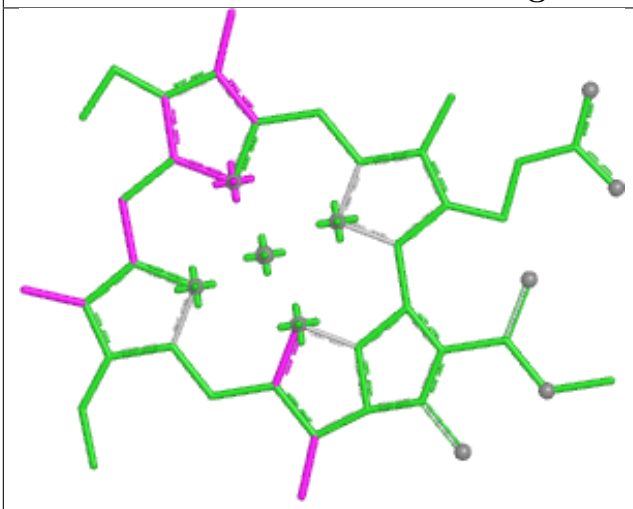


Rings

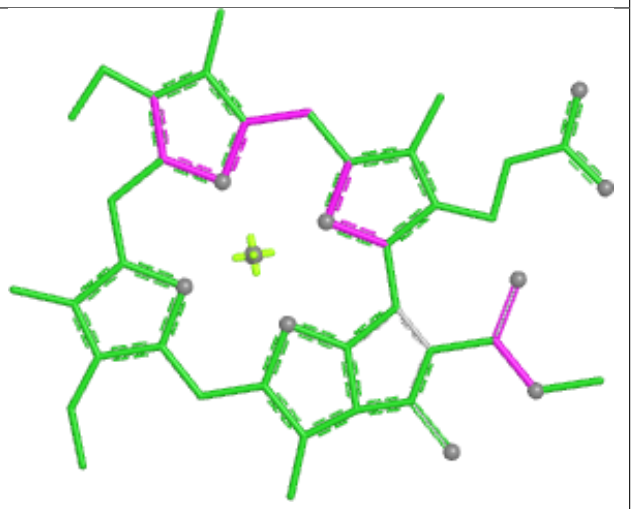
Ligand CLA g 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

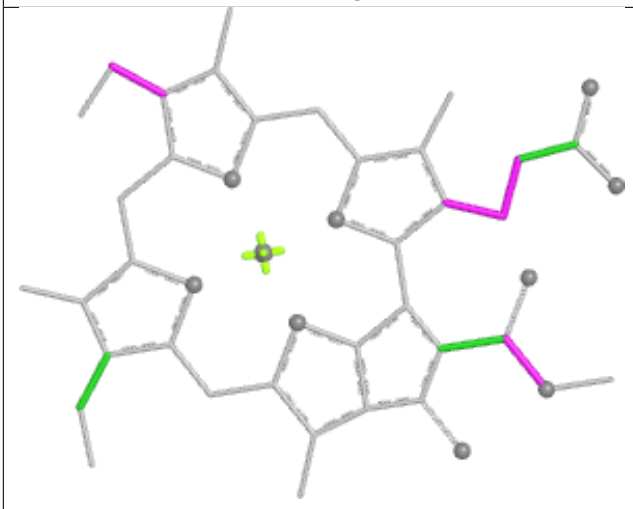
Ligand CLA 4 610



Bond lengths



Bond angles

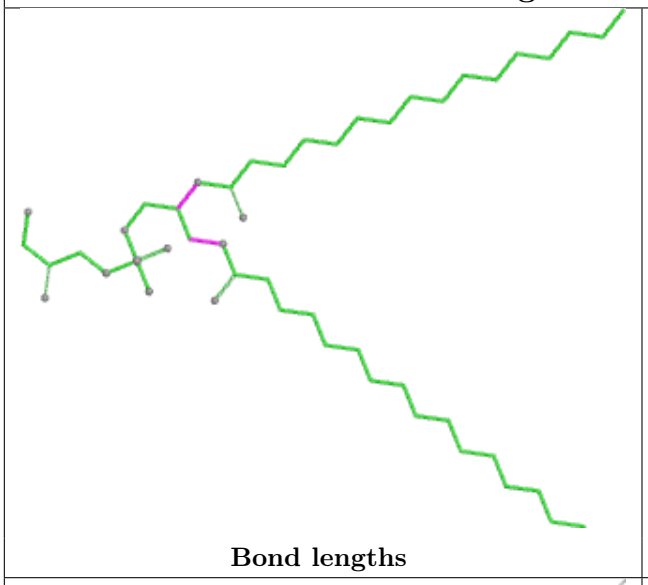


Torsions

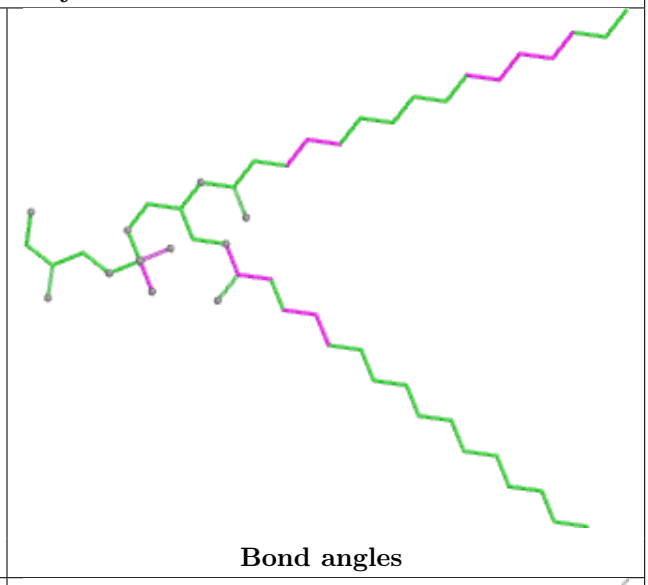


Rings

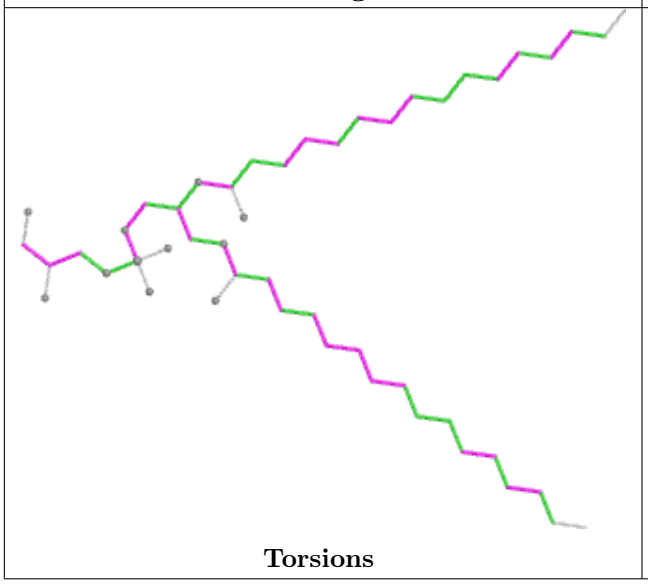
Ligand LHG y 2630



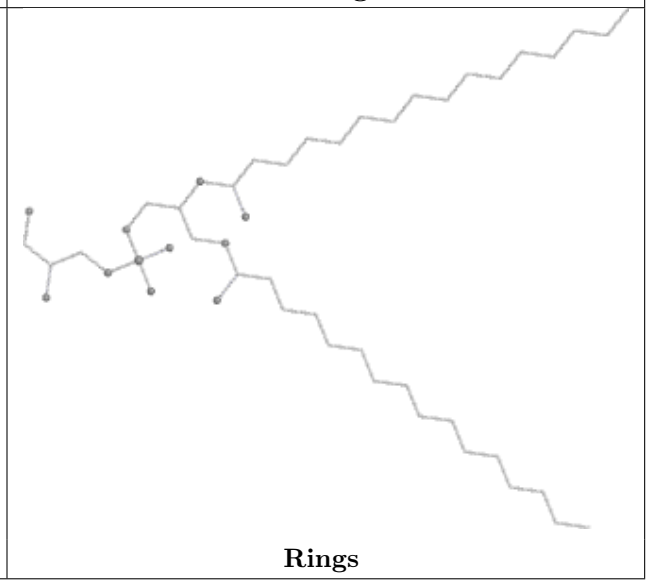
Bond lengths



Bond angles

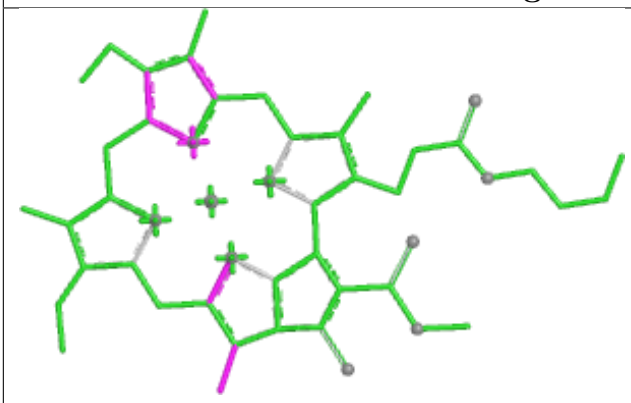


Torsions

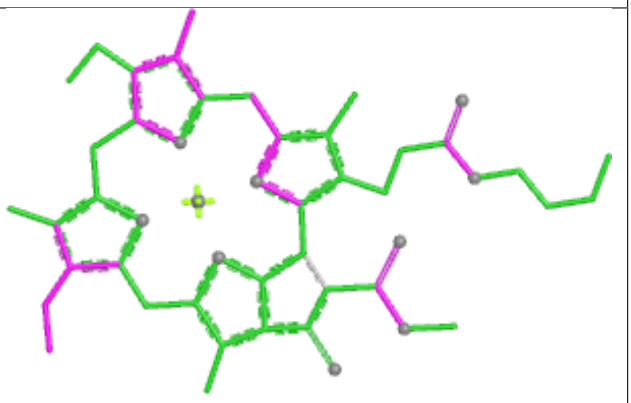


Rings

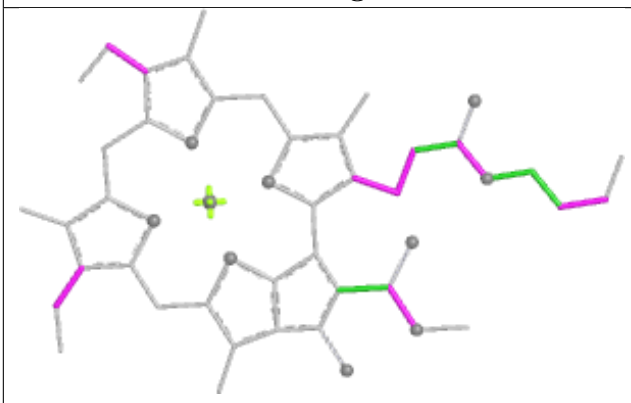
Ligand CLA R 601



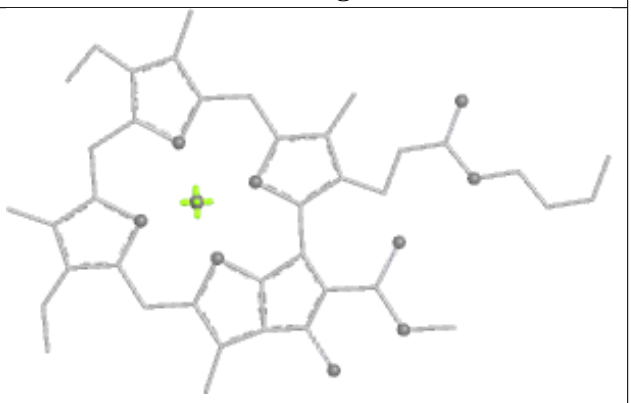
Bond lengths



Bond angles

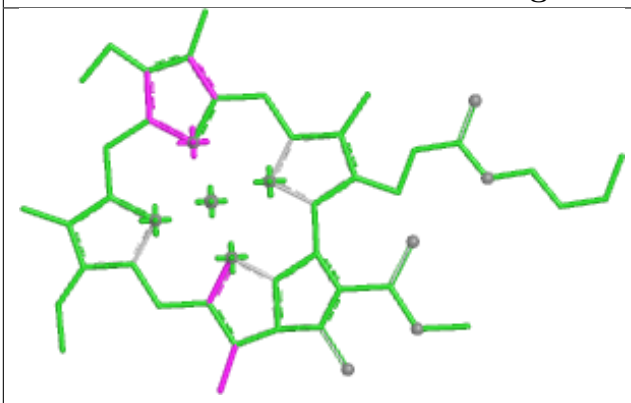


Torsions

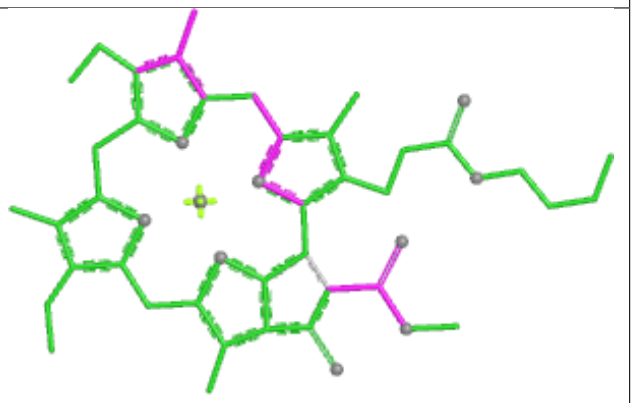


Rings

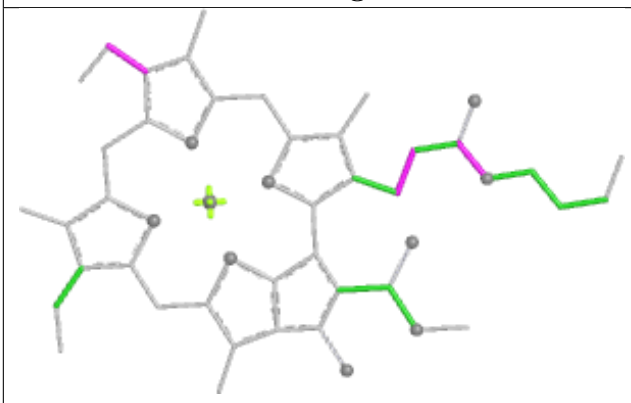
Ligand CLA s 614



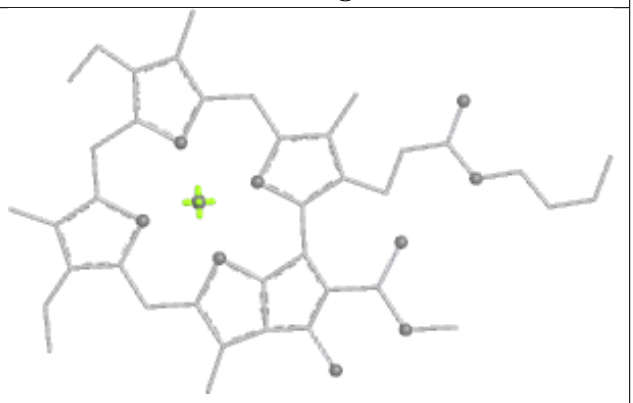
Bond lengths



Bond angles

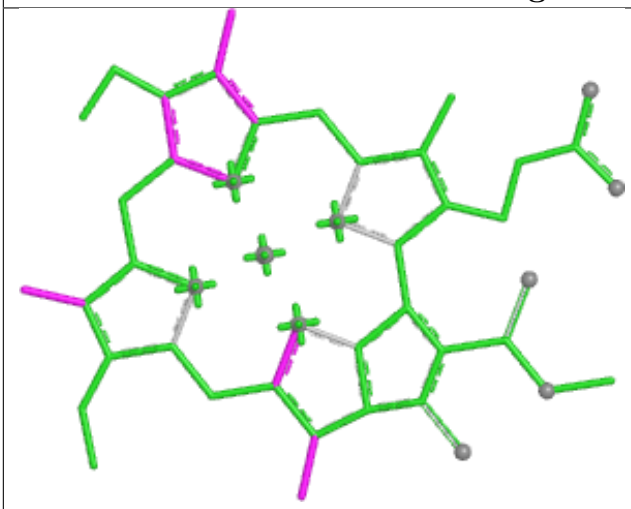


Torsions

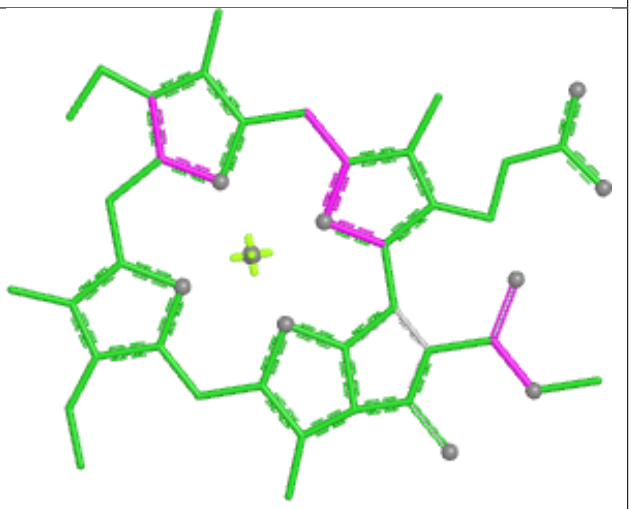


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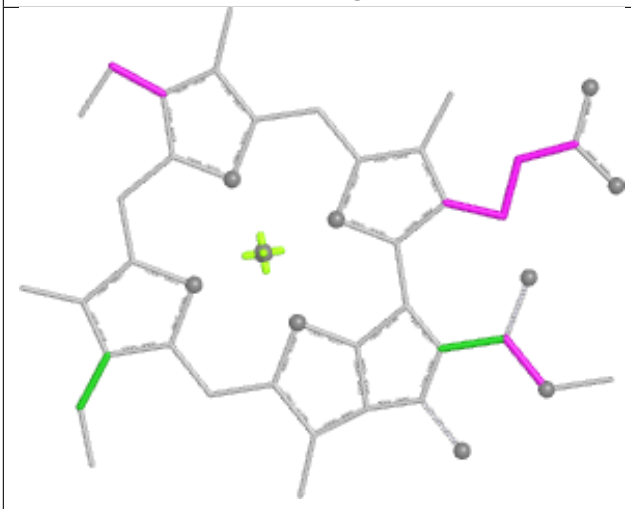
Ligand CLA 4 604



