Full wwPDB EM Validation Report

Mar 10, 2026 – 03:56 AM UTC

PDB ID	:	5XNM / pdb_00005xnm
EMDB ID	:	EMD-6742
Title	:	Structure of unstacked 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	:	3.20 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:

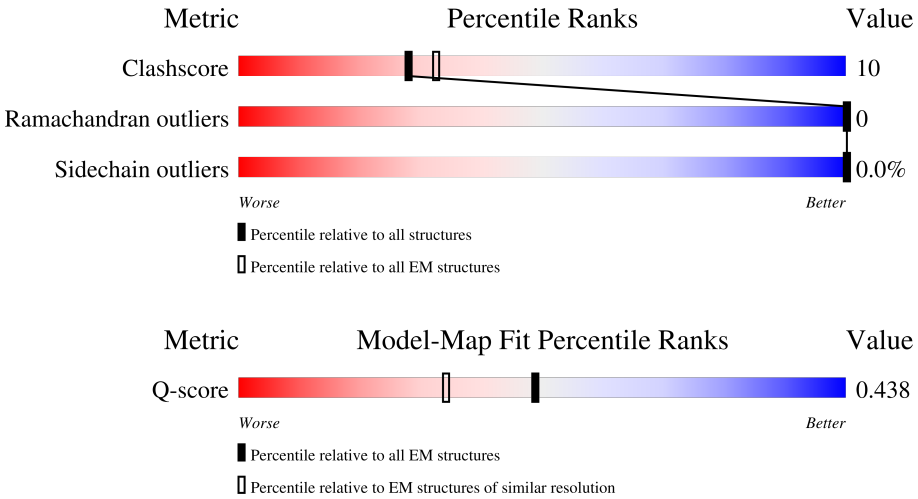
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.20 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	15020 (2.70 - 3.70)

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% 79% 16% 6%
1	2	232	94% 77% 17% 6%
1	5	232	93% 81% 13% 6%
1	6	232	94% 75% 19% 6%

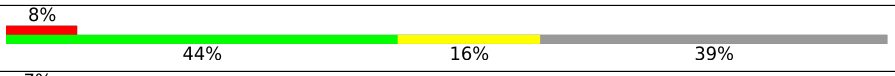
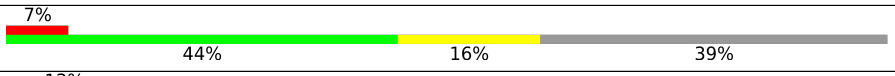
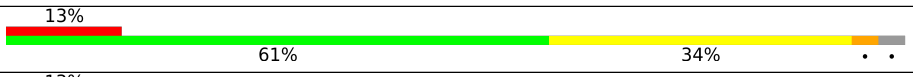
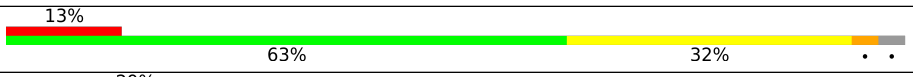
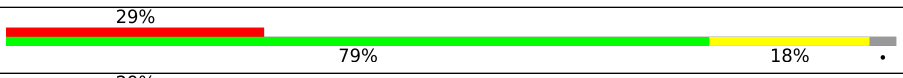
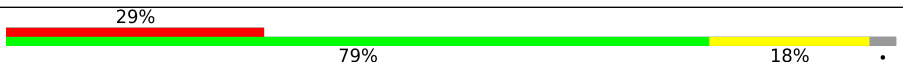
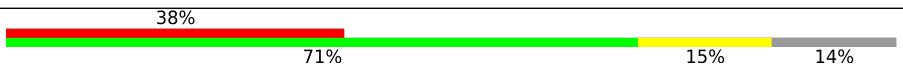
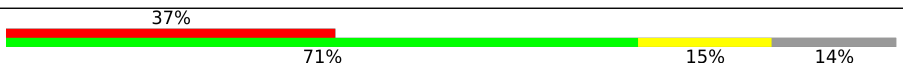
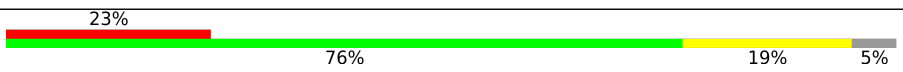
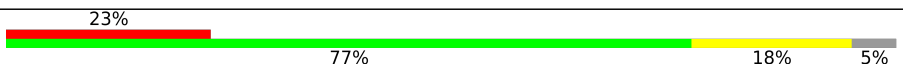
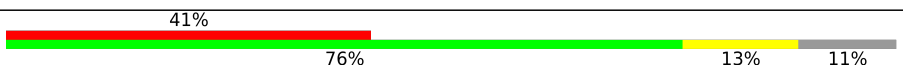
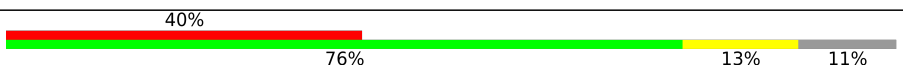
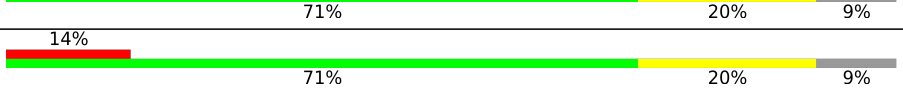
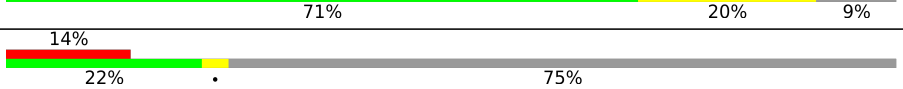
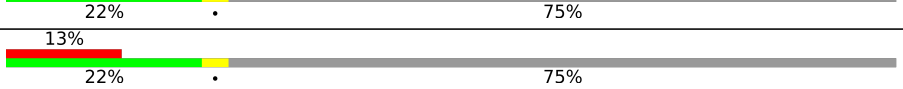
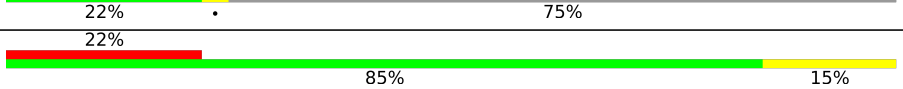
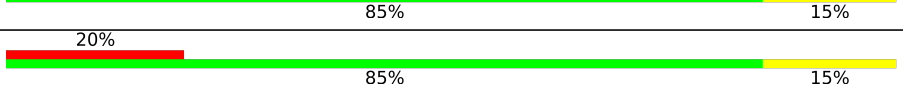
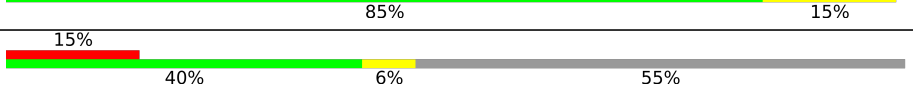
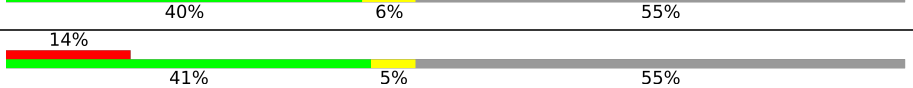
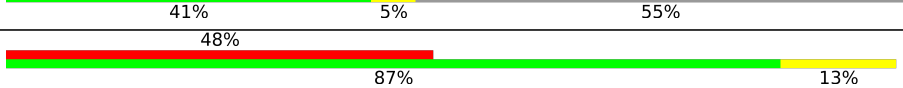
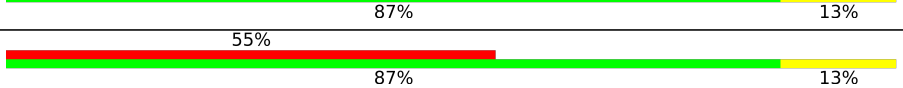
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Mol	Chain	Length	Quality of chain
1	G	232	19% 76% 19% 6%
1	N	232	12% 77% 18% 6%
1	Y	232	5% 76% 18% 6%
1	g	232	19% 75% 19% 6%
1	n	232	12% 76% 19% 6%
1	y	232	5% 77% 18% 6%
2	3	243	90% 76% 15% 9%
2	7	243	90% 75% 15% 9%
3	4	210	92% 74% 20% 6%
3	8	210	93% 71% 22% 6%
4	A	344	8% 81% 16%
4	a	344	7% 81% 16%
5	B	507	11% 81% 18%
5	b	507	10% 82% 17%
6	C	473	11% 79% 15% 5%
6	c	473	12% 79% 16% 5%
7	D	353	7% 76% 20%
7	d	353	7% 76% 20%
8	E	83	30% 81% 10% 10%
8	e	83	34% 81% 10% 10%
9	F	39	13% 64% 13% 23%
9	f	39	13% 64% 13% 23%
10	H	73	14% 71% 11% 18%
10	h	73	12% 73% 10% 18%
11	I	36	78% 17% 6%

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Mol	Chain	Length	Quality of chain
11	i	36	
12	J	40	
12	j	40	
13	K	61	
13	k	61	
14	L	38	
14	l	38	
15	M	34	
15	m	34	
16	O	248	
16	o	248	
17	R	246	
17	r	246	
18	S	244	
18	s	244	
19	T	35	
19	t	35	
20	U	99	
20	u	99	
21	W	54	
21	w	54	
22	X	86	
22	x	86	
23	Z	62	
23	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
24	CHL	1	601	X	-	-	-
24	CHL	1	605	X	-	-	-
24	CHL	1	606	X	-	-	-
24	CHL	1	607	X	-	-	-
24	CHL	1	608	X	-	-	-
24	CHL	1	609	X	-	-	-
24	CHL	2	601	X	-	-	-
24	CHL	2	605	X	-	-	-
24	CHL	2	606	X	-	-	-
24	CHL	2	607	X	-	-	-
24	CHL	2	608	X	-	-	-
24	CHL	2	609	X	-	-	-
24	CHL	3	601	X	-	-	-
24	CHL	3	605	X	-	-	-
24	CHL	3	606	X	-	-	-
24	CHL	3	607	X	-	-	-
24	CHL	3	608	X	-	-	-
24	CHL	3	609	X	-	-	-
24	CHL	4	601	X	-	-	-
24	CHL	4	606	X	-	-	-
24	CHL	4	607	X	-	-	-
24	CHL	4	608	X	-	-	-
24	CHL	4	609	X	-	-	-
24	CHL	5	601	X	-	-	-
24	CHL	5	605	X	-	-	-
24	CHL	5	606	X	-	-	-
24	CHL	5	607	X	-	-	-
24	CHL	5	608	X	-	-	-
24	CHL	5	609	X	-	-	-
24	CHL	6	601	X	-	-	-
24	CHL	6	605	X	-	-	-
24	CHL	6	606	X	-	-	-
24	CHL	6	607	X	-	-	-
24	CHL	6	608	X	-	-	-
24	CHL	6	609	X	-	-	-
24	CHL	7	601	X	-	-	-
24	CHL	7	605	X	-	-	-
24	CHL	7	606	X	-	-	-
24	CHL	7	607	X	-	-	-
24	CHL	7	608	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	n	608	X	-	-	-
24	CHL	n	609	X	-	-	-
24	CHL	r	606	X	-	-	-
24	CHL	r	607	X	-	-	-
24	CHL	r	608	X	-	-	-
24	CHL	r	614	X	-	-	-
24	CHL	s	601	X	-	-	-
24	CHL	s	606	X	-	-	-
24	CHL	s	607	X	-	-	-
24	CHL	s	608	X	-	-	-
24	CHL	y	601	X	-	-	-
24	CHL	y	605	X	-	-	-
24	CHL	y	606	X	-	-	-
24	CHL	y	607	X	-	-	-
24	CHL	y	608	X	-	-	-
24	CHL	y	609	X	-	-	-
25	CLA	1	602	X	-	-	-
25	CLA	1	603	X	-	-	-
25	CLA	1	604	X	-	-	-
25	CLA	1	610	X	-	-	-
25	CLA	1	611	X	-	-	-
25	CLA	1	612	X	-	-	-
25	CLA	1	614	X	-	-	-
25	CLA	2	602	X	-	-	-
25	CLA	2	603	X	-	-	-
25	CLA	2	610	X	-	-	-
25	CLA	2	611	X	-	-	-
25	CLA	2	612	X	-	-	-
25	CLA	3	602	X	-	-	-
25	CLA	3	603	X	-	-	-
25	CLA	3	604	X	-	-	-
25	CLA	3	610	X	-	-	-
25	CLA	3	611	X	-	-	-
25	CLA	3	612	X	-	-	-
25	CLA	3	613	X	-	-	-
25	CLA	3	614	X	-	-	-
25	CLA	4	602	X	-	-	-
25	CLA	4	603	X	-	-	-
25	CLA	4	610	X	-	-	-
25	CLA	4	611	X	-	-	-
25	CLA	4	612	X	-	-	-
25	CLA	5	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	5	603	X	-	-	-
25	CLA	5	604	X	-	-	-
25	CLA	5	610	X	-	-	-
25	CLA	5	611	X	-	-	-
25	CLA	5	612	X	-	-	-
25	CLA	5	614	X	-	-	-
25	CLA	6	602	X	-	-	-
25	CLA	6	603	X	-	-	-
25	CLA	6	610	X	-	-	-
25	CLA	6	611	X	-	-	-
25	CLA	6	612	X	-	-	-
25	CLA	7	602	X	-	-	-
25	CLA	7	603	X	-	-	-
25	CLA	7	604	X	-	-	-
25	CLA	7	610	X	-	-	-
25	CLA	7	611	X	-	-	-
25	CLA	7	612	X	-	-	-
25	CLA	7	613	X	-	-	-
25	CLA	7	614	X	-	-	-
25	CLA	8	602	X	-	-	-
25	CLA	8	603	X	-	-	-
25	CLA	8	610	X	-	-	-
25	CLA	8	611	X	-	-	-
25	CLA	8	612	X	-	-	-
25	CLA	A	405	X	-	-	-
25	CLA	A	406	X	-	-	-
25	CLA	A	407	X	-	-	-
25	CLA	A	410	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	S	614	X	-	-	-
25	CLA	Y	602	X	-	-	-
25	CLA	Y	603	X	-	-	-
25	CLA	Y	604	X	-	-	-
25	CLA	Y	610	X	-	-	-
25	CLA	Y	611	X	-	-	-
25	CLA	Y	612	X	-	-	-
25	CLA	Y	613	X	-	-	-
25	CLA	Y	614	X	-	-	-
25	CLA	a	405	X	-	-	-
25	CLA	a	406	X	-	-	-
25	CLA	a	407	X	-	-	-
25	CLA	a	410	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	b	617	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	d	402	X	-	-	-
25	CLA	g	602	X	-	-	-
25	CLA	g	603	X	-	-	-
25	CLA	g	610	X	-	-	-
25	CLA	g	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	g	612	X	-	-	-
25	CLA	g	614	X	-	-	-
25	CLA	n	602	X	-	-	-
25	CLA	n	603	X	-	-	-
25	CLA	n	604	X	-	-	-
25	CLA	n	610	X	-	-	-
25	CLA	n	611	X	-	-	-
25	CLA	n	612	X	-	-	-
25	CLA	n	613	X	-	-	-
25	CLA	n	614	X	-	-	-
25	CLA	r	601	X	-	-	-
25	CLA	r	602	X	-	-	-
25	CLA	r	603	X	-	-	-
25	CLA	r	604	X	-	-	-
25	CLA	r	609	X	-	-	-
25	CLA	r	610	X	-	-	-
25	CLA	r	611	X	-	-	-
25	CLA	r	612	X	-	-	-
25	CLA	r	613	X	-	-	-
25	CLA	s	602	X	-	-	-
25	CLA	s	603	X	-	-	-
25	CLA	s	604	X	-	-	-
25	CLA	s	609	X	-	-	-
25	CLA	s	610	X	-	-	-
25	CLA	s	611	X	-	-	-
25	CLA	s	612	X	-	-	-
25	CLA	s	613	X	-	-	-
25	CLA	s	614	X	-	-	-
25	CLA	y	602	X	-	-	-
25	CLA	y	603	X	-	-	-
25	CLA	y	604	X	-	-	-
25	CLA	y	610	X	-	-	-
25	CLA	y	611	X	-	-	-
25	CLA	y	612	X	-	-	-
25	CLA	y	613	X	-	-	-
25	CLA	y	614	X	-	-	-

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 92842 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 1534	C 1009	N 247	O 274	S 4	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	340	Total 2703	C 1784	N 443	O 464	S 12	0	0
7	d	340	Total 2703	C 1784	N 443	O 464	S 12	0	0

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

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

- 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	34	Total	C	N	O	0	0
			247	168	38	41		
12	j	34	Total	C	N	O	0	0
			247	168	38	41		

- 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	214	Total 1631	C 1039	N 260	O 329	S 3	0	0
16	o	214	Total 1631	C 1039	N 260	O 329	S 3	0	0

- Molecule 17 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29.

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

- Molecule 18 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26.

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

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

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

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

- Molecule 20 is a protein called Photosystem II luminal extrinsic protein Tn, PsbTn.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	25	Total 193	C 123	N 35	O 32	S 3	0	0
20	u	25	Total 193	C 123	N 35	O 32	S 3	0	0

- Molecule 21 is a protein called Photosystem II reaction center protein W, PSBW.

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

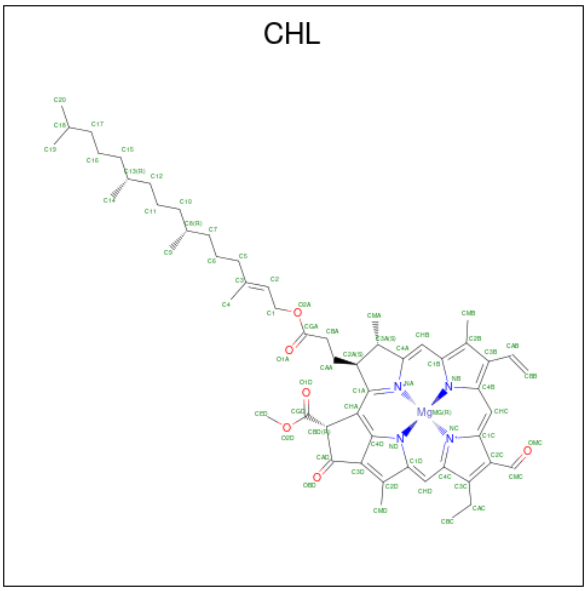
- Molecule 22 is a protein called Photosystem II reaction center protein X.

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

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

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

- Molecule 24 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
24	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
24	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	S	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
24	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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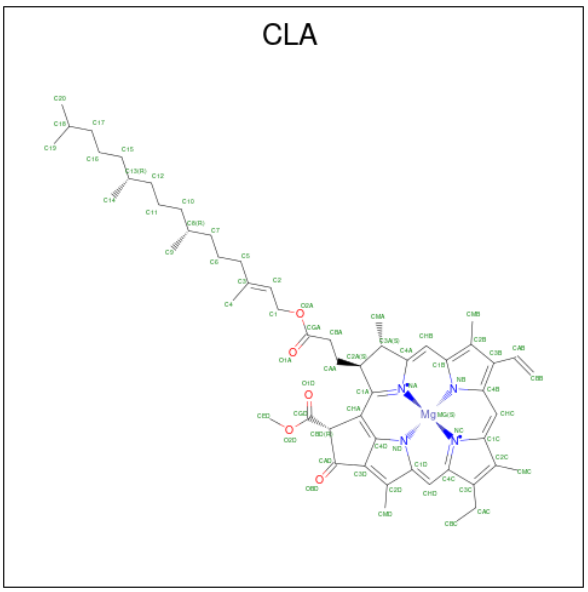
Mol	Chain	Residues	Atoms					AltConf
24	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
25	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

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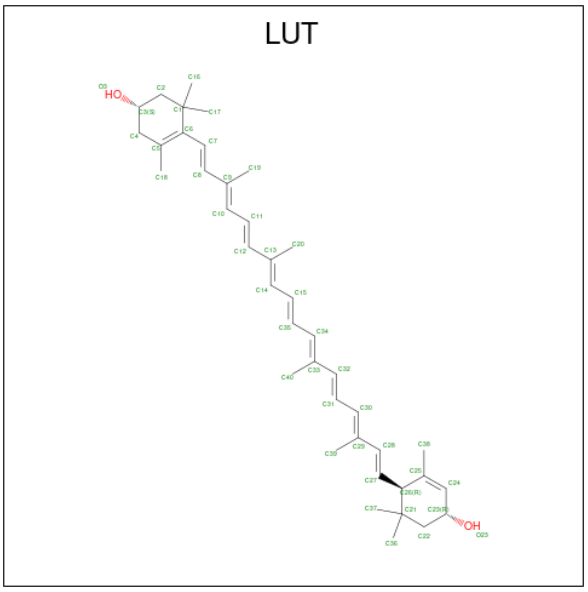
Mol	Chain	Residues	Atoms					AltConf
25	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	n	1	Total	C	Mg	N	O	0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

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

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



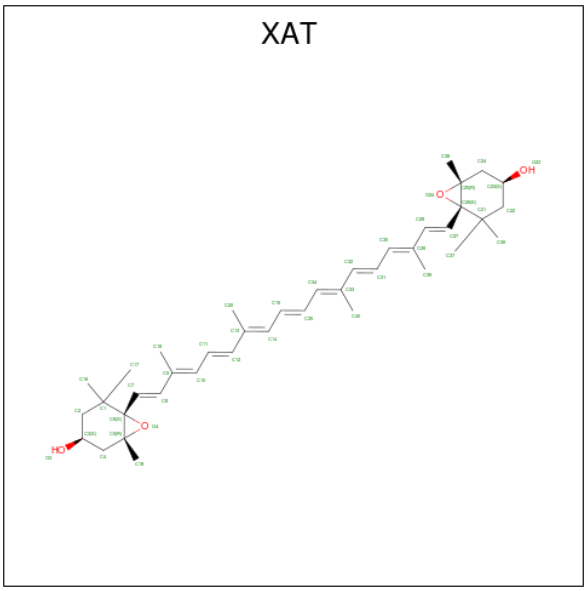
Mol	Chain	Residues	Atoms			AltConf
26	1	1	Total	C	O	0
			42	40	2	
26	1	1	Total	C	O	0
			42	40	2	
26	2	1	Total	C	O	0
			42	40	2	
26	2	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	4	1	Total	C	O	0
			42	40	2	
26	G	1	Total	C	O	0
			42	40	2	
26	G	1	Total	C	O	0
			42	40	2	
26	N	1	Total	C	O	0
			42	40	2	
26	N	1	Total	C	O	0
			42	40	2	
26	R	1	Total	C	O	0
			42	40	2	
26	S	1	Total	C	O	0
			42	40	2	
26	S	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms	AltConf
26	Y	1	Total C O 42 40 2	0
26	Y	1	Total C O 42 40 2	0
26	5	1	Total C O 42 40 2	0
26	5	1	Total C O 42 40 2	0
26	6	1	Total C O 42 40 2	0
26	6	1	Total C O 42 40 2	0
26	7	1	Total C O 42 40 2	0
26	7	1	Total C O 42 40 2	0
26	8	1	Total C O 42 40 2	0
26	g	1	Total C O 42 40 2	0
26	g	1	Total C O 42 40 2	0
26	n	1	Total C O 42 40 2	0
26	n	1	Total C O 42 40 2	0
26	r	1	Total C O 42 40 2	0
26	s	1	Total C O 42 40 2	0
26	s	1	Total C O 42 40 2	0
26	y	1	Total C O 42 40 2	0
26	y	1	Total C O 42 40 2	0

- Molecule 27 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: $C_{40}H_{56}O_4$).



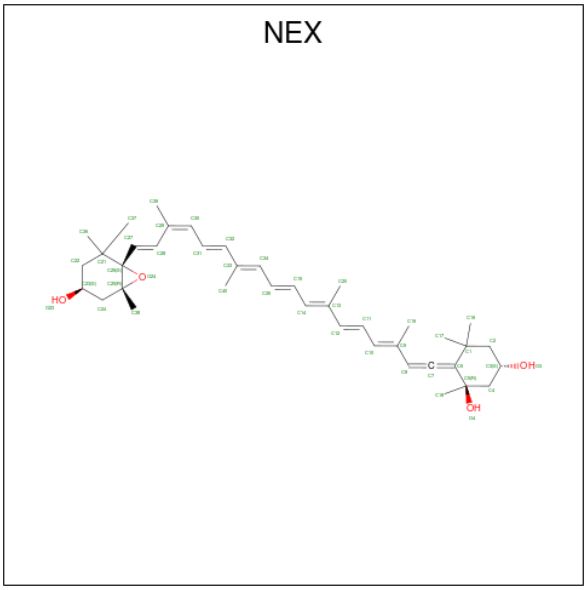
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			44	40	4	
27	2	1	Total	C	O	0
			44	40	4	
27	3	1	Total	C	O	0
			44	40	4	
27	4	1	Total	C	O	0
			44	40	4	
27	G	1	Total	C	O	0
			44	40	4	
27	N	1	Total	C	O	0
			44	40	4	
27	R	1	Total	C	O	0
			44	40	4	
27	Y	1	Total	C	O	0
			44	40	4	
27	5	1	Total	C	O	0
			44	40	4	
27	6	1	Total	C	O	0
			44	40	4	
27	7	1	Total	C	O	0
			44	40	4	
27	8	1	Total	C	O	0
			44	40	4	
27	g	1	Total	C	O	0
			44	40	4	
27	n	1	Total	C	O	0
			44	40	4	

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

- Molecule 28 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: $C_{40}H_{56}O_4$).



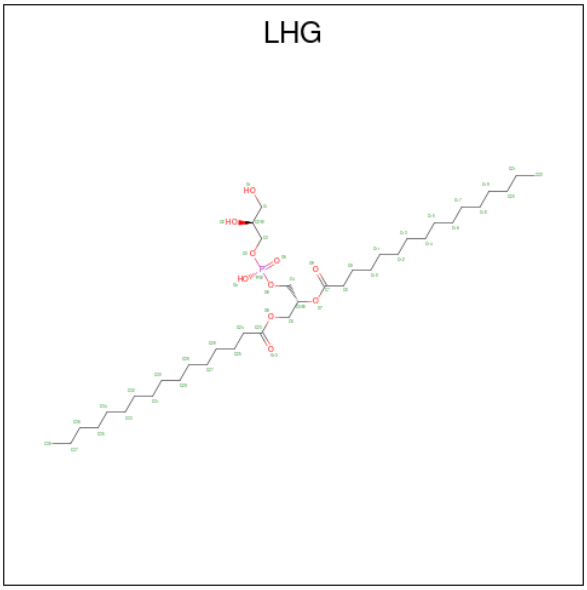
Mol	Chain	Residues	Atoms	AltConf
28	1	1	Total C O 44 40 4	0
28	2	1	Total C O 44 40 4	0
28	3	1	Total C O 44 40 4	0
28	G	1	Total C O 44 40 4	0
28	N	1	Total C O 44 40 4	0
28	R	1	Total C O 44 40 4	0
28	S	1	Total C O 44 40 4	0
28	Y	1	Total C O 44 40 4	0

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

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
29	1	1	Total C O P 41 30 10 1	0
29	2	1	Total C O P 37 26 10 1	0
29	3	1	Total C O P 47 36 10 1	0

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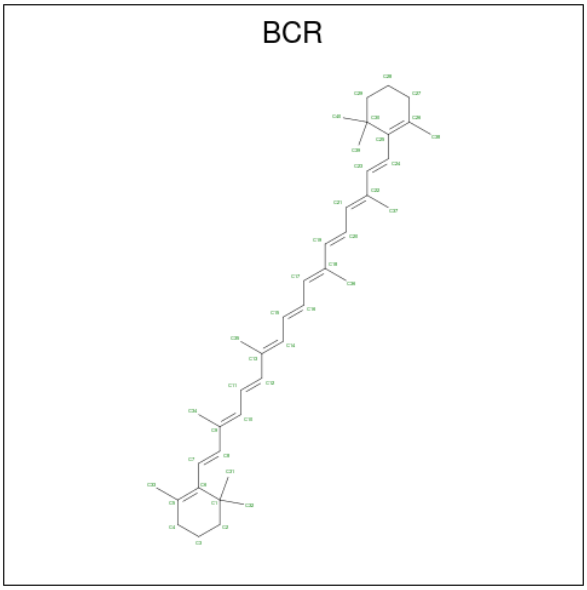
Mol	Chain	Residues	Atoms				AltConf
29	4	1	Total	C	O	P	0
			21	10	10	1	
29	B	1	Total	C	O	P	0
			47	36	10	1	
29	B	1	Total	C	O	P	0
			49	38	10	1	
29	C	1	Total	C	O	P	0
			49	38	10	1	
29	C	1	Total	C	O	P	0
			49	38	10	1	
29	C	1	Total	C	O	P	0
			49	38	10	1	
29	D	1	Total	C	O	P	0
			46	35	10	1	
29	D	1	Total	C	O	P	0
			49	38	10	1	
29	D	1	Total	C	O	P	0
			43	32	10	1	
29	G	1	Total	C	O	P	0
			49	38	10	1	
29	L	1	Total	C	O	P	0
			49	38	10	1	
29	N	1	Total	C	O	P	0
			49	38	10	1	
29	R	1	Total	C	O	P	0
			42	31	10	1	
29	S	1	Total	C	O	P	0
			49	38	10	1	
29	Y	1	Total	C	O	P	0
			49	38	10	1	
29	5	1	Total	C	O	P	0
			41	30	10	1	
29	6	1	Total	C	O	P	0
			37	26	10	1	
29	7	1	Total	C	O	P	0
			47	36	10	1	
29	8	1	Total	C	O	P	0
			21	10	10	1	
29	b	1	Total	C	O	P	0
			47	36	10	1	
29	b	1	Total	C	O	P	0
			49	38	10	1	

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

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



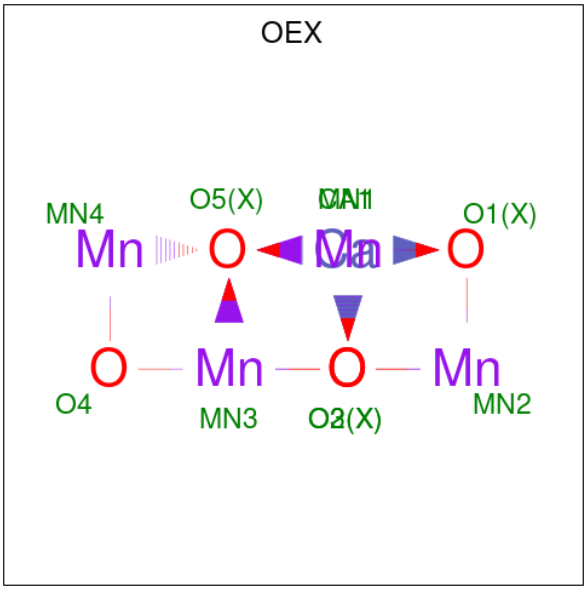
Mol	Chain	Residues	Atoms	AltConf
30	4	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	D	1	Total C 40 40	0
30	H	1	Total C 40 40	0
30	T	1	Total C 40 40	0
30	8	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	d	1	Total C 40 40	0

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

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).

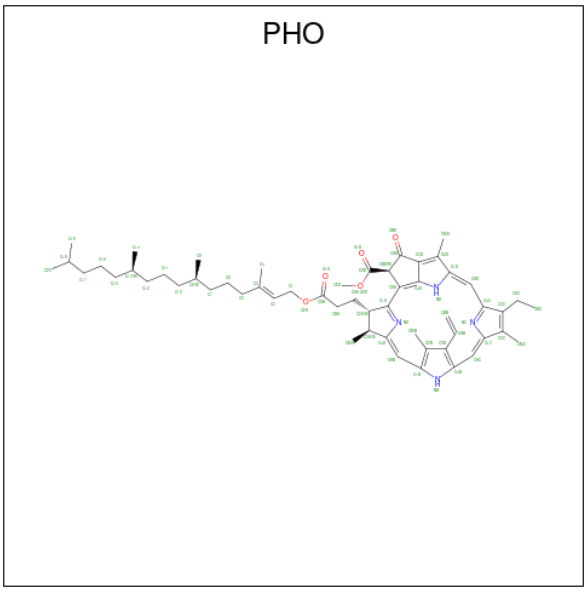


Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total Ca Mn O 10 1 4 5	0
31	a	1	Total Ca Mn O 10 1 4 5	0

- Molecule 32 is FE (II) ION (CCD ID: FE2) (formula: Fe).

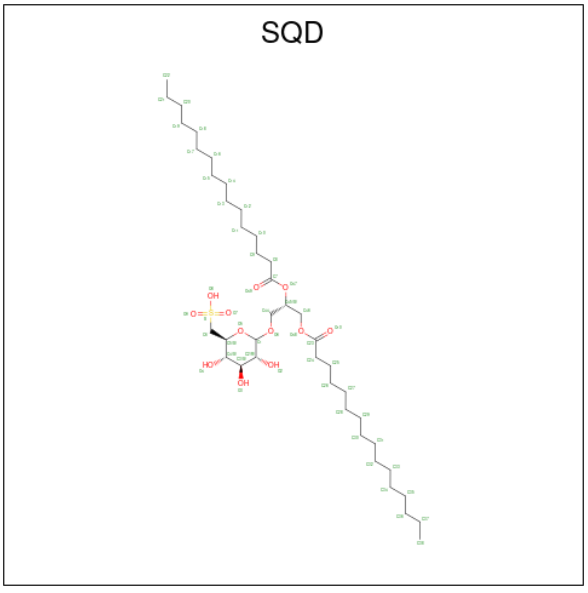
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total Fe 1 1	0
32	a	1	Total Fe 1 1	0

- Molecule 33 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



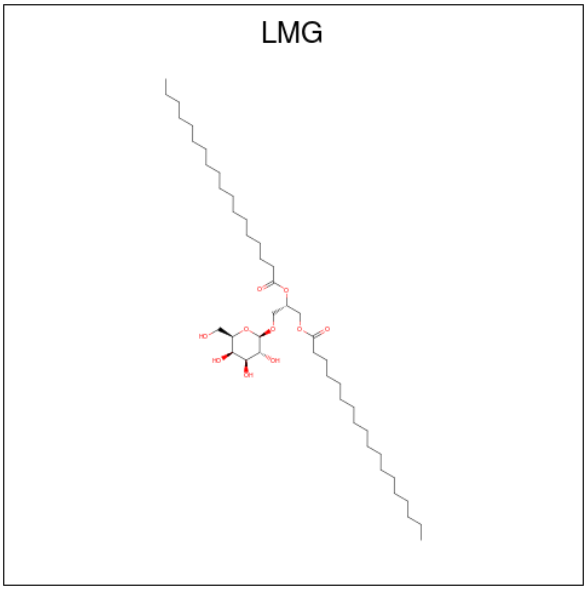
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	N	O	0
			64	55	4	5	
33	A	1	Total	C	N	O	0
			64	55	4	5	
33	a	1	Total	C	N	O	0
			64	55	4	5	
33	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 34 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
34	A	1	Total	C	O	S	0
			50	37	12	1	
34	A	1	Total	C	O	S	0
			54	41	12	1	
34	B	1	Total	C	O	S	0
			54	41	12	1	
34	B	1	Total	C	O	S	0
			42	29	12	1	
34	a	1	Total	C	O	S	0
			50	37	12	1	
34	a	1	Total	C	O	S	0
			54	41	12	1	
34	b	1	Total	C	O	S	0
			54	41	12	1	
34	b	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



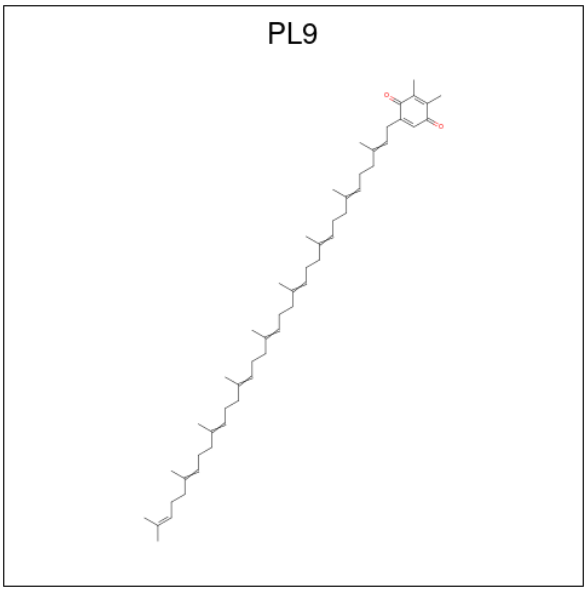
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			48	38	10	
35	A	1	Total	C	O	0
			40	30	10	
35	B	1	Total	C	O	0
			51	41	10	

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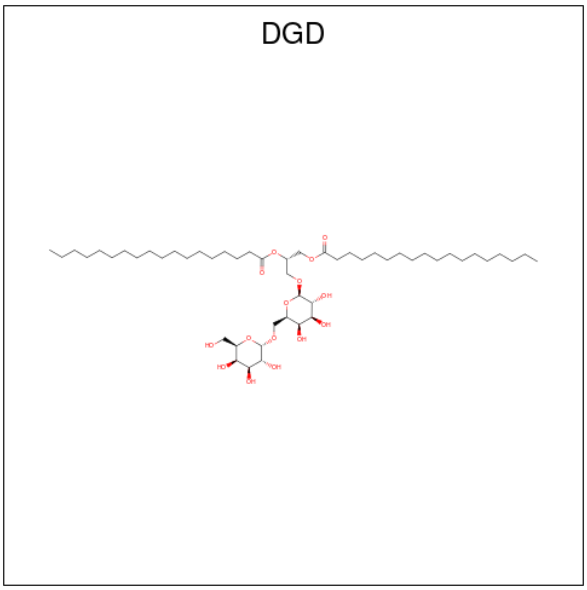
Mol	Chain	Residues	Atoms	AltConf
35	B	1	Total C O 55 45 10	0
35	C	1	Total C O 51 41 10	0
35	D	1	Total C O 46 36 10	0
35	Z	1	Total C O 51 41 10	0
35	a	1	Total C O 48 38 10	0
35	a	1	Total C O 40 30 10	0
35	b	1	Total C O 51 41 10	0
35	b	1	Total C O 55 45 10	0
35	c	1	Total C O 51 41 10	0
35	d	1	Total C O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

- Molecule 36 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
36	A	1	Total C O 13 11 2	0
36	D	1	Total C O 55 53 2	0
36	a	1	Total C O 13 11 2	0
36	d	1	Total C O 55 53 2	0

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



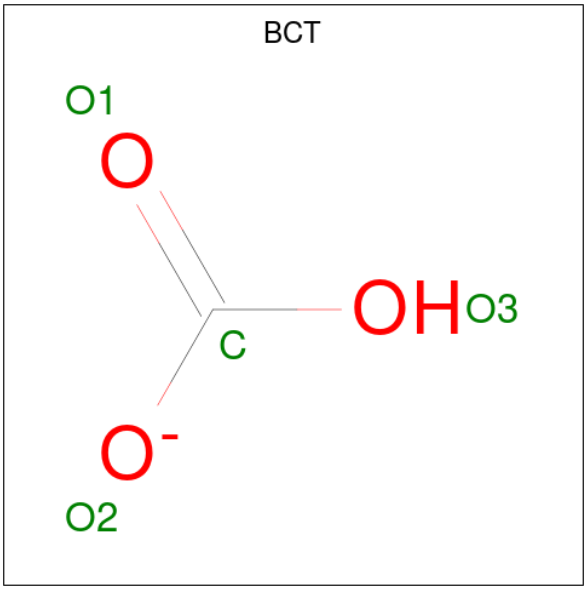
Mol	Chain	Residues	Atoms	AltConf
37	B	1	Total C O 59 44 15	0
37	C	1	Total C O 55 40 15	0
37	C	1	Total C O 62 47 15	0
37	C	1	Total C O 60 45 15	0
37	H	1	Total C O 62 47 15	0
37	b	1	Total C O 59 44 15	0
37	c	1	Total C O 55 40 15	0

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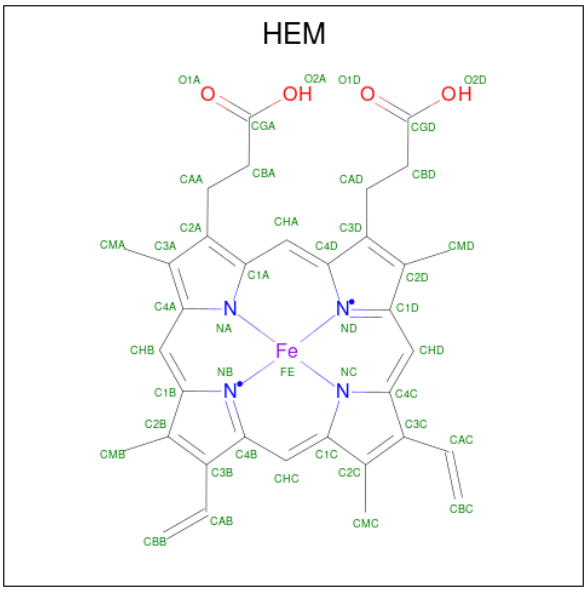
Mol	Chain	Residues	Atoms	AltConf
37	c	1	Total C O 62 47 15	0
37	c	1	Total C O 60 45 15	0
37	h	1	Total C O 62 47 15	0

- Molecule 38 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



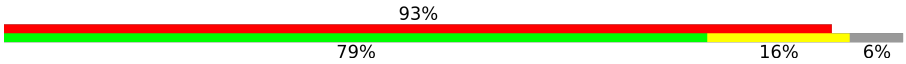
Mol	Chain	Residues	Atoms					AltConf
39	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
39	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

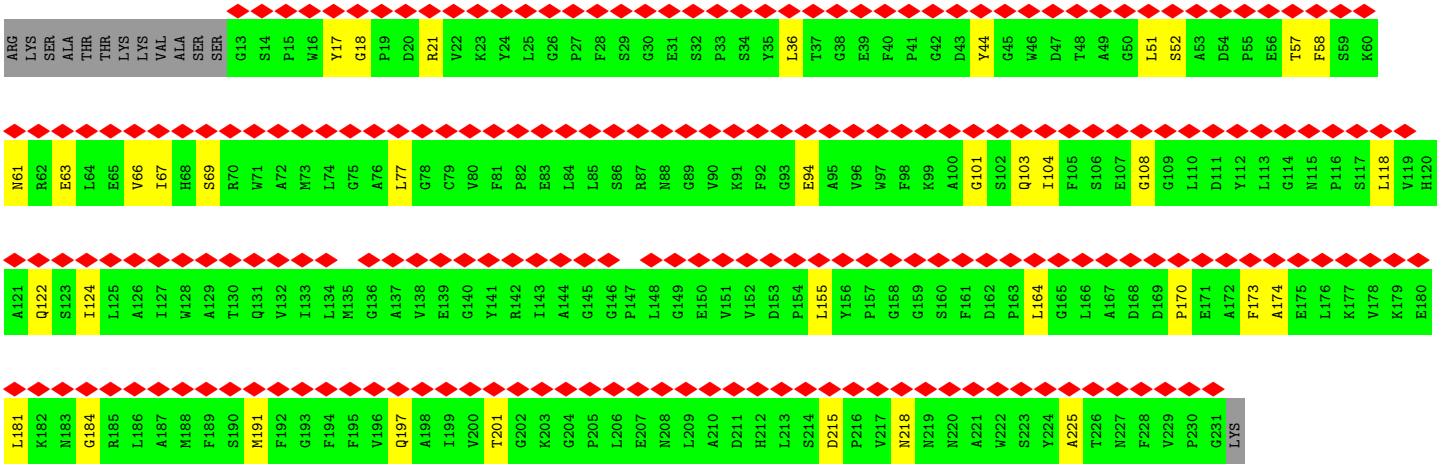
3 Residue-property plots (i)

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

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

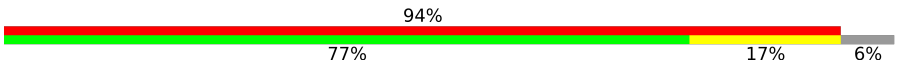
Chain 1:

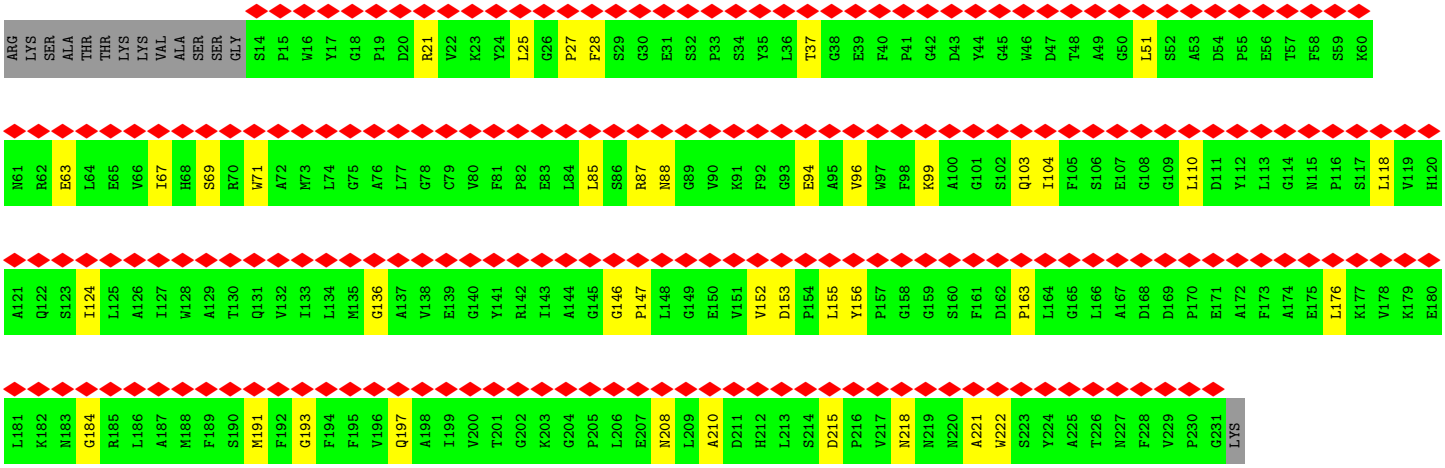




• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

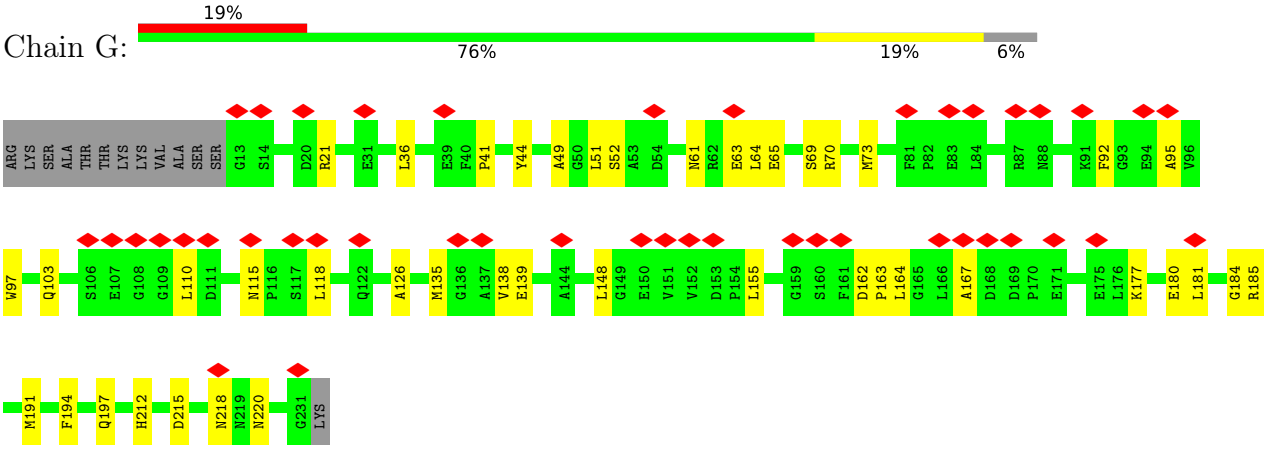
Chain 2:





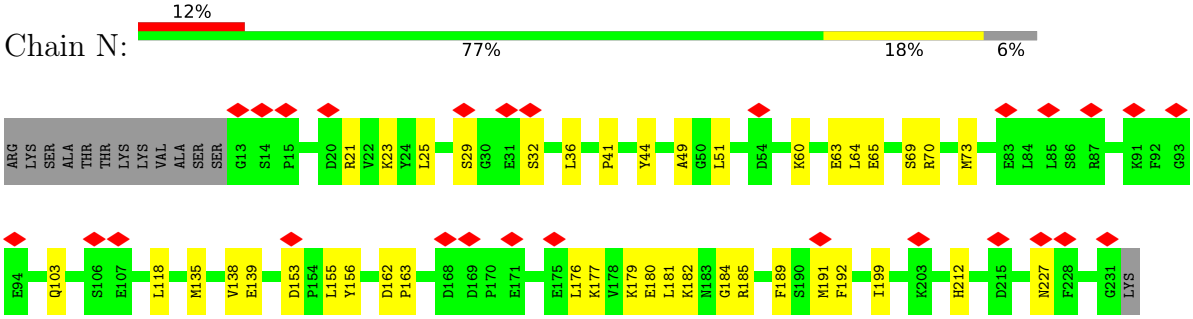
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain G:



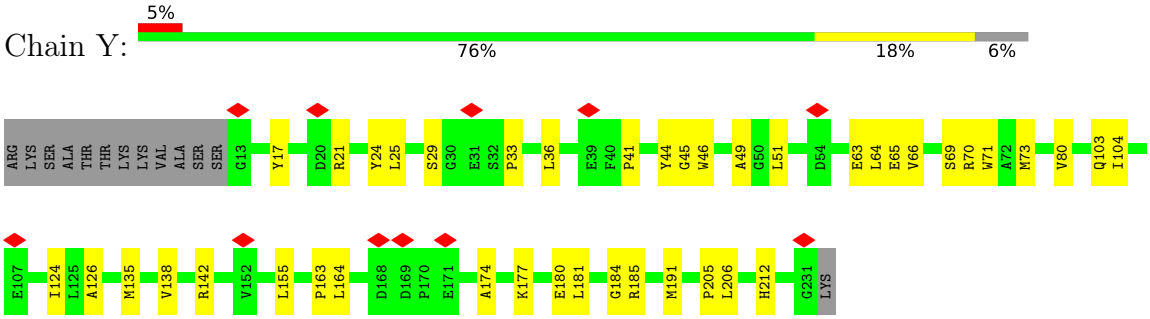
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain N:



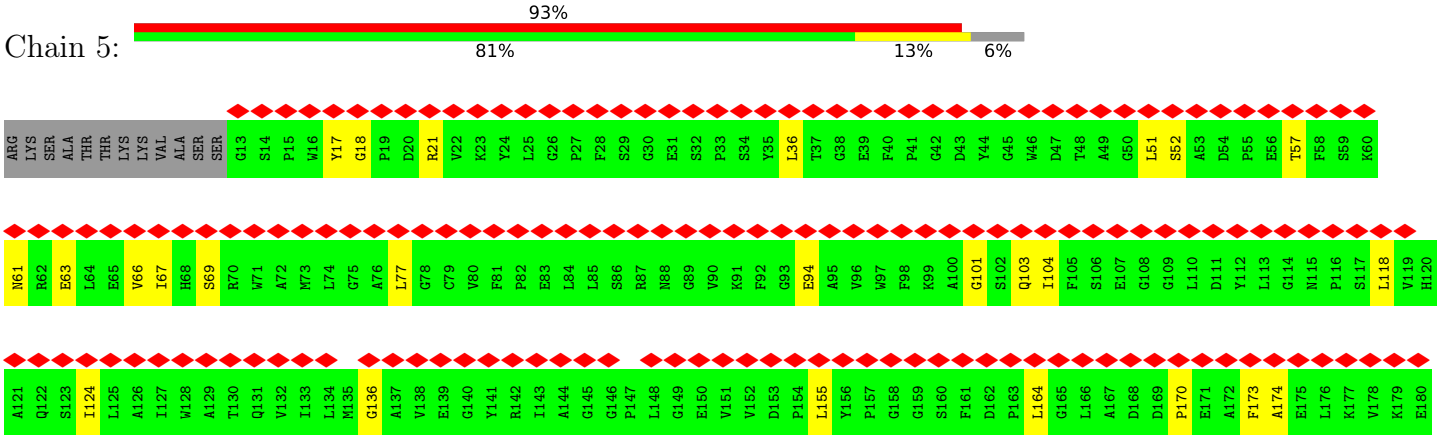
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

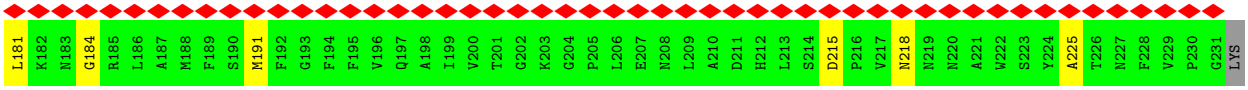
Chain Y:



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

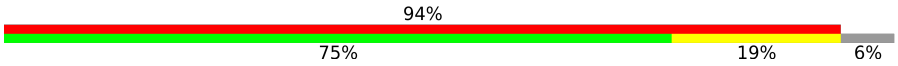
Chain 5:

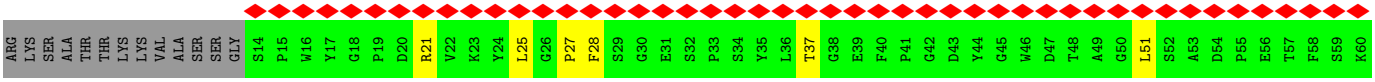


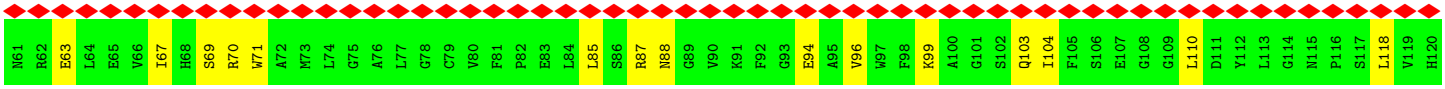


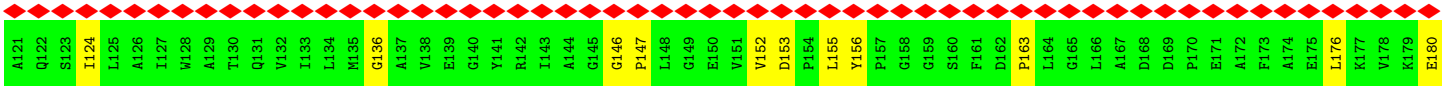
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

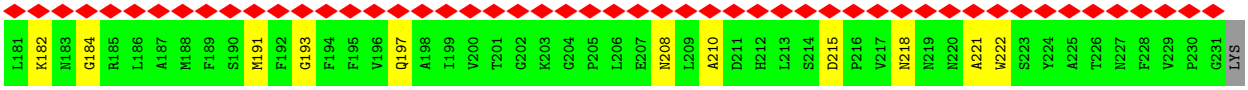
Chain 6:







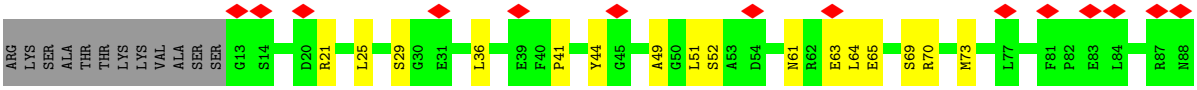


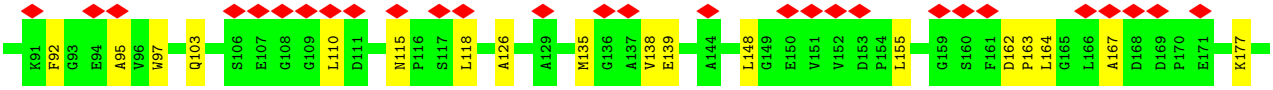


• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain g:





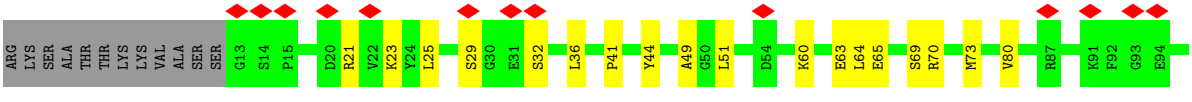




• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain n:

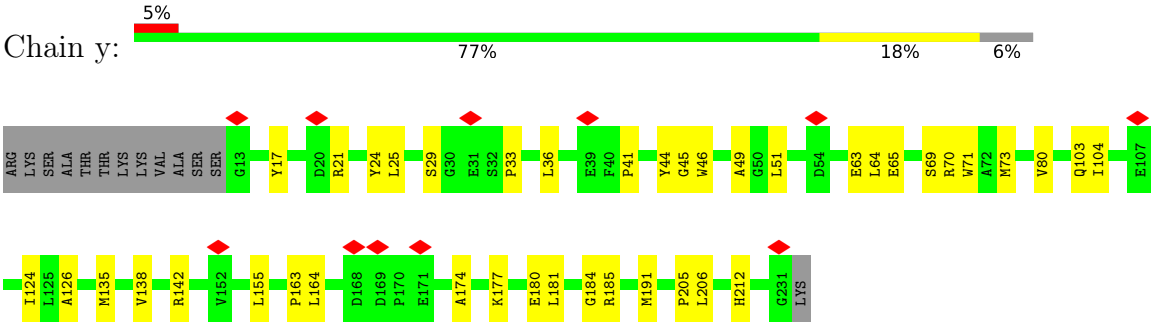






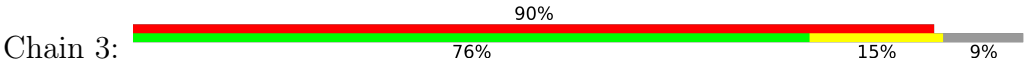
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

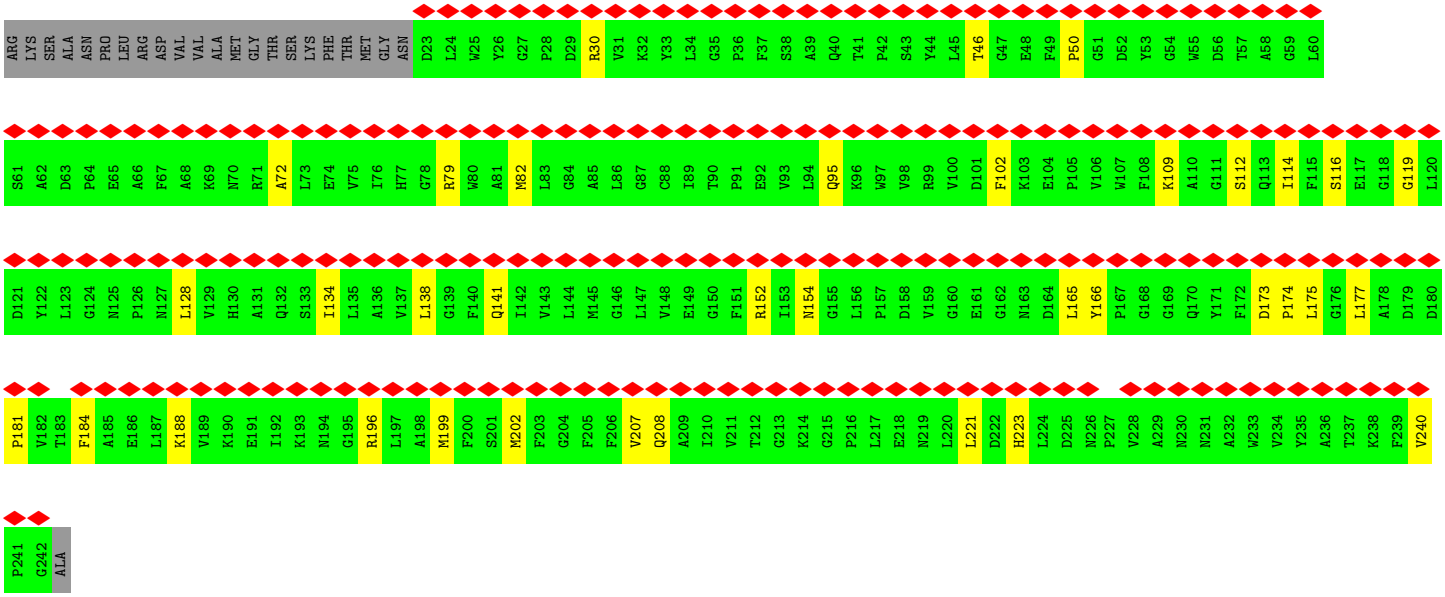
Chain y:



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

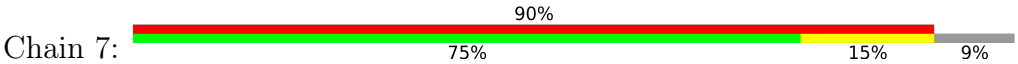
Chain 3:

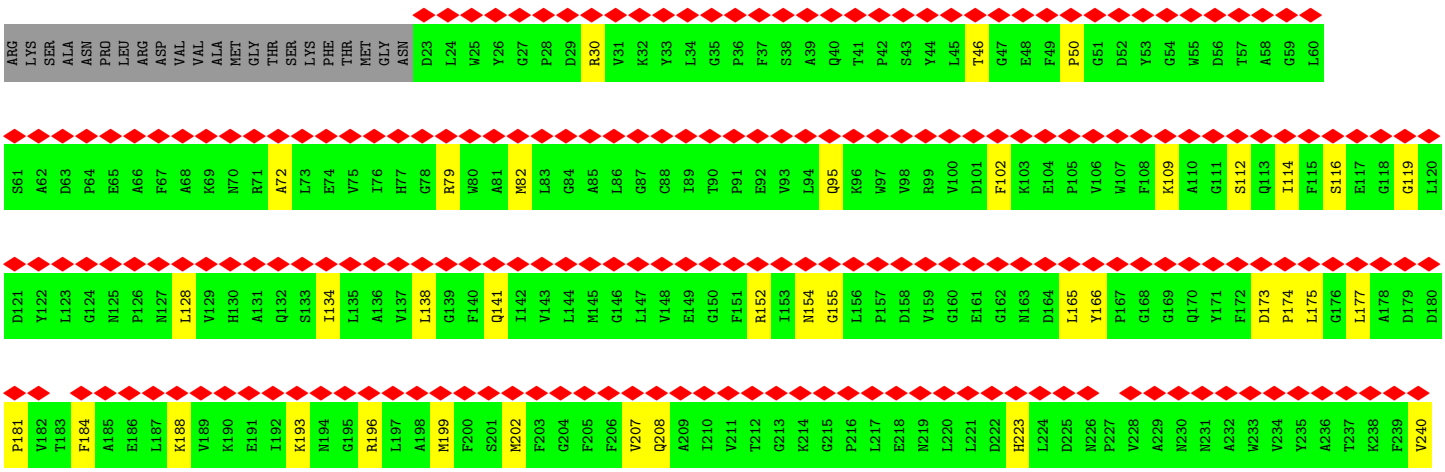




• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 7:

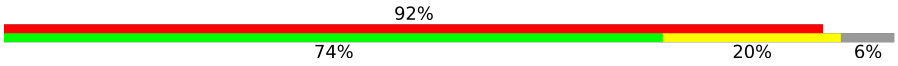


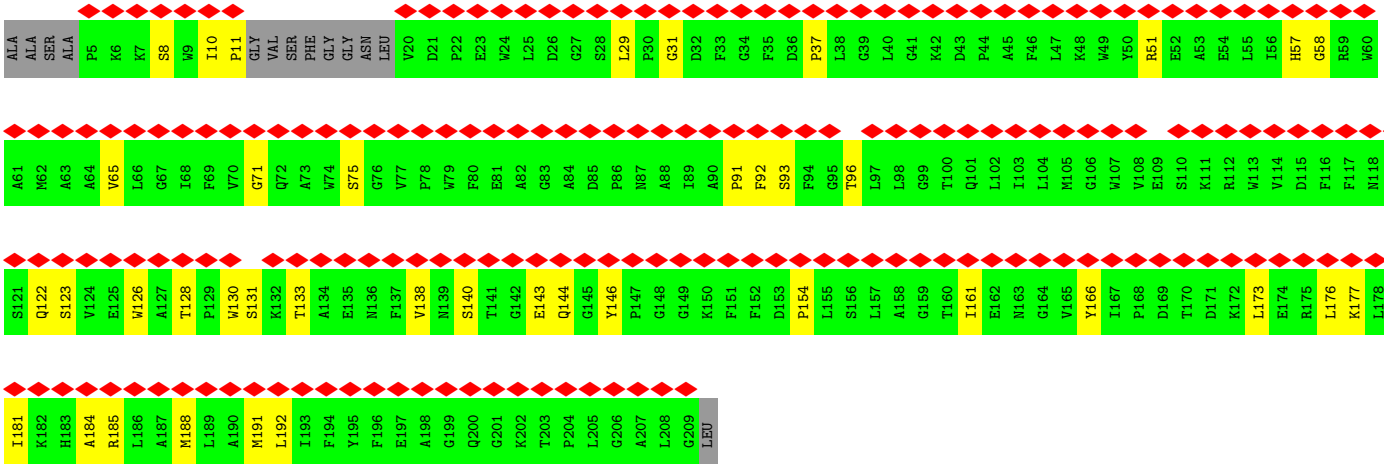




• Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24

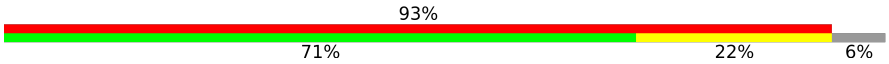
Chain 4:





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

Chain 8:

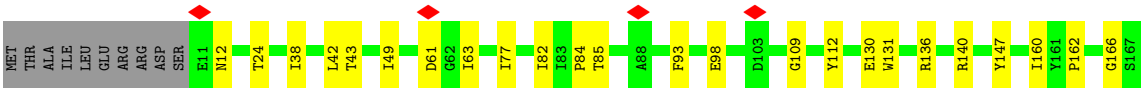


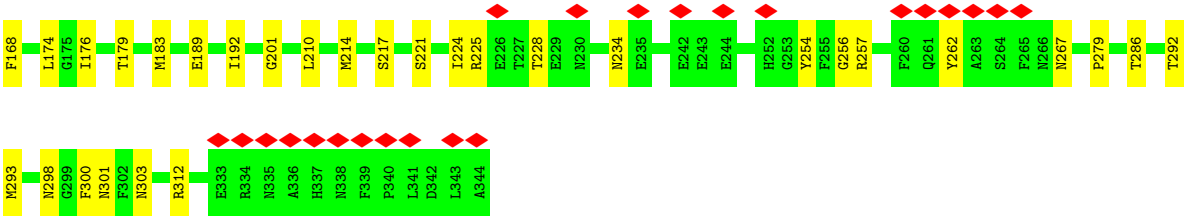


• Molecule 4: Photosystem II protein D1

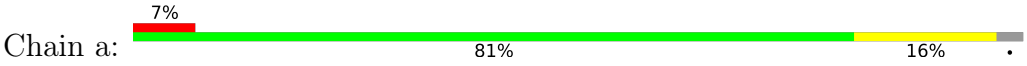
Chain A:

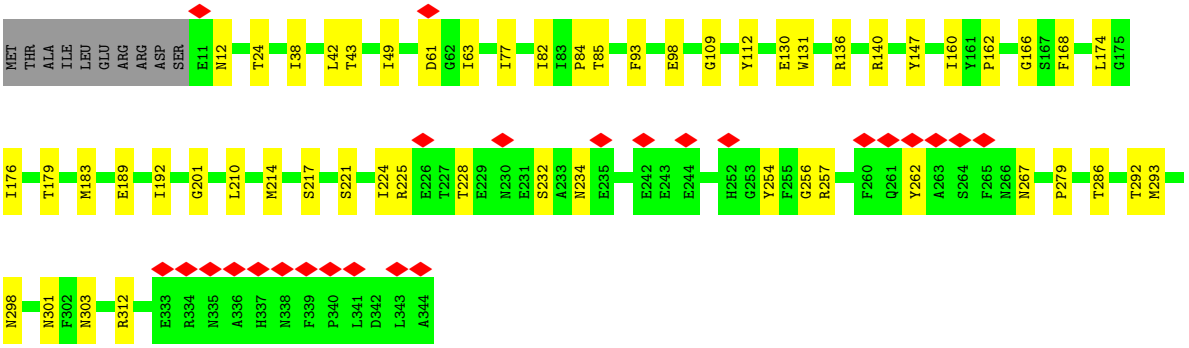




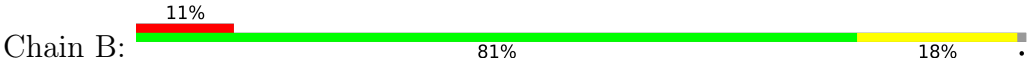


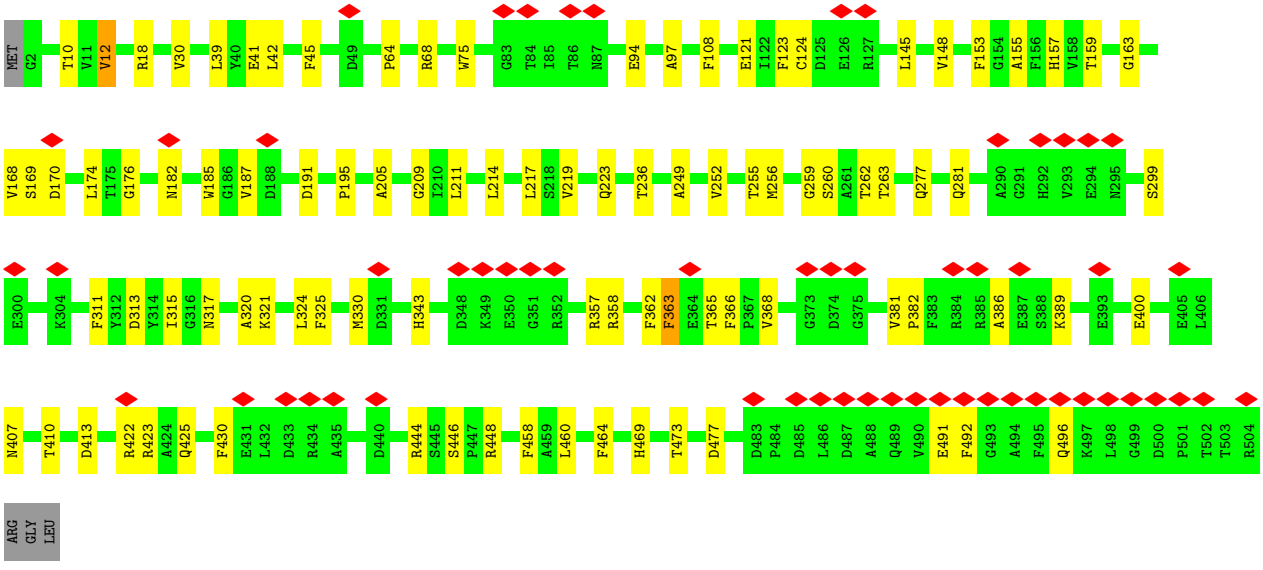
• Molecule 4: Photosystem II protein D1



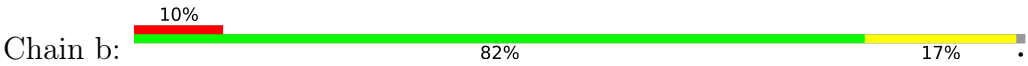


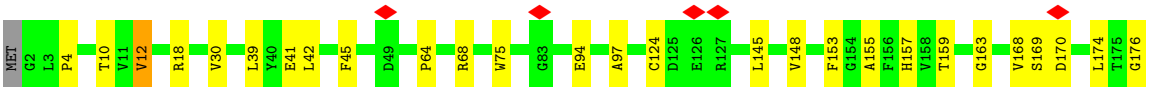
• Molecule 5: Photosystem II CP47 reaction center protein

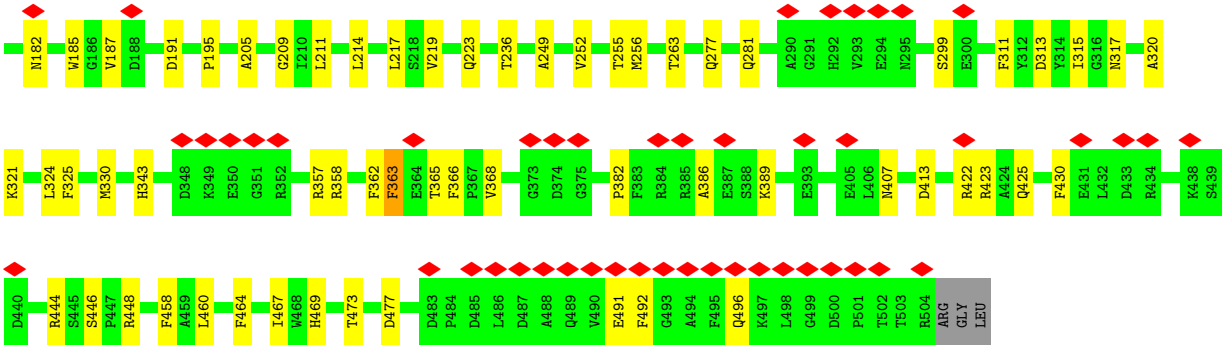




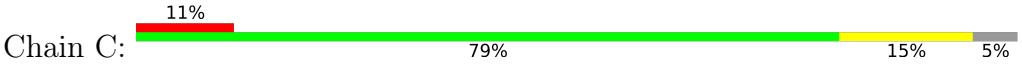
• Molecule 5: Photosystem II CP47 reaction center protein

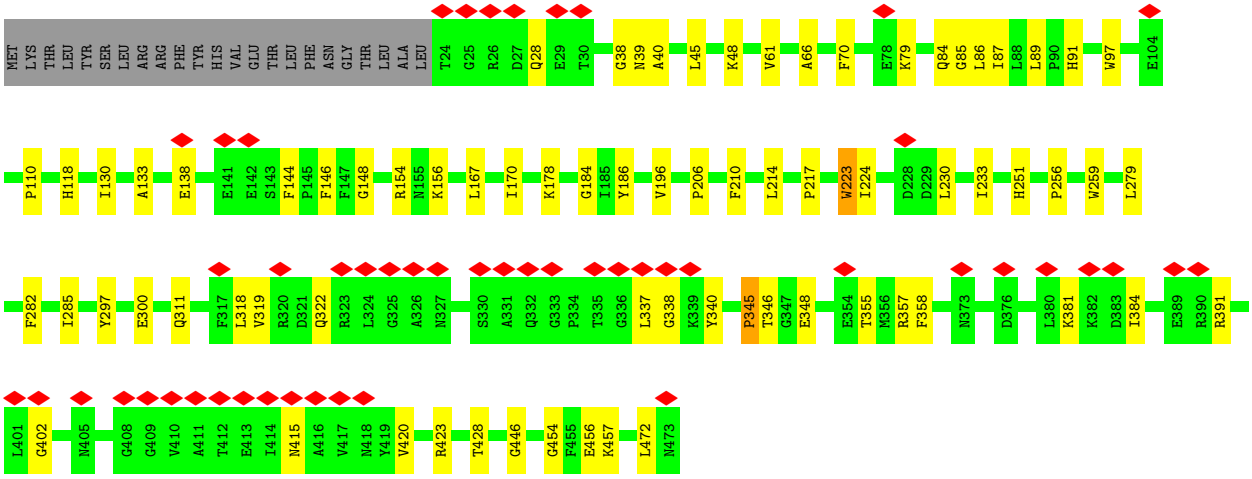




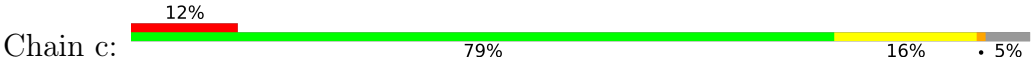


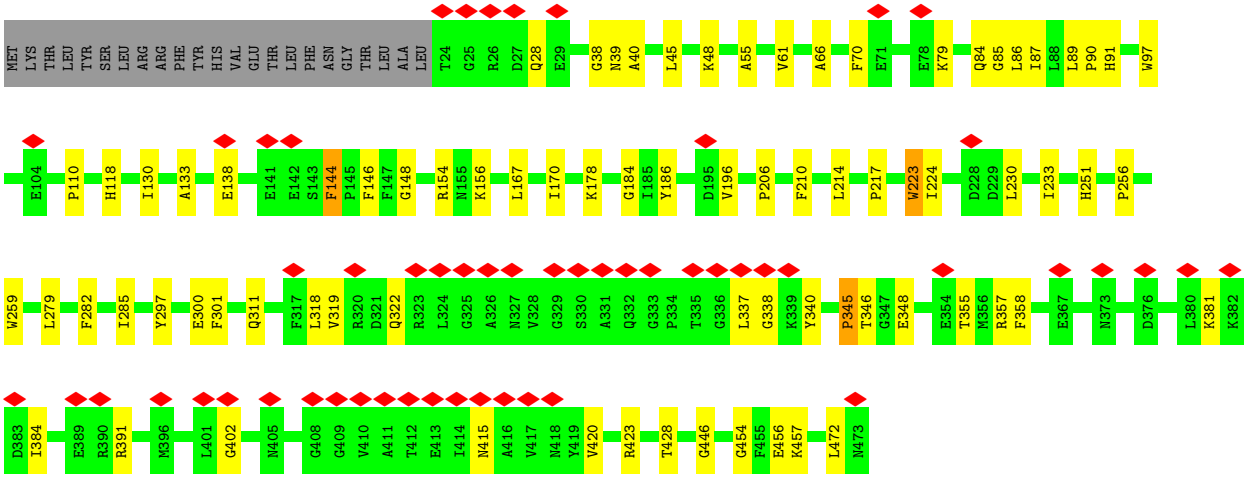
• Molecule 6: Photosystem II CP43 reaction center protein





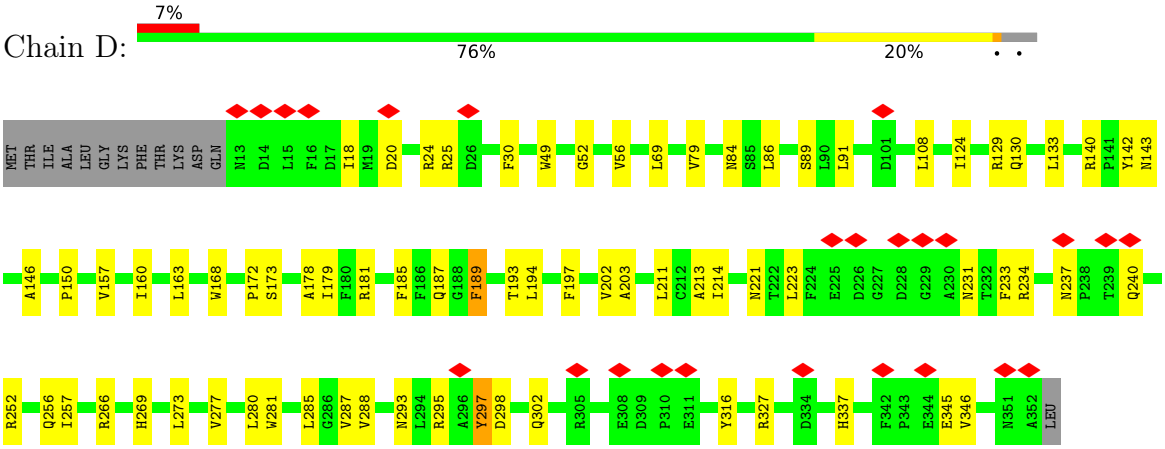
• Molecule 6: Photosystem II CP43 reaction center protein