Bond lengths



Bond angles

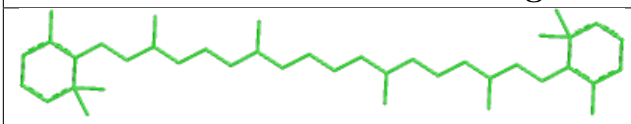


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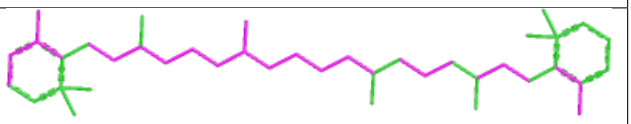


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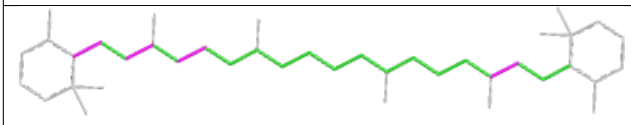
Ligand BCR d 404



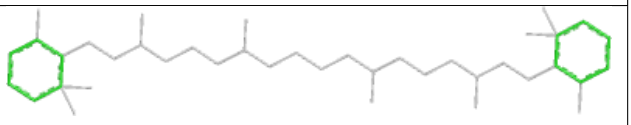
Bond lengths



Bond angles

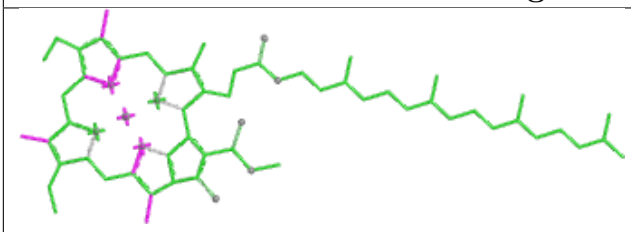


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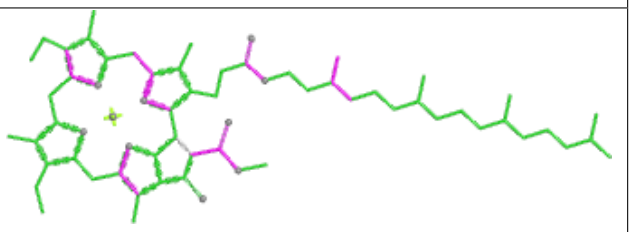


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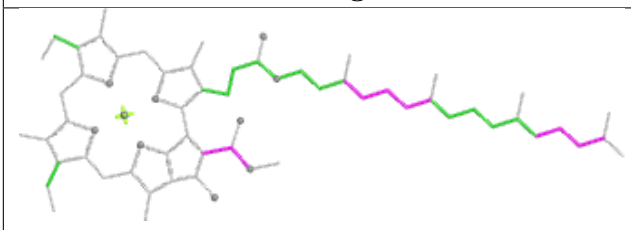
Ligand CLA b 615



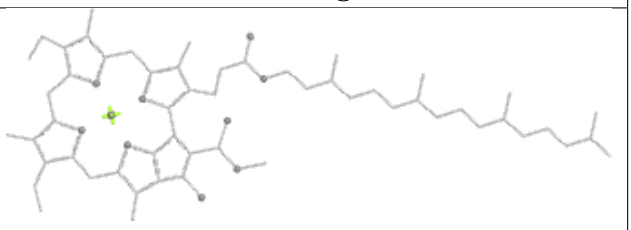
Bond lengths



Bond angles

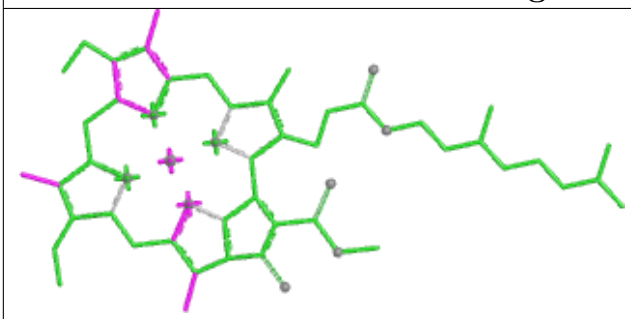


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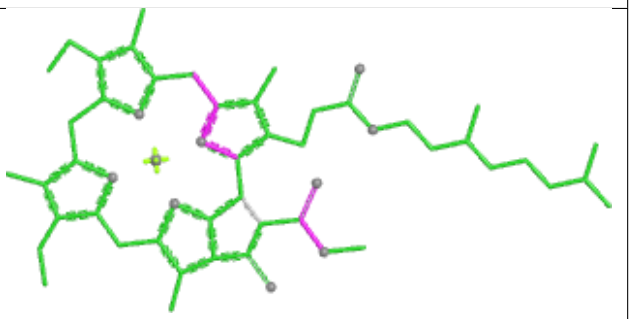


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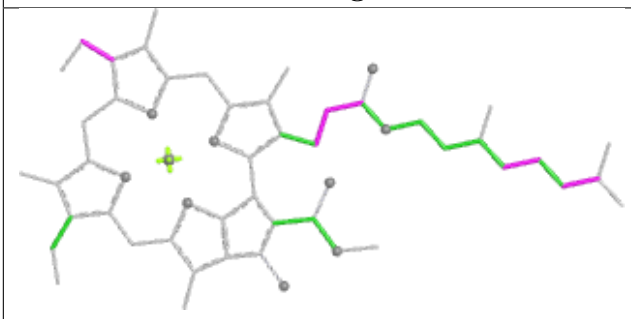
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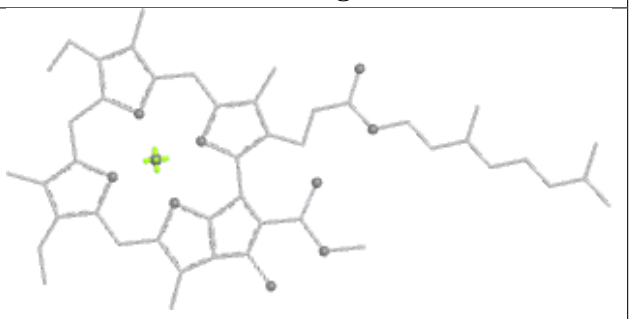
Bond lengths



Bond angles

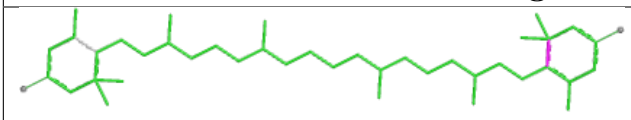


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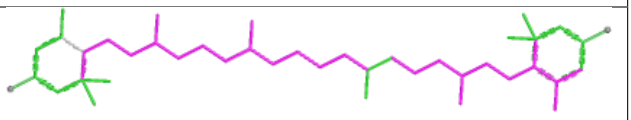


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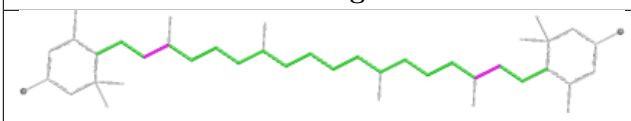
Ligand LUT 4 620



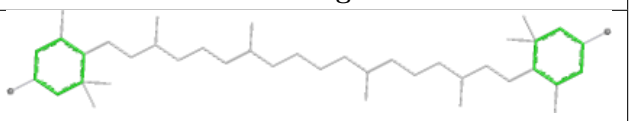
Bond lengths



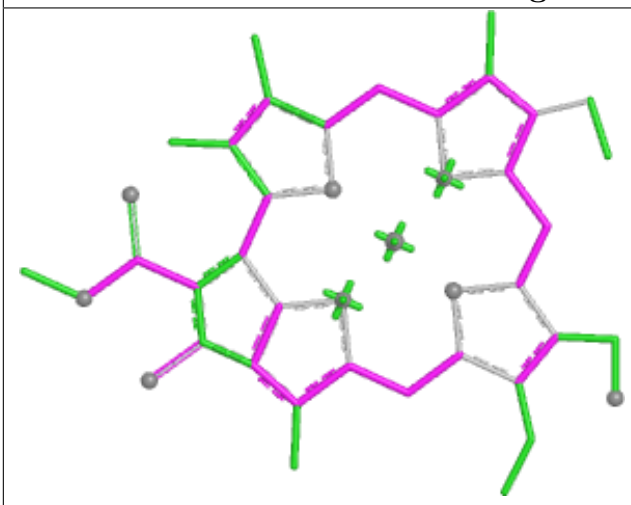
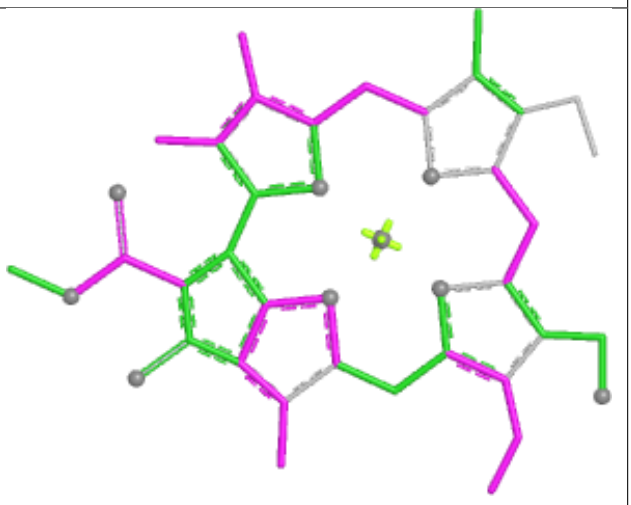
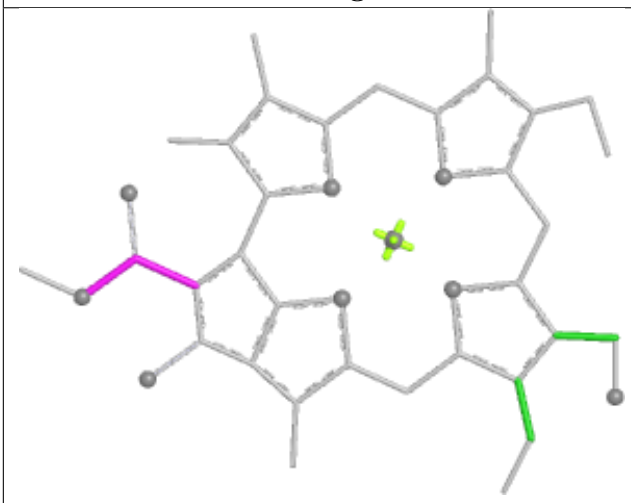
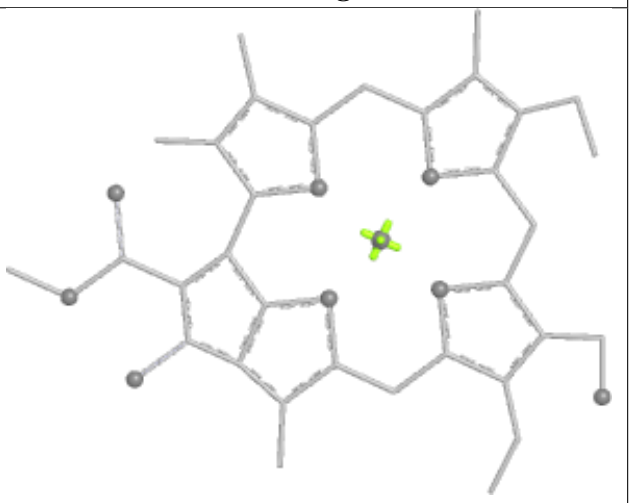
Bond angles



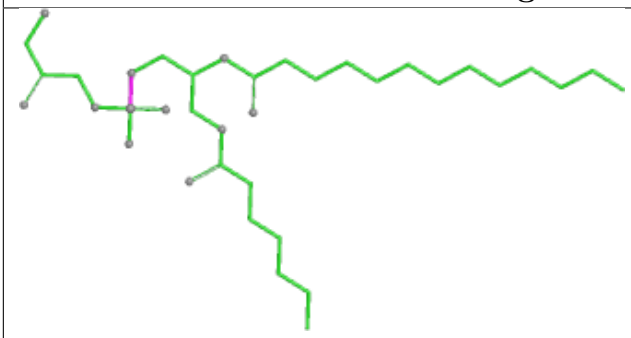
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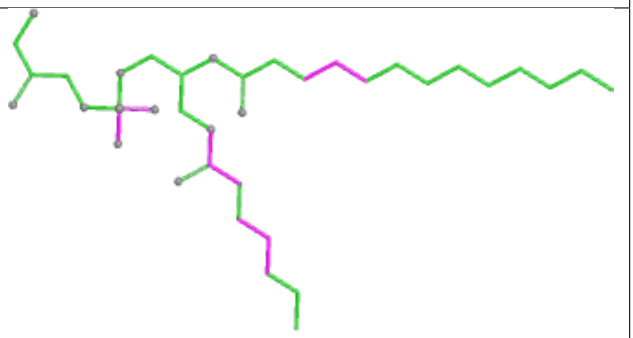
Rings

Ligand CHL r 614	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

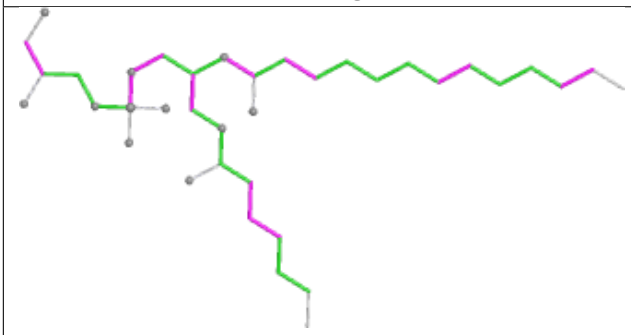
Ligand LHG 2 2630



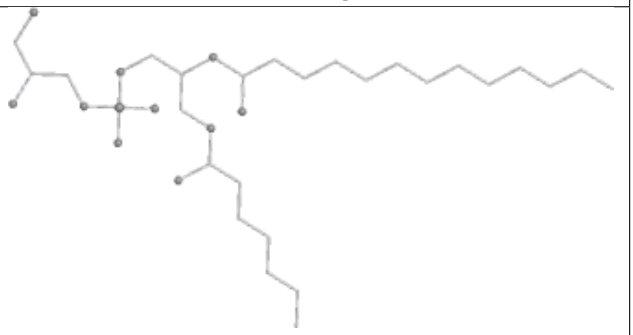
Bond lengths



Bond angles

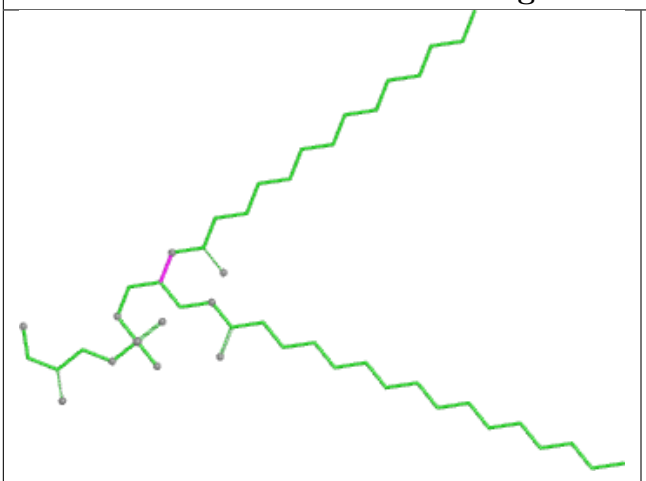


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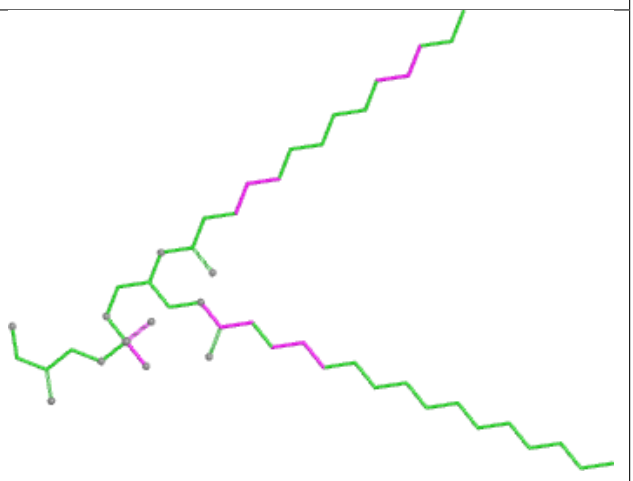


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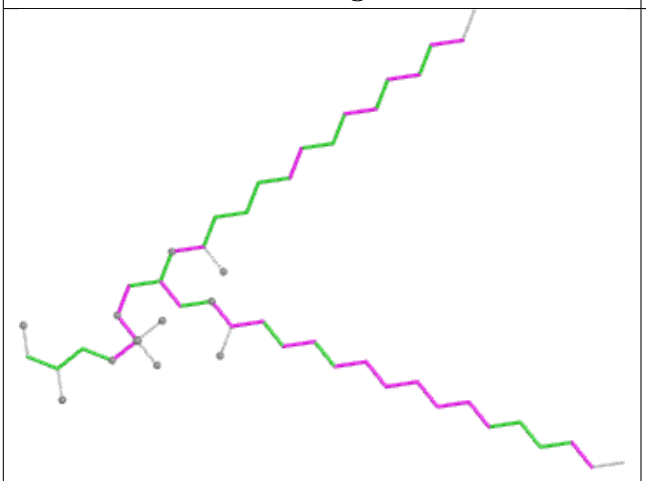
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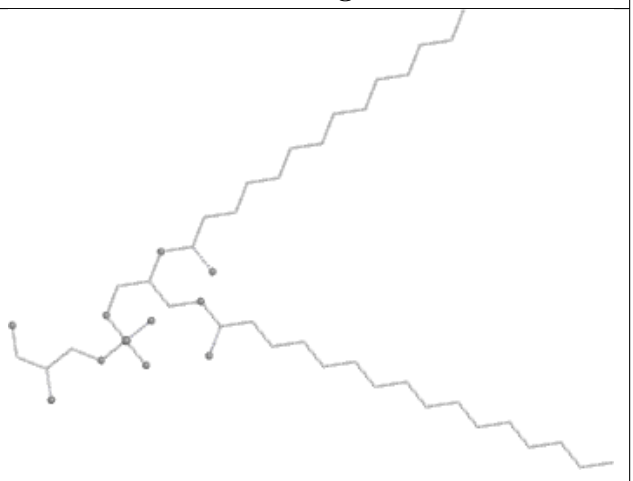
Bond lengths



Bond angles

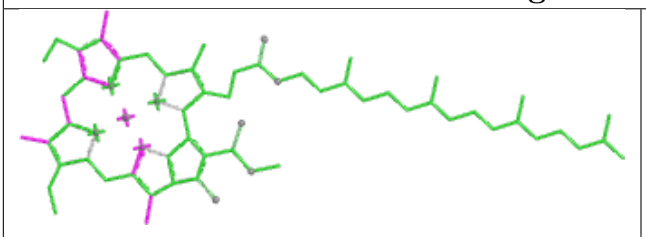


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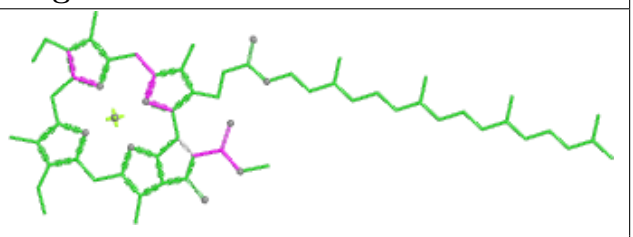


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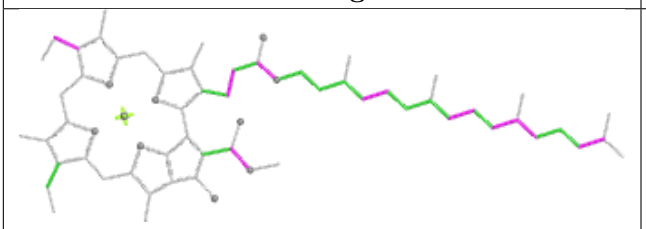
Ligand CLA g 613



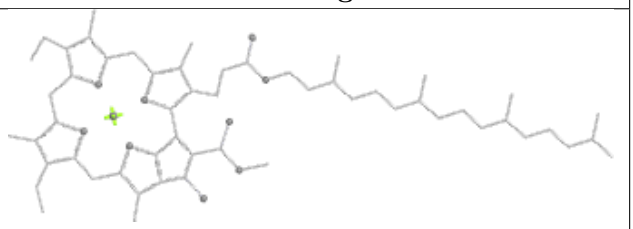
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Bond angles

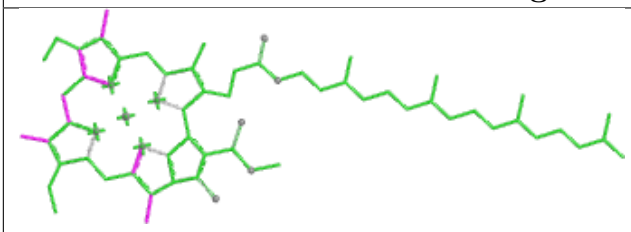


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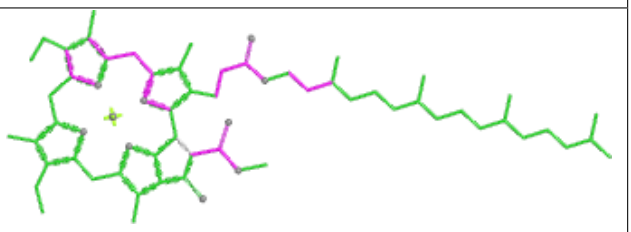


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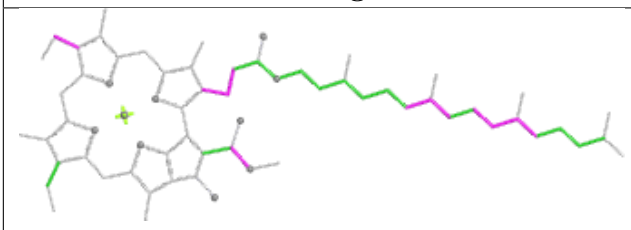
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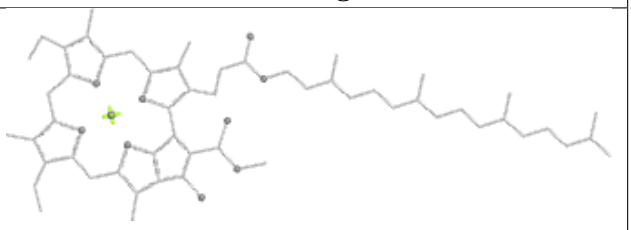
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Bond angles

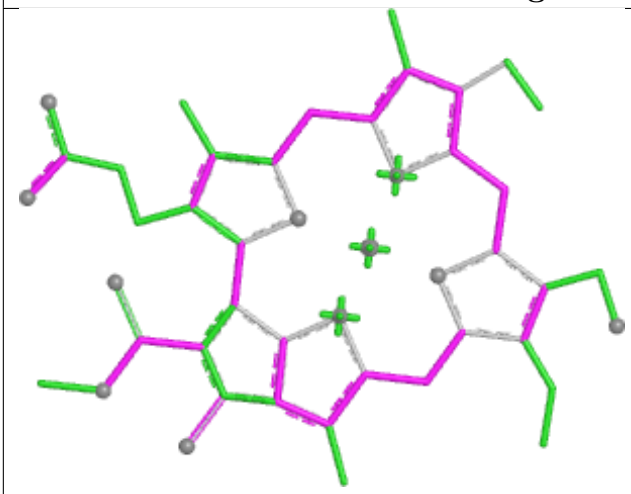


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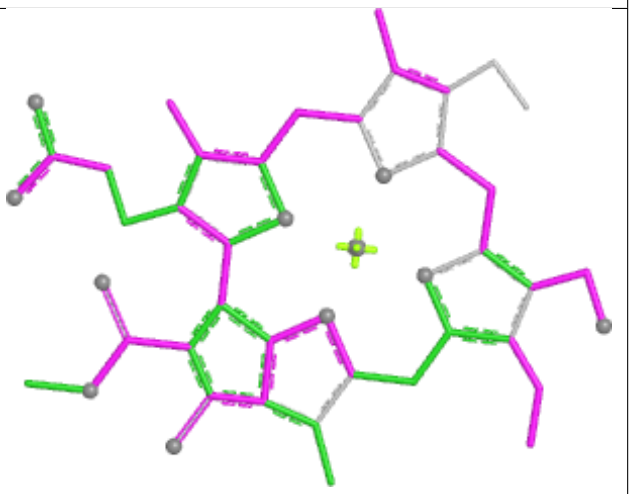


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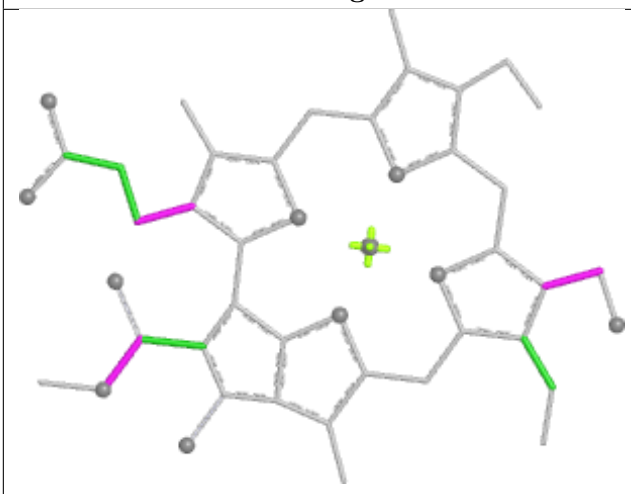
Ligand CHL 4 608



Bond lengths



Bond angles

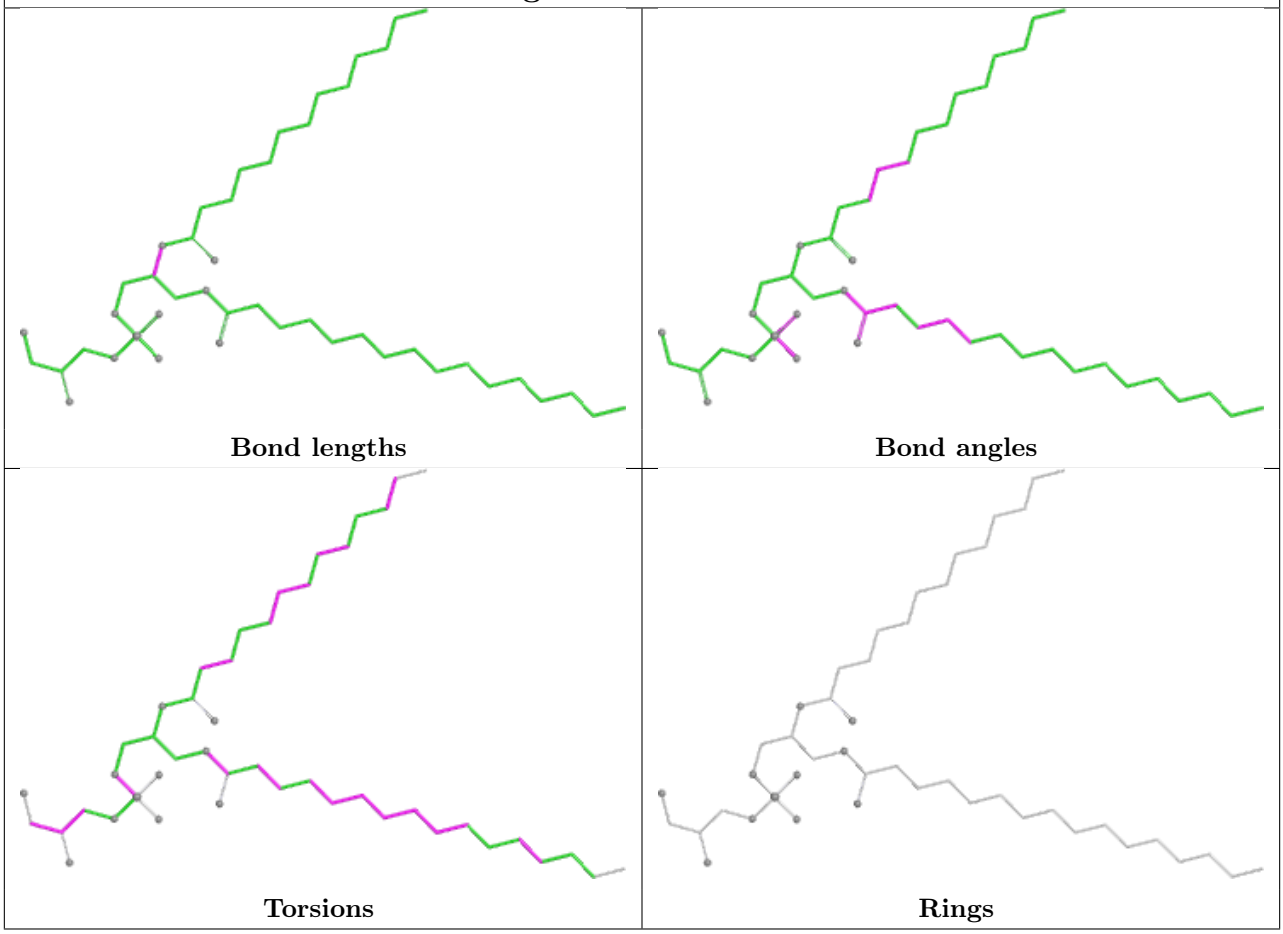


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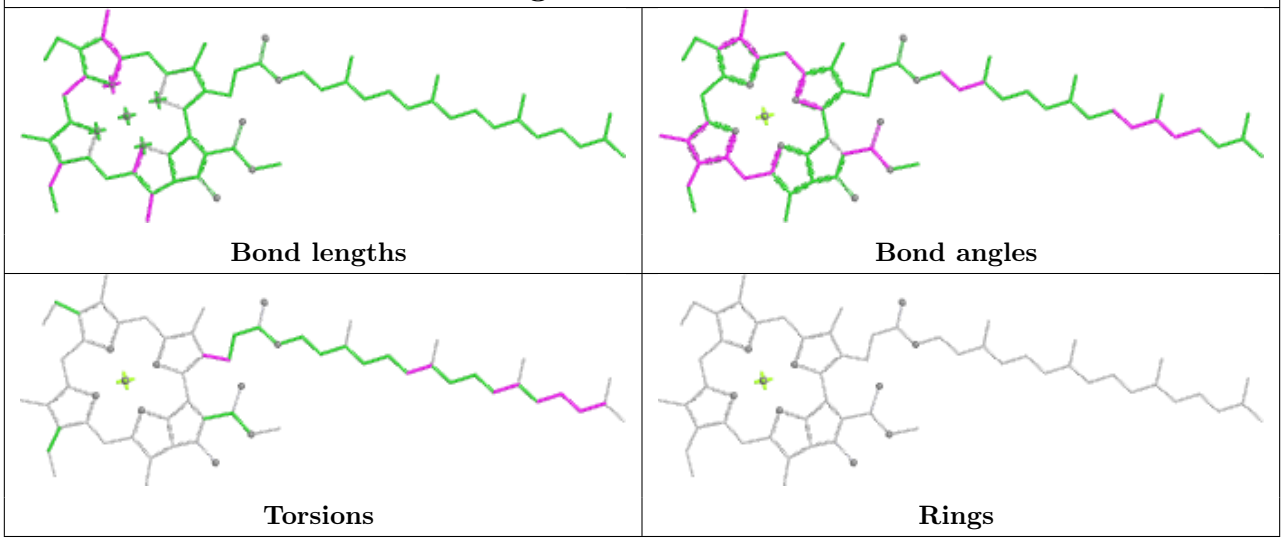


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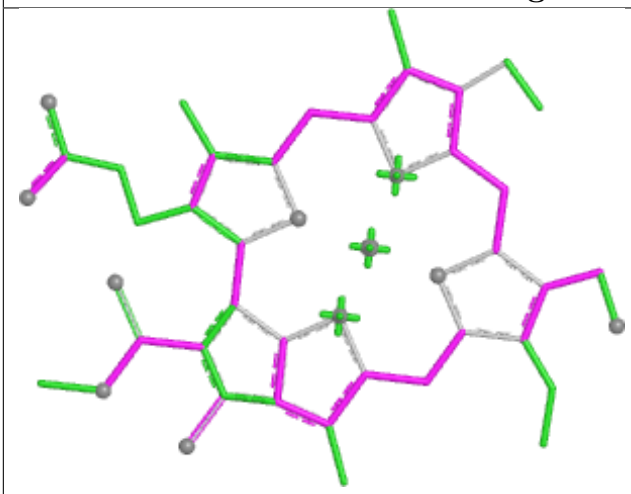
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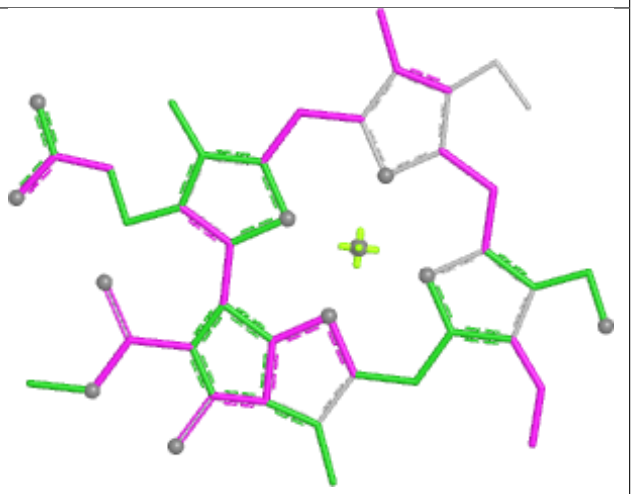
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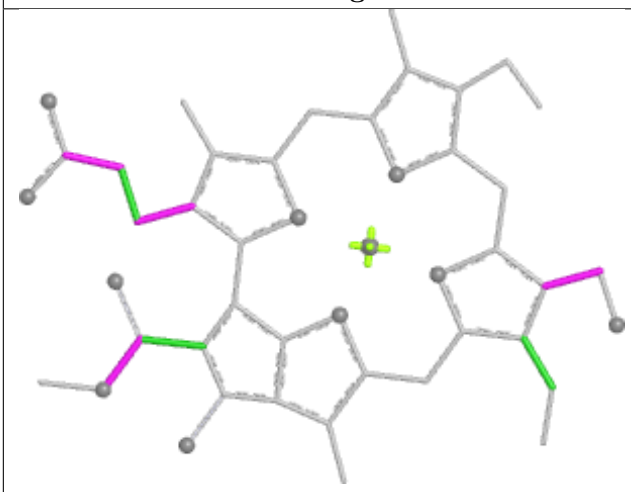
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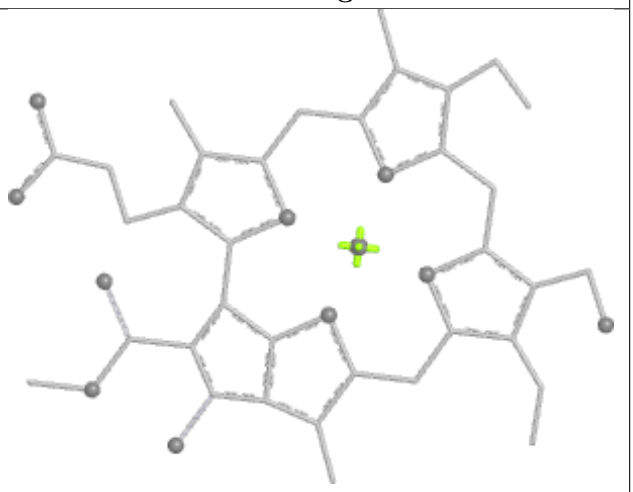
Bond lengths