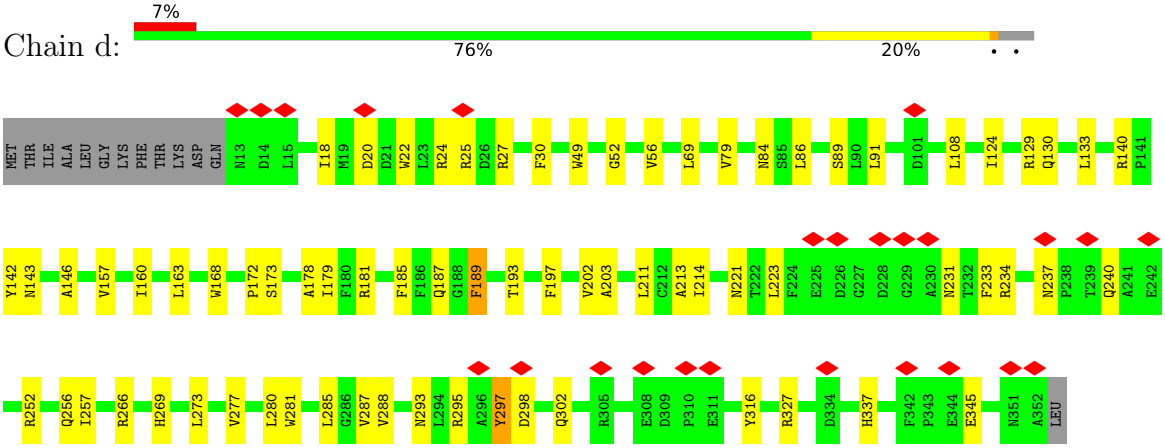
• Molecule 7: Photosystem II D2 protein

Chain D:



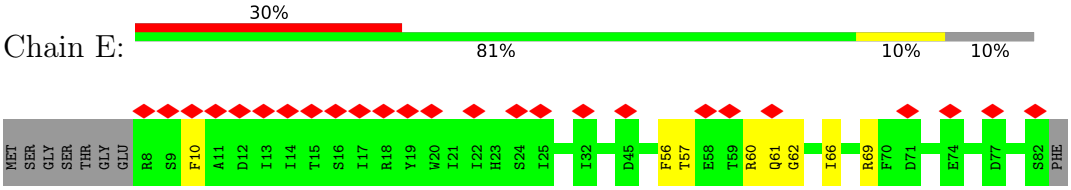
• Molecule 7: Photosystem II D2 protein

Chain d:



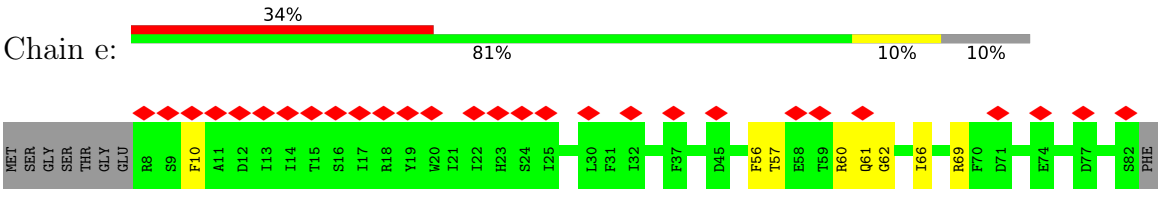
• Molecule 8: Cytochrome b559 subunit alpha

Chain E:



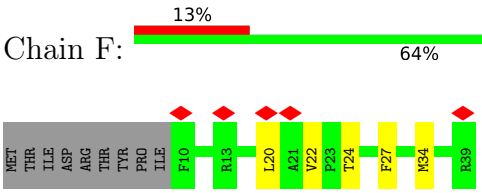
• Molecule 8: Cytochrome b559 subunit alpha

Chain e:



• Molecule 9: Cytochrome b559 subunit beta, PsbF

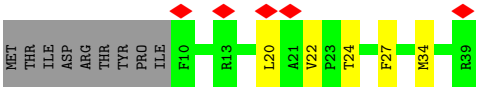
Chain F:



• Molecule 9: Cytochrome b559 subunit beta, PsbF

Chain f:





• Molecule 10: Photosystem II reaction center protein H

Chain H:

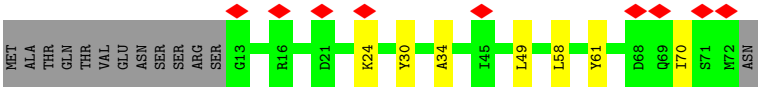




• Molecule 10: Photosystem II reaction center protein H

Chain h:

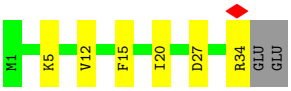




• Molecule 11: Photosystem II reaction center protein I, PsbI

Chain I:

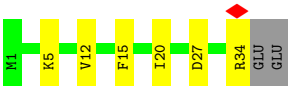




• Molecule 11: Photosystem II reaction center protein I, PsbI

Chain i:

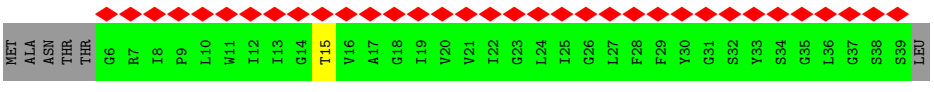




• Molecule 12: Photosystem II reaction center protein J

Chain J:

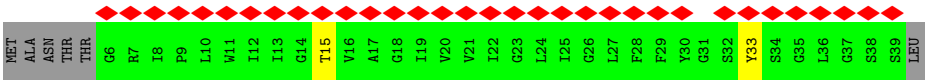




• Molecule 12: Photosystem II reaction center protein J

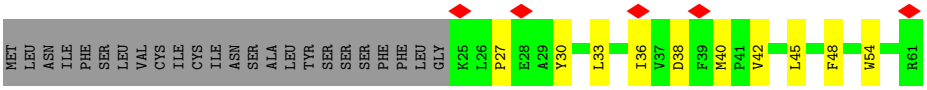
Chain j:





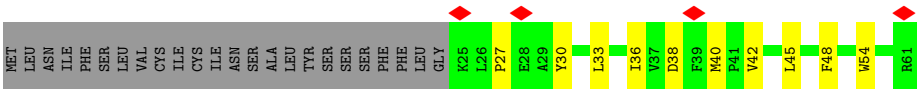
• Molecule 13: Photosystem II reaction center protein K





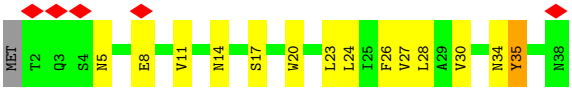
• Molecule 13: Photosystem II reaction center protein K





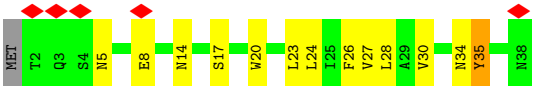
• Molecule 14: Photosystem II reaction center protein L



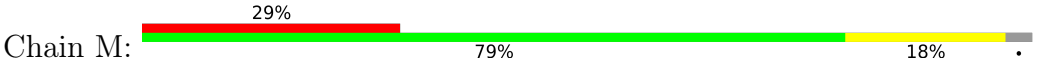


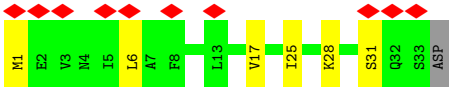
• Molecule 14: Photosystem II reaction center protein L



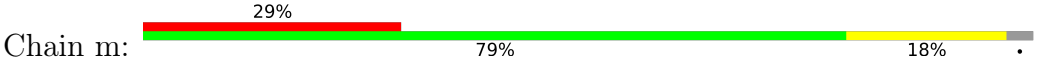


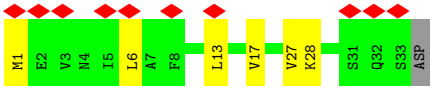
• Molecule 15: Photosystem II reaction center protein M





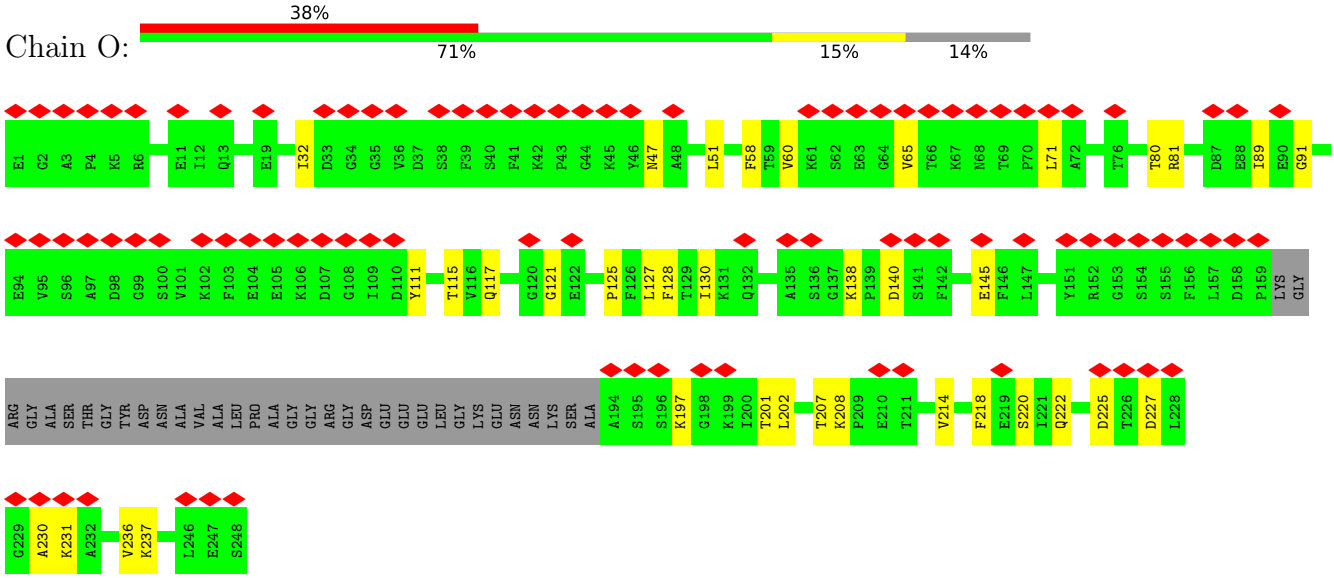
• Molecule 15: Photosystem II reaction center protein M





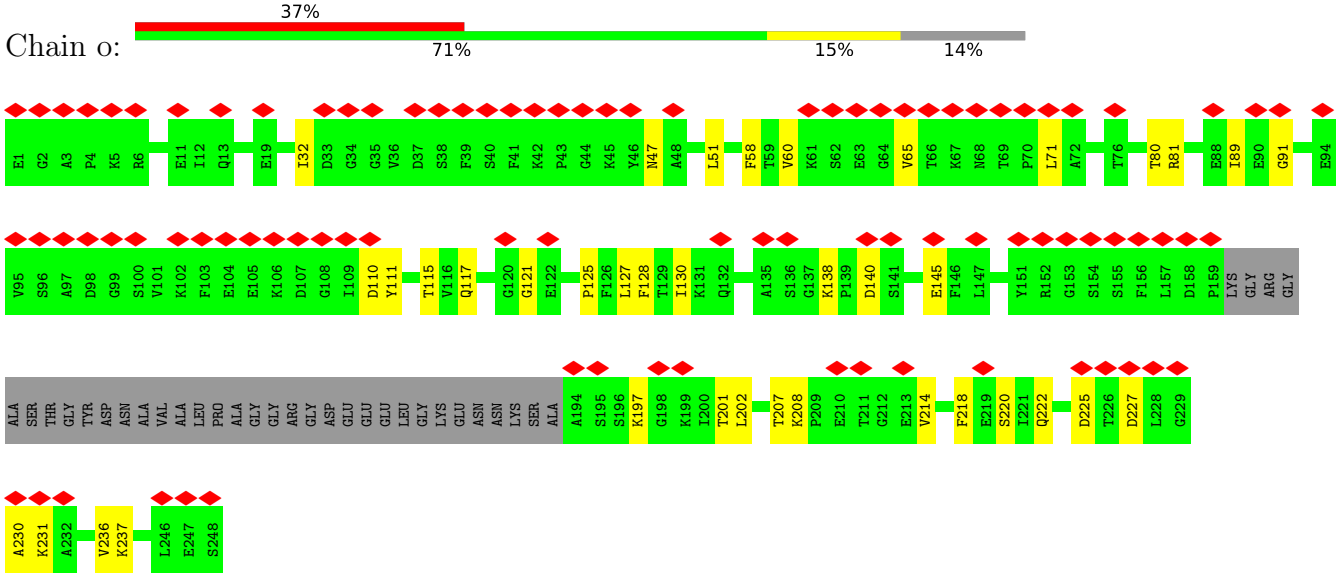
• Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic

Chain O:



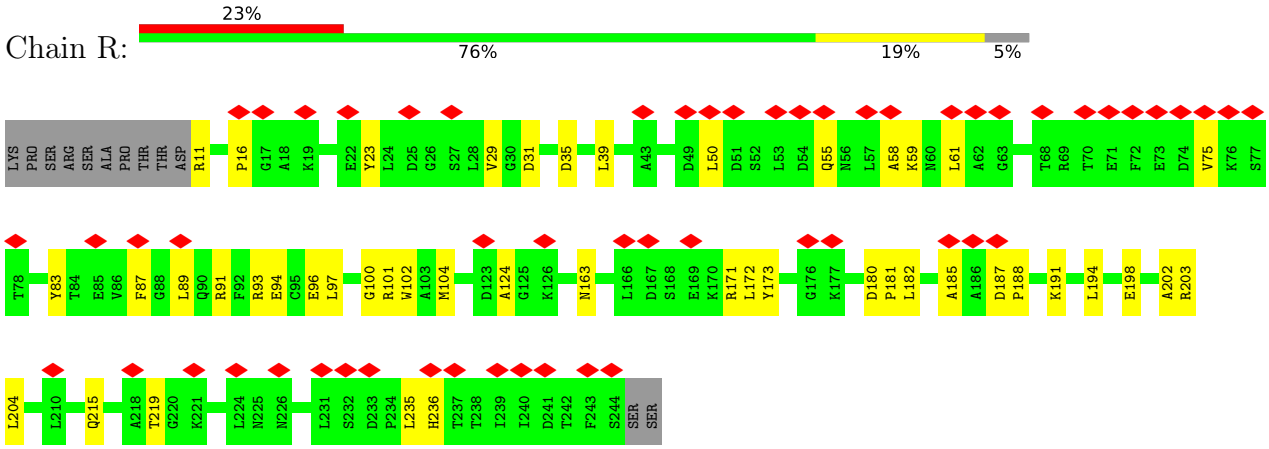
• Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic

Chain o:



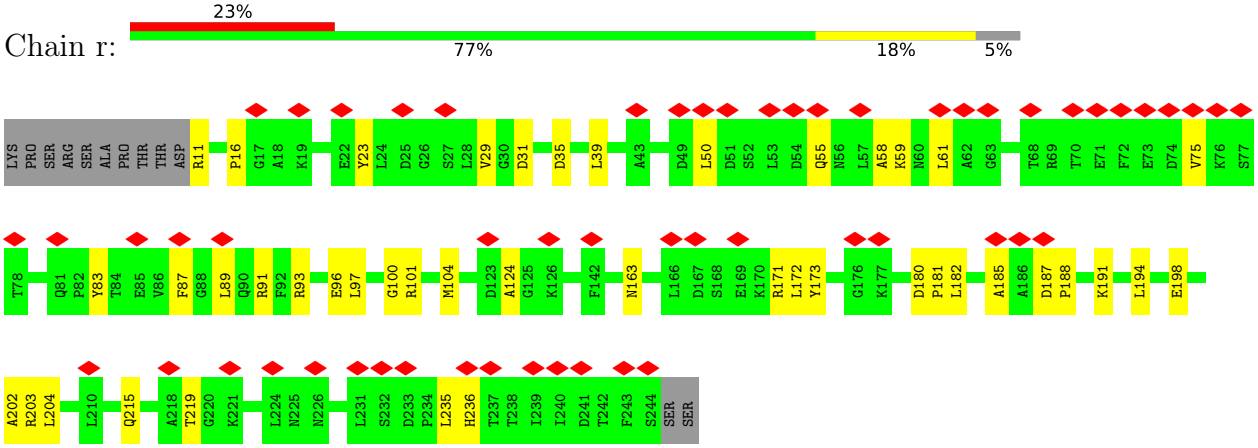
• Molecule 17: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29

Chain R:



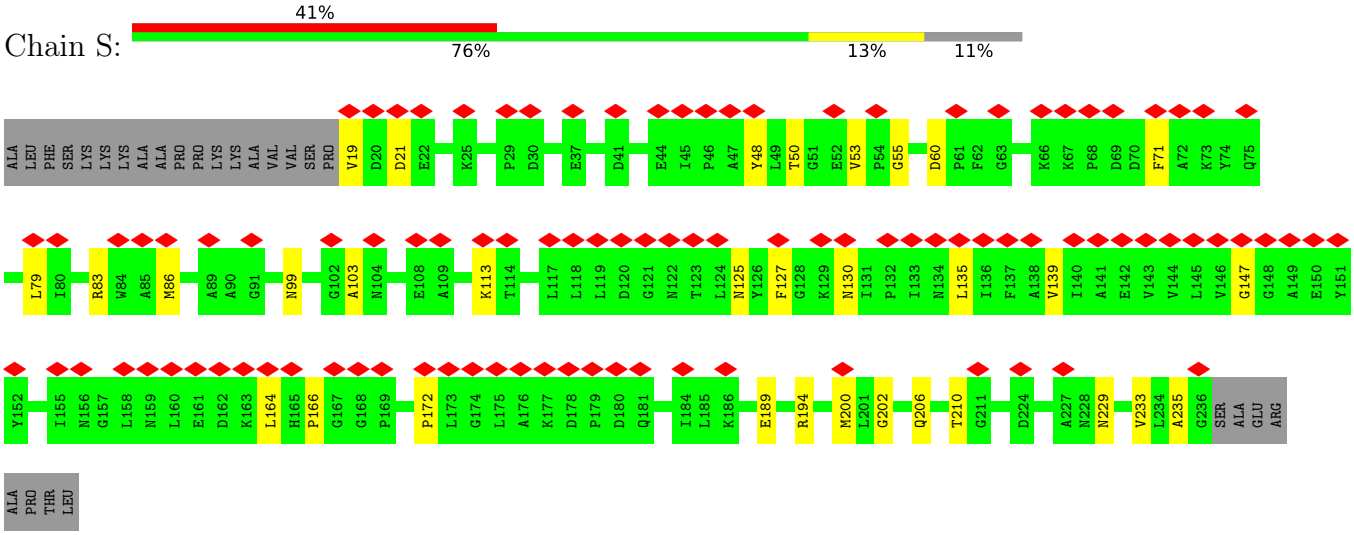
• Molecule 17: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29

Chain r:



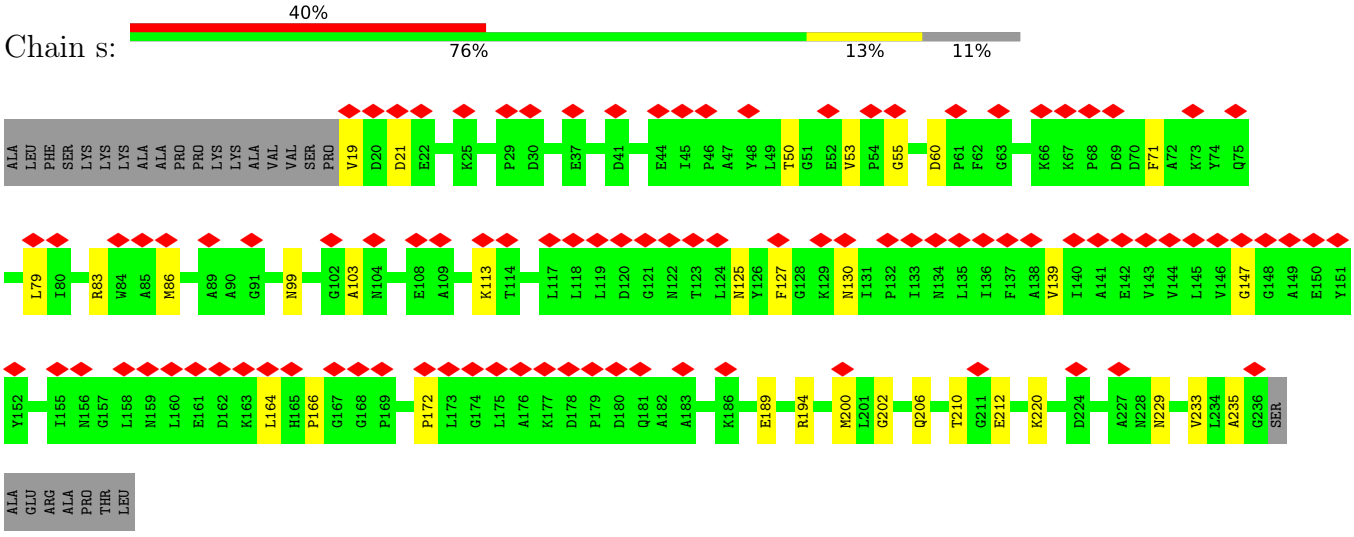
• Molecule 18: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

Chain S:

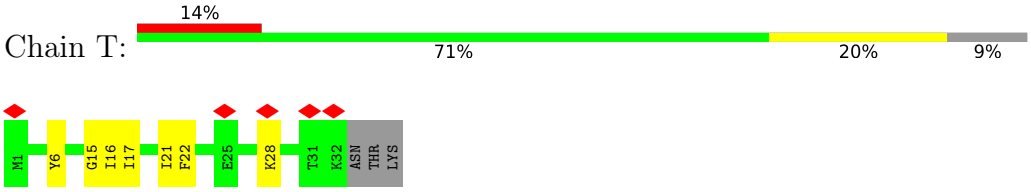


• Molecule 18: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

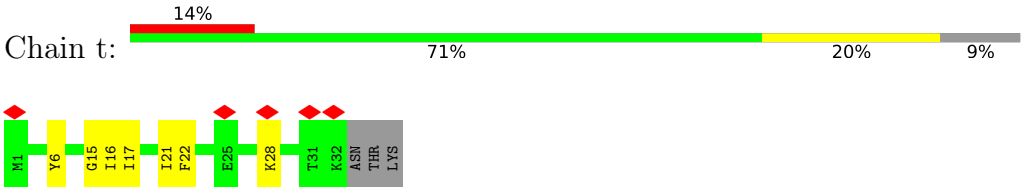
Chain s:



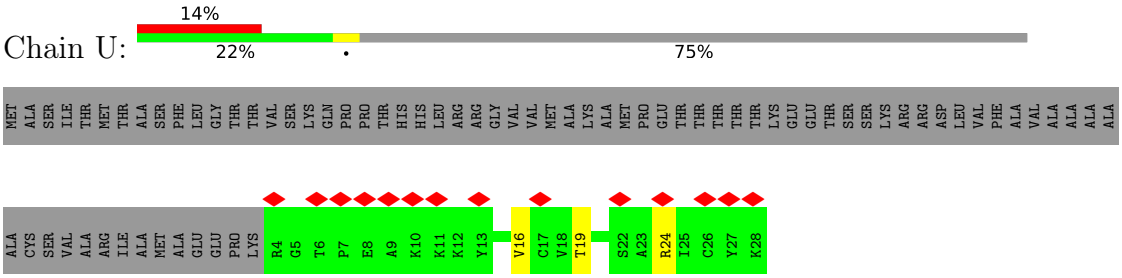
• Molecule 19: Photosystem II reaction center protein T



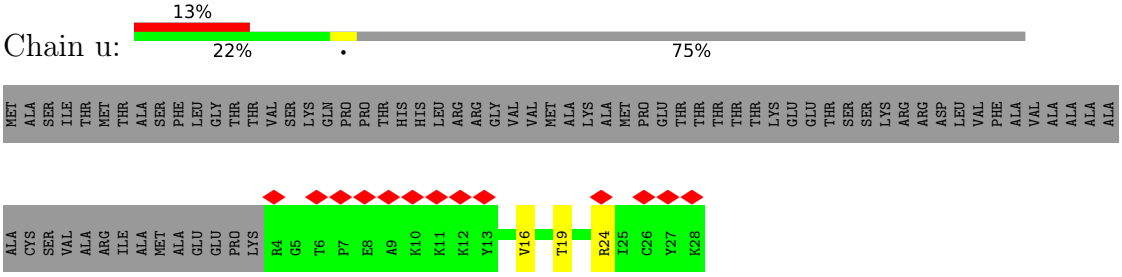
• Molecule 19: Photosystem II reaction center protein T



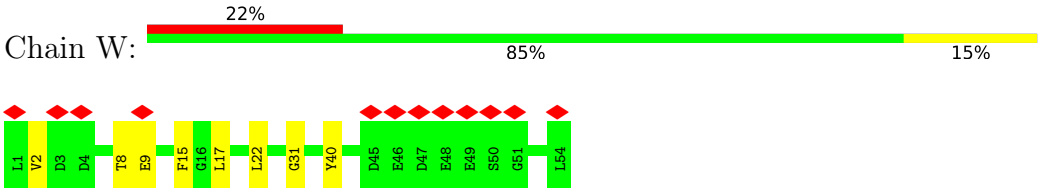
• Molecule 20: Photosystem II luminal extrinsic protein Tn, PsbTn



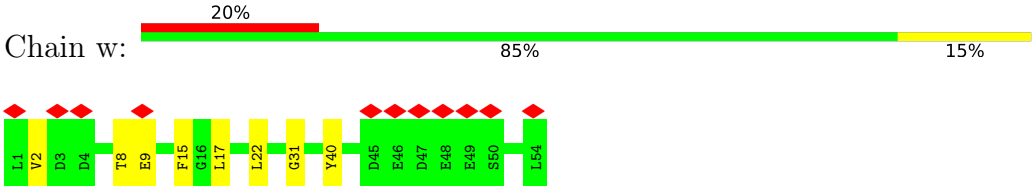
• Molecule 20: Photosystem II luminal extrinsic protein Tn, PsbTn



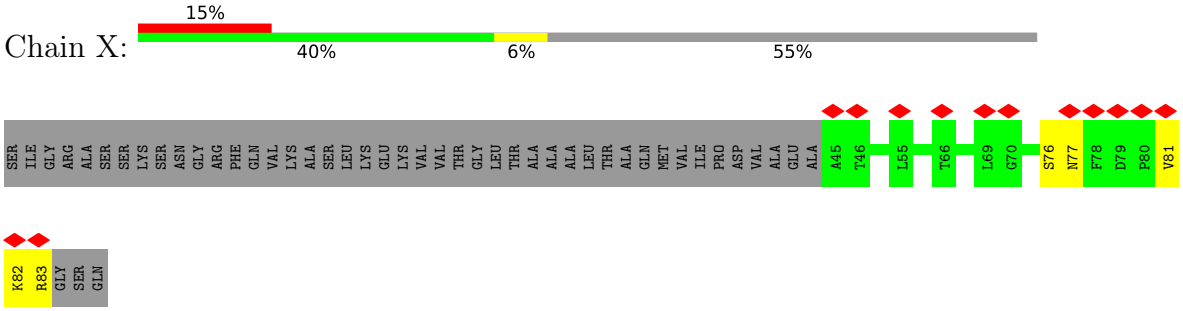
• Molecule 21: Photosystem II reaction center protein W, PSBW



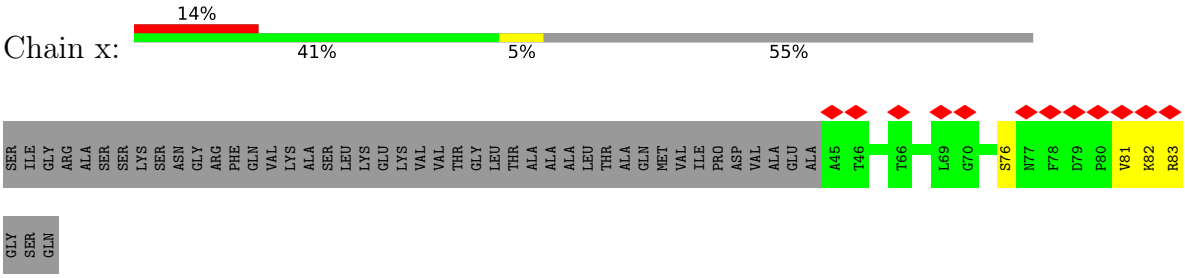
• Molecule 21: Photosystem II reaction center protein W, PSBW



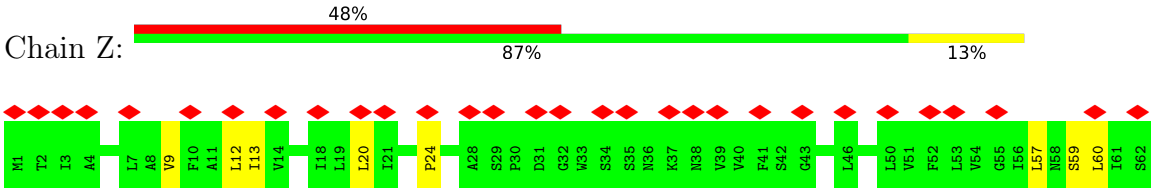
• Molecule 22: Photosystem II reaction center protein X



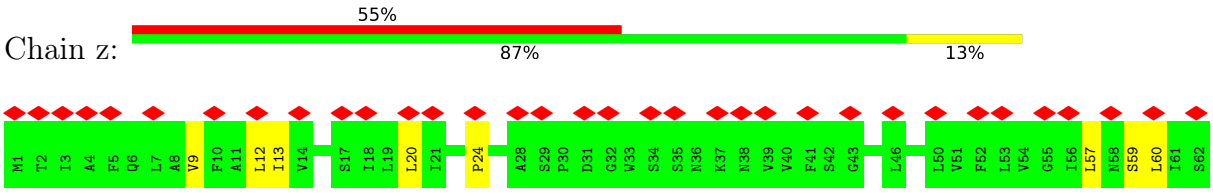
• Molecule 22: Photosystem II reaction center protein X



• Molecule 23: Photosystem II reaction center protein Z



• Molecule 23: Photosystem II reaction center protein Z



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	50237	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	0.118	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.026	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, LMG, SQD, HEM, BCT, XAT, LHG, CLA, NEX, PL9, FE2, PHO, CHL, OEX, BCR, LUT

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	0.42	0/1720	0.55	0/2342
1	2	0.36	0/1716	0.57	1/2337 (0.0%)
1	5	0.42	0/1720	0.55	0/2342
1	6	0.36	0/1716	0.57	1/2337 (0.0%)
1	G	0.41	0/1720	0.54	0/2342
1	N	0.42	0/1720	0.54	1/2342 (0.0%)
1	Y	0.49	0/1720	0.57	0/2342
1	g	0.41	0/1720	0.54	0/2342
1	n	0.42	0/1720	0.54	1/2342 (0.0%)
1	y	0.49	0/1720	0.57	0/2342
2	3	0.42	0/1759	0.58	0/2396
2	7	0.42	0/1759	0.58	0/2396
3	4	0.39	0/1586	0.65	0/2158
3	8	0.39	0/1586	0.66	0/2158
4	A	0.43	0/2697	0.57	0/3677
4	a	0.43	0/2697	0.57	0/3677
5	B	0.51	1/4081 (0.0%)	0.61	1/5556 (0.0%)
5	b	0.51	1/4081 (0.0%)	0.61	1/5556 (0.0%)
6	C	0.34	0/3614	0.57	4/4922 (0.1%)
6	c	0.34	0/3614	0.57	4/4922 (0.1%)
7	D	0.60	0/2795	0.68	3/3812 (0.1%)
7	d	0.60	0/2795	0.68	3/3812 (0.1%)
8	E	0.28	0/630	0.52	0/857
8	e	0.28	0/630	0.52	0/857
9	F	0.45	1/248 (0.4%)	0.51	0/335
9	f	0.44	1/248 (0.4%)	0.51	0/335
10	H	0.45	0/461	0.54	0/626
10	h	0.45	0/461	0.54	0/626
11	I	0.52	0/286	0.67	0/386
11	i	0.53	0/286	0.67	0/386
12	J	0.27	0/253	0.67	0/343
12	j	0.27	0/253	0.67	0/343

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
13	K	0.52	0/318	0.94	2/434 (0.5%)
13	k	0.52	0/318	0.94	2/434 (0.5%)
14	L	0.52	0/319	0.74	1/434 (0.2%)
14	l	0.52	0/319	0.74	1/434 (0.2%)
15	M	0.57	0/260	0.75	0/355
15	m	0.57	0/260	0.75	0/355
16	O	0.39	0/1664	0.55	0/2250
16	o	0.39	0/1664	0.55	0/2250
17	R	0.40	0/1886	0.61	1/2569 (0.0%)
17	r	0.41	0/1886	0.61	1/2569 (0.0%)
18	S	0.27	0/1736	0.55	0/2359
18	s	0.27	0/1736	0.55	0/2359
19	T	0.43	0/269	0.45	0/365
19	t	0.44	0/269	0.46	0/365
20	U	0.33	0/197	0.69	0/264
20	u	0.33	0/197	0.69	0/264
21	W	0.44	0/429	0.54	0/581
21	w	0.44	0/429	0.54	0/581
22	X	0.58	1/279 (0.4%)	0.62	0/380
22	x	0.58	0/279	0.62	0/380
23	Z	0.37	0/474	0.53	0/648
23	z	0.37	0/474	0.53	0/648
All	All	0.44	5/69674 (0.0%)	0.59	28/94824 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	343	HIS	C-N	5.98	1.39	1.33
5	b	343	HIS	C-N	5.98	1.39	1.33
9	F	22	VAL	CA-CB	-5.59	1.51	1.54
9	f	22	VAL	CA-CB	-5.50	1.51	1.54
22	X	77	ASN	CA-C	-5.00	1.46	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	k	42	VAL	CA-C-N	8.86	125.82	120.24
13	k	42	VAL	C-N-CA	8.86	125.82	120.24
13	K	42	VAL	CA-C-N	8.78	125.77	120.24
13	K	42	VAL	C-N-CA	8.78	125.77	120.24
5	B	363	PHE	N-CA-C	6.57	119.31	109.25
5	b	363	PHE	N-CA-C	6.56	119.29	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	d	168	TRP	N-CA-C	-6.45	105.38	113.18
7	D	168	TRP	N-CA-C	-6.44	105.39	113.18
14	L	35	TYR	N-CA-C	6.13	118.04	111.36
17	R	29	VAL	N-CA-C	6.10	116.16	110.42
14	l	35	TYR	N-CA-C	6.09	118.00	111.36
17	r	29	VAL	N-CA-C	6.05	116.11	110.42
7	d	189	PHE	N-CA-C	6.04	117.94	111.36
7	D	189	PHE	N-CA-C	6.03	117.93	111.36
6	C	223	TRP	CB-CA-C	-5.70	109.99	116.54
6	c	223	TRP	CB-CA-C	-5.69	110.00	116.54
6	c	345	PRO	N-CA-C	-5.36	106.08	113.53
6	C	345	PRO	N-CA-C	-5.34	106.11	113.53
6	C	144	PHE	CA-C-N	-5.20	114.31	119.56
6	C	144	PHE	C-N-CA	-5.20	114.31	119.56
7	D	297	TYR	N-CA-C	5.20	116.75	111.14
7	d	297	TYR	N-CA-C	5.18	116.74	111.14
6	c	144	PHE	CA-C-N	-5.14	114.37	119.56
6	c	144	PHE	C-N-CA	-5.14	114.37	119.56
1	n	227	ASN	N-CA-C	5.08	116.82	111.28
1	N	227	ASN	N-CA-C	5.05	116.78	111.28
1	6	152	VAL	N-CA-C	-5.03	106.75	111.48
1	2	152	VAL	N-CA-C	-5.02	106.76	111.48