Bond angles

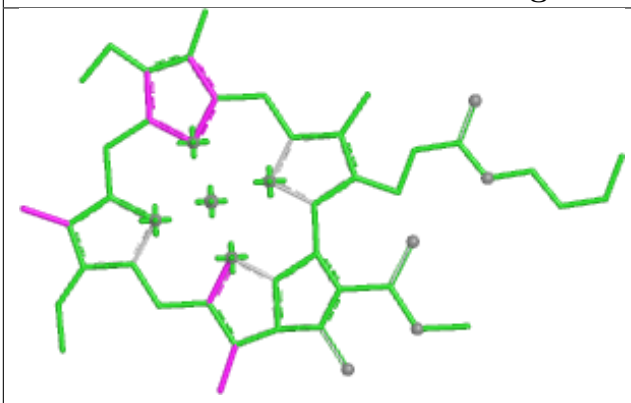


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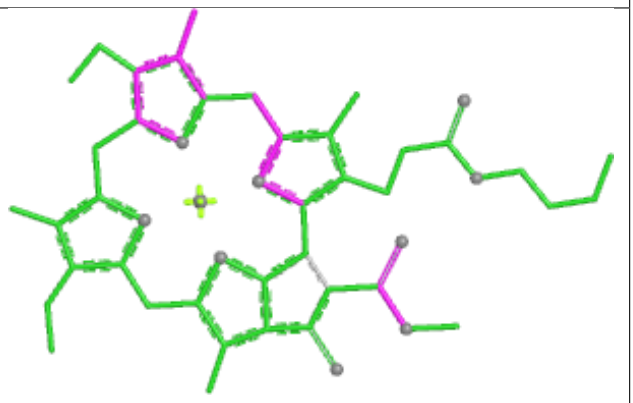


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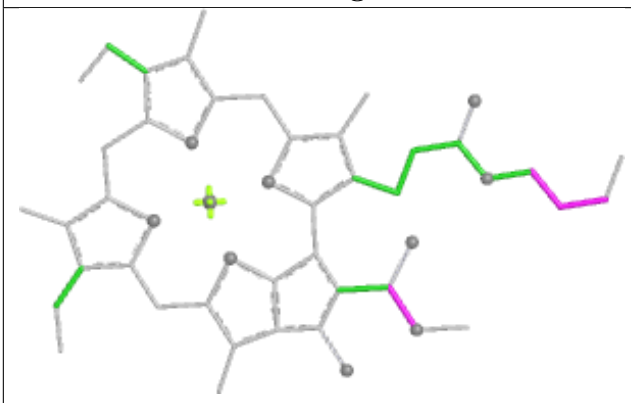
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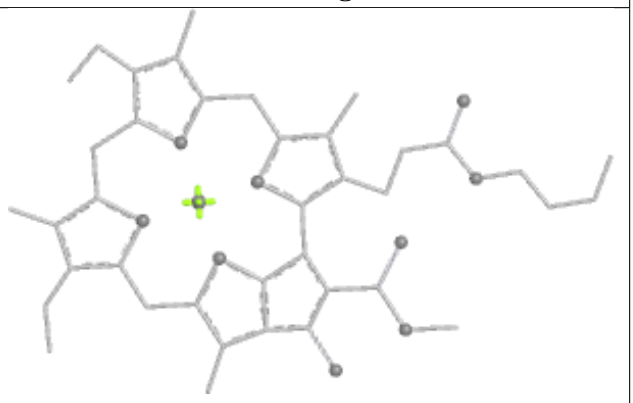
Bond lengths



Bond angles

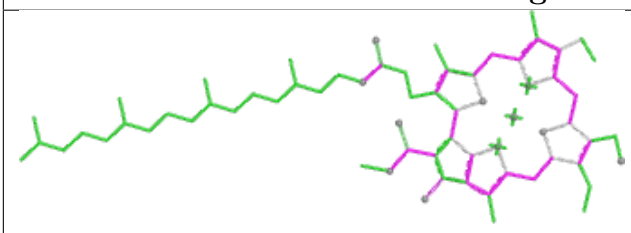


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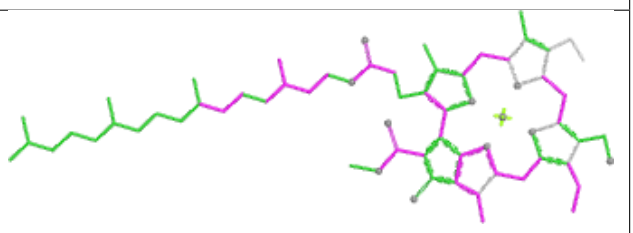


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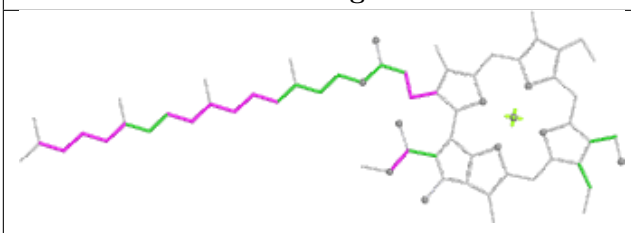
Ligand CHL r 606



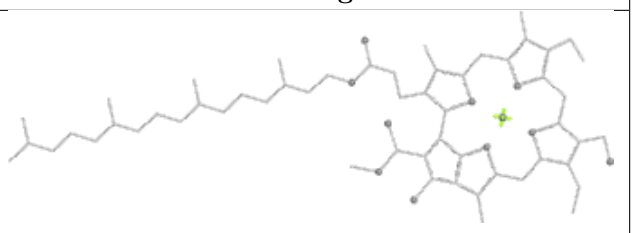
Bond lengths



Bond angles

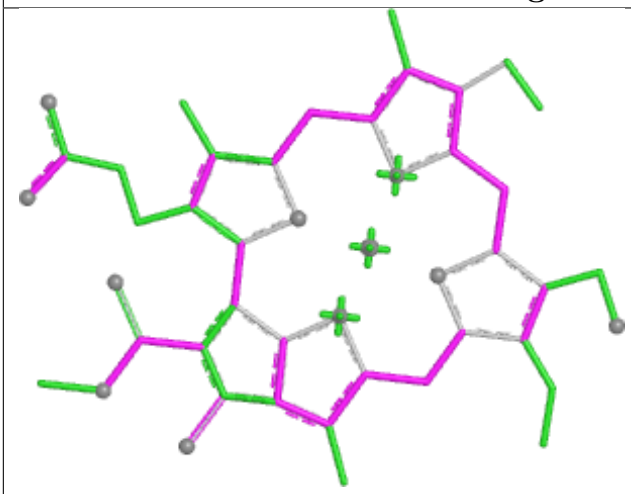


Torsions

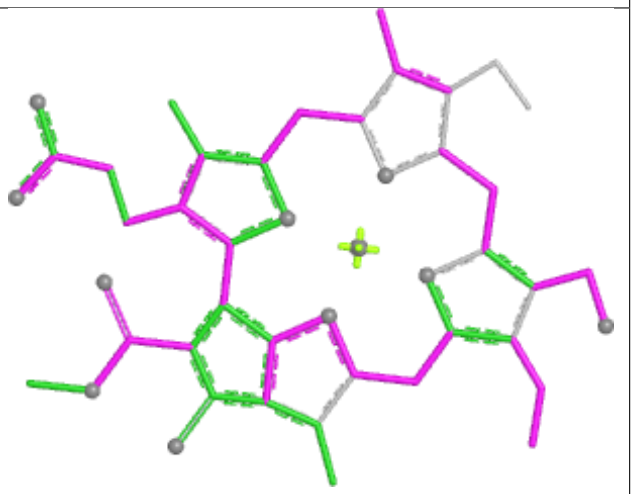


Rings

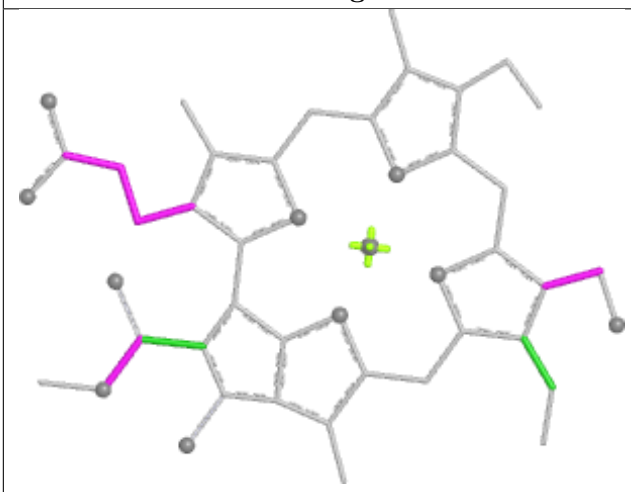
Ligand CHL 3 605



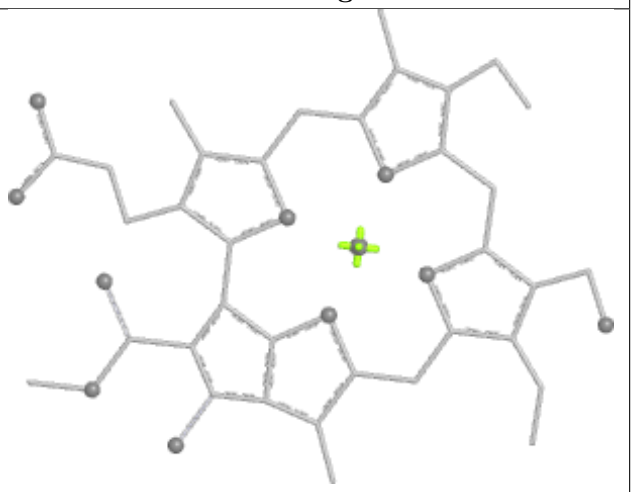
Bond lengths



Bond angles

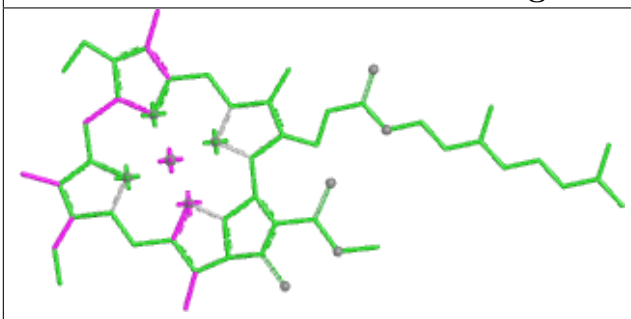


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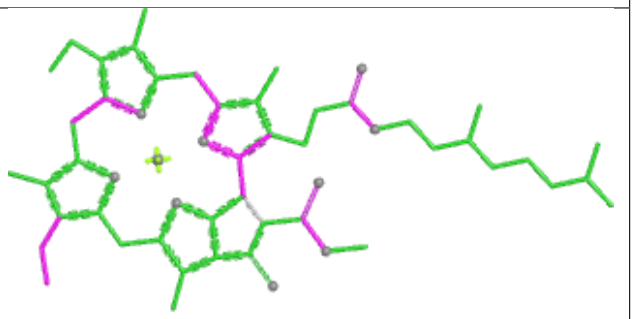


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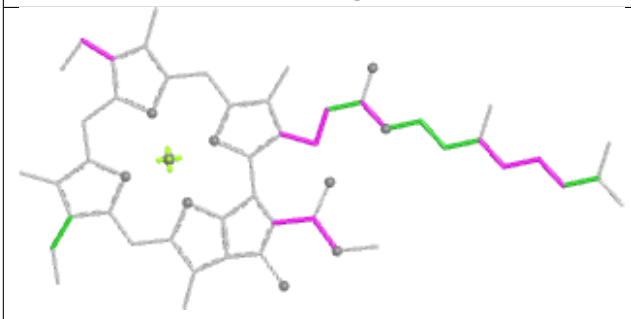
Ligand CLA 3 603



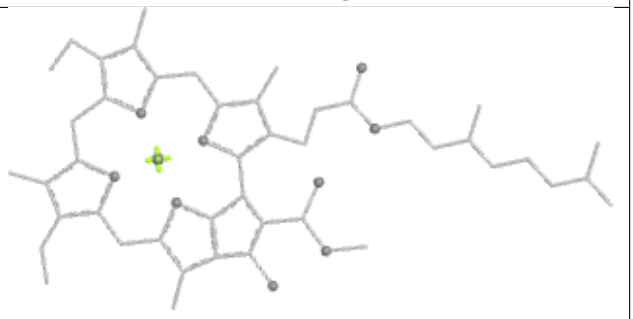
Bond lengths



Bond angles

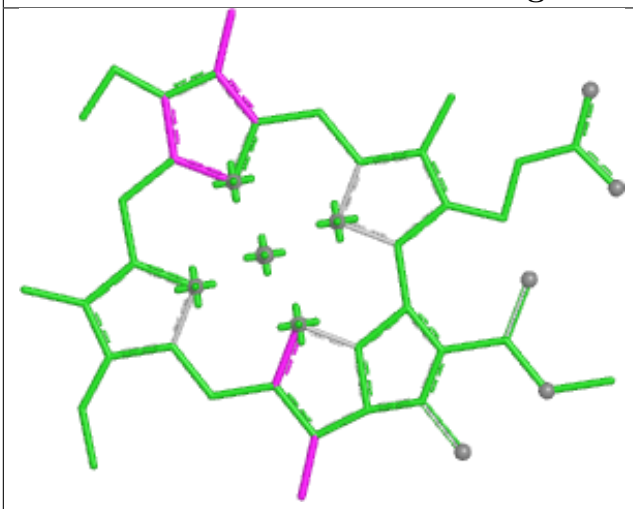


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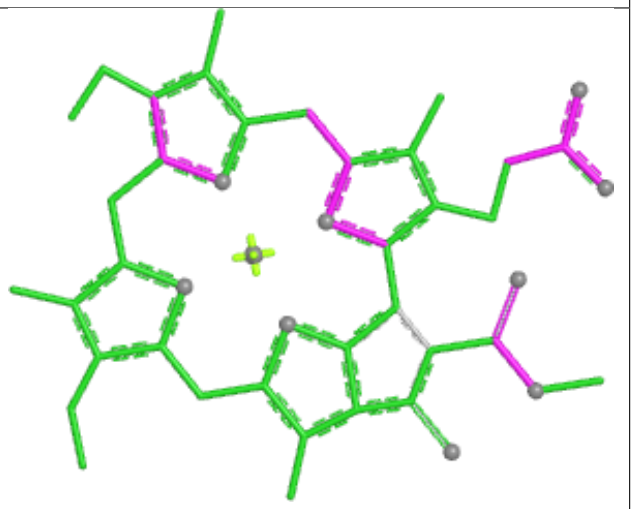


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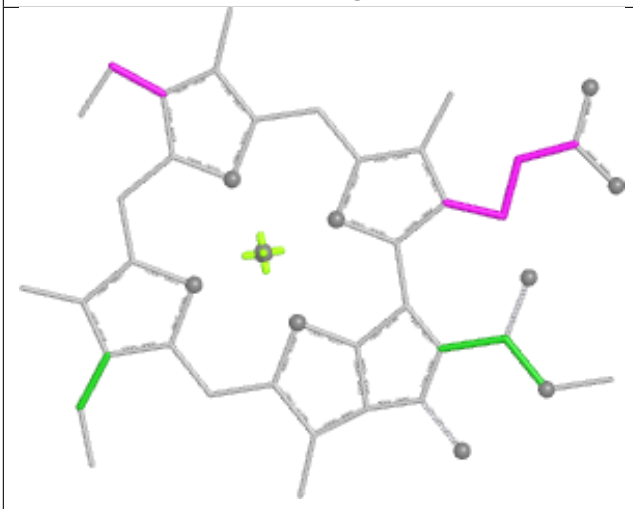
Ligand CLA S 609



Bond lengths



Bond angles

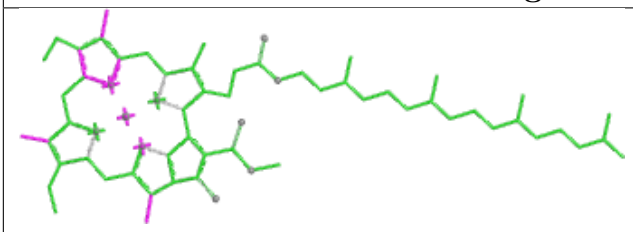


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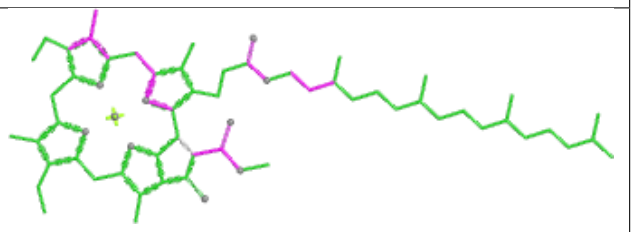


Rings

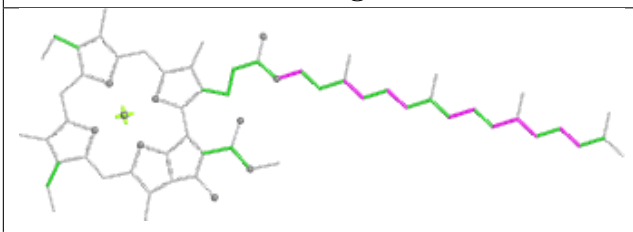
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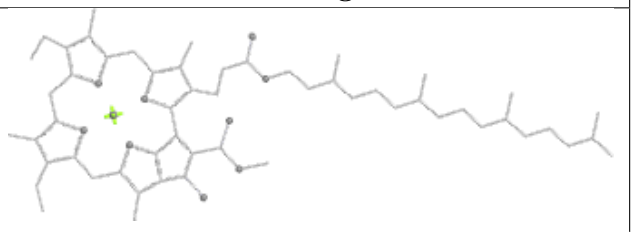
Bond lengths



Bond angles

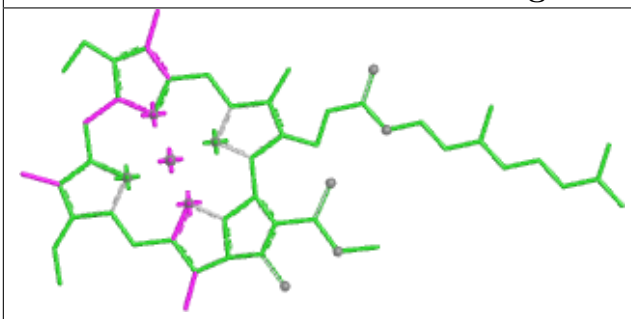


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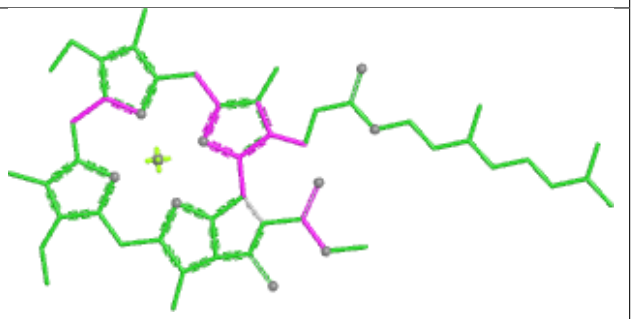


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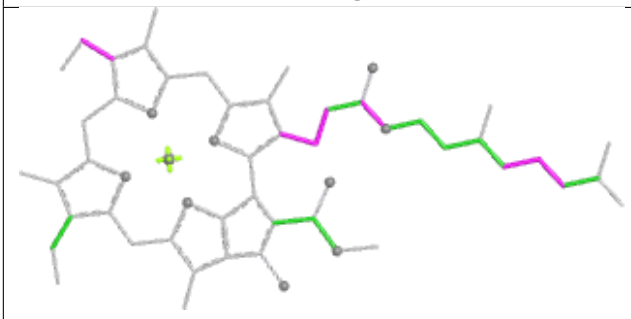
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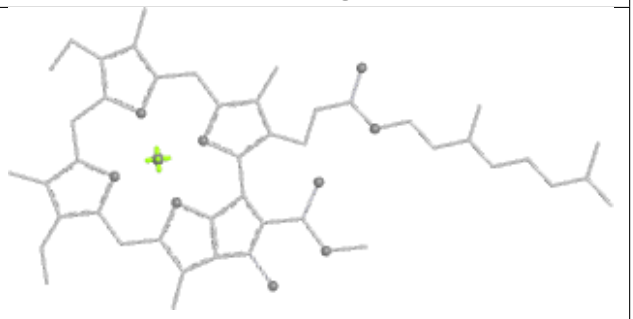
Bond lengths



Bond angles

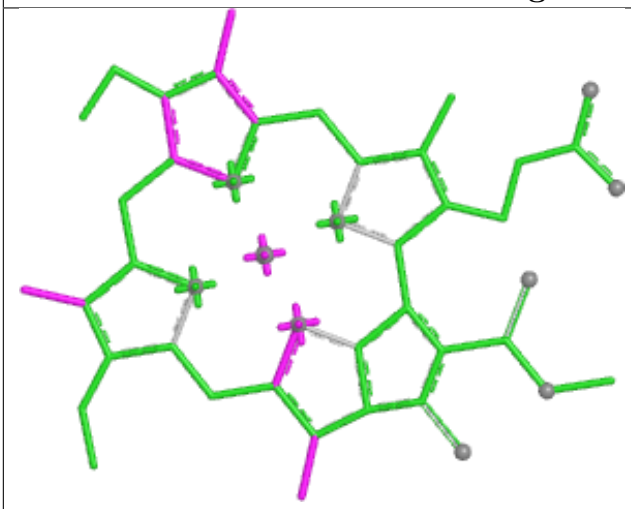


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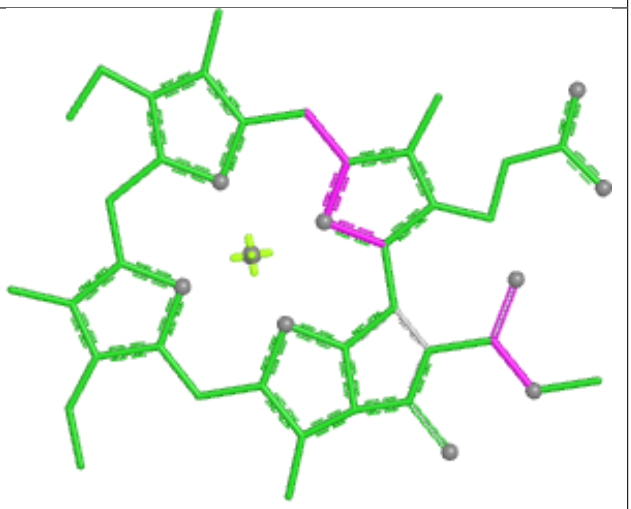


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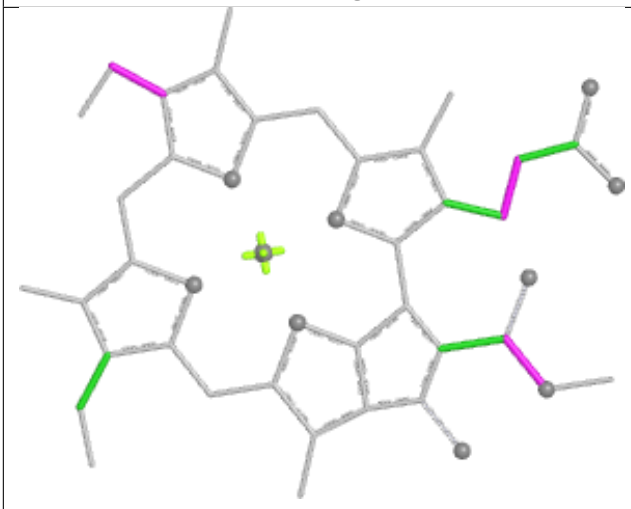
Ligand CLA 2 613



Bond lengths



Bond angles

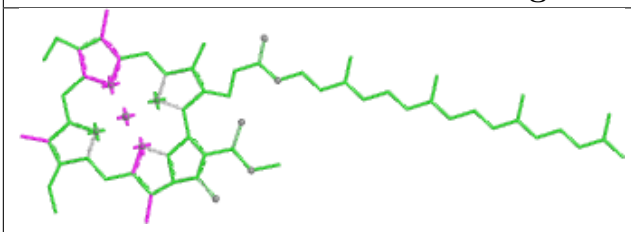


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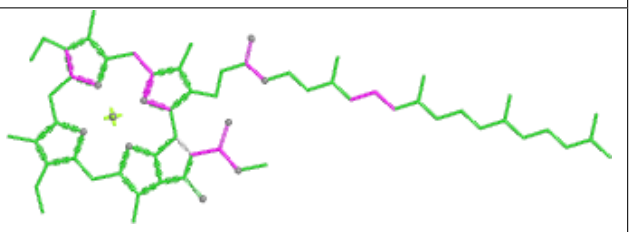


Rings

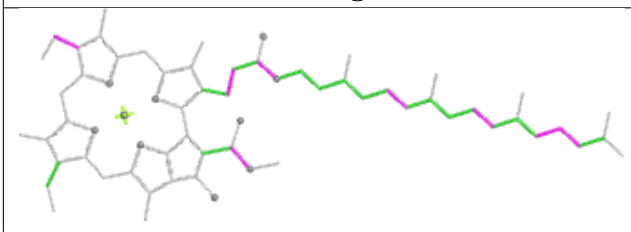
Ligand CLA c 503



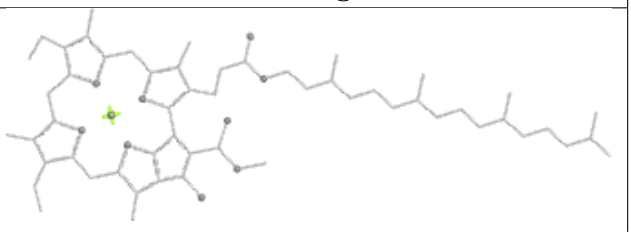
Bond lengths



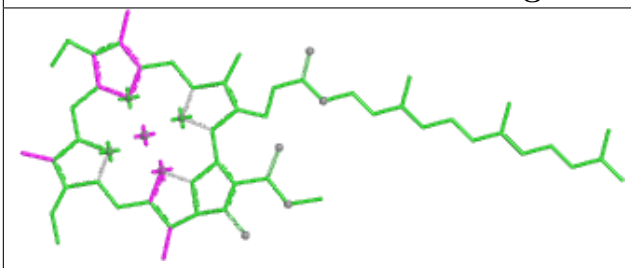
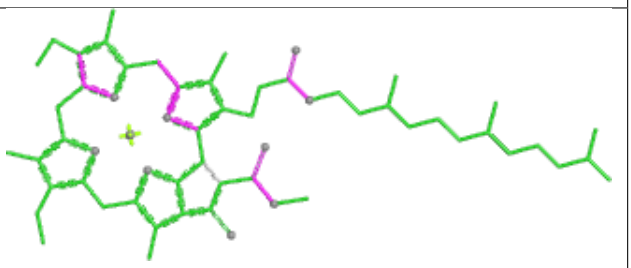
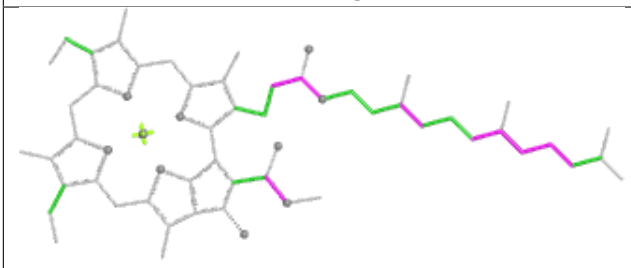
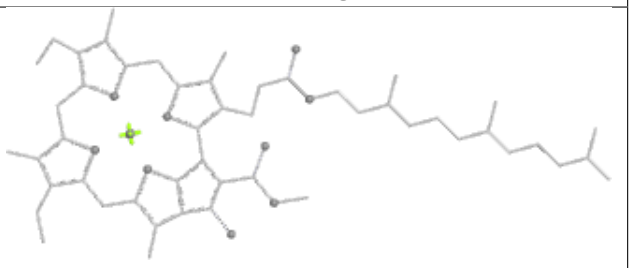
Bond angles

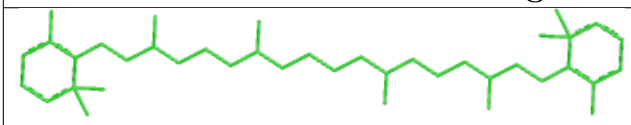
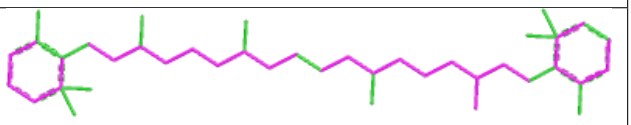
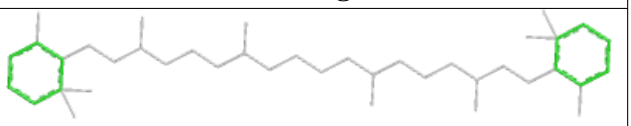


Torsions

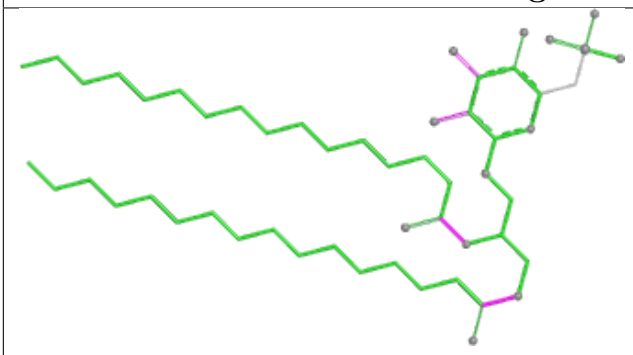


Rings

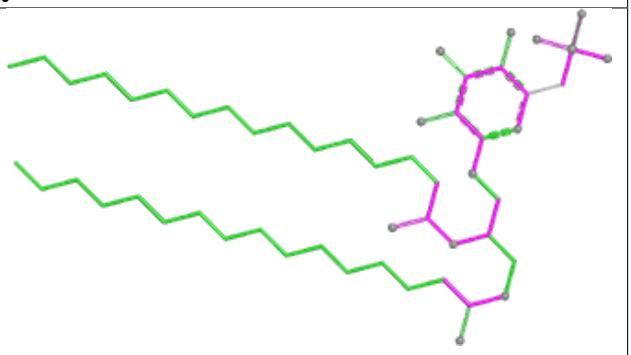
Ligand CLA Y 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 4 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

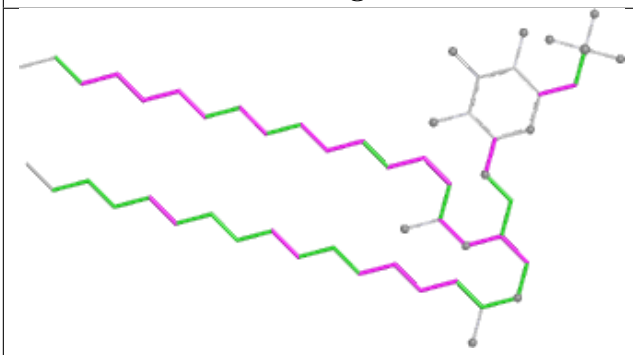
Ligand SQD a 418



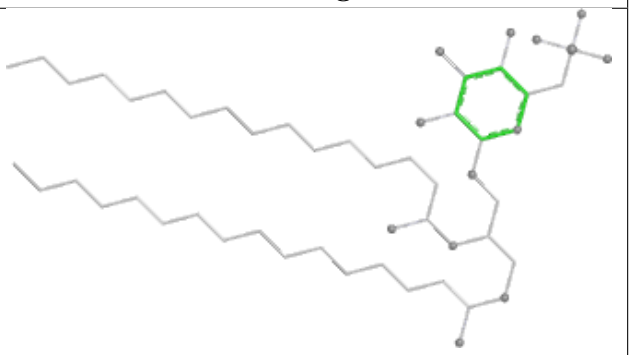
Bond lengths



Bond angles

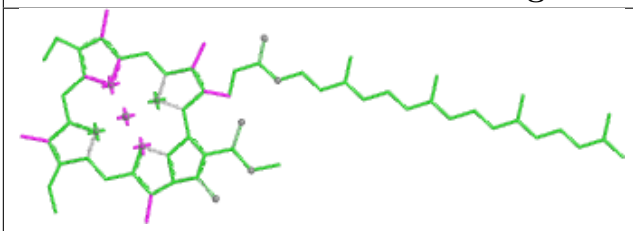


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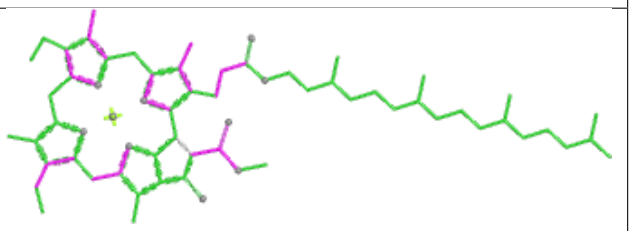


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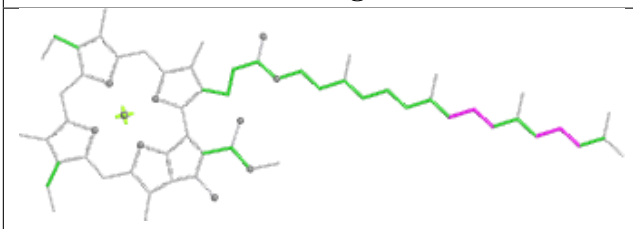
Ligand CLA d 402



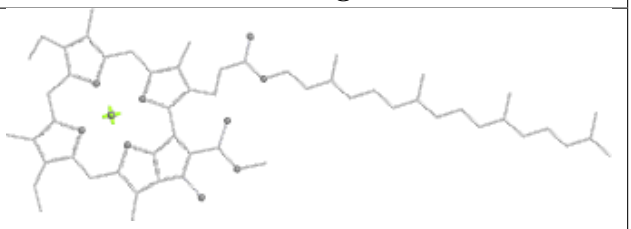
Bond lengths



Bond angles

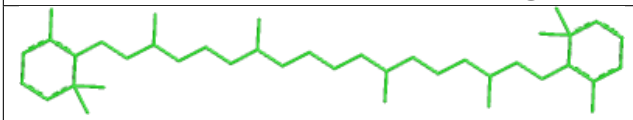


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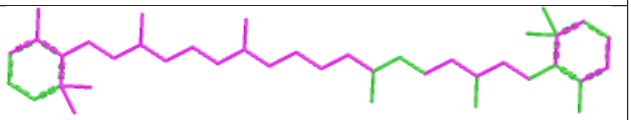