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	29	0
1	5	1668	0	1596	24	0
1	6	1664	0	1593	30	0
1	G	1668	0	1596	37	0
1	N	1668	0	1596	36	0
1	Y	1668	0	1596	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	g	1668	0	1596	39	0
1	n	1668	0	1596	38	0
1	y	1668	0	1596	33	0
2	3	1707	0	1659	29	0
2	7	1707	0	1659	31	0
3	4	1534	0	1486	32	0
3	8	1534	0	1486	36	0
4	A	2616	0	2522	54	0
4	a	2616	0	2522	55	0
5	B	3948	0	3818	83	0
5	b	3948	0	3818	78	0
6	C	3497	0	3422	59	0
6	c	3497	0	3422	62	0
7	D	2703	0	2593	62	0
7	d	2703	0	2593	61	0
8	E	612	0	595	6	0
8	e	612	0	595	7	0
9	F	241	0	246	3	0
9	f	241	0	246	4	0
10	H	452	0	473	12	0
10	h	452	0	473	11	0
11	I	278	0	291	7	0
11	i	278	0	291	7	0
12	J	247	0	258	1	0
12	j	247	0	258	2	0
13	K	306	0	313	13	0
13	k	306	0	313	13	0
14	L	311	0	299	20	0
14	l	311	0	299	18	0
15	M	256	0	284	6	0
15	m	256	0	284	6	0
16	O	1631	0	1625	24	0
16	o	1631	0	1625	25	0
17	R	1835	0	1801	43	0
17	r	1835	0	1801	42	0
18	S	1689	0	1670	25	0
18	s	1689	0	1670	24	0
19	T	261	0	280	9	0
19	t	261	0	280	9	0
20	U	193	0	205	4	0
20	u	193	0	205	4	0
21	W	419	0	402	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	w	419	0	402	8	0
22	X	276	0	301	4	0
22	x	276	0	301	4	0
23	Z	464	0	493	7	0
23	z	464	0	493	7	0
24	1	309	0	244	10	0
24	2	306	0	238	10	0
24	3	316	0	254	15	0
24	4	229	0	152	3	0
24	5	309	0	244	13	0
24	6	306	0	238	11	0
24	7	316	0	254	17	0
24	8	229	0	152	3	0
24	G	355	0	335	15	0
24	N	362	0	350	13	0
24	R	225	0	201	4	0
24	S	196	0	144	5	0
24	Y	362	0	350	16	0
24	g	355	0	335	16	0
24	n	362	0	350	13	0
24	r	225	0	201	3	0
24	s	196	0	144	5	0
24	y	362	0	350	17	0
25	1	412	0	348	12	0
25	2	391	0	314	13	0
25	3	426	0	373	11	0
25	4	270	0	198	4	0
25	5	412	0	348	11	0
25	6	391	0	314	14	0
25	7	426	0	373	13	0
25	8	270	0	198	5	0
25	A	240	0	242	15	0
25	B	1040	0	1152	55	0
25	C	845	0	936	33	0
25	D	130	0	144	9	0
25	G	477	0	477	21	0
25	N	473	0	468	24	0
25	R	543	0	490	22	0
25	S	465	0	393	7	0
25	Y	473	0	468	23	0
25	a	240	0	242	15	0
25	b	1040	0	1152	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	c	845	0	936	33	0
25	d	130	0	144	7	0
25	g	477	0	477	23	0
25	n	473	0	468	24	0
25	r	543	0	490	21	0
25	s	465	0	393	7	0
25	y	473	0	468	20	0
26	1	84	0	112	10	0
26	2	84	0	112	7	0
26	3	84	0	112	11	0
26	4	42	0	56	4	0
26	5	84	0	112	11	0
26	6	84	0	112	7	0
26	7	84	0	112	9	0
26	8	42	0	56	3	0
26	G	84	0	112	14	0
26	N	84	0	112	6	0
26	R	42	0	56	4	0
26	S	84	0	112	7	0
26	Y	84	0	112	9	0
26	g	84	0	112	14	0
26	n	84	0	112	9	0
26	r	42	0	56	4	0
26	s	84	0	112	5	0
26	y	84	0	112	6	0
27	1	44	0	56	4	0
27	2	44	0	56	6	0
27	3	44	0	56	4	0
27	4	44	0	56	5	0
27	5	44	0	56	4	0
27	6	44	0	56	5	0
27	7	44	0	56	7	0
27	8	44	0	56	7	0
27	G	44	0	56	4	0
27	N	44	0	56	6	0
27	R	44	0	56	5	0
27	Y	44	0	56	5	0
27	g	44	0	56	4	0
27	n	44	0	56	7	0
27	r	44	0	56	5	0
27	y	44	0	56	5	0
28	1	44	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	2	44	0	56	2	0
28	3	44	0	56	2	0
28	5	44	0	56	3	0
28	6	44	0	56	0	0
28	7	44	0	56	2	0
28	G	44	0	56	3	0
28	N	44	0	56	3	0
28	R	44	0	56	4	0
28	S	44	0	56	1	0
28	Y	44	0	56	1	0
28	g	44	0	56	2	0
28	n	44	0	56	5	0
28	r	44	0	56	2	0
28	s	44	0	56	1	0
28	y	44	0	56	4	0
29	1	41	0	55	0	0
29	2	37	0	44	2	0
29	3	47	0	67	3	0
29	4	21	0	12	1	0
29	5	41	0	55	0	0
29	6	37	0	44	2	0
29	7	47	0	67	4	0
29	8	21	0	12	1	0
29	B	96	0	141	5	0
29	C	147	0	222	7	0
29	D	138	0	195	19	0
29	G	49	0	74	2	0
29	L	49	0	74	8	0
29	N	49	0	74	4	0
29	R	42	0	57	3	0
29	S	49	0	74	2	0
29	Y	49	0	74	3	0
29	b	96	0	141	5	0
29	c	147	0	222	9	0
29	d	138	0	195	20	0
29	g	49	0	74	4	0
29	l	49	0	74	8	0
29	n	49	0	74	4	0
29	r	42	0	57	3	0
29	s	49	0	74	2	0
29	y	49	0	74	4	0
30	4	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	8	40	0	56	3	0
30	A	40	0	56	2	0
30	B	120	0	168	13	0
30	C	160	0	224	15	0
30	D	40	0	56	4	0
30	H	40	0	56	6	0
30	T	40	0	56	3	0
30	a	40	0	56	3	0
30	b	120	0	168	12	0
30	c	160	0	224	16	0
30	d	40	0	56	7	0
30	h	40	0	56	5	0
30	t	40	0	56	7	0
31	A	10	0	0	2	0
31	a	10	0	0	2	0
32	A	1	0	0	0	0
32	a	1	0	0	0	0
33	A	128	0	148	11	0
33	a	128	0	148	11	0
34	A	104	0	144	8	0
34	B	96	0	126	8	0
34	a	104	0	145	8	0
34	b	96	0	125	7	0
35	A	88	0	116	2	0
35	B	106	0	158	6	0
35	C	51	0	72	1	0
35	D	46	0	62	2	0
35	Z	51	0	72	6	0
35	a	88	0	116	2	0
35	b	106	0	158	6	0
35	c	51	0	72	1	0
35	d	46	0	62	3	0
35	z	51	0	72	5	0
36	A	13	0	7	0	0
36	D	55	0	80	6	0
36	a	13	0	7	0	0
36	d	55	0	80	6	0
37	B	59	0	76	1	0
37	C	177	0	228	7	0
37	H	62	0	80	6	0
37	b	59	0	76	1	0
37	c	177	0	228	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	h	62	0	80	6	0
38	D	4	0	0	1	0
38	d	4	0	0	1	0
39	F	43	0	30	0	0
39	f	43	0	30	0	0
All	All	92842	0	92620	1778	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 (1778) 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)
24:7:606:CHL:HBB2	24:7:607:CHL:HBB1	1.57	0.86
24:3:606:CHL:HBB2	24:3:607:CHL:HBB1	1.57	0.85
25:b:603:CLA:H12	10:h:61:TYR:HD2	1.46	0.80
25:B:603:CLA:H12	10:H:61:TYR:HD2	1.46	0.78
25:1:602:CLA:HAB	26:1:1621:LUT:H32	1.66	0.77
16:O:128:PHE:HA	16:O:222:GLN:HE22	1.50	0.76
25:5:602:CLA:HAB	26:5:1621:LUT:H32	1.66	0.76
16:o:128:PHE:HA	16:o:222:GLN:HE22	1.50	0.75
1:6:191:MET:HE2	26:6:1621:LUT:H10	1.70	0.74
2:3:202:MET:HE2	26:3:1621:LUT:H10	1.69	0.74
1:y:191:MET:HE2	26:y:1621:LUT:H10	1.69	0.74
7:D:86:LEU:HD13	7:D:91:LEU:HD11	1.70	0.74
1:2:191:MET:HE2	26:2:1621:LUT:H10	1.69	0.74
1:Y:191:MET:HE2	26:Y:1621:LUT:H10	1.69	0.73
7:d:86:LEU:HD13	7:d:91:LEU:HD11	1.70	0.72
25:2:610:CLA:H2	26:2:1620:LUT:H28	1.72	0.72
2:7:202:MET:HE2	26:7:1621:LUT:H10	1.69	0.71
1:G:191:MET:HE2	26:G:1621:LUT:H10	1.71	0.71
25:6:610:CLA:H2	26:6:1620:LUT:H28	1.72	0.71
1:g:191:MET:HE2	26:g:1621:LUT:H10	1.71	0.71
30:C:516:BCR:HC21	23:Z:13:ILE:HG23	1.74	0.70
30:C:517:BCR:H332	23:Z:12:LEU:HD23	1.74	0.70
30:c:516:BCR:HC21	23:z:13:ILE:HG23	1.74	0.69
1:N:191:MET:HE2	26:N:1621:LUT:H10	1.73	0.69
1:n:191:MET:HE2	26:n:1621:LUT:H10	1.73	0.69
2:3:95:GLN:HE22	2:3:102:PHE:H	1.39	0.69
1:G:70:ARG:NE	1:G:180:GLU:OE2	2.24	0.69
2:7:95:GLN:HE22	2:7:102:PHE:H	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:c:517:BCR:H332	23:z:12:LEU:HD23	1.74	0.68
33:a:409:PHO:H3A	25:d:402:CLA:H142	1.75	0.68
1:g:70:ARG:NE	1:g:180:GLU:OE2	2.24	0.68
33:A:409:PHO:H3A	25:D:402:CLA:H142	1.75	0.68
6:c:456:GLU:OE2	6:c:457:LYS:NZ	2.26	0.68
17:r:163:ASN:HD22	25:r:616:CLA:HBC3	1.59	0.67
5:B:313:ASP:OD2	5:B:358:ARG:NH2	2.27	0.67
7:D:187:GLN:HB2	25:D:402:CLA:HBC1	1.76	0.67
3:8:91:PRO:HB2	17:r:235:LEU:HD22	1.76	0.67
5:b:18:ARG:NH1	14:l:5:ASN:HD22	1.92	0.67
3:4:91:PRO:HB2	17:R:235:LEU:HD22	1.76	0.67
30:C:517:BCR:H333	23:Z:9:VAL:HG13	1.77	0.67
17:R:163:ASN:HD22	25:R:616:CLA:HBC3	1.59	0.67
18:S:200:MET:HG2	26:S:1621:LUT:H14	1.76	0.67
5:b:313:ASP:OD2	5:b:358:ARG:NH2	2.27	0.67
30:c:517:BCR:H333	23:z:9:VAL:HG13	1.77	0.67
5:B:18:ARG:NH1	14:L:5:ASN:HD22	1.91	0.67
6:C:456:GLU:OE2	6:C:457:LYS:NZ	2.26	0.66
18:s:200:MET:HG2	26:s:1621:LUT:H14	1.76	0.66
5:B:145:LEU:HB3	25:B:605:CLA:H162	1.77	0.66
18:s:139:VAL:HG22	24:s:607:CHL:HBC1	1.77	0.66
7:D:193:THR:HG23	25:D:402:CLA:HBC2	1.78	0.66
7:d:193:THR:HG23	25:d:402:CLA:HBC2	1.78	0.65
7:d:187:GLN:HB2	25:d:402:CLA:HBC1	1.76	0.65
5:b:145:LEU:HB3	25:b:605:CLA:H162	1.77	0.65
14:L:20:TRP:CZ3	14:L:23:LEU:HD23	2.32	0.65
18:S:139:VAL:HG22	24:S:607:CHL:HBC1	1.77	0.65
6:C:38:GLY:HA3	25:C:511:CLA:HMD2	1.79	0.64
18:S:147:GLY:HA2	25:S:609:CLA:HAB	1.79	0.64
25:B:603:CLA:H12	10:H:61:TYR:CD2	2.30	0.64
14:l:20:TRP:CZ3	14:l:23:LEU:HD23	2.32	0.64
4:A:221:SER:HA	7:D:140:ARG:HB2	1.80	0.64
25:a:410:CLA:HAA2	35:a:413:LMG:H112	1.79	0.64
6:c:38:GLY:HA3	25:c:511:CLA:HMD2	1.79	0.64
2:7:208:GLN:HE22	26:7:1620:LUT:H41	1.62	0.64
25:A:410:CLA:HAA2	35:A:413:LMG:H112	1.79	0.64
2:3:208:GLN:HE22	26:3:1620:LUT:H41	1.62	0.64
17:R:93:ARG:NH1	17:R:96:GLU:OE2	2.31	0.64
17:r:93:ARG:NH1	17:r:96:GLU:OE2	2.31	0.64
24:r:606:CHL:HBA2	28:r:623:NEX:H403	1.80	0.64
18:s:147:GLY:HA2	25:s:609:CLA:HAB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:5:610:CLA:H2	26:5:1620:LUT:H28	1.81	0.63
10:H:61:TYR:HD1	10:H:61:TYR:O	1.82	0.63
4:a:82:ILE:HB	4:a:174:LEU:HB2	1.80	0.63
10:h:61:TYR:HD1	10:h:61:TYR:O	1.82	0.63
4:a:221:SER:HA	7:d:140:ARG:HB2	1.80	0.63
34:b:621:SQD:H141	34:b:623:SQD:H122	1.81	0.63
25:g:610:CLA:H52	26:g:1620:LUT:H28	1.81	0.63
3:8:138:VAL:HG22	3:8:140:SER:H	1.63	0.62
25:b:603:CLA:H12	10:h:61:TYR:CD2	2.30	0.62
16:O:117:GLN:HE21	16:O:121:GLY:HA2	1.64	0.62
25:b:608:CLA:H2	35:b:622:LMG:H151	1.81	0.62
3:4:138:VAL:HG22	3:4:140:SER:H	1.63	0.62
16:o:117:GLN:HE21	16:o:121:GLY:HA2	1.64	0.62
27:N:1622:XAT:H363	29:N:2630:LHG:HC41	1.81	0.62
24:R:606:CHL:HBA2	28:R:623:NEX:H403	1.80	0.62
7:D:20:ASP:OD2	7:D:24:ARG:NH1	2.28	0.62
5:B:423:ARG:NH1	5:B:430:PHE:O	2.33	0.62
25:G:610:CLA:H52	26:G:1620:LUT:H28	1.81	0.62
27:n:1622:XAT:H363	29:n:2630:LHG:HC41	1.81	0.62
1:N:118:LEU:HG	18:S:127:PHE:HZ	1.65	0.62
4:a:140:ARG:HB2	7:d:221:ASN:HA	1.82	0.62
34:B:621:SQD:H141	34:B:623:SQD:H122	1.81	0.61
25:1:610:CLA:H2	26:1:1620:LUT:H28	1.81	0.61
4:A:82:ILE:HB	4:A:174:LEU:HB2	1.80	0.61
25:b:603:CLA:H202	37:h:102:DGD:HA72	1.81	0.61
4:A:140:ARG:HB2	7:D:221:ASN:HA	1.82	0.61
25:B:603:CLA:H202	37:H:102:DGD:HA72	1.81	0.61
25:a:410:CLA:H2	11:i:12:VAL:HG11	1.83	0.61
25:1:602:CLA:HBA1	26:1:1621:LUT:H382	1.83	0.61
22:X:81:VAL:HG12	22:X:83:ARG:H	1.65	0.61
1:n:118:LEU:HG	18:s:127:PHE:HZ	1.65	0.61
6:C:402:GLY:HA3	6:C:420:VAL:HG22	1.83	0.61
25:r:602:CLA:H72	27:r:622:XAT:H28	1.83	0.61
25:A:410:CLA:H2	11:I:12:VAL:HG11	1.83	0.61
25:B:608:CLA:H2	35:B:622:LMG:H151	1.81	0.61
7:D:298:ASP:HA	7:D:316:TYR:OH	2.00	0.61
5:b:423:ARG:NH1	5:b:430:PHE:O	2.33	0.61
6:c:86:LEU:HD13	6:c:89:LEU:HD12	1.83	0.61
25:c:511:CLA:H141	23:z:20:LEU:HD22	1.83	0.61
1:6:163:PRO:HD2	26:6:1620:LUT:H23	1.83	0.60
27:7:1622:XAT:H12	29:7:2630:LHG:H191	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:298:ASP:HA	7:d:316:TYR:OH	2.00	0.60
3:4:93:SER:N	17:R:235:LEU:O	2.35	0.60
25:g:613:CLA:H162	25:g:614:CLA:H2	1.83	0.60
25:c:511:CLA:HBA1	30:c:517:BCR:H271	1.84	0.60
1:Y:164:LEU:HD12	26:Y:1620:LUT:H222	1.84	0.60
6:c:402:GLY:HA3	6:c:420:VAL:HG22	1.83	0.60
22:x:81:VAL:HG12	22:x:83:ARG:H	1.65	0.60
6:c:45:LEU:HD22	6:c:138:GLU:HB3	1.84	0.60
1:g:115:ASN:HB3	1:g:118:LEU:HD12	1.84	0.60
1:G:115:ASN:HB3	1:G:118:LEU:HD12	1.84	0.60
2:7:50:PRO:HG3	2:7:188:LYS:HD3	1.83	0.60
5:B:311:PHE:O	5:B:317:ASN:ND2	2.35	0.60
1:G:103:GLN:NE2	25:G:604:CLA:O1D	2.34	0.60
1:2:104:ILE:HG21	1:2:124:ILE:HD13	1.83	0.59
25:C:511:CLA:H141	23:Z:20:LEU:HD22	1.83	0.59
25:R:602:CLA:H72	27:R:622:XAT:H28	1.83	0.59
1:6:104:ILE:HG21	1:6:124:ILE:HD13	1.83	0.59
5:b:311:PHE:O	5:b:317:ASN:ND2	2.35	0.59
27:3:1622:XAT:H12	29:3:2630:LHG:H191	1.83	0.59
4:A:24:THR:O	7:D:256:GLN:NE2	2.30	0.59
6:C:45:LEU:HD22	6:C:138:GLU:HB3	1.84	0.59
1:y:164:LEU:HD12	26:y:1620:LUT:H222	1.84	0.59
1:2:21:ARG:NH1	1:2:37:THR:O	2.35	0.59
1:2:163:PRO:HD2	26:2:1620:LUT:H23	1.83	0.59
5:B:124:CYS:O	10:H:24:LYS:NZ	2.36	0.59
1:6:21:ARG:NH1	1:6:37:THR:O	2.35	0.59
17:R:97:LEU:HB3	17:R:172:LEU:HD11	1.85	0.59
25:5:602:CLA:HBA1	26:5:1621:LUT:H382	1.83	0.59
25:G:613:CLA:H162	25:G:614:CLA:H2	1.83	0.59
5:b:18:ARG:NH2	34:b:621:SQD:O8	2.35	0.59
17:r:97:LEU:HB3	17:r:172:LEU:HD11	1.85	0.59
6:C:86:LEU:HD13	6:C:89:LEU:HD12	1.83	0.59
1:1:103:GLN:HE22	25:1:604:CLA:HED3	1.67	0.59
1:g:103:GLN:NE2	25:g:604:CLA:O1D	2.34	0.59
17:r:23:TYR:HD2	17:r:89:LEU:HD11	1.68	0.59
30:d:404:BCR:H14C	9:f:27:PHE:CD2	2.38	0.59
5:b:389:LYS:N	7:d:345:GLU:OE2	2.36	0.59
1:1:66:VAL:HG22	1:1:181:LEU:HD21	1.85	0.59
25:C:511:CLA:HBA1	30:C:517:BCR:H271	1.84	0.59
2:3:50:PRO:HG3	2:3:188:LYS:HD3	1.83	0.58
30:D:404:BCR:H14C	9:F:27:PHE:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:139:GLU:OE1	24:N:609:CHL:NA	2.36	0.58
16:O:227:ASP:HB3	16:O:230:ALA:HB3	1.85	0.58
17:r:59:LYS:HE2	17:r:61:LEU:HD21	1.85	0.58
1:y:70:ARG:NE	1:y:180:GLU:OE2	2.36	0.58
16:o:207:THR:HG22	16:o:214:VAL:HG22	1.84	0.58
5:B:18:ARG:NH2	34:B:621:SQD:O8	2.36	0.58
30:C:517:BCR:H312	13:K:33:LEU:HD13	1.84	0.58
3:8:93:SER:N	17:r:235:LEU:O	2.35	0.58
17:R:59:LYS:HE2	17:R:61:LEU:HD21	1.85	0.58
3:8:126:TRP:CH2	17:r:16:PRO:HA	2.39	0.58
5:b:124:CYS:O	10:h:24:LYS:NZ	2.36	0.58
6:C:472:LEU:HD21	7:D:256:GLN:HE21	1.68	0.58
2:3:79:ARG:NH1	24:3:608:CHL:OBD	2.36	0.58
16:O:207:THR:HG22	16:O:214:VAL:HG22	1.84	0.58
3:8:93:SER:HB2	17:r:236:HIS:HA	1.86	0.58
6:C:346:THR:OG1	6:C:348:GLU:OE1	2.21	0.58
1:5:66:VAL:HG22	1:5:181:LEU:HD21	1.85	0.58
7:d:108:LEU:HD23	8:e:66:ILE:HD13	1.85	0.58
17:r:101:ARG:NH2	24:r:608:CHL:OBD	2.35	0.58
4:A:77:ILE:HD11	19:T:6:TYR:HB3	1.85	0.58
1:N:23:LYS:NZ	1:N:32:SER:HB3	2.19	0.58
2:7:141:GLN:HE22	24:7:607:CHL:HMC	1.69	0.58
6:c:346:THR:OG1	6:c:348:GLU:OE1	2.21	0.58
16:o:227:ASP:HB3	16:o:230:ALA:HB3	1.85	0.58
2:7:79:ARG:NH1	24:7:608:CHL:OBD	2.36	0.58
3:4:126:TRP:CH2	17:R:16:PRO:HA	2.39	0.57
4:A:201:GLY:HA3	4:A:286:THR:HG23	1.86	0.57
1:Y:70:ARG:NE	1:Y:180:GLU:OE2	2.36	0.57
1:5:103:GLN:HE22	25:5:604:CLA:HED3	1.67	0.57
1:n:23:LYS:NZ	1:n:32:SER:HB3	2.19	0.57
33:A:409:PHO:OBD	7:D:130:GLN:NE2	2.37	0.57
25:3:611:CLA:HAB	27:3:1622:XAT:H221	1.86	0.57
4:A:192:ILE:HG13	4:A:293:MET:HE1	1.86	0.57
7:D:108:LEU:HD23	8:E:66:ILE:HD13	1.85	0.57
29:c:522:LHG:H181	21:w:31:GLY:HA3	1.86	0.57
3:4:93:SER:HB2	17:R:236:HIS:HA	1.85	0.57
4:a:43:THR:HG23	30:a:411:BCR:H362	1.87	0.57
30:c:517:BCR:H312	13:k:33:LEU:HD13	1.85	0.57
4:A:166:GLY:HA3	6:C:358:PHE:HE1	1.70	0.57
29:C:522:LHG:H181	21:W:31:GLY:HA3	1.86	0.57
1:N:64:LEU:HD11	1:Y:49:ALA:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:201:GLY:HA3	4:a:286:THR:HG23	1.86	0.57
1:n:139:GLU:OE1	24:n:609:CHL:NA	2.36	0.57
25:7:611:CLA:HAB	27:7:1622:XAT:H221	1.86	0.57
4:A:43:THR:HG23	30:A:411:BCR:H362	1.87	0.57
30:D:404:BCR:H372	35:D:411:LMG:H292	1.87	0.57
33:a:409:PHO:OBD	7:d:130:GLN:NE2	2.37	0.57
16:o:51:LEU:HB3	16:o:89:ILE:HB	1.86	0.57
1:y:51:LEU:HD13	25:y:602:CLA:H42	1.87	0.57
5:B:389:LYS:N	7:D:345:GLU:OE2	2.36	0.56
6:C:282:PHE:HE1	25:C:501:CLA:H111	1.70	0.56
16:O:51:LEU:HB3	16:O:89:ILE:HB	1.86	0.56
17:R:101:ARG:NH2	24:R:608:CHL:OBD	2.36	0.56
1:5:94:GLU:N	1:5:103:GLN:OE1	2.38	0.56
5:b:256:MET:HA	5:b:263:THR:HG21	1.87	0.56
25:c:511:CLA:C4D	13:k:54:TRP:HH2	2.18	0.56
4:a:77:ILE:HD11	19:t:6:TYR:HB3	1.85	0.56
6:c:472:LEU:HD21	7:d:256:GLN:HE21	1.68	0.56
2:3:109:LYS:HA	24:3:607:CHL:HED3	1.87	0.56
2:3:141:GLN:HE22	24:3:607:CHL:HMC	1.69	0.56
5:B:30:VAL:HG12	25:B:606:CLA:HHD	1.87	0.56
5:B:30:VAL:HG11	25:B:613:CLA:H112	1.87	0.56
17:R:124:ALA:HB1	25:R:604:CLA:HED1	1.86	0.56
3:8:92:PHE:HA	17:r:235:LEU:HB3	1.87	0.56
6:c:282:PHE:HE1	25:c:501:CLA:H111	1.70	0.56
30:d:404:BCR:H372	35:d:411:LMG:H292	1.87	0.56
7:d:20:ASP:OD2	7:d:24:ARG:NH1	2.28	0.56
1:n:70:ARG:NH1	24:n:608:CHL:OBD	2.33	0.56
2:7:175:LEU:HD13	26:7:1620:LUT:H222	1.88	0.56
4:a:166:GLY:HA3	6:c:358:PHE:HE1	1.70	0.56
4:a:192:ILE:HG13	4:a:293:MET:HE1	1.86	0.56
5:b:30:VAL:HG11	25:b:613:CLA:H112	1.87	0.56
1:Y:51:LEU:HD13	25:Y:602:CLA:H42	1.87	0.56
4:a:136:ARG:NH1	11:i:27:ASP:OD1	2.39	0.56
29:d:408:LHG:H152	29:l:101:LHG:H272	1.87	0.56
37:C:519:DGD:HAT2	37:C:520:DGD:HBE1	1.88	0.56
37:c:519:DGD:HAT2	37:c:520:DGD:HBE1	1.88	0.56
29:D:408:LHG:H152	29:L:101:LHG:H272	1.87	0.56
29:c:2630:LHG:H101	25:s:611:CLA:HAB	1.87	0.56
17:r:124:ALA:HB1	25:r:604:CLA:HED1	1.86	0.56
4:a:24:THR:O	7:d:256:GLN:NE2	2.30	0.56
17:R:91:ARG:NH1	25:R:603:CLA:O1A	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:21:ARG:NH2	1:1:36:LEU:O	2.39	0.55
4:A:140:ARG:NH2	29:D:410:LHG:O5	2.39	0.55
1:N:21:ARG:NH2	1:N:36:LEU:O	2.38	0.55
17:R:23:TYR:HD2	17:R:89:LEU:HD11	1.68	0.55
1:n:64:LEU:HD11	1:y:49:ALA:HA	1.87	0.55
5:B:256:MET:HA	5:B:263:THR:HG21	1.87	0.55
25:C:511:CLA:C4D	13:K:54:TRP:HH2	2.18	0.55
3:4:92:PHE:HA	17:R:235:LEU:HB3	1.87	0.55
4:a:42:LEU:HD23	34:a:418:SQD:H212	1.88	0.55
4:A:303:ASN:O	6:C:415:ASN:ND2	2.39	0.55
1:G:69:SER:HB3	1:G:184:GLY:HA3	1.89	0.55
4:a:140:ARG:NH2	29:d:410:LHG:O5	2.39	0.55
1:g:69:SER:HB3	1:g:184:GLY:HA3	1.89	0.55
18:S:202:GLY:O	18:S:206:GLN:HB3	2.07	0.55
2:7:109:LYS:HA	24:7:607:CHL:HED3	1.87	0.55
5:b:30:VAL:HG12	25:b:606:CLA:HHD	1.87	0.55
29:d:409:LHG:O1	29:l:101:LHG:O4	2.25	0.55
25:c:501:CLA:H171	25:c:507:CLA:H122	1.89	0.55
1:1:94:GLU:N	1:1:103:GLN:OE1	2.38	0.55
1:2:193:GLY:O	1:2:197:GLN:HG2	2.07	0.55
29:C:2630:LHG:H101	25:S:611:CLA:HAB	1.87	0.55
25:G:603:CLA:H12	1:N:51:LEU:HD11	1.88	0.55
21:W:17:LEU:HA	21:W:22:LEU:HD23	1.89	0.55
1:N:103:GLN:NE2	25:N:604:CLA:O1D	2.40	0.55
5:b:191:ASP:HB2	10:h:70:ILE:HG12	1.89	0.55
6:c:311:GLN:OE1	6:c:355:THR:OG1	2.25	0.55
25:g:603:CLA:H12	1:n:51:LEU:HD11	1.88	0.55
1:2:215:ASP:OD2	1:2:218:ASN:ND2	2.40	0.55
25:C:513:CLA:H71	29:C:2630:LHG:H122	1.89	0.55
16:O:81:ARG:NH1	21:W:9:GLU:OE2	2.40	0.55
1:5:21:ARG:NH2	1:5:36:LEU:O	2.39	0.55
1:6:193:GLY:O	1:6:197:GLN:HG2	2.07	0.55
4:a:303:ASN:O	6:c:415:ASN:ND2	2.39	0.55
16:o:65:VAL:HA	16:o:71:LEU:HD21	1.90	0.55
24:1:607:CHL:HBB1	24:3:601:CHL:H141	1.90	0.54
1:2:27:PRO:O	2:3:154:ASN:ND2	2.40	0.54
2:3:175:LEU:HD13	26:3:1620:LUT:H222	1.88	0.54
29:B:2631:LHG:H242	29:B:2631:LHG:HC91	1.90	0.54
5:b:357:ARG:NH1	5:b:358:ARG:O	2.40	0.54
5:B:357:ARG:NH1	5:B:358:ARG:O	2.40	0.54
29:D:409:LHG:O1	29:L:101:LHG:O4	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:70:ARG:NE	1:N:180:GLU:OE2	2.38	0.54
25:a:410:CLA:H2	11:i:12:VAL:CG1	2.37	0.54
1:n:21:ARG:NH2	1:n:36:LEU:O	2.38	0.54
1:y:104:ILE:HG21	1:y:124:ILE:HD13	1.90	0.54
5:B:191:ASP:HB2	10:H:70:ILE:HG12	1.89	0.54
6:C:297:TYR:O	6:C:423:ARG:NH2	2.38	0.54
25:C:501:CLA:H171	25:C:507:CLA:H122	1.89	0.54
7:d:142:TYR:OH	29:d:408:LHG:O4	2.26	0.54
16:o:81:ARG:NH1	21:w:9:GLU:OE2	2.40	0.54
21:w:17:LEU:HA	21:w:22:LEU:HD23	1.89	0.54
1:1:164:LEU:HD13	26:1:1620:LUT:H222	1.90	0.54
5:B:256:MET:O	5:B:448:ARG:NH1	2.39	0.54
17:R:182:LEU:HD12	26:R:620:LUT:H222	1.90	0.54
1:6:27:PRO:O	2:7:154:ASN:ND2	2.40	0.54
29:8:2630:LHG:O3	29:8:2630:LHG:O1	2.24	0.54
4:A:42:LEU:HD23	34:A:418:SQD:H212	1.88	0.54
4:a:293:MET:HG2	4:a:298:ASN:HA	1.90	0.54
17:r:182:LEU:HD12	26:r:620:LUT:H222	1.90	0.54
1:5:191:MET:HE2	26:5:1621:LUT:H10	1.89	0.54
1:6:85:LEU:HD23	1:6:88:ASN:HD22	1.73	0.54
25:7:611:CLA:H3A	3:8:131:SER:HA	1.90	0.54
14:l:20:TRP:HA	14:l:20:TRP:CE3	2.43	0.54
3:4:161:ILE:HA	3:4:166:TYR:HA	1.90	0.54
25:A:410:CLA:H2	11:I:12:VAL:CG1	2.37	0.54
6:C:130:ILE:HD11	30:C:517:BCR:H21C	1.90	0.54
25:C:511:CLA:CHA	13:K:54:TRP:HH2	2.21	0.54
1:6:215:ASP:OD2	1:6:218:ASN:ND2	2.40	0.54
24:g:608:CHL:H152	28:g:1623:NEX:H402	1.90	0.54
24:5:607:CHL:HBB1	24:7:601:CHL:H141	1.89	0.54
30:b:618:BCR:H322	35:b:622:LMG:H111	1.90	0.54
25:c:511:CLA:CHA	13:k:54:TRP:HH2	2.21	0.54
17:r:204:LEU:HD13	25:r:611:CLA:HBC1	1.90	0.54
1:2:85:LEU:HD23	1:2:88:ASN:HD22	1.73	0.54
3:4:31:GLY:HA3	3:4:181:ILE:HG21	1.90	0.54
6:C:154:ARG:HB3	6:C:256:PRO:HG2	1.90	0.54
1:5:164:LEU:HD13	26:5:1620:LUT:H222	1.90	0.54
3:8:161:ILE:HA	3:8:166:TYR:HA	1.90	0.54
5:b:358:ARG:HG3	20:u:19:THR:HB	1.90	0.54
1:n:135:MET:HA	1:n:138:VAL:HG22	1.90	0.54
30:B:618:BCR:H322	35:B:622:LMG:H111	1.90	0.53
29:C:523:LHG:HC5	25:Y:611:CLA:H11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:135:MET:HA	1:N:138:VAL:HG22	1.90	0.53
16:O:65:VAL:HA	16:O:71:LEU:HD21	1.90	0.53
17:R:39:LEU:HD12	27:R:622:XAT:H23	1.90	0.53
18:S:125:ASN:ND2	18:S:130:ASN:OD1	2.41	0.53
6:c:154:ARG:HB3	6:c:256:PRO:HG2	1.90	0.53
6:c:223:TRP:HZ3	6:c:285:ILE:CD1	2.22	0.53
25:c:513:CLA:H71	29:c:2630:LHG:H122	1.89	0.53
4:A:136:ARG:NH1	11:I:27:ASP:OD1	2.39	0.53
29:c:523:LHG:HC5	25:y:611:CLA:H11	1.90	0.53
25:3:611:CLA:H3A	3:4:131:SER:HA	1.90	0.53
29:4:2630:LHG:O3	29:4:2630:LHG:O1	2.24	0.53
17:R:204:LEU:HD13	25:R:611:CLA:HBC1	1.90	0.53
1:6:63:GLU:HA	1:6:155:LEU:HD21	1.91	0.53
2:7:112:SER:HB3	24:7:607:CHL:HED2	1.90	0.53
6:C:223:TRP:HZ3	6:C:285:ILE:CD1	2.22	0.53
1:N:70:ARG:NH1	24:N:608:CHL:OBD	2.33	0.53
18:s:202:GLY:O	18:s:206:GLN:HB3	2.07	0.53
29:s:2630:LHG:H282	29:s:2630:LHG:HC91	1.90	0.53
1:1:191:MET:HE2	26:1:1621:LUT:H10	1.89	0.53
4:A:293:MET:HG2	4:A:298:ASN:HA	1.90	0.53
5:B:358:ARG:HG3	20:U:19:THR:HB	1.90	0.53
6:C:311:GLN:OE1	6:C:355:THR:OG1	2.25	0.53
27:2:1622:XAT:H14	29:2:2630:LHG:H171	1.91	0.53
4:A:131:TRP:CZ3	25:C:505:CLA:HAA2	2.44	0.53
36:D:405:PL9:H111	29:D:409:LHG:HC92	1.91	0.53
25:2:603:CLA:HED2	24:2:609:CHL:H93	1.90	0.53
16:O:145:GLU:HB3	16:O:197:LYS:HE2	1.91	0.53
1:Y:80:VAL:HG13	1:Y:206:LEU:HD11	1.90	0.53
3:8:65:VAL:HG21	26:8:620:LUT:H12	1.91	0.53
29:b:2631:LHG:H242	29:b:2631:LHG:HC91	1.90	0.53
1:n:70:ARG:NE	1:n:180:GLU:OE2	2.38	0.53
1:y:80:VAL:HG13	1:y:206:LEU:HD11	1.90	0.53
36:d:405:PL9:H111	29:d:409:LHG:HC92	1.90	0.53
17:r:39:LEU:HD12	27:r:622:XAT:H23	1.90	0.53
1:1:18:GLY:O	1:1:21:ARG:NH1	2.40	0.53
33:A:408:PHO:H51	34:A:418:SQD:H201	1.91	0.53
30:D:404:BCR:H21C	35:D:411:LMG:H372	1.90	0.53
24:G:608:CHL:H152	28:G:1623:NEX:H402	1.90	0.53
24:N:608:CHL:HHC	24:N:608:CHL:HBB1	1.91	0.53
16:O:111:TYR:HD2	16:O:127:LEU:HD11	1.74	0.53
29:S:2630:LHG:H282	29:S:2630:LHG:HC91	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:131:TRP:CZ3	25:c:505:CLA:HAA2	2.44	0.53
33:a:409:PHO:HBC3	7:d:280:LEU:HD22	1.91	0.53
1:y:126:ALA:HB3	24:y:605:CHL:HMC	1.91	0.53
24:G:601:CHL:HHC	24:G:601:CHL:HBB1	1.91	0.53
14:L:20:TRP:HA	14:L:20:TRP:CE3	2.43	0.53
1:Y:104:ILE:HG21	1:Y:124:ILE:HD13	1.90	0.53
6:c:297:TYR:O	6:c:423:ARG:NH2	2.38	0.53
24:g:601:CHL:HHC	24:g:601:CHL:HBB1	1.91	0.53
34:B:623:SQD:H62	14:L:8:GLU:HB2	1.91	0.52
25:N:602:CLA:H203	26:N:1621:LUT:H391	1.90	0.52
3:8:31:GLY:HA3	3:8:181:ILE:HG21	1.90	0.52
1:n:103:GLN:NE2	25:n:604:CLA:O1D	2.40	0.52
1:y:103:GLN:HE22	25:y:604:CLA:HED2	1.74	0.52
4:A:279:PRO:HG2	7:D:213:ALA:HB2	1.91	0.52
33:A:409:PHO:HBC3	7:D:280:LEU:HD22	1.91	0.52
5:B:153:PHE:HB2	25:B:607:CLA:HBB1	1.91	0.52
1:Y:212:HIS:CG	25:Y:613:CLA:HAA2	2.44	0.52
5:b:153:PHE:HB2	25:b:607:CLA:HBB1	1.91	0.52
6:c:79:LYS:HB3	6:c:84:GLN:HE21	1.75	0.52
18:s:99:ASN:ND2	18:s:103:ALA:O	2.42	0.52
24:1:608:CHL:HHC	24:1:608:CHL:HBB1	1.92	0.52
2:3:174:PRO:HD2	26:3:1620:LUT:H23	1.91	0.52
5:B:169:SER:HA	5:B:176:GLY:HA2	1.92	0.52
6:C:223:TRP:HE3	37:C:518:DGD:HB21	1.73	0.52
18:S:99:ASN:ND2	18:S:103:ALA:O	2.42	0.52
25:6:603:CLA:HED2	24:6:609:CHL:H93	1.91	0.52
5:b:255:THR:HG21	25:b:603:CLA:HED1	1.91	0.52
6:c:130:ILE:HD11	30:c:517:BCR:H21C	1.90	0.52
6:c:345:PRO:HB3	16:o:81:ARG:HD3	1.91	0.52
1:y:44:TYR:HE2	24:y:601:CHL:HBC2	1.75	0.52
1:1:52:SER:OG	1:1:61:ASN:ND2	2.43	0.52
1:2:221:ALA:N	25:2:613:CLA:O1A	2.43	0.52
5:B:18:ARG:HH11	14:L:5:ASN:HD22	1.56	0.52
27:6:1622:XAT:H14	29:6:2630:LHG:H171	1.91	0.52
5:b:18:ARG:HH11	14:l:5:ASN:HD22	1.56	0.52
30:d:404:BCR:H21C	35:d:411:LMG:H372	1.90	0.52
1:2:25:LEU:HB3	1:2:28:PHE:HB2	1.91	0.52
1:Y:103:GLN:HE22	25:Y:604:CLA:HED2	1.74	0.52
2:7:174:PRO:HD2	26:7:1620:LUT:H23	1.91	0.52
4:a:162:PRO:HB3	4:a:168:PHE:HA	1.91	0.52
1:n:69:SER:HB3	1:n:184:GLY:HA3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:n:601:CHL:HBB1	24:n:601:CHL:HHC	1.92	0.52
16:o:32:ILE:HG23	16:o:208:LYS:HE2	1.92	0.52
18:s:50:THR:HG22	18:s:50:THR:O	2.09	0.52
5:B:255:THR:HG21	25:B:603:CLA:HED1	1.91	0.52
7:D:142:TYR:OH	29:D:408:LHG:O4	2.26	0.52
14:L:17:SER:HB3	29:L:101:LHG:HC62	1.91	0.52
17:R:75:VAL:HG22	17:R:83:TYR:HE1	1.75	0.52
1:Y:44:TYR:HE2	24:Y:601:CHL:HBC2	1.74	0.52
1:N:69:SER:HB3	1:N:184:GLY:HA3	1.91	0.52
6:c:223:TRP:HE3	37:c:518:DGD:HB21	1.73	0.52
1:g:51:LEU:HD13	25:g:602:CLA:H42	1.91	0.52
25:n:602:CLA:H203	26:n:1621:LUT:H391	1.90	0.52
6:C:251:HIS:HE1	25:C:506:CLA:NA	2.08	0.52
17:R:96:GLU:HB2	25:R:602:CLA:C1B	2.40	0.52
2:7:196:ARG:HA	2:7:199:MET:HE3	1.91	0.52
4:a:85:THR:HA	4:a:109:GLY:HA3	1.91	0.52
5:b:214:LEU:CD1	25:r:609:CLA:H93	2.40	0.52
24:n:608:CHL:HHC	24:n:608:CHL:HBB1	1.91	0.52
1:y:212:HIS:CG	25:y:613:CLA:HAA2	2.44	0.52
3:4:65:VAL:HG21	26:4:620:LUT:H12	1.91	0.52
25:B:615:CLA:H43	34:B:621:SQD:H122	1.91	0.52
18:S:50:THR:HG22	18:S:50:THR:O	2.09	0.52
1:6:25:LEU:HB3	1:6:28:PHE:HB2	1.91	0.52
4:a:279:PRO:HG2	7:d:213:ALA:HB2	1.91	0.52
5:b:256:MET:O	5:b:448:ARG:NH1	2.39	0.52
27:y:1622:XAT:H10	29:y:2630:LHG:H212	1.92	0.52
5:B:214:LEU:CD1	25:R:609:CLA:H93	2.40	0.52
1:N:51:LEU:HD13	25:N:602:CLA:H42	1.90	0.52
24:5:608:CHL:HHC	24:5:608:CHL:HBB1	1.92	0.52
33:a:408:PHO:H51	34:a:418:SQD:H201	1.91	0.52
6:c:322:GLN:HE22	6:c:381:LYS:HA	1.75	0.52
1:1:69:SER:HB3	1:1:184:GLY:HA3	1.92	0.51
1:2:63:GLU:HA	1:2:155:LEU:HD21	1.91	0.51
5:B:155:ALA:O	5:B:159:THR:OG1	2.28	0.51
25:C:503:CLA:HAB	25:C:512:CLA:H41	1.92	0.51
5:b:75:TRP:HB3	37:b:626:DGD:HD5	1.91	0.51
6:c:454:GLY:O	11:i:34:ARG:NH2	2.43	0.51
1:n:51:LEU:HD13	25:n:602:CLA:H42	1.90	0.51
16:o:111:TYR:HD2	16:o:127:LEU:HD11	1.74	0.51
17:r:91:ARG:NH1	25:r:603:CLA:O1A	2.38	0.51
2:3:112:SER:HB3	24:3:607:CHL:HED2	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:511:CLA:C4D	13:K:54:TRP:CH2	2.93	0.51
1:G:51:LEU:HD13	25:G:602:CLA:H42	1.92	0.51
3:8:10:ILE:HG23	3:8:11:PRO:HD3	1.92	0.51
4:a:257:ARG:NH2	5:b:491:GLU:O	2.43	0.51
25:c:503:CLA:HAB	25:c:512:CLA:H41	1.92	0.51
25:c:511:CLA:C4D	13:k:54:TRP:CH2	2.93	0.51
4:A:257:ARG:NH2	5:B:491:GLU:O	2.43	0.51
6:C:322:GLN:HE22	6:C:381:LYS:HA	1.75	0.51
29:C:2630:LHG:H152	29:S:2630:LHG:H111	1.92	0.51
1:Y:69:SER:HB3	1:Y:184:GLY:HA3	1.92	0.51
27:Y:1622:XAT:H10	29:Y:2630:LHG:H212	1.92	0.51
1:6:221:ALA:N	25:6:613:CLA:O1A	2.43	0.51
5:b:169:SER:HA	5:b:176:GLY:HA2	1.92	0.51
4:A:189:GLU:OE2	31:A:401:OEX:O5	2.29	0.51
34:A:412:SQD:H442	7:D:233:PHE:CD2	2.46	0.51
25:B:604:CLA:HAB	25:B:606:CLA:H152	1.92	0.51
1:G:51:LEU:HD11	25:Y:603:CLA:H12	1.93	0.51
1:Y:126:ALA:HB3	24:Y:605:CHL:HMC	1.91	0.51
24:Y:608:CHL:HHC	24:Y:608:CHL:HBB1	1.92	0.51
5:b:155:ALA:O	5:b:159:THR:OG1	2.28	0.51
30:b:619:BCR:HC42	35:b:622:LMG:H341	1.93	0.51
14:l:17:SER:HB3	29:l:101:LHG:HC62	1.91	0.51
16:o:145:GLU:HB3	16:o:197:LYS:HE2	1.90	0.51
1:1:77:LEU:HD13	25:1:612:CLA:HBB2	1.92	0.51
2:3:114:ILE:HG21	2:3:134:ILE:HD13	1.91	0.51
4:A:85:THR:HA	4:A:109:GLY:HA3	1.91	0.51
4:A:162:PRO:HB3	4:A:168:PHE:HA	1.91	0.51
6:C:79:LYS:HB3	6:C:84:GLN:HE21	1.75	0.51
6:C:345:PRO:HB3	16:O:81:ARG:HD3	1.91	0.51
5:b:223:GLN:N	10:h:34:ALA:O	2.44	0.51
25:b:604:CLA:HAB	25:b:606:CLA:H152	1.92	0.51
18:s:125:ASN:ND2	18:s:130:ASN:OD1	2.41	0.51
1:y:69:SER:HB3	1:y:184:GLY:HA3	1.92	0.51
1:2:94:GLU:N	1:2:103:GLN:OE1	2.43	0.51
2:3:196:ARG:HA	2:3:199:MET:HE3	1.92	0.51
25:3:602:CLA:H72	26:3:1621:LUT:H30	1.93	0.51
1:G:21:ARG:NH2	1:G:36:LEU:O	2.41	0.51
16:O:138:LYS:HG2	16:O:140:ASP:H	1.75	0.51
4:a:189:GLU:OE2	31:a:401:OEX:O5	2.29	0.51
6:c:251:HIS:HE1	25:c:506:CLA:NA	2.08	0.51
16:o:138:LYS:HG2	16:o:140:ASP:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:r:96:GLU:HB2	25:r:602:CLA:C1B	2.40	0.51
1:5:77:LEU:HD13	25:5:612:CLA:HBB2	1.92	0.51
3:8:58:GLY:HA3	3:8:184:ALA:HB1	1.93	0.51
1:n:118:LEU:HG	18:s:127:PHE:CZ	2.46	0.51
25:2:602:CLA:HBA1	26:2:1621:LUT:H382	1.93	0.51
3:4:58:GLY:HA3	3:4:184:ALA:HB1	1.93	0.51
34:A:412:SQD:H131	29:D:410:LHG:H142	1.93	0.51
6:C:40:ALA:HB2	25:C:508:CLA:H2A	1.93	0.51
24:N:601:CHL:HBB1	24:N:601:CHL:HHC	1.92	0.51
1:Y:41:PRO:HG3	1:Y:177:LYS:HB3	1.93	0.51
1:5:52:SER:OG	1:5:61:ASN:ND2	2.43	0.51
1:5:69:SER:HB3	1:5:184:GLY:HA3	1.92	0.51
1:6:94:GLU:N	1:6:103:GLN:OE1	2.43	0.51
1:1:51:LEU:HD13	25:1:602:CLA:H42	1.93	0.51
16:O:32:ILE:HG23	16:O:208:LYS:HE2	1.92	0.51
19:T:15:GLY:HA2	30:T:101:BCR:H12C	1.92	0.51
3:8:120:ASP:O	3:8:123:SER:OG	2.28	0.51
34:b:623:SQD:H62	14:l:8:GLU:HB2	1.91	0.51
29:c:2630:LHG:H152	29:s:2630:LHG:H111	1.92	0.51
1:y:135:MET:HA	1:y:138:VAL:HG22	1.93	0.51
25:A:405:CLA:H122	33:A:408:PHO:H3A	1.94	0.51
1:5:51:LEU:HD13	25:5:602:CLA:H42	1.93	0.51
2:7:114:ILE:HG21	2:7:134:ILE:HD13	1.91	0.51
2:7:175:LEU:HB3	2:7:177:LEU:HD13	1.93	0.51
25:7:602:CLA:H72	26:7:1621:LUT:H30	1.93	0.51
25:b:615:CLA:H43	34:b:621:SQD:H122	1.92	0.51
5:B:75:TRP:HB3	37:B:626:DGD:HD5	1.91	0.50
19:T:17:ILE:HG22	30:T:101:BCR:H313	1.93	0.50
34:a:412:SQD:H442	7:d:233:PHE:CD2	2.46	0.50
11:i:5:LYS:HE2	21:w:22:LEU:HD21	1.94	0.50
17:r:75:VAL:HG22	17:r:83:TYR:HE1	1.75	0.50
3:4:120:ASP:O	3:4:123:SER:OG	2.28	0.50
27:6:1622:XAT:H41	24:7:607:CHL:HAA2	1.93	0.50
25:c:503:CLA:HMA3	35:z:101:LMG:H191	1.93	0.50
17:r:100:GLY:HA3	17:r:202:ALA:HB1	1.93	0.50
1:y:41:PRO:HG3	1:y:177:LYS:HB3	1.93	0.50
24:y:608:CHL:HHC	24:y:608:CHL:HBB1	1.92	0.50
5:B:223:GLN:N	10:H:34:ALA:O	2.44	0.50
34:a:412:SQD:H131	29:d:410:LHG:H142	1.93	0.50
25:b:605:CLA:HBD	25:b:605:CLA:HBA1	1.93	0.50
25:b:605:CLA:H91	25:b:607:CLA:HAB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:522:LHG:H192	25:y:612:CLA:H101	1.94	0.50
24:y:601:CHL:HBB1	24:y:601:CHL:HHC	1.93	0.50
30:B:619:BCR:HC42	35:B:622:LMG:H341	1.93	0.50
6:C:148:GLY:O	6:C:156:LYS:NZ	2.44	0.50
5:b:281:GLN:NE2	20:u:19:THR:OG1	2.42	0.50
2:3:175:LEU:HB3	2:3:177:LEU:HD13	1.93	0.50
3:4:10:ILE:HG23	3:4:11:PRO:HD3	1.93	0.50
4:A:98:GLU:OE2	21:W:8:THR:OG1	2.30	0.50
4:A:256:GLY:HA3	5:B:492:PHE:HZ	1.76	0.50
4:A:286:THR:HG21	25:A:405:CLA:HMA3	1.93	0.50
5:B:281:GLN:NE2	20:U:19:THR:OG1	2.42	0.50
24:N:609:CHL:HBB1	24:Y:601:CHL:H51	1.93	0.50
25:B:605:CLA:H91	25:B:607:CLA:HAB	1.92	0.50
25:B:605:CLA:HBD	25:B:605:CLA:HBA1	1.93	0.50
1:Y:103:GLN:NE2	25:Y:604:CLA:O1D	2.44	0.50
24:n:609:CHL:HBB1	24:y:601:CHL:H51	1.93	0.50
17:r:194:LEU:HB3	25:r:610:CLA:H3A	1.93	0.50
19:t:15:GLY:HA2	30:t:101:BCR:H12C	1.92	0.50
3:4:57:HIS:HD2	27:4:622:XAT:H15	1.77	0.50
25:A:410:CLA:H13	35:A:413:LMG:H321	1.94	0.50
18:S:166:PRO:HB3	24:S:608:CHL:HBC2	1.94	0.50
24:Y:601:CHL:HHC	24:Y:601:CHL:HBB1	1.92	0.50
24:8:608:CHL:HHC	24:8:608:CHL:HBB1	1.93	0.50
25:8:612:CLA:HED2	25:8:612:CLA:H2A	1.94	0.50
1:g:51:LEU:HD11	25:y:603:CLA:H12	1.93	0.50
17:r:215:GLN:O	17:r:219:THR:OG1	2.25	0.50
17:R:100:GLY:HA3	17:R:202:ALA:HB1	1.93	0.50
25:S:603:CLA:HED2	25:S:603:CLA:H2A	1.94	0.50
1:Y:135:MET:HA	1:Y:138:VAL:HG22	1.93	0.50
7:d:297:TYR:OH	7:d:327:ARG:NH1	2.42	0.50
1:n:153:ASP:OD2	1:n:156:TYR:N	2.43	0.50
2:3:152:ARG:NH2	24:3:609:CHL:O1D	2.45	0.50
3:4:154:PRO:HD2	26:4:620:LUT:H23	1.94	0.50
25:4:612:CLA:HED2	25:4:612:CLA:H2A	1.94	0.50
29:C:522:LHG:H192	25:Y:612:CLA:H101	1.93	0.50
7:D:30:PHE:O	7:D:129:ARG:NH1	2.37	0.50
1:G:73:MET:SD	25:G:610:CLA:HAB	2.52	0.50
4:a:38:ILE:HG23	34:a:418:SQD:H151	1.94	0.50
30:b:618:BCR:HC41	15:m:6:LEU:HD23	1.94	0.50
1:y:44:TYR:CE2	24:y:601:CHL:HBC2	2.47	0.50
1:2:208:ASN:ND2	25:2:613:CLA:O1D	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:297:TYR:OH	7:D:327:ARG:NH1	2.42	0.49
11:I:5:LYS:HE2	21:W:22:LEU:HD21	1.94	0.49
1:Y:44:TYR:CE2	24:Y:601:CHL:HBC2	2.47	0.49
4:a:256:GLY:HA3	5:b:492:PHE:HZ	1.76	0.49
7:d:30:PHE:O	7:d:129:ARG:NH1	2.37	0.49
1:g:73:MET:SD	25:g:610:CLA:HAB	2.52	0.49
1:g:220:ASN:HB2	25:g:614:CLA:HED1	1.94	0.49
27:2:1622:XAT:H41	24:3:607:CHL:HAA2	1.93	0.49
24:4:608:CHL:HBB1	24:4:608:CHL:HHC	1.93	0.49
25:N:603:CLA:HMD3	24:N:609:CHL:HBA2	1.93	0.49
18:S:83:ARG:NE	18:S:189:GLU:OE2	2.44	0.49
25:a:410:CLA:H13	35:a:413:LMG:H321	1.94	0.49
5:b:330:MET:HA	5:b:444:ARG:HB2	1.93	0.49
1:y:103:GLN:NE2	25:y:604:CLA:O1D	2.44	0.49
6:C:110:PRO:HB3	35:Z:101:LMG:H142	1.94	0.49
7:D:181:ARG:C	7:D:181:ARG:HD3	2.37	0.49
8:E:57:THR:O	8:E:61:GLN:NE2	2.46	0.49
1:G:163:PRO:HD2	26:G:1620:LUT:H23	1.94	0.49
1:N:162:ASP:OD1	26:N:1620:LUT:O23	2.31	0.49
17:R:194:LEU:HB3	25:R:610:CLA:H3A	1.93	0.49
25:Y:611:CLA:HBB1	25:Y:611:CLA:HHC	1.94	0.49
6:c:230:LEU:HD23	6:c:233:ILE:HD12	1.94	0.49
25:n:603:CLA:HMD3	24:n:609:CHL:HBA2	1.93	0.49
4:A:267:ASN:ND2	7:D:233:PHE:O	2.45	0.49
5:B:187:VAL:HG23	25:B:602:CLA:HMD3	1.95	0.49
5:B:362:PHE:HB3	7:D:189:PHE:CD2	2.48	0.49
6:C:230:LEU:HD23	6:C:233:ILE:HD12	1.94	0.49
8:E:60:ARG:NH1	8:E:62:GLY:O	2.45	0.49
1:G:70:ARG:NH1	24:G:608:CHL:OBD	2.38	0.49
25:6:602:CLA:HBA1	26:6:1621:LUT:H382	1.93	0.49
3:8:57:HIS:HD2	27:8:622:XAT:H15	1.77	0.49
4:a:98:GLU:OE2	21:w:8:THR:OG1	2.30	0.49
5:b:10:THR:OG1	17:r:55:GLN:NE2	2.45	0.49
5:b:187:VAL:HG23	25:b:602:CLA:HMD3	1.95	0.49
24:g:607:CHL:HBB1	26:g:1621:LUT:H161	1.94	0.49
25:y:611:CLA:HHC	25:y:611:CLA:HBB1	1.94	0.49
24:1:607:CHL:HAA2	27:3:1622:XAT:H41	1.94	0.49
1:2:222:TRP:HZ2	2:3:138:LEU:HD22	1.78	0.49
5:B:330:MET:HA	5:B:444:ARG:HB2	1.93	0.49
30:B:619:BCR:H14C	30:t:101:BCR:H383	1.95	0.49
24:5:607:CHL:HAA2	27:7:1622:XAT:H41	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:405:CLA:H102	33:a:408:PHO:HAA1	1.95	0.49
8:e:57:THR:O	8:e:61:GLN:NE2	2.46	0.49
1:g:163:PRO:HD2	26:g:1620:LUT:H23	1.94	0.49
25:g:603:CLA:H42	25:y:603:CLA:H41	1.95	0.49
5:b:362:PHE:HB3	7:d:189:PHE:CD2	2.47	0.49
19:t:17:ILE:HG22	30:t:101:BCR:H313	1.93	0.49
5:B:299:SER:HB3	5:B:407:ASN:HD21	1.78	0.49
6:c:110:PRO:HB3	35:z:101:LMG:H142	1.94	0.49
25:s:603:CLA:HED2	25:s:603:CLA:H2A	1.94	0.49
5:B:320:ALA:HB1	7:D:293:ASN:HD22	1.77	0.49
25:G:603:CLA:H42	25:Y:603:CLA:H41	1.95	0.49
1:N:41:PRO:HG3	1:N:177:LYS:HD3	1.94	0.49
17:R:23:TYR:OH	17:R:35:ASP:OD2	2.28	0.49
17:R:187:ASP:OD1	17:R:187:ASP:N	2.37	0.49
1:5:18:GLY:O	1:5:21:ARG:NH1	2.40	0.49
25:a:405:CLA:H122	33:a:408:PHO:H3A	1.94	0.49
25:a:407:CLA:HAB	25:d:402:CLA:H72	1.95	0.49
6:c:40:ALA:HB2	25:c:508:CLA:H2A	1.93	0.49
6:c:148:GLY:O	6:c:156:LYS:NZ	2.44	0.49
1:g:135:MET:HA	1:g:138:VAL:HG22	1.94	0.49
25:n:610:CLA:HBB1	25:n:612:CLA:H3A	1.95	0.49
1:y:73:MET:SD	25:y:610:CLA:HAB	2.53	0.49
3:4:93:SER:CB	17:R:236:HIS:HA	2.43	0.49
4:A:38:ILE:HG23	34:A:418:SQD:H151	1.94	0.49
1:6:222:TRP:HZ2	2:7:138:LEU:HD22	1.78	0.49
5:b:299:SER:HB3	5:b:407:ASN:HD21	1.78	0.49
25:b:615:CLA:H8	30:b:618:BCR:H362	1.95	0.49
27:g:1622:XAT:H1	29:g:2630:LHG:HO1	1.61	0.49
1:n:65:GLU:OE2	1:n:185:ARG:NE	2.43	0.49
17:r:39:LEU:HD13	25:r:602:CLA:H42	1.95	0.49
18:s:83:ARG:NE	18:s:189:GLU:OE2	2.44	0.49
1:y:142:ARG:NH2	24:y:609:CHL:O1D	2.43	0.49
27:3:1622:XAT:H393	29:3:2630:LHG:H101	1.94	0.49
1:G:135:MET:HA	1:G:138:VAL:HG22	1.94	0.49
1:G:220:ASN:HB2	25:G:614:CLA:HED1	1.94	0.49
1:N:23:LYS:HZ1	1:N:32:SER:HB3	1.76	0.49
17:R:180:ASP:OD1	26:R:620:LUT:O23	2.29	0.49
3:8:191:MET:HE2	27:8:622:XAT:H10	1.94	0.49
4:a:176:ILE:HD11	36:d:405:PL9:H452	1.95	0.49
4:a:254:TYR:HE2	7:d:143:ASN:HD22	1.61	0.49
5:b:321:LYS:NZ	5:b:363:PHE:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:602:CLA:HAC1	30:h:101:BCR:H383	1.95	0.49
1:g:64:LEU:HD11	1:n:49:ALA:HA	1.95	0.49
1:n:41:PRO:HG3	1:n:177:LYS:HD3	1.94	0.49
17:r:180:ASP:OD1	26:r:620:LUT:O23	2.29	0.49
4:A:12:ASN:HD21	21:W:40:TYR:HA	1.78	0.48
5:B:362:PHE:HB3	7:D:189:PHE:HD2	1.78	0.48
25:B:603:CLA:C1	10:H:61:TYR:HD2	2.23	0.48
6:C:454:GLY:O	11:I:34:ARG:NH2	2.43	0.48
1:6:176:LEU:HB3	25:6:610:CLA:H3A	1.95	0.48
3:8:93:SER:CB	17:r:236:HIS:HA	2.43	0.48
6:c:28:GLN:NE2	7:d:234:ARG:HD3	2.28	0.48
8:e:60:ARG:NH1	8:e:62:GLY:O	2.45	0.48
18:s:166:PRO:HB3	24:s:608:CHL:HBC2	1.94	0.48
30:B:618:BCR:HC41	15:M:6:LEU:HD23	1.94	0.48
25:C:503:CLA:HMA3	35:Z:101:LMG:H191	1.93	0.48
7:D:25:ARG:NH2	22:X:81:VAL:HG22	2.28	0.48
29:D:409:LHG:H131	14:L:20:TRP:HH2	1.78	0.48
17:R:11:ARG:HH21	17:R:31:ASP:CG	2.21	0.48
1:Y:73:MET:SD	25:Y:610:CLA:HAB	2.53	0.48
1:6:208:ASN:ND2	25:6:613:CLA:O1D	2.45	0.48
25:b:616:CLA:H91	25:b:616:CLA:H172	1.95	0.48
7:d:25:ARG:NH2	22:x:81:VAL:HG22	2.28	0.48
7:d:181:ARG:C	7:d:181:ARG:HD3	2.37	0.48
17:r:101:ARG:HA	17:r:104:MET:HE3	1.95	0.48
1:y:205:PRO:O	26:y:1620:LUT:O3	2.29	0.48
25:B:615:CLA:H8	30:B:618:BCR:H362	1.95	0.48
1:G:139:GLU:OE1	24:G:609:CHL:NA	2.46	0.48
1:N:65:GLU:OE2	1:N:185:ARG:NE	2.43	0.48
2:7:152:ARG:NH2	24:7:609:CHL:O1D	2.45	0.48
1:g:162:ASP:OD1	26:g:1620:LUT:O23	2.32	0.48
1:n:162:ASP:OD1	26:n:1620:LUT:O23	2.31	0.48
18:s:60:ASP:OD1	26:s:1621:LUT:O23	2.30	0.48
4:A:254:TYR:HE2	7:D:143:ASN:HD22	1.61	0.48
17:R:39:LEU:HD13	25:R:602:CLA:H42	1.95	0.48
18:S:60:ASP:OD1	26:S:1621:LUT:O23	2.30	0.48
27:5:1622:XAT:H41	24:6:607:CHL:HAA2	1.95	0.48
3:8:154:PRO:HD2	26:8:620:LUT:H23	1.94	0.48
5:b:320:ALA:HB1	7:d:293:ASN:HD22	1.77	0.48
6:c:223:TRP:CZ3	6:c:285:ILE:CD1	2.97	0.48
25:c:501:CLA:HBB1	25:c:507:CLA:H41	1.95	0.48
1:2:51:LEU:HD13	25:2:602:CLA:H42	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:176:LEU:HB3	25:2:610:CLA:H3A	1.95	0.48
3:4:143:GLU:H	3:4:146:TYR:HB2	1.79	0.48
3:4:191:MET:HE2	27:4:622:XAT:H10	1.94	0.48
5:B:10:THR:OG1	17:R:55:GLN:NE2	2.45	0.48
24:G:607:CHL:HBB1	26:G:1621:LUT:H161	1.94	0.48
27:G:1622:XAT:H1	29:G:2630:LHG:HO1	1.59	0.48
1:N:118:LEU:HG	18:S:127:PHE:CZ	2.46	0.48
27:6:1622:XAT:H31	27:6:1622:XAT:H391	1.71	0.48
3:8:130:TRP:HD1	25:r:611:CLA:HAB	1.78	0.48
6:c:223:TRP:CG	6:c:224:ILE:H	2.32	0.48
1:g:139:GLU:OE1	24:g:609:CHL:NA	2.46	0.48
1:2:103:GLN:HG3	1:2:110:LEU:HD13	1.96	0.48
3:4:130:TRP:HD1	25:R:611:CLA:HAB	1.78	0.48
5:B:321:LYS:NZ	5:B:363:PHE:O	2.46	0.48
6:C:223:TRP:CZ3	6:C:285:ILE:CD1	2.97	0.48
25:N:610:CLA:HBB1	25:N:612:CLA:H3A	1.95	0.48
17:R:101:ARG:HA	17:R:104:MET:HE3	1.95	0.48
1:6:96:VAL:HG12	1:6:99:LYS:H	1.78	0.48
4:a:131:TRP:HE1	6:c:446:GLY:HA2	1.78	0.48
4:a:267:ASN:ND2	7:d:233:PHE:O	2.45	0.48
4:a:286:THR:HG21	25:a:405:CLA:HMA3	1.93	0.48
31:a:401:OEX:O4	6:c:357:ARG:NH2	2.46	0.48
14:l:20:TRP:CZ3	29:l:101:LHG:H161	2.49	0.48
1:n:182:LYS:NZ	29:n:2630:LHG:O4	2.44	0.48
6:C:223:TRP:CG	6:C:224:ILE:H	2.32	0.48
27:7:1622:XAT:H393	29:7:2630:LHG:H101	1.94	0.48
29:d:408:LHG:O9	29:l:101:LHG:HC81	2.13	0.48
1:g:65:GLU:OE2	1:g:185:ARG:NE	2.43	0.48
27:1:1622:XAT:H41	24:2:607:CHL:HAA2	1.95	0.48
5:B:12:VAL:HG12	25:B:613:CLA:HMC1	1.96	0.48
25:C:507:CLA:H142	30:C:515:BCR:H362	1.96	0.48
29:D:408:LHG:O9	29:L:101:LHG:HC81	2.13	0.48
1:G:64:LEU:HD11	1:N:49:ALA:HA	1.95	0.48
14:L:24:LEU:HD23	29:L:101:LHG:H261	1.96	0.48
1:N:153:ASP:OD2	1:N:156:TYR:N	2.43	0.48
1:g:70:ARG:NH1	24:g:608:CHL:OBD	2.38	0.48
1:2:87:ARG:HH12	1:2:210:ALA:HB2	1.79	0.48
5:B:168:VAL:HG13	5:B:195:PRO:HG2	1.95	0.48
1:6:118:LEU:HD23	24:6:605:CHL:HED2	1.96	0.48
18:s:210:THR:HG22	18:s:233:VAL:HG11	1.95	0.48
4:A:131:TRP:HE1	6:C:446:GLY:HA2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:176:ILE:HD11	36:D:405:PL9:H452	1.95	0.48
5:B:41:GLU:O	5:B:45:PHE:N	2.46	0.48
25:B:614:CLA:H41	25:B:614:CLA:H61	1.61	0.48
25:B:616:CLA:H91	25:B:616:CLA:H172	1.95	0.48
6:C:28:GLN:NE2	7:D:234:ARG:HD3	2.28	0.48
7:D:157:VAL:HG22	7:D:287:VAL:HG11	1.96	0.48
1:G:194:PHE:HE1	26:G:1620:LUT:C5	2.27	0.48
7:d:52:GLY:HA3	7:d:79:VAL:HG22	1.96	0.48
29:d:409:LHG:H131	14:l:20:TRP:HH2	1.78	0.48
4:A:301:ASN:OD1	4:A:303:ASN:ND2	2.47	0.47
1:N:179:LYS:HD3	25:N:612:CLA:HAA2	1.96	0.47
4:a:301:ASN:OD1	4:a:303:ASN:ND2	2.47	0.47
33:a:408:PHO:H51	34:a:418:SQD:H223	1.96	0.47
5:b:362:PHE:HB3	7:d:189:PHE:HD2	1.78	0.47
7:d:157:VAL:HG22	7:d:287:VAL:HG11	1.96	0.47
14:l:24:LEU:HD23	29:l:101:LHG:H261	1.96	0.47
25:n:610:CLA:H71	25:n:612:CLA:H101	1.96	0.47
17:r:187:ASP:OD1	17:r:187:ASP:N	2.37	0.47
4:A:84:PRO:HA	4:A:112:TYR:CG	2.49	0.47
25:A:405:CLA:H102	33:A:408:PHO:HAA1	1.95	0.47
18:S:210:THR:HG22	18:S:233:VAL:HG11	1.95	0.47
24:S:606:CHL:HHC	24:S:606:CHL:HBB1	1.96	0.47
1:6:69:SER:HB3	1:6:184:GLY:HA3	1.96	0.47
5:b:41:GLU:O	5:b:45:PHE:N	2.46	0.47
1:g:110:LEU:HD21	25:g:604:CLA:HAA1	1.96	0.47
1:g:194:PHE:HE1	26:g:1620:LUT:H41	1.79	0.47
1:2:96:VAL:HG12	1:2:99:LYS:H	1.78	0.47
24:3:608:CHL:H2A	24:3:608:CHL:HED3	1.97	0.47
25:B:602:CLA:HAC1	30:H:101:BCR:H383	1.95	0.47
25:C:501:CLA:HBB1	25:C:507:CLA:H41	1.95	0.47
1:G:65:GLU:OE2	1:G:185:ARG:NE	2.43	0.47
1:6:51:LEU:HD13	25:6:602:CLA:H42	1.95	0.47
16:o:89:ILE:HD13	16:o:130:ILE:HD11	1.96	0.47
17:r:11:ARG:HH21	17:r:31:ASP:CG	2.21	0.47
24:s:606:CHL:HHC	24:s:606:CHL:HBB1	1.96	0.47
28:1:1623:NEX:H22	25:R:612:CLA:H11	1.97	0.47
16:O:58:PHE:CE2	21:W:2:VAL:HG21	2.50	0.47
16:O:89:ILE:HD13	16:O:130:ILE:HD11	1.96	0.47
16:O:202:LEU:HD23	16:O:218:PHE:HB3	1.96	0.47
2:7:72:ALA:HA	2:7:165:LEU:HD11	1.96	0.47
3:8:37:PRO:HD2	27:8:622:XAT:H242	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:168:VAL:HG13	5:b:195:PRO:HG2	1.95	0.47
25:c:511:CLA:HBA2	13:k:54:TRP:CH2	2.50	0.47
25:1:613:CLA:H2	25:1:613:CLA:H61	1.60	0.47
28:1:1623:NEX:H11	28:1:1623:NEX:H191	1.78	0.47
1:2:153:ASP:OD2	1:2:156:TYR:N	2.43	0.47
2:3:30:ARG:NH1	2:3:46:THR:O	2.48	0.47
2:3:116:SER:OG	2:3:119:GLY:O	2.33	0.47
25:C:508:CLA:HBC2	29:D:410:LHG:H341	1.97	0.47
15:M:31:SER:HB3	15:m:28:LYS:HG3	1.95	0.47
25:N:603:CLA:H91	24:N:609:CHL:H112	1.97	0.47
17:R:215:GLN:O	17:R:219:THR:OG1	2.25	0.47
1:Y:142:ARG:NH2	24:Y:609:CHL:O1D	2.43	0.47
1:Y:163:PRO:HB2	28:r:623:NEX:H22	1.96	0.47
28:5:1623:NEX:H22	25:r:612:CLA:H11	1.97	0.47
24:7:608:CHL:HED3	24:7:608:CHL:H2A	1.97	0.47
4:a:84:PRO:HA	4:a:112:TYR:CG	2.49	0.47
5:b:236:THR:HB	5:b:473:THR:HG21	1.96	0.47
1:2:118:LEU:HD23	24:2:605:CHL:HED2	1.96	0.47
5:B:236:THR:HB	5:B:473:THR:HG21	1.96	0.47
30:B:620:BCR:H271	19:t:22:PHE:HB3	1.97	0.47
7:D:52:GLY:HA3	7:D:79:VAL:HG22	1.96	0.47
1:G:162:ASP:OD1	26:G:1620:LUT:O23	2.32	0.47
25:G:613:CLA:H91	29:G:2630:LHG:H321	1.96	0.47
14:L:26:PHE:CD1	19:T:16:ILE:HD11	2.50	0.47
18:S:19:VAL:HG12	18:S:21:ASP:H	1.79	0.47
3:8:143:GLU:H	3:8:146:TYR:HB2	1.79	0.47
4:a:12:ASN:HD21	21:w:40:TYR:HA	1.78	0.47
5:b:363:PHE:N	5:b:363:PHE:CD1	2.83	0.47
30:c:517:BCR:H281	13:k:54:TRP:CE3	2.50	0.47
24:g:607:CHL:H2	24:g:607:CHL:H62	1.59	0.47
14:l:26:PHE:CD1	19:t:16:ILE:HD11	2.50	0.47
1:n:176:LEU:HD23	1:n:179:LYS:HD2	1.97	0.47
25:n:603:CLA:H91	24:n:609:CHL:H112	1.97	0.47
16:o:58:PHE:CE2	21:w:2:VAL:HG21	2.50	0.47
2:3:128:LEU:HD23	24:3:605:CHL:HED2	1.96	0.47
3:4:37:PRO:HD2	27:4:622:XAT:H242	1.95	0.47
33:A:408:PHO:H51	34:A:418:SQD:H223	1.96	0.47
30:B:618:BCR:H342	30:t:101:BCR:H402	1.97	0.47
6:C:206:PRO:O	6:C:210:PHE:HB2	2.15	0.47
7:D:160:ILE:HG21	7:D:288:VAL:HG22	1.96	0.47
25:N:610:CLA:H71	25:N:612:CLA:H101	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:113:LYS:HA	24:S:607:CHL:HED3	1.96	0.47
1:Y:205:PRO:O	26:Y:1620:LUT:O3	2.29	0.47
25:5:613:CLA:H61	25:5:613:CLA:H2	1.60	0.47
1:6:103:GLN:HG3	1:6:110:LEU:HD13	1.96	0.47
5:b:12:VAL:HG12	25:b:613:CLA:HMC1	1.95	0.47
6:c:259:TRP:HH2	25:c:507:CLA:H201	1.80	0.47
6:c:279:LEU:HD11	25:c:507:CLA:HBA1	1.97	0.47
27:g:1622:XAT:H201	27:g:1622:XAT:H15	1.67	0.47
28:n:1623:NEX:H11	28:n:1623:NEX:H191	1.73	0.47
18:s:19:VAL:HG12	18:s:21:ASP:H	1.79	0.47
18:s:79:LEU:HD13	18:s:164:LEU:HD23	1.96	0.47
1:2:69:SER:HB3	1:2:184:GLY:HA3	1.96	0.47
4:A:61:ASP:HB2	4:A:63:ILE:HG12	1.97	0.47
5:B:219:VAL:HG22	17:R:87:PHE:HZ	1.80	0.47
25:B:605:CLA:HBB1	25:B:614:CLA:HBC2	1.96	0.47
35:B:2633:LMG:H272	25:R:609:CLA:H43	1.97	0.47
30:C:517:BCR:H281	13:K:54:TRP:CE3	2.50	0.47
1:G:110:LEU:HD21	25:G:604:CLA:HAA1	1.96	0.47
1:G:194:PHE:HE1	26:G:1620:LUT:H41	1.79	0.47
14:L:20:TRP:CZ3	29:L:101:LHG:H161	2.49	0.47
7:d:163:LEU:HD13	37:h:102:DGD:HB92	1.97	0.47
18:s:113:LYS:HA	24:s:607:CHL:HED3	1.96	0.47
25:D:403:CLA:H102	25:D:403:CLA:H61	1.72	0.47
28:R:623:NEX:H11	28:R:623:NEX:H191	1.74	0.47
1:6:87:ARG:HH12	1:6:210:ALA:HB2	1.79	0.47
24:7:606:CHL:HBC2	24:7:607:CHL:HHD	1.97	0.47
30:a:411:BCR:H11C	30:a:411:BCR:H341	1.81	0.47
5:b:185:TRP:HD1	24:r:607:CHL:H93	1.80	0.47
6:c:206:PRO:O	6:c:210:PHE:HB2	2.15	0.47
25:c:508:CLA:HBC2	29:d:410:LHG:H341	1.97	0.47
7:d:160:ILE:HG21	7:d:288:VAL:HG22	1.96	0.47
3:4:29:LEU:HD11	3:4:51:ARG:HD3	1.97	0.47
25:A:407:CLA:HAB	25:D:402:CLA:H72	1.95	0.47
5:B:363:PHE:N	5:B:363:PHE:CD1	2.83	0.47
7:D:49:TRP:HA	7:D:79:VAL:HG21	1.96	0.47
27:N:1622:XAT:H201	27:N:1622:XAT:H15	1.62	0.47
30:c:517:BCR:H15C	30:c:517:BCR:H351	1.80	0.47
27:y:1622:XAT:H31	27:y:1622:XAT:H391	1.78	0.47
25:2:610:CLA:H43	25:2:612:CLA:HBA1	1.97	0.46
24:G:601:CHL:H91	24:G:601:CHL:H112	1.79	0.46
18:S:79:LEU:HD13	18:S:164:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:610:CLA:H43	25:6:612:CLA:HBA1	1.97	0.46
25:b:605:CLA:HBB1	25:b:614:CLA:HBC2	1.96	0.46
25:b:614:CLA:H61	25:b:614:CLA:H41	1.61	0.46
25:c:510:CLA:H191	13:k:45:LEU:HD23	1.97	0.46
16:o:220:SER:O	16:o:237:LYS:HA	2.15	0.46
24:y:609:CHL:HHC	24:y:609:CHL:HBB1	1.97	0.46
4:A:292:THR:HG22	6:C:428:THR:HB	1.97	0.46
5:B:148:VAL:HG11	29:B:2631:LHG:H201	1.97	0.46
6:C:87:ILE:O	6:C:91:HIS:ND1	2.48	0.46
25:C:511:CLA:HBA2	13:K:54:TRP:CH2	2.50	0.46
30:C:514:BCR:H351	30:C:514:BCR:H15C	1.78	0.46
2:7:30:ARG:NH1	2:7:46:THR:O	2.48	0.46
25:7:603:CLA:HMD3	24:7:609:CHL:HBA2	1.97	0.46
1:g:194:PHE:HE1	26:g:1620:LUT:C5	2.27	0.46
28:y:1623:NEX:H11	28:y:1623:NEX:H191	1.74	0.46
24:N:606:CHL:HMB1	24:N:609:CHL:HMC	1.97	0.46
16:O:220:SER:O	16:O:237:LYS:HA	2.15	0.46
1:5:17:TYR:HE2	1:5:174:ALA:HB1	1.81	0.46
4:a:61:ASP:HB2	4:a:63:ILE:HG12	1.96	0.46
33:a:408:PHO:H61	33:a:408:PHO:H2	1.56	0.46
6:c:87:ILE:O	6:c:91:HIS:ND1	2.48	0.46
25:c:507:CLA:H142	30:c:515:BCR:H362	1.96	0.46
1:n:25:LEU:HB2	1:n:29:SER:HA	1.98	0.46
25:n:613:CLA:H2	25:n:613:CLA:H61	1.67	0.46
24:y:607:CHL:H62	24:y:607:CHL:H2	1.55	0.46
26:y:1621:LUT:H15	26:y:1621:LUT:H201	1.81	0.46
25:B:611:CLA:H141	25:B:613:CLA:HBD	1.96	0.46
7:D:173:SER:HB2	7:D:178:ALA:HB1	1.98	0.46
27:G:1622:XAT:H31	27:G:1622:XAT:H391	1.73	0.46
24:Y:609:CHL:HHC	24:Y:609:CHL:HBB1	1.97	0.46
2:7:116:SER:OG	2:7:119:GLY:O	2.33	0.46
27:8:622:XAT:H15	27:8:622:XAT:H201	1.82	0.46
1:n:205:PRO:O	26:n:1620:LUT:O3	2.28	0.46
26:n:1621:LUT:H35	26:n:1621:LUT:H401	1.79	0.46
5:B:185:TRP:HD1	24:R:607:CHL:H93	1.80	0.46
35:b:2633:LMG:H272	25:r:609:CLA:H43	1.97	0.46
6:c:91:HIS:NE2	25:c:502:CLA:O1D	2.40	0.46
6:c:223:TRP:HZ3	6:c:285:ILE:HG12	1.80	0.46
16:o:60:VAL:HG22	16:o:236:VAL:HG22	1.97	0.46
16:o:201:THR:O	16:o:218:PHE:HA	2.15	0.46
25:r:613:CLA:H92	29:r:2630:LHG:H171	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:y:602:CLA:H101	26:y:1621:LUT:H371	1.97	0.46
1:1:215:ASP:OD2	1:1:218:ASN:ND2	2.46	0.46
25:A:405:CLA:H191	29:D:409:LHG:H331	1.98	0.46
30:C:515:BCR:H15C	30:C:515:BCR:H351	1.78	0.46
7:D:163:LEU:HD13	37:H:102:DGD:HB92	1.97	0.46
7:D:302:GLN:HG2	15:M:1:MET:HE1	1.98	0.46
9:F:20:LEU:O	9:F:24:THR:OG1	2.31	0.46
10:H:30:TYR:HE2	17:R:50:LEU:HA	1.80	0.46
16:O:60:VAL:HG22	16:O:236:VAL:HG22	1.97	0.46
2:7:128:LEU:HD23	24:7:605:CHL:HED2	1.96	0.46
3:8:71:GLY:O	3:8:75:SER:OG	2.29	0.46
7:d:84:ASN:HD22	7:d:337:HIS:CD2	2.33	0.46
1:g:63:GLU:HA	1:g:155:LEU:HD21	1.98	0.46
25:g:613:CLA:H2	25:g:613:CLA:H61	1.72	0.46
1:n:179:LYS:HD3	25:n:612:CLA:HAA2	1.96	0.46
1:1:17:TYR:HE2	1:1:174:ALA:HB1	1.81	0.46
4:A:224:ILE:O	7:D:266:ARG:NH2	2.43	0.46
25:B:610:CLA:CHC	30:H:101:BCR:HC8	2.45	0.46
25:C:510:CLA:H191	13:K:45:LEU:HD23	1.97	0.46
7:D:84:ASN:HD22	7:D:337:HIS:CD2	2.33	0.46
18:S:55:GLY:HA3	18:S:194:ARG:HH12	1.80	0.46
25:Y:602:CLA:H101	26:Y:1621:LUT:H371	1.97	0.46
25:5:603:CLA:HMD3	24:5:609:CHL:HBA2	1.98	0.46
4:a:130:GLU:HG2	7:d:257:ILE:HG21	1.98	0.46
25:a:406:CLA:H52	36:d:405:PL9:H151	1.98	0.46
25:b:610:CLA:CHC	30:h:101:BCR:HC8	2.45	0.46
7:d:124:ILE:HD11	37:h:102:DGD:HAE1	1.98	0.46
25:g:613:CLA:H91	29:g:2630:LHG:H321	1.96	0.46
16:o:202:LEU:HD23	16:o:218:PHE:HB3	1.96	0.46
1:2:147:PRO:HB2	24:2:608:CHL:HBB2	1.98	0.46
2:3:72:ALA:HA	2:3:165:LEU:HD11	1.96	0.46
6:C:66:ALA:HB1	13:K:40:MET:HB3	1.98	0.46
1:N:25:LEU:HB2	1:N:29:SER:HA	1.98	0.46
1:N:63:GLU:HA	1:N:155:LEU:HD21	1.97	0.46
16:O:201:THR:O	16:O:218:PHE:HA	2.15	0.46
27:R:622:XAT:H35	27:R:622:XAT:H401	1.79	0.46
24:S:606:CHL:HMC	24:S:607:CHL:C1C	2.46	0.46
25:5:610:CLA:CBB	26:5:1620:LUT:H32	2.46	0.46
5:b:219:VAL:HG22	17:r:87:PHE:HZ	1.80	0.46
5:b:315:ILE:HG12	5:b:321:LYS:HG3	1.97	0.46
25:b:613:CLA:H61	25:b:613:CLA:H102	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:c:66:ALA:HB1	13:k:40:MET:HB3	1.98	0.46
6:c:186:TYR:HA	6:c:196:VAL:HA	1.98	0.46
1:g:52:SER:OG	1:g:61:ASN:ND2	2.48	0.46
1:g:148:LEU:HG	24:g:608:CHL:HBB1	1.97	0.46
10:h:30:TYR:HE2	17:r:50:LEU:HA	1.80	0.46
25:4:611:CLA:HBA2	25:4:612:CLA:HMD3	1.98	0.46
25:A:406:CLA:H52	36:D:405:PL9:H151	1.98	0.46
30:B:618:BCR:H15C	30:B:618:BCR:H351	1.79	0.46
30:B:620:BCR:H11C	30:B:620:BCR:H341	1.83	0.46
6:C:338:GLY:HA2	16:O:111:TYR:OH	2.16	0.46
30:C:517:BCR:H15C	30:C:517:BCR:H351	1.80	0.46
7:D:69:LEU:HD13	9:F:34:MET:HE2	1.98	0.46
25:G:603:CLA:HBB1	25:G:603:CLA:HHC	1.98	0.46
16:O:227:ASP:HB2	16:O:231:LYS:HE3	1.97	0.46
1:Y:21:ARG:NH2	1:Y:36:LEU:O	2.44	0.46
25:Y:613:CLA:H2	25:Y:613:CLA:H61	1.67	0.46
25:7:602:CLA:HBA1	26:7:1621:LUT:H382	1.98	0.46
5:b:157:HIS:HE1	25:b:607:CLA:NA	2.14	0.46
18:s:53:VAL:HG21	18:s:71:PHE:HE2	1.80	0.46
25:3:602:CLA:HBA1	26:3:1621:LUT:H382	1.98	0.46
6:C:91:HIS:NE2	25:C:502:CLA:O1D	2.40	0.46
7:D:211:LEU:HA	7:D:214:ILE:HG22	1.98	0.46
13:K:27:PRO:HB2	13:K:30:TYR:HD2	1.80	0.46
18:S:53:VAL:HG21	18:S:71:PHE:HE2	1.80	0.46
4:a:140:ARG:NH1	7:d:223:LEU:HD12	2.30	0.46
5:b:148:VAL:HG11	29:b:2631:LHG:H201	1.97	0.46
7:d:211:LEU:HA	7:d:214:ILE:HG22	1.98	0.46
7:d:302:GLN:HG2	15:m:1:MET:HE1	1.98	0.46
29:d:409:LHG:H321	19:t:21:ILE:HD11	1.97	0.46
1:g:97:TRP:O	26:g:1621:LUT:O3	2.34	0.46
25:g:603:CLA:HHC	25:g:603:CLA:HBB1	1.98	0.46
27:1:1622:XAT:H31	27:1:1622:XAT:H391	1.74	0.45
3:4:173:LEU:HG	3:4:177:LYS:HE3	1.98	0.45
6:C:279:LEU:HD11	25:C:507:CLA:HBA1	1.97	0.45
1:N:176:LEU:HD23	1:N:179:LYS:HD2	1.97	0.45
24:7:606:CHL:HHC	24:7:606:CHL:HBB1	1.98	0.45
27:7:1622:XAT:H11	27:7:1622:XAT:H191	1.80	0.45
25:8:611:CLA:HBA2	25:8:612:CLA:HMD3	1.98	0.45
4:a:49:ILE:HG12	36:d:405:PL9:H501	1.98	0.45
4:a:228:THR:HA	17:r:58:ALA:HA	1.98	0.45
4:a:292:THR:HG22	6:c:428:THR:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:49:TRP:HA	7:d:79:VAL:HG21	1.96	0.45
7:d:69:LEU:HD13	9:f:34:MET:HE2	1.98	0.45
1:n:63:GLU:HA	1:n:155:LEU:HD21	1.98	0.45
24:s:606:CHL:HMC	24:s:607:CHL:C1C	2.46	0.45
24:3:606:CHL:HHC	24:3:606:CHL:HBB1	1.98	0.45
3:4:96:THR:HG21	17:R:235:LEU:HA	1.99	0.45
4:A:140:ARG:NH1	7:D:223:LEU:HD12	2.30	0.45
4:A:312:ARG:NH1	8:E:56:PHE:HB2	2.32	0.45
25:S:604:CLA:HBA2	25:S:604:CLA:H3A	1.79	0.45
24:5:609:CHL:H91	24:5:609:CHL:H112	1.83	0.45
27:7:1622:XAT:H15	27:7:1622:XAT:H201	1.78	0.45
13:k:27:PRO:HB2	13:k:30:TYR:HD2	1.80	0.45
1:1:104:ILE:HG21	1:1:124:ILE:HD13	1.98	0.45
25:1:603:CLA:HMD3	24:1:609:CHL:HBA2	1.98	0.45
5:B:157:HIS:HE1	25:B:607:CLA:NA	2.14	0.45
6:C:186:TYR:HA	6:C:196:VAL:HA	1.98	0.45
7:D:237:ASN:HB3	7:D:240:GLN:HB3	1.98	0.45
1:G:148:LEU:HG	24:G:608:CHL:HBB1	1.97	0.45
1:N:44:TYR:CD2	25:N:602:CLA:HMD2	2.52	0.45
25:R:602:CLA:H101	27:R:622:XAT:H371	1.98	0.45
25:b:611:CLA:H141	25:b:613:CLA:HBD	1.96	0.45
29:b:2630:LHG:H152	29:b:2631:LHG:H162	1.99	0.45
18:s:55:GLY:HA3	18:s:194:ARG:HH12	1.80	0.45
25:2:614:CLA:HBA2	25:2:614:CLA:H3A	1.73	0.45
25:3:603:CLA:HMD3	24:3:609:CHL:HBA2	1.97	0.45
24:3:606:CHL:HBC2	24:3:607:CHL:HHD	1.97	0.45
31:A:401:OEX:O4	6:C:357:ARG:NH2	2.46	0.45
5:B:145:LEU:HD22	25:B:605:CLA:H18	1.98	0.45
29:D:409:LHG:H321	19:T:21:ILE:HD11	1.97	0.45
25:G:602:CLA:H91	25:Y:603:CLA:H8	1.98	0.45
25:G:610:CLA:HBB1	25:G:612:CLA:H3A	1.99	0.45
25:N:603:CLA:H12	1:Y:51:LEU:HD11	1.98	0.45
26:R:620:LUT:H35	26:R:620:LUT:H401	1.84	0.45
24:7:609:CHL:H91	24:7:609:CHL:H112	1.83	0.45
4:a:147:TYR:OH	33:a:408:PHO:O1A	2.31	0.45
5:b:460:LEU:HG	7:d:281:TRP:HZ3	1.82	0.45
26:g:1620:LUT:H401	26:g:1620:LUT:H35	1.78	0.45
24:n:607:CHL:H62	24:n:607:CHL:H2	1.58	0.45
16:o:227:ASP:HB2	16:o:231:LYS:HE3	1.97	0.45
25:r:611:CLA:H3A	25:r:611:CLA:HBA2	1.54	0.45
5:B:211:LEU:HD22	25:R:603:CLA:H111	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:277:GLN:HB3	20:U:24:ARG:HG3	1.98	0.45
5:B:362:PHE:CZ	7:D:185:PHE:HZ	2.34	0.45
6:C:61:VAL:HG13	6:C:118:HIS:HD2	1.82	0.45
6:C:259:TRP:HH2	25:C:507:CLA:H201	1.80	0.45
1:N:192:PHE:CD2	25:N:602:CLA:H171	2.51	0.45
28:N:1623:NEX:H11	28:N:1623:NEX:H191	1.73	0.45
27:5:1622:XAT:H11	27:5:1622:XAT:H191	1.79	0.45
3:8:131:SER:O	3:8:133:THR:OG1	2.24	0.45
5:b:362:PHE:CZ	7:d:185:PHE:HZ	2.34	0.45
30:c:516:BCR:H21C	12:j:15:THR:HG23	1.98	0.45
25:g:610:CLA:HBB1	25:g:612:CLA:H3A	1.99	0.45
27:n:1622:XAT:H31	27:n:1622:XAT:H391	1.73	0.45
4:A:49:ILE:HG12	36:D:405:PL9:H501	1.98	0.45
4:A:130:GLU:HG2	7:D:257:ILE:HG21	1.98	0.45
5:B:315:ILE:HG12	5:B:321:LYS:HG3	1.97	0.45
5:B:368:VAL:HG21	5:B:422:ARG:HG2	1.98	0.45
25:B:602:CLA:H92	25:B:602:CLA:H61	1.81	0.45
25:B:614:CLA:H102	25:B:614:CLA:H62	1.79	0.45
6:C:223:TRP:CE3	6:C:224:ILE:HG12	2.52	0.45
24:Y:601:CHL:H102	27:Y:1622:XAT:H14	1.99	0.45
30:b:619:BCR:H24C	30:b:619:BCR:H371	1.83	0.45
6:c:318:LEU:HD12	6:c:340:TYR:HB3	1.99	0.45
1:n:44:TYR:CD2	25:n:602:CLA:HMD2	2.52	0.45
25:r:602:CLA:H101	27:r:622:XAT:H371	1.98	0.45
1:y:71:TRP:CE2	24:y:608:CHL:HED2	2.52	0.45
26:1:1621:LUT:H201	26:1:1621:LUT:H15	1.80	0.45
3:4:185:ARG:HA	3:4:188:MET:HE3	1.98	0.45
25:B:604:CLA:H62	25:B:604:CLA:H41	1.76	0.45
15:M:28:LYS:HB2	15:m:27:VAL:HG12	1.98	0.45
25:R:613:CLA:H92	29:R:2630:LHG:H171	1.98	0.45
7:d:173:SER:HB2	7:d:178:ALA:HB1	1.98	0.45
25:g:602:CLA:H91	25:y:603:CLA:H8	1.98	0.45
25:g:610:CLA:H62	25:g:610:CLA:H41	1.82	0.45
25:n:603:CLA:H12	1:y:51:LEU:HD11	1.98	0.45
25:n:603:CLA:H92	25:n:603:CLA:H61	1.80	0.45
28:n:1623:NEX:H15	28:n:1623:NEX:H201	1.78	0.45
4:A:228:THR:HA	17:R:58:ALA:HA	1.98	0.45
30:C:516:BCR:H21C	12:J:15:THR:HG23	1.98	0.45
1:G:97:TRP:O	26:G:1621:LUT:O3	2.34	0.45
3:8:29:LEU:HD11	3:8:51:ARG:HD3	1.97	0.45
3:8:185:ARG:HA	3:8:188:MET:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:410:CLA:HAB	11:i:15:PHE:CD2	2.52	0.45
25:b:612:CLA:H112	25:b:612:CLA:H72	1.74	0.45
7:d:18:ILE:HG22	22:x:76:SER:HB3	1.99	0.45
24:n:606:CHL:HMB1	24:n:609:CHL:HMC	1.97	0.45
1:1:108:GLY:O	1:1:122:GLN:NE2	2.39	0.45
24:1:607:CHL:H91	24:1:607:CHL:H112	1.79	0.45
25:1:610:CLA:CBB	26:1:1620:LUT:H32	2.46	0.45
3:4:131:SER:O	3:4:133:THR:OG1	2.24	0.45
25:B:613:CLA:H3A	25:B:613:CLA:HBA2	1.58	0.45
25:B:616:CLA:HBA1	25:B:616:CLA:H3A	1.77	0.45
30:H:101:BCR:H371	30:H:101:BCR:H24C	1.76	0.45
4:a:224:ILE:O	7:d:266:ARG:NH2	2.43	0.45
5:b:211:LEU:HD22	25:r:603:CLA:H111	1.97	0.45
5:b:368:VAL:HG21	5:b:422:ARG:HG2	1.99	0.45
30:b:618:BCR:H11C	30:b:618:BCR:H341	1.87	0.45
6:c:85:GLY:HA3	37:c:519:DGD:HE2	1.99	0.45
30:c:514:BCR:H15C	30:c:514:BCR:H351	1.78	0.45
1:g:21:ARG:NH2	1:g:36:LEU:O	2.42	0.45
1:n:192:PHE:CD2	25:n:602:CLA:H171	2.51	0.45
1:y:65:GLU:OE2	1:y:185:ARG:NE	2.47	0.45
34:B:621:SQD:H271	34:B:623:SQD:H102	1.99	0.45
29:D:409:LHG:C28	19:T:17:ILE:HG23	2.47	0.45
26:G:1621:LUT:H15	26:G:1621:LUT:H201	1.81	0.45
24:7:601:CHL:HAC1	29:7:2630:LHG:HC2	1.99	0.45
1:n:212:HIS:CG	25:n:613:CLA:HAA2	2.52	0.45
25:s:613:CLA:H61	25:s:613:CLA:H2	1.70	0.45
25:y:612:CLA:H142	25:y:612:CLA:H111	1.78	0.45
33:A:408:PHO:H2	33:A:408:PHO:H61	1.56	0.44
25:A:410:CLA:HAB	11:I:15:PHE:CD2	2.52	0.44
7:D:91:LEU:HA	7:D:91:LEU:HD23	1.81	0.44
1:G:49:ALA:HA	1:Y:64:LEU:HD11	1.98	0.44
24:Y:607:CHL:H62	24:Y:607:CHL:H2	1.55	0.44
25:Y:612:CLA:H142	25:Y:612:CLA:H111	1.78	0.44
3:8:96:THR:HG21	17:r:235:LEU:HA	1.99	0.44
4:a:160:ILE:HD11	37:c:518:DGD:HBT2	1.99	0.44
5:b:145:LEU:HD22	25:b:605:CLA:H18	1.98	0.44
28:s:1623:NEX:H11	28:s:1623:NEX:H191	1.76	0.44
24:2:606:CHL:HBC2	24:2:607:CHL:HHD	1.98	0.44
7:D:124:ILE:HD11	37:H:102:DGD:HAE1	1.98	0.44
29:D:409:LHG:H272	29:D:409:LHG:H141	1.99	0.44
24:N:606:CHL:HBA2	28:N:1623:NEX:H31	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:R:623:NEX:H22	1:y:163:PRO:HB2	2.00	0.44
1:Y:63:GLU:HA	1:Y:155:LEU:HD21	1.99	0.44
3:8:173:LEU:HG	3:8:177:LYS:HE3	1.98	0.44
5:b:277:GLN:HB3	20:u:24:ARG:HG3	1.98	0.44
6:c:338:GLY:HA2	16:o:111:TYR:OH	2.16	0.44
29:d:409:LHG:H272	29:d:409:LHG:H141	1.99	0.44
25:y:603:CLA:H3A	25:y:603:CLA:HBA1	1.64	0.44
4:A:160:ILE:HD11	37:C:518:DGD:HBT2	1.99	0.44
6:C:223:TRP:HZ3	6:C:285:ILE:HG12	1.80	0.44
7:D:18:ILE:HG22	22:X:76:SER:HB3	1.99	0.44
1:G:63:GLU:HA	1:G:155:LEU:HD21	1.98	0.44
27:Y:1622:XAT:H15	27:Y:1622:XAT:H201	1.65	0.44
1:5:104:ILE:HG21	1:5:124:ILE:HD13	1.98	0.44
4:a:42:LEU:CD2	34:a:418:SQD:H212	2.47	0.44
7:d:22:TRP:O	7:d:27:ARG:NH2	2.39	0.44
29:d:410:LHG:H121	29:d:410:LHG:H312	1.99	0.44
1:g:49:ALA:HA	1:y:64:LEU:HD11	1.99	0.44
27:g:1622:XAT:H391	27:g:1622:XAT:H31	1.73	0.44
10:h:49:LEU:HB3	30:h:101:BCR:H14C	1.99	0.44
2:3:207:VAL:HG11	25:3:613:CLA:HAC2	2.00	0.44
4:A:147:TYR:OH	33:A:408:PHO:O1A	2.31	0.44
6:C:39:ASN:ND2	25:C:510:CLA:O1A	2.49	0.44
26:G:1621:LUT:H35	26:G:1621:LUT:H401	1.79	0.44
30:T:101:BCR:H341	30:T:101:BCR:H11C	1.77	0.44
1:Y:71:TRP:CE2	24:Y:608:CHL:HED2	2.52	0.44
24:6:606:CHL:HBC2	24:6:607:CHL:HHD	1.98	0.44
34:b:621:SQD:H271	34:b:623:SQD:H102	1.99	0.44
6:c:214:LEU:HD22	21:w:15:PHE:CZ	2.53	0.44
7:d:237:ASN:HB3	7:d:240:GLN:HB3	1.98	0.44
1:g:126:ALA:HB3	24:g:605:CHL:HMC	1.99	0.44
28:y:1623:NEX:H35	28:y:1623:NEX:H401	1.73	0.44
24:3:606:CHL:HMB2	24:3:609:CHL:HMC	2.00	0.44
3:4:71:GLY:O	3:4:75:SER:OG	2.29	0.44
5:B:363:PHE:HB3	5:B:365:THR:O	2.18	0.44
5:B:460:LEU:HG	7:D:281:TRP:HZ3	1.82	0.44
25:B:611:CLA:H11	25:B:613:CLA:H191	1.99	0.44
7:D:194:LEU:O	14:L:35:TYR:OH	2.32	0.44
26:G:1620:LUT:H35	26:G:1620:LUT:H401	1.78	0.44
1:N:212:HIS:CG	25:N:613:CLA:HAA2	2.52	0.44
16:O:125:PRO:HG2	16:O:225:ASP:HB3	2.00	0.44
1:6:136:GLY:HA2	24:6:609:CHL:HAB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:147:PRO:HB2	24:6:608:CHL:HBB2	1.98	0.44
6:c:61:VAL:HG13	6:c:118:HIS:HD2	1.82	0.44
30:c:515:BCR:H15C	30:c:515:BCR:H351	1.78	0.44
25:d:403:CLA:H61	25:d:403:CLA:H102	1.72	0.44
25:g:611:CLA:H61	25:g:611:CLA:H41	1.86	0.44
25:n:611:CLA:H92	25:n:611:CLA:H61	1.81	0.44
25:n:613:CLA:H121	27:n:1622:XAT:H34	1.99	0.44
27:2:1622:XAT:H35	27:2:1622:XAT:H401	1.88	0.44
3:4:51:ARG:HH21	3:4:144:GLN:HB2	1.82	0.44
5:B:362:PHE:O	7:D:295:ARG:NH1	2.51	0.44
25:B:602:CLA:H12	25:B:602:CLA:H52	1.76	0.44
6:C:85:GLY:HA3	37:C:519:DGD:HE2	1.99	0.44
25:G:610:CLA:H62	25:G:610:CLA:H41	1.82	0.44
27:N:1622:XAT:H391	27:N:1622:XAT:H31	1.73	0.44
35:Z:101:LMG:HC91	35:Z:101:LMG:H291	1.80	0.44
4:a:312:ARG:NH1	8:e:56:PHE:HB2	2.32	0.44
25:b:611:CLA:H11	25:b:613:CLA:H191	1.99	0.44
6:c:223:TRP:CE3	6:c:224:ILE:HG12	2.52	0.44
24:g:607:CHL:H143	24:g:607:CHL:H111	1.71	0.44
30:h:101:BCR:H15C	30:h:101:BCR:H351	1.79	0.44
14:l:30:VAL:O	14:l:34:ASN:ND2	2.51	0.44
5:B:170:ASP:HB3	5:B:174:LEU:H	1.83	0.44
5:B:205:ALA:O	5:B:209:GLY:N	2.45	0.44
5:B:325:PHE:CG	14:L:35:TYR:HB3	2.53	0.44
6:C:28:GLN:HE22	7:D:231:ASN:HD22	1.66	0.44
6:C:214:LEU:HD22	21:W:15:PHE:CZ	2.53	0.44
25:N:613:CLA:H121	27:N:1622:XAT:H34	1.99	0.44
28:N:1623:NEX:H15	28:N:1623:NEX:H201	1.78	0.44
24:Y:608:CHL:H11	26:Y:1620:LUT:H383	1.99	0.44
28:5:1623:NEX:H15	28:5:1623:NEX:H201	1.90	0.44
25:a:405:CLA:H191	29:d:409:LHG:H331	1.98	0.44
5:b:325:PHE:CG	14:l:35:TYR:HB3	2.53	0.44
24:n:606:CHL:HBA2	28:n:1623:NEX:H31	1.99	0.44
27:n:1622:XAT:H201	27:n:1622:XAT:H15	1.62	0.44
16:o:47:ASN:HA	16:o:91:GLY:O	2.17	0.44
29:B:2630:LHG:H152	29:B:2631:LHG:H162	1.99	0.44
1:G:52:SER:OG	1:G:61:ASN:ND2	2.48	0.44
27:G:1622:XAT:H201	27:G:1622:XAT:H15	1.67	0.44
27:N:1622:XAT:H361	29:N:2630:LHG:HC92	2.00	0.44
16:O:47:ASN:HA	16:O:91:GLY:O	2.17	0.44
17:R:187:ASP:HA	17:R:188:PRO:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:S:603:CLA:HBA1	25:S:603:CLA:H3A	1.87	0.44
26:5:1621:LUT:H35	26:5:1621:LUT:H401	1.84	0.44
4:a:24:THR:O	7:d:252:ARG:NH2	2.47	0.44
6:c:28:GLN:HE22	7:d:231:ASN:HD22	1.66	0.44
25:c:510:CLA:H193	25:c:510:CLA:H162	1.80	0.44
29:d:409:LHG:C28	19:t:17:ILE:HG23	2.47	0.44
24:g:606:CHL:HMB1	24:g:609:CHL:HMC	1.99	0.44
1:y:63:GLU:HA	1:y:155:LEU:HD21	1.99	0.44
28:2:1623:NEX:H201	28:2:1623:NEX:H15	1.71	0.44
24:4:601:CHL:HBA1	24:4:601:CHL:H3A	1.76	0.44
7:D:52:GLY:HA2	7:D:56:VAL:HB	1.99	0.44
1:G:126:ALA:HB3	24:G:605:CHL:HMC	1.99	0.44
14:L:30:VAL:O	14:L:34:ASN:ND2	2.51	0.44
1:N:199:ILE:HG13	24:N:607:CHL:H42	2.00	0.44
28:7:1623:NEX:H11	28:7:1623:NEX:H191	1.80	0.44
5:b:363:PHE:HB3	5:b:365:THR:O	2.18	0.44
18:s:212:GLU:OE2	18:s:220:LYS:NZ	2.42	0.44
24:3:601:CHL:HAC1	29:3:2630:LHG:HC2	1.99	0.43
5:B:400:GLU:OE1	5:B:410:THR:OG1	2.26	0.43
25:B:612:CLA:H112	25:B:612:CLA:H72	1.74	0.43
6:C:318:LEU:HD12	6:C:340:TYR:HB3	1.99	0.43
25:N:602:CLA:H172	25:N:602:CLA:H13	1.81	0.43
1:5:215:ASP:OD2	1:5:218:ASN:ND2	2.46	0.43
24:8:606:CHL:HBA2	30:8:623:BCR:H19C	2.00	0.43
4:a:225:ARG:HD3	17:r:58:ALA:HB1	1.99	0.43
1:g:215:ASP:OD2	1:g:218:ASN:HB2	2.18	0.43
17:r:181:PRO:HD2	26:r:620:LUT:H23	1.99	0.43
4:A:42:LEU:HD23	34:A:418:SQD:C21	2.48	0.43
24:N:607:CHL:H111	24:N:607:CHL:H143	1.74	0.43
18:S:172:PRO:HD2	26:S:1620:LUT:H23	2.00	0.43
1:Y:17:TYR:CE2	1:Y:174:ALA:HB1	2.54	0.43
27:Y:1622:XAT:H11	27:Y:1622:XAT:H191	1.81	0.43
26:7:1620:LUT:H35	26:7:1620:LUT:H401	1.86	0.43
5:b:324:LEU:HD21	7:d:197:PHE:HE2	1.83	0.43
6:c:39:ASN:ND2	25:c:510:CLA:O1A	2.49	0.43
7:d:89:SER:HB3	8:e:69:ARG:NH2	2.33	0.43
4:A:42:LEU:CD2	34:A:418:SQD:H212	2.47	0.43
25:B:604:CLA:H2	25:B:606:CLA:H91	2.00	0.43
25:B:615:CLA:H91	25:B:615:CLA:H112	1.86	0.43
25:D:403:CLA:H62	25:D:403:CLA:H41	1.79	0.43
1:G:148:LEU:N	24:G:608:CHL:OMC	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:G:606:CHL:HMB1	24:G:609:CHL:HMC	1.99	0.43
25:G:611:CLA:H91	25:G:611:CLA:H112	1.79	0.43
18:S:86:MET:SD	25:S:610:CLA:HAB	2.59	0.43
4:a:217:SER:HA	7:d:273:LEU:HD12	1.99	0.43
7:d:52:GLY:HA2	7:d:56:VAL:HB	1.99	0.43
29:d:409:LHG:HC2	14:l:14:ASN:HD21	1.84	0.43
29:d:409:LHG:H252	14:l:23:LEU:HD22	2.00	0.43
1:n:23:LYS:HZ1	1:n:32:SER:HB3	1.83	0.43
1:n:199:ILE:HG13	24:n:607:CHL:H42	2.00	0.43
27:n:1622:XAT:H361	29:n:2630:LHG:HC92	2.00	0.43
17:r:75:VAL:HG11	17:r:171:ARG:HD2	2.00	0.43
24:y:601:CHL:H102	27:y:1622:XAT:H14	1.99	0.43
1:2:136:GLY:HA2	24:2:609:CHL:HAB	2.00	0.43
27:2:1622:XAT:H31	27:2:1622:XAT:H391	1.71	0.43
5:B:324:LEU:HD21	7:D:197:PHE:HE2	1.83	0.43
29:D:410:LHG:H312	29:D:410:LHG:H121	1.99	0.43
28:G:1623:NEX:H11	28:G:1623:NEX:H191	1.76	0.43
10:H:49:LEU:HB3	30:H:101:BCR:H14C	1.99	0.43
17:R:181:PRO:HD2	26:R:620:LUT:H23	1.99	0.43
25:R:611:CLA:H3A	25:R:611:CLA:HBA2	1.54	0.43
4:a:254:TYR:CD1	7:d:133:LEU:HG	2.53	0.43
5:b:170:ASP:HB3	5:b:174:LEU:H	1.82	0.43
5:b:281:GLN:HG2	20:u:16:VAL:HG22	2.01	0.43
1:g:148:LEU:N	24:g:608:CHL:OMC	2.52	0.43
24:y:608:CHL:H11	26:y:1620:LUT:H383	1.99	0.43
24:4:606:CHL:HBA2	30:4:623:BCR:H19C	2.00	0.43
26:4:620:LUT:H15	26:4:620:LUT:H201	1.79	0.43
25:B:611:CLA:H102	25:B:616:CLA:HAA1	2.00	0.43
25:C:510:CLA:HBA1	25:C:510:CLA:H11	1.76	0.43
17:R:185:ALA:HB1	17:R:191:LYS:HG3	2.00	0.43
26:S:1620:LUT:H35	26:S:1620:LUT:H401	1.79	0.43
25:c:506:CLA:H41	25:c:506:CLA:H62	1.81	0.43
18:s:86:MET:SD	25:s:610:CLA:HAB	2.59	0.43
5:B:366:PHE:O	5:B:425:GLN:NE2	2.49	0.43
25:B:604:CLA:H193	25:B:604:CLA:H162	1.84	0.43
7:D:202:VAL:HG22	25:D:402:CLA:C1B	2.49	0.43
1:G:164:LEU:HD12	26:G:1620:LUT:H222	2.01	0.43
1:G:215:ASP:OD2	1:G:218:ASN:HB2	2.18	0.43
18:S:202:GLY:O	18:S:206:GLN:CB	2.66	0.43
1:5:170:PRO:HA	1:5:173:PHE:HB3	2.00	0.43
28:5:1623:NEX:H11	28:5:1623:NEX:H191	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:7:606:CHL:HMB2	24:7:609:CHL:HMC	2.00	0.43
4:a:42:LEU:HD23	34:a:418:SQD:C21	2.48	0.43
25:b:611:CLA:H102	25:b:616:CLA:HAA1	2.00	0.43
25:b:613:CLA:H122	25:b:613:CLA:H162	1.88	0.43
1:g:164:LEU:HD12	26:g:1620:LUT:H222	2.01	0.43
25:A:406:CLA:H121	25:A:406:CLA:HMA1	2.01	0.43
5:B:260:SER:OG	5:B:262:THR:OG1	2.34	0.43
29:D:409:LHG:H252	14:L:23:LEU:HD22	2.00	0.43
1:G:181:LEU:HD23	1:G:181:LEU:HA	1.87	0.43
26:Y:1621:LUT:H35	26:Y:1621:LUT:H401	1.77	0.43
25:5:602:CLA:H93	25:5:602:CLA:H111	1.85	0.43
1:g:92:PHE:HB2	1:g:95:ALA:HB2	2.00	0.43
27:2:1622:XAT:H363	29:2:2630:LHG:HC41	2.01	0.43
5:B:330:MET:HE3	5:B:446:SER:N	2.34	0.43
5:B:413:ASP:OD1	5:B:413:ASP:N	2.51	0.43
6:C:217:PRO:HG3	37:C:518:DGD:HA71	2.01	0.43
7:D:89:SER:HB3	8:E:69:ARG:NH2	2.33	0.43
17:R:75:VAL:HG11	17:R:171:ARG:HD2	2.00	0.43
25:a:406:CLA:HMA1	25:a:406:CLA:H121	2.01	0.43
27:r:622:XAT:H35	27:r:622:XAT:H401	1.78	0.43
1:1:44:TYR:N	25:1:602:CLA:OBD	2.40	0.43
26:3:1620:LUT:H35	26:3:1620:LUT:H401	1.86	0.43
5:B:249:ALA:HA	5:B:252:VAL:HG22	2.01	0.43
5:B:281:GLN:HG2	20:U:16:VAL:HG22	2.01	0.43
30:B:620:BCR:H15C	30:B:620:BCR:H351	1.85	0.43
1:G:44:TYR:CD2	25:G:602:CLA:HMD2	2.54	0.43
26:N:1621:LUT:H401	26:N:1621:LUT:H35	1.79	0.43
26:8:620:LUT:H35	26:8:620:LUT:H401	1.80	0.43
4:a:63:ILE:HA	6:c:337:LEU:HD11	2.01	0.43
5:b:362:PHE:O	7:d:295:ARG:NH1	2.51	0.43
25:b:604:CLA:H193	25:b:604:CLA:H162	1.84	0.43
37:h:102:DGD:HB91	37:h:102:DGD:HB62	1.66	0.43
26:r:620:LUT:H35	26:r:620:LUT:H401	1.84	0.43
25:1:603:CLA:H3A	25:1:603:CLA:HBA1	1.78	0.43
26:1:1620:LUT:H15	26:1:1620:LUT:H201	1.86	0.43
4:A:225:ARG:HD3	17:R:58:ALA:HB1	1.99	0.43
30:B:619:BCR:H24C	30:B:619:BCR:H371	1.84	0.43
24:G:601:CHL:H152	24:Y:607:CHL:HBB1	2.01	0.43
1:Y:25:LEU:HB2	1:Y:29:SER:HA	2.01	0.43
26:Y:1620:LUT:H35	26:Y:1620:LUT:H401	1.86	0.43
3:8:122:GLN:H	17:r:16:PRO:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:477:ASP:OD1	5:b:477:ASP:N	2.52	0.43
25:b:604:CLA:H2	25:b:606:CLA:H91	2.00	0.43
25:c:510:CLA:H11	25:c:510:CLA:HBA1	1.76	0.43
29:d:409:LHG:H281	19:t:17:ILE:HG23	2.01	0.43
1:g:44:TYR:CD2	25:g:602:CLA:HMD2	2.53	0.43
24:g:601:CHL:H152	24:y:607:CHL:HBB1	2.01	0.43
27:g:1622:XAT:H11	27:g:1622:XAT:H191	1.93	0.43
17:r:23:TYR:OH	17:r:35:ASP:OD2	2.28	0.43
24:1:606:CHL:HMB1	24:1:609:CHL:HMC	2.01	0.42
1:2:96:VAL:HB	1:2:99:LYS:HB2	2.01	0.42
2:3:166:TYR:HB3	25:3:610:CLA:HED2	2.01	0.42
25:B:608:CLA:H192	14:L:28:LEU:HD11	2.01	0.42
25:B:617:CLA:H11	25:B:617:CLA:H51	1.90	0.42
30:H:101:BCR:H15C	30:H:101:BCR:H351	1.79	0.42
1:N:73:MET:SD	25:N:610:CLA:HAB	2.59	0.42
25:N:611:CLA:H61	25:N:611:CLA:H92	1.81	0.42
1:6:71:TRP:CE2	24:6:608:CHL:HED2	2.54	0.42
1:6:96:VAL:HB	1:6:99:LYS:HB2	2.01	0.42
24:6:609:CHL:H93	24:6:609:CHL:H61	1.84	0.42
2:7:181:PRO:HA	2:7:184:PHE:HB3	2.02	0.42
28:7:1623:NEX:H201	28:7:1623:NEX:H15	1.67	0.42
3:8:51:ARG:HH21	3:8:144:GLN:HB2	1.82	0.42
25:a:405:CLA:C3	33:a:408:PHO:HBB1	2.49	0.42
30:b:619:BCR:H15C	30:b:619:BCR:H351	1.79	0.42
30:b:619:BCR:H361	30:b:619:BCR:H20C	1.86	0.42
1:g:63:GLU:HA	1:g:155:LEU:HD11	2.00	0.42
3:4:192:LEU:HD13	25:4:603:CLA:HBB2	2.01	0.42
4:A:254:TYR:CD1	7:D:133:LEU:HG	2.53	0.42
6:C:223:TRP:CG	6:C:224:ILE:N	2.87	0.42
25:C:510:CLA:H162	25:C:510:CLA:H193	1.80	0.42
25:N:610:CLA:H41	25:N:610:CLA:H62	1.86	0.42
26:g:1621:LUT:H372	25:y:603:CLA:HED3	2.01	0.42
26:s:1620:LUT:H35	26:s:1620:LUT:H401	1.79	0.42
25:2:604:CLA:HBA1	24:2:606:CHL:C1D	2.49	0.42
27:2:1622:XAT:H202	2:3:138:LEU:HD21	2.01	0.42
4:A:217:SER:HA	7:D:273:LEU:HD12	1.99	0.42
6:C:319:VAL:HG22	6:C:384:ILE:HD13	2.02	0.42
29:D:409:LHG:HC2	14:L:14:ASN:HD21	1.84	0.42
30:H:101:BCR:H20C	30:H:101:BCR:H361	1.82	0.42
25:N:613:CLA:H91	29:N:2630:LHG:H321	2.01	0.42
19:T:22:PHE:HB3	30:b:620:BCR:H271	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:603:CLA:H3A	25:Y:603:CLA:HBA1	1.64	0.42
25:Y:610:CLA:H91	25:Y:610:CLA:H111	1.89	0.42
27:8:622:XAT:H35	27:8:622:XAT:H401	1.85	0.42
4:a:210:LEU:O	4:a:214:MET:HB2	2.20	0.42
25:b:608:CLA:H192	14:l:28:LEU:HD11	2.02	0.42
1:g:212:HIS:CG	25:g:613:CLA:HAA2	2.55	0.42
16:o:125:PRO:HG2	16:o:225:ASP:HB3	2.00	0.42
18:s:202:GLY:O	18:s:206:GLN:CB	2.66	0.42
1:y:36:LEU:HD13	1:y:45:GLY:HA2	2.00	0.42
25:y:602:CLA:H172	25:y:602:CLA:H13	1.84	0.42
1:1:170:PRO:HA	1:1:173:PHE:HB3	2.00	0.42
26:4:620:LUT:H401	26:4:620:LUT:H35	1.80	0.42
1:Y:36:LEU:HD13	1:Y:45:GLY:HA2	2.01	0.42
2:7:207:VAL:HG11	25:7:613:CLA:HAC2	2.00	0.42
25:b:603:CLA:H62	25:b:603:CLA:H41	1.75	0.42
30:b:618:BCR:H15C	30:b:618:BCR:H351	1.79	0.42
36:d:405:PL9:H401	29:d:409:LHG:H212	2.01	0.42
25:n:602:CLA:H172	25:n:602:CLA:H13	1.81	0.42
1:1:225:ALA:HA	27:1:1622:XAT:H42	2.02	0.42
1:2:71:TRP:CE2	24:2:608:CHL:HED2	2.54	0.42
25:B:607:CLA:H161	25:B:607:CLA:H141	1.85	0.42
25:B:611:CLA:HBD	25:B:611:CLA:H143	2.00	0.42
29:B:2630:LHG:H131	29:B:2631:LHG:H162	2.01	0.42
7:D:172:PRO:HB3	7:D:179:ILE:HD12	2.01	0.42
1:G:63:GLU:HA	1:G:155:LEU:HD11	2.01	0.42
26:G:1620:LUT:H15	26:G:1620:LUT:H201	1.88	0.42
28:G:1623:NEX:H15	28:G:1623:NEX:H201	1.81	0.42
25:Y:603:CLA:H2	25:Y:603:CLA:H61	1.81	0.42
5:b:330:MET:HE3	5:b:446:SER:N	2.34	0.42
25:b:611:CLA:H143	25:b:611:CLA:HBD	2.00	0.42
6:c:144:PHE:O	6:c:148:GLY:N	2.52	0.42
7:d:146:ALA:HA	7:d:277:VAL:HG21	2.02	0.42
7:d:202:VAL:HG22	25:d:402:CLA:C1B	2.49	0.42
1:n:73:MET:SD	25:n:610:CLA:HAB	2.59	0.42
25:3:613:CLA:H61	25:3:613:CLA:H2	1.81	0.42
7:D:203:ALA:HB2	36:D:405:PL9:H353	2.02	0.42
1:G:92:PHE:HB2	1:G:95:ALA:HB2	2.01	0.42
1:G:212:HIS:CG	25:G:613:CLA:HAA2	2.55	0.42
25:G:613:CLA:H2	25:G:613:CLA:H61	1.72	0.42
14:L:20:TRP:HZ3	14:L:23:LEU:HD23	1.78	0.42
14:L:27:VAL:HG11	29:L:101:LHG:H201	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:44:TYR:HE2	24:Y:601:CHL:CBC	2.32	0.42
25:a:410:CLA:H112	25:a:410:CLA:H72	1.81	0.42
6:c:223:TRP:CG	6:c:224:ILE:N	2.87	0.42
7:d:172:PRO:HB3	7:d:179:ILE:HD12	2.01	0.42
30:d:404:BCR:H15C	30:d:404:BCR:H351	1.91	0.42
26:g:1621:LUT:H35	26:g:1621:LUT:H401	1.79	0.42
25:n:602:CLA:HBA1	26:n:1621:LUT:H382	2.01	0.42
1:2:146:GLY:HA3	1:2:147:PRO:HD3	1.85	0.42
3:4:8:SER:HB2	3:4:11:PRO:HD2	2.01	0.42
4:A:24:THR:O	7:D:252:ARG:NH2	2.47	0.42
4:A:63:ILE:HA	6:C:337:LEU:HD11	2.01	0.42
5:B:382:PRO:HB3	5:B:386:ALA:HB3	2.01	0.42
35:B:622:LMG:H242	7:D:285:LEU:HD23	2.02	0.42
24:G:601:CHL:H62	24:G:601:CHL:H41	1.82	0.42
13:K:45:LEU:O	13:K:48:PHE:HB3	2.20	0.42
1:N:182:LYS:NZ	29:N:2630:LHG:O4	2.44	0.42
1:5:225:ALA:HA	27:5:1622:XAT:H42	2.02	0.42
5:b:249:ALA:HA	5:b:252:VAL:HG22	2.01	0.42
5:b:413:ASP:N	5:b:413:ASP:OD1	2.51	0.42
25:b:605:CLA:H93	25:b:606:CLA:HAB	2.02	0.42
35:c:521:LMG:H361	13:k:45:LEU:HD11	2.01	0.42
25:n:613:CLA:H91	29:n:2630:LHG:H321	2.01	0.42
17:r:203:ARG:HB2	29:r:2630:LHG:H241	2.02	0.42
1:y:24:TYR:CG	1:y:46:TRP:HB2	2.55	0.42
1:y:181:LEU:HD23	1:y:181:LEU:HA	1.81	0.42
27:4:622:XAT:H35	27:4:622:XAT:H401	1.85	0.42
4:A:234:ASN:HD21	29:D:408:LHG:HC11	1.85	0.42
25:B:605:CLA:H93	25:B:606:CLA:HAB	2.02	0.42
25:C:506:CLA:H71	11:I:20:ILE:HD13	2.02	0.42
7:D:146:ALA:HA	7:D:277:VAL:HG21	2.02	0.42
16:O:80:THR:O	16:O:81:ARG:HB2	2.19	0.42
26:Y:1621:LUT:H15	26:Y:1621:LUT:H201	1.82	0.42
27:Y:1622:XAT:H12	29:Y:2630:LHG:H191	2.02	0.42
1:5:181:LEU:HD23	1:5:181:LEU:HA	1.81	0.42
3:8:8:SER:HB2	3:8:11:PRO:HD2	2.01	0.42
3:8:192:LEU:HD13	25:8:603:CLA:HBB2	2.01	0.42
4:a:234:ASN:HD21	29:d:408:LHG:HC11	1.85	0.42
5:b:182:ASN:HA	35:b:2633:LMG:HC62	2.02	0.42
5:b:214:LEU:HD12	25:r:609:CLA:H93	2.02	0.42
5:b:469:HIS:HE1	25:b:612:CLA:NA	2.18	0.42
25:b:603:CLA:H42	37:h:102:DGD:HB41	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:c:217:PRO:HG3	37:c:518:DGD:HA71	2.01	0.42
7:d:203:ALA:HB2	36:d:405:PL9:H353	2.02	0.42
1:n:65:GLU:O	1:n:69:SER:OG	2.30	0.42
1:y:25:LEU:HB2	1:y:29:SER:HA	2.01	0.42
1:1:118:LEU:HD23	1:1:118:LEU:HA	1.86	0.42
28:2:1623:NEX:H35	28:2:1623:NEX:H401	1.90	0.42
28:3:1623:NEX:H15	28:3:1623:NEX:H201	1.67	0.42
3:4:122:GLN:H	17:R:16:PRO:HB2	1.84	0.42
4:A:210:LEU:O	4:A:214:MET:HB2	2.20	0.42
5:B:182:ASN:HA	35:B:2633:LMG:HC62	2.02	0.42
25:B:603:CLA:H93	25:B:603:CLA:H61	1.78	0.42
24:G:607:CHL:HAA2	27:N:1622:XAT:H41	2.01	0.42
17:R:203:ARG:HB2	29:R:2630:LHG:H241	2.02	0.42
25:R:613:CLA:H111	29:R:2630:LHG:H292	2.02	0.42
1:Y:65:GLU:OE2	1:Y:185:ARG:NE	2.47	0.42
1:6:146:GLY:HA3	1:6:147:PRO:HD3	1.85	0.42
25:6:604:CLA:HBA1	24:6:606:CHL:C1D	2.49	0.42
3:8:128:THR:OG1	3:8:133:THR:N	2.53	0.42
5:b:42:LEU:HD13	5:b:94:GLU:HG3	2.02	0.42
25:b:615:CLA:H91	25:b:615:CLA:H112	1.87	0.42
24:g:601:CHL:H112	24:g:601:CHL:H91	1.79	0.42
26:g:1621:LUT:H15	26:g:1621:LUT:H201	1.81	0.42
17:r:185:ALA:HB1	17:r:191:LYS:HG3	2.00	0.42
18:s:229:ASN:ND2	35:z:101:LMG:H342	2.35	0.42
1:y:44:TYR:HE2	24:y:601:CHL:CBC	2.32	0.42
28:y:1623:NEX:H15	28:y:1623:NEX:H201	1.84	0.42
30:4:623:BCR:H351	30:4:623:BCR:H15C	1.76	0.42
5:B:469:HIS:HE1	25:B:612:CLA:NA	2.18	0.42
25:B:613:CLA:H61	25:B:613:CLA:H102	1.62	0.42
30:B:619:BCR:H14C	30:t:101:BCR:C38	2.50	0.42
6:C:167:LEU:HD23	6:C:170:ILE:HD12	2.02	0.42
25:C:504:CLA:H42	37:C:519:DGD:HB32	2.02	0.42
26:G:1621:LUT:H372	25:Y:603:CLA:HED3	2.01	0.42
24:N:607:CHL:H62	24:N:607:CHL:H2	1.59	0.42
1:5:63:GLU:HA	1:5:155:LEU:HD11	2.01	0.42
27:6:1622:XAT:H363	29:6:2630:LHG:HC41	2.01	0.42
2:7:166:TYR:HB3	25:7:610:CLA:HED2	2.01	0.42
3:8:85:ASP:HB3	3:8:88:ALA:HB2	2.02	0.42
30:8:623:BCR:H11C	30:8:623:BCR:H341	1.85	0.42
5:b:496:GLN:HE22	22:x:82:LYS:HB2	1.85	0.42
30:c:517:BCR:H24C	30:c:517:BCR:H371	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:65:GLU:O	1:g:69:SER:OG	2.34	0.42
13:k:45:LEU:O	13:k:48:PHE:HB3	2.20	0.42
14:l:27:VAL:HG11	29:l:101:LHG:H201	2.02	0.42
27:r:622:XAT:H15	27:r:622:XAT:H201	1.87	0.42
18:s:172:PRO:HD2	26:s:1620:LUT:H23	2.00	0.42
26:2:1620:LUT:H15	26:2:1620:LUT:H201	1.85	0.41
4:A:179:THR:O	4:A:183:MET:HG3	2.20	0.41
6:C:70:PHE:CD1	13:K:38:ASP:HA	2.55	0.41
6:C:97:TRP:NE1	35:Z:101:LMG:H151	2.35	0.41
30:C:517:BCR:H371	30:C:517:BCR:H24C	1.75	0.41
1:N:189:PHE:HD1	25:N:602:CLA:H201	1.85	0.41
1:Y:24:TYR:CG	1:Y:46:TRP:HB2	2.55	0.41
1:6:67:ILE:HG22	24:6:609:CHL:HMD2	2.02	0.41
1:6:153:ASP:OD2	1:6:156:TYR:N	2.43	0.41
5:b:217:LEU:HB3	25:r:616:CLA:HBA2	2.02	0.41
5:b:467:ILE:HD13	5:b:467:ILE:HA	1.91	0.41
6:c:48:LYS:NZ	6:c:133:ALA:O	2.52	0.41
6:c:70:PHE:CD1	13:k:38:ASP:HA	2.55	0.41
6:c:97:TRP:NE1	35:z:101:LMG:H151	2.35	0.41
25:c:504:CLA:H42	37:c:519:DGD:HB32	2.02	0.41
1:g:197:GLN:HG3	25:g:613:CLA:C1D	2.50	0.41
10:h:58:LEU:HD11	37:h:102:DGD:HA31	2.02	0.41
26:n:1620:LUT:H35	26:n:1620:LUT:H401	1.80	0.41
25:s:604:CLA:H3A	25:s:604:CLA:HBA2	1.80	0.41
25:A:405:CLA:C3	33:A:408:PHO:HBB1	2.49	0.41
5:B:214:LEU:HD12	25:R:609:CLA:H93	2.02	0.41
34:B:623:SQD:H312	15:M:17:VAL:HG13	2.01	0.41
25:C:513:CLA:H203	25:C:513:CLA:H161	1.84	0.41
7:D:150:PRO:HB3	25:D:402:CLA:H41	2.02	0.41
36:D:405:PL9:H401	29:D:409:LHG:H212	2.01	0.41
17:R:83:TYR:OH	17:R:94:GLU:OE1	2.25	0.41
5:b:64:PRO:O	5:b:68:ARG:HB2	2.20	0.41
5:b:458:PHE:HB3	25:b:605:CLA:HBC2	2.02	0.41
25:b:614:CLA:H102	25:b:614:CLA:H62	1.79	0.41
6:c:319:VAL:HG22	6:c:384:ILE:HD13	2.02	0.41
26:s:1621:LUT:H401	26:s:1621:LUT:H35	1.81	0.41
1:y:17:TYR:CE2	1:y:174:ALA:HB1	2.54	0.41
2:3:181:PRO:HA	2:3:184:PHE:HB3	2.02	0.41
26:3:1620:LUT:H31	26:3:1620:LUT:H391	1.94	0.41
25:A:406:CLA:H111	25:A:406:CLA:H152	1.84	0.41
25:B:608:CLA:HAC2	30:t:101:BCR:H272	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:615:CLA:H92	25:B:615:CLA:H61	1.94	0.41
6:C:48:LYS:NZ	6:C:133:ALA:O	2.52	0.41
30:D:404:BCR:H11C	30:D:404:BCR:H341	1.94	0.41
13:K:33:LEU:HD22	13:K:36:ILE:HD11	2.02	0.41
26:S:1620:LUT:H31	26:S:1620:LUT:H391	1.94	0.41
26:5:1620:LUT:H31	26:5:1620:LUT:H391	1.88	0.41
26:5:1620:LUT:H35	26:5:1620:LUT:H401	1.77	0.41
25:6:602:CLA:CBB	26:6:1621:LUT:H32	2.50	0.41
25:6:612:CLA:HBB1	26:6:1620:LUT:C13	2.50	0.41
30:8:623:BCR:H15C	30:8:623:BCR:H351	1.76	0.41
25:g:610:CLA:H13	25:g:610:CLA:H172	1.86	0.41
14:l:17:SER:OG	29:l:101:LHG:HC42	2.21	0.41
14:l:20:TRP:HZ3	14:l:23:LEU:HD23	1.78	0.41
1:1:57:THR:HG22	1:1:61:ASN:HD21	1.85	0.41
25:2:602:CLA:CBB	26:2:1621:LUT:H32	2.50	0.41
2:3:79:ARG:HA	2:3:82:MET:HE3	2.02	0.41
25:3:610:CLA:CBB	26:3:1620:LUT:H32	2.51	0.41
30:A:411:BCR:H24C	30:A:411:BCR:H371	1.79	0.41
5:B:108:PHE:CE2	30:t:101:BCR:H353	2.54	0.41
5:B:121:GLU:HG3	10:H:16:ARG:HD3	2.03	0.41
25:B:603:CLA:H42	37:H:102:DGD:HB41	2.01	0.41
25:B:611:CLA:H51	25:B:611:CLA:H8	1.93	0.41
6:C:110:PRO:HG3	35:Z:101:LMG:H121	2.03	0.41
14:L:17:SER:OG	29:L:101:LHG:HC42	2.21	0.41
17:R:173:TYR:HE1	17:R:198:GLU:OE2	2.03	0.41
18:S:235:ALA:HB2	23:Z:59:SER:HB3	2.03	0.41
25:S:613:CLA:H61	25:S:613:CLA:H2	1.70	0.41
26:S:1621:LUT:H15	26:S:1621:LUT:H201	1.93	0.41
25:Y:602:CLA:H13	25:Y:602:CLA:H172	1.84	0.41
25:Y:602:CLA:H193	25:Y:602:CLA:H161	1.85	0.41
25:5:612:CLA:HBB1	26:5:1620:LUT:H35	2.03	0.41
5:b:157:HIS:HA	5:b:163:GLY:HA3	2.02	0.41
35:b:622:LMG:H242	7:d:285:LEU:HD23	2.02	0.41
30:d:404:BCR:H11C	30:d:404:BCR:H341	1.95	0.41
1:g:41:PRO:HG3	1:g:177:LYS:HB3	2.02	0.41
28:g:1623:NEX:H35	28:g:1623:NEX:H401	1.95	0.41
16:o:80:THR:HG23	16:o:115:THR:HB	2.03	0.41
25:y:603:CLA:HHC	25:y:603:CLA:HBB1	2.03	0.41
25:1:612:CLA:HBB1	26:1:1620:LUT:H35	2.03	0.41
5:B:64:PRO:O	5:B:68:ARG:HB2	2.20	0.41
29:B:2631:LHG:H161	29:B:2631:LHG:H341	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:501:CLA:HBB1	25:C:501:CLA:HHC	2.02	0.41
1:G:41:PRO:HG3	1:G:177:LYS:HB3	2.03	0.41
1:G:197:GLN:HG3	25:G:613:CLA:C1D	2.50	0.41
25:G:610:CLA:H172	25:G:610:CLA:H13	1.86	0.41
10:H:58:LEU:HD11	37:H:102:DGD:HA31	2.02	0.41
18:S:229:ASN:ND2	35:Z:101:LMG:H342	2.35	0.41
24:Y:601:CHL:HMA3	29:Y:2630:LHG:H121	2.03	0.41
1:5:67:ILE:HG22	24:5:609:CHL:HMD2	2.03	0.41
1:5:118:LEU:HD23	1:5:118:LEU:HA	1.86	0.41
30:a:411:BCR:H15C	30:a:411:BCR:H351	1.85	0.41
5:b:382:PRO:HB3	5:b:386:ALA:HB3	2.01	0.41
25:b:610:CLA:HHC	25:b:610:CLA:HAB	1.89	0.41
25:b:616:CLA:H2	25:b:616:CLA:H61	1.80	0.41
34:b:623:SQD:H312	15:m:17:VAL:HG13	2.02	0.41
29:b:2630:LHG:H131	29:b:2631:LHG:H162	2.01	0.41
6:c:110:PRO:HG3	35:z:101:LMG:H121	2.03	0.41
37:c:520:DGD:O1B	12:j:33:TYR:OH	2.32	0.41
29:c:2630:LHG:H223	25:s:614:CLA:H2	2.02	0.41
7:d:269:HIS:CE1	38:d:401:BCT:O3	2.73	0.41
1:1:63:GLU:HA	1:1:155:LEU:HD11	2.01	0.41
26:1:1620:LUT:H35	26:1:1620:LUT:H401	1.77	0.41
25:2:603:CLA:H3A	25:2:603:CLA:HBA1	1.80	0.41
25:2:612:CLA:HBB1	26:2:1620:LUT:C13	2.51	0.41
1:N:163:PRO:HD2	26:N:1620:LUT:H23	2.03	0.41
1:5:118:LEU:HD23	24:5:605:CHL:HED2	2.03	0.41
26:5:1620:LUT:H15	26:5:1620:LUT:H201	1.86	0.41
3:8:36:ASP:OD1	27:8:622:XAT:O23	2.32	0.41
5:b:205:ALA:O	5:b:209:GLY:N	2.45	0.41
25:b:606:CLA:H92	25:b:606:CLA:H61	1.93	0.41
25:c:501:CLA:HBB1	25:c:501:CLA:HHC	2.02	0.41
7:d:89:SER:HB3	8:e:69:ARG:HH21	1.86	0.41
1:g:41:PRO:HG3	1:g:177:LYS:HD3	2.03	0.41
1:g:167:ALA:HB2	25:g:610:CLA:HAA1	2.01	0.41
25:g:612:CLA:H142	25:g:612:CLA:H111	1.85	0.41
27:n:1622:XAT:H11	27:n:1622:XAT:H191	1.87	0.41
16:o:80:THR:O	16:o:81:ARG:HB2	2.19	0.41
17:r:187:ASP:HA	17:r:188:PRO:HD3	1.82	0.41
1:1:52:SER:HB3	1:1:58:PHE:HD1	1.85	0.41
24:2:606:CHL:HMB2	24:2:609:CHL:HMC	2.03	0.41
26:3:1621:LUT:H15	26:3:1621:LUT:H201	1.94	0.41
5:B:464:PHE:HD2	25:B:612:CLA:HAC2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:409:LHG:H281	19:T:17:ILE:HG23	2.01	0.41
14:L:11:VAL:HG11	15:M:25:ILE:HD12	2.02	0.41
1:N:192:PHE:CE2	25:N:602:CLA:H171	2.55	0.41
27:R:622:XAT:H173	27:R:622:XAT:H3	1.91	0.41
18:S:48:TYR:OH	18:S:60:ASP:OD2	2.38	0.41
25:Y:602:CLA:H203	26:Y:1621:LUT:H391	2.03	0.41
4:a:179:THR:O	4:a:183:MET:HG3	2.20	0.41
5:b:39:LEU:HG	5:b:97:ALA:HB1	2.03	0.41
25:b:605:CLA:H72	25:b:605:CLA:H111	1.92	0.41
6:c:146:PHE:HB3	29:c:2630:LHG:HC12	2.03	0.41
25:c:511:CLA:H8	23:z:24:PRO:HB3	2.03	0.41
28:n:1623:NEX:H35	28:n:1623:NEX:H401	1.90	0.41
16:o:110:ASP:OD1	16:o:110:ASP:N	2.53	0.41
18:s:235:ALA:HB2	23:z:59:SER:HB3	2.03	0.41
24:1:607:CHL:HED1	2:3:240:VAL:HG13	2.02	0.41
2:3:221:LEU:HD13	2:3:221:LEU:HA	1.95	0.41
4:A:300:PHE:HE1	37:C:520:DGD:HB31	1.85	0.41
35:C:521:LMG:H361	13:K:45:LEU:HD11	2.01	0.41
7:D:269:HIS:CE1	38:D:401:BCT:O3	2.73	0.41
27:G:1622:XAT:H11	27:G:1622:XAT:H191	1.93	0.41
1:N:63:GLU:HA	1:N:155:LEU:HD11	2.03	0.41
25:R:612:CLA:HHC	25:R:612:CLA:HBB1	2.03	0.41
25:Y:603:CLA:HHC	25:Y:603:CLA:HBB1	2.03	0.41
24:Y:607:CHL:H91	24:Y:607:CHL:H111	1.95	0.41
1:5:136:GLY:HA2	24:5:609:CHL:HAB	2.03	0.41
24:5:606:CHL:HMB1	24:5:609:CHL:HMC	2.01	0.41
24:5:607:CHL:H112	24:5:607:CHL:H91	1.79	0.41
27:6:1622:XAT:H202	2:7:138:LEU:HD21	2.01	0.41
25:7:610:CLA:CBB	26:7:1620:LUT:H32	2.51	0.41
25:c:511:CLA:H93	30:c:517:BCR:H23C	2.03	0.41
25:c:513:CLA:H11	30:c:514:BCR:H381	2.02	0.41
1:n:176:LEU:HB3	25:n:610:CLA:H3A	2.03	0.41
1:n:192:PHE:CE2	25:n:602:CLA:H171	2.55	0.41
17:r:173:TYR:HE1	17:r:198:GLU:OE2	2.03	0.41
27:y:1622:XAT:H15	27:y:1622:XAT:H201	1.65	0.41
1:1:101:GLY:HA2	24:1:606:CHL:HAC2	2.03	0.41
1:2:67:ILE:HG22	24:2:609:CHL:HMD2	2.02	0.41
1:2:155:LEU:HA	1:2:155:LEU:HD23	1.89	0.41
2:3:223:HIS:CG	25:3:613:CLA:HAA2	2.56	0.41
4:A:262:TYR:CE2	8:E:10:PHE:HD2	2.39	0.41
5:B:123:PHE:HE1	25:B:616:CLA:HBC3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:217:LEU:HB3	25:R:616:CLA:HBA2	2.02	0.41
30:B:618:BCR:H282	34:B:621:SQD:H82	2.02	0.41
6:C:146:PHE:HB3	29:C:2630:LHG:HC12	2.03	0.41
6:C:300:GLU:HG3	6:C:391:ARG:HH12	1.86	0.41
25:C:511:CLA:H8	23:Z:24:PRO:HB3	2.03	0.41
24:G:607:CHL:H143	24:G:607:CHL:H111	1.71	0.41
1:N:181:LEU:HA	1:N:181:LEU:HD23	1.88	0.41
25:N:602:CLA:HBA1	26:N:1621:LUT:H382	2.01	0.41
25:N:611:CLA:H62	25:N:612:CLA:C1D	2.51	0.41
1:5:101:GLY:HA2	24:5:606:CHL:HAC2	2.03	0.41
1:6:70:ARG:NE	1:6:180:GLU:OE2	2.45	0.41
2:7:223:HIS:CG	25:7:613:CLA:HAA2	2.56	0.41
25:7:602:CLA:H93	25:7:602:CLA:H111	1.86	0.41
4:a:262:TYR:CE2	8:e:10:PHE:HD2	2.39	0.41
5:b:313:ASP:CG	5:b:358:ARG:HH12	2.29	0.41
5:b:464:PHE:HD2	25:b:612:CLA:HAC2	1.85	0.41
25:b:603:CLA:C1	10:h:61:TYR:HD2	2.23	0.41
25:b:612:CLA:H61	25:b:612:CLA:H2	1.81	0.41
25:b:615:CLA:H192	15:m:13:LEU:HD21	2.03	0.41
25:b:616:CLA:HBA1	25:b:616:CLA:H3A	1.77	0.41
30:b:620:BCR:H15C	30:b:620:BCR:H351	1.85	0.41
6:c:90:PRO:HB3	6:c:301:PHE:HB3	2.03	0.41
25:c:506:CLA:H71	11:i:20:ILE:HD13	2.02	0.41
30:d:404:BCR:H382	35:d:411:LMG:H341	2.03	0.41
24:g:606:CHL:HMB1	24:g:609:CHL:HAC1	2.03	0.41
24:g:607:CHL:HAA2	27:n:1622:XAT:H41	2.02	0.41
26:g:1620:LUT:H15	26:g:1620:LUT:H201	1.88	0.41
1:n:80:VAL:HG13	1:n:206:LEU:HD11	2.03	0.41
24:n:608:CHL:H152	28:n:1623:NEX:H402	2.03	0.41
25:n:611:CLA:H62	25:n:612:CLA:C1D	2.51	0.41
25:r:602:CLA:H93	25:r:602:CLA:H111	1.95	0.41
25:r:612:CLA:HHC	25:r:612:CLA:HBB1	2.03	0.41
5:B:39:LEU:HG	5:B:97:ALA:HB1	2.03	0.41
25:B:603:CLA:H62	25:B:603:CLA:H41	1.75	0.41
24:G:607:CHL:H2	24:G:607:CHL:H62	1.59	0.41
25:Y:612:CLA:H61	25:Y:612:CLA:H102	1.87	0.41
28:Y:1623:NEX:H401	28:Y:1623:NEX:H35	1.72	0.41
1:5:57:THR:HG22	1:5:61:ASN:HD21	1.85	0.41
25:7:603:CLA:H92	25:7:603:CLA:H61	1.93	0.41
3:8:176:LEU:HB3	25:8:610:CLA:H3A	2.02	0.41
25:b:603:CLA:H61	25:b:603:CLA:H93	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:b:2631:LHG:H341	29:b:2631:LHG:H161	2.03	0.41
6:c:178:LYS:NZ	6:c:184:GLY:O	2.54	0.41
6:c:300:GLU:HG3	6:c:391:ARG:HH12	1.86	0.41
25:d:403:CLA:H41	25:d:403:CLA:H62	1.79	0.41
19:t:28:LYS:HE2	19:t:28:LYS:HB2	1.90	0.41
24:y:606:CHL:HBA2	28:y:1623:NEX:H403	2.03	0.41
1:1:67:ILE:HG22	24:1:609:CHL:HMD2	2.03	0.40
3:4:176:LEU:HB3	25:4:610:CLA:H3A	2.02	0.40
33:A:409:PHO:H61	33:A:409:PHO:H41	1.78	0.40
5:B:157:HIS:HA	5:B:163:GLY:HA3	2.02	0.40
5:B:259:GLY:O	10:H:61:TYR:OH	2.39	0.40
6:C:178:LYS:NZ	6:C:184:GLY:O	2.54	0.40
1:G:167:ALA:HB2	25:G:610:CLA:HAA1	2.01	0.40
24:N:606:CHL:HMC	24:N:607:CHL:NC	2.36	0.40
25:R:616:CLA:HBA2	25:R:616:CLA:H3A	1.87	0.40
18:S:135:LEU:O	18:S:139:VAL:HG23	2.21	0.40
25:6:604:CLA:H3A	25:6:604:CLA:HBA2	1.85	0.40
26:6:1620:LUT:H31	26:6:1620:LUT:H391	1.91	0.40
2:7:173:ASP:OD1	26:7:1620:LUT:O23	2.24	0.40
25:7:610:CLA:HBB1	25:7:610:CLA:H52	2.03	0.40
25:b:602:CLA:H12	25:b:602:CLA:H52	1.76	0.40
25:b:614:CLA:H3A	25:b:614:CLA:HBA1	1.90	0.40
6:c:167:LEU:HD23	6:c:170:ILE:HD12	2.02	0.40
30:h:101:BCR:H24C	30:h:101:BCR:H371	1.76	0.40
1:n:189:PHE:HD1	25:n:602:CLA:H201	1.85	0.40
24:n:607:CHL:HHB	24:n:607:CHL:HMA1	1.82	0.40
27:1:1622:XAT:H201	27:1:1622:XAT:H15	1.76	0.40
2:3:173:ASP:OD1	26:3:1620:LUT:O23	2.24	0.40
28:3:1623:NEX:H35	28:3:1623:NEX:H401	1.87	0.40
30:4:623:BCR:H11C	30:4:623:BCR:H341	1.85	0.40
5:B:42:LEU:HD13	5:B:94:GLU:HG3	2.02	0.40
5:B:313:ASP:CG	5:B:358:ARG:HH12	2.29	0.40
5:B:458:PHE:HB3	25:B:605:CLA:HBC2	2.02	0.40
5:B:477:ASP:OD1	5:B:477:ASP:N	2.52	0.40
5:B:496:GLN:HE22	22:X:82:LYS:HB2	1.85	0.40
25:D:402:CLA:H143	25:D:402:CLA:H161	1.89	0.40
25:N:603:CLA:H92	25:N:603:CLA:H61	1.81	0.40
17:R:102:TRP:CE2	24:R:608:CHL:HED2	2.56	0.40
1:6:182:LYS:HZ3	25:6:611:CLA:CGD	2.35	0.40
25:6:614:CLA:HBA2	25:6:614:CLA:H3A	1.73	0.40
27:7:1622:XAT:H35	27:7:1622:XAT:H401	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:203:THR:HG22	3:8:205:LEU:H	1.86	0.40
25:b:603:CLA:H143	25:b:603:CLA:H111	1.98	0.40
9:f:20:LEU:O	9:f:24:THR:OG1	2.31	0.40
25:r:613:CLA:H111	29:r:2630:LHG:H292	2.02	0.40
3:4:128:THR:OG1	3:4:133:THR:N	2.53	0.40
25:C:513:CLA:H11	30:C:514:BCR:H381	2.02	0.40
37:H:102:DGD:HB62	37:H:102:DGD:HB91	1.66	0.40
1:N:60:LYS:NZ	1:Y:33:PRO:HG3	2.37	0.40
28:S:1623:NEX:H35	28:S:1623:NEX:H401	1.85	0.40
1:Y:66:VAL:HG22	1:Y:181:LEU:HD21	2.03	0.40
2:7:128:LEU:HD23	2:7:128:LEU:HA	1.90	0.40
4:a:93:PHE:HZ	25:a:410:CLA:HAA1	1.86	0.40
5:b:366:PHE:HD2	5:b:425:GLN:HE21	1.68	0.40
30:b:619:BCR:H11C	30:b:619:BCR:H341	1.89	0.40
6:c:55:ALA:HB1	30:c:517:BCR:H373	2.04	0.40
29:c:522:LHG:HC81	25:y:611:CLA:H51	2.04	0.40
30:d:404:BCR:H12C	9:f:27:PHE:CE2	2.57	0.40
1:g:25:LEU:HB2	1:g:29:SER:HA	2.04	0.40
25:g:603:CLA:H92	25:g:603:CLA:H61	1.85	0.40
29:g:2630:LHG:H332	29:g:2630:LHG:H361	1.97	0.40
1:n:60:LYS:NZ	1:y:33:PRO:HG3	2.37	0.40
25:y:611:CLA:C1B	29:y:2630:LHG:HC31	2.52	0.40
25:y:613:CLA:H61	25:y:613:CLA:H2	1.67	0.40
5:B:381:VAL:O	7:D:346:VAL:HG12	2.22	0.40
25:B:615:CLA:H93	34:B:623:SQD:H292	2.03	0.40
25:C:510:CLA:H2	25:C:510:CLA:H61	1.93	0.40
25:N:613:CLA:H61	25:N:613:CLA:H2	1.67	0.40
19:T:28:LYS:HB2	19:T:28:LYS:HE2	1.90	0.40
1:Y:63:GLU:HA	1:Y:155:LEU:HD11	2.03	0.40
24:5:609:CHL:H42	25:7:602:CLA:H143	2.02	0.40
27:5:1622:XAT:H31	27:5:1622:XAT:H391	1.74	0.40
2:7:79:ARG:HA	2:7:82:MET:HE3	2.02	0.40
2:7:193:LYS:HZ1	29:7:2630:LHG:P	2.45	0.40
3:8:81:GLU:HA	24:8:607:CHL:HED2	2.03	0.40
25:8:604:CLA:C2B	27:8:622:XAT:H183	2.52	0.40
4:a:232:SER:HB2	5:b:4:PRO:HG3	2.04	0.40
4:a:234:ASN:ND2	29:d:408:LHG:HC11	2.37	0.40
33:a:409:PHO:H3A	33:a:409:PHO:HBA1	1.83	0.40
25:b:602:CLA:H92	25:b:602:CLA:H61	1.81	0.40
7:d:298:ASP:OD1	7:d:298:ASP:N	2.52	0.40
13:k:33:LEU:HD22	13:k:36:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:163:PRO:HD2	26:n:1620:LUT:H23	2.02	0.40
1:y:21:ARG:NH2	1:y:36:LEU:O	2.44	0.40
24:y:601:CHL:H101	24:y:601:CHL:H61	1.85	0.40
24:y:601:CHL:HMA3	29:y:2630:LHG:H121	2.03	0.40
27:y:1622:XAT:H12	29:y:2630:LHG:H191	2.02	0.40
23:z:57:LEU:HD23	23:z:60:LEU:HD12	2.03	0.40
1:1:197:GLN:O	1:1:201:THR:OG1	2.32	0.40
24:1:609:CHL:H42	25:3:602:CLA:H143	2.02	0.40
28:1:1623:NEX:H35	28:1:1623:NEX:H401	1.93	0.40
27:4:622:XAT:H15	27:4:622:XAT:H201	1.82	0.40
4:A:93:PHE:HZ	25:A:410:CLA:HAA1	1.86	0.40
5:B:366:PHE:HD2	5:B:425:GLN:HE21	1.68	0.40
25:B:613:CLA:H111	25:B:614:CLA:HAB	2.04	0.40
25:C:511:CLA:H93	30:C:517:BCR:H23C	2.03	0.40
16:O:80:THR:HG23	16:O:115:THR:HB	2.03	0.40
25:R:609:CLA:HAA2	25:R:616:CLA:C1D	2.52	0.40
28:R:623:NEX:H35	28:R:623:NEX:H401	1.94	0.40
26:S:1621:LUT:H401	26:S:1621:LUT:H35	1.81	0.40
23:Z:57:LEU:HD23	23:Z:60:LEU:HD12	2.03	0.40
24:5:607:CHL:HED1	2:7:240:VAL:HG13	2.02	0.40
24:6:606:CHL:HMB2	24:6:609:CHL:HMC	2.03	0.40
2:7:155:GLY:HA2	24:7:608:CHL:HAC1	2.04	0.40
5:b:10:THR:HG22	25:b:612:CLA:HMA2	2.03	0.40
25:b:615:CLA:H93	34:b:623:SQD:H292	2.03	0.40
25:c:513:CLA:H203	25:c:513:CLA:H161	1.84	0.40
24:g:601:CHL:HMA3	29:g:2630:LHG:H121	2.02	0.40
10:h:30:TYR:CE2	17:r:50:LEU:HG	2.57	0.40
26:n:1620:LUT:H15	26:n:1620:LUT:H201	1.88	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%)	211 (97%)	6 (3%)	0	100	100
1	2	216/232 (93%)	211 (98%)	5 (2%)	0	100	100
1	5	217/232 (94%)	211 (97%)	6 (3%)	0	100	100
1	6	216/232 (93%)	211 (98%)	5 (2%)	0	100	100
1	G	217/232 (94%)	214 (99%)	3 (1%)	0	100	100
1	N	217/232 (94%)	215 (99%)	2 (1%)	0	100	100
1	Y	217/232 (94%)	215 (99%)	2 (1%)	0	100	100
1	g	217/232 (94%)	214 (99%)	3 (1%)	0	100	100
1	n	217/232 (94%)	215 (99%)	2 (1%)	0	100	100
1	y	217/232 (94%)	215 (99%)	2 (1%)	0	100	100
2	3	218/243 (90%)	208 (95%)	10 (5%)	0	100	100
2	7	218/243 (90%)	208 (95%)	10 (5%)	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%)	324 (98%)	8 (2%)	0	100	100
4	a	332/344 (96%)	324 (98%)	8 (2%)	0	100	100
5	B	501/507 (99%)	488 (97%)	13 (3%)	0	100	100
5	b	501/507 (99%)	488 (97%)	13 (3%)	0	100	100
6	C	448/473 (95%)	441 (98%)	7 (2%)	0	100	100
6	c	448/473 (95%)	441 (98%)	7 (2%)	0	100	100
7	D	338/353 (96%)	332 (98%)	6 (2%)	0	100	100
7	d	338/353 (96%)	332 (98%)	6 (2%)	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
9	f	28/39 (72%)	28 (100%)	0	0	100	100
10	H	58/73 (80%)	57 (98%)	1 (2%)	0	100	100
10	h	58/73 (80%)	57 (98%)	1 (2%)	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	32/40 (80%)	32 (100%)	0	0	100	100
12	j	32/40 (80%)	32 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	31 (100%)	0	0	100	100
15	m	31/34 (91%)	31 (100%)	0	0	100	100
16	O	210/248 (85%)	203 (97%)	7 (3%)	0	100	100
16	o	210/248 (85%)	203 (97%)	7 (3%)	0	100	100
17	R	232/246 (94%)	226 (97%)	6 (3%)	0	100	100
17	r	232/246 (94%)	226 (97%)	6 (3%)	0	100	100
18	S	216/244 (88%)	206 (95%)	10 (5%)	0	100	100
18	s	216/244 (88%)	206 (95%)	10 (5%)	0	100	100
19	T	30/35 (86%)	30 (100%)	0	0	100	100
19	t	30/35 (86%)	30 (100%)	0	0	100	100
20	U	23/99 (23%)	22 (96%)	1 (4%)	0	100	100
20	u	23/99 (23%)	22 (96%)	1 (4%)	0	100	100
21	W	52/54 (96%)	52 (100%)	0	0	100	100
21	w	52/54 (96%)	52 (100%)	0	0	100	100
22	X	37/86 (43%)	37 (100%)	0	0	100	100
22	x	37/86 (43%)	37 (100%)	0	0	100	100
23	Z	60/62 (97%)	60 (100%)	0	0	100	100
23	z	60/62 (97%)	60 (100%)	0	0	100	100
All	All	8596/9536 (90%)	8394 (98%)	202 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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	88
5	b	400/403 (99%)	399 (100%)	1 (0%)	86	88
6	C	352/373 (94%)	352 (100%)	0	100	100
6	c	352/373 (94%)	352 (100%)	0	100	100
7	D	274/285 (96%)	274 (100%)	0	100	100
7	d	274/285 (96%)	274 (100%)	0	100	100
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	25/30 (83%)	25 (100%)	0	100	100
12	j	25/30 (83%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	182/204 (89%)	182 (100%)	0	100	100
16	o	182/204 (89%)	182 (100%)	0	100	100
17	R	191/202 (95%)	191 (100%)	0	100	100
17	r	191/202 (95%)	191 (100%)	0	100	100
18	S	170/190 (90%)	170 (100%)	0	100	100
18	s	170/190 (90%)	170 (100%)	0	100	100
19	T	29/32 (91%)	29 (100%)	0	100	100
19	t	29/32 (91%)	29 (100%)	0	100	100
20	U	21/80 (26%)	21 (100%)	0	100	100
20	u	21/80 (26%)	21 (100%)	0	100	100
21	W	44/44 (100%)	44 (100%)	0	100	100
21	w	44/44 (100%)	44 (100%)	0	100	100
22	X	32/67 (48%)	32 (100%)	0	100	100
22	x	32/67 (48%)	32 (100%)	0	100	100
23	Z	54/54 (100%)	54 (100%)	0	100	100
23	z	54/54 (100%)	54 (100%)	0	100	100
All	All	6992/7658 (91%)	6990 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	12	VAL
5	b	12	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) 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	219	ASN
3	4	72	GLN
4	A	234	ASN
4	A	303	ASN
4	A	315	ASN
4	A	335	ASN
5	B	216	HIS
5	B	274	GLN
5	B	296	GLN
5	B	343	HIS
6	C	28	GLN
6	C	322	GLN
6	C	398	HIS
6	C	415	ASN
7	D	13	ASN
7	D	84	ASN
7	D	143	ASN
7	D	187	GLN
7	D	264	ASN
7	D	323	ASN
7	D	351	ASN
1	G	61	ASN
14	L	5	ASN
14	L	10	ASN
16	O	47	ASN
16	O	74	GLN
16	O	117	GLN
16	O	222	GLN
17	R	47	GLN
17	R	226	ASN
17	R	236	HIS
18	S	165	HIS
1	5	61	ASN
1	6	61	ASN
1	6	88	ASN
2	7	70	ASN
2	7	95	GLN
2	7	219	ASN
3	8	72	GLN