Rings

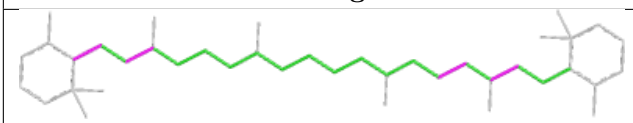
Ligand BCR C 516



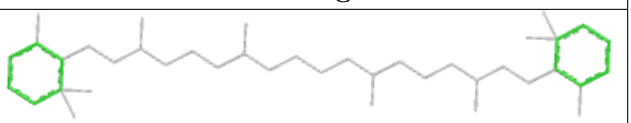
Bond lengths



Bond angles

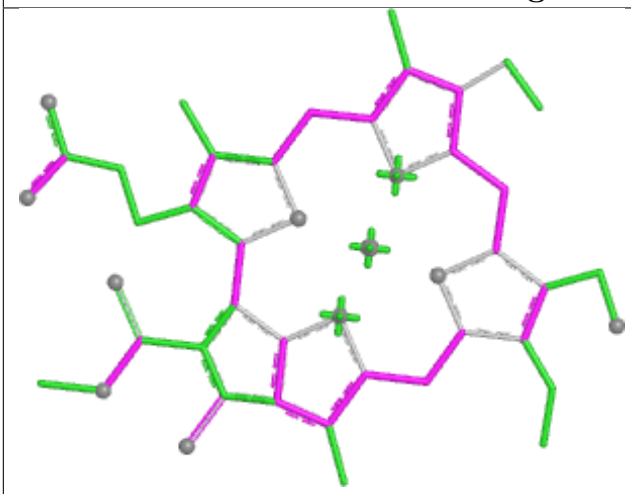


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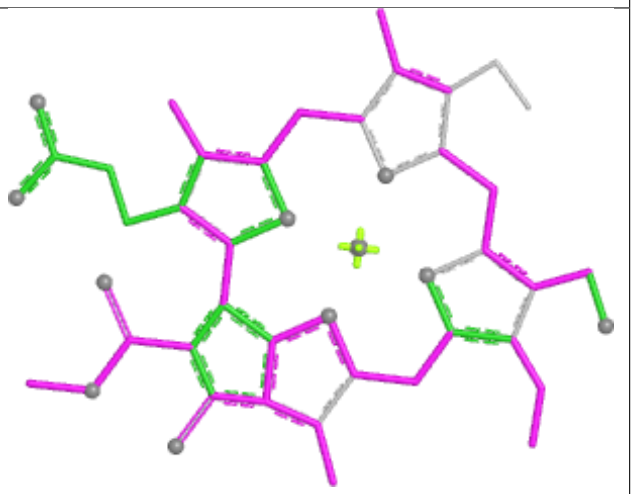


Rings

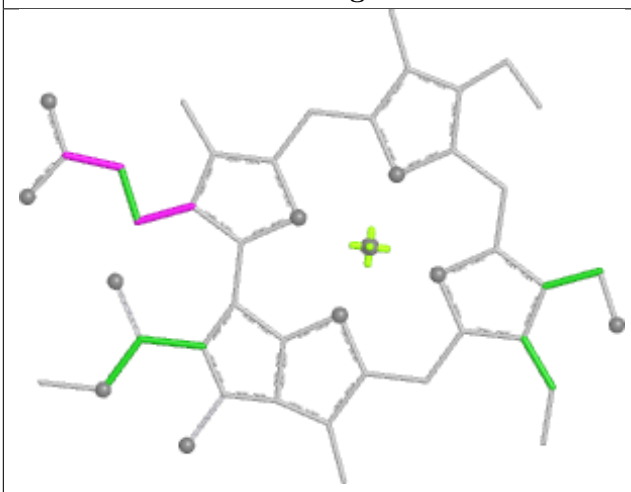
Ligand CHL 2 601



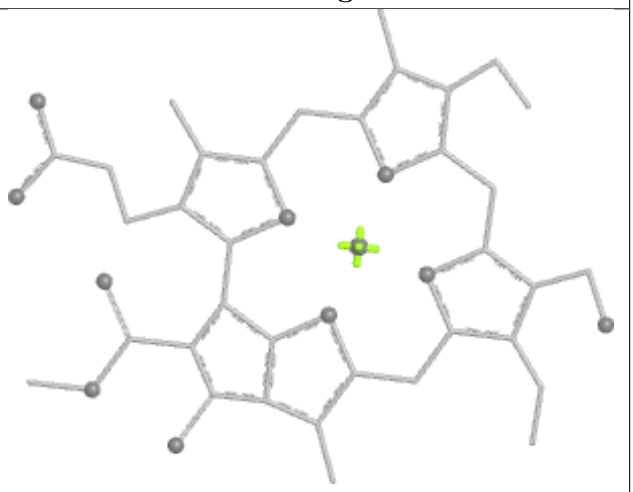
Bond lengths



Bond angles

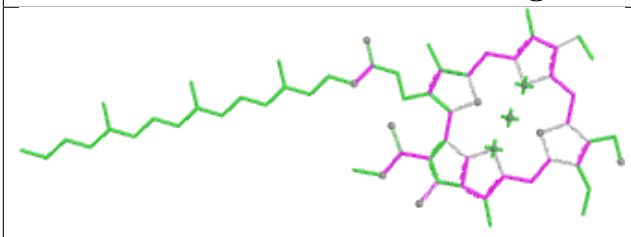


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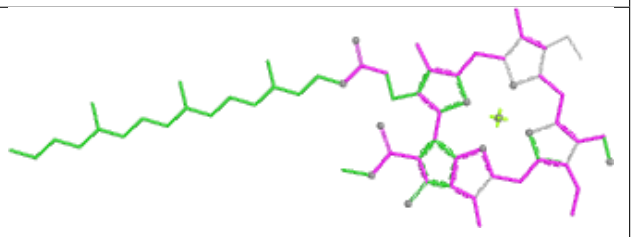


Rings

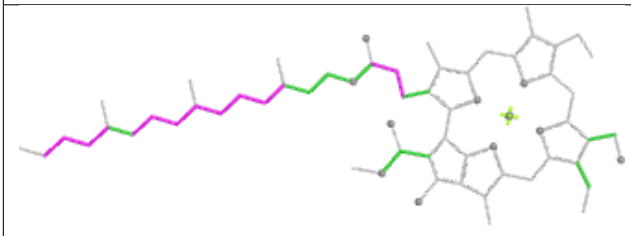
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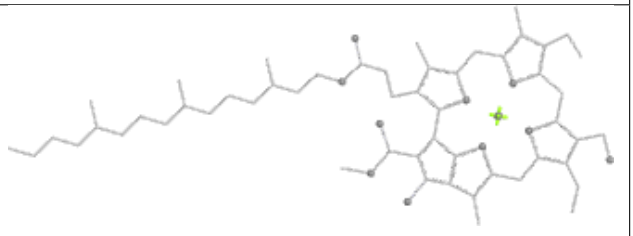
Bond lengths



Bond angles

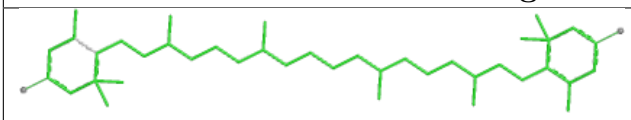


Torsions

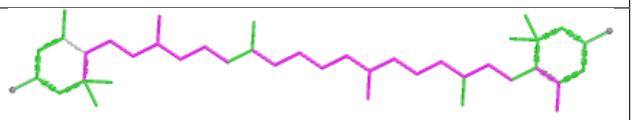


Rings

Ligand LUT 3 1620



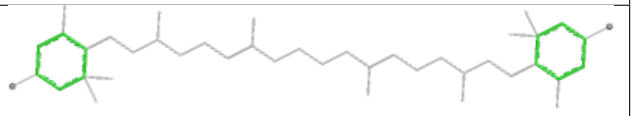
Bond lengths



Bond angles

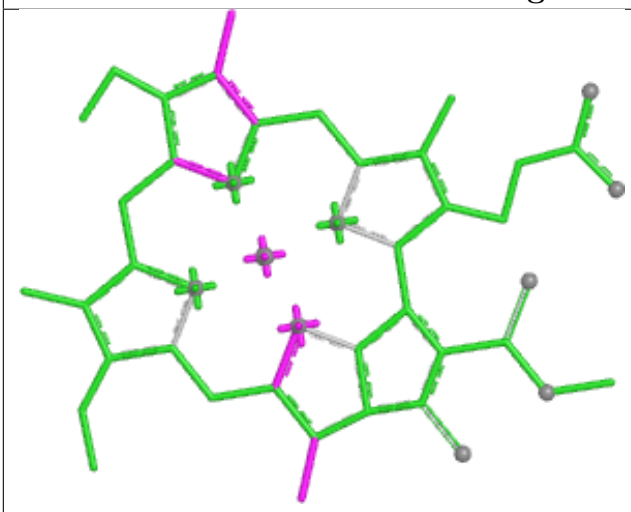


Torsions

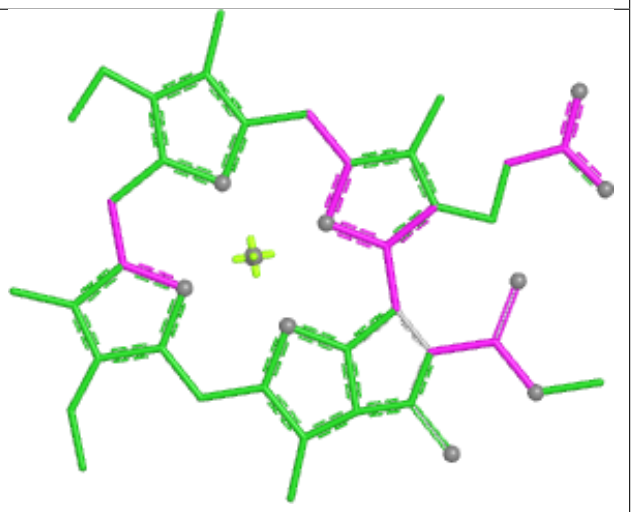


Rings

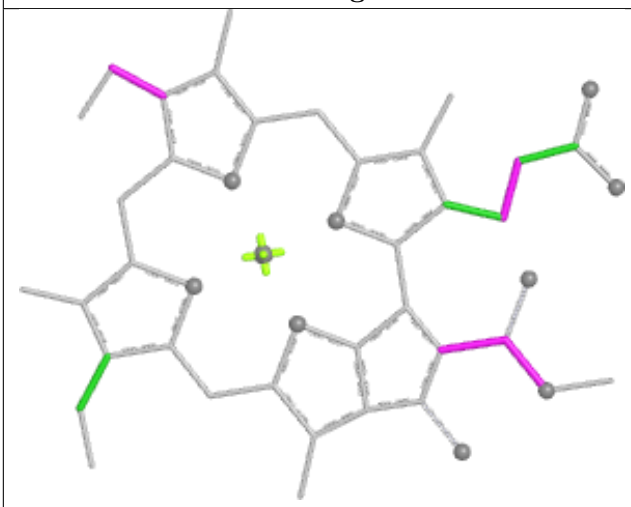
Ligand CLA S 603



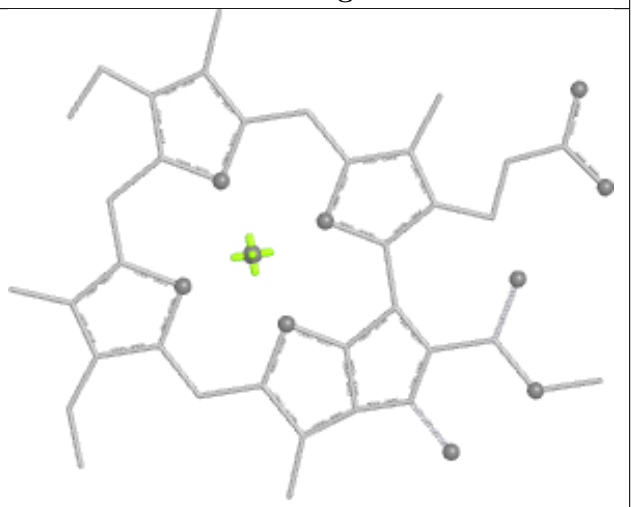
Bond lengths



Bond angles

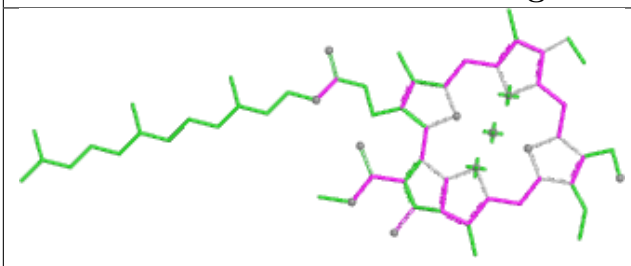


Torsions

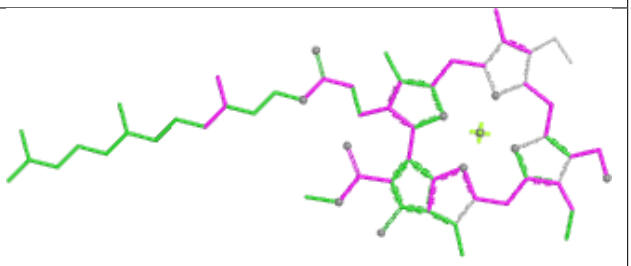


Rings

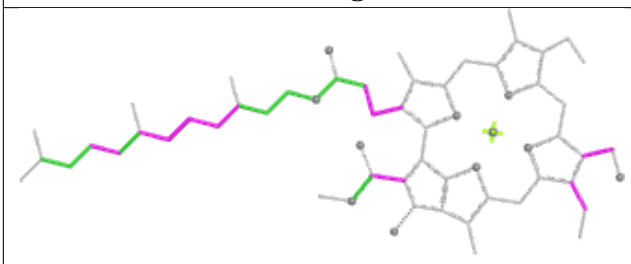
Ligand CHL 2 607



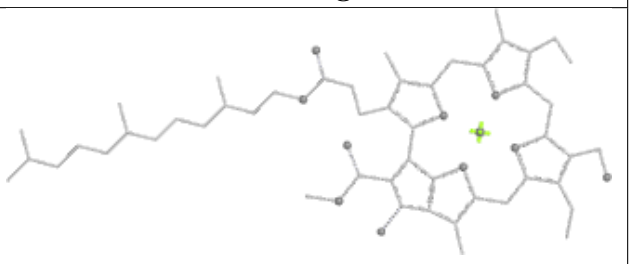
Bond lengths



Bond angles

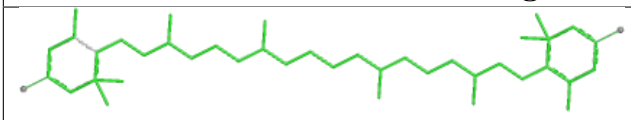


Torsions

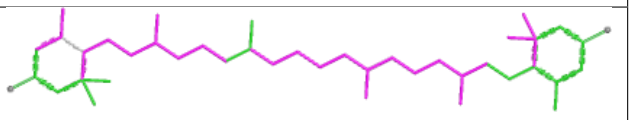


Rings

Ligand LUT s 1621



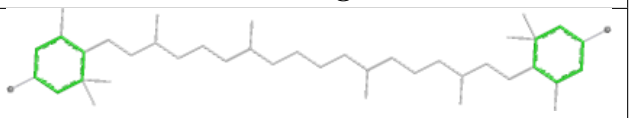
Bond lengths



Bond angles

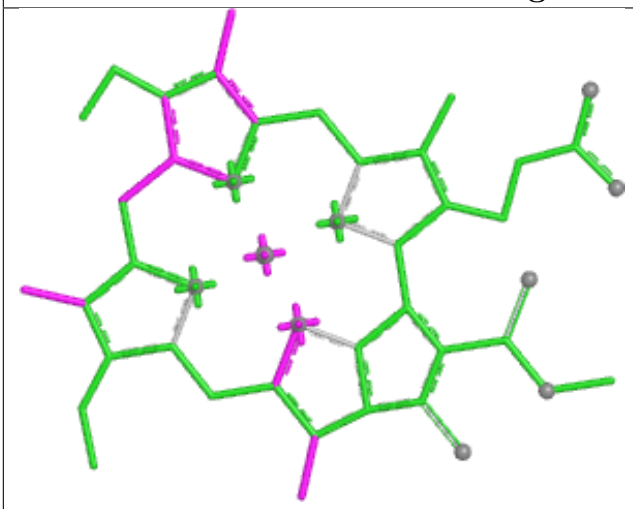


Torsions

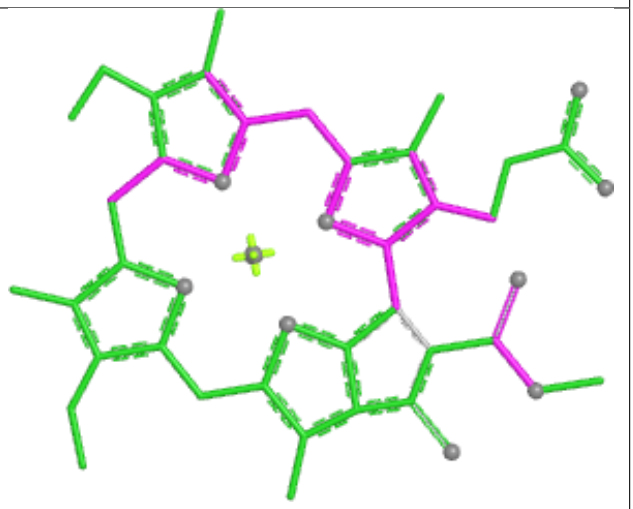


Rings

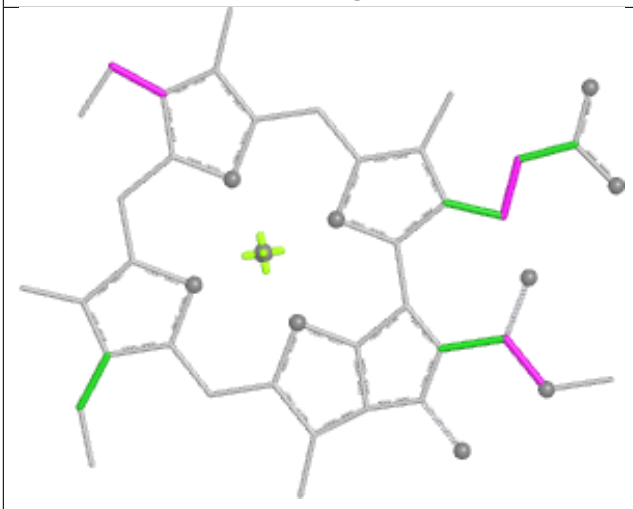
Ligand CLA 5 612



Bond lengths



Bond angles

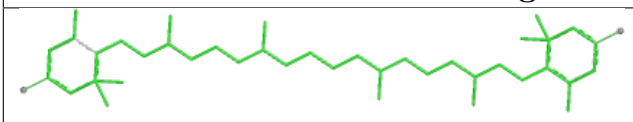


Torsions

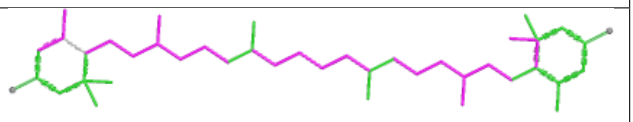


Rings

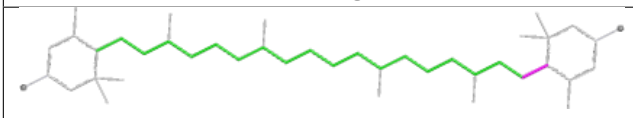
Ligand LUT n 1620



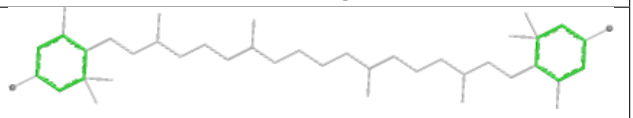
Bond lengths



Bond angles

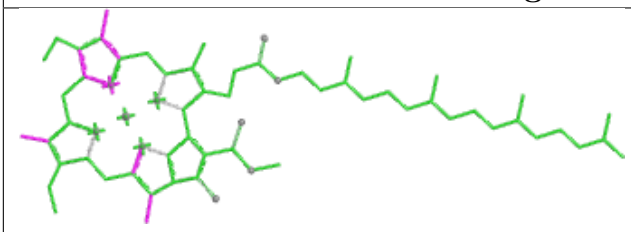


Torsions

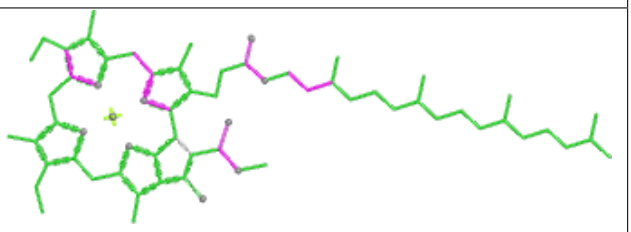


Rings

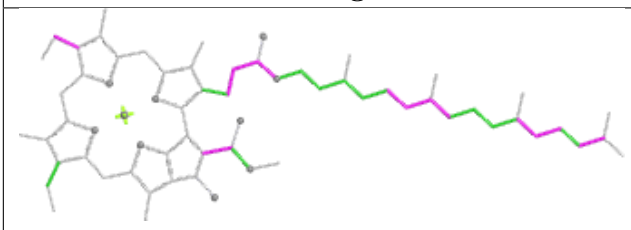
Ligand CLA B 602



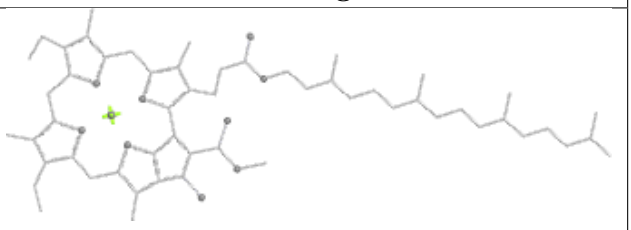
Bond lengths



Bond angles

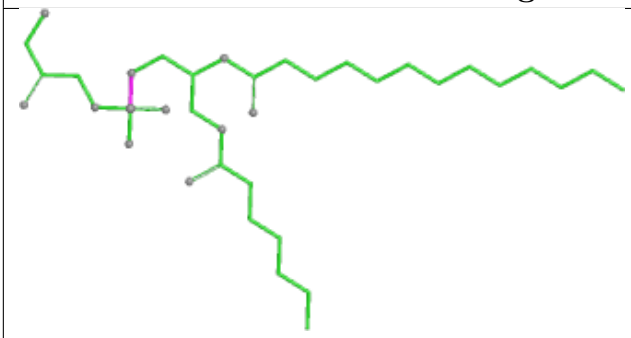


Torsions

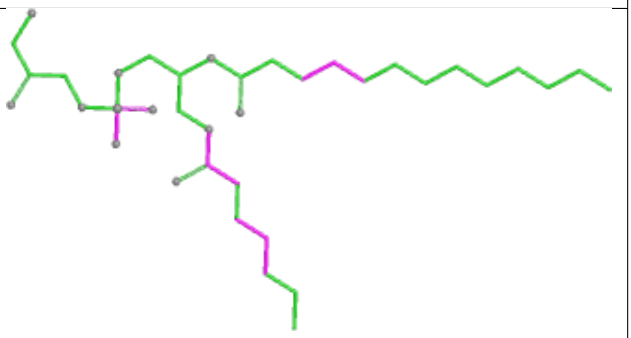


Rings

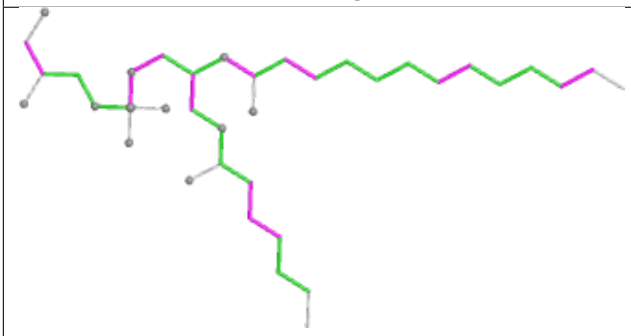
Ligand LHG 6 2630



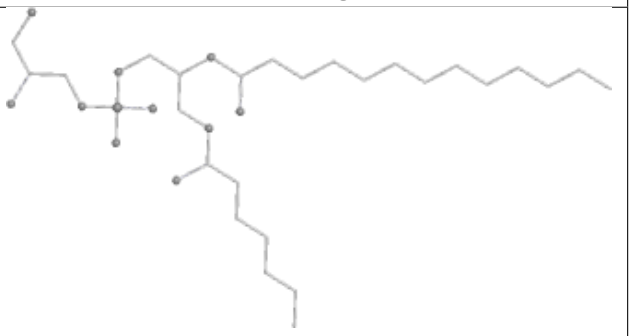
Bond lengths



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.

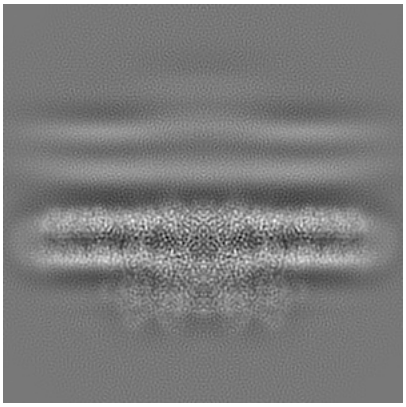
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6741. These allow visual inspection of the internal detail of the map and identification of artifacts.

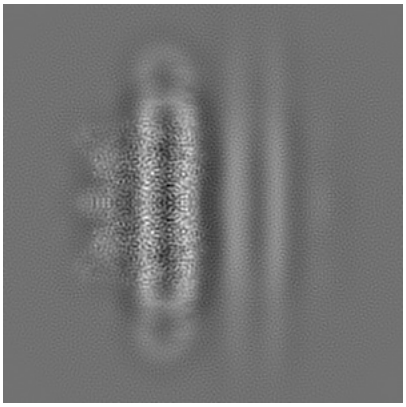
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

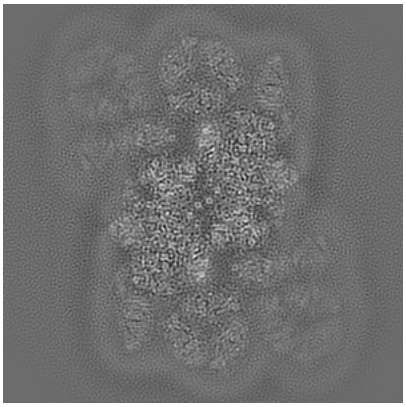
6.1.1 Primary map



X



Y

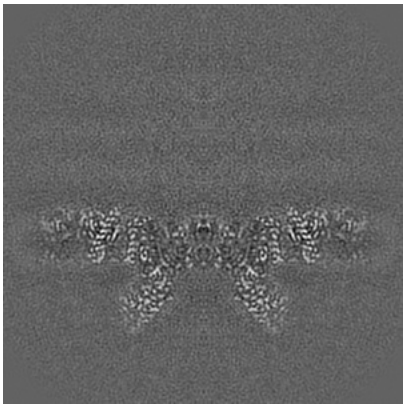


Z

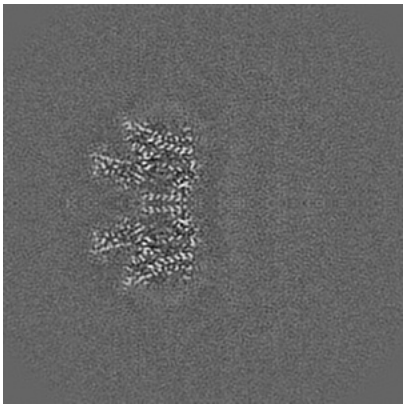
The images above show the map projected in three orthogonal directions.

6.2 Central slices

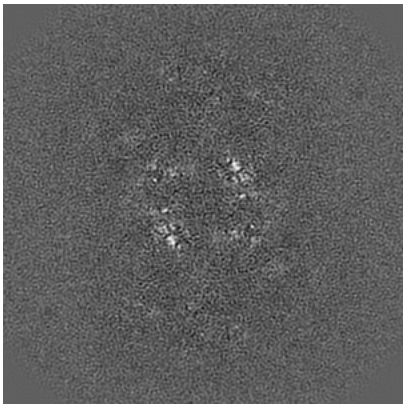
6.2.1 Primary map



X Index: 150



Y Index: 150

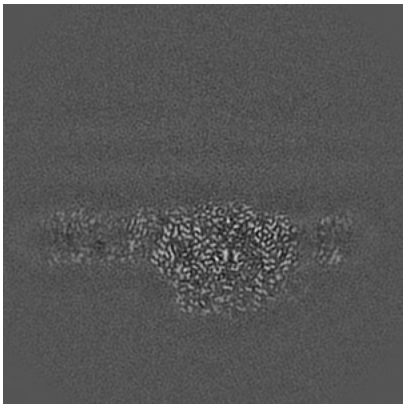


Z Index: 150

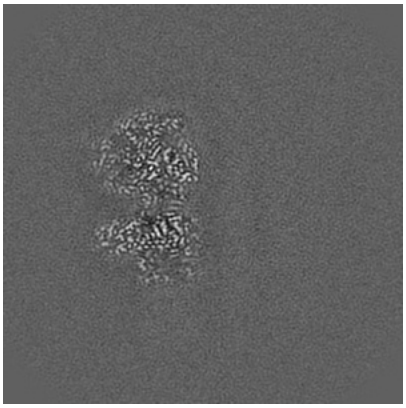
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

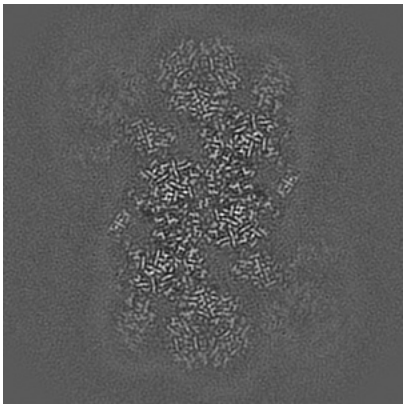
6.3.1 Primary map



X Index: 178



Y Index: 162

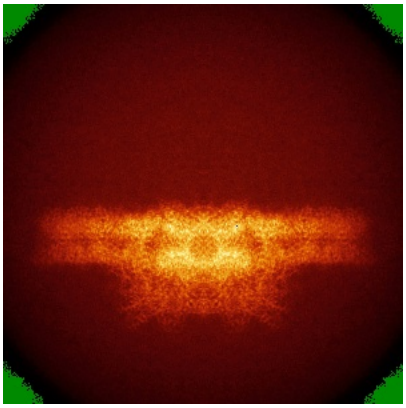


Z Index: 130

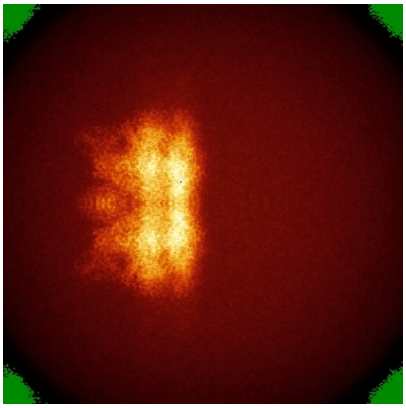
The images above show the largest variance slices of the map in three orthogonal directions.

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

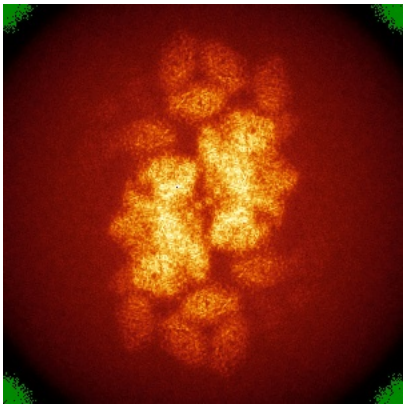
6.4.1 Primary map



X



Y



Z

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 17.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

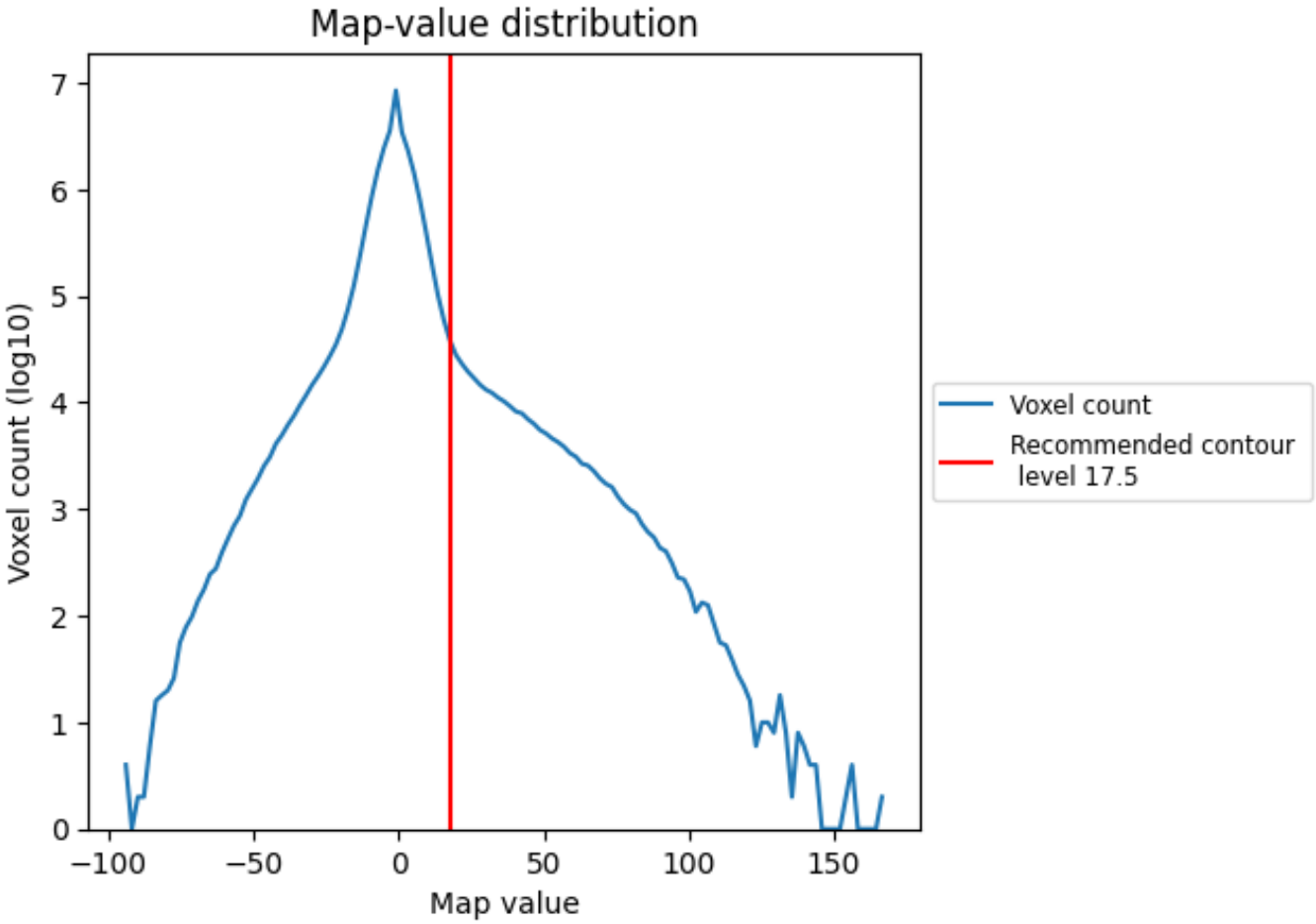
6.6 Mask visualisation (i)