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Mol	Chain	Res	Type
4	a	234	ASN
4	a	303	ASN
4	a	315	ASN
4	a	335	ASN
5	b	216	HIS
5	b	274	GLN
5	b	296	GLN
5	b	343	HIS
6	c	28	GLN
6	c	322	GLN
6	c	398	HIS
6	c	415	ASN
7	d	13	ASN
7	d	84	ASN
7	d	143	ASN
7	d	264	ASN
7	d	351	ASN
1	g	61	ASN
14	l	5	ASN
14	l	10	ASN
14	l	34	ASN
16	o	47	ASN
16	o	74	GLN
16	o	222	GLN
17	r	47	GLN
17	r	226	ASN
17	r	236	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 486 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
24	CHL	Y	605	1	42,56,74	3.83	19 (45%)	36,92,114	2.76	12 (33%)
25	CLA	C	511	6	69,73,73	1.18	7 (10%)	82,113,113	1.21	7 (8%)
24	CHL	3	601	2	58,72,74	3.21	20 (34%)	55,111,114	2.73	18 (32%)
29	LHG	d	408	-	45,45,48	0.86	1 (2%)	48,51,54	1.40	5 (10%)
24	CHL	G	601	1	60,74,74	3.20	19 (31%)	58,114,114	2.58	20 (34%)
25	CLA	5	612	1	49,53,73	1.39	8 (16%)	58,89,113	1.50	9 (15%)
28	NEX	7	1623	-	40,46,46	1.00	2 (5%)	50,70,70	2.32	16 (32%)
25	CLA	a	406	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	7 (8%)
25	CLA	3	610	2	64,68,73	1.21	8 (12%)	76,107,113	1.15	7 (9%)
25	CLA	2	613	1	49,53,73	1.36	7 (14%)	58,89,113	1.26	7 (12%)
24	CHL	s	607	-	52,66,74	3.59	19 (36%)	48,104,114	2.64	18 (37%)
26	LUT	y	1620	-	42,43,43	0.95	1 (2%)	51,60,60	2.08	21 (41%)
25	CLA	5	602	1	65,69,73	1.22	10 (15%)	77,108,113	1.18	6 (7%)
24	CHL	7	606	-	40,54,74	4.07	20 (50%)	34,90,114	3.03	13 (38%)
30	BCR	C	515	-	41,41,41	0.70	0	56,56,56	1.92	17 (30%)
25	CLA	B	617	5	69,73,73	1.19	8 (11%)	82,113,113	1.31	7 (8%)
25	CLA	2	611	29	49,53,73	1.35	8 (16%)	58,89,113	1.42	7 (12%)
34	SQD	a	418	-	52,54,54	0.90	3 (5%)	62,65,65	1.60	11 (17%)
39	HEM	F	101	9,8	50,50,50	1.36	8 (16%)	67,82,82	1.04	3 (4%)
24	CHL	Y	608	-	60,74,74	3.17	19 (31%)	58,114,114	2.36	14 (24%)
29	LHG	Y	2630	25	48,48,48	0.84	2 (4%)	51,54,54	1.28	6 (11%)
28	NEX	G	1623	-	40,46,46	1.09	3 (7%)	50,70,70	2.38	16 (32%)
24	CHL	g	608	-	60,74,74	3.31	19 (31%)	58,114,114	2.43	14 (24%)
24	CHL	S	601	18	40,54,74	4.04	19 (47%)	34,90,114	3.02	15 (44%)
24	CHL	R	606	-	60,74,74	3.27	19 (31%)	58,114,114	2.47	18 (31%)
25	CLA	6	611	29	49,53,73	1.35	8 (16%)	58,89,113	1.42	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	b	607	5	69,73,73	1.20	9 (13%)	82,113,113	1.29	8 (9%)
25	CLA	c	507	-	69,73,73	1.14	8 (11%)	82,113,113	1.40	10 (12%)
25	CLA	b	614	5	69,73,73	1.23	9 (13%)	82,113,113	1.35	9 (10%)
24	CHL	3	607	-	47,61,74	3.71	19 (40%)	41,98,114	2.43	15 (36%)
25	CLA	2	614	1	49,53,73	1.35	9 (18%)	58,89,113	1.29	7 (12%)
38	BCT	D	401	32	3,3,3	1.17	0	2,3,3	4.25	2 (100%)
25	CLA	C	509	6	69,73,73	1.16	8 (11%)	82,113,113	1.29	7 (8%)
24	CHL	3	606	-	40,54,74	4.06	20 (50%)	34,90,114	3.02	13 (38%)
25	CLA	C	510	6	69,73,73	1.16	8 (11%)	82,113,113	1.27	9 (10%)
25	CLA	r	609	17	62,66,73	1.20	9 (14%)	73,104,113	1.23	4 (5%)
26	LUT	n	1621	-	42,43,43	0.92	1 (2%)	51,60,60	1.99	15 (29%)
25	CLA	y	612	1	64,68,73	1.24	9 (14%)	76,107,113	1.30	9 (11%)
27	XAT	2	1622	-	41,47,47	0.97	2 (4%)	54,74,74	2.77	23 (42%)
25	CLA	g	611	29	64,68,73	1.19	10 (15%)	76,107,113	1.28	4 (5%)
25	CLA	1	614	1	49,53,73	1.36	9 (18%)	58,89,113	1.30	7 (12%)
27	XAT	N	1622	-	41,47,47	0.92	2 (4%)	54,74,74	2.90	24 (44%)
25	CLA	b	617	5	69,73,73	1.19	8 (11%)	82,113,113	1.31	7 (8%)
30	BCR	C	517	-	41,41,41	0.72	0	56,56,56	2.12	13 (23%)
34	SQD	A	412	-	48,50,54	0.98	6 (12%)	58,61,65	1.61	9 (15%)
24	CHL	r	606	-	60,74,74	3.28	19 (31%)	58,114,114	2.47	18 (31%)
24	CHL	2	609	1	55,69,74	3.37	20 (36%)	52,108,114	2.51	17 (32%)
25	CLA	n	611	29	64,68,73	1.18	7 (10%)	76,107,113	1.32	6 (7%)
27	XAT	6	1622	-	41,47,47	0.97	2 (4%)	54,74,74	2.77	23 (42%)
28	NEX	r	623	-	40,46,46	1.14	3 (7%)	50,70,70	2.44	20 (40%)
24	CHL	5	605	1	40,54,74	3.97	20 (50%)	34,90,114	2.66	10 (29%)
24	CHL	g	607	-	60,74,74	3.24	19 (31%)	58,114,114	2.23	13 (22%)
25	CLA	7	614	2	52,56,73	1.34	6 (11%)	61,92,113	1.31	6 (9%)
29	LHG	D	410	-	42,42,48	0.68	1 (2%)	45,48,54	1.26	4 (8%)
24	CHL	r	607	-	50,64,74	3.61	19 (38%)	46,102,114	2.61	19 (41%)
25	CLA	N	603	1	69,73,73	1.20	10 (14%)	82,113,113	1.32	11 (13%)
24	CHL	n	601	1	60,74,74	3.27	19 (31%)	58,114,114	2.54	18 (31%)
25	CLA	s	603	18	49,53,73	1.39	5 (10%)	58,89,113	1.40	5 (8%)
24	CHL	n	607	-	60,74,74	3.19	19 (31%)	58,114,114	2.39	12 (20%)
29	LHG	C	523	-	48,48,48	0.66	2 (4%)	51,54,54	1.26	6 (11%)
25	CLA	S	610	18	59,63,73	1.24	8 (13%)	70,101,113	1.26	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	7	613	2	62,66,73	1.22	10 (16%)	73,104,113	1.28	4 (5%)
25	CLA	4	610	3	49,53,73	1.36	9 (18%)	58,89,113	1.23	7 (12%)
24	CHL	2	608	-	40,54,74	4.02	20 (50%)	34,90,114	2.80	10 (29%)
25	CLA	B	605	5	69,73,73	1.28	13 (18%)	82,113,113	1.73	17 (20%)
25	CLA	8	602	3	49,53,73	1.30	9 (18%)	58,89,113	1.46	7 (12%)
26	LUT	3	1621	-	42,43,43	0.86	1 (2%)	51,60,60	1.70	12 (23%)
25	CLA	5	603	1	59,63,73	1.27	10 (16%)	70,101,113	1.42	7 (10%)
25	CLA	a	405	4	69,73,73	1.20	10 (14%)	82,113,113	1.25	5 (6%)
24	CHL	G	608	-	60,74,74	3.31	19 (31%)	58,114,114	2.43	14 (24%)
25	CLA	c	508	6	69,73,73	1.16	7 (10%)	82,113,113	1.33	7 (8%)
35	LMG	D	411	-	46,46,55	0.85	1 (2%)	54,54,63	1.38	6 (11%)
29	LHG	7	2630	25	46,46,48	0.81	1 (2%)	49,52,54	1.33	4 (8%)
25	CLA	R	602	17	64,68,73	1.18	8 (12%)	76,107,113	1.31	8 (10%)
25	CLA	2	610	1	54,58,73	1.27	7 (12%)	64,95,113	1.14	4 (6%)
26	LUT	1	1620	-	42,43,43	0.80	0	51,60,60	1.99	14 (27%)
30	BCR	B	620	-	41,41,41	0.85	1 (2%)	56,56,56	2.03	15 (26%)
27	XAT	R	622	-	41,47,47	1.01	3 (7%)	54,74,74	2.63	19 (35%)
25	CLA	7	604	-	49,53,73	1.35	8 (16%)	58,89,113	1.28	4 (6%)
25	CLA	R	613	17	64,68,73	1.21	6 (9%)	76,107,113	1.35	5 (6%)
29	LHG	B	2630	-	46,46,48	0.71	2 (4%)	49,52,54	1.24	5 (10%)
26	LUT	6	1620	-	42,43,43	0.72	0	51,60,60	1.89	14 (27%)
25	CLA	S	609	18	49,53,73	1.40	5 (10%)	58,89,113	1.27	6 (10%)
25	CLA	B	604	5	69,73,73	1.24	9 (13%)	82,113,113	1.25	9 (10%)
25	CLA	y	603	1	69,73,73	1.20	9 (13%)	82,113,113	1.33	10 (12%)
30	BCR	8	623	-	41,41,41	0.73	0	56,56,56	2.20	15 (26%)
25	CLA	7	612	2	49,53,73	1.39	10 (20%)	58,89,113	1.39	6 (10%)
29	LHG	R	2630	25	41,41,48	0.75	1 (2%)	44,47,54	1.36	6 (13%)
25	CLA	r	616	17	49,53,73	1.37	10 (20%)	58,89,113	1.40	5 (8%)
28	NEX	Y	1623	-	40,46,46	1.25	4 (10%)	50,70,70	2.61	20 (40%)
28	NEX	1	1623	-	40,46,46	1.25	4 (10%)	50,70,70	2.49	18 (36%)
29	LHG	4	2630	25	20,20,48	0.89	1 (5%)	23,26,54	1.36	2 (8%)
38	BCT	d	401	32	3,3,3	1.17	0	2,3,3	4.24	2 (100%)
30	BCR	b	619	-	41,41,41	0.74	0	56,56,56	1.89	17 (30%)
24	CHL	N	609	1	60,74,74	3.17	20 (33%)	58,114,114	2.35	20 (34%)
37	DGD	b	626	-	60,60,67	0.97	1 (1%)	74,74,81	1.39	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	BCR	c	516	-	41,41,41	0.65	0	56,56,56	1.96	14 (25%)
29	LHG	c	523	-	48,48,48	0.66	2 (4%)	51,54,54	1.26	6 (11%)
37	DGD	C	519	-	63,63,67	0.99	4 (6%)	77,77,81	1.38	11 (14%)
24	CHL	y	607	-	60,74,74	3.17	19 (31%)	58,114,114	2.29	12 (20%)
25	CLA	3	614	2	52,56,73	1.34	6 (11%)	61,92,113	1.31	6 (9%)
24	CHL	R	614	17	36,50,74	4.27	17 (47%)	29,85,114	2.58	12 (41%)
25	CLA	Y	603	1	69,73,73	1.20	9 (13%)	82,113,113	1.33	10 (12%)
24	CHL	1	601	1	40,54,74	3.94	20 (50%)	34,90,114	2.84	14 (41%)
25	CLA	n	603	1	69,73,73	1.20	10 (14%)	82,113,113	1.33	9 (10%)
24	CHL	S	607	-	52,66,74	3.59	19 (36%)	48,104,114	2.64	18 (37%)
24	CHL	3	608	-	40,54,74	3.95	20 (50%)	34,90,114	2.85	13 (38%)
25	CLA	n	604	-	54,58,73	1.35	9 (16%)	64,95,113	1.38	9 (14%)
35	LMG	C	521	-	51,51,55	0.75	1 (1%)	59,59,63	1.31	6 (10%)
25	CLA	5	611	29	49,53,73	1.35	10 (20%)	58,89,113	1.44	4 (6%)
25	CLA	1	610	1	60,64,73	1.19	6 (10%)	71,102,113	1.20	9 (12%)
27	XAT	g	1622	-	41,47,47	0.99	2 (4%)	54,74,74	2.74	20 (37%)
24	CHL	N	607	-	60,74,74	3.19	19 (31%)	58,114,114	2.38	12 (20%)
25	CLA	y	610	1	64,68,73	1.21	7 (10%)	76,107,113	1.19	10 (13%)
26	LUT	n	1620	-	42,43,43	0.80	1 (2%)	51,60,60	1.99	17 (33%)
29	LHG	N	2630	25	48,48,48	0.78	1 (2%)	51,54,54	1.34	7 (13%)
25	CLA	g	614	1	52,56,73	1.31	9 (17%)	61,92,113	1.18	5 (8%)
27	XAT	G	1622	-	41,47,47	0.99	2 (4%)	54,74,74	2.73	20 (37%)
36	PL9	D	405	-	55,55,55	2.28	18 (32%)	68,69,69	1.58	14 (20%)
29	LHG	D	409	-	48,48,48	0.83	1 (2%)	51,54,54	1.35	7 (13%)
24	CHL	4	601	3	39,53,74	4.31	18 (46%)	33,89,114	2.10	12 (36%)
28	NEX	n	1623	-	40,46,46	1.16	4 (10%)	50,70,70	2.29	16 (32%)
30	BCR	T	101	-	41,41,41	0.83	1 (2%)	56,56,56	2.65	22 (39%)
25	CLA	Y	610	1	64,68,73	1.21	7 (10%)	76,107,113	1.19	10 (13%)
25	CLA	7	611	29	59,63,73	1.29	10 (16%)	70,101,113	1.35	8 (11%)
25	CLA	A	410	4	64,68,73	1.18	8 (12%)	76,107,113	1.35	8 (10%)
29	LHG	d	410	-	42,42,48	0.68	1 (2%)	45,48,54	1.26	4 (8%)
30	BCR	t	101	-	41,41,41	0.82	1 (2%)	56,56,56	2.65	22 (39%)
29	LHG	L	101	-	48,48,48	0.79	1 (2%)	51,54,54	1.33	6 (11%)
25	CLA	C	506	6	69,73,73	1.20	8 (11%)	82,113,113	1.25	6 (7%)
25	CLA	S	612	18	53,57,73	1.30	6 (11%)	61,93,113	1.31	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	3	603	2	59,63,73	1.24	11 (18%)	70,101,113	1.45	8 (11%)
25	CLA	R	604	-	52,56,73	1.33	10 (19%)	61,92,113	1.44	10 (16%)
24	CHL	7	609	2	55,69,74	3.46	19 (34%)	52,108,114	2.29	15 (28%)
29	LHG	G	2630	25	48,48,48	0.80	1 (2%)	51,54,54	1.33	6 (11%)
28	NEX	3	1623	-	40,46,46	1.00	2 (5%)	50,70,70	2.32	16 (32%)
25	CLA	2	612	1	49,53,73	1.37	9 (18%)	58,89,113	1.36	8 (13%)
24	CHL	7	607	-	47,61,74	3.71	19 (40%)	41,98,114	2.43	15 (36%)
24	CHL	8	601	3	39,53,74	4.30	19 (48%)	33,89,114	2.10	12 (36%)
30	BCR	C	514	-	41,41,41	0.70	0	56,56,56	1.75	13 (23%)
35	LMG	b	622	-	51,51,55	0.89	2 (3%)	59,59,63	1.41	6 (10%)
26	LUT	S	1621	-	42,43,43	0.71	0	51,60,60	1.87	15 (29%)
26	LUT	5	1620	-	42,43,43	0.81	0	51,60,60	1.99	14 (27%)
27	XAT	8	622	-	41,47,47	0.93	2 (4%)	54,74,74	2.63	21 (38%)
29	LHG	b	2631	-	48,48,48	0.67	1 (2%)	51,54,54	1.25	6 (11%)
30	BCR	d	404	-	41,41,41	0.71	1 (2%)	56,56,56	1.95	16 (28%)
25	CLA	R	601	17	53,57,73	1.30	10 (18%)	61,93,113	1.56	9 (14%)
24	CHL	y	606	-	44,58,74	3.57	20 (45%)	37,94,114	3.00	15 (40%)
25	CLA	D	402	7	69,73,73	1.22	9 (13%)	82,113,113	1.35	10 (12%)
30	BCR	D	404	-	41,41,41	0.71	1 (2%)	56,56,56	1.95	16 (28%)
34	SQD	a	412	-	48,50,54	0.98	5 (10%)	58,61,65	1.61	9 (15%)
24	CHL	1	609	1	56,70,74	3.37	20 (35%)	53,109,114	2.29	14 (26%)
25	CLA	c	501	6	69,73,73	1.17	7 (10%)	82,113,113	1.11	7 (8%)
26	LUT	S	1620	-	42,43,43	0.67	0	51,60,60	1.94	16 (31%)
25	CLA	B	614	5	69,73,73	1.23	9 (13%)	82,113,113	1.35	9 (10%)
24	CHL	6	605	1	40,54,74	4.11	19 (47%)	34,90,114	2.58	12 (35%)
28	NEX	5	1623	-	40,46,46	1.24	4 (10%)	50,70,70	2.49	19 (38%)
25	CLA	2	602	1	65,69,73	1.20	9 (13%)	77,108,113	1.21	8 (10%)
24	CHL	6	609	1	55,69,74	3.37	20 (36%)	52,108,114	2.51	17 (32%)
29	LHG	y	2630	25	48,48,48	0.85	2 (4%)	51,54,54	1.28	6 (11%)
28	NEX	S	1623	-	40,46,46	1.06	3 (7%)	50,70,70	2.26	17 (34%)
24	CHL	4	606	-	40,54,74	4.08	19 (47%)	34,90,114	2.95	13 (38%)
26	LUT	R	620	-	42,43,43	0.88	2 (4%)	51,60,60	2.14	21 (41%)
27	XAT	y	1622	-	41,47,47	1.01	3 (7%)	54,74,74	2.96	21 (38%)
24	CHL	4	609	3	40,54,74	3.93	19 (47%)	34,90,114	2.93	14 (41%)
25	CLA	Y	611	29	64,68,73	1.25	9 (14%)	76,107,113	1.24	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	DGD	c	519	-	63,63,67	0.99	4 (6%)	77,77,81	1.39	11 (14%)
25	CLA	s	604	-	54,58,73	1.31	5 (9%)	64,95,113	1.41	7 (10%)
24	CHL	7	608	-	40,54,74	3.94	20 (50%)	34,90,114	2.84	13 (38%)
24	CHL	r	608	-	55,69,74	3.24	19 (34%)	52,108,114	2.62	14 (26%)
29	LHG	D	408	-	45,45,48	0.86	1 (2%)	48,51,54	1.40	5 (10%)
26	LUT	4	620	-	42,43,43	0.87	2 (4%)	51,60,60	2.27	17 (33%)
26	LUT	y	1621	-	42,43,43	0.97	2 (4%)	51,60,60	1.98	17 (33%)
24	CHL	4	608	-	40,54,74	3.96	20 (50%)	34,90,114	3.06	15 (44%)
25	CLA	C	505	6	69,73,73	1.15	7 (10%)	82,113,113	1.34	8 (9%)
35	LMG	A	413	-	48,48,55	0.78	1 (2%)	56,56,63	1.31	5 (8%)
24	CHL	3	605	2	40,54,74	4.04	19 (47%)	34,90,114	2.84	13 (38%)
24	CHL	5	607	-	57,71,74	3.38	20 (35%)	54,110,114	2.53	19 (35%)
24	CHL	8	606	-	40,54,74	4.08	19 (47%)	34,90,114	2.95	13 (38%)
39	HEM	f	101	9,8	50,50,50	1.36	8 (16%)	67,82,82	1.04	3 (4%)
25	CLA	5	610	1	60,64,73	1.18	5 (8%)	71,102,113	1.20	9 (12%)
25	CLA	s	609	18	49,53,73	1.40	5 (10%)	58,89,113	1.27	6 (10%)
25	CLA	7	610	2	64,68,73	1.21	7 (10%)	76,107,113	1.15	7 (9%)
26	LUT	Y	1621	-	42,43,43	0.97	2 (4%)	51,60,60	1.98	17 (33%)
24	CHL	Y	607	-	60,74,74	3.17	19 (31%)	58,114,114	2.29	12 (20%)
25	CLA	s	610	18	59,63,73	1.24	8 (13%)	70,101,113	1.26	10 (14%)
25	CLA	r	602	17	64,68,73	1.18	8 (12%)	76,107,113	1.31	8 (10%)
26	LUT	1	1621	-	42,43,43	0.92	2 (4%)	51,60,60	1.97	15 (29%)
25	CLA	b	612	5	69,73,73	1.27	7 (10%)	82,113,113	1.49	12 (14%)
25	CLA	R	611	29	53,57,73	1.31	9 (16%)	61,93,113	1.23	6 (9%)
30	BCR	c	517	-	41,41,41	0.72	0	56,56,56	2.13	13 (23%)
27	XAT	n	1622	-	41,47,47	0.93	2 (4%)	54,74,74	2.90	23 (42%)
25	CLA	g	604	-	54,58,73	1.36	9 (16%)	64,95,113	1.37	6 (9%)
24	CHL	3	609	2	55,69,74	3.46	20 (36%)	52,108,114	2.29	15 (28%)
29	LHG	b	2630	-	46,46,48	0.70	2 (4%)	49,52,54	1.24	5 (10%)
25	CLA	S	603	18	49,53,73	1.39	5 (10%)	58,89,113	1.40	5 (8%)
25	CLA	y	613	1	69,73,73	1.20	10 (14%)	82,113,113	1.54	8 (9%)
24	CHL	N	605	1	42,56,74	3.91	18 (42%)	36,92,114	2.87	15 (41%)
30	BCR	H	101	-	41,41,41	0.84	2 (4%)	56,56,56	2.04	13 (23%)
24	CHL	n	609	1	60,74,74	3.17	20 (33%)	58,114,114	2.35	19 (32%)
24	CHL	g	609	1	55,69,74	3.38	20 (36%)	52,108,114	2.45	16 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	b	613	5	69,73,73	1.26	8 (11%)	82,113,113	1.52	12 (14%)
25	CLA	r	612	17	53,57,73	1.32	9 (16%)	61,93,113	1.43	6 (9%)
33	PHO	a	408	-	58,69,69	2.06	12 (20%)	55,99,99	1.69	9 (16%)
25	CLA	b	610	5	69,73,73	1.17	10 (14%)	82,113,113	1.31	9 (10%)
25	CLA	Y	612	1	64,68,73	1.24	9 (14%)	76,107,113	1.30	9 (11%)
25	CLA	c	512	6	69,73,73	1.15	6 (8%)	82,113,113	1.22	5 (6%)
24	CHL	5	606	-	40,54,74	3.86	20 (50%)	34,90,114	3.00	11 (32%)
25	CLA	1	613	1	59,63,73	1.25	9 (15%)	70,101,113	1.30	8 (11%)
25	CLA	c	509	6	69,73,73	1.16	8 (11%)	82,113,113	1.29	7 (8%)
26	LUT	s	1621	-	42,43,43	0.71	0	51,60,60	1.86	15 (29%)
25	CLA	r	610	17	69,73,73	1.11	7 (10%)	82,113,113	1.22	7 (8%)
25	CLA	N	612	1	64,68,73	1.19	8 (12%)	76,107,113	1.30	6 (7%)
25	CLA	g	602	1	69,73,73	1.19	10 (14%)	82,113,113	1.37	9 (10%)
25	CLA	s	611	29	60,64,73	1.23	6 (10%)	71,102,113	1.21	5 (7%)
33	PHO	A	409	-	58,69,69	2.05	11 (18%)	55,99,99	1.69	9 (16%)
25	CLA	G	610	1	68,72,73	1.14	7 (10%)	80,111,113	1.23	9 (11%)
26	LUT	5	1621	-	42,43,43	0.92	2 (4%)	51,60,60	1.97	15 (29%)
25	CLA	R	609	17	62,66,73	1.20	10 (16%)	73,104,113	1.23	4 (5%)
37	DGD	C	518	-	56,56,67	0.99	4 (7%)	70,70,81	1.54	12 (17%)
25	CLA	d	402	7	69,73,73	1.22	9 (13%)	82,113,113	1.35	10 (12%)
27	XAT	r	622	-	41,47,47	1.01	3 (7%)	54,74,74	2.63	19 (35%)
25	CLA	4	611	29	49,53,73	1.34	8 (16%)	58,89,113	1.26	6 (10%)
25	CLA	c	511	6	69,73,73	1.19	7 (10%)	82,113,113	1.22	7 (8%)
25	CLA	C	503	6	69,73,73	1.18	9 (13%)	82,113,113	1.21	5 (6%)
25	CLA	B	606	5	69,73,73	1.23	10 (14%)	82,113,113	1.44	6 (7%)
25	CLA	s	612	18	53,57,73	1.30	6 (11%)	61,93,113	1.31	6 (9%)
24	CHL	6	606	-	40,54,74	3.95	19 (47%)	34,90,114	2.88	13 (38%)
25	CLA	B	611	-	69,73,73	1.20	8 (11%)	82,113,113	1.40	13 (15%)
25	CLA	g	610	1	68,72,73	1.15	7 (10%)	80,111,113	1.23	9 (11%)
24	CHL	1	608	-	40,54,74	3.95	20 (50%)	34,90,114	2.93	12 (35%)
25	CLA	b	609	5	69,73,73	1.13	8 (11%)	82,113,113	1.41	8 (9%)
35	LMG	Z	101	-	51,51,55	0.88	3 (5%)	59,59,63	1.29	6 (10%)
24	CHL	y	608	-	60,74,74	3.17	19 (31%)	58,114,114	2.36	14 (24%)
25	CLA	6	612	1	49,53,73	1.37	9 (18%)	58,89,113	1.36	8 (13%)
25	CLA	y	604	-	54,58,73	1.37	9 (16%)	64,95,113	1.40	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	y	614	1	52,56,73	1.33	8 (15%)	61,92,113	1.33	6 (9%)
25	CLA	3	612	2	49,53,73	1.39	10 (20%)	58,89,113	1.39	6 (10%)
24	CHL	2	601	1	40,54,74	4.07	20 (50%)	34,90,114	2.85	16 (47%)
26	LUT	2	1621	-	42,43,43	0.79	1 (2%)	51,60,60	1.87	18 (35%)
24	CHL	2	607	-	55,69,74	3.47	20 (36%)	52,108,114	1.95	14 (26%)
25	CLA	b	616	5	69,73,73	1.15	9 (13%)	82,113,113	1.34	8 (9%)
24	CHL	G	609	1	55,69,74	3.37	20 (36%)	52,108,114	2.45	16 (30%)
25	CLA	B	616	5	69,73,73	1.16	9 (13%)	82,113,113	1.34	8 (9%)
29	LHG	6	2630	25	36,36,48	0.75	1 (2%)	39,42,54	1.29	4 (10%)
29	LHG	3	2630	25	46,46,48	0.81	1 (2%)	49,52,54	1.33	4 (8%)
25	CLA	Y	604	-	54,58,73	1.36	9 (16%)	64,95,113	1.40	10 (15%)
29	LHG	B	2631	-	48,48,48	0.67	1 (2%)	51,54,54	1.25	6 (11%)
24	CHL	G	607	-	60,74,74	3.23	19 (31%)	58,114,114	2.23	13 (22%)
24	CHL	1	607	-	57,71,74	3.38	20 (35%)	54,110,114	2.53	19 (35%)
26	LUT	Y	1620	-	42,43,43	0.94	1 (2%)	51,60,60	2.08	21 (41%)
25	CLA	6	604	-	49,53,73	1.36	9 (18%)	58,89,113	1.41	10 (17%)
26	LUT	s	1620	-	42,43,43	0.67	0	51,60,60	1.93	16 (31%)
24	CHL	s	601	18	40,54,74	4.03	19 (47%)	34,90,114	3.03	15 (44%)
25	CLA	3	613	2	62,66,73	1.22	10 (16%)	73,104,113	1.28	4 (5%)
25	CLA	b	602	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	7 (8%)
24	CHL	S	606	-	40,54,74	4.20	18 (45%)	34,90,114	2.86	14 (41%)
24	CHL	r	614	17	36,50,74	4.27	17 (47%)	29,85,114	2.58	12 (41%)
25	CLA	b	604	5	69,73,73	1.24	9 (13%)	82,113,113	1.25	10 (12%)
25	CLA	4	612	3	49,53,73	1.36	9 (18%)	58,89,113	1.40	7 (12%)
24	CHL	S	608	-	40,54,74	4.18	19 (47%)	34,90,114	2.42	11 (32%)
25	CLA	B	603	5	69,73,73	1.17	9 (13%)	82,113,113	1.15	5 (6%)
29	LHG	S	2630	25	48,48,48	0.67	1 (2%)	51,54,54	1.28	7 (13%)
35	LMG	c	521	-	51,51,55	0.75	1 (1%)	59,59,63	1.31	6 (10%)
25	CLA	N	613	1	64,68,73	1.20	8 (12%)	76,107,113	1.51	7 (9%)
25	CLA	7	603	2	59,63,73	1.24	11 (18%)	70,101,113	1.44	8 (11%)
25	CLA	r	603	17	64,68,73	1.20	9 (14%)	76,107,113	1.31	9 (11%)
25	CLA	s	613	18	59,63,73	1.25	7 (11%)	70,101,113	1.22	5 (7%)
25	CLA	S	613	18	59,63,73	1.24	7 (11%)	70,101,113	1.22	5 (7%)
24	CHL	1	605	1	40,54,74	3.98	20 (50%)	34,90,114	2.66	10 (29%)
30	BCR	b	620	-	41,41,41	0.85	1 (2%)	56,56,56	2.04	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	6	614	1	49,53,73	1.34	9 (18%)	58,89,113	1.29	7 (12%)
24	CHL	N	606	-	44,58,74	3.57	20 (45%)	37,94,114	2.94	15 (40%)
34	SQD	b	621	-	52,54,54	0.92	2 (3%)	62,65,65	1.65	10 (16%)
35	LMG	b	2633	-	55,55,55	0.74	0	63,63,63	1.36	6 (9%)
25	CLA	g	612	1	64,68,73	1.21	9 (14%)	76,107,113	1.25	7 (9%)
25	CLA	6	613	1	49,53,73	1.35	7 (14%)	58,89,113	1.26	6 (10%)
25	CLA	8	612	3	49,53,73	1.37	9 (18%)	58,89,113	1.40	7 (12%)
25	CLA	B	612	5	69,73,73	1.27	9 (13%)	82,113,113	1.50	14 (17%)
29	LHG	d	409	-	48,48,48	0.83	1 (2%)	51,54,54	1.35	7 (13%)
25	CLA	C	512	6	69,73,73	1.15	6 (8%)	82,113,113	1.22	5 (6%)
24	CHL	G	605	1	40,54,74	4.04	19 (47%)	34,90,114	2.87	12 (35%)
24	CHL	y	601	1	60,74,74	3.17	20 (33%)	58,114,114	2.77	19 (32%)
25	CLA	4	604	-	49,53,73	1.36	9 (18%)	58,89,113	1.37	6 (10%)
29	LHG	8	2630	25	20,20,48	0.89	1 (5%)	23,26,54	1.36	2 (8%)
26	LUT	G	1620	-	42,43,43	0.78	1 (2%)	51,60,60	1.96	14 (27%)
25	CLA	B	602	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	7 (8%)
30	BCR	a	411	-	41,41,41	0.72	0	56,56,56	1.87	12 (21%)
25	CLA	R	616	17	49,53,73	1.38	10 (20%)	58,89,113	1.40	5 (8%)
25	CLA	n	614	1	52,56,73	1.28	8 (15%)	61,92,113	1.33	7 (11%)
25	CLA	G	611	29	64,68,73	1.19	10 (15%)	76,107,113	1.28	4 (5%)
25	CLA	N	602	1	69,73,73	1.17	9 (13%)	82,113,113	1.27	9 (10%)
25	CLA	2	603	1	59,63,73	1.26	9 (15%)	70,101,113	1.37	6 (8%)
24	CHL	Y	601	1	60,74,74	3.17	20 (33%)	58,114,114	2.77	19 (32%)
25	CLA	C	513	6	69,73,73	1.13	6 (8%)	82,113,113	1.30	9 (10%)
30	BCR	c	514	-	41,41,41	0.70	0	56,56,56	1.75	14 (25%)
25	CLA	B	610	5	69,73,73	1.17	10 (14%)	82,113,113	1.31	9 (10%)
24	CHL	5	608	-	40,54,74	3.95	20 (50%)	34,90,114	2.92	11 (32%)
26	LUT	g	1620	-	42,43,43	0.77	0	51,60,60	1.96	14 (27%)
24	CHL	g	601	1	60,74,74	3.20	19 (31%)	58,114,114	2.58	20 (34%)
25	CLA	A	406	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	8 (9%)
37	DGD	H	102	-	63,63,67	1.20	6 (9%)	77,77,81	1.52	10 (12%)
24	CHL	y	605	1	42,56,74	3.82	19 (45%)	36,92,114	2.76	12 (33%)
26	LUT	g	1621	-	42,43,43	0.92	2 (4%)	51,60,60	2.00	17 (33%)
30	BCR	B	619	-	41,41,41	0.75	0	56,56,56	1.89	17 (30%)
25	CLA	8	604	-	49,53,73	1.36	9 (18%)	58,89,113	1.37	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	LUT	2	1620	-	42,43,43	0.72	0	51,60,60	1.88	14 (27%)
30	BCR	A	411	-	41,41,41	0.72	0	56,56,56	1.87	12 (21%)
25	CLA	G	603	1	69,73,73	1.19	9 (13%)	82,113,113	1.34	9 (10%)
28	NEX	2	1623	-	40,46,46	1.10	3 (7%)	50,70,70	2.28	14 (28%)
25	CLA	y	611	29	64,68,73	1.25	9 (14%)	76,107,113	1.24	7 (9%)
24	CHL	y	609	1	60,74,74	3.22	20 (33%)	58,114,114	2.40	17 (29%)
25	CLA	S	614	18	53,57,73	1.27	6 (11%)	61,93,113	1.35	6 (9%)
24	CHL	s	606	-	40,54,74	4.20	18 (45%)	34,90,114	2.86	14 (41%)
24	CHL	6	607	-	55,69,74	3.46	20 (36%)	52,108,114	1.95	15 (28%)
25	CLA	B	608	-	69,73,73	1.19	9 (13%)	82,113,113	1.29	7 (8%)
24	CHL	6	608	-	40,54,74	4.02	20 (50%)	34,90,114	2.78	10 (29%)
25	CLA	1	611	29	49,53,73	1.35	10 (20%)	58,89,113	1.44	4 (6%)
27	XAT	1	1622	-	41,47,47	0.93	2 (4%)	54,74,74	2.64	20 (37%)
25	CLA	c	506	6	69,73,73	1.20	9 (13%)	82,113,113	1.25	6 (7%)
28	NEX	s	1623	-	40,46,46	1.06	3 (7%)	50,70,70	2.26	16 (32%)
25	CLA	6	610	1	54,58,73	1.27	8 (14%)	64,95,113	1.14	4 (6%)
24	CHL	1	606	-	40,54,74	3.87	20 (50%)	34,90,114	3.00	11 (32%)
24	CHL	s	608	-	40,54,74	4.17	19 (47%)	34,90,114	2.41	11 (32%)
31	OEX	A	401	6,4	0,15,15	-	-	-		
25	CLA	c	505	6	69,73,73	1.15	7 (10%)	82,113,113	1.34	8 (9%)
35	LMG	a	415	-	40,40,55	0.87	0	48,48,63	1.32	6 (12%)
29	LHG	c	522	-	48,48,48	0.68	1 (2%)	51,54,54	1.29	6 (11%)
25	CLA	D	403	7	69,73,73	1.16	10 (14%)	82,113,113	1.25	7 (8%)
26	LUT	8	620	-	42,43,43	0.86	2 (4%)	51,60,60	2.27	17 (33%)
25	CLA	1	603	1	59,63,73	1.27	10 (16%)	70,101,113	1.42	7 (10%)
25	CLA	S	604	-	54,58,73	1.31	8 (14%)	64,95,113	1.41	7 (10%)
29	LHG	C	2630	-	48,48,48	0.67	1 (2%)	51,54,54	1.31	6 (11%)
25	CLA	b	615	5	69,73,73	1.17	7 (10%)	82,113,113	1.19	9 (10%)
35	LMG	d	411	-	46,46,55	0.85	2 (4%)	54,54,63	1.38	6 (11%)
25	CLA	b	611	-	69,73,73	1.20	8 (11%)	82,113,113	1.40	13 (15%)
34	SQD	b	623	-	40,42,54	1.10	5 (12%)	50,53,65	1.67	11 (22%)
25	CLA	c	510	6	69,73,73	1.16	8 (11%)	82,113,113	1.27	9 (10%)
25	CLA	N	611	29	64,68,73	1.18	7 (10%)	76,107,113	1.32	6 (7%)
24	CHL	Y	606	-	44,58,74	3.56	20 (45%)	37,94,114	2.99	15 (40%)
34	SQD	B	621	-	52,54,54	0.92	3 (5%)	62,65,65	1.65	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LHG	l	101	-	48,48,48	0.79	1 (2%)	51,54,54	1.33	6 (11%)
29	LHG	r	2630	25	41,41,48	0.75	1 (2%)	44,47,54	1.36	6 (13%)
25	CLA	7	602	2	64,68,73	1.21	9 (14%)	76,107,113	1.20	7 (9%)
30	BCR	h	101	-	41,41,41	0.84	2 (4%)	56,56,56	2.04	13 (23%)
25	CLA	G	612	1	64,68,73	1.21	9 (14%)	76,107,113	1.25	7 (9%)
25	CLA	b	608	-	69,73,73	1.19	10 (14%)	82,113,113	1.29	7 (8%)
25	CLA	d	403	7	69,73,73	1.15	9 (13%)	82,113,113	1.25	7 (8%)
27	XAT	Y	1622	-	41,47,47	1.01	2 (4%)	54,74,74	2.96	21 (38%)
36	PL9	d	405	-	55,55,55	2.27	18 (32%)	68,69,69	1.58	13 (19%)
25	CLA	4	602	3	49,53,73	1.30	8 (16%)	58,89,113	1.46	7 (12%)
30	BCR	c	515	-	41,41,41	0.70	0	56,56,56	1.93	17 (30%)
24	CHL	5	601	1	40,54,74	3.94	20 (50%)	34,90,114	2.85	14 (41%)
28	NEX	y	1623	-	40,46,46	1.25	4 (10%)	50,70,70	2.62	20 (40%)
24	CHL	4	607	-	40,54,74	4.03	19 (47%)	34,90,114	2.58	14 (41%)
29	LHG	C	522	-	48,48,48	0.68	1 (2%)	51,54,54	1.29	6 (11%)
25	CLA	C	502	6	69,73,73	1.15	6 (8%)	82,113,113	1.41	7 (8%)
33	PHO	a	409	-	58,69,69	2.05	11 (18%)	55,99,99	1.69	8 (14%)
24	CHL	g	605	1	40,54,74	4.03	19 (47%)	34,90,114	2.87	12 (35%)
25	CLA	1	612	1	49,53,73	1.39	9 (18%)	58,89,113	1.49	9 (15%)
25	CLA	A	407	-	54,58,73	1.29	8 (14%)	64,95,113	1.29	4 (6%)
25	CLA	N	614	1	52,56,73	1.28	8 (15%)	61,92,113	1.34	7 (11%)
25	CLA	G	614	1	52,56,73	1.31	9 (17%)	61,92,113	1.19	5 (8%)
25	CLA	3	611	29	59,63,73	1.30	10 (16%)	70,101,113	1.35	8 (11%)
25	CLA	G	613	1	69,73,73	1.18	10 (14%)	82,113,113	1.34	4 (4%)
24	CHL	8	608	-	40,54,74	3.95	20 (50%)	34,90,114	3.06	15 (44%)
25	CLA	b	605	5	69,73,73	1.28	13 (18%)	82,113,113	1.73	17 (20%)
24	CHL	g	606	-	44,58,74	3.70	19 (43%)	37,94,114	2.80	15 (40%)
25	CLA	B	615	5	69,73,73	1.17	7 (10%)	82,113,113	1.19	9 (10%)
24	CHL	n	605	1	42,56,74	3.91	18 (42%)	36,92,114	2.88	15 (41%)
29	LHG	s	2630	25	48,48,48	0.67	1 (2%)	51,54,54	1.28	7 (13%)
24	CHL	2	605	1	40,54,74	4.11	19 (47%)	34,90,114	2.58	12 (35%)
29	LHG	1	2630	25	40,40,48	0.77	1 (2%)	43,46,54	1.35	6 (13%)
25	CLA	n	610	1	69,73,73	1.12	7 (10%)	82,113,113	1.23	9 (10%)
24	CHL	8	607	-	40,54,74	4.02	19 (47%)	34,90,114	2.59	14 (41%)
25	CLA	B	609	5	69,73,73	1.13	7 (10%)	82,113,113	1.41	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	R	608	-	55,69,74	3.24	19 (34%)	52,108,114	2.62	15 (28%)
25	CLA	C	507	-	69,73,73	1.14	8 (11%)	82,113,113	1.40	10 (12%)
25	CLA	5	614	1	49,53,73	1.36	9 (18%)	58,89,113	1.30	7 (12%)
25	CLA	b	606	5	69,73,73	1.24	10 (14%)	82,113,113	1.44	6 (7%)
37	DGD	C	520	-	61,61,67	0.98	3 (4%)	75,75,81	1.43	10 (13%)
24	CHL	n	606	-	44,58,74	3.57	20 (45%)	37,94,114	2.94	15 (40%)
26	LUT	N	1620	-	42,43,43	0.80	1 (2%)	51,60,60	2.00	17 (33%)
25	CLA	A	405	4	69,73,73	1.20	9 (13%)	82,113,113	1.26	5 (6%)
26	LUT	N	1621	-	42,43,43	0.92	1 (2%)	51,60,60	1.99	15 (29%)
25	CLA	c	513	6	69,73,73	1.13	6 (8%)	82,113,113	1.30	10 (12%)
24	CHL	R	607	-	50,64,74	3.62	19 (38%)	46,102,114	2.60	19 (41%)
27	XAT	5	1622	-	41,47,47	0.93	2 (4%)	54,74,74	2.63	20 (37%)
37	DGD	c	518	-	56,56,67	0.99	4 (7%)	70,70,81	1.54	12 (17%)
35	LMG	a	413	-	48,48,55	0.78	1 (2%)	56,56,63	1.30	4 (7%)
25	CLA	8	611	29	49,53,73	1.34	8 (16%)	58,89,113	1.26	6 (10%)
26	LUT	3	1620	-	42,43,43	0.85	1 (2%)	51,60,60	2.19	21 (41%)
25	CLA	c	503	6	69,73,73	1.18	9 (13%)	82,113,113	1.21	5 (6%)
26	LUT	6	1621	-	42,43,43	0.79	1 (2%)	51,60,60	1.87	18 (35%)
25	CLA	3	604	-	49,53,73	1.35	8 (16%)	58,89,113	1.28	4 (6%)
25	CLA	G	602	1	69,73,73	1.18	10 (14%)	82,113,113	1.37	9 (10%)
24	CHL	n	608	-	60,74,74	3.24	19 (31%)	58,114,114	2.53	14 (24%)
37	DGD	h	102	-	63,63,67	1.20	6 (9%)	77,77,81	1.52	10 (12%)
24	CHL	5	609	1	56,70,74	3.37	20 (35%)	53,109,114	2.29	14 (26%)
36	PL9	a	414	-	13,13,55	0.73	0	17,17,69	2.31	4 (23%)
25	CLA	r	613	17	64,68,73	1.21	6 (9%)	76,107,113	1.36	5 (6%)
28	NEX	N	1623	-	40,46,46	1.17	4 (10%)	50,70,70	2.29	16 (32%)
25	CLA	S	611	29	60,64,73	1.23	6 (10%)	71,102,113	1.22	5 (7%)
30	BCR	b	618	-	41,41,41	0.92	1 (2%)	56,56,56	2.01	13 (23%)
33	PHO	A	408	-	58,69,69	2.07	12 (20%)	55,99,99	1.68	9 (16%)
25	CLA	R	612	17	53,57,73	1.32	9 (16%)	61,93,113	1.43	6 (9%)
24	CHL	N	601	1	60,74,74	3.27	19 (31%)	58,114,114	2.54	18 (31%)
25	CLA	N	604	-	54,58,73	1.36	9 (16%)	64,95,113	1.39	9 (14%)
28	NEX	R	623	-	40,46,46	1.14	3 (7%)	50,70,70	2.45	20 (40%)
24	CHL	G	606	-	44,58,74	3.71	19 (43%)	37,94,114	2.80	15 (40%)
25	CLA	1	602	1	65,69,73	1.23	10 (15%)	77,108,113	1.18	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	2	606	-	40,54,74	3.95	19 (47%)	34,90,114	2.89	13 (38%)
35	LMG	B	622	-	51,51,55	0.89	2 (3%)	59,59,63	1.41	6 (10%)
25	CLA	N	610	1	69,73,73	1.12	7 (10%)	82,113,113	1.23	9 (10%)
25	CLA	8	610	3	49,53,73	1.36	9 (18%)	58,89,113	1.23	7 (12%)
25	CLA	y	602	1	69,73,73	1.20	8 (11%)	82,113,113	1.25	10 (12%)
25	CLA	r	604	-	52,56,73	1.34	10 (19%)	61,92,113	1.44	10 (16%)
25	CLA	6	602	1	65,69,73	1.20	9 (13%)	77,108,113	1.21	8 (10%)
36	PL9	A	414	-	13,13,55	0.74	0	17,17,69	2.30	4 (23%)
26	LUT	7	1620	-	42,43,43	0.85	1 (2%)	51,60,60	2.20	21 (41%)
25	CLA	R	610	17	69,73,73	1.11	7 (10%)	82,113,113	1.23	7 (8%)
24	CHL	6	601	1	40,54,74	4.06	20 (50%)	34,90,114	2.84	16 (47%)
25	CLA	b	603	5	69,73,73	1.16	9 (13%)	82,113,113	1.15	4 (4%)
25	CLA	G	604	-	54,58,73	1.35	8 (14%)	64,95,113	1.37	6 (9%)
25	CLA	1	604	-	54,58,73	1.32	9 (16%)	64,95,113	1.36	7 (10%)
25	CLA	Y	614	1	52,56,73	1.33	8 (15%)	61,92,113	1.32	6 (9%)
30	BCR	C	516	-	41,41,41	0.66	0	56,56,56	1.96	14 (25%)
24	CHL	7	601	2	58,72,74	3.21	20 (34%)	55,111,114	2.72	18 (32%)
34	SQD	B	623	-	40,42,54	1.10	5 (12%)	50,53,65	1.67	11 (22%)
25	CLA	Y	613	1	69,73,73	1.20	10 (14%)	82,113,113	1.55	8 (9%)
26	LUT	7	1621	-	42,43,43	0.86	1 (2%)	51,60,60	1.70	12 (23%)
25	CLA	n	613	1	64,68,73	1.21	8 (12%)	76,107,113	1.51	7 (9%)
25	CLA	g	613	1	69,73,73	1.18	10 (14%)	82,113,113	1.34	4 (4%)
24	CHL	Y	609	1	60,74,74	3.22	20 (33%)	58,114,114	2.40	17 (29%)
25	CLA	c	502	6	69,73,73	1.15	5 (7%)	82,113,113	1.41	8 (9%)
28	NEX	6	1623	-	40,46,46	1.10	3 (7%)	50,70,70	2.28	14 (28%)
37	DGD	c	520	-	61,61,67	0.98	3 (4%)	75,75,81	1.43	10 (13%)
25	CLA	4	603	3	49,53,73	1.37	9 (18%)	58,89,113	1.38	5 (8%)
25	CLA	S	602	18	65,69,73	1.20	8 (12%)	77,108,113	1.22	8 (10%)
29	LHG	n	2630	25	48,48,48	0.78	1 (2%)	51,54,54	1.34	7 (13%)
25	CLA	n	612	1	64,68,73	1.18	8 (12%)	76,107,113	1.30	6 (7%)
25	CLA	a	410	4	64,68,73	1.17	8 (12%)	76,107,113	1.35	8 (10%)
24	CHL	N	608	-	60,74,74	3.24	19 (31%)	58,114,114	2.53	15 (25%)
24	CHL	8	609	3	40,54,74	3.93	19 (47%)	34,90,114	2.93	14 (41%)
25	CLA	Y	602	1	69,73,73	1.20	8 (11%)	82,113,113	1.24	10 (12%)
34	SQD	A	418	-	52,54,54	0.90	3 (5%)	62,65,65	1.60	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LHG	2	2630	25	36,36,48	0.76	1 (2%)	39,42,54	1.29	4 (10%)
25	CLA	5	613	1	59,63,73	1.25	9 (15%)	70,101,113	1.29	8 (11%)
35	LMG	B	2633	-	55,55,55	0.74	0	63,63,63	1.36	6 (9%)
35	LMG	A	415	-	40,40,55	0.87	0	48,48,63	1.32	6 (12%)
25	CLA	2	604	-	49,53,73	1.36	9 (18%)	58,89,113	1.41	10 (17%)
25	CLA	B	613	5	69,73,73	1.26	8 (11%)	82,113,113	1.52	12 (14%)
25	CLA	8	603	3	49,53,73	1.37	9 (18%)	58,89,113	1.38	5 (8%)
27	XAT	3	1622	-	41,47,47	1.03	2 (4%)	54,74,74	2.96	26 (48%)
25	CLA	C	508	6	69,73,73	1.16	7 (10%)	82,113,113	1.33	7 (8%)
35	LMG	z	101	-	51,51,55	0.87	3 (5%)	59,59,63	1.29	6 (10%)
26	LUT	G	1621	-	42,43,43	0.92	2 (4%)	51,60,60	2.00	16 (31%)
25	CLA	6	603	1	59,63,73	1.27	9 (15%)	70,101,113	1.38	6 (8%)
27	XAT	4	622	-	41,47,47	0.93	2 (4%)	54,74,74	2.62	21 (38%)
25	CLA	c	504	-	69,73,73	1.15	7 (10%)	82,113,113	1.21	5 (6%)
25	CLA	C	501	6	69,73,73	1.17	7 (10%)	82,113,113	1.11	7 (8%)
25	CLA	R	603	17	64,68,73	1.20	9 (14%)	76,107,113	1.31	9 (11%)
29	LHG	5	2630	25	40,40,48	0.77	1 (2%)	43,46,54	1.35	6 (13%)
31	OEX	a	401	6,4	0,15,15	-	-	-		
25	CLA	s	602	18	65,69,73	1.20	8 (12%)	77,108,113	1.22	8 (10%)
26	LUT	r	620	-	42,43,43	0.87	2 (4%)	51,60,60	2.14	21 (41%)
25	CLA	s	614	18	53,57,73	1.27	5 (9%)	61,93,113	1.34	6 (9%)
37	DGD	B	626	-	60,60,67	0.97	1 (1%)	74,74,81	1.38	6 (8%)
28	NEX	g	1623	-	40,46,46	1.09	3 (7%)	50,70,70	2.37	16 (32%)
25	CLA	5	604	-	54,58,73	1.32	9 (16%)	64,95,113	1.35	7 (10%)
25	CLA	n	602	1	69,73,73	1.17	9 (13%)	82,113,113	1.27	9 (10%)
29	LHG	g	2630	25	48,48,48	0.80	1 (2%)	51,54,54	1.33	6 (11%)
25	CLA	g	603	1	69,73,73	1.19	9 (13%)	82,113,113	1.34	9 (10%)
25	CLA	r	601	17	53,57,73	1.30	10 (18%)	61,93,113	1.55	9 (14%)
27	XAT	7	1622	-	41,47,47	1.03	2 (4%)	54,74,74	2.96	26 (48%)
30	BCR	4	623	-	41,41,41	0.72	0	56,56,56	2.20	15 (26%)
25	CLA	r	611	29	53,57,73	1.32	9 (16%)	61,93,113	1.23	6 (9%)
29	LHG	c	2630	-	48,48,48	0.67	1 (2%)	51,54,54	1.31	6 (11%)
24	CHL	7	605	2	40,54,74	4.05	19 (47%)	34,90,114	2.84	13 (38%)
25	CLA	3	602	2	64,68,73	1.20	9 (14%)	76,107,113	1.20	7 (9%)
25	CLA	C	504	-	69,73,73	1.15	7 (10%)	82,113,113	1.21	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	a	407	-	54,58,73	1.29	8 (14%)	64,95,113	1.29	4 (6%)
30	BCR	B	618	-	41,41,41	0.92	1 (2%)	56,56,56	2.01	13 (23%)
25	CLA	B	607	5	69,73,73	1.20	9 (13%)	82,113,113	1.29	8 (9%)

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
24	CHL	Y	605	1	3/3/16/26	6/18/116/137	-
25	CLA	C	511	6	-	10/39/115/115	-
24	CHL	3	601	2	4/4/19/26	12/37/135/137	-
29	LHG	d	408	-	-	17/50/50/53	-
24	CHL	G	601	1	4/4/20/26	17/39/137/137	-
25	CLA	5	612	1	1/1/11/20	6/15/91/115	-
28	NEX	7	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	a	406	-	1/1/15/20	2/39/115/115	-
25	CLA	3	610	2	1/1/14/20	6/33/109/115	-
25	CLA	2	613	1	-	5/15/91/115	-
24	CHL	s	607	-	4/4/18/26	13/30/128/137	-
26	LUT	y	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	5	602	1	1/1/14/20	10/35/111/115	-
24	CHL	7	606	-	3/3/16/26	5/15/113/137	-
30	BCR	C	515	-	-	6/29/63/63	0/2/2/2
25	CLA	B	617	5	1/1/15/20	19/39/115/115	-
25	CLA	2	611	29	1/1/11/20	4/15/91/115	-
34	SQD	a	418	-	-	21/49/69/69	0/1/1/1
39	HEM	F	101	9,8	-	1/14/54/54	-
24	CHL	Y	608	-	4/4/20/26	16/39/137/137	-
29	LHG	Y	2630	25	-	19/53/53/53	-
28	NEX	G	1623	-	-	5/27/83/83	0/3/3/3
24	CHL	g	608	-	4/4/20/26	18/39/137/137	-
24	CHL	S	601	18	3/3/16/26	6/15/113/137	-
24	CHL	R	606	-	4/4/20/26	22/39/137/137	-
25	CLA	6	611	29	1/1/11/20	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	607	5	1/1/15/20	12/39/115/115	-
25	CLA	c	507	-	1/1/15/20	21/39/115/115	-
24	CHL	3	607	-	3/3/17/26	13/24/122/137	-
25	CLA	b	614	5	1/1/15/20	13/39/115/115	-
25	CLA	2	614	1	-	8/15/91/115	-
25	CLA	C	509	6	1/1/15/20	7/39/115/115	-
24	CHL	3	606	-	3/3/16/26	5/15/113/137	-
25	CLA	C	510	6	1/1/15/20	16/39/115/115	-
25	CLA	r	609	17	1/1/13/20	2/31/107/115	-
26	LUT	n	1621	-	-	1/29/67/67	0/2/2/2
25	CLA	y	612	1	1/1/14/20	14/33/109/115	-
27	XAT	2	1622	-	-	4/31/93/93	0/4/4/4
25	CLA	g	611	29	1/1/14/20	12/33/109/115	-
25	CLA	1	614	1	1/1/11/20	5/15/91/115	-
27	XAT	N	1622	-	-	3/31/93/93	0/4/4/4
25	CLA	b	617	5	1/1/15/20	19/39/115/115	-
30	BCR	C	517	-	-	4/29/63/63	0/2/2/2
34	SQD	A	412	-	-	18/45/65/69	0/1/1/1
24	CHL	r	606	-	4/4/20/26	22/39/137/137	-
24	CHL	2	609	1	4/4/19/26	13/33/131/137	-
25	CLA	n	611	29	1/1/14/20	9/33/109/115	-
27	XAT	6	1622	-	-	4/31/93/93	0/4/4/4
28	NEX	r	623	-	-	4/27/83/83	0/3/3/3
24	CHL	5	605	1	3/3/16/26	8/15/113/137	-
24	CHL	g	607	-	4/4/20/26	12/39/137/137	-
25	CLA	7	614	2	1/1/11/20	5/19/95/115	-
29	LHG	D	410	-	-	24/47/47/53	-
24	CHL	r	607	-	4/4/18/26	8/27/125/137	-
25	CLA	N	603	1	1/1/15/20	13/39/115/115	-
24	CHL	n	601	1	4/4/20/26	19/39/137/137	-
25	CLA	s	603	18	1/1/11/20	6/15/91/115	-
24	CHL	n	607	-	4/4/20/26	15/39/137/137	-
29	LHG	C	523	-	-	20/53/53/53	-
25	CLA	S	610	18	1/1/13/20	6/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	7	613	2	1/1/13/20	8/31/107/115	-
25	CLA	4	610	3	1/1/11/20	6/15/91/115	-
24	CHL	2	608	-	3/3/16/26	7/15/113/137	-
25	CLA	B	605	5	1/1/15/20	13/39/115/115	-
25	CLA	8	602	3	1/1/11/20	4/15/91/115	-
26	LUT	3	1621	-	-	3/29/67/67	0/2/2/2
25	CLA	5	603	1	1/1/13/20	11/27/103/115	-
25	CLA	a	405	4	1/1/15/20	10/39/115/115	-
24	CHL	G	608	-	4/4/20/26	18/39/137/137	-
25	CLA	c	508	6	1/1/15/20	8/39/115/115	-
35	LMG	D	411	-	-	15/41/61/70	0/1/1/1
29	LHG	7	2630	25	-	23/51/51/53	-
25	CLA	R	602	17	1/1/14/20	7/33/109/115	-
25	CLA	2	610	1	1/1/12/20	5/21/97/115	-
26	LUT	1	1620	-	-	2/29/67/67	0/2/2/2
30	BCR	B	620	-	-	6/29/63/63	0/2/2/2
27	XAT	R	622	-	-	5/31/93/93	0/4/4/4
25	CLA	7	604	-	1/1/11/20	10/15/91/115	-
25	CLA	R	613	17	1/1/14/20	11/33/109/115	-
29	LHG	B	2630	-	-	30/51/51/53	-
26	LUT	6	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	S	609	18	1/1/11/20	9/15/91/115	-
25	CLA	B	604	5	1/1/15/20	11/39/115/115	-
25	CLA	y	603	1	1/1/15/20	11/39/115/115	-
30	BCR	8	623	-	-	11/29/63/63	0/2/2/2
25	CLA	7	612	2	1/1/11/20	6/15/91/115	-
29	LHG	R	2630	25	-	15/46/46/53	-
25	CLA	r	616	17	-	6/15/91/115	-
28	NEX	Y	1623	-	-	3/27/83/83	0/3/3/3
28	NEX	1	1623	-	-	8/27/83/83	0/3/3/3
29	LHG	4	2630	25	-	8/23/23/53	-
30	BCR	b	619	-	-	2/29/63/63	0/2/2/2
24	CHL	N	609	1	4/4/20/26	17/39/137/137	-
37	DGD	b	626	-	-	22/48/88/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	c	516	-	-	9/29/63/63	0/2/2/2
29	LHG	c	523	-	-	20/53/53/53	-
37	DGD	C	519	-	-	26/51/91/95	0/2/2/2
24	CHL	y	607	-	4/4/20/26	15/39/137/137	-
25	CLA	3	614	2	1/1/11/20	5/19/95/115	-
24	CHL	R	614	17	3/3/15/26	4/10/108/137	-
25	CLA	Y	603	1	1/1/15/20	11/39/115/115	-
24	CHL	1	601	1	3/3/16/26	6/15/113/137	-
25	CLA	n	603	1	1/1/15/20	13/39/115/115	-
24	CHL	S	607	-	4/4/18/26	13/30/128/137	-
24	CHL	3	608	-	3/3/16/26	8/15/113/137	-
25	CLA	n	604	-	1/1/12/20	3/21/97/115	-
35	LMG	C	521	-	-	21/46/66/70	0/1/1/1
25	CLA	5	611	29	1/1/11/20	7/15/91/115	-
25	CLA	1	610	1	1/1/13/20	4/29/105/115	-
27	XAT	g	1622	-	-	2/31/93/93	0/4/4/4
24	CHL	N	607	-	4/4/20/26	15/39/137/137	-
25	CLA	y	610	1	1/1/14/20	9/33/109/115	-
26	LUT	n	1620	-	-	2/29/67/67	0/2/2/2
29	LHG	N	2630	25	-	24/53/53/53	-
25	CLA	g	614	1	1/1/11/20	7/19/95/115	-
27	XAT	G	1622	-	-	2/31/93/93	0/4/4/4
36	PL9	D	405	-	-	8/53/73/73	0/1/1/1
29	LHG	D	409	-	-	19/53/53/53	-
24	CHL	4	601	3	3/3/16/26	3/13/111/137	-
28	NEX	n	1623	-	-	5/27/83/83	0/3/3/3
30	BCR	T	101	-	-	13/29/63/63	0/2/2/2
25	CLA	Y	610	1	1/1/14/20	9/33/109/115	-
25	CLA	7	611	29	1/1/13/20	11/27/103/115	-
25	CLA	A	410	4	1/1/14/20	9/33/109/115	-
29	LHG	d	410	-	-	24/47/47/53	-
30	BCR	t	101	-	-	13/29/63/63	0/2/2/2
29	LHG	L	101	-	-	20/53/53/53	-
25	CLA	C	506	6	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	S	612	18	1/1/11/20	3/20/96/115	-
25	CLA	3	603	2	1/1/13/20	10/27/103/115	-
25	CLA	R	604	-	1/1/11/20	4/19/95/115	-
24	CHL	7	609	2	4/4/19/26	14/33/131/137	-
29	LHG	G	2630	25	-	25/53/53/53	-
28	NEX	3	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	2	612	1	1/1/11/20	8/15/91/115	-
24	CHL	7	607	-	3/3/17/26	13/24/122/137	-
24	CHL	8	601	3	3/3/16/26	3/13/111/137	-
30	BCR	C	514	-	-	2/29/63/63	0/2/2/2
35	LMG	b	622	-	-	23/46/66/70	0/1/1/1
26	LUT	S	1621	-	-	3/29/67/67	0/2/2/2
26	LUT	5	1620	-	-	2/29/67/67	0/2/2/2
27	XAT	8	622	-	-	2/31/93/93	0/4/4/4
29	LHG	b	2631	-	-	19/53/53/53	-
30	BCR	d	404	-	-	5/29/63/63	0/2/2/2
25	CLA	R	601	17	1/1/11/20	9/20/96/115	-
24	CHL	y	606	-	3/3/16/26	5/20/118/137	-
25	CLA	D	402	7	1/1/15/20	5/39/115/115	-
30	BCR	D	404	-	-	5/29/63/63	0/2/2/2
34	SQD	a	412	-	-	18/45/65/69	0/1/1/1
24	CHL	1	609	1	4/4/19/26	13/35/133/137	-
25	CLA	c	501	6	1/1/15/20	12/39/115/115	-
26	LUT	S	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	B	614	5	1/1/15/20	13/39/115/115	-
24	CHL	6	605	1	3/3/16/26	8/15/113/137	-
28	NEX	5	1623	-	-	8/27/83/83	0/3/3/3
25	CLA	2	602	1	1/1/14/20	13/35/111/115	-
24	CHL	6	609	1	4/4/19/26	13/33/131/137	-
29	LHG	y	2630	25	-	19/53/53/53	-
28	NEX	S	1623	-	-	5/27/83/83	0/3/3/3
24	CHL	4	606	-	3/3/16/26	6/15/113/137	-
26	LUT	R	620	-	-	2/29/67/67	0/2/2/2
27	XAT	y	1622	-	-	3/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	4	609	3	3/3/16/26	6/15/113/137	-
25	CLA	Y	611	29	1/1/14/20	8/33/109/115	-
37	DGD	c	519	-	-	26/51/91/95	0/2/2/2
25	CLA	s	604	-	1/1/12/20	6/21/97/115	-
24	CHL	7	608	-	3/3/16/26	8/15/113/137	-
24	CHL	r	608	-	4/4/19/26	15/33/131/137	-
29	LHG	D	408	-	-	17/50/50/53	-
26	LUT	4	620	-	-	5/29/67/67	0/2/2/2
26	LUT	y	1621	-	-	1/29/67/67	0/2/2/2
24	CHL	4	608	-	3/3/16/26	10/15/113/137	-
25	CLA	C	505	6	-	10/39/115/115	-
35	LMG	A	413	-	-	18/43/63/70	0/1/1/1
24	CHL	3	605	2	3/3/16/26	9/15/113/137	-
24	CHL	5	607	-	4/4/19/26	20/36/134/137	-
24	CHL	8	606	-	3/3/16/26	6/15/113/137	-
39	HEM	f	101	9,8	-	1/14/54/54	-
25	CLA	5	610	1	1/1/13/20	4/29/105/115	-
25	CLA	s	609	18	1/1/11/20	9/15/91/115	-
25	CLA	7	610	2	1/1/14/20	6/33/109/115	-
26	LUT	Y	1621	-	-	1/29/67/67	0/2/2/2
24	CHL	Y	607	-	4/4/20/26	15/39/137/137	-
25	CLA	s	610	18	1/1/13/20	6/27/103/115	-
25	CLA	r	602	17	1/1/14/20	7/33/109/115	-
26	LUT	1	1621	-	-	5/29/67/67	0/2/2/2
25	CLA	b	612	5	1/1/15/20	10/39/115/115	-
25	CLA	R	611	29	1/1/11/20	11/20/96/115	-
30	BCR	c	517	-	-	4/29/63/63	0/2/2/2
27	XAT	n	1622	-	-	3/31/93/93	0/4/4/4
25	CLA	g	604	-	-	7/21/97/115	-
24	CHL	3	609	2	4/4/19/26	14/33/131/137	-
29	LHG	b	2630	-	-	30/51/51/53	-
25	CLA	S	603	18	1/1/11/20	6/15/91/115	-
25	CLA	y	613	1	1/1/15/20	10/39/115/115	-
24	CHL	N	605	1	3/3/16/26	8/18/116/137	-
30	BCR	H	101	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	n	609	1	4/4/20/26	17/39/137/137	-
24	CHL	g	609	1	4/4/19/26	12/33/131/137	-
25	CLA	b	613	5	1/1/15/20	14/39/115/115	-
25	CLA	r	612	17	1/1/11/20	6/20/96/115	-
33	PHO	a	408	-	-	6/37/103/103	0/5/6/6
25	CLA	b	610	5	-	6/39/115/115	-
25	CLA	Y	612	1	1/1/14/20	14/33/109/115	-
25	CLA	c	512	6	1/1/15/20	9/39/115/115	-
24	CHL	5	606	-	3/3/16/26	7/15/113/137	-
25	CLA	1	613	1	-	8/27/103/115	-
25	CLA	c	509	6	1/1/15/20	7/39/115/115	-
26	LUT	s	1621	-	-	3/29/67/67	0/2/2/2
25	CLA	r	610	17	1/1/15/20	14/39/115/115	-
25	CLA	N	612	1	1/1/14/20	10/33/109/115	-
25	CLA	g	602	1	1/1/15/20	11/39/115/115	-
25	CLA	s	611	29	1/1/13/20	9/29/105/115	-
33	PHO	A	409	-	-	8/37/103/103	0/5/6/6
25	CLA	G	610	1	1/1/14/20	13/38/114/115	-
26	LUT	5	1621	-	-	5/29/67/67	0/2/2/2
25	CLA	R	609	17	1/1/13/20	2/31/107/115	-
37	DGD	C	518	-	-	16/44/84/95	0/2/2/2
25	CLA	d	402	7	1/1/15/20	5/39/115/115	-
27	XAT	r	622	-	-	5/31/93/93	0/4/4/4
25	CLA	4	611	29	1/1/11/20	8/15/91/115	-
25	CLA	c	511	6	-	10/39/115/115	-
25	CLA	C	503	6	1/1/15/20	11/39/115/115	-
25	CLA	B	606	5	1/1/15/20	16/39/115/115	-
25	CLA	s	612	18	1/1/11/20	3/20/96/115	-
24	CHL	6	606	-	3/3/16/26	5/15/113/137	-
25	CLA	B	611	-	1/1/15/20	10/39/115/115	-
25	CLA	g	610	1	1/1/14/20	13/38/114/115	-
24	CHL	1	608	-	3/3/16/26	3/15/113/137	-
25	CLA	b	609	5	1/1/15/20	5/39/115/115	-
35	LMG	Z	101	-	-	22/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	y	608	-	4/4/20/26	16/39/137/137	-
25	CLA	6	612	1	1/1/11/20	8/15/91/115	-
25	CLA	y	604	-	1/1/12/20	4/21/97/115	-
25	CLA	y	614	1	1/1/11/20	5/19/95/115	-
25	CLA	3	612	2	1/1/11/20	6/15/91/115	-
24	CHL	2	601	1	3/3/16/26	6/15/113/137	-
26	LUT	2	1621	-	-	0/29/67/67	0/2/2/2
24	CHL	2	607	-	4/4/19/26	20/33/131/137	-
25	CLA	b	616	5	1/1/15/20	14/39/115/115	-
24	CHL	G	609	1	4/4/19/26	12/33/131/137	-
25	CLA	B	616	5	1/1/15/20	14/39/115/115	-
29	LHG	6	2630	25	-	14/41/41/53	-
29	LHG	3	2630	25	-	23/51/51/53	-
25	CLA	Y	604	-	1/1/12/20	4/21/97/115	-
29	LHG	B	2631	-	-	19/53/53/53	-
24	CHL	G	607	-	4/4/20/26	12/39/137/137	-
24	CHL	1	607	-	4/4/19/26	20/36/134/137	-
26	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	6	604	-	-	7/15/91/115	-
26	LUT	s	1620	-	-	2/29/67/67	0/2/2/2
24	CHL	s	601	18	3/3/16/26	6/15/113/137	-
25	CLA	3	613	2	1/1/13/20	8/31/107/115	-
25	CLA	b	602	-	1/1/15/20	15/39/115/115	-
24	CHL	S	606	-	3/3/16/26	8/15/113/137	-
24	CHL	r	614	17	3/3/15/26	4/10/108/137	-
25	CLA	b	604	5	1/1/15/20	11/39/115/115	-
25	CLA	4	612	3	1/1/11/20	8/15/91/115	-
24	CHL	S	608	-	3/3/16/26	6/15/113/137	-
25	CLA	B	603	5	1/1/15/20	12/39/115/115	-
29	LHG	S	2630	25	-	24/53/53/53	-
35	LMG	c	521	-	-	21/46/66/70	0/1/1/1
25	CLA	N	613	1	1/1/14/20	7/33/109/115	-
25	CLA	7	603	2	1/1/13/20	10/27/103/115	-
25	CLA	r	603	17	1/1/14/20	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	s	613	18	1/1/13/20	2/27/103/115	-
25	CLA	S	613	18	1/1/13/20	2/27/103/115	-
24	CHL	1	605	1	3/3/16/26	8/15/113/137	-
30	BCR	b	620	-	-	6/29/63/63	0/2/2/2
25	CLA	6	614	1	-	8/15/91/115	-
24	CHL	N	606	-	3/3/16/26	8/20/118/137	-
34	SQD	b	621	-	-	18/49/69/69	0/1/1/1
35	LMG	b	2633	-	-	21/50/70/70	0/1/1/1
25	CLA	g	612	1	1/1/14/20	12/33/109/115	-
25	CLA	6	613	1	-	5/15/91/115	-
25	CLA	8	612	3	1/1/11/20	8/15/91/115	-
25	CLA	B	612	5	1/1/15/20	10/39/115/115	-
29	LHG	d	409	-	-	19/53/53/53	-
25	CLA	C	512	6	1/1/15/20	9/39/115/115	-
24	CHL	G	605	1	3/3/16/26	8/15/113/137	-
24	CHL	y	601	1	4/4/20/26	15/39/137/137	-
25	CLA	4	604	-	-	9/15/91/115	-
29	LHG	8	2630	25	-	8/23/23/53	-
26	LUT	G	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	B	602	-	1/1/15/20	15/39/115/115	-
30	BCR	a	411	-	-	2/29/63/63	0/2/2/2
25	CLA	R	616	17	-	6/15/91/115	-
25	CLA	n	614	1	1/1/11/20	6/19/95/115	-
25	CLA	G	611	29	1/1/14/20	12/33/109/115	-
25	CLA	N	602	1	1/1/15/20	12/39/115/115	-
25	CLA	2	603	1	1/1/13/20	14/27/103/115	-
24	CHL	Y	601	1	4/4/20/26	15/39/137/137	-
25	CLA	C	513	6	-	13/39/115/115	-
30	BCR	c	514	-	-	2/29/63/63	0/2/2/2
25	CLA	B	610	5	-	6/39/115/115	-
24	CHL	5	608	-	3/3/16/26	3/15/113/137	-
26	LUT	g	1620	-	-	2/29/67/67	0/2/2/2
24	CHL	g	601	1	4/4/20/26	17/39/137/137	-
25	CLA	A	406	-	1/1/15/20	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGD	H	102	-	-	25/51/91/95	0/2/2/2
24	CHL	y	605	1	3/3/16/26	6/18/116/137	-
26	LUT	g	1621	-	-	1/29/67/67	0/2/2/2
30	BCR	B	619	-	-	2/29/63/63	0/2/2/2
25	CLA	8	604	-	-	9/15/91/115	-
26	LUT	2	1620	-	-	2/29/67/67	0/2/2/2
30	BCR	A	411	-	-	2/29/63/63	0/2/2/2
25	CLA	G	603	1	1/1/15/20	10/39/115/115	-
28	NEX	2	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	y	611	29	1/1/14/20	8/33/109/115	-
24	CHL	y	609	1	4/4/20/26	14/39/137/137	-
25	CLA	S	614	18	1/1/11/20	5/20/96/115	-
24	CHL	s	606	-	3/3/16/26	8/15/113/137	-
24	CHL	6	607	-	4/4/19/26	20/33/131/137	-
25	CLA	B	608	-	1/1/15/20	12/39/115/115	-
24	CHL	6	608	-	3/3/16/26	7/15/113/137	-
25	CLA	1	611	29	1/1/11/20	7/15/91/115	-
27	XAT	1	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	c	506	6	-	16/39/115/115	-
28	NEX	s	1623	-	-	5/27/83/83	0/3/3/3
25	CLA	6	610	1	1/1/12/20	5/21/97/115	-
24	CHL	1	606	-	3/3/16/26	7/15/113/137	-
24	CHL	s	608	-	3/3/16/26	6/15/113/137	-
25	CLA	c	505	6	-	10/39/115/115	-
35	LMG	a	415	-	-	11/35/55/70	0/1/1/1
29	LHG	c	522	-	-	20/53/53/53	-
25	CLA	D	403	7	-	13/39/115/115	-
26	LUT	8	620	-	-	5/29/67/67	0/2/2/2
25	CLA	1	603	1	1/1/13/20	11/27/103/115	-
25	CLA	S	604	-	1/1/12/20	6/21/97/115	-
29	LHG	C	2630	-	-	27/53/53/53	-
25	CLA	b	615	5	1/1/15/20	14/39/115/115	-
35	LMG	d	411	-	-	15/41/61/70	0/1/1/1
25	CLA	b	611	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	SQD	b	623	-	-	18/37/57/69	0/1/1/1
25	CLA	c	510	6	1/1/15/20	16/39/115/115	-
25	CLA	N	611	29	1/1/14/20	9/33/109/115	-
24	CHL	Y	606	-	3/3/16/26	5/20/118/137	-
34	SQD	B	621	-	-	18/49/69/69	0/1/1/1
29	LHG	l	101	-	-	20/53/53/53	-
29	LHG	r	2630	25	-	15/46/46/53	-
25	CLA	7	602	2	1/1/14/20	15/33/109/115	-
30	BCR	h	101	-	-	3/29/63/63	0/2/2/2
25	CLA	G	612	1	1/1/14/20	12/33/109/115	-
25	CLA	b	608	-	1/1/15/20	12/39/115/115	-
25	CLA	d	403	7	-	13/39/115/115	-
27	XAT	Y	1622	-	-	3/31/93/93	0/4/4/4
36	PL9	d	405	-	-	8/53/73/73	0/1/1/1
25	CLA	4	602	3	1/1/11/20	4/15/91/115	-
30	BCR	c	515	-	-	6/29/63/63	0/2/2/2
24	CHL	5	601	1	3/3/16/26	6/15/113/137	-
28	NEX	y	1623	-	-	3/27/83/83	0/3/3/3
24	CHL	4	607	-	3/3/16/26	8/15/113/137	-
29	LHG	C	522	-	-	20/53/53/53	-
25	CLA	C	502	6	1/1/15/20	19/39/115/115	-
33	PHO	a	409	-	-	8/37/103/103	0/5/6/6
24	CHL	g	605	1	3/3/16/26	8/15/113/137	-
25	CLA	1	612	1	1/1/11/20	6/15/91/115	-
25	CLA	A	407	-	1/1/12/20	5/21/97/115	-
25	CLA	N	614	1	1/1/11/20	6/19/95/115	-
25	CLA	G	614	1	1/1/11/20	7/19/95/115	-
25	CLA	3	611	29	1/1/13/20	11/27/103/115	-
25	CLA	G	613	1	-	13/39/115/115	-
24	CHL	8	608	-	3/3/16/26	10/15/113/137	-
25	CLA	b	605	5	1/1/15/20	13/39/115/115	-
24	CHL	g	606	-	3/3/16/26	8/20/118/137	-
25	CLA	B	615	5	1/1/15/20	14/39/115/115	-
24	CHL	n	605	1	3/3/16/26	8/18/116/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	s	2630	25	-	24/53/53/53	-
24	CHL	2	605	1	3/3/16/26	8/15/113/137	-
29	LHG	1	2630	25	-	9/45/45/53	-
25	CLA	n	610	1	1/1/15/20	11/39/115/115	-
24	CHL	8	607	-	3/3/16/26	8/15/113/137	-
25	CLA	B	609	5	1/1/15/20	5/39/115/115	-
24	CHL	R	608	-	4/4/19/26	15/33/131/137	-
25	CLA	C	507	-	1/1/15/20	21/39/115/115	-
25	CLA	5	614	1	1/1/11/20	5/15/91/115	-
25	CLA	b	606	5	1/1/15/20	16/39/115/115	-
37	DGD	C	520	-	-	29/49/89/95	0/2/2/2
24	CHL	n	606	-	3/3/16/26	8/20/118/137	-
26	LUT	N	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	A	405	4	1/1/15/20	10/39/115/115	-
26	LUT	N	1621	-	-	1/29/67/67	0/2/2/2
25	CLA	c	513	6	-	13/39/115/115	-
24	CHL	R	607	-	4/4/18/26	8/27/125/137	-
27	XAT	5	1622	-	-	2/31/93/93	0/4/4/4
37	DGD	c	518	-	-	16/44/84/95	0/2/2/2
35	LMG	a	413	-	-	18/43/63/70	0/1/1/1
25	CLA	8	611	29	1/1/11/20	8/15/91/115	-
26	LUT	3	1620	-	-	1/29/67/67	0/2/2/2
25	CLA	c	503	6	1/1/15/20	11/39/115/115	-
26	LUT	6	1621	-	-	0/29/67/67	0/2/2/2
25	CLA	3	604	-	1/1/11/20	10/15/91/115	-
25	CLA	G	602	1	1/1/15/20	11/39/115/115	-
24	CHL	n	608	-	4/4/20/26	14/39/137/137	-
37	DGD	h	102	-	-	25/51/91/95	0/2/2/2
24	CHL	5	609	1	4/4/19/26	13/35/133/137	-
36	PL9	a	414	-	-	1/5/18/73	0/1/1/1
25	CLA	r	613	17	1/1/14/20	11/33/109/115	-
28	NEX	N	1623	-	-	5/27/83/83	0/3/3/3
25	CLA	S	611	29	1/1/13/20	9/29/105/115	-
30	BCR	b	618	-	-	4/29/63/63	0/2/2/2
33	PHO	A	408	-	-	6/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	R	612	17	1/1/11/20	6/20/96/115	-
24	CHL	N	601	1	4/4/20/26	19/39/137/137	-
25	CLA	N	604	-	1/1/12/20	3/21/97/115	-
28	NEX	R	623	-	-	4/27/83/83	0/3/3/3
24	CHL	G	606	-	3/3/16/26	8/20/118/137	-
25	CLA	1	602	1	1/1/14/20	10/35/111/115	-
24	CHL	2	606	-	3/3/16/26	5/15/113/137	-
35	LMG	B	622	-	-	23/46/66/70	0/1/1/1
25	CLA	N	610	1	1/1/15/20	11/39/115/115	-
25	CLA	8	610	3	1/1/11/20	6/15/91/115	-
25	CLA	y	602	1	1/1/15/20	13/39/115/115	-
25	CLA	r	604	-	1/1/11/20	4/19/95/115	-
25	CLA	6	602	1	1/1/14/20	13/35/111/115	-
36	PL9	A	414	-	-	1/5/18/73	0/1/1/1
26	LUT	7	1620	-	-	1/29/67/67	0/2/2/2
25	CLA	R	610	17	1/1/15/20	14/39/115/115	-
24	CHL	6	601	1	3/3/16/26	6/15/113/137	-
25	CLA	b	603	5	1/1/15/20	12/39/115/115	-
25	CLA	G	604	-	-	7/21/97/115	-
25	CLA	1	604	-	1/1/12/20	10/21/97/115	-
25	CLA	Y	614	1	1/1/11/20	5/19/95/115	-
30	BCR	C	516	-	-	9/29/63/63	0/2/2/2
24	CHL	7	601	2	4/4/19/26	12/37/135/137	-
34	SQD	B	623	-	-	18/37/57/69	0/1/1/1
25	CLA	Y	613	1	1/1/15/20	10/39/115/115	-
26	LUT	7	1621	-	-	3/29/67/67	0/2/2/2
25	CLA	n	613	1	1/1/14/20	7/33/109/115	-
25	CLA	g	613	1	-	13/39/115/115	-
24	CHL	Y	609	1	4/4/20/26	14/39/137/137	-
25	CLA	c	502	6	1/1/15/20	19/39/115/115	-
28	NEX	6	1623	-	-	4/27/83/83	0/3/3/3
37	DGD	c	520	-	-	29/49/89/95	0/2/2/2
25	CLA	4	603	3	1/1/11/20	6/15/91/115	-
25	CLA	S	602	18	1/1/14/20	15/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	n	2630	25	-	24/53/53/53	-
25	CLA	n	612	1	1/1/14/20	10/33/109/115	-
25	CLA	a	410	4	1/1/14/20	9/33/109/115	-
24	CHL	N	608	-	4/4/20/26	14/39/137/137	-
24	CHL	8	609	3	3/3/16/26	6/15/113/137	-
25	CLA	Y	602	1	1/1/15/20	14/39/115/115	-
34	SQD	A	418	-	-	21/49/69/69	0/1/1/1
29	LHG	2	2630	25	-	14/41/41/53	-
25	CLA	5	613	1	-	8/27/103/115	-
35	LMG	B	2633	-	-	21/50/70/70	0/1/1/1
35	LMG	A	415	-	-	11/35/55/70	0/1/1/1
25	CLA	B	613	5	1/1/15/20	14/39/115/115	-
25	CLA	2	604	-	-	7/15/91/115	-
25	CLA	8	603	3	1/1/11/20	6/15/91/115	-
27	XAT	3	1622	-	-	1/31/93/93	0/4/4/4
25	CLA	C	508	6	1/1/15/20	8/39/115/115	-
35	LMG	z	101	-	-	22/46/66/70	0/1/1/1
26	LUT	G	1621	-	-	1/29/67/67	0/2/2/2
25	CLA	6	603	1	1/1/13/20	14/27/103/115	-
27	XAT	4	622	-	-	2/31/93/93	0/4/4/4
25	CLA	c	504	-	1/1/15/20	11/39/115/115	-
25	CLA	C	501	6	1/1/15/20	12/39/115/115	-
25	CLA	R	603	17	1/1/14/20	13/33/109/115	-
29	LHG	5	2630	25	-	9/45/45/53	-
25	CLA	s	602	18	1/1/14/20	15/35/111/115	-
26	LUT	r	620	-	-	2/29/67/67	0/2/2/2
25	CLA	s	614	18	1/1/11/20	5/20/96/115	-
37	DGD	B	626	-	-	22/48/88/95	0/2/2/2
28	NEX	g	1623	-	-	6/27/83/83	0/3/3/3
25	CLA	5	604	-	1/1/12/20	10/21/97/115	-
25	CLA	n	602	1	1/1/15/20	13/39/115/115	-
29	LHG	g	2630	25	-	25/53/53/53	-
25	CLA	g	603	1	1/1/15/20	10/39/115/115	-
25	CLA	r	601	17	1/1/11/20	9/20/96/115	-
27	XAT	7	1622	-	-	1/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	4	623	-	-	11/29/63/63	0/2/2/2
25	CLA	r	611	29	1/1/11/20	11/20/96/115	-
29	LHG	c	2630	-	-	27/53/53/53	-
24	CHL	7	605	2	3/3/16/26	9/15/113/137	-
25	CLA	3	602	2	1/1/14/20	15/33/109/115	-
25	CLA	C	504	-	1/1/15/20	11/39/115/115	-
25	CLA	a	407	-	1/1/12/20	5/21/97/115	-
30	BCR	B	618	-	-	4/29/63/63	0/2/2/2
25	CLA	B	607	5	1/1/15/20	12/39/115/115	-