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

7 Map analysis

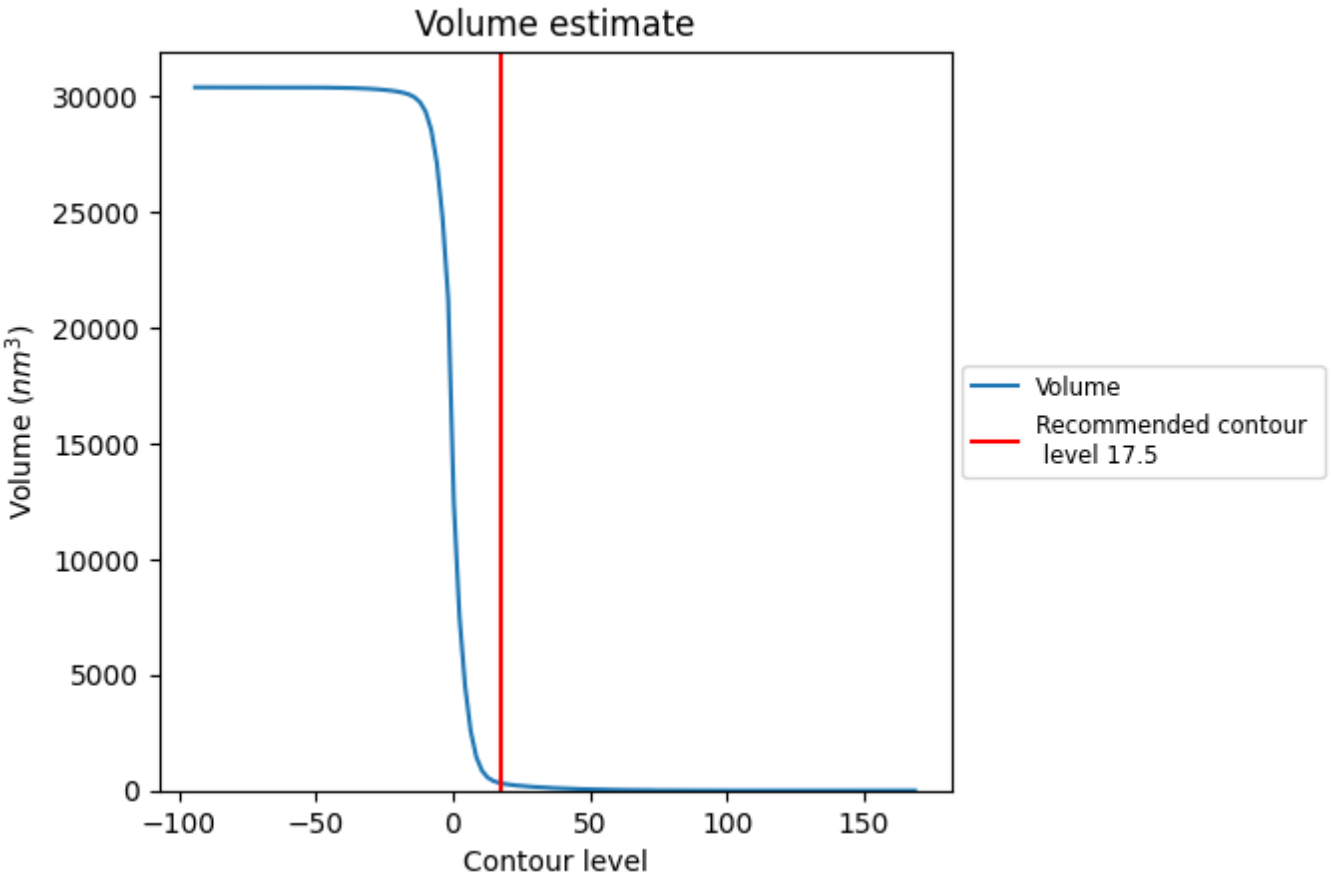
This section contains the results of statistical analysis of the map.

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.

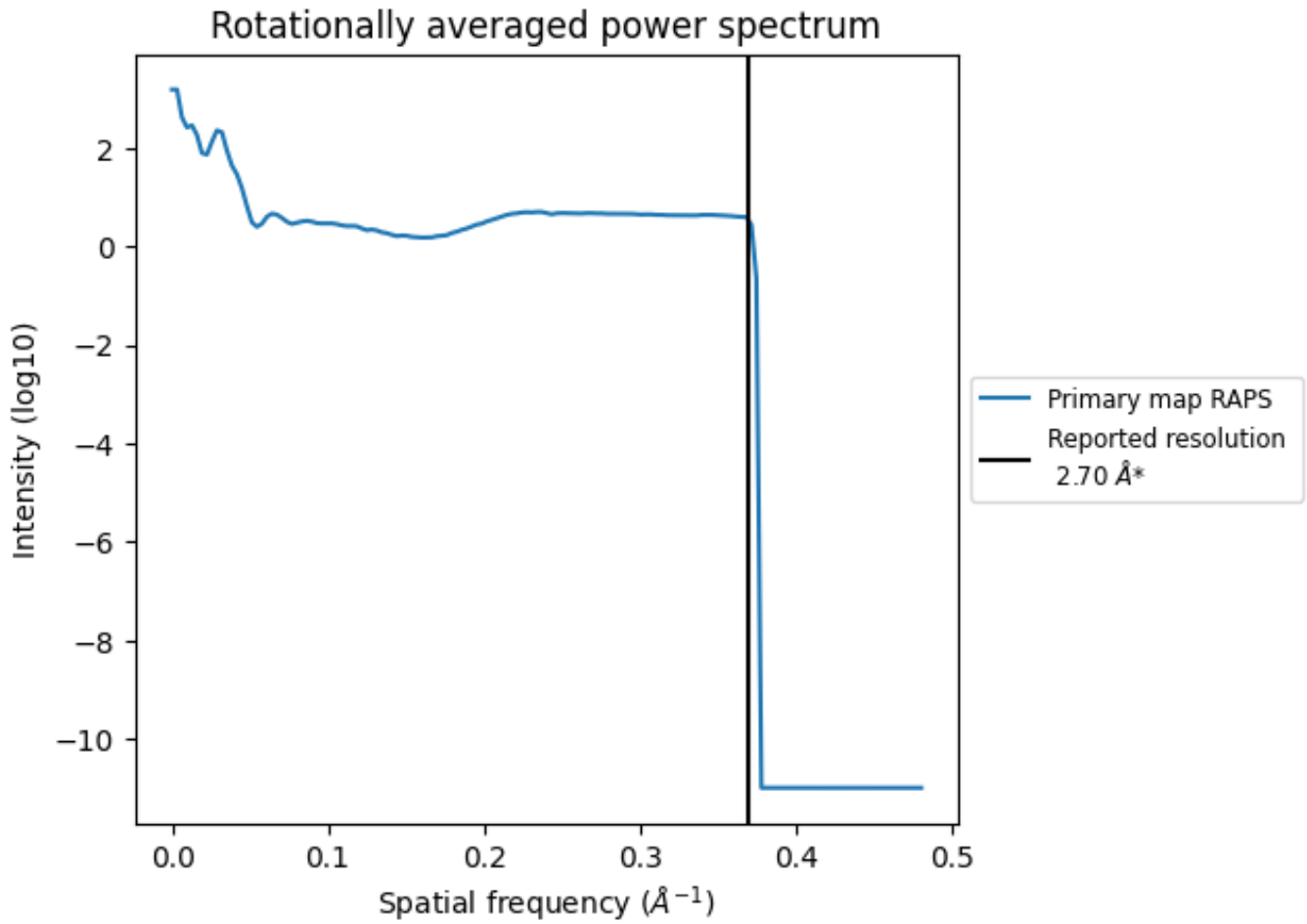
7.2 Volume estimate



The volume at the recommended contour level is 319 nm^3; this corresponds to an approximate mass of 288 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 0.370 Å^{-1}

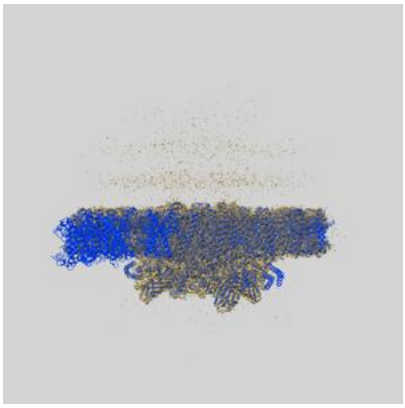
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

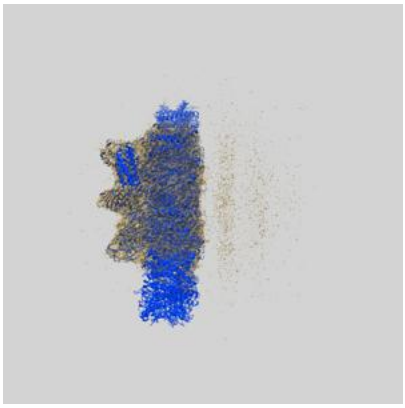
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6741 and PDB model 5XNL. Per-residue inclusion information can be found in section 3 on page 52.

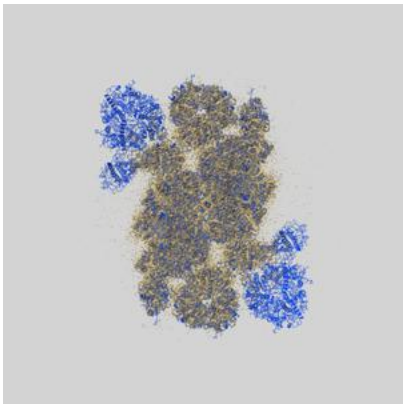
9.1 Map-model overlay



X



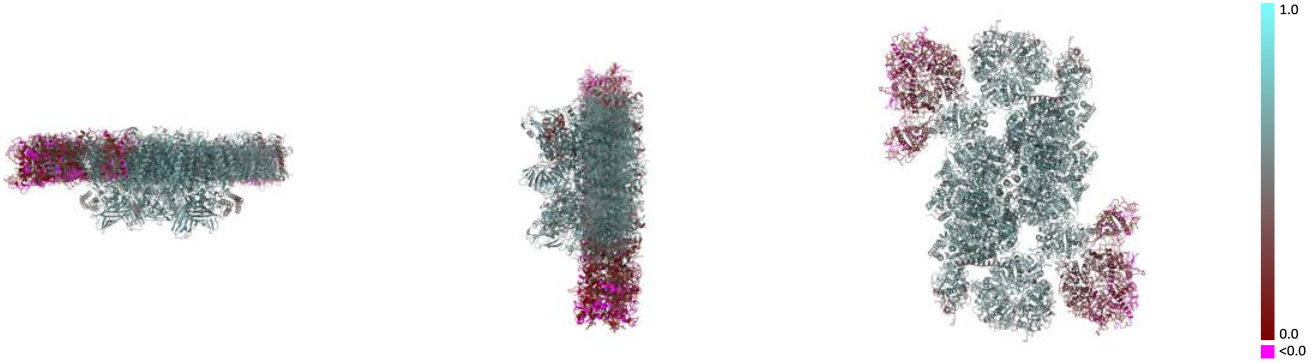
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 17.5 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.

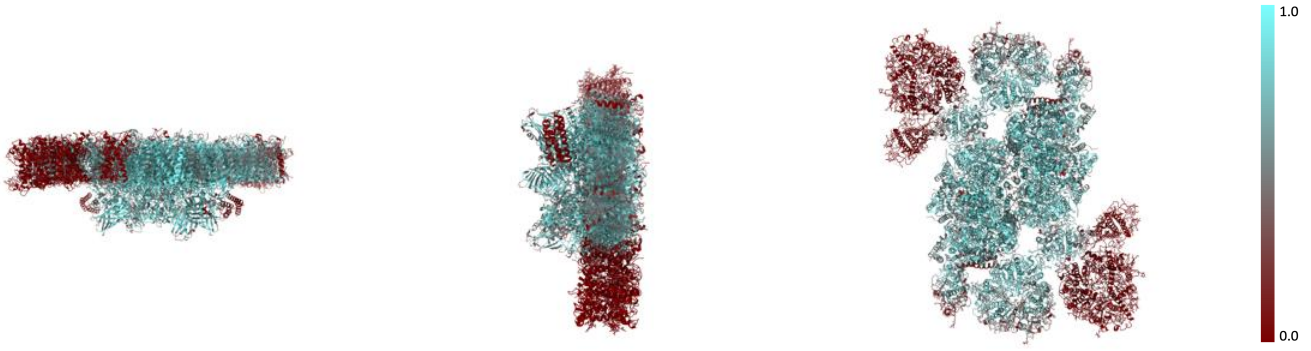
9.2 Q-score mapped to coordinate model (i)



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.

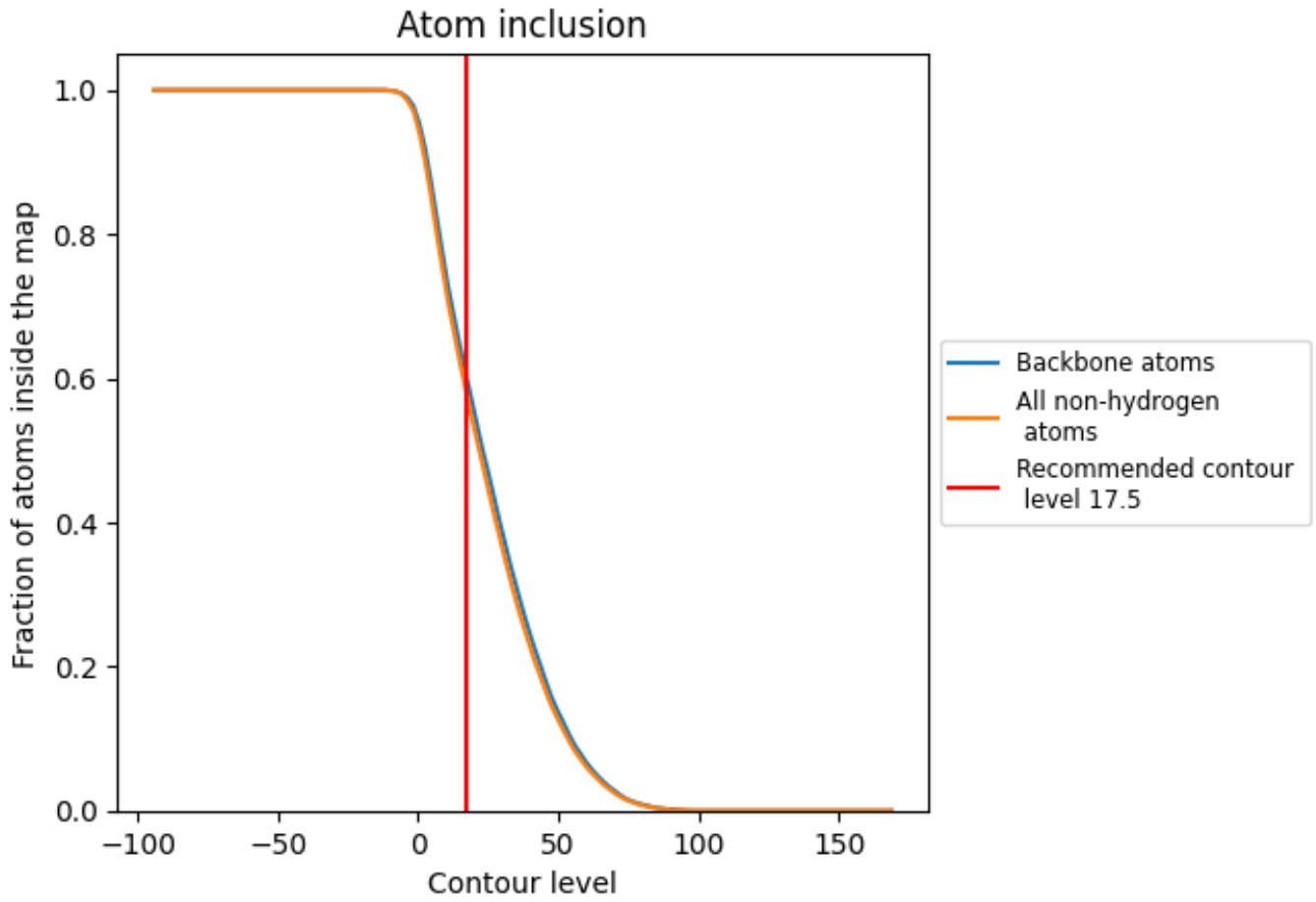
9.3 Atom inclusion mapped to coordinate model (i)



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 (17.5).

9.4 Atom inclusion (i)



At the recommended contour level, 60% of all backbone atoms, 57% 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 (17.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5740	0.5080
1	0.0440	0.2350
2	0.0000	0.0900
3	0.0190	0.2140
4	0.0370	0.1910
5	0.0440	0.2370
6	0.0000	0.0880
7	0.0190	0.2130
8	0.0370	0.1890
A	0.8730	0.6430
B	0.8090	0.6200
C	0.8210	0.6290
D	0.8650	0.6370
E	0.7800	0.6010
F	0.7890	0.6140
G	0.5390	0.5460
H	0.8030	0.6150
I	0.8750	0.6340
J	0.6810	0.5830
K	0.7320	0.5880
L	0.8080	0.6190
M	0.6740	0.5720
N	0.6000	0.5620
O	0.7230	0.5810
P	0.6240	0.5760
Q	0.0760	0.4090
R	0.6350	0.5630
S	0.5200	0.5220
T	0.7010	0.6000
W	0.6930	0.5860
X	0.5880	0.5550
Y	0.7970	0.6100
Z	0.5570	0.5360
a	0.8720	0.6420
b	0.8080	0.6200



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Chain	Atom inclusion	Q-score
c	0.8200	0.6300
d	0.8640	0.6370
e	0.7800	0.6010
f	0.7930	0.6130
g	0.5410	0.5450
h	0.8010	0.6110
i	0.8750	0.6330
j	0.6770	0.5810
k	0.7320	0.5800
l	0.8060	0.6240
m	0.6670	0.5710
n	0.5990	0.5610
o	0.7210	0.5820
p	0.6260	0.5770
q	0.0770	0.4070
r	0.6360	0.5650
s	0.5220	0.5210
t	0.6880	0.6000
w	0.6930	0.5880
x	0.5880	0.5590
y	0.7970	0.6110
z	0.5540	0.5340