All (4058) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	601	CHL	C2C-C3C	10.88	1.46	1.36
24	S	608	CHL	C2C-C3C	10.86	1.46	1.36
24	s	608	CHL	C2C-C3C	10.84	1.46	1.36
24	8	601	CHL	C2C-C3C	10.83	1.46	1.36
24	2	605	CHL	C2C-C3C	10.60	1.46	1.36
24	6	605	CHL	C2C-C3C	10.58	1.46	1.36
24	3	608	CHL	C2C-C3C	10.42	1.46	1.36
24	6	608	CHL	C2C-C3C	10.41	1.46	1.36
24	2	608	CHL	C2C-C3C	10.39	1.46	1.36
24	7	608	CHL	C2C-C3C	10.38	1.46	1.36
24	3	609	CHL	C2C-C3C	10.33	1.46	1.36
24	7	609	CHL	C2C-C3C	10.31	1.46	1.36
24	4	606	CHL	C2C-C3C	10.29	1.46	1.36
24	8	606	CHL	C2C-C3C	10.27	1.46	1.36
24	2	606	CHL	C2C-C3C	10.26	1.46	1.36
24	s	606	CHL	C2C-C3C	10.26	1.46	1.36
24	6	607	CHL	C2C-C3C	10.25	1.46	1.36
24	r	606	CHL	C2C-C3C	10.25	1.46	1.36
24	S	606	CHL	C2C-C3C	10.24	1.46	1.36
24	2	607	CHL	C2C-C3C	10.22	1.46	1.36
24	6	606	CHL	C2C-C3C	10.22	1.46	1.36
24	R	606	CHL	C2C-C3C	10.17	1.46	1.36
24	7	605	CHL	C2C-C3C	10.11	1.46	1.36
24	r	614	CHL	C1D-C2D	10.10	1.51	1.39
24	3	605	CHL	C2C-C3C	10.06	1.46	1.36
24	R	614	CHL	C1D-C2D	10.05	1.51	1.39
24	s	606	CHL	C1D-C2D	10.02	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	609	CHL	C2C-C3C	10.01	1.46	1.36
24	1	605	CHL	C2C-C3C	10.00	1.46	1.36
24	1	609	CHL	C2C-C3C	10.00	1.46	1.36
24	S	606	CHL	C1D-C2D	9.99	1.50	1.39
24	1	606	CHL	C2C-C3C	9.98	1.46	1.36
24	s	608	CHL	C1D-C2D	9.97	1.50	1.39
24	r	614	CHL	C2C-C3C	9.97	1.46	1.36
24	S	608	CHL	C1D-C2D	9.97	1.50	1.39
24	5	605	CHL	C2C-C3C	9.97	1.46	1.36
24	R	614	CHL	C2C-C3C	9.96	1.46	1.36
24	G	605	CHL	C2C-C3C	9.95	1.46	1.36
24	g	605	CHL	C2C-C3C	9.93	1.46	1.36
24	5	606	CHL	C2C-C3C	9.87	1.45	1.36
24	g	609	CHL	C2C-C3C	9.87	1.45	1.36
24	G	609	CHL	C2C-C3C	9.84	1.45	1.36
24	g	608	CHL	C2C-C3C	9.83	1.45	1.36
24	s	607	CHL	C2C-C3C	9.81	1.45	1.36
24	G	608	CHL	C2C-C3C	9.80	1.45	1.36
24	2	601	CHL	C2C-C3C	9.79	1.45	1.36
24	S	607	CHL	C2C-C3C	9.79	1.45	1.36
24	5	608	CHL	C2C-C3C	9.78	1.45	1.36
24	1	608	CHL	C2C-C3C	9.77	1.45	1.36
24	S	601	CHL	C2C-C3C	9.74	1.45	1.36
24	8	601	CHL	C1D-C2D	9.74	1.50	1.39
24	s	601	CHL	C1D-C2D	9.73	1.50	1.39
24	S	601	CHL	C1D-C2D	9.72	1.50	1.39
24	6	601	CHL	C2C-C3C	9.72	1.45	1.36
24	s	601	CHL	C2C-C3C	9.72	1.45	1.36
24	R	607	CHL	C2C-C3C	9.71	1.45	1.36
24	r	607	CHL	C2C-C3C	9.71	1.45	1.36
24	4	601	CHL	C1D-C2D	9.71	1.50	1.39
24	4	607	CHL	C2C-C3C	9.70	1.45	1.36
24	5	607	CHL	C2C-C3C	9.69	1.45	1.36
24	1	607	CHL	C2C-C3C	9.68	1.45	1.36
24	6	601	CHL	C1D-C2D	9.68	1.50	1.39
24	7	606	CHL	C2C-C3C	9.67	1.45	1.36
24	8	607	CHL	C2C-C3C	9.66	1.45	1.36
24	n	605	CHL	C2C-C3C	9.65	1.45	1.36
24	N	605	CHL	C2C-C3C	9.65	1.45	1.36
24	5	607	CHL	C1D-C2D	9.65	1.50	1.39
24	3	606	CHL	C2C-C3C	9.64	1.45	1.36
24	2	601	CHL	C1D-C2D	9.63	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	605	CHL	C1D-C2D	9.62	1.50	1.39
24	1	607	CHL	C1D-C2D	9.60	1.50	1.39
24	5	609	CHL	C1D-C2D	9.59	1.50	1.39
24	1	609	CHL	C1D-C2D	9.58	1.50	1.39
24	g	605	CHL	C1D-C2D	9.58	1.50	1.39
24	G	606	CHL	C2C-C3C	9.57	1.45	1.36
24	g	606	CHL	C2C-C3C	9.54	1.45	1.36
24	R	607	CHL	C1D-C2D	9.54	1.50	1.39
24	4	609	CHL	C2C-C3C	9.52	1.45	1.36
24	r	607	CHL	C1D-C2D	9.52	1.50	1.39
24	n	607	CHL	C2C-C3C	9.51	1.45	1.36
24	7	609	CHL	C1D-C2D	9.49	1.50	1.39
24	N	601	CHL	C2C-C3C	9.49	1.45	1.36
24	8	609	CHL	C2C-C3C	9.47	1.45	1.36
24	6	609	CHL	C1D-C2D	9.46	1.50	1.39
24	N	607	CHL	C2C-C3C	9.45	1.45	1.36
24	Y	607	CHL	C2C-C3C	9.45	1.45	1.36
24	2	609	CHL	C1D-C2D	9.45	1.50	1.39
24	s	607	CHL	C1D-C2D	9.45	1.50	1.39
24	S	607	CHL	C1D-C2D	9.45	1.50	1.39
24	4	607	CHL	C1D-C2D	9.43	1.50	1.39
24	y	607	CHL	C2C-C3C	9.43	1.45	1.36
24	3	609	CHL	C1D-C2D	9.42	1.50	1.39
24	n	601	CHL	C2C-C3C	9.42	1.45	1.36
24	3	605	CHL	C1D-C2D	9.42	1.50	1.39
24	1	601	CHL	C2C-C3C	9.40	1.45	1.36
24	7	605	CHL	C1D-C2D	9.39	1.50	1.39
24	8	606	CHL	C1D-C2D	9.38	1.50	1.39
24	Y	605	CHL	C2C-C3C	9.38	1.45	1.36
24	5	601	CHL	C2C-C3C	9.36	1.45	1.36
24	y	605	CHL	C2C-C3C	9.36	1.45	1.36
24	1	601	CHL	C1D-C2D	9.35	1.50	1.39
24	8	607	CHL	C1D-C2D	9.35	1.50	1.39
24	n	609	CHL	C2C-C3C	9.34	1.45	1.36
24	N	609	CHL	C2C-C3C	9.33	1.45	1.36
24	8	609	CHL	C1D-C2D	9.33	1.50	1.39
24	5	601	CHL	C1D-C2D	9.33	1.50	1.39
24	y	608	CHL	C2C-C3C	9.33	1.45	1.36
24	N	601	CHL	C1D-C2D	9.32	1.50	1.39
24	Y	608	CHL	C2C-C3C	9.32	1.45	1.36
24	4	606	CHL	C1D-C2D	9.31	1.50	1.39
24	n	601	CHL	C1D-C2D	9.30	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	608	CHL	C2C-C3C	9.29	1.45	1.36
24	4	609	CHL	C1D-C2D	9.29	1.50	1.39
24	N	608	CHL	C2C-C3C	9.27	1.45	1.36
24	g	608	CHL	C1D-C2D	9.27	1.50	1.39
24	G	608	CHL	C1D-C2D	9.25	1.50	1.39
24	G	606	CHL	C1D-C2D	9.25	1.50	1.39
24	6	608	CHL	C1D-C2D	9.24	1.50	1.39
24	N	609	CHL	C1D-C2D	9.24	1.50	1.39
24	g	606	CHL	C1D-C2D	9.24	1.50	1.39
24	2	609	CHL	C2C-C3C	9.23	1.45	1.36
24	6	609	CHL	C2C-C3C	9.23	1.45	1.36
24	n	609	CHL	C1D-C2D	9.22	1.50	1.39
24	2	608	CHL	C1D-C2D	9.22	1.50	1.39
24	3	607	CHL	C1D-C2D	9.22	1.50	1.39
24	r	606	CHL	C1D-C2D	9.20	1.50	1.39
24	6	605	CHL	C1D-C2D	9.20	1.50	1.39
24	G	601	CHL	C1D-C2D	9.19	1.50	1.39
24	g	607	CHL	C2C-C3C	9.18	1.45	1.36
24	2	605	CHL	C1D-C2D	9.18	1.50	1.39
24	Y	609	CHL	C2C-C3C	9.18	1.45	1.36
24	g	601	CHL	C1D-C2D	9.17	1.50	1.39
24	4	601	CHL	C1A-CHA	9.17	1.50	1.40
24	7	607	CHL	C2C-C3C	9.16	1.45	1.36
24	g	609	CHL	C1D-C2D	9.16	1.50	1.39
24	3	607	CHL	C2C-C3C	9.15	1.45	1.36
24	3	606	CHL	C1D-C2D	9.14	1.50	1.39
24	7	606	CHL	C1D-C2D	9.14	1.50	1.39
24	N	605	CHL	C1D-C2D	9.14	1.50	1.39
24	7	607	CHL	C1D-C2D	9.13	1.50	1.39
24	G	607	CHL	C2C-C3C	9.13	1.45	1.36
24	y	609	CHL	C2C-C3C	9.13	1.45	1.36
24	G	609	CHL	C1D-C2D	9.13	1.50	1.39
24	g	607	CHL	C1D-C2D	9.13	1.49	1.39
24	1	605	CHL	C1D-C2D	9.13	1.49	1.39
24	R	606	CHL	C1D-C2D	9.12	1.49	1.39
24	8	601	CHL	C1A-CHA	9.11	1.50	1.40
24	7	601	CHL	C1D-C2D	9.10	1.49	1.39
24	n	605	CHL	C1D-C2D	9.10	1.49	1.39
24	s	607	CHL	C1A-CHA	9.08	1.50	1.40
24	Y	605	CHL	C1D-C2D	9.07	1.49	1.39
24	5	605	CHL	C1D-C2D	9.07	1.49	1.39
24	3	601	CHL	C1D-C2D	9.07	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	605	CHL	C1D-C2D	9.07	1.49	1.39
24	y	609	CHL	C1D-C2D	9.06	1.49	1.39
24	G	607	CHL	C1D-C2D	9.06	1.49	1.39
24	Y	609	CHL	C1D-C2D	9.06	1.49	1.39
24	Y	601	CHL	C1D-C2D	9.04	1.49	1.39
24	n	607	CHL	C1A-CHA	9.03	1.50	1.40
24	S	607	CHL	C1A-CHA	9.02	1.50	1.40
24	N	607	CHL	C1A-CHA	9.00	1.50	1.40
24	y	601	CHL	C1D-C2D	8.99	1.49	1.39
24	N	608	CHL	C1D-C2D	8.93	1.49	1.39
24	2	606	CHL	C1D-C2D	8.92	1.49	1.39
24	2	607	CHL	C1D-C2D	8.92	1.49	1.39
24	7	608	CHL	C1D-C2D	8.90	1.49	1.39
24	n	608	CHL	C1D-C2D	8.89	1.49	1.39
24	4	608	CHL	C2C-C3C	8.88	1.45	1.36
33	a	409	PHO	C1B-C2B	8.87	1.49	1.39
33	A	409	PHO	C1B-C2B	8.87	1.49	1.39
24	6	606	CHL	C1D-C2D	8.87	1.49	1.39
24	6	607	CHL	C1D-C2D	8.87	1.49	1.39
24	4	608	CHL	C1D-C2D	8.86	1.49	1.39
24	3	608	CHL	C1D-C2D	8.86	1.49	1.39
33	A	408	PHO	C1B-C2B	8.83	1.49	1.39
24	5	608	CHL	C1D-C2D	8.82	1.49	1.39
24	1	608	CHL	C1D-C2D	8.81	1.49	1.39
24	8	608	CHL	C1D-C2D	8.80	1.49	1.39
24	8	608	CHL	C2C-C3C	8.80	1.44	1.36
33	a	408	PHO	C1B-C2B	8.78	1.49	1.39
24	7	601	CHL	C2C-C3C	8.78	1.44	1.36
24	3	601	CHL	C2C-C3C	8.74	1.44	1.36
24	S	606	CHL	C3B-C4B	8.69	1.49	1.41
24	s	606	CHL	C3B-C4B	8.69	1.49	1.41
24	g	601	CHL	C2C-C3C	8.68	1.44	1.36
24	G	601	CHL	C2C-C3C	8.66	1.44	1.36
24	S	608	CHL	C1A-CHA	8.61	1.49	1.40
24	N	607	CHL	C1D-C2D	8.61	1.49	1.39
24	N	606	CHL	C1D-C2D	8.58	1.49	1.39
24	n	607	CHL	C1D-C2D	8.58	1.49	1.39
24	y	606	CHL	C2C-C3C	8.57	1.44	1.36
24	s	608	CHL	C1A-CHA	8.56	1.49	1.40
24	Y	606	CHL	C2C-C3C	8.55	1.44	1.36
24	n	606	CHL	C1D-C2D	8.55	1.49	1.39
24	s	607	CHL	C1B-C2B	8.54	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	606	CHL	C2C-C3C	8.53	1.44	1.36
24	n	606	CHL	C2C-C3C	8.52	1.44	1.36
24	S	607	CHL	C1B-C2B	8.52	1.49	1.39
24	S	608	CHL	C1B-C2B	8.50	1.49	1.39
24	s	608	CHL	C1B-C2B	8.49	1.49	1.39
24	1	606	CHL	C1D-C2D	8.48	1.49	1.39
24	r	608	CHL	C2C-C3C	8.48	1.44	1.36
24	R	608	CHL	C2C-C3C	8.46	1.44	1.36
24	5	606	CHL	C1D-C2D	8.45	1.49	1.39
24	y	607	CHL	C1A-CHA	8.44	1.49	1.40
24	Y	607	CHL	C1A-CHA	8.41	1.49	1.40
24	Y	601	CHL	C2C-C3C	8.40	1.44	1.36
24	y	601	CHL	C2C-C3C	8.40	1.44	1.36
24	Y	608	CHL	C1D-C2D	8.37	1.49	1.39
24	Y	607	CHL	C1D-C2D	8.36	1.49	1.39
24	y	608	CHL	C1D-C2D	8.31	1.49	1.39
24	y	607	CHL	C1D-C2D	8.30	1.49	1.39
24	s	606	CHL	C1A-CHA	8.30	1.49	1.40
24	S	606	CHL	C1A-CHA	8.28	1.49	1.40
24	g	605	CHL	C1B-C2B	8.26	1.48	1.39
24	G	605	CHL	C1B-C2B	8.24	1.48	1.39
24	8	601	CHL	C1B-C2B	8.23	1.48	1.39
24	4	601	CHL	C1B-C2B	8.21	1.48	1.39
24	r	614	CHL	C1B-C2B	8.20	1.48	1.39
24	2	605	CHL	C1B-C2B	8.19	1.48	1.39
33	a	409	PHO	C3B-C4B	8.18	1.49	1.41
33	A	409	PHO	C3B-C4B	8.17	1.49	1.41
24	6	605	CHL	C1B-C2B	8.16	1.48	1.39
24	2	608	CHL	C1B-C2B	8.15	1.48	1.39
24	6	608	CHL	C1B-C2B	8.15	1.48	1.39
24	R	614	CHL	C1B-C2B	8.15	1.48	1.39
24	3	607	CHL	C1A-CHA	8.14	1.49	1.40
24	g	608	CHL	C3B-C4B	8.14	1.49	1.41
24	2	607	CHL	C1B-C2B	8.14	1.48	1.39
24	7	607	CHL	C1A-CHA	8.13	1.49	1.40
24	G	608	CHL	C3B-C4B	8.12	1.49	1.41
24	r	608	CHL	C1D-C2D	8.11	1.48	1.39
24	6	607	CHL	C1B-C2B	8.10	1.48	1.39
24	1	605	CHL	C1B-C2B	8.09	1.48	1.39
33	A	408	PHO	C3B-C4B	8.08	1.49	1.41
24	n	605	CHL	C1A-CHA	8.07	1.49	1.40
24	R	608	CHL	C1D-C2D	8.06	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	605	CHL	C1B-C2B	8.06	1.48	1.39
24	N	605	CHL	C1A-CHA	8.06	1.49	1.40
24	g	607	CHL	C1A-CHA	8.05	1.49	1.40
33	a	408	PHO	C3B-C4B	8.04	1.49	1.41
24	N	608	CHL	C3B-C4B	8.03	1.49	1.41
24	8	608	CHL	C1B-C2B	8.03	1.48	1.39
24	R	608	CHL	C1A-CHA	8.00	1.49	1.40
24	4	608	CHL	C1B-C2B	8.00	1.48	1.39
24	G	607	CHL	C1A-CHA	8.00	1.49	1.40
24	n	608	CHL	C3B-C4B	7.98	1.49	1.41
24	S	606	CHL	C1B-C2B	7.96	1.48	1.39
24	r	608	CHL	C1A-CHA	7.96	1.49	1.40
24	3	605	CHL	C1B-C2B	7.95	1.48	1.39
24	s	606	CHL	C1B-C2B	7.95	1.48	1.39
24	7	605	CHL	C1B-C2B	7.94	1.48	1.39
24	1	601	CHL	C1B-C2B	7.92	1.48	1.39
24	5	601	CHL	C1B-C2B	7.91	1.48	1.39
24	Y	605	CHL	C1A-CHA	7.88	1.49	1.40
24	y	605	CHL	C1A-CHA	7.86	1.48	1.40
24	R	614	CHL	C1A-CHA	7.84	1.48	1.40
24	n	601	CHL	C3B-C4B	7.83	1.49	1.41
24	3	606	CHL	C3B-C4B	7.82	1.49	1.41
24	2	607	CHL	C1A-CHA	7.81	1.48	1.40
24	y	606	CHL	C1A-CHA	7.81	1.48	1.40
24	5	607	CHL	C1A-CHA	7.80	1.48	1.40
24	1	607	CHL	C1A-CHA	7.80	1.48	1.40
24	N	601	CHL	C3B-C4B	7.80	1.49	1.41
24	6	607	CHL	C1A-CHA	7.80	1.48	1.40
24	r	614	CHL	C1A-CHA	7.78	1.48	1.40
24	6	601	CHL	C1B-C2B	7.78	1.48	1.39
24	7	606	CHL	C3B-C4B	7.77	1.49	1.41
24	g	609	CHL	C1A-CHA	7.77	1.48	1.40
24	Y	606	CHL	C1A-CHA	7.76	1.48	1.40
24	G	601	CHL	C3B-C4B	7.76	1.48	1.41
24	G	609	CHL	C1A-CHA	7.75	1.48	1.40
24	7	607	CHL	C1B-C2B	7.75	1.48	1.39
24	g	601	CHL	C3B-C4B	7.74	1.48	1.41
24	2	601	CHL	C1B-C2B	7.73	1.48	1.39
24	3	607	CHL	C1B-C2B	7.72	1.48	1.39
24	G	608	CHL	C1B-C2B	7.70	1.48	1.39
24	g	608	CHL	C1A-CHA	7.70	1.48	1.40
24	2	608	CHL	C1A-CHA	7.69	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	607	CHL	C1B-C2B	7.69	1.48	1.39
24	G	605	CHL	C1A-CHA	7.68	1.48	1.40
24	6	608	CHL	C1A-CHA	7.68	1.48	1.40
24	S	601	CHL	C1B-C2B	7.68	1.48	1.39
24	g	607	CHL	C1B-C2B	7.67	1.48	1.39
24	n	608	CHL	C1A-CHA	7.67	1.48	1.40
24	s	601	CHL	C1B-C2B	7.66	1.48	1.39
24	N	608	CHL	C1A-CHA	7.65	1.48	1.40
24	g	605	CHL	C1A-CHA	7.65	1.48	1.40
24	n	607	CHL	C1B-C2B	7.65	1.48	1.39
24	n	605	CHL	C1B-C2B	7.64	1.48	1.39
24	N	607	CHL	C1B-C2B	7.64	1.48	1.39
24	G	608	CHL	C1A-CHA	7.64	1.48	1.40
24	r	607	CHL	C3B-C4B	7.64	1.48	1.41
24	8	609	CHL	C1B-C2B	7.64	1.48	1.39
24	y	601	CHL	C1B-C2B	7.64	1.48	1.39
24	g	608	CHL	C1B-C2B	7.63	1.48	1.39
24	Y	601	CHL	C1B-C2B	7.63	1.48	1.39
24	R	607	CHL	C1A-CHA	7.62	1.48	1.40
24	Y	605	CHL	C1B-C2B	7.62	1.48	1.39
24	N	605	CHL	C1B-C2B	7.61	1.48	1.39
24	y	608	CHL	C3B-C4B	7.61	1.48	1.41
24	R	607	CHL	C3B-C4B	7.61	1.48	1.41
24	8	607	CHL	C1B-C2B	7.61	1.48	1.39
24	4	607	CHL	C1B-C2B	7.60	1.48	1.39
24	4	609	CHL	C1B-C2B	7.60	1.48	1.39
24	r	607	CHL	C1A-CHA	7.60	1.48	1.40
24	N	601	CHL	C1B-C2B	7.59	1.48	1.39
24	n	601	CHL	C1B-C2B	7.59	1.48	1.39
24	Y	608	CHL	C3B-C4B	7.59	1.48	1.41
24	2	605	CHL	C1A-CHA	7.59	1.48	1.40
24	R	607	CHL	C1B-C2B	7.58	1.48	1.39
36	D	405	PL9	C3-C4	-7.58	1.37	1.49
36	d	405	PL9	C3-C4	-7.58	1.37	1.49
24	6	605	CHL	C1A-CHA	7.57	1.48	1.40
24	y	606	CHL	C1D-C2D	7.57	1.48	1.39
24	Y	606	CHL	C1D-C2D	7.57	1.48	1.39
24	y	605	CHL	C1B-C2B	7.57	1.48	1.39
24	1	608	CHL	C3B-C4B	7.54	1.48	1.41
24	6	601	CHL	C3B-C4B	7.54	1.48	1.41
24	6	606	CHL	C1A-CHA	7.54	1.48	1.40
24	4	609	CHL	C1A-CHA	7.53	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	601	CHL	C3B-C4B	7.53	1.48	1.41
24	8	609	CHL	C1A-CHA	7.52	1.48	1.40
24	7	601	CHL	C1B-C2B	7.52	1.48	1.39
24	8	606	CHL	C3B-C4B	7.52	1.48	1.41
24	5	608	CHL	C3B-C4B	7.51	1.48	1.41
24	3	601	CHL	C1B-C2B	7.51	1.48	1.39
24	3	607	CHL	C3B-C4B	7.51	1.48	1.41
24	r	607	CHL	C1B-C2B	7.50	1.48	1.39
24	4	606	CHL	C3B-C4B	7.50	1.48	1.41
24	7	607	CHL	C3B-C4B	7.50	1.48	1.41
24	2	606	CHL	C1A-CHA	7.49	1.48	1.40
24	5	606	CHL	C1A-CHA	7.49	1.48	1.40
24	S	601	CHL	C3B-C4B	7.49	1.48	1.41
24	4	601	CHL	C3B-C4B	7.48	1.48	1.41
24	Y	601	CHL	C3B-C4B	7.46	1.48	1.41
24	1	606	CHL	C1A-CHA	7.46	1.48	1.40
24	S	608	CHL	C3B-C4B	7.44	1.48	1.41
24	4	608	CHL	C3B-C4B	7.43	1.48	1.41
24	8	601	CHL	C3B-C4B	7.43	1.48	1.41
24	y	601	CHL	C3B-C4B	7.43	1.48	1.41
24	s	601	CHL	C3B-C4B	7.43	1.48	1.41
24	n	608	CHL	C1B-C2B	7.42	1.48	1.39
24	8	608	CHL	C3B-C4B	7.41	1.48	1.41
24	Y	606	CHL	C1B-C2B	7.39	1.48	1.39
24	N	608	CHL	C1B-C2B	7.39	1.48	1.39
24	R	608	CHL	C1B-C2B	7.39	1.48	1.39
24	r	608	CHL	C1B-C2B	7.39	1.48	1.39
24	y	606	CHL	C1B-C2B	7.37	1.47	1.39
24	y	608	CHL	C1A-CHA	7.37	1.48	1.40
24	Y	608	CHL	C1A-CHA	7.36	1.48	1.40
24	s	608	CHL	C3B-C4B	7.36	1.48	1.41
24	3	609	CHL	C1B-C2B	7.35	1.47	1.39
24	S	607	CHL	C3B-C4B	7.33	1.48	1.41
24	7	609	CHL	C1B-C2B	7.32	1.47	1.39
24	3	605	CHL	C1A-CHA	7.31	1.48	1.40
24	N	605	CHL	C3B-C4B	7.31	1.48	1.41
24	7	605	CHL	C1A-CHA	7.31	1.48	1.40
24	2	609	CHL	C1A-CHA	7.30	1.48	1.40
24	8	606	CHL	C1A-CHA	7.27	1.48	1.40
24	4	607	CHL	C1A-CHA	7.26	1.48	1.40
24	s	607	CHL	C3B-C4B	7.25	1.48	1.41
24	4	606	CHL	C1B-C2B	7.24	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	609	CHL	C1A-CHA	7.24	1.48	1.40
24	n	605	CHL	C3B-C4B	7.23	1.48	1.41
24	y	609	CHL	C3B-C4B	7.23	1.48	1.41
24	8	607	CHL	C1A-CHA	7.23	1.48	1.40
24	4	606	CHL	C1A-CHA	7.22	1.48	1.40
24	5	607	CHL	C3B-C4B	7.22	1.48	1.41
24	y	608	CHL	C1B-C2B	7.22	1.47	1.39
24	Y	608	CHL	C1B-C2B	7.21	1.47	1.39
24	8	606	CHL	C1B-C2B	7.21	1.47	1.39
24	g	609	CHL	C1B-C2B	7.20	1.47	1.39
24	r	606	CHL	C1A-CHA	7.19	1.48	1.40
24	1	607	CHL	C3B-C4B	7.19	1.48	1.41
24	G	601	CHL	C1B-C2B	7.18	1.47	1.39
24	G	606	CHL	C1A-CHA	7.18	1.48	1.40
24	G	609	CHL	C1B-C2B	7.17	1.47	1.39
24	g	606	CHL	C1A-CHA	7.16	1.48	1.40
24	Y	609	CHL	C3B-C4B	7.15	1.48	1.41
24	R	606	CHL	C1A-CHA	7.15	1.48	1.40
24	R	606	CHL	C3B-C4B	7.15	1.48	1.41
24	5	607	CHL	C1B-C2B	7.15	1.47	1.39
24	g	601	CHL	C1B-C2B	7.14	1.47	1.39
24	r	606	CHL	C3B-C4B	7.13	1.48	1.41
24	S	601	CHL	C1A-CHA	7.13	1.48	1.40
24	3	608	CHL	C1B-C2B	7.12	1.47	1.39
24	n	606	CHL	C1A-CHA	7.12	1.48	1.40
24	1	607	CHL	C1B-C2B	7.11	1.47	1.39
24	7	608	CHL	C1B-C2B	7.11	1.47	1.39
24	7	606	CHL	C1B-C2B	7.10	1.47	1.39
24	Y	609	CHL	C1A-CHA	7.09	1.48	1.40
24	s	601	CHL	C1A-CHA	7.09	1.48	1.40
24	y	609	CHL	C1A-CHA	7.07	1.48	1.40
24	N	606	CHL	C1A-CHA	7.07	1.48	1.40
24	7	608	CHL	C1A-CHA	7.06	1.48	1.40
24	g	607	CHL	C3B-C4B	7.06	1.48	1.41
24	3	606	CHL	C1B-C2B	7.06	1.47	1.39
24	4	607	CHL	C3B-C4B	7.06	1.48	1.41
24	3	608	CHL	C1A-CHA	7.05	1.48	1.40
24	2	606	CHL	C1B-C2B	7.05	1.47	1.39
24	6	606	CHL	C1B-C2B	7.03	1.47	1.39
24	8	607	CHL	C3B-C4B	7.03	1.48	1.41
24	4	608	CHL	C1A-CHA	7.02	1.48	1.40
24	5	605	CHL	C1A-CHA	7.02	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	609	CHL	C1A-CHA	7.00	1.48	1.40
24	8	608	CHL	C1A-CHA	6.99	1.48	1.40
24	G	607	CHL	C3B-C4B	6.98	1.48	1.41
24	3	609	CHL	C1A-CHA	6.98	1.47	1.40
24	5	609	CHL	C1A-CHA	6.96	1.47	1.40
24	N	609	CHL	C1A-CHA	6.96	1.47	1.40
24	1	609	CHL	C1A-CHA	6.95	1.47	1.40
24	n	609	CHL	C1A-CHA	6.94	1.47	1.40
24	y	607	CHL	C1B-C2B	6.94	1.47	1.39
24	Y	607	CHL	C1B-C2B	6.93	1.47	1.39
24	1	605	CHL	C1A-CHA	6.92	1.47	1.40
24	6	605	CHL	C3B-C4B	6.90	1.48	1.41
24	2	605	CHL	C3B-C4B	6.89	1.48	1.41
24	7	605	CHL	C3B-C4B	6.89	1.48	1.41
24	R	606	CHL	C1B-C2B	6.88	1.47	1.39
24	Y	601	CHL	C3D-C4D	-6.87	1.31	1.41
24	r	606	CHL	C1B-C2B	6.87	1.47	1.39
24	7	609	CHL	C3B-C4B	6.87	1.48	1.41
24	y	601	CHL	C3D-C4D	-6.86	1.31	1.41
24	3	605	CHL	C3B-C4B	6.86	1.48	1.41
24	1	608	CHL	C1A-CHA	6.85	1.47	1.40
24	3	609	CHL	C3B-C4B	6.83	1.48	1.41
24	1	606	CHL	C1B-C2B	6.82	1.47	1.39
24	5	608	CHL	C1A-CHA	6.80	1.47	1.40
24	G	605	CHL	C3B-C4B	6.80	1.48	1.41
24	n	609	CHL	C3A-C2A	-6.79	1.48	1.54
24	2	609	CHL	C1B-C2B	6.79	1.47	1.39
24	6	609	CHL	C1B-C2B	6.78	1.47	1.39
24	Y	609	CHL	C1B-C2B	6.78	1.47	1.39
24	5	606	CHL	C1B-C2B	6.77	1.47	1.39
24	y	609	CHL	C1B-C2B	6.76	1.47	1.39
24	G	601	CHL	C1A-CHA	6.76	1.47	1.40
24	g	601	CHL	C1A-CHA	6.75	1.47	1.40
24	g	605	CHL	C3B-C4B	6.75	1.48	1.41
24	7	601	CHL	C1A-CHA	6.75	1.47	1.40
24	N	609	CHL	C3A-C2A	-6.73	1.48	1.54
24	6	601	CHL	C1A-CHA	6.73	1.47	1.40
24	2	601	CHL	C1A-CHA	6.73	1.47	1.40
24	R	614	CHL	C3B-C4B	6.72	1.47	1.41
24	3	601	CHL	C1A-CHA	6.69	1.47	1.40
24	7	606	CHL	C3D-C4D	-6.67	1.31	1.41
24	g	609	CHL	C3B-C4B	6.66	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	608	CHL	C3B-C4B	6.64	1.47	1.41
24	r	614	CHL	C3B-C4B	6.64	1.47	1.41
24	2	601	CHL	C3A-C2A	-6.63	1.49	1.54
24	r	608	CHL	C3B-C4B	6.63	1.47	1.41
24	3	606	CHL	C3D-C4D	-6.62	1.31	1.41
24	G	609	CHL	C3B-C4B	6.62	1.47	1.41
24	Y	609	CHL	C3D-C4D	-6.62	1.31	1.41
24	N	601	CHL	C1A-CHA	6.62	1.47	1.40
24	n	601	CHL	C1A-CHA	6.62	1.47	1.40
24	1	601	CHL	C3D-C4D	-6.62	1.31	1.41
24	5	601	CHL	C1A-CHA	6.61	1.47	1.40
24	y	609	CHL	C3D-C4D	-6.60	1.31	1.41
24	y	605	CHL	C3B-C4B	6.60	1.47	1.41
24	3	601	CHL	C3D-C4D	-6.59	1.31	1.41
24	7	608	CHL	C3B-C4B	6.58	1.47	1.41
24	7	601	CHL	C3D-C4D	-6.58	1.31	1.41
24	5	601	CHL	C3D-C4D	-6.57	1.31	1.41
24	1	605	CHL	C3B-C4B	6.57	1.47	1.41
24	Y	605	CHL	C3B-C4B	6.57	1.47	1.41
24	5	608	CHL	C3D-C4D	-6.55	1.31	1.41
24	g	601	CHL	C3D-C4D	-6.54	1.31	1.41
24	3	608	CHL	C3B-C4B	6.54	1.47	1.41
24	G	601	CHL	C3D-C4D	-6.54	1.31	1.41
24	1	601	CHL	C1A-CHA	6.54	1.47	1.40
24	6	601	CHL	C3A-C2A	-6.54	1.49	1.54
24	5	605	CHL	C3B-C4B	6.53	1.47	1.41
24	1	608	CHL	C3D-C4D	-6.53	1.31	1.41
24	G	606	CHL	C1B-C2B	6.53	1.47	1.39
24	g	606	CHL	C1B-C2B	6.52	1.47	1.39
24	n	606	CHL	C1B-C2B	6.52	1.47	1.39
24	1	607	CHL	C3A-C2A	-6.51	1.49	1.54
24	5	609	CHL	C3D-C4D	-6.50	1.31	1.41
24	1	609	CHL	C3D-C4D	-6.49	1.31	1.41
24	N	606	CHL	C1B-C2B	6.47	1.46	1.39
24	n	608	CHL	C3D-C4D	-6.45	1.31	1.41
24	n	606	CHL	C3D-C4D	-6.43	1.31	1.41
24	7	606	CHL	C1A-CHA	6.41	1.47	1.40
24	5	607	CHL	C3A-C2A	-6.41	1.49	1.54
24	N	608	CHL	C3D-C4D	-6.41	1.31	1.41
24	N	606	CHL	C3D-C4D	-6.40	1.31	1.41
24	4	608	CHL	C3A-C2A	-6.40	1.49	1.54
24	8	608	CHL	C3A-C2A	-6.40	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	608	CHL	C3D-C4D	-6.38	1.31	1.41
24	4	608	CHL	C3D-C4D	-6.37	1.31	1.41
24	y	608	CHL	C3D-C4D	-6.37	1.31	1.41
24	3	606	CHL	C3A-C2A	-6.36	1.49	1.54
24	3	606	CHL	C1A-CHA	6.35	1.47	1.40
24	y	606	CHL	C3D-C4D	-6.34	1.31	1.41
24	Y	608	CHL	C3D-C4D	-6.33	1.31	1.41
24	6	608	CHL	C3B-C4B	6.33	1.47	1.41
24	7	606	CHL	C3A-C2A	-6.32	1.49	1.54
24	y	607	CHL	C3B-C4B	6.32	1.47	1.41
24	n	609	CHL	C1B-C2B	6.32	1.46	1.39
24	Y	606	CHL	C3D-C4D	-6.32	1.31	1.41
24	n	601	CHL	C3D-C4D	-6.31	1.31	1.41
24	n	609	CHL	C3D-C4D	-6.31	1.31	1.41
24	N	609	CHL	C3B-C4B	6.30	1.47	1.41
24	Y	607	CHL	C3B-C4B	6.30	1.47	1.41
24	N	609	CHL	C3D-C4D	-6.30	1.31	1.41
24	N	601	CHL	C3D-C4D	-6.30	1.31	1.41
24	N	609	CHL	C1B-C2B	6.30	1.46	1.39
24	n	609	CHL	C3B-C4B	6.29	1.47	1.41
24	5	608	CHL	C1B-C2B	6.29	1.46	1.39
24	1	608	CHL	C3A-C2A	-6.28	1.49	1.54
24	R	608	CHL	C3D-C4D	-6.28	1.31	1.41
24	r	608	CHL	C3D-C4D	-6.28	1.32	1.41
24	5	608	CHL	C3A-C2A	-6.27	1.49	1.54
24	G	606	CHL	C3B-C4B	6.25	1.47	1.41
24	6	609	CHL	C3B-C4B	6.24	1.47	1.41
24	6	601	CHL	C3D-C4D	-6.24	1.32	1.41
24	2	601	CHL	C3D-C4D	-6.24	1.32	1.41
24	2	608	CHL	C3B-C4B	6.23	1.47	1.41
24	1	608	CHL	C1B-C2B	6.23	1.46	1.39
24	6	609	CHL	C3A-C2A	-6.22	1.49	1.54
24	3	609	CHL	C3D-C4D	-6.21	1.32	1.41
24	5	601	CHL	C3B-C4B	6.20	1.47	1.41
24	2	607	CHL	C3B-C4B	6.20	1.47	1.41
24	4	606	CHL	C3A-C2A	-6.20	1.49	1.54
24	5	609	CHL	C1B-C2B	6.19	1.46	1.39
24	3	601	CHL	C3B-C4B	6.19	1.47	1.41
24	g	606	CHL	C3B-C4B	6.19	1.47	1.41
24	1	609	CHL	C1B-C2B	6.18	1.46	1.39
24	8	609	CHL	C3B-C4B	6.17	1.47	1.41
24	7	609	CHL	C3D-C4D	-6.17	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	606	CHL	C3A-C2A	-6.16	1.49	1.54
24	1	601	CHL	C3B-C4B	6.16	1.47	1.41
24	2	609	CHL	C3B-C4B	6.16	1.47	1.41
24	4	609	CHL	C3B-C4B	6.16	1.47	1.41
24	6	607	CHL	C3B-C4B	6.15	1.47	1.41
24	R	606	CHL	C3A-C2A	-6.14	1.49	1.54
24	g	609	CHL	C3D-C4D	-6.14	1.32	1.41
24	7	601	CHL	C3B-C4B	6.14	1.47	1.41
24	2	609	CHL	C3A-C2A	-6.13	1.49	1.54
24	5	609	CHL	C3A-C2A	-6.13	1.49	1.54
24	G	609	CHL	C3D-C4D	-6.13	1.32	1.41
24	1	606	CHL	C3D-C4D	-6.12	1.32	1.41
24	1	609	CHL	C3A-C2A	-6.12	1.49	1.54
24	Y	601	CHL	C1A-CHA	6.11	1.46	1.40
24	G	608	CHL	C3D-C4D	-6.10	1.32	1.41
24	5	605	CHL	C3D-C4D	-6.10	1.32	1.41
24	y	601	CHL	C1A-CHA	6.10	1.46	1.40
24	5	606	CHL	C3D-C4D	-6.09	1.32	1.41
24	3	608	CHL	C3D-C4D	-6.08	1.32	1.41
24	2	607	CHL	C3D-C4D	-6.08	1.32	1.41
24	g	608	CHL	C3D-C4D	-6.08	1.32	1.41
24	7	608	CHL	C3D-C4D	-6.07	1.32	1.41
24	r	606	CHL	C3A-C2A	-6.06	1.49	1.54
24	g	606	CHL	C3D-C4D	-6.06	1.32	1.41
24	6	607	CHL	C3D-C4D	-6.06	1.32	1.41
24	N	607	CHL	C3B-C4B	6.05	1.47	1.41
24	G	606	CHL	C3D-C4D	-6.05	1.32	1.41
24	2	609	CHL	C3D-C4D	-6.05	1.32	1.41
24	1	605	CHL	C3D-C4D	-6.05	1.32	1.41
24	1	609	CHL	C3B-C4B	6.04	1.47	1.41
24	6	609	CHL	C3D-C4D	-6.04	1.32	1.41
24	r	606	CHL	C3D-C4D	-6.04	1.32	1.41
24	n	606	CHL	C3A-C2A	-6.03	1.49	1.54
24	n	607	CHL	C3B-C4B	6.02	1.47	1.41
24	y	607	CHL	C3D-C4D	-6.02	1.32	1.41
24	g	609	CHL	C3A-C2A	-6.02	1.49	1.54
24	1	606	CHL	C3B-C4B	6.02	1.47	1.41
24	7	607	CHL	C3D-C4D	-6.02	1.32	1.41
24	6	606	CHL	C3B-C4B	6.02	1.47	1.41
24	5	609	CHL	C3B-C4B	6.01	1.47	1.41
24	2	606	CHL	C3B-C4B	6.01	1.47	1.41
24	1	607	CHL	C3D-C4D	-6.01	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	609	CHL	C3A-C2A	-6.00	1.49	1.54
24	Y	607	CHL	C3D-C4D	-6.00	1.32	1.41
24	G	609	CHL	C3A-C2A	-6.00	1.49	1.54
24	Y	607	CHL	C3A-C2A	-6.00	1.49	1.54
24	R	606	CHL	C3D-C4D	-5.99	1.32	1.41
24	Y	609	CHL	C3A-C2A	-5.99	1.49	1.54
24	5	606	CHL	C3B-C4B	5.99	1.47	1.41
24	N	606	CHL	C3A-C2A	-5.97	1.49	1.54
24	8	609	CHL	C3D-C4D	-5.96	1.32	1.41
24	3	607	CHL	C3D-C4D	-5.96	1.32	1.41
24	5	607	CHL	C3D-C4D	-5.96	1.32	1.41
24	y	607	CHL	C3A-C2A	-5.95	1.49	1.54
24	r	607	CHL	C3D-C4D	-5.95	1.32	1.41
24	R	607	CHL	C3D-C4D	-5.95	1.32	1.41
24	Y	605	CHL	C3D-C4D	-5.95	1.32	1.41
24	y	606	CHL	C3A-C2A	-5.95	1.49	1.54
24	N	608	CHL	C3A-C2A	-5.94	1.49	1.54
24	Y	606	CHL	C3A-C2A	-5.93	1.49	1.54
24	y	605	CHL	C3D-C4D	-5.93	1.32	1.41
24	4	609	CHL	C3D-C4D	-5.92	1.32	1.41
24	6	606	CHL	C3A-C2A	-5.91	1.49	1.54
24	n	608	CHL	C3A-C2A	-5.90	1.49	1.54
24	N	605	CHL	C3D-C4D	-5.90	1.32	1.41
24	n	605	CHL	C3D-C4D	-5.88	1.32	1.41
24	2	606	CHL	C3D-C4D	-5.88	1.32	1.41
24	4	609	CHL	C3A-C2A	-5.86	1.49	1.54
24	6	608	CHL	C3A-C2A	-5.86	1.49	1.54
24	6	606	CHL	C3D-C4D	-5.84	1.32	1.41
24	8	607	CHL	C3D-C4D	-5.84	1.32	1.41
24	4	606	CHL	C3D-C4D	-5.84	1.32	1.41
24	2	608	CHL	C3A-C2A	-5.84	1.49	1.54
24	8	606	CHL	C3D-C4D	-5.84	1.32	1.41
24	4	607	CHL	C3D-C4D	-5.84	1.32	1.41
24	2	606	CHL	C3A-C2A	-5.83	1.49	1.54
24	8	609	CHL	C3A-C2A	-5.82	1.49	1.54
24	R	614	CHL	C3D-C4D	-5.81	1.32	1.41
24	5	609	CHL	CHB-C4A	-5.80	1.31	1.38
24	7	605	CHL	C3D-C4D	-5.80	1.32	1.41
24	g	607	CHL	C3D-C4D	-5.80	1.32	1.41
24	1	609	CHL	CHB-C4A	-5.79	1.31	1.38
24	6	608	CHL	C3D-C4D	-5.79	1.32	1.41
24	r	614	CHL	C3D-C4D	-5.79	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	608	CHL	C3D-C4D	-5.77	1.32	1.41
24	g	606	CHL	C3A-C2A	-5.77	1.49	1.54
24	R	608	CHL	C3A-C2A	-5.76	1.49	1.54
24	G	607	CHL	C3D-C4D	-5.76	1.32	1.41
24	n	607	CHL	C3A-C2A	-5.75	1.49	1.54
24	3	608	CHL	C3A-C2A	-5.75	1.49	1.54
24	N	607	CHL	C3A-C2A	-5.75	1.49	1.54
24	7	606	CHL	CHB-C4A	-5.75	1.31	1.38
24	3	605	CHL	C3D-C4D	-5.75	1.32	1.41
24	s	601	CHL	C3D-C4D	-5.75	1.32	1.41
24	S	601	CHL	C3D-C4D	-5.74	1.32	1.41
24	3	606	CHL	CHB-C4A	-5.73	1.31	1.38
24	r	608	CHL	C3A-C2A	-5.73	1.49	1.54
24	G	606	CHL	C3A-C2A	-5.72	1.49	1.54
24	7	608	CHL	C3A-C2A	-5.72	1.49	1.54
24	g	607	CHL	C3A-C2A	-5.71	1.49	1.54
24	N	609	CHL	CHB-C4A	-5.70	1.31	1.38
24	y	601	CHL	C3A-C2A	-5.70	1.49	1.54
24	n	609	CHL	CHB-C4A	-5.70	1.31	1.38
36	D	405	PL9	C6-C1	-5.70	1.39	1.48
24	Y	601	CHL	C3A-C2A	-5.70	1.49	1.54
36	d	405	PL9	C6-C1	-5.69	1.39	1.48
24	G	607	CHL	C3A-C2A	-5.68	1.49	1.54
24	3	605	CHL	C3A-C2A	-5.68	1.49	1.54
24	g	605	CHL	C3D-C4D	-5.67	1.32	1.41
24	Y	606	CHL	C3B-C4B	5.66	1.46	1.41
24	Y	608	CHL	C3A-C2A	-5.66	1.49	1.54
24	7	605	CHL	C3A-C2A	-5.66	1.49	1.54
24	y	606	CHL	C3B-C4B	5.65	1.46	1.41
24	y	608	CHL	C3A-C2A	-5.65	1.49	1.54
24	G	605	CHL	C3D-C4D	-5.65	1.32	1.41
24	N	607	CHL	C3D-C4D	-5.62	1.33	1.41
24	6	605	CHL	C3D-C4D	-5.61	1.33	1.41
24	n	607	CHL	C3D-C4D	-5.60	1.33	1.41
24	1	606	CHL	C3A-C2A	-5.60	1.49	1.54
24	2	605	CHL	C3D-C4D	-5.59	1.33	1.41
24	5	608	CHL	CHB-C4A	-5.58	1.31	1.38
24	2	607	CHL	C3A-C2A	-5.57	1.49	1.54
24	1	601	CHL	C3A-C2A	-5.57	1.49	1.54
24	3	601	CHL	C3A-C2A	-5.56	1.49	1.54
24	G	609	CHL	CHB-C4A	-5.56	1.31	1.38
24	4	607	CHL	C3A-C2A	-5.55	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	605	CHL	C3A-C2A	-5.54	1.49	1.54
24	g	609	CHL	CHB-C4A	-5.54	1.31	1.38
24	5	606	CHL	C3A-C2A	-5.54	1.49	1.54
24	6	607	CHL	C3A-C2A	-5.53	1.49	1.54
24	1	608	CHL	CHB-C4A	-5.53	1.31	1.38
24	7	601	CHL	C3A-C2A	-5.53	1.49	1.54
24	y	609	CHL	CHB-C4A	-5.52	1.32	1.38
24	2	605	CHL	C3A-C2A	-5.51	1.49	1.54
24	N	606	CHL	C3B-C4B	5.51	1.46	1.41
24	5	601	CHL	C3A-C2A	-5.51	1.50	1.54
24	1	607	CHL	CHB-C4A	-5.51	1.32	1.38
24	S	608	CHL	C3D-C4D	-5.50	1.33	1.41
24	Y	609	CHL	CHB-C4A	-5.50	1.32	1.38
24	G	608	CHL	C3A-C2A	-5.50	1.50	1.54
24	5	607	CHL	CHB-C4A	-5.50	1.32	1.38
24	g	601	CHL	CHB-C4A	-5.49	1.32	1.38
24	G	601	CHL	CHB-C4A	-5.49	1.32	1.38
24	8	607	CHL	C3A-C2A	-5.49	1.50	1.54
24	s	608	CHL	C3D-C4D	-5.48	1.33	1.41
24	7	601	CHL	CHB-C4A	-5.48	1.32	1.38
24	n	606	CHL	C3B-C4B	5.46	1.46	1.41
24	3	601	CHL	CHB-C4A	-5.46	1.32	1.38
24	r	606	CHL	CHB-C4A	-5.46	1.32	1.38
24	n	601	CHL	C3A-C2A	-5.45	1.50	1.54
24	g	608	CHL	C3A-C2A	-5.44	1.50	1.54
24	N	601	CHL	C3A-C2A	-5.43	1.50	1.54
24	R	606	CHL	CHB-C4A	-5.43	1.32	1.38
24	G	601	CHL	C3A-C2A	-5.41	1.50	1.54
24	4	601	CHL	C3D-C4D	-5.40	1.33	1.41
24	g	601	CHL	C3A-C2A	-5.40	1.50	1.54
24	8	601	CHL	C3D-C4D	-5.37	1.33	1.41
24	8	606	CHL	CHB-C4A	-5.37	1.32	1.38
24	4	606	CHL	CHB-C4A	-5.36	1.32	1.38
24	8	601	CHL	C3B-C2B	5.34	1.47	1.40
24	3	609	CHL	C3A-C2A	-5.34	1.50	1.54
24	G	607	CHL	CHB-C4A	-5.33	1.32	1.38
24	n	605	CHL	CHB-C4A	-5.33	1.32	1.38
24	Y	601	CHL	CHB-C4A	-5.33	1.32	1.38
24	N	605	CHL	CHB-C4A	-5.31	1.32	1.38
24	y	601	CHL	CHB-C4A	-5.31	1.32	1.38
24	g	607	CHL	CHB-C4A	-5.31	1.32	1.38
24	s	601	CHL	C3A-C2A	-5.30	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	609	CHL	C3A-C2A	-5.30	1.50	1.54
24	7	609	CHL	CHB-C4A	-5.28	1.32	1.38
24	S	601	CHL	C3A-C2A	-5.28	1.50	1.54
24	y	607	CHL	CHB-C4A	-5.27	1.32	1.38
24	3	609	CHL	CHB-C4A	-5.27	1.32	1.38
24	4	601	CHL	C3B-C2B	5.27	1.47	1.40
24	S	606	CHL	C3D-C4D	-5.26	1.33	1.41
24	6	606	CHL	CHB-C4A	-5.24	1.32	1.38
24	s	606	CHL	C3D-C4D	-5.24	1.33	1.41
24	7	607	CHL	C3A-C2A	-5.23	1.50	1.54
24	Y	607	CHL	CHB-C4A	-5.23	1.32	1.38
24	2	606	CHL	CHB-C4A	-5.23	1.32	1.38
24	3	607	CHL	C3A-C2A	-5.23	1.50	1.54
24	n	606	CHL	CHB-C4A	-5.20	1.32	1.38
24	s	606	CHL	CHC-C4B	5.18	1.48	1.39
24	Y	605	CHL	C3A-C2A	-5.18	1.50	1.54
24	S	606	CHL	CHC-C4B	5.17	1.48	1.39
24	n	605	CHL	C3A-C2A	-5.16	1.50	1.54
24	6	609	CHL	CHB-C4A	-5.16	1.32	1.38
24	N	605	CHL	C3A-C2A	-5.15	1.50	1.54
24	S	607	CHL	O2D-CGD	5.15	1.45	1.33
24	8	609	CHL	CHB-C4A	-5.15	1.32	1.38
24	N	606	CHL	CHB-C4A	-5.15	1.32	1.38
24	s	601	CHL	CHB-C4A	-5.14	1.32	1.38
24	s	607	CHL	O2D-CGD	5.14	1.45	1.33
24	S	601	CHL	CHB-C4A	-5.14	1.32	1.38
24	g	606	CHL	CHB-C4A	-5.14	1.32	1.38
24	2	609	CHL	CHB-C4A	-5.14	1.32	1.38
24	4	609	CHL	CHB-C4A	-5.14	1.32	1.38
24	Y	608	CHL	CHB-C4A	-5.14	1.32	1.38
24	2	607	CHL	CHB-C4A	-5.13	1.32	1.38
24	G	606	CHL	CHB-C4A	-5.12	1.32	1.38
24	6	607	CHL	CHB-C4A	-5.11	1.32	1.38
24	s	607	CHL	C3D-C4D	-5.10	1.33	1.41
24	r	614	CHL	OBD-CAD	5.10	1.29	1.22
24	N	608	CHL	CHB-C4A	-5.09	1.32	1.38
24	y	605	CHL	C3A-C2A	-5.09	1.50	1.54
24	n	608	CHL	CHB-C4A	-5.09	1.32	1.38
24	S	607	CHL	C3D-C4D	-5.09	1.33	1.41
24	y	608	CHL	CHB-C4A	-5.09	1.32	1.38
24	s	607	CHL	OBD-CAD	5.09	1.29	1.22
24	3	607	CHL	CHB-C4A	-5.08	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	607	CHL	O2D-CGD	5.07	1.45	1.33
24	8	609	CHL	O2D-CGD	5.07	1.45	1.33
24	n	605	CHL	OBD-CAD	5.07	1.29	1.22
24	2	607	CHL	O2D-CGD	5.07	1.45	1.33
24	R	614	CHL	OBD-CAD	5.07	1.28	1.22
24	4	609	CHL	O2D-CGD	5.06	1.45	1.33
24	N	605	CHL	OBD-CAD	5.06	1.28	1.22
24	S	607	CHL	OBD-CAD	5.06	1.28	1.22
24	7	607	CHL	CHB-C4A	-5.05	1.32	1.38
24	S	608	CHL	C3B-C2B	5.03	1.47	1.40
24	5	605	CHL	C3A-C2A	-5.03	1.50	1.54
24	S	601	CHL	O2D-CGD	5.03	1.45	1.33
24	s	608	CHL	C3B-C2B	5.03	1.47	1.40
24	5	606	CHL	CHB-C4A	-5.02	1.32	1.38
24	R	607	CHL	CHB-C4A	-5.02	1.32	1.38
24	1	606	CHL	CHB-C4A	-5.02	1.32	1.38
24	3	608	CHL	CHB-C4A	-5.02	1.32	1.38
24	7	608	CHL	CHB-C4A	-5.01	1.32	1.38
24	s	601	CHL	O2D-CGD	5.01	1.45	1.33
24	r	608	CHL	CHB-C4A	-5.01	1.32	1.38
36	D	405	PL9	C7-C3	-5.00	1.44	1.51
24	7	605	CHL	CHB-C4A	-4.99	1.32	1.38
24	3	605	CHL	CHB-C4A	-4.99	1.32	1.38
24	y	605	CHL	CHB-C4A	-4.99	1.32	1.38
36	d	405	PL9	C7-C3	-4.98	1.44	1.51
24	1	605	CHL	C3A-C2A	-4.98	1.50	1.54
24	Y	605	CHL	CHB-C4A	-4.98	1.32	1.38
24	R	608	CHL	CHB-C4A	-4.97	1.32	1.38
24	R	607	CHL	O2D-CGD	4.97	1.45	1.33
24	r	607	CHL	CHB-C4A	-4.97	1.32	1.38
24	6	605	CHL	O2D-CGD	4.96	1.45	1.33
24	g	605	CHL	O2D-CGD	4.96	1.45	1.33
24	r	607	CHL	O2D-CGD	4.96	1.45	1.33
24	2	601	CHL	O2D-CGD	4.96	1.45	1.33
24	n	601	CHL	O2D-CGD	4.96	1.45	1.33
24	N	601	CHL	O2D-CGD	4.96	1.45	1.33
24	2	605	CHL	O2D-CGD	4.95	1.45	1.33
24	6	601	CHL	O2D-CGD	4.95	1.45	1.33
24	G	605	CHL	O2D-CGD	4.95	1.45	1.33
24	s	606	CHL	O2D-CGD	4.95	1.45	1.33
24	g	608	CHL	O2D-CGD	4.94	1.45	1.33
24	S	608	CHL	O2D-CGD	4.93	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	608	CHL	O2D-CGD	4.93	1.45	1.33
24	s	608	CHL	O2D-CGD	4.93	1.45	1.33
24	4	607	CHL	CHB-C4A	-4.93	1.32	1.38
24	S	606	CHL	O2D-CGD	4.92	1.45	1.33
24	6	606	CHL	O2D-CGD	4.92	1.45	1.33
24	3	605	CHL	O2D-CGD	4.92	1.45	1.33
24	2	605	CHL	CHB-C4A	-4.92	1.32	1.38
24	7	606	CHL	O2D-CGD	4.91	1.45	1.33
24	R	614	CHL	C2A-C3A	-4.91	1.50	1.54
24	r	607	CHL	C3A-C2A	-4.91	1.50	1.54
24	2	609	CHL	O2D-CGD	4.91	1.45	1.33
24	3	606	CHL	O2D-CGD	4.91	1.45	1.33
24	7	605	CHL	O2D-CGD	4.91	1.45	1.33
24	1	605	CHL	CHB-C4A	-4.91	1.32	1.38
24	6	605	CHL	CHB-C4A	-4.91	1.32	1.38
24	4	608	CHL	O2D-CGD	4.90	1.45	1.33
24	2	606	CHL	O2D-CGD	4.90	1.45	1.33
24	R	607	CHL	OBD-CAD	4.89	1.28	1.22
24	S	606	CHL	C3B-C2B	4.89	1.47	1.40
24	r	614	CHL	C2A-C3A	-4.89	1.50	1.54
24	8	607	CHL	CHB-C4A	-4.89	1.32	1.38
24	6	609	CHL	O2D-CGD	4.89	1.45	1.33
24	g	601	CHL	O2D-CGD	4.89	1.45	1.33
24	G	601	CHL	O2D-CGD	4.89	1.45	1.33
24	R	607	CHL	C3A-C2A	-4.89	1.50	1.54
24	r	607	CHL	OBD-CAD	4.89	1.28	1.22
24	8	608	CHL	O2D-CGD	4.88	1.45	1.33
24	g	605	CHL	C3A-C2A	-4.88	1.50	1.54
24	5	605	CHL	CHB-C4A	-4.87	1.32	1.38
24	4	601	CHL	OBD-CAD	4.87	1.28	1.22
24	g	607	CHL	O2D-CGD	4.87	1.45	1.33
24	n	607	CHL	CHB-C4A	-4.86	1.32	1.38
24	G	607	CHL	O2D-CGD	4.86	1.45	1.33
24	2	601	CHL	CHB-C4A	-4.86	1.32	1.38
24	s	606	CHL	C3B-C2B	4.86	1.46	1.40
24	5	605	CHL	O2D-CGD	4.85	1.45	1.33
24	4	608	CHL	CHB-C4A	-4.85	1.32	1.38
24	6	605	CHL	OBD-CAD	4.84	1.28	1.22
24	7	606	CHL	CHC-C4B	4.84	1.47	1.39
24	4	601	CHL	CHC-C4B	4.84	1.47	1.39
24	1	605	CHL	O2D-CGD	4.84	1.45	1.33
24	8	606	CHL	O2D-CGD	4.84	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	607	CHL	CHB-C4A	-4.84	1.32	1.38
24	G	606	CHL	O2D-CGD	4.84	1.45	1.33
24	g	606	CHL	O2D-CGD	4.84	1.45	1.33
24	6	601	CHL	CHB-C4A	-4.83	1.32	1.38
24	n	606	CHL	O2D-CGD	4.83	1.45	1.33
24	4	606	CHL	O2D-CGD	4.83	1.45	1.33
24	8	601	CHL	CHC-C4B	4.82	1.47	1.39
24	N	607	CHL	O2D-CGD	4.82	1.45	1.33
24	n	607	CHL	O2D-CGD	4.82	1.45	1.33
24	G	605	CHL	OBD-CAD	4.81	1.28	1.22
24	2	608	CHL	O2D-CGD	4.81	1.45	1.33
24	5	606	CHL	O2D-CGD	4.81	1.45	1.33
24	G	605	CHL	C3A-C2A	-4.81	1.50	1.54
24	8	601	CHL	OBD-CAD	4.81	1.28	1.22
24	g	605	CHL	OBD-CAD	4.81	1.28	1.22
24	r	606	CHL	O2D-CGD	4.81	1.45	1.33
24	y	606	CHL	CHB-C4A	-4.81	1.32	1.38
24	2	605	CHL	OBD-CAD	4.81	1.28	1.22
24	Y	606	CHL	CHB-C4A	-4.81	1.32	1.38
24	1	606	CHL	O2D-CGD	4.80	1.45	1.33
24	3	606	CHL	CHC-C4B	4.80	1.47	1.39
24	2	608	CHL	CHB-C4A	-4.80	1.32	1.38
24	N	606	CHL	O2D-CGD	4.80	1.45	1.33
24	4	601	CHL	CHD-C1D	4.80	1.47	1.39
24	6	608	CHL	O2D-CGD	4.79	1.45	1.33
24	8	608	CHL	CHB-C4A	-4.79	1.32	1.38
24	R	606	CHL	O2D-CGD	4.79	1.45	1.33
24	7	601	CHL	O2D-CGD	4.79	1.45	1.33
24	n	601	CHL	CHB-C4A	-4.79	1.32	1.38
24	4	607	CHL	O2D-CGD	4.79	1.45	1.33
24	8	607	CHL	O2D-CGD	4.78	1.45	1.33
24	6	608	CHL	CHB-C4A	-4.78	1.32	1.38
24	S	601	CHL	CHC-C4B	4.78	1.47	1.39
24	3	601	CHL	O2D-CGD	4.78	1.45	1.33
24	Y	605	CHL	O2D-CGD	4.77	1.45	1.33
24	S	606	CHL	OBD-CAD	4.77	1.28	1.22
24	8	601	CHL	CHD-C1D	4.77	1.47	1.39
24	N	601	CHL	CHB-C4A	-4.77	1.32	1.38
24	s	606	CHL	OBD-CAD	4.76	1.28	1.22
24	Y	606	CHL	O2D-CGD	4.76	1.44	1.33
24	4	608	CHL	CHB-C1B	4.75	1.47	1.39
24	r	614	CHL	O2D-CGD	4.75	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	614	CHL	O2D-CGD	4.75	1.44	1.33
24	s	601	CHL	CHC-C4B	4.75	1.47	1.39
24	4	601	CHL	O2D-CGD	4.75	1.45	1.30
24	1	601	CHL	CHB-C4A	-4.75	1.32	1.38
24	4	601	CHL	CHD-C4C	4.75	1.48	1.39
24	s	607	CHL	C3B-C2B	4.75	1.46	1.40
24	8	601	CHL	O2D-CGD	4.74	1.45	1.30
24	r	614	CHL	CHB-C4A	-4.74	1.32	1.38
24	3	608	CHL	O2D-CGD	4.74	1.44	1.33
24	8	601	CHL	CHD-C4C	4.73	1.48	1.39
24	g	609	CHL	O2D-CGD	4.73	1.44	1.33
24	y	606	CHL	O2D-CGD	4.73	1.44	1.33
24	y	605	CHL	O2D-CGD	4.73	1.44	1.33
24	n	608	CHL	O2D-CGD	4.73	1.44	1.33
24	s	606	CHL	CHB-C1B	4.73	1.47	1.39
24	N	608	CHL	O2D-CGD	4.73	1.44	1.33
24	7	608	CHL	O2D-CGD	4.72	1.44	1.33
24	8	608	CHL	CHB-C1B	4.72	1.47	1.39
24	G	607	CHL	OBD-CAD	4.72	1.28	1.22
24	6	605	CHL	CHC-C4B	4.72	1.47	1.39
24	R	614	CHL	C3B-C2B	4.72	1.46	1.40
24	2	605	CHL	CHC-C4B	4.71	1.47	1.39
24	7	609	CHL	O2D-CGD	4.71	1.44	1.33
24	3	609	CHL	C3B-C2B	4.71	1.46	1.40
24	G	605	CHL	C3B-C2B	4.71	1.46	1.40
24	n	605	CHL	O2D-CGD	4.71	1.44	1.33
24	r	614	CHL	C3B-C2B	4.71	1.46	1.40
24	2	605	CHL	C3B-C2B	4.71	1.46	1.40
24	S	607	CHL	C3B-C2B	4.71	1.46	1.40
24	g	605	CHL	C3B-C2B	4.71	1.46	1.40
24	G	609	CHL	O2D-CGD	4.71	1.44	1.33
24	g	607	CHL	OBD-CAD	4.70	1.28	1.22
24	S	606	CHL	CHB-C1B	4.70	1.47	1.39
24	R	614	CHL	CHB-C4A	-4.70	1.33	1.38
24	7	609	CHL	C3B-C2B	4.69	1.46	1.40
24	g	608	CHL	CHC-C4B	4.69	1.47	1.39
24	5	601	CHL	CHB-C4A	-4.69	1.33	1.38
24	r	614	CHL	CHC-C4B	4.68	1.47	1.39
24	G	608	CHL	CHB-C4A	-4.68	1.33	1.38
24	g	608	CHL	CHB-C4A	-4.68	1.33	1.38
24	5	608	CHL	O2D-CGD	4.68	1.44	1.33
24	R	614	CHL	CHC-C4B	4.68	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	609	CHL	O2D-CGD	4.68	1.44	1.33
24	N	605	CHL	O2D-CGD	4.68	1.44	1.33
24	6	605	CHL	C3B-C2B	4.67	1.46	1.40
24	G	608	CHL	CHC-C4B	4.67	1.47	1.39
24	1	601	CHL	O2D-CGD	4.67	1.44	1.33
24	n	609	CHL	O2D-CGD	4.67	1.44	1.33
24	3	609	CHL	O2D-CGD	4.67	1.44	1.33
24	1	607	CHL	O2D-CGD	4.66	1.44	1.33
24	y	601	CHL	O2D-CGD	4.65	1.44	1.33
24	5	607	CHL	O2D-CGD	4.65	1.44	1.33
24	7	607	CHL	O2D-CGD	4.65	1.44	1.33
24	y	609	CHL	O2D-CGD	4.65	1.44	1.33
24	8	607	CHL	OBD-CAD	4.64	1.28	1.22
24	n	601	CHL	CHC-C4B	4.64	1.47	1.39
24	S	601	CHL	O2A-CGA	4.64	1.46	1.30
24	1	608	CHL	O2D-CGD	4.64	1.44	1.33
24	5	601	CHL	O2D-CGD	4.64	1.44	1.33
24	3	607	CHL	O2D-CGD	4.63	1.44	1.33
24	8	609	CHL	OBD-CAD	4.63	1.28	1.22
24	Y	601	CHL	O2D-CGD	4.63	1.44	1.33
24	4	607	CHL	OBD-CAD	4.63	1.28	1.22
24	Y	609	CHL	O2D-CGD	4.63	1.44	1.33
24	S	608	CHL	CHB-C1B	4.63	1.47	1.39
24	7	605	CHL	OBD-CAD	4.63	1.28	1.22
24	3	605	CHL	O2A-CGA	4.63	1.46	1.30
24	s	601	CHL	O2A-CGA	4.63	1.46	1.30
24	7	605	CHL	O2A-CGA	4.63	1.46	1.30
24	4	601	CHL	CHB-C1B	4.63	1.47	1.39
24	N	601	CHL	CHC-C4B	4.62	1.47	1.39
24	1	609	CHL	CHD-C1D	4.62	1.47	1.39
24	3	605	CHL	OBD-CAD	4.62	1.28	1.22
24	4	609	CHL	OBD-CAD	4.62	1.28	1.22
24	8	601	CHL	CHB-C4A	-4.61	1.33	1.38
24	1	605	CHL	OBD-CAD	4.61	1.28	1.22
24	n	601	CHL	C3B-C2B	4.61	1.46	1.40
24	5	605	CHL	OBD-CAD	4.61	1.28	1.22
24	r	614	CHL	CHC-C1C	4.61	1.48	1.39
24	G	608	CHL	C3B-C2B	4.61	1.46	1.40
24	8	601	CHL	CHB-C1B	4.61	1.47	1.39
24	g	608	CHL	C3B-C2B	4.60	1.46	1.40
24	6	607	CHL	C3B-C2B	4.60	1.46	1.40
24	r	614	CHL	CHB-C1B	4.60	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	614	CHL	CHC-C1C	4.60	1.48	1.39
24	5	608	CHL	CHC-C4B	4.59	1.47	1.39
24	s	608	CHL	CHB-C1B	4.59	1.47	1.39
24	8	606	CHL	OBD-CAD	4.59	1.28	1.22
24	s	606	CHL	O2A-CGA	4.58	1.46	1.30
24	6	607	CHL	OBD-CAD	4.58	1.28	1.22
24	5	609	CHL	CHD-C1D	4.58	1.47	1.39
24	G	605	CHL	O2A-CGA	4.58	1.46	1.30
24	1	608	CHL	CHC-C4B	4.58	1.47	1.39
24	R	614	CHL	CHB-C1B	4.58	1.47	1.39
37	h	102	DGD	O2D-C2D	-4.58	1.31	1.43
24	y	607	CHL	O2D-CGD	4.58	1.44	1.33
24	g	605	CHL	O2A-CGA	4.58	1.46	1.30
24	S	606	CHL	O2A-CGA	4.58	1.45	1.30
24	Y	607	CHL	O2D-CGD	4.58	1.44	1.33
37	H	102	DGD	O2D-C2D	-4.58	1.31	1.43
24	4	601	CHL	CHB-C4A	-4.58	1.33	1.38
24	1	609	CHL	O2D-CGD	4.58	1.44	1.33
24	4	606	CHL	OBD-CAD	4.57	1.28	1.22
24	S	606	CHL	C3A-C2A	-4.57	1.50	1.54
24	7	608	CHL	CHC-C4B	4.57	1.47	1.39
24	2	607	CHL	C3B-C2B	4.57	1.46	1.40
24	5	601	CHL	O2A-CGA	4.56	1.45	1.30
24	R	608	CHL	O2D-CGD	4.56	1.44	1.33
24	4	607	CHL	C3B-C2B	4.56	1.46	1.40
24	7	609	CHL	OBD-CAD	4.56	1.28	1.22
24	4	601	CHL	CHC-C1C	4.56	1.48	1.39
24	4	606	CHL	CHC-C4B	4.56	1.47	1.39
24	6	608	CHL	O2A-CGA	4.56	1.45	1.30
24	8	601	CHL	CHC-C1C	4.56	1.48	1.39
24	2	608	CHL	O2A-CGA	4.56	1.45	1.30
24	6	605	CHL	O2A-CGA	4.56	1.45	1.30
24	2	606	CHL	O2A-CGA	4.55	1.45	1.30
24	2	605	CHL	O2A-CGA	4.55	1.45	1.30
24	3	608	CHL	CHC-C4B	4.55	1.47	1.39
24	S	608	CHL	O2A-CGA	4.55	1.45	1.30
24	8	601	CHL	O2A-CGA	4.55	1.45	1.30
24	N	601	CHL	C3B-C2B	4.55	1.46	1.40
24	5	609	CHL	O2D-CGD	4.55	1.44	1.33
24	2	601	CHL	C3B-C2B	4.54	1.46	1.40
24	4	601	CHL	O2A-CGA	4.54	1.45	1.30
24	1	601	CHL	O2A-CGA	4.54	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	608	CHL	O2D-CGD	4.54	1.44	1.33
24	6	606	CHL	OBD-CAD	4.54	1.28	1.22
24	s	608	CHL	O2A-CGA	4.54	1.45	1.30
24	7	606	CHL	OBD-CAD	4.54	1.28	1.22
24	n	601	CHL	CHD-C4C	4.54	1.48	1.39
24	6	606	CHL	O2A-CGA	4.54	1.45	1.30
24	6	601	CHL	O2A-CGA	4.54	1.45	1.30
24	8	606	CHL	CHC-C4B	4.54	1.47	1.39
24	2	607	CHL	OBD-CAD	4.53	1.28	1.22
24	6	609	CHL	OBD-CAD	4.53	1.28	1.22
24	2	606	CHL	OBD-CAD	4.53	1.28	1.22
24	5	605	CHL	C3B-C2B	4.53	1.46	1.40
24	3	609	CHL	OBD-CAD	4.53	1.28	1.22
24	2	609	CHL	OBD-CAD	4.52	1.28	1.22
24	6	601	CHL	C3B-C2B	4.52	1.46	1.40
24	s	606	CHL	C3A-C2A	-4.52	1.50	1.54
24	5	609	CHL	CHD-C4C	4.52	1.48	1.39
24	8	609	CHL	O2A-CGA	4.52	1.45	1.30
24	S	601	CHL	OBD-CAD	4.52	1.28	1.22
24	5	606	CHL	O2A-CGA	4.52	1.45	1.30
24	s	601	CHL	OBD-CAD	4.52	1.28	1.22
24	y	607	CHL	OBD-CAD	4.52	1.28	1.22
24	8	607	CHL	O2A-CGA	4.52	1.45	1.30
24	1	609	CHL	CHD-C4C	4.52	1.48	1.39
24	2	601	CHL	O2A-CGA	4.52	1.45	1.30
24	G	605	CHL	CHB-C4A	-4.51	1.33	1.38
24	4	607	CHL	O2A-CGA	4.51	1.45	1.30
24	4	609	CHL	O2A-CGA	4.51	1.45	1.30
24	1	605	CHL	C3B-C2B	4.51	1.46	1.40
24	1	606	CHL	O2A-CGA	4.51	1.45	1.30
24	3	607	CHL	OBD-CAD	4.51	1.28	1.22
24	r	606	CHL	OBD-CAD	4.51	1.28	1.22
24	y	608	CHL	O2D-CGD	4.51	1.44	1.33
24	1	607	CHL	OBD-CAD	4.51	1.28	1.22
24	1	608	CHL	O2A-CGA	4.50	1.45	1.30
24	N	601	CHL	CHD-C4C	4.50	1.48	1.39
24	Y	608	CHL	O2D-CGD	4.50	1.44	1.33
24	8	607	CHL	C3B-C2B	4.50	1.46	1.40
24	3	609	CHL	CHD-C1D	4.50	1.46	1.39
24	r	614	CHL	CHD-C4C	4.50	1.48	1.39
24	7	608	CHL	O2A-CGA	4.50	1.45	1.30
24	3	606	CHL	O2A-CGA	4.50	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	606	CHL	OBD-CAD	4.50	1.28	1.22
24	3	608	CHL	O2A-CGA	4.50	1.45	1.30
24	7	609	CHL	CHD-C1D	4.50	1.46	1.39
24	3	606	CHL	OBD-CAD	4.49	1.28	1.22
24	5	606	CHL	CHC-C4B	4.49	1.46	1.39
24	g	605	CHL	CHB-C4A	-4.49	1.33	1.38
24	N	607	CHL	OBD-CAD	4.49	1.28	1.22
24	2	607	CHL	CHD-C1D	4.49	1.46	1.39
24	7	606	CHL	O2A-CGA	4.49	1.45	1.30
24	N	606	CHL	O2A-CGA	4.49	1.46	1.33
24	n	606	CHL	O2A-CGA	4.48	1.46	1.33
24	5	608	CHL	O2A-CGA	4.48	1.45	1.30
24	1	606	CHL	CHC-C4B	4.48	1.46	1.39
24	y	605	CHL	OBD-CAD	4.48	1.28	1.22
24	7	605	CHL	C3B-C2B	4.48	1.46	1.40
24	R	606	CHL	OBD-CAD	4.48	1.28	1.22
24	6	607	CHL	CHD-C1D	4.48	1.46	1.39
24	3	605	CHL	C3B-C2B	4.47	1.46	1.40
24	Y	605	CHL	OBD-CAD	4.47	1.28	1.22
24	1	605	CHL	O2A-CGA	4.47	1.45	1.30
24	G	606	CHL	OBD-CAD	4.47	1.28	1.22
24	5	606	CHL	OBD-CAD	4.47	1.28	1.22
24	7	607	CHL	OBD-CAD	4.47	1.28	1.22
24	1	606	CHL	OBD-CAD	4.46	1.28	1.22
24	R	614	CHL	CHD-C4C	4.46	1.47	1.39
24	5	605	CHL	O2A-CGA	4.46	1.45	1.30
24	5	607	CHL	OBD-CAD	4.46	1.28	1.22
24	Y	607	CHL	OBD-CAD	4.46	1.28	1.22
24	7	609	CHL	CHD-C4C	4.45	1.47	1.39
24	2	601	CHL	CHB-C1B	4.45	1.46	1.39
24	6	601	CHL	OBD-CAD	4.45	1.28	1.22
24	n	607	CHL	OBD-CAD	4.44	1.28	1.22
24	3	609	CHL	O2A-CGA	4.44	1.46	1.33
24	4	607	CHL	CHD-C4C	4.44	1.47	1.39
24	2	601	CHL	OBD-CAD	4.44	1.28	1.22
24	6	601	CHL	CHB-C1B	4.44	1.46	1.39
24	1	605	CHL	CHB-C1B	4.43	1.46	1.39
24	4	607	CHL	CHB-C1B	4.43	1.46	1.39
24	N	601	CHL	CHB-C1B	4.43	1.46	1.39
24	4	606	CHL	O2A-CGA	4.43	1.45	1.30
24	7	609	CHL	O2A-CGA	4.43	1.46	1.33
24	3	608	CHL	CHC-C1C	4.42	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	605	CHL	CHB-C1B	4.42	1.46	1.39
24	7	607	CHL	CHC-C4B	4.42	1.46	1.39
24	S	608	CHL	OBD-CAD	4.42	1.28	1.22
24	s	608	CHL	OBD-CAD	4.42	1.28	1.22
24	8	606	CHL	O2A-CGA	4.42	1.45	1.30
24	S	608	CHL	CHD-C4C	4.42	1.47	1.39
24	s	608	CHL	CHD-C4C	4.42	1.47	1.39
24	N	608	CHL	CHC-C4B	4.41	1.46	1.39
24	3	609	CHL	CHD-C4C	4.41	1.47	1.39
24	8	607	CHL	CHD-C4C	4.41	1.47	1.39
24	N	605	CHL	CHD-C1D	4.41	1.46	1.39
24	n	605	CHL	CHD-C1D	4.41	1.46	1.39
24	n	608	CHL	CHC-C4B	4.41	1.46	1.39
24	s	607	CHL	O2A-CGA	4.41	1.46	1.33
24	S	607	CHL	O2A-CGA	4.41	1.46	1.33
24	8	607	CHL	CHB-C1B	4.41	1.46	1.39
24	3	607	CHL	CHC-C4B	4.40	1.46	1.39
24	1	609	CHL	OBD-CAD	4.40	1.28	1.22
24	n	601	CHL	CHB-C1B	4.40	1.46	1.39
24	2	607	CHL	CHD-C4C	4.39	1.47	1.39
24	R	614	CHL	CHD-C1D	4.39	1.46	1.39
24	7	608	CHL	CHC-C1C	4.39	1.47	1.39
24	8	608	CHL	O2A-CGA	4.39	1.45	1.30
24	n	605	CHL	CHC-C4B	4.39	1.46	1.39
24	S	607	CHL	CHB-C4A	-4.38	1.33	1.38
24	3	609	CHL	CHB-C1B	4.38	1.46	1.39
24	4	608	CHL	O2A-CGA	4.38	1.45	1.30
28	Y	1623	NEX	C7-C6	-4.38	1.25	1.30
24	5	609	CHL	OBD-CAD	4.38	1.28	1.22
24	6	607	CHL	CHD-C4C	4.38	1.47	1.39
24	N	605	CHL	CHC-C4B	4.38	1.46	1.39
28	y	1623	NEX	C7-C6	-4.38	1.25	1.30
24	S	601	CHL	CHC-C1C	4.38	1.47	1.39
24	r	607	CHL	C3B-C2B	4.37	1.46	1.40
24	g	608	CHL	OBD-CAD	4.37	1.28	1.22
24	g	601	CHL	CHD-C4C	4.37	1.47	1.39
24	s	601	CHL	CHC-C1C	4.37	1.47	1.39
24	N	609	CHL	O2A-CGA	4.37	1.46	1.33
24	4	606	CHL	C3B-C2B	4.36	1.46	1.40
24	G	608	CHL	OBD-CAD	4.36	1.28	1.22
24	n	609	CHL	O2A-CGA	4.36	1.46	1.33
24	G	601	CHL	CHD-C4C	4.36	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	605	CHL	CHD-C1D	4.36	1.46	1.39
24	S	608	CHL	CHD-C1D	4.35	1.46	1.39
24	g	605	CHL	CHD-C1D	4.35	1.46	1.39
24	7	609	CHL	CHB-C1B	4.35	1.46	1.39
24	S	601	CHL	CHD-C4C	4.35	1.47	1.39
24	r	614	CHL	CHD-C1D	4.35	1.46	1.39
36	D	405	PL9	C7-C8	-4.35	1.43	1.50
24	R	607	CHL	C3B-C2B	4.34	1.46	1.40
24	g	605	CHL	CHB-C1B	4.34	1.46	1.39
24	g	608	CHL	CHC-C1C	4.34	1.47	1.39
24	s	601	CHL	CHD-C4C	4.34	1.47	1.39
24	y	608	CHL	CHC-C4B	4.34	1.46	1.39
24	s	607	CHL	CHB-C4A	-4.34	1.33	1.38
24	G	607	CHL	CHC-C1C	4.33	1.47	1.39
24	7	607	CHL	O2A-CGA	4.33	1.46	1.33
24	2	601	CHL	CHC-C4B	4.33	1.46	1.39
24	1	601	CHL	CHB-C1B	4.33	1.46	1.39
24	2	609	CHL	CHB-C1B	4.33	1.46	1.39
24	g	601	CHL	CHC-C4B	4.33	1.46	1.39
24	s	608	CHL	CHD-C1D	4.33	1.46	1.39
24	7	605	CHL	CHC-C4B	4.32	1.46	1.39
24	6	605	CHL	CHB-C1B	4.32	1.46	1.39
24	N	601	CHL	O2A-CGA	4.32	1.45	1.33
24	2	609	CHL	C3B-C2B	4.32	1.46	1.40
24	2	605	CHL	CHB-C1B	4.32	1.46	1.39
24	G	606	CHL	CHC-C4B	4.32	1.46	1.39
24	6	601	CHL	CHC-C4B	4.32	1.46	1.39
24	n	601	CHL	O2A-CGA	4.32	1.45	1.33
24	G	601	CHL	CHC-C4B	4.32	1.46	1.39
24	S	607	CHL	CHB-C1B	4.32	1.46	1.39
24	3	607	CHL	O2A-CGA	4.31	1.45	1.33
24	R	606	CHL	CHC-C4B	4.31	1.46	1.39
24	g	605	CHL	CHC-C4B	4.31	1.46	1.39
24	6	609	CHL	CHB-C1B	4.31	1.46	1.39
24	G	605	CHL	CHC-C4B	4.31	1.46	1.39
24	7	607	CHL	CHC-C1C	4.31	1.47	1.39
24	S	607	CHL	CHC-C4B	4.31	1.46	1.39
24	g	606	CHL	CHC-C4B	4.31	1.46	1.39
24	G	608	CHL	CHC-C1C	4.31	1.47	1.39
24	8	606	CHL	C3B-C2B	4.31	1.46	1.40
24	g	607	CHL	CHC-C1C	4.31	1.47	1.39
24	Y	608	CHL	CHC-C4B	4.31	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	605	CHL	CHC-C4B	4.31	1.46	1.39
24	G	605	CHL	CHB-C1B	4.30	1.46	1.39
24	3	607	CHL	CHC-C1C	4.30	1.47	1.39
24	s	607	CHL	CHC-C4B	4.30	1.46	1.39
24	Y	606	CHL	O2A-CGA	4.30	1.45	1.33
24	s	607	CHL	CHB-C1B	4.30	1.46	1.39
24	y	606	CHL	O2A-CGA	4.30	1.45	1.33
36	d	405	PL9	C7-C8	-4.30	1.43	1.50
24	S	606	CHL	CHD-C1D	4.30	1.46	1.39
24	R	607	CHL	CHD-C4C	4.29	1.47	1.39
24	5	601	CHL	CHB-C1B	4.29	1.46	1.39
24	6	608	CHL	CHC-C4B	4.29	1.46	1.39
24	N	607	CHL	O2A-CGA	4.29	1.45	1.33
24	s	606	CHL	CHD-C1D	4.29	1.46	1.39
24	2	608	CHL	OBD-CAD	4.29	1.27	1.22
24	G	609	CHL	CHD-C1D	4.28	1.46	1.39
24	r	608	CHL	O2A-CGA	4.28	1.45	1.33
24	g	608	CHL	CHB-C1B	4.28	1.46	1.39
24	5	601	CHL	C3B-C2B	4.28	1.46	1.40
24	S	608	CHL	C3A-C2A	-4.28	1.51	1.54
24	8	607	CHL	CHC-C4B	4.28	1.46	1.39
24	n	607	CHL	O2A-CGA	4.28	1.45	1.33
24	S	606	CHL	CHC-C1C	4.28	1.47	1.39
24	2	608	CHL	CHC-C4B	4.28	1.46	1.39
24	1	601	CHL	OBD-CAD	4.28	1.27	1.22
24	N	609	CHL	CHD-C1D	4.28	1.46	1.39
24	y	606	CHL	CHB-C1B	4.28	1.46	1.39
24	g	609	CHL	CHD-C1D	4.28	1.46	1.39
24	Y	606	CHL	CHB-C1B	4.28	1.46	1.39
24	r	606	CHL	CHC-C4B	4.27	1.46	1.39
24	1	601	CHL	CHD-C4C	4.27	1.47	1.39
24	s	608	CHL	C3A-C2A	-4.27	1.51	1.54
24	r	607	CHL	CHD-C4C	4.27	1.47	1.39
24	S	606	CHL	CHB-C4A	-4.27	1.33	1.38
24	G	608	CHL	CHB-C1B	4.27	1.46	1.39
24	4	607	CHL	CHC-C4B	4.27	1.46	1.39
28	1	1623	NEX	C7-C6	-4.26	1.25	1.30
24	s	606	CHL	CHD-C4C	4.26	1.47	1.39
24	S	606	CHL	CHD-C4C	4.26	1.47	1.39
24	s	606	CHL	CHB-C4A	-4.26	1.33	1.38
24	s	601	CHL	CHD-C1D	4.26	1.46	1.39
24	6	608	CHL	OBD-CAD	4.26	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	5	1623	NEX	C7-C6	-4.26	1.25	1.30
24	5	601	CHL	OBD-CAD	4.26	1.27	1.22
24	6	609	CHL	C3B-C2B	4.26	1.46	1.40
24	5	601	CHL	CHD-C4C	4.26	1.47	1.39
24	7	608	CHL	CHB-C1B	4.25	1.46	1.39
24	S	608	CHL	CHC-C4B	4.25	1.46	1.39
24	G	606	CHL	C3B-C2B	4.25	1.46	1.40
24	R	608	CHL	O2A-CGA	4.25	1.45	1.33
24	3	605	CHL	CHB-C1B	4.25	1.46	1.39
24	7	605	CHL	CHB-C1B	4.25	1.46	1.39
24	3	608	CHL	CHB-C1B	4.25	1.46	1.39
24	1	607	CHL	O2A-CGA	4.25	1.45	1.33
24	Y	609	CHL	CHD-C1D	4.24	1.46	1.39
24	n	609	CHL	CHD-C1D	4.24	1.46	1.39
24	5	609	CHL	O2A-CGA	4.24	1.45	1.33
24	s	606	CHL	CHC-C1C	4.24	1.47	1.39
24	R	606	CHL	O2A-CGA	4.24	1.45	1.33
24	6	605	CHL	CHD-C4C	4.24	1.47	1.39
24	y	609	CHL	CHD-C1D	4.24	1.46	1.39
24	r	606	CHL	O2A-CGA	4.24	1.45	1.33
24	N	605	CHL	O2A-CGA	4.24	1.45	1.33
24	y	609	CHL	O2A-CGA	4.24	1.45	1.33
24	2	605	CHL	CHD-C4C	4.24	1.47	1.39
24	2	607	CHL	CHB-C1B	4.24	1.46	1.39
24	n	605	CHL	O2A-CGA	4.24	1.45	1.33
24	N	605	CHL	CHD-C4C	4.24	1.47	1.39
24	s	608	CHL	CHC-C4B	4.24	1.46	1.39
24	8	601	CHL	C3D-C2D	4.23	1.46	1.39
24	1	601	CHL	C3B-C2B	4.23	1.46	1.40
24	g	605	CHL	CHD-C4C	4.23	1.47	1.39
24	6	607	CHL	CHB-C1B	4.23	1.46	1.39
24	1	609	CHL	O2A-CGA	4.23	1.45	1.33
24	4	608	CHL	C3B-C2B	4.23	1.46	1.40
24	Y	609	CHL	O2A-CGA	4.23	1.45	1.33
24	6	609	CHL	O2A-CGA	4.23	1.45	1.33
24	r	608	CHL	CHC-C4B	4.23	1.46	1.39
24	8	608	CHL	C3B-C2B	4.23	1.46	1.40
24	S	601	CHL	CHD-C1D	4.23	1.46	1.39
24	G	605	CHL	CHD-C4C	4.22	1.47	1.39
24	g	608	CHL	O2A-CGA	4.22	1.45	1.33
24	y	601	CHL	CHD-C4C	4.22	1.47	1.39
24	n	605	CHL	CHD-C4C	4.22	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	609	CHL	O2A-CGA	4.22	1.45	1.33
24	G	608	CHL	O2A-CGA	4.22	1.45	1.33
24	2	609	CHL	O2A-CGA	4.21	1.45	1.33
24	5	607	CHL	O2A-CGA	4.21	1.45	1.33
25	B	612	CLA	CMC-C2C	-4.21	1.42	1.50
24	2	605	CHL	CHC-C1C	4.21	1.47	1.39
24	2	608	CHL	C3B-C2B	4.21	1.46	1.40
25	b	612	CLA	CMC-C2C	-4.21	1.42	1.50
24	4	601	CHL	C3D-C2D	4.21	1.46	1.39
24	6	606	CHL	CHD-C1D	4.21	1.46	1.39
24	Y	601	CHL	CHD-C4C	4.21	1.47	1.39
24	g	606	CHL	C3B-C2B	4.21	1.46	1.40
24	3	606	CHL	CHD-C1D	4.21	1.46	1.39
24	s	608	CHL	CHC-C1C	4.21	1.47	1.39
24	2	606	CHL	CHD-C1D	4.20	1.46	1.39
24	G	609	CHL	O2A-CGA	4.20	1.45	1.33
24	8	607	CHL	CHD-C1D	4.20	1.46	1.39
24	8	609	CHL	CHC-C4B	4.20	1.46	1.39
24	5	608	CHL	CHC-C1C	4.20	1.47	1.39
24	6	601	CHL	CHD-C4C	4.20	1.47	1.39
24	7	606	CHL	CHD-C1D	4.20	1.46	1.39
24	2	601	CHL	CHD-C4C	4.20	1.47	1.39
24	6	605	CHL	CHC-C1C	4.20	1.47	1.39
24	S	607	CHL	CHD-C4C	4.20	1.47	1.39
24	3	607	CHL	CHB-C1B	4.19	1.46	1.39
24	6	608	CHL	C3B-C2B	4.19	1.46	1.40
24	4	609	CHL	CHC-C4B	4.19	1.46	1.39
24	S	608	CHL	CHC-C1C	4.19	1.47	1.39
24	4	607	CHL	CHD-C1D	4.19	1.46	1.39
24	R	608	CHL	CHC-C4B	4.19	1.46	1.39
24	g	609	CHL	CHD-C4C	4.19	1.47	1.39
24	3	601	CHL	O2A-CGA	4.18	1.45	1.33
24	7	607	CHL	CHB-C1B	4.18	1.46	1.39
24	g	606	CHL	O2A-CGA	4.18	1.45	1.33
24	Y	605	CHL	O2A-CGA	4.18	1.45	1.33
24	2	609	CHL	CHD-C4C	4.18	1.47	1.39
24	s	607	CHL	CHD-C4C	4.18	1.47	1.39
24	G	606	CHL	CHD-C4C	4.18	1.47	1.39
24	G	606	CHL	O2A-CGA	4.18	1.45	1.33
24	s	607	CHL	C3A-C2A	-4.18	1.51	1.54
24	6	609	CHL	CHD-C4C	4.17	1.47	1.39
24	y	605	CHL	O2A-CGA	4.17	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	607	CHL	C3B-C2B	4.17	1.46	1.40
24	2	607	CHL	CHC-C1C	4.17	1.47	1.39
24	1	608	CHL	CHC-C1C	4.17	1.47	1.39
24	7	606	CHL	CHD-C4C	4.17	1.47	1.39
24	7	601	CHL	O2A-CGA	4.17	1.45	1.33
24	n	609	CHL	CHD-C4C	4.16	1.47	1.39
24	6	607	CHL	CHC-C1C	4.15	1.47	1.39
24	Y	608	CHL	CHB-C1B	4.15	1.46	1.39
24	G	609	CHL	CHD-C4C	4.15	1.47	1.39
24	R	607	CHL	CHC-C4B	4.15	1.46	1.39
24	6	606	CHL	CHB-C1B	4.15	1.46	1.39
24	2	609	CHL	CHC-C4B	4.15	1.46	1.39
24	S	607	CHL	C3A-C2A	-4.15	1.51	1.54
24	7	607	CHL	C3B-C2B	4.14	1.46	1.40
24	r	607	CHL	O2A-CGA	4.14	1.45	1.33
24	2	606	CHL	CHB-C1B	4.14	1.46	1.39
24	S	607	CHL	CHD-C1D	4.14	1.46	1.39
24	6	609	CHL	CHC-C4B	4.14	1.46	1.39
24	y	608	CHL	CHB-C1B	4.14	1.46	1.39
24	g	606	CHL	CHD-C4C	4.13	1.47	1.39
24	R	607	CHL	O2A-CGA	4.13	1.45	1.33
24	R	607	CHL	CHB-C1B	4.13	1.46	1.39
24	N	609	CHL	CHD-C4C	4.13	1.47	1.39
24	n	605	CHL	CHC-C1C	4.13	1.47	1.39
24	y	601	CHL	CHC-C4B	4.13	1.46	1.39
24	7	601	CHL	CHC-C1C	4.12	1.47	1.39
24	7	606	CHL	CHC-C1C	4.12	1.47	1.39
24	R	608	CHL	CHB-C1B	4.12	1.46	1.39
24	r	606	CHL	CHC-C1C	4.12	1.47	1.39
24	s	607	CHL	CHD-C1D	4.12	1.46	1.39
24	3	606	CHL	CHC-C1C	4.11	1.47	1.39
24	3	606	CHL	C3B-C2B	4.11	1.45	1.40
24	N	605	CHL	CHC-C1C	4.11	1.47	1.39
24	6	607	CHL	O2A-CGA	4.11	1.45	1.33
24	r	607	CHL	CHC-C4B	4.11	1.46	1.39
24	r	608	CHL	CHB-C1B	4.11	1.46	1.39
24	Y	601	CHL	CHC-C4B	4.11	1.46	1.39
24	8	608	CHL	CHC-C4B	4.11	1.46	1.39
24	7	606	CHL	C3B-C2B	4.11	1.45	1.40
24	3	606	CHL	CHD-C4C	4.11	1.47	1.39
24	2	607	CHL	O2A-CGA	4.11	1.45	1.33
24	3	601	CHL	CHC-C1C	4.10	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	607	CHL	CHD-C1D	4.10	1.46	1.39
24	3	609	CHL	CHC-C4B	4.10	1.46	1.39
24	5	607	CHL	CHD-C4C	4.10	1.47	1.39
24	n	601	CHL	OBD-CAD	4.10	1.27	1.22
24	r	607	CHL	CHB-C1B	4.10	1.46	1.39
24	Y	605	CHL	C3B-C2B	4.10	1.45	1.40
24	N	608	CHL	CHB-C1B	4.10	1.46	1.39
24	Y	605	CHL	CHC-C4B	4.09	1.46	1.39
24	R	606	CHL	CHC-C1C	4.09	1.47	1.39
24	n	605	CHL	C3B-C2B	4.09	1.45	1.40
24	N	606	CHL	CHB-C1B	4.09	1.46	1.39
24	4	608	CHL	CHC-C4B	4.09	1.46	1.39
24	g	601	CHL	O2A-CGA	4.09	1.45	1.33
24	r	608	CHL	C3B-C2B	4.09	1.45	1.40
24	1	607	CHL	CHD-C1D	4.09	1.46	1.39
24	R	607	CHL	CHD-C1D	4.09	1.46	1.39
24	R	608	CHL	C3B-C2B	4.09	1.45	1.40
24	N	601	CHL	OBD-CAD	4.09	1.27	1.22
24	1	607	CHL	CHD-C4C	4.08	1.47	1.39
24	5	605	CHL	CHD-C4C	4.08	1.47	1.39
24	y	605	CHL	C3B-C2B	4.08	1.45	1.40
24	g	609	CHL	OBD-CAD	4.08	1.27	1.22
24	7	609	CHL	CHC-C4B	4.08	1.46	1.39
24	s	601	CHL	C3B-C2B	4.08	1.45	1.40
24	S	608	CHL	CHB-C4A	-4.08	1.33	1.38
24	7	608	CHL	C3B-C2B	4.08	1.45	1.40
24	n	606	CHL	CHB-C1B	4.08	1.46	1.39
24	1	601	CHL	CHC-C4B	4.08	1.46	1.39
24	1	609	CHL	CHB-C1B	4.08	1.46	1.39
24	G	609	CHL	OBD-CAD	4.08	1.27	1.22
24	5	607	CHL	CHD-C1D	4.07	1.46	1.39
24	y	605	CHL	CHC-C4B	4.07	1.46	1.39
24	5	601	CHL	CHC-C4B	4.07	1.46	1.39
24	y	608	CHL	O2A-CGA	4.07	1.45	1.33
24	3	605	CHL	CHD-C4C	4.07	1.47	1.39
24	g	605	CHL	CHC-C1C	4.07	1.47	1.39
24	y	605	CHL	CHD-C1D	4.07	1.46	1.39
24	Y	605	CHL	CHD-C1D	4.07	1.46	1.39
24	S	606	CHL	C3D-C2D	4.07	1.46	1.39
24	6	608	CHL	CHB-C1B	4.07	1.46	1.39
24	1	605	CHL	CHD-C4C	4.07	1.47	1.39
24	Y	608	CHL	O2A-CGA	4.07	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	607	CHL	O2A-CGA	4.07	1.45	1.33
24	N	608	CHL	O2A-CGA	4.07	1.45	1.33
24	3	601	CHL	OBD-CAD	4.07	1.27	1.22
24	G	601	CHL	O2A-CGA	4.06	1.45	1.33
24	Y	607	CHL	CHC-C4B	4.06	1.46	1.39
24	y	601	CHL	CHB-C1B	4.06	1.46	1.39
24	s	606	CHL	C3D-C2D	4.06	1.46	1.39
24	5	609	CHL	CHB-C1B	4.06	1.46	1.39
24	7	605	CHL	CHD-C4C	4.06	1.47	1.39
24	r	607	CHL	CHC-C1C	4.06	1.47	1.39
24	g	607	CHL	CHC-C4B	4.06	1.46	1.39
24	G	607	CHL	CHC-C4B	4.06	1.46	1.39
24	y	607	CHL	CHC-C4B	4.05	1.46	1.39
24	n	608	CHL	CHB-C1B	4.05	1.46	1.39
24	7	608	CHL	CHD-C4C	4.05	1.47	1.39
24	2	608	CHL	CHB-C1B	4.05	1.46	1.39
24	n	608	CHL	O2A-CGA	4.05	1.45	1.33
24	G	601	CHL	C3B-C2B	4.05	1.45	1.40
24	g	608	CHL	CHD-C4C	4.05	1.47	1.39
24	Y	601	CHL	CHB-C1B	4.05	1.46	1.39
24	7	601	CHL	OBD-CAD	4.04	1.27	1.22
24	g	607	CHL	O2A-CGA	4.04	1.45	1.33
24	n	606	CHL	CHC-C4B	4.04	1.46	1.39
24	G	608	CHL	CHD-C4C	4.04	1.47	1.39
24	y	609	CHL	CHD-C4C	4.04	1.47	1.39
24	4	606	CHL	CHD-C1D	4.04	1.46	1.39
24	G	605	CHL	CHC-C1C	4.04	1.47	1.39
24	4	606	CHL	CHD-C4C	4.04	1.47	1.39
24	R	607	CHL	CHC-C1C	4.04	1.47	1.39
24	N	605	CHL	C3B-C2B	4.04	1.45	1.40
24	S	601	CHL	C3B-C2B	4.04	1.45	1.40
24	s	608	CHL	CHB-C4A	-4.04	1.33	1.38
24	3	608	CHL	CHD-C4C	4.03	1.47	1.39
24	g	601	CHL	C3B-C2B	4.03	1.45	1.40
24	y	605	CHL	CHB-C1B	4.03	1.46	1.39
24	Y	609	CHL	CHD-C4C	4.03	1.47	1.39
24	8	606	CHL	CHC-C1C	4.03	1.47	1.39
24	Y	605	CHL	CHB-C1B	4.03	1.46	1.39
24	3	608	CHL	C3B-C2B	4.02	1.45	1.40
24	y	609	CHL	CHC-C4B	4.02	1.46	1.39
24	5	606	CHL	C3B-C2B	4.02	1.45	1.40
24	4	606	CHL	CHC-C1C	4.02	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	606	CHL	CHD-C4C	4.02	1.47	1.39
24	s	607	CHL	CHC-C1C	4.02	1.47	1.39
24	Y	609	CHL	CHC-C4B	4.02	1.46	1.39
24	s	601	CHL	CHB-C1B	4.02	1.46	1.39
24	2	606	CHL	CHD-C4C	4.02	1.47	1.39
24	8	607	CHL	CHC-C1C	4.01	1.47	1.39
24	8	606	CHL	CHB-C1B	4.01	1.46	1.39
24	6	606	CHL	CHD-C4C	4.01	1.47	1.39
24	N	606	CHL	CHC-C4B	4.01	1.46	1.39
24	6	608	CHL	CHD-C4C	4.01	1.47	1.39
24	6	606	CHL	CHC-C4B	4.01	1.46	1.39
24	7	601	CHL	CHC-C4B	4.01	1.46	1.39
24	2	609	CHL	CHD-C1D	4.01	1.46	1.39
24	4	607	CHL	CHC-C1C	4.00	1.47	1.39
24	2	608	CHL	CHD-C4C	4.00	1.47	1.39
24	g	606	CHL	CHD-C1D	4.00	1.46	1.39
24	N	607	CHL	C3B-C2B	4.00	1.45	1.40
24	1	606	CHL	C3B-C2B	4.00	1.45	1.40
24	2	606	CHL	CHC-C4B	4.00	1.46	1.39
24	Y	607	CHL	O2A-CGA	4.00	1.45	1.33
24	8	606	CHL	CHD-C1D	4.00	1.46	1.39
24	N	608	CHL	CHC-C1C	4.00	1.47	1.39
24	4	606	CHL	CHB-C1B	4.00	1.46	1.39
24	S	601	CHL	CHB-C1B	4.00	1.46	1.39
24	S	607	CHL	CHC-C1C	4.00	1.47	1.39
24	Y	601	CHL	O2A-CGA	4.00	1.45	1.33
24	7	606	CHL	CHB-C1B	4.00	1.46	1.39
24	3	606	CHL	CHB-C1B	3.99	1.46	1.39
24	G	606	CHL	CHD-C1D	3.99	1.46	1.39
24	3	601	CHL	CHC-C4B	3.99	1.46	1.39
24	Y	609	CHL	OBD-CAD	3.99	1.27	1.22
24	R	606	CHL	CHD-C4C	3.99	1.47	1.39
24	1	605	CHL	CHC-C4B	3.99	1.46	1.39
24	4	609	CHL	CHD-C4C	3.99	1.47	1.39
24	6	609	CHL	CHD-C1D	3.99	1.46	1.39
24	y	601	CHL	O2A-CGA	3.99	1.45	1.33
24	7	608	CHL	OBD-CAD	3.99	1.27	1.22
24	6	607	CHL	CHC-C4B	3.98	1.46	1.39
24	r	606	CHL	C3B-C2B	3.98	1.45	1.40
24	y	607	CHL	O2A-CGA	3.98	1.45	1.33
24	7	601	CHL	C3B-C2B	3.98	1.45	1.40
24	R	606	CHL	C3B-C2B	3.98	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	608	CHL	CHC-C1C	3.98	1.47	1.39
24	3	608	CHL	OBD-CAD	3.98	1.27	1.22
24	r	606	CHL	CHD-C4C	3.97	1.47	1.39
24	2	609	CHL	CHC-C1C	3.97	1.47	1.39
24	8	609	CHL	CHD-C4C	3.97	1.47	1.39
24	5	608	CHL	CHB-C1B	3.97	1.46	1.39
24	y	605	CHL	CHD-C4C	3.96	1.47	1.39
24	S	607	CHL	C3D-C2D	3.96	1.46	1.39
24	1	608	CHL	CHB-C1B	3.96	1.46	1.39
24	1	609	CHL	C3B-C2B	3.96	1.45	1.40
24	6	606	CHL	C3B-C2B	3.96	1.45	1.40
24	G	606	CHL	CHC-C1C	3.96	1.47	1.39
24	g	606	CHL	CHC-C1C	3.96	1.47	1.39
24	N	609	CHL	OBD-CAD	3.96	1.27	1.22
24	2	607	CHL	CHC-C4B	3.95	1.46	1.39
24	Y	608	CHL	C3B-C2B	3.95	1.45	1.40
24	n	607	CHL	C3B-C2B	3.95	1.45	1.40
24	3	607	CHL	CHD-C1D	3.95	1.46	1.39
24	Y	605	CHL	CHD-C4C	3.95	1.46	1.39
24	2	605	CHL	CHD-C1D	3.94	1.46	1.39
24	1	606	CHL	CHC-C1C	3.94	1.46	1.39
24	R	606	CHL	CHD-C1D	3.94	1.46	1.39
24	n	609	CHL	OBD-CAD	3.94	1.27	1.22
24	y	608	CHL	C3B-C2B	3.94	1.45	1.40
24	6	609	CHL	CHC-C1C	3.94	1.46	1.39
24	s	607	CHL	C3D-C2D	3.94	1.46	1.39
24	y	609	CHL	OBD-CAD	3.94	1.27	1.22
24	5	606	CHL	CHC-C1C	3.93	1.46	1.39
24	5	605	CHL	CHC-C4B	3.93	1.46	1.39
24	y	609	CHL	CHB-C1B	3.93	1.46	1.39
24	y	607	CHL	CHC-C1C	3.93	1.46	1.39
24	7	607	CHL	CHD-C1D	3.93	1.46	1.39
24	3	601	CHL	C3B-C2B	3.93	1.45	1.40
24	5	609	CHL	C3B-C2B	3.92	1.45	1.40
24	6	605	CHL	CHD-C1D	3.92	1.46	1.39
24	4	609	CHL	CHB-C1B	3.92	1.46	1.39
24	r	606	CHL	CHD-C1D	3.92	1.46	1.39
24	8	609	CHL	CHB-C1B	3.92	1.46	1.39
24	Y	606	CHL	OBD-CAD	3.92	1.27	1.22
24	Y	608	CHL	CHC-C1C	3.92	1.46	1.39
24	y	608	CHL	CHC-C1C	3.91	1.46	1.39
24	2	606	CHL	C3B-C2B	3.91	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	608	CHL	CHD-C4C	3.91	1.46	1.39
24	5	606	CHL	CHB-C1B	3.91	1.46	1.39
24	R	608	CHL	CHC-C1C	3.91	1.46	1.39
24	y	606	CHL	OBD-CAD	3.91	1.27	1.22
24	Y	601	CHL	C3B-C2B	3.91	1.45	1.40
24	Y	607	CHL	CHC-C1C	3.90	1.46	1.39
24	y	601	CHL	C3B-C2B	3.90	1.45	1.40
24	G	606	CHL	CHB-C1B	3.90	1.45	1.39
24	Y	609	CHL	CHB-C1B	3.90	1.45	1.39
24	N	606	CHL	OBD-CAD	3.90	1.27	1.22
24	r	606	CHL	CHB-C1B	3.89	1.45	1.39
24	5	605	CHL	CHC-C1C	3.89	1.46	1.39
24	n	608	CHL	CHD-C4C	3.89	1.46	1.39
24	n	607	CHL	CHC-C1C	3.89	1.46	1.39
24	Y	606	CHL	CHC-C4B	3.89	1.45	1.39
24	r	608	CHL	CHC-C1C	3.89	1.46	1.39
24	Y	605	CHL	CHC-C1C	3.89	1.46	1.39
24	Y	609	CHL	C3B-C2B	3.89	1.45	1.40
24	7	601	CHL	CHD-C4C	3.88	1.46	1.39
24	1	608	CHL	OBD-CAD	3.88	1.27	1.22
24	g	606	CHL	CHB-C1B	3.87	1.45	1.39
24	y	605	CHL	CHC-C1C	3.87	1.46	1.39
24	3	601	CHL	CHD-C4C	3.87	1.46	1.39
24	n	605	CHL	CHB-C1B	3.87	1.45	1.39
24	N	607	CHL	CHC-C1C	3.87	1.46	1.39
24	4	609	CHL	C3B-C2B	3.87	1.45	1.40
24	y	609	CHL	C3B-C2B	3.87	1.45	1.40
24	5	608	CHL	OBD-CAD	3.87	1.27	1.22
24	1	601	CHL	CHD-C1D	3.87	1.45	1.39
24	g	607	CHL	C3B-C2B	3.87	1.45	1.40
24	G	609	CHL	C3B-C2B	3.87	1.45	1.40
24	G	607	CHL	C3B-C2B	3.86	1.45	1.40
24	1	606	CHL	CHB-C1B	3.86	1.45	1.39
24	5	601	CHL	CHD-C1D	3.86	1.45	1.39
24	1	605	CHL	CHC-C1C	3.86	1.46	1.39
24	g	601	CHL	CHB-C1B	3.86	1.45	1.39
24	R	606	CHL	CHB-C1B	3.86	1.45	1.39
24	3	609	CHL	CHC-C1C	3.86	1.46	1.39
24	y	601	CHL	CHC-C1C	3.86	1.46	1.39
24	y	606	CHL	CHC-C4B	3.85	1.45	1.39
24	7	609	CHL	CHC-C1C	3.85	1.46	1.39
24	8	609	CHL	C3B-C2B	3.85	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	609	CHL	CHD-C1D	3.85	1.45	1.39
24	7	605	CHL	CHD-C1D	3.85	1.45	1.39
24	n	606	CHL	OBD-CAD	3.85	1.27	1.22
24	N	601	CHL	CHC-C1C	3.85	1.46	1.39
24	G	601	CHL	CHB-C1B	3.84	1.45	1.39
24	N	605	CHL	CHB-C1B	3.84	1.45	1.39
24	y	607	CHL	CBD-CGD	-3.84	1.47	1.52
24	1	605	CHL	CHD-C1D	3.84	1.45	1.39
24	3	605	CHL	CHD-C1D	3.84	1.45	1.39
24	N	608	CHL	C3B-C2B	3.83	1.45	1.40
24	S	608	CHL	C3D-C2D	3.83	1.46	1.39
24	n	608	CHL	C3B-C2B	3.83	1.45	1.40
24	2	601	CHL	CHD-C1D	3.83	1.45	1.39
24	Y	601	CHL	CHC-C1C	3.83	1.46	1.39
24	G	607	CHL	CHB-C1B	3.83	1.45	1.39
24	g	609	CHL	C3B-C2B	3.83	1.45	1.40
24	n	606	CHL	C3B-C2B	3.82	1.45	1.40
24	Y	607	CHL	CBD-CGD	-3.82	1.47	1.52
24	n	601	CHL	CHC-C1C	3.82	1.46	1.39
24	4	608	CHL	CHD-C4C	3.82	1.46	1.39
24	4	608	CHL	CHC-C1C	3.81	1.46	1.39
24	y	608	CHL	OBD-CAD	3.80	1.27	1.22
24	6	608	CHL	CHC-C1C	3.80	1.46	1.39
24	5	601	CHL	CHC-C1C	3.80	1.46	1.39
24	g	607	CHL	CHB-C1B	3.80	1.45	1.39
24	2	608	CHL	CHD-C1D	3.80	1.45	1.39
24	s	608	CHL	C3D-C2D	3.80	1.46	1.39
24	N	606	CHL	C3B-C2B	3.80	1.45	1.40
24	8	608	CHL	CHC-C1C	3.80	1.46	1.39
25	R	613	CLA	C1D-ND	3.80	1.42	1.37
24	2	608	CHL	CHC-C1C	3.79	1.46	1.39
24	g	608	CHL	CHD-C1D	3.79	1.45	1.39
25	r	613	CLA	C1D-ND	3.79	1.42	1.37
24	6	601	CHL	CHD-C1D	3.79	1.45	1.39
24	5	607	CHL	CHC-C1C	3.79	1.46	1.39
24	8	609	CHL	CHD-C1D	3.79	1.45	1.39
24	5	605	CHL	CHD-C1D	3.79	1.45	1.39
24	n	601	CHL	CHD-C1D	3.78	1.45	1.39
24	g	601	CHL	CHD-C1D	3.78	1.45	1.39
24	G	608	CHL	CHD-C1D	3.78	1.45	1.39
24	8	608	CHL	CHD-C4C	3.78	1.46	1.39
24	3	605	CHL	C3D-C2D	3.78	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	605	CHL	C3D-C2D	3.77	1.46	1.39
24	7	607	CHL	CHD-C4C	3.77	1.46	1.39
24	1	607	CHL	CHC-C4B	3.77	1.45	1.39
24	5	607	CHL	CHB-C1B	3.77	1.45	1.39
24	1	601	CHL	CHC-C1C	3.77	1.46	1.39
24	N	601	CHL	CHD-C1D	3.77	1.45	1.39
24	6	608	CHL	CHD-C1D	3.77	1.45	1.39
24	n	606	CHL	CHD-C4C	3.77	1.46	1.39
24	N	606	CHL	CHD-C1D	3.77	1.45	1.39
24	1	607	CHL	CHC-C1C	3.76	1.46	1.39
24	G	607	CHL	CHD-C4C	3.76	1.46	1.39
24	G	601	CHL	CHD-C1D	3.76	1.45	1.39
24	5	608	CHL	CBD-CGD	-3.76	1.47	1.52
24	n	607	CHL	CHC-C4B	3.76	1.45	1.39
24	Y	608	CHL	OBD-CAD	3.76	1.27	1.22
24	y	607	CHL	C3B-C2B	3.76	1.45	1.40
24	N	606	CHL	CHD-C4C	3.76	1.46	1.39
24	N	607	CHL	CHC-C4B	3.76	1.45	1.39
24	5	605	CHL	C3D-C2D	3.76	1.46	1.39
24	5	608	CHL	CHD-C4C	3.75	1.46	1.39
37	h	102	DGD	O5D-C6D	-3.75	1.37	1.43
24	7	605	CHL	C3D-C2D	3.75	1.46	1.39
24	g	607	CHL	CHD-C4C	3.75	1.46	1.39
37	H	102	DGD	O5D-C6D	-3.75	1.37	1.43
24	5	607	CHL	CHC-C4B	3.74	1.45	1.39
24	Y	607	CHL	C3B-C2B	3.74	1.45	1.40
24	1	608	CHL	CBD-CGD	-3.74	1.47	1.52
24	1	607	CHL	CHB-C1B	3.74	1.45	1.39
24	2	605	CHL	C3D-C2D	3.74	1.46	1.39
24	1	608	CHL	CHD-C4C	3.74	1.46	1.39
24	8	609	CHL	CHC-C1C	3.74	1.46	1.39
29	d	409	LHG	O7-C5	-3.74	1.37	1.46
24	1	605	CHL	C3D-C2D	3.74	1.46	1.39
24	n	606	CHL	CHD-C1D	3.74	1.45	1.39
24	y	606	CHL	C3B-C2B	3.73	1.45	1.40
24	3	607	CHL	CHD-C4C	3.73	1.46	1.39
24	n	608	CHL	OBD-CAD	3.73	1.27	1.22
24	g	609	CHL	CHB-C1B	3.73	1.45	1.39
24	G	609	CHL	CHB-C1B	3.73	1.45	1.39
24	N	608	CHL	OBD-CAD	3.73	1.27	1.22
25	s	609	CLA	C1D-ND	3.72	1.42	1.37
25	S	609	CLA	C1D-ND	3.72	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	609	CHL	CHC-C1C	3.72	1.46	1.39
24	3	605	CHL	CHC-C1C	3.72	1.46	1.39
29	D	409	LHG	O7-C5	-3.71	1.37	1.46
24	7	605	CHL	CHC-C1C	3.71	1.46	1.39
24	Y	606	CHL	C3B-C2B	3.71	1.45	1.40
24	g	605	CHL	C3D-C2D	3.68	1.45	1.39
24	6	607	CHL	C3D-C2D	3.68	1.45	1.39
24	2	606	CHL	CHC-C1C	3.68	1.46	1.39
24	G	605	CHL	C3D-C2D	3.68	1.45	1.39
24	6	606	CHL	CHC-C1C	3.67	1.46	1.39
24	2	607	CHL	C3D-C2D	3.67	1.45	1.39
29	l	101	LHG	O7-C5	-3.66	1.38	1.46
29	L	101	LHG	O7-C5	-3.66	1.38	1.46
24	N	606	CHL	CHC-C1C	3.65	1.46	1.39
25	s	604	CLA	C1D-ND	3.65	1.42	1.37
24	N	607	CHL	CHB-C1B	3.65	1.45	1.39
24	5	606	CHL	CHD-C1D	3.65	1.45	1.39
24	n	607	CHL	CHB-C1B	3.65	1.45	1.39
24	g	607	CHL	CHD-C1D	3.65	1.45	1.39
24	g	601	CHL	OBD-CAD	3.64	1.27	1.22
24	1	609	CHL	CHC-C1C	3.64	1.46	1.39
24	R	614	CHL	C3D-C2D	3.64	1.45	1.39
24	n	606	CHL	CHC-C1C	3.64	1.46	1.39
24	5	609	CHL	CHC-C1C	3.64	1.46	1.39
24	n	609	CHL	C3B-C2B	3.64	1.45	1.40
24	G	601	CHL	OBD-CAD	3.63	1.27	1.22
24	G	607	CHL	CHD-C1D	3.63	1.45	1.39
24	1	607	CHL	C3B-C2B	3.63	1.45	1.40
24	7	601	CHL	CHB-C1B	3.63	1.45	1.39
24	6	601	CHL	CHC-C1C	3.62	1.46	1.39
24	3	601	CHL	CHB-C1B	3.62	1.45	1.39
24	2	601	CHL	CHC-C1C	3.62	1.46	1.39
24	G	601	CHL	CHC-C1C	3.62	1.46	1.39
24	5	607	CHL	C3B-C2B	3.62	1.45	1.40
24	4	607	CHL	C3D-C2D	3.62	1.45	1.39
24	S	601	CHL	C3D-C2D	3.61	1.45	1.39
28	N	1623	NEX	C7-C6	-3.61	1.26	1.30
24	Y	608	CHL	CHD-C4C	3.61	1.46	1.39
24	g	601	CHL	CHC-C1C	3.61	1.46	1.39
24	N	609	CHL	C3B-C2B	3.60	1.45	1.40
24	y	608	CHL	CHD-C4C	3.60	1.46	1.39
24	s	601	CHL	C3D-C2D	3.60	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	601	CHL	CBD-CGD	-3.60	1.48	1.52
24	1	606	CHL	CHD-C1D	3.59	1.45	1.39
24	1	606	CHL	CHD-C4C	3.59	1.46	1.39
24	5	601	CHL	CBD-CGD	-3.59	1.48	1.52
24	r	614	CHL	C3D-C2D	3.59	1.45	1.39
24	5	606	CHL	CHD-C4C	3.58	1.46	1.39
24	y	607	CHL	CHD-C4C	3.58	1.46	1.39
24	8	607	CHL	C3D-C2D	3.58	1.45	1.39
25	y	604	CLA	CMB-C2B	-3.58	1.43	1.50
24	Y	607	CHL	CHD-C4C	3.57	1.46	1.39
25	S	604	CLA	C1D-ND	3.57	1.42	1.37
28	n	1623	NEX	C7-C6	-3.57	1.26	1.30
36	D	405	PL9	C53-C6	-3.57	1.43	1.50
25	s	603	CLA	C1D-ND	3.56	1.42	1.37
24	Y	601	CHL	OBD-CAD	3.56	1.27	1.22
24	y	601	CHL	CBD-CGD	-3.56	1.48	1.52
25	Y	604	CLA	CMB-C2B	-3.56	1.43	1.50
24	N	607	CHL	CHD-C4C	3.55	1.46	1.39
24	1	608	CHL	CHD-C1D	3.54	1.45	1.39
36	d	405	PL9	C53-C6	-3.54	1.43	1.50
24	Y	601	CHL	CBD-CGD	-3.54	1.48	1.52
24	8	608	CHL	OBD-CAD	3.54	1.26	1.22
24	1	607	CHL	CBD-CGD	-3.54	1.48	1.52
25	S	603	CLA	C1D-ND	3.54	1.42	1.37
24	y	606	CHL	CHD-C4C	3.53	1.46	1.39
25	7	614	CLA	C1D-ND	3.53	1.42	1.37
28	r	623	NEX	C7-C6	-3.53	1.26	1.30
24	n	608	CHL	CHD-C1D	3.53	1.45	1.39
24	4	608	CHL	OBD-CAD	3.52	1.26	1.22
24	n	607	CHL	CHD-C4C	3.52	1.46	1.39
24	y	601	CHL	OBD-CAD	3.52	1.26	1.22
28	R	623	NEX	C7-C6	-3.52	1.26	1.30
24	Y	606	CHL	CHD-C4C	3.52	1.46	1.39
24	5	607	CHL	CBD-CGD	-3.52	1.48	1.52
24	5	608	CHL	CHD-C1D	3.52	1.45	1.39
25	S	610	CLA	C1D-ND	3.52	1.42	1.37
25	s	610	CLA	C1D-ND	3.52	1.42	1.37
25	3	614	CLA	C4B-NB	3.52	1.42	1.37
24	y	605	CHL	C3D-C2D	3.52	1.45	1.39
25	3	614	CLA	C1D-ND	3.51	1.42	1.37
24	4	606	CHL	C3D-C2D	3.51	1.45	1.39
24	N	608	CHL	CHD-C1D	3.51	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	608	CHL	CHD-C4C	3.51	1.46	1.39
24	1	609	CHL	CBD-CGD	-3.51	1.48	1.52
24	5	609	CHL	CBD-CGD	-3.51	1.48	1.52
24	G	609	CHL	CHC-C4B	3.51	1.45	1.39
24	6	609	CHL	C3D-C2D	3.50	1.45	1.39
24	2	609	CHL	C3D-C2D	3.50	1.45	1.39
24	8	606	CHL	C3D-C2D	3.49	1.45	1.39
25	7	614	CLA	C4B-NB	3.49	1.42	1.37
24	Y	605	CHL	C3D-C2D	3.49	1.45	1.39
24	3	601	CHL	CHD-C1D	3.49	1.45	1.39
24	r	608	CHL	CHD-C4C	3.49	1.46	1.39
25	s	602	CLA	C1D-ND	3.49	1.42	1.37
28	1	1623	NEX	C7-C8	-3.48	1.26	1.31
24	3	601	CHL	CBD-CGD	-3.47	1.48	1.52
33	a	409	PHO	C4D-CHA	3.47	1.44	1.39
28	5	1623	NEX	C7-C8	-3.47	1.26	1.31
24	7	601	CHL	CHD-C1D	3.47	1.45	1.39
24	7	607	CHL	C3D-C2D	3.46	1.45	1.39
25	B	613	CLA	CMD-C2D	-3.46	1.43	1.50
24	g	609	CHL	CHC-C4B	3.46	1.45	1.39
24	n	607	CHL	CHD-C1D	3.46	1.45	1.39
33	A	409	PHO	C4D-CHA	3.45	1.44	1.39
24	5	609	CHL	CHC-C4B	3.45	1.45	1.39
24	N	607	CHL	CHD-C1D	3.44	1.45	1.39
24	8	601	CHL	C3A-C2A	-3.44	1.51	1.54
25	b	613	CLA	CMD-C2D	-3.44	1.43	1.50
24	4	601	CHL	C3A-C2A	-3.44	1.51	1.54
24	y	607	CHL	CHB-C1B	3.44	1.45	1.39
24	3	607	CHL	C3D-C2D	3.43	1.45	1.39
24	r	607	CHL	C3D-C2D	3.43	1.45	1.39
24	y	607	CHL	CHD-C1D	3.43	1.45	1.39
24	8	608	CHL	CHD-C1D	3.43	1.45	1.39
24	5	608	CHL	C3B-C2B	3.42	1.45	1.40
25	c	511	CLA	C1D-ND	3.42	1.42	1.37
24	G	607	CHL	C3D-C2D	3.42	1.45	1.39
29	G	2630	LHG	O7-C5	-3.42	1.38	1.46
37	h	102	DGD	O2G-C2G	-3.42	1.38	1.46
29	g	2630	LHG	O7-C5	-3.41	1.38	1.46
24	1	608	CHL	C3B-C2B	3.41	1.45	1.40
24	4	608	CHL	CHD-C1D	3.41	1.45	1.39
24	n	605	CHL	C3D-C2D	3.41	1.45	1.39
25	C	511	CLA	C1D-ND	3.41	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	507	CLA	C1D-ND	3.41	1.42	1.37
24	7	601	CHL	CBD-CGD	-3.41	1.48	1.52
24	1	609	CHL	CHC-C4B	3.41	1.45	1.39
25	C	513	CLA	C1D-ND	3.41	1.42	1.37
25	S	602	CLA	C1D-ND	3.41	1.42	1.37
25	N	604	CLA	CMB-C2B	-3.41	1.43	1.50
24	Y	609	CHL	CHC-C1C	3.40	1.45	1.39
25	C	507	CLA	C1D-ND	3.40	1.42	1.37
24	y	609	CHL	CHC-C1C	3.40	1.45	1.39
25	C	503	CLA	C1D-ND	3.40	1.42	1.37
24	R	607	CHL	C3D-C2D	3.40	1.45	1.39
24	g	607	CHL	C3D-C2D	3.40	1.45	1.39
24	3	609	CHL	C3D-C2D	3.40	1.45	1.39
24	Y	607	CHL	CHB-C1B	3.40	1.45	1.39
37	H	102	DGD	O2G-C2G	-3.40	1.38	1.46
24	Y	607	CHL	CHD-C1D	3.40	1.45	1.39
25	c	504	CLA	C1D-ND	3.39	1.42	1.37
25	n	604	CLA	CMB-C2B	-3.39	1.43	1.50
25	c	502	CLA	C1D-ND	3.39	1.42	1.37
24	8	608	CHL	CBD-CGD	-3.39	1.48	1.52
25	c	503	CLA	C1D-ND	3.38	1.42	1.37
28	s	1623	NEX	C7-C8	-3.38	1.26	1.31
25	C	508	CLA	C1D-ND	3.38	1.42	1.37
25	c	508	CLA	C1D-ND	3.38	1.42	1.37
24	N	609	CHL	C3D-C2D	3.38	1.45	1.39
25	c	513	CLA	C1D-ND	3.38	1.42	1.37
24	4	608	CHL	CBD-CGD	-3.37	1.48	1.52
24	N	605	CHL	C3D-C2D	3.37	1.45	1.39
24	7	609	CHL	C3D-C2D	3.37	1.45	1.39
28	S	1623	NEX	C7-C8	-3.37	1.26	1.31
24	r	608	CHL	CBD-CGD	-3.37	1.48	1.52
25	C	504	CLA	C1D-ND	3.36	1.42	1.37
25	c	506	CLA	C1D-ND	3.35	1.42	1.37
25	s	611	CLA	C1D-ND	3.35	1.42	1.37
25	S	611	CLA	C1D-ND	3.35	1.42	1.37
25	C	501	CLA	C4B-NB	3.35	1.42	1.37
25	7	611	CLA	CMB-C2B	-3.34	1.43	1.50
25	s	602	CLA	C4B-NB	3.33	1.42	1.37
24	6	608	CHL	C3D-C2D	3.33	1.45	1.39
25	S	602	CLA	C4B-NB	3.33	1.42	1.37
24	R	608	CHL	CBD-CGD	-3.33	1.48	1.52
25	C	502	CLA	C1D-ND	3.33	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	611	CLA	CMB-C2B	-3.33	1.43	1.50
36	d	405	PL9	C52-C5	-3.32	1.44	1.50
24	r	608	CHL	OBD-CAD	3.32	1.26	1.22
24	R	608	CHL	OBD-CAD	3.32	1.26	1.22
24	n	609	CHL	CHB-C1B	3.32	1.45	1.39
24	6	609	CHL	CBD-CGD	-3.32	1.48	1.52
25	C	506	CLA	C1D-ND	3.32	1.42	1.37
24	n	609	CHL	C3D-C2D	3.32	1.45	1.39
36	D	405	PL9	C52-C5	-3.32	1.44	1.50
24	N	609	CHL	CHB-C1B	3.32	1.45	1.39
24	2	608	CHL	C3D-C2D	3.32	1.45	1.39
24	Y	606	CHL	CHD-C1D	3.32	1.45	1.39
24	6	606	CHL	C3D-C2D	3.32	1.45	1.39
24	2	609	CHL	CBD-CGD	-3.31	1.48	1.52
24	3	607	CHL	CBD-CGD	-3.31	1.48	1.52
24	y	606	CHL	CHD-C1D	3.31	1.45	1.39
24	2	606	CHL	C3D-C2D	3.30	1.45	1.39
25	c	501	CLA	C4B-NB	3.30	1.42	1.37
25	G	604	CLA	CMB-C2B	-3.30	1.44	1.50
24	y	608	CHL	CBD-CGD	-3.29	1.48	1.52
24	7	607	CHL	CBD-CGD	-3.29	1.48	1.52
25	g	604	CLA	CMB-C2B	-3.29	1.44	1.50
24	Y	606	CHL	CBD-CGD	-3.29	1.48	1.52
28	r	623	NEX	C7-C8	-3.28	1.26	1.31
25	S	609	CLA	C4B-NB	3.28	1.42	1.37
33	A	408	PHO	C4D-CHA	3.27	1.44	1.39
24	8	606	CHL	CBD-CGD	-3.27	1.48	1.52
28	2	1623	NEX	C7-C8	-3.27	1.26	1.31
36	d	405	PL9	C36-C34	-3.27	1.44	1.51
24	4	606	CHL	CBD-CGD	-3.27	1.48	1.52
29	D	408	LHG	O7-C5	-3.27	1.38	1.46
24	y	606	CHL	CBD-CGD	-3.27	1.48	1.52
24	N	601	CHL	C3D-C2D	3.26	1.45	1.39
24	y	601	CHL	CHD-C1D	3.26	1.44	1.39
33	a	408	PHO	C4D-CHA	3.26	1.44	1.39
36	D	405	PL9	C36-C34	-3.26	1.44	1.51
24	y	609	CHL	CBD-CGD	-3.26	1.48	1.52
28	R	623	NEX	C7-C8	-3.26	1.26	1.31
24	N	609	CHL	CHC-C4B	3.26	1.44	1.39
28	G	1623	NEX	C7-C6	-3.26	1.26	1.30
25	s	609	CLA	C4B-NB	3.26	1.42	1.37
24	Y	601	CHL	CHD-C1D	3.25	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	604	CLA	C1D-ND	3.25	1.42	1.37
24	R	606	CHL	C3D-C2D	3.25	1.45	1.39
24	5	606	CHL	CBD-CGD	-3.25	1.48	1.52
24	n	601	CHL	C3D-C2D	3.25	1.45	1.39
24	Y	608	CHL	CBD-CGD	-3.25	1.48	1.52
24	g	609	CHL	C3D-C2D	3.24	1.45	1.39
24	1	606	CHL	CBD-CGD	-3.24	1.48	1.52
29	d	408	LHG	O7-C5	-3.24	1.39	1.46
28	6	1623	NEX	C7-C8	-3.24	1.26	1.31
25	c	505	CLA	C1D-ND	3.24	1.42	1.37
24	n	609	CHL	CHC-C4B	3.23	1.44	1.39
24	r	606	CHL	C3D-C2D	3.23	1.45	1.39
24	g	609	CHL	CHC-C1C	3.23	1.45	1.39
24	y	606	CHL	CHC-C1C	3.23	1.45	1.39
24	G	609	CHL	CHC-C1C	3.23	1.45	1.39
24	Y	609	CHL	CBD-CGD	-3.23	1.48	1.52
25	s	613	CLA	C1D-ND	3.23	1.42	1.37
24	y	608	CHL	CHD-C1D	3.22	1.44	1.39
24	8	609	CHL	C3D-C2D	3.22	1.45	1.39
24	Y	608	CHL	CHD-C1D	3.22	1.44	1.39
25	s	603	CLA	C4B-NB	3.21	1.42	1.37
24	G	609	CHL	C3D-C2D	3.21	1.45	1.39
24	8	608	CHL	C3D-C2D	3.21	1.45	1.39
25	b	604	CLA	CMB-C2B	-3.21	1.44	1.50
25	C	505	CLA	C1D-ND	3.21	1.42	1.37
25	2	604	CLA	C1D-ND	3.20	1.42	1.37
25	B	617	CLA	CMC-C2C	-3.20	1.44	1.50
24	3	608	CHL	CBD-CGD	-3.20	1.48	1.52
24	1	609	CHL	C3D-C2D	3.20	1.45	1.39
24	Y	606	CHL	CHC-C1C	3.20	1.45	1.39
25	B	604	CLA	CMB-C2B	-3.20	1.44	1.50
24	4	608	CHL	C3D-C2D	3.20	1.45	1.39
25	b	617	CLA	CMC-C2C	-3.20	1.44	1.50
39	F	101	HEM	CAC-C3C	3.19	1.55	1.47
24	5	609	CHL	C3D-C2D	3.19	1.45	1.39
25	G	603	CLA	C4B-NB	3.19	1.42	1.37
39	f	101	HEM	CAC-C3C	3.19	1.55	1.47
25	n	613	CLA	C4B-NB	3.19	1.42	1.37
25	5	612	CLA	C1D-ND	3.19	1.42	1.37
24	4	609	CHL	C3D-C2D	3.19	1.45	1.39
24	2	608	CHL	CBD-CGD	-3.19	1.48	1.52
24	3	608	CHL	CHD-C1D	3.19	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	603	CLA	C4B-NB	3.18	1.42	1.37
25	S	613	CLA	C1D-ND	3.18	1.42	1.37
24	7	608	CHL	CBD-CGD	-3.18	1.48	1.52
24	7	609	CHL	CBD-CGD	-3.18	1.48	1.52
28	g	1623	NEX	C7-C6	-3.18	1.26	1.30
29	y	2630	LHG	O7-C5	-3.18	1.39	1.46
25	G	612	CLA	C1D-ND	3.18	1.42	1.37
25	N	613	CLA	C4B-NB	3.18	1.42	1.37
25	S	612	CLA	C1D-ND	3.17	1.42	1.37
25	g	612	CLA	C1D-ND	3.17	1.42	1.37
25	S	614	CLA	C1D-ND	3.17	1.42	1.37
25	g	603	CLA	C4B-NB	3.17	1.42	1.37
24	3	605	CHL	CBD-CGD	-3.16	1.48	1.52
25	c	512	CLA	C1D-ND	3.16	1.42	1.37
25	s	612	CLA	C1D-ND	3.16	1.42	1.37
24	6	608	CHL	CBD-CGD	-3.16	1.48	1.52
24	3	609	CHL	CBD-CGD	-3.16	1.48	1.52
25	y	613	CLA	C1D-ND	3.15	1.42	1.37
29	3	2630	LHG	O7-C5	-3.15	1.39	1.46
25	A	406	CLA	C1D-ND	3.15	1.42	1.37
25	B	605	CLA	CMD-C2D	-3.15	1.44	1.50
29	7	2630	LHG	O7-C5	-3.14	1.39	1.46
25	a	406	CLA	C1D-ND	3.14	1.42	1.37
29	Y	2630	LHG	O7-C5	-3.14	1.39	1.46
29	n	2630	LHG	O7-C5	-3.14	1.39	1.46
25	b	605	CLA	CMD-C2D	-3.14	1.44	1.50
24	7	605	CHL	CBD-CGD	-3.14	1.48	1.52
25	c	501	CLA	C1D-ND	3.14	1.42	1.37
25	1	604	CLA	CMB-C2B	-3.14	1.44	1.50
39	f	101	HEM	CAB-C3B	3.14	1.55	1.47
25	B	615	CLA	CMD-C2D	-3.14	1.44	1.50
25	5	604	CLA	CMB-C2B	-3.14	1.44	1.50
25	C	501	CLA	C1D-ND	3.14	1.42	1.37
39	F	101	HEM	CAB-C3B	3.13	1.55	1.47
29	N	2630	LHG	O7-C5	-3.13	1.39	1.46
25	s	614	CLA	C1D-ND	3.13	1.42	1.37
25	C	512	CLA	C1D-ND	3.13	1.42	1.37
28	N	1623	NEX	C7-C8	-3.12	1.26	1.31
24	Y	609	CHL	C3D-C2D	3.12	1.45	1.39
25	1	612	CLA	C1D-ND	3.12	1.42	1.37
25	s	612	CLA	C4B-NB	3.12	1.42	1.37
24	7	608	CHL	CHD-C1D	3.12	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	609	CHL	C3D-C2D	3.12	1.45	1.39
25	S	612	CLA	C4B-NB	3.12	1.42	1.37
24	g	601	CHL	C3D-C2D	3.11	1.45	1.39
28	6	1623	NEX	C7-C6	-3.11	1.27	1.30
28	n	1623	NEX	C7-C8	-3.11	1.26	1.31
25	Y	613	CLA	C1D-ND	3.10	1.41	1.37
24	G	606	CHL	C3D-C2D	3.10	1.44	1.39
25	b	615	CLA	CMD-C2D	-3.10	1.44	1.50
28	2	1623	NEX	C7-C6	-3.09	1.27	1.30
24	n	607	CHL	CBD-CGD	-3.08	1.48	1.52
24	G	601	CHL	C3D-C2D	3.08	1.44	1.39
33	A	408	PHO	C1D-C2D	3.08	1.42	1.39
24	g	606	CHL	C3D-C2D	3.08	1.44	1.39
25	c	504	CLA	C4B-NB	3.07	1.41	1.37
25	c	509	CLA	C1D-ND	3.07	1.41	1.37
25	C	509	CLA	C1D-ND	3.06	1.41	1.37
25	4	611	CLA	C1D-ND	3.06	1.41	1.37
33	a	408	PHO	C1D-C2D	3.06	1.42	1.39
25	2	612	CLA	C1D-ND	3.06	1.41	1.37
34	b	623	SQD	O48-C23	3.06	1.42	1.33
25	C	510	CLA	C1D-ND	3.06	1.41	1.37
24	R	607	CHL	CBD-CGD	-3.05	1.48	1.52
34	B	623	SQD	O48-C23	3.05	1.42	1.33
25	a	405	CLA	CMC-C2C	-3.05	1.44	1.50
25	C	506	CLA	CMB-C2B	-3.05	1.44	1.50
24	r	607	CHL	CBD-CGD	-3.04	1.48	1.52
25	8	611	CLA	C1D-ND	3.04	1.41	1.37
25	c	506	CLA	CMB-C2B	-3.04	1.44	1.50
25	N	612	CLA	C1D-ND	3.04	1.41	1.37
24	n	607	CHL	C3D-C2D	3.04	1.44	1.39
25	S	610	CLA	C4B-NB	3.04	1.41	1.37
33	A	409	PHO	C1D-C2D	3.04	1.42	1.39
25	A	405	CLA	CMC-C2C	-3.03	1.44	1.50
25	s	610	CLA	C4B-NB	3.03	1.41	1.37
25	c	510	CLA	C1D-ND	3.03	1.41	1.37
25	6	612	CLA	C1D-ND	3.03	1.41	1.37
25	S	613	CLA	C4B-NB	3.03	1.41	1.37
24	r	606	CHL	CBD-CGD	-3.03	1.48	1.52
25	s	611	CLA	C4B-NB	3.03	1.41	1.37
33	a	409	PHO	C1D-C2D	3.02	1.42	1.39
34	b	623	SQD	O47-C7	3.02	1.42	1.34
24	R	606	CHL	CBD-CGD	-3.02	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	612	CLA	C1D-ND	3.02	1.41	1.37
25	C	504	CLA	C4B-NB	3.02	1.41	1.37
24	N	607	CHL	CBD-CGD	-3.02	1.48	1.52
25	s	604	CLA	C4B-NB	3.02	1.41	1.37
34	B	623	SQD	O47-C7	3.02	1.42	1.34
24	N	607	CHL	C3D-C2D	3.02	1.44	1.39
25	N	614	CLA	C1D-ND	3.02	1.41	1.37
25	S	611	CLA	C4B-NB	3.02	1.41	1.37
25	c	511	CLA	C4B-NB	3.01	1.41	1.37
25	s	613	CLA	C4B-NB	3.01	1.41	1.37
24	1	606	CHL	C3D-C2D	3.01	1.44	1.39
24	g	601	CHL	CBD-CGD	-3.01	1.48	1.52
25	6	612	CLA	C4B-NB	3.01	1.41	1.37
25	A	407	CLA	C1D-ND	3.01	1.41	1.37
25	S	604	CLA	C4B-NB	3.00	1.41	1.37
28	y	1623	NEX	C7-C8	-3.00	1.27	1.31
24	8	607	CHL	CBD-CGD	-3.00	1.48	1.52
25	n	612	CLA	C1D-ND	2.99	1.41	1.37
25	N	611	CLA	C1D-ND	2.99	1.41	1.37
33	A	409	PHO	CMC-C2C	-2.99	1.46	1.50
25	B	613	CLA	MG-ND	-2.99	1.99	2.05
25	B	612	CLA	CMB-C2B	-2.99	1.44	1.50
33	a	409	PHO	CMC-C2C	-2.99	1.46	1.50
25	B	607	CLA	C1D-ND	2.99	1.41	1.37
25	b	612	CLA	CMB-C2B	-2.98	1.44	1.50
25	B	602	CLA	C1D-ND	2.98	1.41	1.37
24	5	606	CHL	C3D-C2D	2.98	1.44	1.39
25	N	613	CLA	C1D-ND	2.98	1.41	1.37
25	n	614	CLA	C1D-ND	2.98	1.41	1.37
25	b	613	CLA	MG-ND	-2.98	1.99	2.05
25	b	602	CLA	C1D-ND	2.98	1.41	1.37
24	G	601	CHL	CBD-CGD	-2.98	1.48	1.52
25	2	613	CLA	C4B-NB	2.98	1.41	1.37
36	d	405	PL9	C26-C24	-2.98	1.45	1.51
25	2	612	CLA	C4B-NB	2.98	1.41	1.37
25	b	607	CLA	C1D-ND	2.98	1.41	1.37
25	b	604	CLA	MG-NB	-2.97	1.99	2.05
25	C	503	CLA	C4B-NB	2.97	1.41	1.37
25	c	503	CLA	C4B-NB	2.97	1.41	1.37
24	Y	606	CHL	C3D-C2D	2.97	1.44	1.39
28	Y	1623	NEX	C7-C8	-2.97	1.27	1.31
25	C	511	CLA	C4B-NB	2.97	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	506	CLA	C4B-NB	2.96	1.41	1.37
24	2	601	CHL	CBD-CGD	-2.96	1.48	1.52
36	d	405	PL9	C16-C14	-2.96	1.45	1.51
25	a	407	CLA	C1D-ND	2.96	1.41	1.37
24	N	609	CHL	CBD-CGD	-2.96	1.48	1.52
36	D	405	PL9	C26-C24	-2.96	1.45	1.51
24	6	601	CHL	CBD-CGD	-2.96	1.48	1.52
24	y	606	CHL	C3D-C2D	2.96	1.44	1.39
24	r	608	CHL	CHD-C1D	2.96	1.44	1.39
25	c	501	CLA	C3B-C4B	2.96	1.51	1.42
29	R	2630	LHG	O7-C5	-2.96	1.39	1.46
29	r	2630	LHG	O7-C5	-2.95	1.39	1.46
29	c	522	LHG	O7-C5	-2.95	1.39	1.46
25	B	604	CLA	MG-NB	-2.95	1.99	2.05
24	g	608	CHL	C3D-C2D	2.95	1.44	1.39
25	B	606	CLA	C1D-ND	2.95	1.41	1.37
25	N	610	CLA	C1D-ND	2.95	1.41	1.37
25	n	611	CLA	C1D-ND	2.95	1.41	1.37
24	R	608	CHL	CHD-C1D	2.95	1.44	1.39
29	C	522	LHG	O7-C5	-2.95	1.39	1.46
34	a	418	SQD	O47-C7	2.95	1.42	1.34
25	d	402	CLA	CMD-C2D	-2.95	1.44	1.50
25	n	613	CLA	C1D-ND	2.95	1.41	1.37
25	b	606	CLA	C1D-ND	2.94	1.41	1.37
25	r	612	CLA	C4B-NB	2.94	1.41	1.37
25	g	602	CLA	CMC-C2C	-2.94	1.44	1.50
25	C	501	CLA	C3B-C4B	2.94	1.51	1.42
34	B	621	SQD	O47-C7	2.94	1.42	1.34
25	c	506	CLA	C4B-NB	2.94	1.41	1.37
25	r	612	CLA	C1D-ND	2.94	1.41	1.37
33	A	408	PHO	CMC-C2C	-2.94	1.46	1.50
36	D	405	PL9	C16-C14	-2.93	1.45	1.51
25	g	610	CLA	C1D-ND	2.93	1.41	1.37
24	G	608	CHL	C3D-C2D	2.92	1.44	1.39
25	D	402	CLA	CMD-C2D	-2.92	1.44	1.50
25	6	613	CLA	C4B-NB	2.92	1.41	1.37
24	n	609	CHL	CHC-C1C	2.92	1.45	1.39
24	n	609	CHL	CBD-CGD	-2.92	1.48	1.52
34	A	418	SQD	O47-C7	2.92	1.42	1.34
26	y	1621	LUT	C22-C21	-2.92	1.51	1.54
25	r	611	CLA	C1D-ND	2.92	1.41	1.37
34	b	621	SQD	O47-C7	2.92	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	602	CLA	C1D-ND	2.92	1.41	1.37
28	s	1623	NEX	C7-C6	-2.92	1.27	1.30
25	G	610	CLA	C1D-ND	2.92	1.41	1.37
29	s	2630	LHG	O7-C5	-2.92	1.39	1.46
36	d	405	PL9	C11-C9	-2.91	1.45	1.51
25	b	605	CLA	CMB-C2B	-2.91	1.44	1.50
25	C	512	CLA	C4B-NB	2.91	1.41	1.37
25	R	612	CLA	C4B-NB	2.91	1.41	1.37
29	S	2630	LHG	O7-C5	-2.91	1.39	1.46
25	G	614	CLA	C1D-ND	2.91	1.41	1.37
24	1	607	CHL	C3D-C2D	2.91	1.44	1.39
24	N	609	CHL	CHC-C1C	2.91	1.44	1.39
25	N	602	CLA	C1D-ND	2.91	1.41	1.37
33	a	408	PHO	CMC-C2C	-2.91	1.46	1.50
24	N	608	CHL	C3D-C2D	2.91	1.44	1.39
25	R	611	CLA	C1D-ND	2.91	1.41	1.37
25	c	512	CLA	C4B-NB	2.91	1.41	1.37
25	d	402	CLA	CMC-C2C	-2.90	1.44	1.50
34	b	621	SQD	O48-C23	2.90	1.41	1.33
24	4	607	CHL	CBD-CGD	-2.90	1.48	1.52
25	n	610	CLA	C1D-ND	2.90	1.41	1.37
25	G	602	CLA	CMC-C2C	-2.89	1.44	1.50
25	5	614	CLA	C1D-ND	2.89	1.41	1.37
24	5	607	CHL	C3D-C2D	2.89	1.44	1.39
36	d	405	PL9	C41-C39	-2.89	1.45	1.51
34	B	621	SQD	O48-C23	2.89	1.41	1.33
28	S	1623	NEX	C7-C6	-2.89	1.27	1.30
25	D	402	CLA	CMC-C2C	-2.89	1.44	1.50
36	D	405	PL9	C41-C39	-2.88	1.45	1.51
25	B	605	CLA	CMB-C2B	-2.88	1.44	1.50
24	n	608	CHL	C3D-C2D	2.88	1.44	1.39
25	2	614	CLA	C1D-ND	2.88	1.41	1.37
24	6	606	CHL	CBD-CGD	-2.88	1.48	1.52
24	n	606	CHL	CBD-CGD	-2.88	1.48	1.52
25	b	611	CLA	MG-NB	-2.88	2.00	2.05
36	D	405	PL9	C11-C9	-2.88	1.45	1.51
26	Y	1621	LUT	C22-C21	-2.88	1.51	1.54
25	G	613	CLA	C4B-NB	2.88	1.41	1.37
25	g	613	CLA	C4B-NB	2.88	1.41	1.37
25	n	613	CLA	C1B-C2B	2.88	1.49	1.43
25	g	614	CLA	C1D-ND	2.88	1.41	1.37
25	G	604	CLA	C1D-ND	2.88	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	611	CLA	MG-NB	-2.87	2.00	2.05
25	6	603	CLA	C1D-ND	2.87	1.41	1.37
25	n	603	CLA	CMD-C2D	-2.87	1.44	1.50
25	B	613	CLA	MG-NB	-2.87	2.00	2.05
25	1	614	CLA	C1D-ND	2.87	1.41	1.37
25	3	611	CLA	CMD-C2D	-2.87	1.44	1.50
24	2	606	CHL	CBD-CGD	-2.87	1.48	1.52
25	N	613	CLA	C1B-C2B	2.87	1.49	1.43
25	6	611	CLA	C1D-ND	2.87	1.41	1.37
25	b	613	CLA	MG-NB	-2.87	2.00	2.05
25	R	601	CLA	C4B-NB	2.86	1.41	1.37
25	8	610	CLA	CMC-C2C	-2.86	1.44	1.50
33	A	408	PHO	C4D-ND	-2.86	1.34	1.38
25	2	611	CLA	C1D-ND	2.86	1.41	1.37
25	c	505	CLA	C4B-NB	2.86	1.41	1.37
25	y	611	CLA	C4B-NB	2.86	1.41	1.37
34	a	412	SQD	O48-C23	2.86	1.41	1.33
34	A	412	SQD	O48-C23	2.86	1.41	1.33
25	7	611	CLA	CMD-C2D	-2.86	1.44	1.50
25	g	604	CLA	C1D-ND	2.86	1.41	1.37
25	y	610	CLA	CMC-C2C	-2.86	1.44	1.50
25	Y	602	CLA	CMC-C2C	-2.85	1.44	1.50
25	3	604	CLA	C1D-ND	2.85	1.41	1.37
34	a	418	SQD	O48-C23	2.85	1.41	1.33
24	G	607	CHL	CBD-CGD	-2.85	1.48	1.52
24	n	608	CHL	CBD-CGD	-2.85	1.48	1.52
25	Y	611	CLA	C4B-NB	2.85	1.41	1.37
25	4	610	CLA	CMC-C2C	-2.85	1.44	1.50
25	g	613	CLA	C1D-ND	2.85	1.41	1.37
24	N	608	CHL	CBD-CGD	-2.85	1.48	1.52
33	A	409	PHO	CMD-C2D	-2.84	1.45	1.51
25	r	601	CLA	C1D-ND	2.84	1.41	1.37
25	4	604	CLA	C1D-ND	2.84	1.41	1.37
25	c	510	CLA	CMD-C2D	-2.84	1.44	1.50
25	S	614	CLA	C4B-NB	2.84	1.41	1.37
25	A	405	CLA	C1D-ND	2.84	1.41	1.37
25	C	510	CLA	C4B-NB	2.84	1.41	1.37
25	y	602	CLA	CMC-C2C	-2.84	1.45	1.50
25	N	603	CLA	CMD-C2D	-2.84	1.45	1.50
34	A	418	SQD	O48-C23	2.84	1.41	1.33
25	7	604	CLA	C1D-ND	2.84	1.41	1.37
25	8	604	CLA	C1D-ND	2.84	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	608	CHL	C3D-C2D	2.83	1.44	1.39
25	R	604	CLA	C1D-ND	2.83	1.41	1.37
25	G	604	CLA	C4B-NB	2.83	1.41	1.37
25	2	603	CLA	C1D-ND	2.83	1.41	1.37
25	r	604	CLA	C1D-ND	2.83	1.41	1.37
25	6	614	CLA	C1D-ND	2.83	1.41	1.37
25	s	614	CLA	C4B-NB	2.83	1.41	1.37
33	a	408	PHO	C4D-ND	-2.83	1.34	1.38
28	7	1623	NEX	C7-C8	-2.83	1.27	1.31
25	C	510	CLA	CMD-C2D	-2.83	1.45	1.50
25	C	505	CLA	C4B-NB	2.83	1.41	1.37
25	r	601	CLA	C4B-NB	2.82	1.41	1.37
25	g	604	CLA	C4B-NB	2.82	1.41	1.37
28	3	1623	NEX	C7-C8	-2.82	1.27	1.31
25	b	613	CLA	CMC-C2C	-2.82	1.45	1.50
33	a	409	PHO	CMD-C2D	-2.82	1.46	1.51
25	4	603	CLA	C1D-ND	2.82	1.41	1.37
24	3	608	CHL	C3D-C2D	2.82	1.44	1.39
24	y	607	CHL	C3D-C2D	2.81	1.44	1.39
24	2	605	CHL	CBD-CGD	-2.81	1.49	1.52
25	g	602	CLA	C1D-ND	2.81	1.41	1.37
25	Y	610	CLA	CMC-C2C	-2.81	1.45	1.50
25	8	603	CLA	C1D-ND	2.81	1.41	1.37
25	7	613	CLA	C1D-ND	2.81	1.41	1.37
24	g	607	CHL	CBD-CGD	-2.81	1.49	1.52
25	3	613	CLA	C1D-ND	2.81	1.41	1.37
25	c	510	CLA	C4B-NB	2.81	1.41	1.37
25	b	610	CLA	CMD-C2D	-2.81	1.45	1.50
25	G	611	CLA	C1D-ND	2.81	1.41	1.37
25	1	611	CLA	C1D-ND	2.81	1.41	1.37
25	y	611	CLA	C1D-ND	2.81	1.41	1.37
25	B	613	CLA	CMC-C2C	-2.81	1.45	1.50
25	G	613	CLA	C1D-ND	2.80	1.41	1.37
24	3	601	CHL	C3D-C2D	2.80	1.44	1.39
24	7	606	CHL	C3D-C2D	2.80	1.44	1.39
24	N	606	CHL	CBD-CGD	-2.80	1.49	1.52
25	G	602	CLA	C1D-ND	2.80	1.41	1.37
25	4	610	CLA	CMD-C2D	-2.80	1.45	1.50
24	5	608	CHL	C3D-C2D	2.80	1.44	1.39
24	6	605	CHL	CBD-CGD	-2.80	1.49	1.52
25	7	602	CLA	CMC-C2C	-2.80	1.45	1.50
24	7	606	CHL	CBD-CGD	-2.80	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	606	CHL	C3D-C2D	2.80	1.44	1.39
25	y	613	CLA	MG-ND	-2.80	2.00	2.05
25	8	610	CLA	CMD-C2D	-2.80	1.45	1.50
25	2	610	CLA	C1D-ND	2.80	1.41	1.37
24	Y	608	CHL	C3D-C2D	2.80	1.44	1.39
25	b	604	CLA	MG-ND	-2.80	2.00	2.05
25	4	603	CLA	C4B-NB	2.79	1.41	1.37
24	1	608	CHL	C3D-C2D	2.79	1.44	1.39
24	7	608	CHL	C3D-C2D	2.79	1.44	1.39
24	R	608	CHL	C3D-C2D	2.79	1.44	1.39
25	3	612	CLA	CMD-C2D	-2.79	1.45	1.50
25	B	604	CLA	C1B-NB	-2.79	1.34	1.37
25	6	610	CLA	C1D-ND	2.79	1.41	1.37
33	A	408	PHO	CMD-C2D	-2.79	1.46	1.51
25	g	611	CLA	C1D-ND	2.78	1.41	1.37
25	b	613	CLA	C1B-NB	-2.78	1.34	1.37
25	B	610	CLA	CMD-C2D	-2.78	1.45	1.50
25	a	405	CLA	C1D-ND	2.78	1.41	1.37
25	n	603	CLA	C1D-ND	2.78	1.41	1.37
25	b	603	CLA	MG-NB	-2.78	2.00	2.05
25	c	502	CLA	C1B-C2B	2.78	1.49	1.43
26	N	1621	LUT	C22-C21	-2.78	1.51	1.54
25	5	611	CLA	C1D-ND	2.78	1.41	1.37
24	7	601	CHL	C3D-C2D	2.78	1.44	1.39
33	a	408	PHO	CMD-C2D	-2.78	1.46	1.51
24	n	606	CHL	C3D-C2D	2.78	1.44	1.39
24	Y	607	CHL	C3D-C2D	2.78	1.44	1.39
25	B	613	CLA	CMA-C3A	-2.78	1.47	1.53
25	R	601	CLA	C1D-ND	2.78	1.41	1.37
25	B	604	CLA	MG-ND	-2.78	2.00	2.05
25	7	612	CLA	CMD-C2D	-2.77	1.45	1.50
25	3	602	CLA	CMC-C2C	-2.77	1.45	1.50
25	B	608	CLA	CMC-C2C	-2.77	1.45	1.50
26	n	1621	LUT	C22-C21	-2.77	1.51	1.54
25	r	613	CLA	CMB-C2B	-2.77	1.45	1.50
25	c	507	CLA	C1B-C2B	2.77	1.49	1.43
25	B	617	CLA	C1D-ND	2.77	1.41	1.37
25	B	603	CLA	MG-NB	-2.77	2.00	2.05
25	r	610	CLA	C1D-ND	2.77	1.41	1.37
25	r	611	CLA	C4B-NB	2.77	1.41	1.37
24	r	608	CHL	C3D-C2D	2.77	1.44	1.39
25	C	502	CLA	C1B-C2B	2.77	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	613	CLA	C1B-NB	-2.77	1.34	1.37
25	R	616	CLA	C4B-NB	2.76	1.41	1.37
25	Y	613	CLA	MG-ND	-2.76	2.00	2.05
25	Y	602	CLA	C1D-ND	2.76	1.41	1.37
26	y	1620	LUT	C22-C21	-2.76	1.51	1.54
24	N	606	CHL	C3D-C2D	2.76	1.44	1.39
25	5	613	CLA	C1D-ND	2.76	1.41	1.37
26	5	1621	LUT	C1-C6	-2.76	1.50	1.53
25	b	604	CLA	C1B-NB	-2.76	1.34	1.37
25	y	604	CLA	C4B-NB	2.76	1.41	1.37
25	B	607	CLA	CMC-C2C	-2.76	1.45	1.50
39	f	101	HEM	FE-NB	2.76	2.03	1.94
25	b	608	CLA	CMC-C2C	-2.76	1.45	1.50
25	Y	611	CLA	C1D-ND	2.76	1.41	1.37
25	2	602	CLA	CMC-C2C	-2.76	1.45	1.50
25	b	613	CLA	CMA-C3A	-2.76	1.47	1.53
25	y	614	CLA	CMD-C2D	-2.76	1.45	1.50
25	8	612	CLA	C1D-ND	2.76	1.41	1.37
25	C	507	CLA	C1B-C2B	2.76	1.49	1.43
25	Y	614	CLA	CMD-C2D	-2.76	1.45	1.50
25	Y	611	CLA	CMD-C2D	-2.75	1.45	1.50
25	s	603	CLA	C1B-C2B	2.75	1.49	1.43
25	N	603	CLA	C1D-ND	2.75	1.41	1.37
25	3	603	CLA	CMD-C2D	-2.75	1.45	1.50
26	8	620	LUT	C22-C21	-2.75	1.51	1.54
24	3	606	CHL	CBD-CGD	-2.75	1.49	1.52
25	R	613	CLA	CMB-C2B	-2.75	1.45	1.50
25	r	616	CLA	C1D-ND	2.75	1.41	1.37
25	R	610	CLA	C1D-ND	2.75	1.41	1.37
35	b	622	LMG	O8-C9	-2.75	1.39	1.45
25	b	612	CLA	CMD-C2D	-2.75	1.45	1.50
33	A	408	PHO	CMB-C2B	-2.75	1.46	1.51
25	y	611	CLA	CMD-C2D	-2.75	1.45	1.50
25	b	617	CLA	C1D-ND	2.75	1.41	1.37
25	B	605	CLA	MG-NB	-2.75	2.00	2.05
33	a	408	PHO	CMB-C2B	-2.75	1.46	1.51
25	B	602	CLA	CMD-C2D	-2.75	1.45	1.50
25	N	604	CLA	C4B-NB	2.75	1.41	1.37
25	n	611	CLA	C4B-NB	2.75	1.41	1.37
25	S	603	CLA	C1B-C2B	2.75	1.49	1.43
25	7	604	CLA	C4B-NB	2.74	1.41	1.37
25	6	602	CLA	CMC-C2C	-2.74	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	602	CLA	C1D-ND	2.74	1.41	1.37
39	F	101	HEM	FE-NB	2.74	2.03	1.94
25	b	607	CLA	CMB-C2B	-2.74	1.45	1.50
25	b	608	CLA	CMB-C2B	-2.74	1.45	1.50
25	5	612	CLA	C4B-NB	2.74	1.41	1.37
25	d	402	CLA	MG-NB	-2.74	2.00	2.05
25	7	603	CLA	CMD-C2D	-2.74	1.45	1.50
25	R	616	CLA	C1D-ND	2.74	1.41	1.37
25	B	614	CLA	CMB-C2B	-2.74	1.45	1.50
26	4	620	LUT	C22-C21	-2.74	1.51	1.54
25	b	607	CLA	CMC-C2C	-2.74	1.45	1.50
25	3	611	CLA	MG-NB	-2.74	2.00	2.05
26	Y	1620	LUT	C22-C21	-2.73	1.51	1.54
25	8	603	CLA	C4B-NB	2.73	1.41	1.37
25	n	604	CLA	C4B-NB	2.73	1.41	1.37
25	R	611	CLA	C4B-NB	2.73	1.41	1.37
25	Y	604	CLA	C4B-NB	2.73	1.41	1.37
35	B	622	LMG	O8-C9	-2.73	1.39	1.45
25	3	604	CLA	C4B-NB	2.73	1.41	1.37
25	g	613	CLA	MG-ND	-2.73	2.00	2.05
25	4	612	CLA	C1D-ND	2.73	1.41	1.37
25	B	608	CLA	C1D-ND	2.73	1.41	1.37
25	D	403	CLA	C1D-ND	2.73	1.41	1.37
25	1	612	CLA	C4B-NB	2.73	1.41	1.37
25	B	607	CLA	CMB-C2B	-2.73	1.45	1.50
25	8	612	CLA	C4B-NB	2.72	1.41	1.37
25	Y	603	CLA	CMD-C2D	-2.72	1.45	1.50
25	7	613	CLA	C4B-NB	2.72	1.41	1.37
25	b	605	CLA	MG-NB	-2.72	2.00	2.05
25	5	610	CLA	C1D-ND	2.72	1.41	1.37
26	G	1621	LUT	C22-C21	-2.72	1.51	1.54
25	1	613	CLA	C1D-ND	2.72	1.41	1.37
25	b	608	CLA	C1D-ND	2.72	1.41	1.37
25	s	612	CLA	C1B-C2B	2.72	1.49	1.43
25	c	513	CLA	C4B-NB	2.72	1.41	1.37
25	r	603	CLA	MG-ND	-2.72	2.00	2.05
25	B	608	CLA	CMB-C2B	-2.71	1.45	1.50
34	A	412	SQD	O47-C7	2.71	1.41	1.34
26	g	1621	LUT	C22-C21	-2.71	1.51	1.54
25	b	602	CLA	CMD-C2D	-2.71	1.45	1.50
25	c	502	CLA	C4B-NB	2.71	1.41	1.37
24	2	601	CHL	C3D-C2D	2.71	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	612	CLA	CMD-C2D	-2.71	1.45	1.50
25	G	613	CLA	MG-ND	-2.71	2.00	2.05
37	h	102	DGD	O4D-C4D	-2.71	1.36	1.43
25	B	605	CLA	C1D-ND	2.71	1.41	1.37
25	b	605	CLA	C1D-ND	2.71	1.41	1.37
25	D	402	CLA	MG-NB	-2.71	2.00	2.05
25	c	508	CLA	CMB-C2B	-2.71	1.45	1.50
29	c	2630	LHG	O7-C5	-2.71	1.40	1.46
25	d	403	CLA	C1D-ND	2.70	1.41	1.37
25	C	508	CLA	CMB-C2B	-2.70	1.45	1.50
25	6	613	CLA	MG-ND	-2.70	2.00	2.05
34	a	412	SQD	O47-C7	2.70	1.41	1.34
25	1	610	CLA	C1D-ND	2.70	1.41	1.37
25	b	614	CLA	CMB-C2B	-2.70	1.45	1.50
37	H	102	DGD	O4D-C4D	-2.70	1.36	1.43
25	R	603	CLA	MG-ND	-2.70	2.00	2.05
29	C	2630	LHG	O7-C5	-2.70	1.40	1.46
25	5	613	CLA	MG-ND	-2.70	2.00	2.05
25	4	611	CLA	C4B-NB	2.70	1.41	1.37
25	4	612	CLA	C4B-NB	2.70	1.41	1.37
25	y	603	CLA	CMD-C2D	-2.70	1.45	1.50
25	c	509	CLA	C4B-NB	2.70	1.41	1.37
25	7	611	CLA	MG-NB	-2.70	2.00	2.05
37	c	520	DGD	O5D-C6D	-2.70	1.39	1.43
24	g	609	CHL	CBD-CGD	-2.69	1.49	1.52
25	G	612	CLA	C4B-NB	2.69	1.41	1.37
35	B	622	LMG	O7-C8	-2.69	1.40	1.46
25	8	611	CLA	C4B-NB	2.69	1.41	1.37
24	Y	605	CHL	CBD-CGD	-2.69	1.49	1.52
25	r	616	CLA	C4B-NB	2.69	1.41	1.37
25	r	616	CLA	CMB-C2B	-2.69	1.45	1.50
24	6	601	CHL	C3D-C2D	2.69	1.44	1.39
25	1	613	CLA	MG-ND	-2.69	2.00	2.05
25	N	611	CLA	C4B-NB	2.69	1.41	1.37
26	1	1621	LUT	C1-C6	-2.69	1.50	1.53
25	n	611	CLA	C1B-C2B	2.69	1.49	1.43
25	C	502	CLA	C4B-NB	2.69	1.41	1.37
25	C	513	CLA	C4B-NB	2.68	1.41	1.37
36	d	405	PL9	C2-C1	-2.68	1.37	1.44
35	b	622	LMG	O7-C8	-2.68	1.40	1.46
25	2	613	CLA	MG-ND	-2.68	2.00	2.05
25	b	606	CLA	CMD-C2D	-2.68	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	616	CLA	C1D-ND	2.68	1.41	1.37
25	N	611	CLA	C1B-C2B	2.68	1.49	1.43
25	S	612	CLA	C1B-C2B	2.68	1.49	1.43
37	C	520	DGD	O5D-C6D	-2.68	1.39	1.43
30	b	620	BCR	C1-C6	-2.68	1.50	1.53
25	C	509	CLA	C4B-NB	2.67	1.41	1.37
25	y	603	CLA	C4B-NB	2.67	1.41	1.37
36	d	405	PL9	C35-C34	-2.67	1.44	1.50
25	3	613	CLA	C4B-NB	2.67	1.41	1.37
30	B	620	BCR	C1-C6	-2.67	1.50	1.53
25	n	614	CLA	C1B-C2B	2.67	1.49	1.43
25	g	612	CLA	C4B-NB	2.67	1.41	1.37
25	b	606	CLA	CMB-C2B	-2.67	1.45	1.50
25	C	512	CLA	C1B-C2B	2.67	1.49	1.43
25	N	614	CLA	C1B-C2B	2.66	1.49	1.43
25	b	605	CLA	MG-ND	-2.66	2.00	2.05
33	a	409	PHO	C4D-ND	-2.66	1.34	1.38
25	B	605	CLA	C1B-NB	-2.66	1.34	1.37
25	y	604	CLA	MG-NB	-2.66	2.00	2.05
25	B	606	CLA	CMD-C2D	-2.66	1.45	1.50
25	B	616	CLA	CMC-C2C	-2.66	1.45	1.50
25	b	616	CLA	CMC-C2C	-2.66	1.45	1.50
36	D	405	PL9	C2-C1	-2.66	1.37	1.44
25	2	614	CLA	C4B-NB	2.66	1.41	1.37
26	3	1620	LUT	C22-C21	-2.66	1.51	1.54
36	D	405	PL9	C35-C34	-2.66	1.44	1.50
25	B	606	CLA	CMB-C2B	-2.66	1.45	1.50
25	c	512	CLA	C1B-C2B	2.66	1.49	1.43
37	c	519	DGD	O1G-C1G	-2.66	1.39	1.45
25	R	616	CLA	CMB-C2B	-2.66	1.45	1.50
24	G	609	CHL	CBD-CGD	-2.66	1.49	1.52
25	N	602	CLA	CMC-C2C	-2.66	1.45	1.50
25	n	602	CLA	CMC-C2C	-2.66	1.45	1.50
25	B	614	CLA	CMC-C2C	-2.66	1.45	1.50
37	C	519	DGD	O1G-C1G	-2.65	1.39	1.45
25	4	610	CLA	C1D-ND	2.65	1.41	1.37
25	2	613	CLA	CMD-C2D	-2.65	1.45	1.50
25	B	606	CLA	CMC-C2C	-2.65	1.45	1.50
25	5	614	CLA	C4B-NB	2.65	1.41	1.37
25	6	613	CLA	CMD-C2D	-2.65	1.45	1.50
25	Y	604	CLA	MG-NB	-2.65	2.00	2.05
25	1	602	CLA	C1D-ND	2.65	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	605	CLA	MG-ND	-2.65	2.00	2.05
25	r	604	CLA	CMD-C2D	-2.65	1.45	1.50
25	g	603	CLA	C3B-C4B	2.65	1.50	1.42
25	R	604	CLA	CMD-C2D	-2.65	1.45	1.50
25	G	603	CLA	C3B-C4B	2.65	1.50	1.42
25	y	604	CLA	C1B-NB	-2.65	1.34	1.37
25	b	615	CLA	CMC-C2C	-2.65	1.45	1.50
25	1	603	CLA	CMB-C2B	-2.65	1.45	1.50
25	Y	610	CLA	C1D-ND	2.65	1.41	1.37
27	7	1622	XAT	O4-C5	-2.65	1.42	1.46
25	1	614	CLA	C4B-NB	2.65	1.41	1.37
25	Y	603	CLA	C1D-ND	2.65	1.41	1.37
25	b	605	CLA	C1B-NB	-2.65	1.34	1.37
25	Y	603	CLA	C4B-NB	2.64	1.41	1.37
25	B	604	CLA	CMD-C2D	-2.64	1.45	1.50
33	A	409	PHO	CAC-C3C	-2.64	1.47	1.51
25	6	614	CLA	C4B-NB	2.64	1.41	1.37
25	b	611	CLA	CMD-C2D	-2.64	1.45	1.50
25	1	613	CLA	C4B-NB	2.64	1.41	1.37
25	y	603	CLA	C1D-ND	2.64	1.41	1.37
33	A	409	PHO	C4D-ND	-2.64	1.34	1.38
26	7	1620	LUT	C22-C21	-2.64	1.51	1.54
25	y	614	CLA	C1D-ND	2.64	1.41	1.37
25	Y	604	CLA	C1B-NB	-2.64	1.34	1.37
25	5	603	CLA	CMB-C2B	-2.64	1.45	1.50
25	b	614	CLA	CMC-C2C	-2.64	1.45	1.50
25	C	513	CLA	C1B-C2B	2.63	1.49	1.43
27	3	1622	XAT	O4-C5	-2.63	1.42	1.46
25	B	611	CLA	CMD-C2D	-2.63	1.45	1.50
25	8	610	CLA	C1D-ND	2.63	1.41	1.37
36	D	405	PL9	C46-C44	-2.63	1.45	1.51
36	d	405	PL9	C46-C44	-2.63	1.45	1.51
25	a	405	CLA	CMD-C2D	-2.63	1.45	1.50
25	Y	614	CLA	C1D-ND	2.63	1.41	1.37
37	c	518	DGD	O1G-C1G	-2.63	1.39	1.45
25	b	604	CLA	CMD-C2D	-2.63	1.45	1.50
25	N	604	CLA	C1B-NB	-2.63	1.34	1.37
25	s	609	CLA	C1B-C2B	2.63	1.49	1.43
25	b	606	CLA	CMC-C2C	-2.63	1.45	1.50
25	5	602	CLA	C1D-ND	2.63	1.41	1.37
25	c	507	CLA	C4B-NB	2.63	1.41	1.37
25	7	602	CLA	C1B-C2B	2.63	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	407	CLA	C4B-NB	2.63	1.41	1.37
25	Y	613	CLA	C4B-NB	2.63	1.41	1.37
25	S	614	CLA	C1B-C2B	2.63	1.49	1.43
36	D	405	PL9	C21-C19	-2.63	1.45	1.51
25	b	613	CLA	CMB-C2B	-2.63	1.45	1.50
25	a	407	CLA	C4B-NB	2.62	1.41	1.37
25	b	608	CLA	CMD-C2D	-2.62	1.45	1.50
25	b	607	CLA	C4B-NB	2.62	1.41	1.37
25	y	610	CLA	C1D-ND	2.62	1.41	1.37
25	S	609	CLA	C1B-C2B	2.62	1.49	1.43
25	y	613	CLA	C4B-NB	2.62	1.41	1.37
24	n	601	CHL	CBD-CGD	-2.62	1.49	1.52
37	C	518	DGD	O1G-C1G	-2.62	1.39	1.45
25	Y	612	CLA	CMD-C2D	-2.62	1.45	1.50
33	a	409	PHO	CAC-C3C	-2.62	1.47	1.51
24	N	601	CHL	CBD-CGD	-2.62	1.49	1.52
24	g	606	CHL	CBD-CGD	-2.62	1.49	1.52
25	B	611	CLA	MG-ND	-2.62	2.00	2.05
36	d	405	PL9	C21-C19	-2.62	1.45	1.51
39	F	101	HEM	FE-ND	2.62	2.03	1.94
24	y	605	CHL	CBD-CGD	-2.62	1.49	1.52
25	s	614	CLA	C1B-C2B	2.62	1.49	1.43
25	7	610	CLA	C1D-ND	2.62	1.41	1.37
25	g	613	CLA	MG-NB	-2.62	2.00	2.05
25	8	603	CLA	CMD-C2D	-2.62	1.45	1.50
25	G	603	CLA	C1D-ND	2.62	1.41	1.37
25	4	603	CLA	CMD-C2D	-2.62	1.45	1.50
25	B	613	CLA	CMB-C2B	-2.62	1.45	1.50
27	r	622	XAT	O4-C5	-2.62	1.42	1.46
25	c	505	CLA	CMD-C2D	-2.62	1.45	1.50
25	N	612	CLA	C4B-NB	2.62	1.41	1.37
25	b	609	CLA	CMD-C2D	-2.61	1.45	1.50
25	c	513	CLA	C1B-C2B	2.61	1.49	1.43
25	Y	611	CLA	C3B-C4B	2.61	1.50	1.42
25	N	604	CLA	C1D-ND	2.61	1.41	1.37
24	G	606	CHL	CBD-CGD	-2.61	1.49	1.52
25	n	604	CLA	C1D-ND	2.61	1.41	1.37
25	b	611	CLA	MG-ND	-2.61	2.00	2.05
25	B	614	CLA	MG-NB	-2.61	2.00	2.05
25	n	612	CLA	C4B-NB	2.61	1.41	1.37
25	5	613	CLA	C4B-NB	2.61	1.41	1.37
25	G	611	CLA	MG-NB	-2.61	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	610	CLA	C1D-ND	2.61	1.41	1.37
25	y	612	CLA	C4B-NB	2.61	1.41	1.37
25	B	615	CLA	CMC-C2C	-2.61	1.45	1.50
25	b	616	CLA	C1D-ND	2.61	1.41	1.37
25	B	609	CLA	CMD-C2D	-2.61	1.45	1.50
25	B	608	CLA	CMD-C2D	-2.61	1.45	1.50
33	a	408	PHO	CBD-CGD	-2.61	1.49	1.52
25	G	613	CLA	MG-NB	-2.61	2.00	2.05
26	G	1621	LUT	C1-C6	-2.61	1.50	1.53
39	f	101	HEM	FE-ND	2.61	2.02	1.94
29	5	2630	LHG	O7-C5	-2.60	1.40	1.46
25	D	403	CLA	CMD-C2D	-2.60	1.45	1.50
27	R	622	XAT	O4-C5	-2.60	1.42	1.46
25	3	610	CLA	MG-NB	-2.60	2.00	2.05
25	g	611	CLA	MG-NB	-2.60	2.00	2.05
25	n	604	CLA	C1B-NB	-2.60	1.34	1.37
25	A	405	CLA	CMD-C2D	-2.60	1.45	1.50
25	6	611	CLA	C4B-NB	2.60	1.41	1.37
25	3	602	CLA	C1B-C2B	2.60	1.49	1.43
25	Y	612	CLA	C4B-NB	2.60	1.41	1.37
25	b	615	CLA	MG-NB	-2.60	2.00	2.05
25	7	610	CLA	MG-NB	-2.60	2.00	2.05
25	7	614	CLA	C3B-C4B	2.60	1.50	1.42
25	7	602	CLA	CMD-C2D	-2.60	1.45	1.50
25	5	604	CLA	MG-NB	-2.60	2.00	2.05
24	4	609	CHL	CBD-CGD	-2.60	1.49	1.52
26	g	1621	LUT	C1-C6	-2.60	1.50	1.53
28	g	1623	NEX	C7-C8	-2.60	1.27	1.31
26	R	620	LUT	C1-C6	-2.60	1.50	1.53
25	y	611	CLA	C3B-C4B	2.60	1.50	1.42
29	1	2630	LHG	O7-C5	-2.60	1.40	1.46
25	C	505	CLA	C1B-C2B	2.60	1.49	1.43
25	N	613	CLA	MG-ND	-2.59	2.00	2.05
25	8	602	CLA	C1D-ND	2.59	1.41	1.37
25	R	612	CLA	C3B-C4B	2.59	1.50	1.42
28	1	1623	NEX	O24-C25	-2.59	1.42	1.46
29	B	2630	LHG	O7-C5	-2.59	1.40	1.46
25	3	614	CLA	C3B-C4B	2.59	1.50	1.42
25	1	604	CLA	MG-NB	-2.59	2.00	2.05
25	Y	613	CLA	C1B-C2B	2.59	1.49	1.43
25	y	613	CLA	MG-NB	-2.59	2.00	2.05
25	c	511	CLA	C1B-C2B	2.59	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	616	CLA	C1B-C2B	2.59	1.49	1.43
25	b	614	CLA	MG-NB	-2.59	2.00	2.05
25	C	509	CLA	CMD-C2D	-2.59	1.45	1.50
25	C	508	CLA	C4B-NB	2.59	1.41	1.37
25	3	602	CLA	CMD-C2D	-2.58	1.45	1.50
25	C	511	CLA	C1B-C2B	2.58	1.49	1.43
25	Y	613	CLA	MG-NB	-2.58	2.00	2.05
25	r	616	CLA	C1B-C2B	2.58	1.49	1.43
25	Y	602	CLA	CMD-C2D	-2.58	1.45	1.50
25	d	403	CLA	CMD-C2D	-2.58	1.45	1.50
28	5	1623	NEX	O24-C25	-2.58	1.42	1.46
25	y	612	CLA	CMD-C2D	-2.58	1.45	1.50
25	3	604	CLA	CMB-C2B	-2.57	1.45	1.50
25	7	604	CLA	CMB-C2B	-2.57	1.45	1.50
25	r	612	CLA	C3B-C4B	2.57	1.50	1.42
25	B	615	CLA	MG-NB	-2.57	2.00	2.05
29	b	2630	LHG	O7-C5	-2.57	1.40	1.46
25	2	611	CLA	C4B-NB	2.57	1.41	1.37
25	c	505	CLA	C1B-C2B	2.57	1.49	1.43
25	B	607	CLA	C4B-NB	2.57	1.41	1.37
25	a	410	CLA	C1D-ND	2.57	1.41	1.37
25	C	505	CLA	CMD-C2D	-2.57	1.45	1.50
35	D	411	LMG	O7-C8	-2.57	1.40	1.46
24	8	609	CHL	CBD-CGD	-2.57	1.49	1.52
25	5	603	CLA	C1D-ND	2.57	1.41	1.37
25	n	613	CLA	MG-ND	-2.57	2.00	2.05
25	y	613	CLA	C1B-C2B	2.57	1.49	1.43
28	G	1623	NEX	C7-C8	-2.57	1.27	1.31
25	G	613	CLA	C1B-C2B	2.57	1.49	1.43
25	b	615	CLA	C1D-ND	2.57	1.41	1.37
25	B	615	CLA	C1B-NB	-2.56	1.34	1.37
25	4	602	CLA	C1D-ND	2.56	1.41	1.37
25	G	614	CLA	C4B-NB	2.56	1.41	1.37
25	y	602	CLA	CMD-C2D	-2.56	1.45	1.50
25	b	607	CLA	CMD-C2D	-2.56	1.45	1.50
25	g	603	CLA	C1D-ND	2.56	1.41	1.37
33	A	409	PHO	CMB-C2B	-2.56	1.46	1.51
25	C	507	CLA	C4B-NB	2.56	1.41	1.37
25	Y	612	CLA	C1D-ND	2.56	1.41	1.37
25	3	613	CLA	C1B-C2B	2.56	1.49	1.43
25	g	613	CLA	C1B-C2B	2.56	1.49	1.43
25	A	410	CLA	CMD-C2D	-2.56	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	610	CLA	CMB-C2B	-2.56	1.45	1.50
25	g	614	CLA	C4B-NB	2.56	1.41	1.37
25	3	603	CLA	MG-ND	-2.56	2.00	2.05
25	B	607	CLA	CMD-C2D	-2.56	1.45	1.50
25	7	603	CLA	C1D-ND	2.56	1.41	1.37
25	b	615	CLA	C1B-NB	-2.56	1.34	1.37
25	c	508	CLA	C4B-NB	2.56	1.41	1.37
25	1	602	CLA	CMC-C2C	-2.56	1.45	1.50
25	4	602	CLA	C4B-NB	2.55	1.41	1.37
25	6	603	CLA	C4B-NB	2.55	1.41	1.37
25	n	612	CLA	C1B-C2B	2.55	1.49	1.43
25	2	603	CLA	C4B-NB	2.55	1.41	1.37
39	F	101	HEM	FE-NA	2.55	2.03	1.95
25	r	604	CLA	CMB-C2B	-2.55	1.45	1.50
25	7	611	CLA	MG-ND	-2.55	2.00	2.05
25	5	604	CLA	MG-ND	-2.55	2.00	2.05
28	R	623	NEX	O24-C25	-2.55	1.42	1.46
25	N	612	CLA	C1B-C2B	2.55	1.49	1.43
25	B	610	CLA	CMB-C2B	-2.55	1.45	1.50
25	B	617	CLA	C1B-C2B	2.55	1.49	1.43
25	y	612	CLA	C1D-ND	2.55	1.41	1.37
25	3	603	CLA	C1D-ND	2.55	1.41	1.37
25	B	615	CLA	C1D-ND	2.55	1.41	1.37
25	Y	610	CLA	CMD-C2D	-2.55	1.45	1.50
25	c	509	CLA	CMD-C2D	-2.55	1.45	1.50
25	N	603	CLA	C4B-NB	2.55	1.41	1.37
25	A	406	CLA	CMB-C2B	-2.55	1.45	1.50
25	g	604	CLA	MG-NB	-2.55	2.00	2.05
25	b	617	CLA	C1B-C2B	2.55	1.49	1.43
33	A	408	PHO	CBD-CGD	-2.55	1.49	1.52
25	d	402	CLA	CMB-C2B	-2.55	1.45	1.50
25	A	406	CLA	C4B-NB	2.55	1.41	1.37
25	y	612	CLA	CMB-C2B	-2.55	1.45	1.50
25	2	611	CLA	MG-NB	-2.55	2.00	2.05
25	4	604	CLA	CMB-C2B	-2.55	1.45	1.50
25	D	402	CLA	CMB-C2B	-2.55	1.45	1.50
25	7	603	CLA	MG-ND	-2.54	2.00	2.05
25	r	602	CLA	CMC-C2C	-2.54	1.45	1.50
25	B	609	CLA	C1B-NB	-2.54	1.34	1.37
28	Y	1623	NEX	O24-C25	-2.54	1.42	1.46
25	1	603	CLA	C1D-ND	2.54	1.41	1.37
25	3	611	CLA	MG-ND	-2.54	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r	620	LUT	C1-C6	-2.54	1.50	1.53
25	a	410	CLA	CMD-C2D	-2.54	1.45	1.50
33	a	409	PHO	CMB-C2B	-2.54	1.46	1.51
25	a	406	CLA	CMB-C2B	-2.54	1.45	1.50
24	6	607	CHL	CBD-CGD	-2.54	1.49	1.52
25	b	610	CLA	CMB-C2B	-2.54	1.45	1.50
25	7	613	CLA	C1B-C2B	2.54	1.49	1.43
25	c	508	CLA	CMC-C2C	-2.54	1.45	1.50
35	d	411	LMG	O7-C8	-2.54	1.40	1.46
25	N	604	CLA	CMD-C2D	-2.54	1.45	1.50
25	G	612	CLA	CMD-C2D	-2.54	1.45	1.50
25	5	603	CLA	MG-ND	-2.54	2.00	2.05
25	S	604	CLA	C1B-C2B	2.54	1.49	1.43
39	f	101	HEM	FE-NA	2.53	2.03	1.95
25	s	604	CLA	C1B-C2B	2.53	1.49	1.43
25	Y	610	CLA	CMB-C2B	-2.53	1.45	1.50
25	y	610	CLA	CMD-C2D	-2.53	1.45	1.50
24	2	607	CHL	CBD-CGD	-2.53	1.49	1.52
27	g	1622	XAT	O4-C5	-2.53	1.42	1.46
25	R	604	CLA	CMB-C2B	-2.53	1.45	1.50
25	B	603	CLA	C1D-ND	2.53	1.41	1.37
25	y	603	CLA	MG-ND	-2.53	2.00	2.05
25	5	614	CLA	CMD-C2D	-2.53	1.45	1.50
25	C	509	CLA	C1B-C2B	2.53	1.49	1.43
25	b	617	CLA	C1B-NB	-2.53	1.34	1.37
25	5	602	CLA	CMC-C2C	-2.53	1.45	1.50
25	Y	602	CLA	CMB-C2B	-2.53	1.45	1.50
25	6	610	CLA	C4B-NB	2.53	1.41	1.37
25	b	609	CLA	C1B-NB	-2.53	1.34	1.37
25	8	602	CLA	C4B-NB	2.53	1.41	1.37
25	b	617	CLA	CMB-C2B	-2.53	1.45	1.50
25	B	614	CLA	C1B-NB	-2.53	1.34	1.37
25	r	603	CLA	MG-NB	-2.53	2.00	2.05
25	2	602	CLA	C4B-NB	2.53	1.41	1.37
25	B	616	CLA	C4B-NB	2.53	1.41	1.37
25	b	610	CLA	C1D-ND	2.53	1.41	1.37
25	b	616	CLA	C4B-NB	2.53	1.41	1.37
24	5	605	CHL	CBD-CGD	-2.53	1.49	1.52
25	R	602	CLA	C1D-ND	2.53	1.41	1.37
25	1	603	CLA	MG-ND	-2.53	2.00	2.05
25	1	604	CLA	MG-ND	-2.53	2.00	2.05
25	r	602	CLA	C1D-ND	2.53	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	508	CLA	CMC-C2C	-2.53	1.45	1.50
25	A	410	CLA	C1D-ND	2.52	1.41	1.37
25	R	603	CLA	C4B-NB	2.52	1.41	1.37
25	b	603	CLA	C1D-ND	2.52	1.41	1.37
25	B	617	CLA	CMD-C2D	-2.52	1.45	1.50
25	R	609	CLA	C1D-ND	2.52	1.41	1.37
25	8	604	CLA	CMB-C2B	-2.52	1.45	1.50
25	Y	603	CLA	MG-ND	-2.52	2.00	2.05
25	y	604	CLA	CMC-C2C	-2.52	1.45	1.50
25	g	612	CLA	CMD-C2D	-2.52	1.45	1.50
25	B	610	CLA	C1D-ND	2.52	1.41	1.37
25	S	611	CLA	C1B-C2B	2.52	1.49	1.43
25	6	603	CLA	MG-ND	-2.52	2.00	2.05
25	6	611	CLA	MG-NB	-2.52	2.00	2.05
25	B	617	CLA	C1B-NB	-2.52	1.34	1.37
26	3	1621	LUT	C22-C21	-2.52	1.51	1.54
25	Y	611	CLA	CMB-C2B	-2.52	1.45	1.50
25	6	602	CLA	C4B-NB	2.52	1.41	1.37
25	2	603	CLA	MG-ND	-2.52	2.00	2.05
25	B	609	CLA	MG-NB	-2.52	2.00	2.05
25	s	611	CLA	C1B-C2B	2.52	1.49	1.43
25	R	603	CLA	MG-NB	-2.52	2.00	2.05
25	R	610	CLA	CMD-C2D	-2.52	1.45	1.50
25	7	611	CLA	C4B-NB	2.52	1.41	1.37
25	7	613	CLA	CMD-C2D	-2.51	1.45	1.50
25	b	617	CLA	CMD-C2D	-2.51	1.45	1.50
26	7	1621	LUT	C22-C21	-2.51	1.51	1.54
25	c	509	CLA	C1B-C2B	2.51	1.49	1.43
25	y	611	CLA	CMB-C2B	-2.51	1.45	1.50
24	1	605	CHL	CBD-CGD	-2.51	1.49	1.52
25	N	603	CLA	C3B-C4B	2.51	1.50	1.42
25	4	611	CLA	C1B-C2B	2.51	1.49	1.43
25	6	613	CLA	C1D-ND	2.51	1.41	1.37
25	Y	612	CLA	CMB-C2B	-2.51	1.45	1.50
28	y	1623	NEX	O24-C25	-2.51	1.43	1.46
25	G	604	CLA	MG-NB	-2.51	2.00	2.05
25	2	613	CLA	C1D-ND	2.51	1.41	1.37
25	R	602	CLA	CMC-C2C	-2.51	1.45	1.50
25	D	403	CLA	MG-NB	-2.51	2.00	2.05
25	2	610	CLA	C4B-NB	2.51	1.41	1.37
25	B	617	CLA	CMB-C2B	-2.51	1.45	1.50
27	G	1622	XAT	O4-C5	-2.51	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	407	CLA	CMD-C2D	-2.51	1.45	1.50
25	6	602	CLA	CMD-C2D	-2.51	1.45	1.50
25	y	602	CLA	CMB-C2B	-2.51	1.45	1.50
25	S	613	CLA	C1B-C2B	2.51	1.49	1.43
25	8	611	CLA	C1B-C2B	2.51	1.49	1.43
24	1	601	CHL	C3D-C2D	2.50	1.43	1.39
25	5	604	CLA	CMD-C2D	-2.50	1.45	1.50
25	n	604	CLA	CMD-C2D	-2.50	1.45	1.50
25	s	613	CLA	C1B-C2B	2.50	1.49	1.43
25	3	611	CLA	C1D-ND	2.50	1.41	1.37
25	r	609	CLA	C1D-ND	2.50	1.41	1.37
25	B	609	CLA	CMC-C2C	-2.50	1.45	1.50
25	Y	612	CLA	MG-ND	-2.50	2.00	2.05
25	y	612	CLA	MG-ND	-2.50	2.00	2.05
25	G	611	CLA	C4B-NB	2.50	1.41	1.37
25	b	614	CLA	C1B-NB	-2.50	1.34	1.37
25	2	602	CLA	CMD-C2D	-2.50	1.45	1.50
25	r	603	CLA	C4B-NB	2.50	1.41	1.37
25	3	611	CLA	C4B-NB	2.50	1.41	1.37
25	1	614	CLA	CMD-C2D	-2.50	1.45	1.50
25	n	603	CLA	C3B-C4B	2.50	1.50	1.42
25	d	403	CLA	MG-NB	-2.50	2.00	2.05
25	3	613	CLA	CMD-C2D	-2.49	1.45	1.50
25	b	611	CLA	CMB-C2B	-2.49	1.45	1.50
25	7	613	CLA	MG-ND	-2.49	2.00	2.05
25	y	614	CLA	MG-NB	-2.49	2.00	2.05
25	Y	604	CLA	CMC-C2C	-2.49	1.45	1.50
25	5	602	CLA	CMD-C2D	-2.49	1.45	1.50
28	r	623	NEX	O24-C25	-2.49	1.43	1.46
25	b	609	CLA	CMC-C2C	-2.49	1.45	1.50
25	B	616	CLA	CMD-C2D	-2.49	1.45	1.50
25	3	613	CLA	MG-ND	-2.49	2.00	2.05
25	r	610	CLA	C4B-NB	2.49	1.41	1.37
25	a	407	CLA	CMD-C2D	-2.49	1.45	1.50
25	6	603	CLA	CMD-C2D	-2.49	1.45	1.50
24	5	601	CHL	C3D-C2D	2.49	1.43	1.39
25	B	611	CLA	CMB-C2B	-2.49	1.45	1.50
25	a	407	CLA	CMB-C2B	-2.49	1.45	1.50
25	r	610	CLA	CMD-C2D	-2.48	1.45	1.50
25	n	603	CLA	C4B-NB	2.48	1.41	1.37
25	S	602	CLA	C1B-C2B	2.48	1.49	1.43
25	N	604	CLA	MG-NB	-2.48	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	603	CLA	MG-ND	-2.48	2.00	2.05
25	1	602	CLA	CMD-C2D	-2.48	1.45	1.50
25	3	612	CLA	MG-NB	-2.48	2.00	2.05
25	5	604	CLA	C4B-NB	2.48	1.41	1.37
25	7	612	CLA	MG-NB	-2.48	2.00	2.05
25	b	609	CLA	MG-NB	-2.48	2.00	2.05
25	n	604	CLA	MG-NB	-2.48	2.00	2.05
25	y	614	CLA	C4B-NB	2.48	1.41	1.37
25	C	503	CLA	C1B-C2B	2.48	1.48	1.43
27	4	622	XAT	O4-C5	-2.48	1.43	1.46
25	4	612	CLA	CMD-C2D	-2.48	1.45	1.50
25	a	406	CLA	C4B-NB	2.48	1.41	1.37
25	A	406	CLA	CMD-C2D	-2.48	1.45	1.50
27	8	622	XAT	O4-C5	-2.48	1.43	1.46
25	2	603	CLA	CMD-C2D	-2.48	1.45	1.50
25	Y	614	CLA	MG-NB	-2.48	2.00	2.05
25	8	603	CLA	MG-ND	-2.47	2.00	2.05
25	b	616	CLA	CMD-C2D	-2.47	1.45	1.50
25	g	611	CLA	C4B-NB	2.47	1.41	1.37
27	y	1622	XAT	O4-C5	-2.47	1.43	1.46
36	d	405	PL9	C31-C29	-2.47	1.46	1.51
25	8	612	CLA	CMD-C2D	-2.47	1.45	1.50
25	Y	612	CLA	CMC-C2C	-2.47	1.45	1.50
25	B	614	CLA	CMD-C2D	-2.47	1.45	1.50
25	b	610	CLA	C1B-C2B	2.47	1.48	1.43
37	C	520	DGD	O1G-C1G	-2.47	1.39	1.45
25	B	604	CLA	C1D-ND	2.47	1.41	1.37
25	1	604	CLA	CMD-C2D	-2.47	1.45	1.50
25	7	612	CLA	CMC-C2C	-2.47	1.45	1.50
25	Y	614	CLA	C4B-NB	2.47	1.41	1.37
25	Y	614	CLA	MG-ND	-2.47	2.00	2.05
27	5	1622	XAT	O4-C5	-2.47	1.43	1.46
36	D	405	PL9	C31-C29	-2.46	1.46	1.51
25	3	612	CLA	MG-ND	-2.46	2.00	2.05
25	6	614	CLA	CMD-C2D	-2.46	1.45	1.50
27	Y	1622	XAT	O4-C5	-2.46	1.43	1.46
25	1	602	CLA	MG-ND	-2.46	2.00	2.05
25	b	604	CLA	C1D-ND	2.46	1.41	1.37
25	a	406	CLA	CMD-C2D	-2.46	1.45	1.50
25	r	603	CLA	CMB-C2B	-2.46	1.45	1.50
25	6	611	CLA	MG-ND	-2.46	2.00	2.05
25	C	510	CLA	C1B-C2B	2.46	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	614	CLA	CMD-C2D	-2.46	1.45	1.50
25	N	612	CLA	CMD-C2D	-2.46	1.45	1.50
25	g	614	CLA	CMD-C2D	-2.46	1.45	1.50
37	c	520	DGD	O1G-C1G	-2.46	1.39	1.45
25	1	604	CLA	C4B-NB	2.46	1.41	1.37
25	2	602	CLA	MG-NB	-2.46	2.00	2.05
25	R	610	CLA	C4B-NB	2.46	1.41	1.37
25	y	614	CLA	MG-ND	-2.46	2.00	2.05
27	n	1622	XAT	O4-C5	-2.46	1.43	1.46
25	G	614	CLA	CMD-C2D	-2.45	1.45	1.50
25	c	503	CLA	C1B-C2B	2.45	1.48	1.43
25	c	510	CLA	C1B-C2B	2.45	1.48	1.43
25	A	407	CLA	CMB-C2B	-2.45	1.45	1.50
25	r	603	CLA	CMD-C2D	-2.45	1.45	1.50
25	s	602	CLA	C1B-C2B	2.45	1.48	1.43
25	5	602	CLA	MG-ND	-2.45	2.00	2.05
25	7	610	CLA	CMB-C2B	-2.45	1.45	1.50
25	r	602	CLA	CMD-C2D	-2.45	1.45	1.50
25	y	612	CLA	CMC-C2C	-2.45	1.45	1.50
25	r	609	CLA	CMD-C2D	-2.45	1.45	1.50
25	B	610	CLA	C1B-C2B	2.45	1.48	1.43
26	N	1620	LUT	C22-C21	-2.45	1.51	1.54
25	2	611	CLA	MG-ND	-2.45	2.00	2.05
27	1	1622	XAT	O4-C5	-2.45	1.43	1.46
25	7	611	CLA	C1D-ND	2.45	1.41	1.37
25	R	603	CLA	CMD-C2D	-2.45	1.45	1.50
25	B	602	CLA	C4B-NB	2.45	1.41	1.37
25	1	604	CLA	C1D-ND	2.45	1.41	1.37
25	7	612	CLA	MG-ND	-2.45	2.00	2.05
25	R	609	CLA	CMD-C2D	-2.45	1.45	1.50
25	N	602	CLA	CMB-C2B	-2.44	1.45	1.50
25	5	604	CLA	C1D-ND	2.44	1.41	1.37
25	b	609	CLA	C1D-ND	2.44	1.41	1.37
25	R	602	CLA	CMD-C2D	-2.44	1.45	1.50
25	g	610	CLA	CMC-C2C	-2.44	1.45	1.50
25	3	612	CLA	C1D-ND	2.44	1.41	1.37
25	b	614	CLA	C1D-ND	2.44	1.41	1.37
25	3	610	CLA	CMB-C2B	-2.44	1.45	1.50
25	R	603	CLA	CMB-C2B	-2.44	1.45	1.50
25	g	602	CLA	CMD-C2D	-2.44	1.45	1.50
25	n	610	CLA	CMC-C2C	-2.44	1.45	1.50
25	G	602	CLA	CMD-C2D	-2.44	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	614	CLA	CMD-C2D	-2.44	1.45	1.50
25	Y	603	CLA	C3B-C4B	2.44	1.49	1.42
25	B	603	CLA	CMD-C2D	-2.44	1.45	1.50
25	1	603	CLA	CMD-C2D	-2.43	1.45	1.50
25	6	602	CLA	MG-NB	-2.43	2.01	2.05
25	y	603	CLA	C3B-C4B	2.43	1.49	1.42
25	N	610	CLA	CMC-C2C	-2.43	1.45	1.50
25	r	603	CLA	C1D-ND	2.43	1.41	1.37
26	1	1621	LUT	C22-C21	-2.43	1.51	1.54
25	5	602	CLA	MG-NB	-2.43	2.01	2.05
24	y	601	CHL	CHA-CBD	-2.43	1.48	1.51
25	Y	611	CLA	MG-NB	-2.43	2.01	2.05
25	5	611	CLA	MG-NB	-2.43	2.01	2.05
25	g	604	CLA	CMD-C2D	-2.43	1.45	1.50
25	B	614	CLA	C1D-ND	2.43	1.41	1.37
25	3	612	CLA	CMC-C2C	-2.43	1.45	1.50
25	G	610	CLA	CMC-C2C	-2.43	1.45	1.50
25	5	603	CLA	CMD-C2D	-2.43	1.45	1.50
24	Y	601	CHL	CHA-CBD	-2.43	1.48	1.51
25	b	609	CLA	MG-ND	-2.43	2.01	2.05
25	n	602	CLA	CMB-C2B	-2.42	1.45	1.50
25	b	602	CLA	C4B-NB	2.42	1.41	1.37
25	4	610	CLA	MG-NB	-2.42	2.01	2.05
25	G	602	CLA	CMB-C2B	-2.42	1.45	1.50
27	7	1622	XAT	O24-C25	-2.42	1.43	1.46
25	1	611	CLA	MG-NB	-2.42	2.01	2.05
25	Y	603	CLA	CMB-C2B	-2.42	1.45	1.50
24	1	608	CHL	CHA-CBD	-2.42	1.48	1.51
25	7	602	CLA	MG-ND	-2.42	2.01	2.05
25	G	604	CLA	CMD-C2D	-2.42	1.45	1.50
25	n	612	CLA	CMD-C2D	-2.42	1.45	1.50
25	R	603	CLA	C1D-ND	2.42	1.41	1.37
25	2	604	CLA	C4B-NB	2.42	1.41	1.37
25	B	609	CLA	C1D-ND	2.42	1.41	1.37
25	N	614	CLA	C4B-NB	2.42	1.41	1.37
25	5	613	CLA	CMD-C2D	-2.42	1.45	1.50
29	B	2631	LHG	O7-C5	-2.42	1.40	1.46
25	8	610	CLA	MG-NB	-2.41	2.01	2.05
25	r	603	CLA	CMC-C2C	-2.41	1.45	1.50
25	8	612	CLA	MG-NB	-2.41	2.01	2.05
25	1	613	CLA	CMD-C2D	-2.41	1.45	1.50
25	g	612	CLA	C1B-C2B	2.41	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	608	CHL	CBD-CGD	-2.41	1.49	1.52
25	n	614	CLA	C4B-NB	2.41	1.41	1.37
28	7	1623	NEX	O24-C25	-2.41	1.43	1.46
25	B	610	CLA	MG-NB	-2.41	2.01	2.05
29	b	2631	LHG	O7-C5	-2.41	1.40	1.46
25	r	602	CLA	MG-NB	-2.41	2.01	2.05
25	r	604	CLA	MG-NB	-2.41	2.01	2.05
25	1	612	CLA	CMC-C2C	-2.41	1.45	1.50
25	R	603	CLA	CMC-C2C	-2.41	1.45	1.50
25	y	603	CLA	CMB-C2B	-2.41	1.45	1.50
25	b	603	CLA	CMD-C2D	-2.41	1.45	1.50
28	n	1623	NEX	O24-C25	-2.41	1.43	1.46
25	N	604	CLA	CMC-C2C	-2.40	1.45	1.50
25	Y	602	CLA	MG-NB	-2.40	2.01	2.05
25	y	602	CLA	MG-NB	-2.40	2.01	2.05
25	r	612	CLA	CMD-C2D	-2.40	1.45	1.50
25	4	612	CLA	MG-NB	-2.40	2.01	2.05
25	y	611	CLA	MG-NB	-2.40	2.01	2.05
28	3	1623	NEX	O24-C25	-2.40	1.43	1.46
25	3	602	CLA	MG-ND	-2.40	2.01	2.05
25	B	611	CLA	CMC-C2C	-2.40	1.45	1.50
25	r	604	CLA	MG-ND	-2.40	2.01	2.05
25	R	604	CLA	MG-NB	-2.40	2.01	2.05
26	y	1621	LUT	C1-C6	-2.40	1.50	1.53
25	5	612	CLA	CMC-C2C	-2.40	1.45	1.50
25	G	612	CLA	C1B-C2B	2.40	1.48	1.43
33	a	408	PHO	C3B-C2B	-2.40	1.37	1.40
25	g	602	CLA	CMB-C2B	-2.40	1.45	1.50
28	N	1623	NEX	O24-C25	-2.40	1.43	1.46
26	n	1620	LUT	C22-C21	-2.40	1.51	1.54
25	R	612	CLA	CMD-C2D	-2.40	1.45	1.50
25	b	610	CLA	MG-NB	-2.40	2.01	2.05
25	5	603	CLA	CMC-C2C	-2.39	1.45	1.50
25	7	612	CLA	C1D-ND	2.39	1.41	1.37
25	2	610	CLA	CMC-C2C	-2.39	1.45	1.50
25	1	602	CLA	MG-NB	-2.39	2.01	2.05
25	6	603	CLA	CMC-C2C	-2.39	1.45	1.50
25	b	614	CLA	MG-ND	-2.39	2.01	2.05
25	R	616	CLA	MG-NB	-2.39	2.01	2.05
25	B	608	CLA	C1B-NB	-2.39	1.34	1.37
25	G	603	CLA	CMB-C2B	-2.39	1.45	1.50
25	R	611	CLA	C1B-C2B	2.39	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	603	CLA	MG-ND	-2.39	2.01	2.05
25	r	611	CLA	C1B-C2B	2.39	1.48	1.43
25	2	603	CLA	CMC-C2C	-2.39	1.45	1.50
37	C	518	DGD	O5D-C6D	-2.39	1.39	1.43
27	N	1622	XAT	O4-C5	-2.39	1.43	1.46
24	g	608	CHL	CBD-CGD	-2.39	1.49	1.52
25	R	604	CLA	MG-ND	-2.39	2.01	2.05
25	3	613	CLA	CMB-C2B	-2.39	1.45	1.50
25	N	603	CLA	CMB-C2B	-2.39	1.45	1.50
25	g	603	CLA	CMB-C2B	-2.39	1.45	1.50
25	A	405	CLA	C1B-C2B	2.39	1.48	1.43
25	1	611	CLA	C4B-NB	2.39	1.41	1.37
25	G	603	CLA	MG-ND	-2.39	2.01	2.05
26	R	620	LUT	C22-C21	-2.39	1.51	1.54
29	6	2630	LHG	O7-C5	-2.39	1.41	1.46
25	g	611	CLA	CMD-C2D	-2.38	1.45	1.50
25	b	608	CLA	C1B-NB	-2.38	1.34	1.37
25	n	602	CLA	C4B-NB	2.38	1.41	1.37
25	n	604	CLA	CMC-C2C	-2.38	1.45	1.50
25	6	604	CLA	C4B-NB	2.38	1.41	1.37
25	b	611	CLA	C1D-ND	2.38	1.41	1.37
25	1	603	CLA	CMC-C2C	-2.38	1.45	1.50
33	A	408	PHO	C3B-C2B	-2.38	1.37	1.40
25	6	610	CLA	CMB-C2B	-2.38	1.45	1.50
25	a	405	CLA	C1B-C2B	2.38	1.48	1.43
25	R	602	CLA	MG-NB	-2.38	2.01	2.05
29	2	2630	LHG	O7-C5	-2.38	1.41	1.46
25	N	602	CLA	C1B-C2B	2.38	1.48	1.43
25	6	603	CLA	C1B-C2B	2.38	1.48	1.43
25	N	602	CLA	C4B-NB	2.38	1.41	1.37
25	Y	604	CLA	CMD-C2D	-2.38	1.45	1.50
25	Y	603	CLA	C1B-NB	-2.38	1.34	1.37
25	B	609	CLA	MG-ND	-2.38	2.01	2.05
25	A	405	CLA	MG-NB	-2.38	2.01	2.05
25	A	410	CLA	CMB-C2B	-2.38	1.45	1.50
25	2	614	CLA	MG-NB	-2.38	2.01	2.05
25	2	610	CLA	CMB-C2B	-2.38	1.45	1.50
25	y	604	CLA	CMD-C2D	-2.38	1.45	1.50
26	5	1621	LUT	C22-C21	-2.38	1.51	1.54
25	G	614	CLA	C1B-C2B	2.37	1.48	1.43
24	5	608	CHL	CHA-CBD	-2.37	1.48	1.51
25	B	614	CLA	MG-ND	-2.37	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	614	CLA	CMB-C2B	-2.37	1.45	1.50
25	5	612	CLA	MG-ND	-2.37	2.01	2.05
25	6	610	CLA	CMC-C2C	-2.37	1.45	1.50
25	C	501	CLA	CMD-C2D	-2.37	1.45	1.50
25	n	602	CLA	C1B-C2B	2.37	1.48	1.43
25	C	512	CLA	CMD-C2D	-2.37	1.45	1.50
25	3	610	CLA	C4B-NB	2.37	1.41	1.37
25	1	610	CLA	MG-NB	-2.37	2.01	2.05
25	a	405	CLA	MG-NB	-2.37	2.01	2.05
25	Y	611	CLA	CMC-C2C	-2.37	1.45	1.50
29	c	523	LHG	O7-C5	-2.37	1.41	1.46
25	r	610	CLA	CMB-C2B	-2.37	1.45	1.50
25	Y	614	CLA	C1B-C2B	2.37	1.48	1.43
25	A	410	CLA	MG-NB	-2.37	2.01	2.05
25	4	603	CLA	C1B-C2B	2.37	1.48	1.43
25	7	612	CLA	CMB-C2B	-2.37	1.45	1.50
25	b	611	CLA	CMC-C2C	-2.37	1.45	1.50
25	n	603	CLA	CMB-C2B	-2.37	1.45	1.50
25	b	604	CLA	CMC-C2C	-2.37	1.45	1.50
37	c	518	DGD	O5D-C6D	-2.37	1.39	1.43
25	6	614	CLA	MG-NB	-2.37	2.01	2.05
25	B	615	CLA	CMB-C2B	-2.37	1.45	1.50
25	b	615	CLA	CMB-C2B	-2.37	1.45	1.50
25	R	610	CLA	CMB-C2B	-2.36	1.45	1.50
25	g	614	CLA	C1B-C2B	2.36	1.48	1.43
25	y	612	CLA	MG-NB	-2.36	2.01	2.05
25	B	604	CLA	CMC-C2C	-2.36	1.45	1.50
25	Y	612	CLA	MG-NB	-2.36	2.01	2.05
25	R	610	CLA	CMC-C2C	-2.36	1.45	1.50
25	B	602	CLA	MG-NB	-2.36	2.01	2.05
25	Y	614	CLA	CMB-C2B	-2.36	1.45	1.50
25	1	613	CLA	CMB-C2B	-2.36	1.45	1.50
25	D	403	CLA	CMB-C2B	-2.36	1.45	1.50
25	8	604	CLA	C4B-NB	2.36	1.41	1.37
25	5	611	CLA	CMB-C2B	-2.36	1.45	1.50
25	y	611	CLA	CMC-C2C	-2.36	1.45	1.50
25	6	611	CLA	CMD-C2D	-2.36	1.45	1.50
25	r	616	CLA	MG-NB	-2.36	2.01	2.05
25	A	405	CLA	MG-ND	-2.35	2.01	2.05
25	d	403	CLA	MG-ND	-2.35	2.01	2.05
25	2	612	CLA	CMB-C2B	-2.35	1.45	1.50
25	y	614	CLA	C1B-C2B	2.35	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	603	CLA	C1B-C2B	2.35	1.48	1.43
26	Y	1621	LUT	C1-C6	-2.35	1.50	1.53
25	D	402	CLA	MG-ND	-2.35	2.01	2.05
27	3	1622	XAT	O24-C25	-2.35	1.43	1.46
28	g	1623	NEX	O24-C25	-2.35	1.43	1.46
25	2	611	CLA	CMD-C2D	-2.35	1.46	1.50
25	7	613	CLA	CMB-C2B	-2.35	1.46	1.50
25	8	603	CLA	C1B-C2B	2.35	1.48	1.43
25	Y	604	CLA	C1D-ND	2.35	1.40	1.37
25	a	410	CLA	CMB-C2B	-2.35	1.46	1.50
25	1	612	CLA	CMD-C2D	-2.35	1.46	1.50
25	3	610	CLA	CMC-C2C	-2.35	1.46	1.50
25	y	611	CLA	MG-ND	-2.35	2.01	2.05
25	3	612	CLA	CMB-C2B	-2.35	1.46	1.50
25	5	613	CLA	CMB-C2B	-2.35	1.46	1.50
25	B	605	CLA	CMC-C2C	-2.35	1.46	1.50
25	6	612	CLA	CMB-C2B	-2.35	1.46	1.50
25	R	613	CLA	C4B-NB	2.35	1.40	1.37
25	7	604	CLA	C1B-C2B	2.35	1.48	1.43
25	a	410	CLA	MG-NB	-2.35	2.01	2.05
25	G	614	CLA	MG-NB	-2.35	2.01	2.05
25	c	512	CLA	CMD-C2D	-2.35	1.46	1.50
25	D	402	CLA	CAA-C2A	-2.34	1.49	1.54
25	g	610	CLA	CMB-C2B	-2.34	1.46	1.50
25	B	611	CLA	C1B-NB	-2.34	1.34	1.37
37	H	102	DGD	O3E-C3E	-2.34	1.37	1.43
25	6	604	CLA	CMC-C2C	-2.34	1.46	1.50
25	c	509	CLA	CMB-C2B	-2.34	1.46	1.50
37	C	519	DGD	O2G-C2G	-2.34	1.41	1.46
25	4	604	CLA	MG-NB	-2.34	2.01	2.05
25	d	403	CLA	CMB-C2B	-2.34	1.46	1.50
25	r	611	CLA	MG-NB	-2.34	2.01	2.05
25	4	604	CLA	C4B-NB	2.34	1.40	1.37
25	5	611	CLA	C4B-NB	2.34	1.40	1.37
25	b	610	CLA	C1B-NB	-2.34	1.34	1.37
25	5	610	CLA	CMC-C2C	-2.34	1.46	1.50
25	8	604	CLA	MG-NB	-2.34	2.01	2.05
25	c	504	CLA	C1B-C2B	2.34	1.48	1.43
25	G	610	CLA	CMB-C2B	-2.34	1.46	1.50
25	r	610	CLA	CMC-C2C	-2.34	1.46	1.50
25	a	405	CLA	MG-ND	-2.34	2.01	2.05
37	C	518	DGD	O2G-C2G	-2.34	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	402	CLA	MG-ND	-2.34	2.01	2.05
25	B	611	CLA	C1D-ND	2.34	1.40	1.37
29	C	523	LHG	O7-C5	-2.34	1.41	1.46
25	1	612	CLA	MG-ND	-2.34	2.01	2.05
25	g	604	CLA	CMC-C2C	-2.34	1.46	1.50
25	R	601	CLA	CHC-C1C	2.34	1.43	1.38
25	C	504	CLA	C1B-C2B	2.34	1.48	1.43
25	4	611	CLA	CMD-C2D	-2.34	1.46	1.50
24	1	609	CHL	CHA-CBD	-2.34	1.48	1.51
25	b	611	CLA	C1B-NB	-2.34	1.34	1.37
25	y	603	CLA	C1B-NB	-2.34	1.34	1.37
37	h	102	DGD	O3E-C3E	-2.34	1.37	1.43
25	7	610	CLA	C4B-NB	2.33	1.40	1.37
25	N	604	CLA	MG-ND	-2.33	2.01	2.05
35	Z	101	LMG	C7-C8	2.33	1.58	1.50
25	D	403	CLA	MG-ND	-2.33	2.01	2.05
25	R	612	CLA	CMB-C2B	-2.33	1.46	1.50
37	c	519	DGD	O2G-C2G	-2.33	1.41	1.46
25	G	611	CLA	CMD-C2D	-2.33	1.46	1.50
25	5	610	CLA	MG-NB	-2.33	2.01	2.05
25	8	610	CLA	C4B-NB	2.33	1.40	1.37
25	r	601	CLA	C3B-C4B	2.33	1.49	1.42
25	c	501	CLA	CMD-C2D	-2.33	1.46	1.50
25	B	608	CLA	MG-NB	-2.33	2.01	2.05
25	C	501	CLA	CMB-C2B	-2.33	1.46	1.50
25	7	610	CLA	CMD-C2D	-2.33	1.46	1.50
25	4	610	CLA	C4B-NB	2.33	1.40	1.37
25	r	613	CLA	C4B-NB	2.33	1.40	1.37
25	b	612	CLA	MG-NB	-2.33	2.01	2.05
25	g	611	CLA	CMB-C2B	-2.33	1.46	1.50
25	3	610	CLA	CMD-C2D	-2.33	1.46	1.50
25	R	609	CLA	CMB-C2B	-2.33	1.46	1.50
25	6	604	CLA	CMB-C2B	-2.33	1.46	1.50
25	g	614	CLA	MG-NB	-2.33	2.01	2.05
25	7	602	CLA	C4B-NB	2.33	1.40	1.37
25	2	604	CLA	CMB-C2B	-2.33	1.46	1.50
25	G	604	CLA	CMC-C2C	-2.33	1.46	1.50
25	r	609	CLA	CMC-C2C	-2.33	1.46	1.50
25	b	605	CLA	CMC-C2C	-2.33	1.46	1.50
25	n	603	CLA	MG-ND	-2.33	2.01	2.05
25	N	602	CLA	CMD-C2D	-2.33	1.46	1.50
25	n	602	CLA	CMD-C2D	-2.33	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	613	CLA	CHC-C4B	-2.33	1.34	1.39
25	r	604	CLA	C4B-NB	2.33	1.40	1.37
25	C	509	CLA	CMB-C2B	-2.33	1.46	1.50
25	c	501	CLA	CMB-C2B	-2.33	1.46	1.50
25	n	612	CLA	CMC-C2C	-2.33	1.46	1.50
24	y	601	CHL	C3D-C2D	2.32	1.43	1.39
25	b	610	CLA	CMC-C2C	-2.32	1.46	1.50
25	1	612	CLA	CMB-C2B	-2.32	1.46	1.50
25	R	611	CLA	MG-NB	-2.32	2.01	2.05
25	1	611	CLA	CMB-C2B	-2.32	1.46	1.50
25	7	610	CLA	MG-ND	-2.32	2.01	2.05
25	B	616	CLA	CMB-C2B	-2.32	1.46	1.50
25	g	610	CLA	CMD-C2D	-2.32	1.46	1.50
25	3	604	CLA	C1B-C2B	2.32	1.48	1.43
25	1	610	CLA	CMC-C2C	-2.32	1.46	1.50
25	n	604	CLA	MG-ND	-2.32	2.01	2.05
25	7	603	CLA	CMC-C2C	-2.32	1.46	1.50
25	y	613	CLA	CHC-C4B	-2.32	1.34	1.39
25	3	612	CLA	C1B-NB	-2.32	1.34	1.37
37	c	518	DGD	O2G-C2G	-2.32	1.41	1.46
25	b	602	CLA	MG-NB	-2.32	2.01	2.05
25	3	614	CLA	C1B-C2B	2.32	1.48	1.43
25	S	614	CLA	CMD-C2D	-2.32	1.46	1.50
25	d	402	CLA	CAA-C2A	-2.32	1.49	1.54
25	N	612	CLA	CMC-C2C	-2.32	1.46	1.50
25	2	610	CLA	CMD-C2D	-2.32	1.46	1.50
25	3	603	CLA	CMC-C2C	-2.32	1.46	1.50
25	C	504	CLA	CMB-C2B	-2.32	1.46	1.50
25	7	610	CLA	CMC-C2C	-2.32	1.46	1.50
25	G	611	CLA	CMB-C2B	-2.32	1.46	1.50
25	8	611	CLA	CMD-C2D	-2.32	1.46	1.50
25	R	611	CLA	MG-ND	-2.32	2.01	2.05
25	b	608	CLA	MG-NB	-2.32	2.01	2.05
26	r	620	LUT	C22-C21	-2.32	1.51	1.54
25	2	604	CLA	CMC-C2C	-2.32	1.46	1.50
25	B	612	CLA	MG-NB	-2.32	2.01	2.05
25	b	604	CLA	C4B-NB	2.32	1.40	1.37
24	Y	601	CHL	C3D-C2D	2.32	1.43	1.39
25	N	603	CLA	MG-ND	-2.32	2.01	2.05
25	b	616	CLA	C1B-C2B	2.32	1.48	1.43
35	z	101	LMG	C7-C8	2.32	1.58	1.50
25	B	608	CLA	C4B-NB	2.32	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	613	CLA	CMB-C2B	-2.31	1.46	1.50
25	5	612	CLA	CMD-C2D	-2.31	1.46	1.50
25	5	602	CLA	C4B-NB	2.31	1.40	1.37
25	y	604	CLA	C1D-ND	2.31	1.40	1.37
25	7	613	CLA	CMC-C2C	-2.31	1.46	1.50
25	n	603	CLA	CMC-C2C	-2.31	1.46	1.50
25	r	612	CLA	CMB-C2B	-2.31	1.46	1.50
25	R	609	CLA	C4B-NB	2.31	1.40	1.37
25	3	610	CLA	MG-ND	-2.31	2.01	2.05
25	2	611	CLA	C1B-C2B	2.31	1.48	1.43
25	B	616	CLA	C1B-C2B	2.31	1.48	1.43
25	N	610	CLA	C1B-C2B	2.31	1.48	1.43
25	B	612	CLA	C1B-NB	-2.31	1.34	1.37
25	R	609	CLA	CMC-C2C	-2.31	1.46	1.50
25	s	614	CLA	CMD-C2D	-2.31	1.46	1.50
25	Y	611	CLA	MG-ND	-2.31	2.01	2.05
25	r	609	CLA	CMB-C2B	-2.31	1.46	1.50
25	Y	602	CLA	C1B-C2B	2.31	1.48	1.43
25	5	602	CLA	CMB-C2B	-2.31	1.46	1.50
25	1	602	CLA	CMB-C2B	-2.31	1.46	1.50
25	b	616	CLA	CMB-C2B	-2.31	1.46	1.50
25	A	406	CLA	C1B-C2B	2.31	1.48	1.43
25	b	611	CLA	C4B-NB	2.31	1.40	1.37
25	7	603	CLA	CMB-C2B	-2.31	1.46	1.50
25	y	604	CLA	MG-ND	-2.31	2.01	2.05
25	b	608	CLA	C4B-NB	2.31	1.40	1.37
28	G	1623	NEX	O24-C25	-2.31	1.43	1.46
25	2	613	CLA	C1B-C2B	2.31	1.48	1.43
25	r	611	CLA	MG-ND	-2.31	2.01	2.05
25	n	610	CLA	C1B-C2B	2.31	1.48	1.43
25	3	613	CLA	CMC-C2C	-2.31	1.46	1.50
25	r	601	CLA	CHC-C1C	2.31	1.43	1.38
25	6	610	CLA	CMD-C2D	-2.31	1.46	1.50
25	B	610	CLA	CMC-C2C	-2.31	1.46	1.50
25	R	601	CLA	C3B-C4B	2.31	1.49	1.42
34	a	412	SQD	O47-C45	-2.30	1.41	1.46
27	r	622	XAT	C2-C1	-2.30	1.51	1.54
25	C	502	CLA	CMB-C2B	-2.30	1.46	1.50
25	s	602	CLA	C3B-C4B	2.30	1.49	1.42
25	r	609	CLA	C4B-NB	2.30	1.40	1.37
25	c	504	CLA	CMB-C2B	-2.30	1.46	1.50
25	4	604	CLA	MG-ND	-2.30	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	618	BCR	C30-C25	-2.30	1.50	1.53
25	s	602	CLA	CMC-C2C	-2.30	1.46	1.50
25	8	604	CLA	CMD-C2D	-2.30	1.46	1.50
25	2	602	CLA	C1B-C2B	2.30	1.48	1.43
30	B	618	BCR	C30-C25	-2.30	1.50	1.53
25	a	406	CLA	C1B-C2B	2.30	1.48	1.43
25	3	611	CLA	CHC-C4B	-2.30	1.34	1.39
36	D	405	PL9	C5-C4	-2.30	1.39	1.47
25	r	604	CLA	C1B-NB	-2.30	1.34	1.37
25	G	610	CLA	MG-NB	-2.30	2.01	2.05
25	6	611	CLA	C1B-C2B	2.30	1.48	1.43
25	g	610	CLA	C1B-C2B	2.30	1.48	1.43
25	2	604	CLA	MG-NB	-2.30	2.01	2.05
25	4	604	CLA	CMD-C2D	-2.30	1.46	1.50
25	B	610	CLA	C1B-NB	-2.30	1.34	1.37
25	d	403	CLA	CMC-C2C	-2.30	1.46	1.50
25	4	612	CLA	C3B-C4B	2.30	1.49	1.42
25	6	613	CLA	C1B-C2B	2.30	1.48	1.43
25	S	602	CLA	C3B-C4B	2.30	1.49	1.42
25	Y	604	CLA	MG-ND	-2.30	2.01	2.05
25	N	603	CLA	CMC-C2C	-2.30	1.46	1.50
27	R	622	XAT	C2-C1	-2.29	1.51	1.54
25	2	604	CLA	C1B-C2B	2.29	1.48	1.43
25	3	614	CLA	CMB-C2B	-2.29	1.46	1.50
25	6	604	CLA	MG-NB	-2.29	2.01	2.05
25	3	611	CLA	C1B-NB	-2.29	1.34	1.37
25	G	611	CLA	MG-ND	-2.29	2.01	2.05
25	g	610	CLA	MG-NB	-2.29	2.01	2.05
25	8	612	CLA	CMC-C2C	-2.29	1.46	1.50
25	n	610	CLA	CMB-C2B	-2.29	1.46	1.50
25	R	604	CLA	C4B-NB	2.29	1.40	1.37
25	r	612	CLA	C1B-C2B	2.29	1.48	1.43
25	7	602	CLA	MG-NB	-2.29	2.01	2.05
25	g	610	CLA	C4B-NB	2.29	1.40	1.37
24	5	609	CHL	CHA-CBD	-2.29	1.49	1.51
25	8	612	CLA	C3B-C4B	2.29	1.49	1.42
34	A	412	SQD	O47-C45	-2.29	1.41	1.46
25	6	602	CLA	C1B-C2B	2.29	1.48	1.43
25	5	611	CLA	C1B-C2B	2.29	1.48	1.43
25	c	508	CLA	C1B-C2B	2.29	1.48	1.43
25	S	602	CLA	CMC-C2C	-2.29	1.46	1.50
36	d	405	PL9	C5-C4	-2.29	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	410	CLA	C4B-NB	2.29	1.40	1.37
25	5	612	CLA	C1B-C2B	2.29	1.48	1.43
25	7	611	CLA	CHC-C4B	-2.29	1.34	1.39
25	B	603	CLA	CMB-C2B	-2.29	1.46	1.50
25	2	604	CLA	CMD-C2D	-2.29	1.46	1.50
25	n	602	CLA	MG-NB	-2.29	2.01	2.05
25	R	604	CLA	C1B-NB	-2.29	1.34	1.37
25	4	612	CLA	CMC-C2C	-2.29	1.46	1.50
25	b	603	CLA	CMB-C2B	-2.29	1.46	1.50
25	7	611	CLA	C1B-NB	-2.28	1.34	1.37
25	1	612	CLA	C1B-C2B	2.28	1.48	1.43
25	g	602	CLA	C1B-C2B	2.28	1.48	1.43
37	b	626	DGD	O2G-C2G	-2.28	1.41	1.46
25	G	610	CLA	CMD-C2D	-2.28	1.46	1.50
25	5	611	CLA	CMC-C2C	-2.28	1.46	1.50
25	N	602	CLA	MG-NB	-2.28	2.01	2.05
25	1	603	CLA	CAC-C3C	-2.28	1.45	1.51
25	1	611	CLA	CMC-C2C	-2.28	1.46	1.50
25	N	610	CLA	CMB-C2B	-2.28	1.46	1.50
25	8	604	CLA	MG-ND	-2.28	2.01	2.05
25	5	603	CLA	CAC-C3C	-2.28	1.45	1.51
25	1	602	CLA	C4B-NB	2.28	1.40	1.37
25	8	602	CLA	CMC-C2C	-2.28	1.46	1.50
25	6	612	CLA	C1B-C2B	2.28	1.48	1.43
25	g	613	CLA	CMD-C2D	-2.28	1.46	1.50
25	G	602	CLA	C1B-C2B	2.28	1.48	1.43
25	7	612	CLA	C1B-NB	-2.28	1.34	1.37
25	B	610	CLA	MG-ND	-2.28	2.01	2.05
25	6	604	CLA	C1B-C2B	2.28	1.48	1.43
25	a	407	CLA	C1B-C2B	2.28	1.48	1.43
25	y	614	CLA	CMC-C2C	-2.28	1.46	1.50
25	g	611	CLA	MG-ND	-2.28	2.01	2.05
25	5	612	CLA	CHC-C4B	-2.28	1.34	1.39
25	r	616	CLA	CMD-C2D	-2.28	1.46	1.50
25	N	611	CLA	CMB-C2B	-2.28	1.46	1.50
25	7	614	CLA	C1B-C2B	2.28	1.48	1.43
25	G	611	CLA	C1B-C2B	2.28	1.48	1.43
25	7	602	CLA	C1B-NB	-2.28	1.34	1.37
25	B	602	CLA	CMB-C2B	-2.28	1.46	1.50
25	Y	614	CLA	CMC-C2C	-2.28	1.46	1.50
25	B	608	CLA	MG-ND	-2.28	2.01	2.05
25	g	611	CLA	C1B-C2B	2.28	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	8	622	XAT	O24-C25	-2.27	1.43	1.46
25	8	610	CLA	MG-ND	-2.27	2.01	2.05
25	S	613	CLA	CMB-C2B	-2.27	1.46	1.50
25	r	602	CLA	C1B-C2B	2.27	1.48	1.43
25	3	602	CLA	MG-NB	-2.27	2.01	2.05
25	4	610	CLA	MG-ND	-2.27	2.01	2.05
25	b	603	CLA	C4B-NB	2.27	1.40	1.37
25	5	603	CLA	CHC-C4B	-2.27	1.34	1.39
25	A	407	CLA	C1B-C2B	2.27	1.48	1.43
25	Y	603	CLA	CMC-C2C	-2.27	1.46	1.50
25	y	602	CLA	C1B-C2B	2.27	1.48	1.43
25	1	611	CLA	C1B-C2B	2.27	1.48	1.43
26	4	620	LUT	C1-C6	-2.27	1.50	1.53
25	4	602	CLA	CMB-C2B	-2.27	1.46	1.50
25	g	612	CLA	CMC-C2C	-2.27	1.46	1.50
25	n	610	CLA	CMD-C2D	-2.27	1.46	1.50
25	y	613	CLA	CMB-C2B	-2.27	1.46	1.50
25	5	612	CLA	CMB-C2B	-2.27	1.46	1.50
25	c	502	CLA	CMB-C2B	-2.27	1.46	1.50
37	B	626	DGD	O2G-C2G	-2.27	1.41	1.46
25	C	508	CLA	C1B-C2B	2.27	1.48	1.43
25	3	603	CLA	CMB-C2B	-2.27	1.46	1.50
25	G	613	CLA	CMD-C2D	-2.27	1.46	1.50
25	b	612	CLA	C1B-NB	-2.27	1.34	1.37
25	2	612	CLA	C1B-C2B	2.27	1.48	1.43
25	D	403	CLA	CMC-C2C	-2.27	1.46	1.50
25	b	602	CLA	CMB-C2B	-2.27	1.46	1.50
25	a	406	CLA	CAC-C3C	-2.27	1.45	1.51
25	C	506	CLA	C1B-C2B	2.27	1.48	1.43
25	A	406	CLA	CAC-C3C	-2.27	1.45	1.51
25	3	602	CLA	C4B-NB	2.27	1.40	1.37
25	4	602	CLA	CMC-C2C	-2.27	1.46	1.50
25	G	603	CLA	CMD-C2D	-2.27	1.46	1.50
25	N	610	CLA	MG-NB	-2.27	2.01	2.05
25	1	613	CLA	C1B-C2B	2.27	1.48	1.43
25	R	612	CLA	C1B-C2B	2.27	1.48	1.43
25	8	612	CLA	C1B-C2B	2.27	1.48	1.43
25	3	602	CLA	C1B-NB	-2.27	1.34	1.37
25	B	603	CLA	C4B-NB	2.27	1.40	1.37
35	a	413	LMG	O7-C8	-2.27	1.41	1.46
39	f	101	HEM	FE-NC	2.27	2.02	1.95
25	1	603	CLA	CHC-C4B	-2.27	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	603	CLA	CMD-C2D	-2.26	1.46	1.50
25	s	612	CLA	CMD-C2D	-2.26	1.46	1.50
25	Y	613	CLA	CMB-C2B	-2.26	1.46	1.50
25	8	602	CLA	CMB-C2B	-2.26	1.46	1.50
25	1	612	CLA	CHC-C4B	-2.26	1.34	1.39
25	R	601	CLA	C1B-C2B	2.26	1.48	1.43
25	G	610	CLA	C4B-NB	2.26	1.40	1.37
24	8	608	CHL	CHA-CBD	-2.26	1.49	1.51
25	G	610	CLA	C1B-C2B	2.26	1.48	1.43
25	G	614	CLA	CMC-C2C	-2.26	1.46	1.50
25	1	604	CLA	CMC-C2C	-2.26	1.46	1.50
25	N	610	CLA	CMD-C2D	-2.26	1.46	1.50
25	B	602	CLA	C1B-C2B	2.26	1.48	1.43
25	S	612	CLA	CMD-C2D	-2.26	1.46	1.50
25	S	604	CLA	C3B-C4B	2.26	1.49	1.42
25	5	613	CLA	C1B-C2B	2.26	1.48	1.43
25	C	506	CLA	MG-NB	-2.26	2.01	2.05
25	n	610	CLA	MG-NB	-2.26	2.01	2.05
25	B	604	CLA	C4B-NB	2.26	1.40	1.37
25	c	506	CLA	C1B-C2B	2.26	1.48	1.43
25	b	608	CLA	MG-ND	-2.26	2.01	2.05
25	b	610	CLA	MG-ND	-2.26	2.01	2.05
25	R	604	CLA	CMC-C2C	-2.26	1.46	1.50
25	B	617	CLA	CHC-C4B	-2.26	1.34	1.39
25	R	602	CLA	C1B-C2B	2.26	1.48	1.43
25	a	410	CLA	C4B-NB	2.26	1.40	1.37
24	S	601	CHL	CBD-CGD	-2.26	1.49	1.52
35	A	413	LMG	O7-C8	-2.26	1.41	1.46
25	s	614	CLA	C3B-C4B	2.26	1.49	1.42
25	s	604	CLA	C3B-C4B	2.26	1.49	1.42
25	B	611	CLA	C4B-NB	2.26	1.40	1.37
25	G	612	CLA	CMC-C2C	-2.26	1.46	1.50
25	N	612	CLA	CMB-C2B	-2.26	1.46	1.50
25	N	610	CLA	C4B-NB	2.26	1.40	1.37
25	4	603	CLA	CMC-C2C	-2.26	1.46	1.50
25	n	614	CLA	CMB-C2B	-2.26	1.46	1.50
25	N	602	CLA	MG-ND	-2.26	2.01	2.05
25	c	506	CLA	MG-NB	-2.26	2.01	2.05
25	g	602	CLA	MG-NB	-2.26	2.01	2.05
25	r	601	CLA	C1B-C2B	2.26	1.48	1.43
39	F	101	HEM	FE-NC	2.25	2.02	1.95
25	1	611	CLA	MG-ND	-2.25	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	602	CLA	MG-ND	-2.25	2.01	2.05
25	3	613	CLA	CHC-C4B	-2.25	1.34	1.39
25	N	614	CLA	CMD-C2D	-2.25	1.46	1.50
25	5	604	CLA	CMC-C2C	-2.25	1.46	1.50
25	6	614	CLA	CMB-C2B	-2.25	1.46	1.50
25	g	614	CLA	CMC-C2C	-2.25	1.46	1.50
27	1	1622	XAT	O24-C25	-2.25	1.43	1.46
25	8	603	CLA	CMC-C2C	-2.25	1.46	1.50
25	s	612	CLA	C3B-C4B	2.25	1.49	1.42
25	5	611	CLA	CMD-C2D	-2.25	1.46	1.50
25	6	602	CLA	MG-ND	-2.25	2.01	2.05
25	R	616	CLA	CMC-C2C	-2.25	1.46	1.50
25	G	602	CLA	MG-NB	-2.25	2.01	2.05
25	G	603	CLA	CMC-C2C	-2.25	1.46	1.50
25	6	610	CLA	C1B-C2B	2.25	1.48	1.43
25	7	613	CLA	CHC-C4B	-2.25	1.34	1.39
24	s	601	CHL	CBD-CGD	-2.25	1.49	1.52
25	B	606	CLA	MG-NB	-2.25	2.01	2.05
25	7	614	CLA	CMB-C2B	-2.25	1.46	1.50
25	2	614	CLA	CMB-C2B	-2.25	1.46	1.50
25	n	610	CLA	C4B-NB	2.25	1.40	1.37
25	6	604	CLA	CMD-C2D	-2.25	1.46	1.50
25	n	612	CLA	CMB-C2B	-2.25	1.46	1.50
25	b	617	CLA	CHC-C4B	-2.24	1.34	1.39
25	N	611	CLA	CMD-C2D	-2.24	1.46	1.50
25	5	614	CLA	CMB-C2B	-2.24	1.46	1.50
25	B	612	CLA	MG-ND	-2.24	2.01	2.05
25	2	610	CLA	C1B-C2B	2.24	1.48	1.43
33	a	408	PHO	CAC-C3C	-2.24	1.47	1.51
25	1	614	CLA	MG-ND	-2.24	2.01	2.05
25	n	611	CLA	CMB-C2B	-2.24	1.46	1.50
25	a	410	CLA	C1B-C2B	2.24	1.48	1.43
25	a	410	CLA	CMC-C2C	-2.24	1.46	1.50
25	y	603	CLA	CMC-C2C	-2.24	1.46	1.50
25	A	410	CLA	CMC-C2C	-2.24	1.46	1.50
25	5	603	CLA	C1B-C2B	2.24	1.48	1.43
25	n	602	CLA	MG-ND	-2.24	2.01	2.05
25	2	613	CLA	CMB-C2B	-2.24	1.46	1.50
25	7	602	CLA	CMB-C2B	-2.24	1.46	1.50
25	b	602	CLA	C1B-C2B	2.24	1.48	1.43
25	6	610	CLA	MG-NB	-2.24	2.01	2.05
25	1	603	CLA	C1B-C2B	2.24	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	614	CLA	CMB-C2B	-2.24	1.46	1.50
25	5	614	CLA	MG-ND	-2.24	2.01	2.05
25	r	604	CLA	CMC-C2C	-2.24	1.46	1.50
25	G	604	CLA	MG-ND	-2.24	2.01	2.05
33	A	408	PHO	CAC-C3C	-2.24	1.47	1.51
25	B	607	CLA	MG-NB	-2.24	2.01	2.05
25	8	602	CLA	C3B-C4B	2.24	1.49	1.42
25	R	616	CLA	CMD-C2D	-2.24	1.46	1.50
25	y	612	CLA	C3B-C4B	2.24	1.49	1.42
25	Y	602	CLA	MG-ND	-2.24	2.01	2.05
25	b	606	CLA	MG-NB	-2.24	2.01	2.05
25	8	603	CLA	CMB-C2B	-2.24	1.46	1.50
25	4	603	CLA	CMB-C2B	-2.23	1.46	1.50
25	r	616	CLA	CMC-C2C	-2.23	1.46	1.50
25	g	604	CLA	C1B-NB	-2.23	1.34	1.37
25	S	612	CLA	C3B-C4B	2.23	1.49	1.42
25	3	612	CLA	C4B-NB	2.23	1.40	1.37
25	6	612	CLA	CMD-C2D	-2.23	1.46	1.50
25	A	410	CLA	C1B-C2B	2.23	1.48	1.43
25	Y	612	CLA	C3B-C4B	2.23	1.49	1.42
25	b	606	CLA	C1B-C2B	2.23	1.48	1.43
25	y	602	CLA	C1B-NB	-2.23	1.34	1.37
35	Z	101	LMG	C4-C5	2.23	1.57	1.53
25	S	614	CLA	C3B-C4B	2.23	1.49	1.42
25	R	611	CLA	CMB-C2B	-2.23	1.46	1.50
25	G	604	CLA	C1B-NB	-2.23	1.34	1.37
25	7	603	CLA	C1B-C2B	2.23	1.48	1.43
25	b	607	CLA	MG-NB	-2.23	2.01	2.05
25	n	614	CLA	CMD-C2D	-2.23	1.46	1.50
25	C	506	CLA	CMD-C2D	-2.23	1.46	1.50
25	b	602	CLA	CMC-C2C	-2.23	1.46	1.50
25	R	603	CLA	C1B-C2B	2.23	1.48	1.43
25	A	405	CLA	C4B-NB	2.23	1.40	1.37
25	Y	602	CLA	C1B-NB	-2.23	1.34	1.37
25	4	612	CLA	C1B-C2B	2.23	1.48	1.43
25	r	603	CLA	C1B-C2B	2.23	1.48	1.43
25	c	506	CLA	CMD-C2D	-2.23	1.46	1.50
25	4	602	CLA	C3B-C4B	2.23	1.49	1.42
27	5	1622	XAT	O24-C25	-2.23	1.43	1.46
25	g	613	CLA	CHC-C4B	-2.23	1.34	1.39
25	N	614	CLA	CMB-C2B	-2.23	1.46	1.50
26	8	620	LUT	C1-C6	-2.23	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	611	CLA	CMB-C2B	-2.23	1.46	1.50
27	4	622	XAT	O24-C25	-2.23	1.43	1.46
25	B	605	CLA	CHC-C4B	-2.23	1.34	1.39
25	2	612	CLA	C3B-C4B	2.22	1.49	1.42
25	7	604	CLA	CMC-C2C	-2.22	1.46	1.50
25	B	606	CLA	C1B-C2B	2.22	1.48	1.43
25	b	605	CLA	CHC-C4B	-2.22	1.34	1.39
25	C	511	CLA	C3B-C4B	2.22	1.49	1.42
25	B	614	CLA	CAA-C2A	-2.22	1.50	1.54
25	y	602	CLA	MG-ND	-2.22	2.01	2.05
29	d	410	LHG	O7-C5	-2.22	1.41	1.46
25	G	613	CLA	CHC-C4B	-2.22	1.34	1.39
25	c	511	CLA	C3B-C4B	2.22	1.49	1.42
25	3	602	CLA	CMB-C2B	-2.22	1.46	1.50
25	y	603	CLA	CAC-C3C	-2.22	1.45	1.51
25	3	612	CLA	C1B-C2B	2.22	1.48	1.43
25	b	607	CLA	C1B-NB	-2.22	1.34	1.37
25	g	602	CLA	C4B-NB	2.22	1.40	1.37
24	4	608	CHL	CHA-CBD	-2.22	1.49	1.51
25	1	610	CLA	CMD-C2D	-2.22	1.46	1.50
30	T	101	BCR	C1-C6	-2.22	1.50	1.53
25	1	613	CLA	CMC-C2C	-2.22	1.46	1.50
25	G	603	CLA	CAC-C3C	-2.22	1.45	1.51
25	G	614	CLA	MG-ND	-2.22	2.01	2.05
25	6	613	CLA	CMB-C2B	-2.22	1.46	1.50
25	8	604	CLA	CMC-C2C	-2.22	1.46	1.50
30	t	101	BCR	C1-C6	-2.22	1.50	1.53
25	5	610	CLA	CMD-C2D	-2.22	1.46	1.50
25	n	611	CLA	CMD-C2D	-2.22	1.46	1.50
25	3	603	CLA	C1B-C2B	2.22	1.48	1.43
35	z	101	LMG	C4-C5	2.22	1.57	1.53
36	D	405	PL9	C10-C9	-2.22	1.45	1.50
25	g	603	CLA	CAC-C3C	-2.22	1.45	1.51
25	3	604	CLA	CMC-C2C	-2.22	1.46	1.50
25	g	603	CLA	CMC-C2C	-2.22	1.46	1.50
25	r	609	CLA	C3B-C4B	2.22	1.49	1.42
25	1	611	CLA	CMD-C2D	-2.21	1.46	1.50
25	b	603	CLA	CMC-C2C	-2.21	1.46	1.50
25	7	612	CLA	C1B-C2B	2.21	1.48	1.43
25	B	603	CLA	CMC-C2C	-2.21	1.46	1.50
25	b	614	CLA	CAA-C2A	-2.21	1.50	1.54
25	4	604	CLA	CMC-C2C	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	602	CLA	C1D-ND	2.21	1.40	1.37
25	r	602	CLA	C4B-NB	2.21	1.40	1.37
36	d	405	PL9	C10-C9	-2.21	1.45	1.50
24	5	606	CHL	MG-ND	-2.21	2.01	2.05
25	3	602	CLA	C1D-ND	2.21	1.40	1.37
25	R	609	CLA	C3B-C4B	2.21	1.49	1.42
25	r	611	CLA	CMD-C2D	-2.21	1.46	1.50
25	1	610	CLA	CMB-C2B	-2.21	1.46	1.50
25	2	612	CLA	CMD-C2D	-2.21	1.46	1.50
25	7	602	CLA	C1D-ND	2.21	1.40	1.37
25	R	612	CLA	MG-ND	-2.21	2.01	2.05
25	6	604	CLA	MG-ND	-2.21	2.01	2.05
25	6	612	CLA	C3B-C4B	2.21	1.49	1.42
25	B	602	CLA	CMC-C2C	-2.21	1.46	1.50
25	S	602	CLA	CMD-C2D	-2.21	1.46	1.50
25	s	602	CLA	CMD-C2D	-2.21	1.46	1.50
25	6	602	CLA	C1D-ND	2.21	1.40	1.37
25	B	615	CLA	MG-ND	-2.21	2.01	2.05
25	3	603	CLA	CAC-C3C	-2.21	1.45	1.51
25	B	607	CLA	C1B-NB	-2.21	1.35	1.37
25	5	611	CLA	MG-ND	-2.21	2.01	2.05
25	2	610	CLA	MG-NB	-2.21	2.01	2.05
25	b	612	CLA	MG-ND	-2.20	2.01	2.05
25	r	609	CLA	C1B-C2B	2.20	1.48	1.43
25	3	604	CLA	CMD-C2D	-2.20	1.46	1.50
25	7	604	CLA	CMD-C2D	-2.20	1.46	1.50
28	5	1623	NEX	C22-C21	-2.20	1.51	1.54
25	5	610	CLA	CMB-C2B	-2.20	1.46	1.50
25	5	613	CLA	CMC-C2C	-2.20	1.46	1.50
25	D	403	CLA	C1B-C2B	2.20	1.48	1.43
25	7	603	CLA	CAC-C3C	-2.20	1.45	1.51
25	s	609	CLA	C3B-C4B	2.20	1.49	1.42
25	4	604	CLA	C1B-NB	-2.20	1.35	1.37
24	y	609	CHL	CMA-C3A	-2.20	1.49	1.53
25	c	510	CLA	C3B-C4B	2.20	1.49	1.42
25	N	614	CLA	CMC-C2C	-2.20	1.46	1.50
25	S	609	CLA	C3B-C4B	2.20	1.49	1.42
24	3	606	CHL	CHA-CBD	-2.20	1.49	1.51
25	C	511	CLA	CMD-C2D	-2.20	1.46	1.50
25	Y	603	CLA	CAC-C3C	-2.20	1.45	1.51
25	7	612	CLA	C4B-NB	2.20	1.40	1.37
25	G	602	CLA	C4B-NB	2.20	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	606	CLA	C1B-NB	-2.20	1.35	1.37
25	R	611	CLA	CMD-C2D	-2.20	1.46	1.50
25	Y	613	CLA	C1B-NB	-2.20	1.35	1.37
25	g	614	CLA	MG-ND	-2.20	2.01	2.05
25	g	604	CLA	MG-ND	-2.20	2.01	2.05
25	n	603	CLA	CAC-C3C	-2.20	1.45	1.51
25	b	615	CLA	MG-ND	-2.19	2.01	2.05
25	c	503	CLA	C3B-C4B	2.19	1.49	1.42
25	C	510	CLA	C3B-C4B	2.19	1.49	1.42
25	4	602	CLA	MG-NB	-2.19	2.01	2.05
28	1	1623	NEX	C22-C21	-2.19	1.51	1.54
25	d	403	CLA	C1B-C2B	2.19	1.48	1.43
25	C	503	CLA	C3B-C4B	2.19	1.49	1.42
25	8	602	CLA	MG-NB	-2.19	2.01	2.05
34	A	412	SQD	O2-C2	-2.19	1.37	1.43
35	Z	101	LMG	C4-C3	2.19	1.58	1.52
25	N	603	CLA	CAC-C3C	-2.19	1.45	1.51
25	1	602	CLA	C1B-C2B	2.19	1.48	1.43
37	c	520	DGD	O2G-C2G	-2.19	1.41	1.46
25	c	507	CLA	CMD-C2D	-2.19	1.46	1.50
25	g	613	CLA	CMC-C2C	-2.19	1.46	1.50
25	s	610	CLA	C1B-C2B	2.19	1.48	1.43
25	R	602	CLA	C4B-NB	2.19	1.40	1.37
24	1	606	CHL	MG-ND	-2.19	2.01	2.05
25	5	614	CLA	MG-NB	-2.19	2.01	2.05
27	g	1622	XAT	O24-C25	-2.19	1.43	1.46
29	D	410	LHG	O7-C5	-2.19	1.41	1.46
34	a	412	SQD	O2-C2	-2.19	1.37	1.43
25	G	614	CLA	CMB-C2B	-2.19	1.46	1.50
25	S	603	CLA	C3B-C4B	2.19	1.49	1.42
25	a	405	CLA	C4B-NB	2.19	1.40	1.37
25	2	604	CLA	CHC-C4B	-2.19	1.34	1.39
25	6	604	CLA	CHC-C4B	-2.19	1.34	1.39
25	2	611	CLA	CMB-C2B	-2.19	1.46	1.50
25	c	511	CLA	CMD-C2D	-2.19	1.46	1.50
25	r	612	CLA	MG-ND	-2.18	2.01	2.05
25	n	611	CLA	MG-NB	-2.18	2.01	2.05
25	s	603	CLA	C3B-C4B	2.18	1.49	1.42
25	n	614	CLA	CMC-C2C	-2.18	1.46	1.50
25	B	606	CLA	C1B-NB	-2.18	1.35	1.37
25	s	613	CLA	CMD-C2D	-2.18	1.46	1.50
25	1	614	CLA	MG-NB	-2.18	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	603	CLA	MG-NB	-2.18	2.01	2.05
25	R	609	CLA	C1B-C2B	2.18	1.48	1.43
25	g	614	CLA	CMB-C2B	-2.18	1.46	1.50
25	D	402	CLA	C4B-NB	2.18	1.40	1.37
25	2	603	CLA	CMB-C2B	-2.18	1.46	1.50
25	6	603	CLA	CMB-C2B	-2.18	1.46	1.50
25	G	602	CLA	MG-ND	-2.18	2.01	2.05
25	r	611	CLA	C3B-C4B	2.18	1.49	1.42
25	G	613	CLA	CMC-C2C	-2.18	1.46	1.50
25	n	611	CLA	CMC-C2C	-2.18	1.46	1.50
25	6	612	CLA	MG-ND	-2.18	2.01	2.05
25	Y	604	CLA	C3B-C4B	2.18	1.49	1.42
25	R	611	CLA	C3B-C4B	2.18	1.49	1.42
25	b	605	CLA	C1B-C2B	2.18	1.48	1.43
25	S	611	CLA	CMD-C2D	-2.18	1.46	1.50
25	r	604	CLA	C1B-C2B	2.18	1.48	1.43
37	C	520	DGD	O2G-C2G	-2.17	1.41	1.46
27	G	1622	XAT	O24-C25	-2.17	1.43	1.46
35	z	101	LMG	C4-C3	2.17	1.58	1.52
25	2	613	CLA	CMC-C2C	-2.17	1.46	1.50
25	C	506	CLA	CMC-C2C	-2.17	1.46	1.50
25	r	612	CLA	CMC-C2C	-2.17	1.46	1.50
25	n	612	CLA	CHC-C4B	-2.17	1.34	1.39
25	y	604	CLA	C3B-C4B	2.17	1.49	1.42
25	N	612	CLA	CHC-C4B	-2.17	1.34	1.39
25	N	611	CLA	MG-NB	-2.17	2.01	2.05
25	7	614	CLA	CMD-C2D	-2.17	1.46	1.50
25	R	616	CLA	C1B-NB	-2.17	1.35	1.37
25	2	612	CLA	MG-ND	-2.17	2.01	2.05
25	b	606	CLA	CAC-C3C	-2.17	1.45	1.51
25	1	603	CLA	MG-NB	-2.17	2.01	2.05
25	d	402	CLA	C4B-NB	2.17	1.40	1.37
25	2	603	CLA	C3B-C4B	2.17	1.49	1.42
25	6	603	CLA	C3B-C4B	2.17	1.49	1.42
25	5	602	CLA	C1B-C2B	2.17	1.48	1.43
25	B	606	CLA	CAC-C3C	-2.17	1.45	1.51
25	C	507	CLA	CMD-C2D	-2.17	1.46	1.50
25	6	611	CLA	CMB-C2B	-2.17	1.46	1.50
37	H	102	DGD	O2E-C2E	-2.17	1.37	1.43
37	h	102	DGD	O2E-C2E	-2.17	1.37	1.43
25	2	611	CLA	CMC-C2C	-2.17	1.46	1.50
25	R	612	CLA	CMC-C2C	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	607	CHL	C4A-C3A	-2.17	1.46	1.51
25	S	610	CLA	C1B-C2B	2.17	1.48	1.43
25	g	603	CLA	C1B-NB	-2.17	1.35	1.37
25	6	613	CLA	CMC-C2C	-2.17	1.46	1.50
25	c	512	CLA	C3B-C4B	2.17	1.49	1.42
25	B	605	CLA	C1B-C2B	2.17	1.48	1.43
25	B	606	CLA	CHC-C4B	-2.17	1.34	1.39
24	1	607	CHL	C4A-C3A	-2.16	1.46	1.51
25	C	513	CLA	CMC-C2C	-2.16	1.46	1.50
25	c	506	CLA	CMC-C2C	-2.16	1.46	1.50
24	7	606	CHL	CHA-CBD	-2.16	1.49	1.51
25	b	606	CLA	CHC-C4B	-2.16	1.34	1.39
25	r	613	CLA	CHC-C4B	-2.16	1.34	1.39
35	c	521	LMG	O7-C8	-2.16	1.41	1.46
25	2	604	CLA	MG-ND	-2.16	2.01	2.05
25	3	603	CLA	MG-NB	-2.16	2.01	2.05
25	S	613	CLA	CMD-C2D	-2.16	1.46	1.50
25	6	611	CLA	CMC-C2C	-2.16	1.46	1.50
27	y	1622	XAT	O24-C25	-2.16	1.43	1.46
25	2	614	CLA	C1B-C2B	2.16	1.48	1.43
25	6	602	CLA	CMB-C2B	-2.16	1.46	1.50
25	s	611	CLA	CMD-C2D	-2.16	1.46	1.50
25	r	616	CLA	C1B-NB	-2.16	1.35	1.37
25	1	613	CLA	CHC-C4B	-2.16	1.34	1.39
25	6	614	CLA	C1B-C2B	2.16	1.48	1.43
24	3	608	CHL	CMC-C2C	2.16	1.49	1.44
25	C	512	CLA	C3B-C4B	2.16	1.49	1.42
25	s	610	CLA	CMB-C2B	-2.16	1.46	1.50
25	Y	610	CLA	C4B-NB	2.16	1.40	1.37
25	r	609	CLA	MG-NB	-2.16	2.01	2.05
25	C	501	CLA	CMC-C2C	-2.16	1.46	1.50
25	S	611	CLA	C3B-C4B	2.16	1.49	1.42
25	4	612	CLA	MG-ND	-2.15	2.01	2.05
25	8	604	CLA	C1B-NB	-2.15	1.35	1.37
25	8	612	CLA	MG-ND	-2.15	2.01	2.05
30	H	101	BCR	C30-C25	-2.15	1.51	1.53
25	r	612	CLA	MG-NB	-2.15	2.01	2.05
25	b	609	CLA	CMB-C2B	-2.15	1.46	1.50
25	2	614	CLA	MG-ND	-2.15	2.01	2.05
25	R	604	CLA	C1B-C2B	2.15	1.48	1.43
24	Y	609	CHL	CMA-C3A	-2.15	1.49	1.53
25	r	601	CLA	CMB-C2B	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	610	CLA	C3B-C4B	2.15	1.49	1.42
25	c	513	CLA	CMC-C2C	-2.15	1.46	1.50
25	N	612	CLA	MG-ND	-2.15	2.01	2.05
24	6	601	CHL	CMC-C2C	2.15	1.49	1.44
25	B	606	CLA	MG-ND	-2.15	2.01	2.05
25	B	602	CLA	C3B-C4B	2.15	1.49	1.42
25	R	601	CLA	CMB-C2B	-2.15	1.46	1.50
25	S	610	CLA	C3B-C4B	2.15	1.49	1.42
25	C	503	CLA	CMD-C2D	-2.15	1.46	1.50
25	7	603	CLA	MG-NB	-2.15	2.01	2.05
25	b	617	CLA	MG-NB	-2.15	2.01	2.05
25	B	617	CLA	MG-NB	-2.15	2.01	2.05
28	6	1623	NEX	O24-C25	-2.15	1.43	1.46
25	3	614	CLA	CMD-C2D	-2.15	1.46	1.50
27	Y	1622	XAT	O24-C25	-2.15	1.43	1.46
25	b	606	CLA	MG-ND	-2.15	2.01	2.05
27	2	1622	XAT	O24-C25	-2.15	1.43	1.46
25	s	611	CLA	C3B-C4B	2.15	1.49	1.42
25	8	603	CLA	C3B-C4B	2.15	1.49	1.42
25	R	613	CLA	CHC-C4B	-2.15	1.34	1.39
25	1	614	CLA	CMC-C2C	-2.14	1.46	1.50
25	y	610	CLA	C3B-C4B	2.14	1.49	1.42
25	c	504	CLA	CMC-C2C	-2.14	1.46	1.50
24	7	608	CHL	CMC-C2C	2.14	1.49	1.44
25	s	611	CLA	CMB-C2B	-2.14	1.46	1.50
25	g	602	CLA	MG-ND	-2.14	2.01	2.05
25	3	603	CLA	C4B-NB	2.14	1.40	1.37
25	G	611	CLA	CMC-C2C	-2.14	1.46	1.50
25	5	614	CLA	CMC-C2C	-2.14	1.46	1.50
25	6	614	CLA	CMC-C2C	-2.14	1.46	1.50
37	C	518	DGD	O3E-C3E	-2.14	1.37	1.43
25	B	609	CLA	CMB-C2B	-2.14	1.46	1.50
25	C	505	CLA	CMC-C2C	-2.14	1.46	1.50
25	R	601	CLA	CMD-C2D	-2.14	1.46	1.50
25	C	505	CLA	CMB-C2B	-2.14	1.46	1.50
25	C	508	CLA	CMD-C2D	-2.14	1.46	1.50
24	N	606	CHL	MG-ND	-2.14	2.01	2.05
24	y	606	CHL	MG-ND	-2.14	2.01	2.05
25	g	612	CLA	MG-ND	-2.14	2.01	2.05
25	B	607	CLA	C1B-C2B	2.14	1.48	1.43
29	B	2630	LHG	P-O6	2.14	1.67	1.59
24	6	609	CHL	CHA-CBD	-2.14	1.49	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	614	CLA	C3B-C4B	2.14	1.49	1.42
25	G	612	CLA	MG-ND	-2.14	2.01	2.05
25	5	614	CLA	C1B-C2B	2.14	1.48	1.43
39	f	101	HEM	CMB-C2B	2.14	1.55	1.50
25	4	611	CLA	CMB-C2B	-2.14	1.46	1.50
25	g	611	CLA	CMC-C2C	-2.14	1.46	1.50
24	2	601	CHL	CMC-C2C	2.14	1.49	1.44
25	c	503	CLA	CMD-C2D	-2.14	1.46	1.50
25	R	609	CLA	MG-ND	-2.14	2.01	2.05
25	Y	610	CLA	C3B-C4B	2.14	1.49	1.42
25	C	513	CLA	CMD-C2D	-2.14	1.46	1.50
25	Y	610	CLA	MG-NB	-2.14	2.01	2.05
25	6	614	CLA	MG-ND	-2.14	2.01	2.05
25	C	511	CLA	CMB-C2B	-2.13	1.46	1.50
25	8	611	CLA	CMB-C2B	-2.13	1.46	1.50
25	B	602	CLA	MG-ND	-2.13	2.01	2.05
37	c	518	DGD	O3E-C3E	-2.13	1.37	1.43
25	y	610	CLA	MG-NB	-2.13	2.01	2.05
25	b	607	CLA	C1B-C2B	2.13	1.48	1.43
25	S	610	CLA	CMB-C2B	-2.13	1.46	1.50
25	8	610	CLA	CMB-C2B	-2.13	1.46	1.50
25	b	602	CLA	C3B-C4B	2.13	1.49	1.42
25	r	601	CLA	CMD-C2D	-2.13	1.46	1.50
25	g	612	CLA	C3B-C4B	2.13	1.49	1.42
25	N	611	CLA	CMC-C2C	-2.13	1.46	1.50
25	C	504	CLA	C3B-C4B	2.13	1.49	1.42
25	a	410	CLA	MG-ND	-2.13	2.01	2.05
29	y	2630	LHG	O8-C6	-2.13	1.40	1.45
27	6	1622	XAT	O4-C5	-2.13	1.43	1.46
25	S	603	CLA	CMD-C2D	-2.13	1.46	1.50
25	c	501	CLA	CMC-C2C	-2.13	1.46	1.50
25	c	505	CLA	CMC-C2C	-2.13	1.46	1.50
25	c	508	CLA	CMD-C2D	-2.13	1.46	1.50
25	s	603	CLA	CMD-C2D	-2.13	1.46	1.50
25	1	602	CLA	C1B-NB	-2.13	1.35	1.37
24	n	606	CHL	MG-ND	-2.13	2.01	2.05
25	n	612	CLA	MG-ND	-2.13	2.01	2.05
25	2	602	CLA	CMB-C2B	-2.13	1.46	1.50
25	C	504	CLA	CMC-C2C	-2.13	1.46	1.50
25	7	612	CLA	CHC-C4B	-2.13	1.34	1.39
25	4	610	CLA	CMB-C2B	-2.13	1.46	1.50
25	6	614	CLA	C3B-C4B	2.13	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	602	CLA	MG-ND	-2.13	2.01	2.05
34	B	623	SQD	O3-C3	-2.13	1.37	1.43
25	b	603	CLA	C1B-NB	-2.13	1.35	1.37
25	y	611	CLA	C1B-NB	-2.13	1.35	1.37
25	1	614	CLA	C1B-C2B	2.13	1.48	1.43
25	3	603	CLA	CHC-C4B	-2.13	1.34	1.39
25	R	609	CLA	MG-NB	-2.13	2.01	2.05
25	s	602	CLA	CMB-C2B	-2.13	1.46	1.50
35	C	521	LMG	O7-C8	-2.13	1.41	1.46
25	5	603	CLA	C1B-NB	-2.13	1.35	1.37
34	b	623	SQD	O3-C3	-2.13	1.37	1.43
25	6	602	CLA	C3B-C4B	2.13	1.48	1.42
25	n	604	CLA	C3B-C4B	2.13	1.48	1.42
25	3	612	CLA	CHC-C4B	-2.13	1.34	1.39
25	G	612	CLA	C3B-C4B	2.13	1.48	1.42
24	G	609	CHL	CMC-C2C	2.13	1.49	1.44
37	c	519	DGD	C4E-C3E	2.12	1.57	1.52
25	Y	611	CLA	C1B-NB	-2.12	1.35	1.37
25	S	604	CLA	CMB-C2B	-2.12	1.46	1.50
25	A	410	CLA	MG-ND	-2.12	2.01	2.05
24	2	609	CHL	CHA-CBD	-2.12	1.49	1.51
25	B	612	CLA	C4B-NB	2.12	1.40	1.37
25	4	603	CLA	MG-NB	-2.12	2.01	2.05
25	7	611	CLA	CMC-C2C	-2.12	1.46	1.50
25	y	613	CLA	CMC-C2C	-2.12	1.46	1.50
25	4	603	CLA	C3B-C4B	2.12	1.48	1.42
25	y	613	CLA	C1B-NB	-2.12	1.35	1.37
25	8	611	CLA	MG-NB	-2.12	2.01	2.05
25	5	613	CLA	CHC-C4B	-2.12	1.34	1.39
25	7	603	CLA	CHC-C4B	-2.12	1.34	1.39
25	b	616	CLA	CHC-C4B	-2.12	1.34	1.39
39	F	101	HEM	CMB-C2B	2.12	1.55	1.50
29	b	2630	LHG	P-O6	2.12	1.67	1.59
25	B	616	CLA	CHC-C4B	-2.12	1.34	1.39
25	A	407	CLA	CMC-C2C	-2.12	1.46	1.50
25	c	505	CLA	CMB-C2B	-2.12	1.46	1.50
37	C	519	DGD	C4E-C3E	2.12	1.57	1.52
27	6	1622	XAT	O24-C25	-2.12	1.43	1.46
30	h	101	BCR	C30-C25	-2.12	1.51	1.53
25	y	612	CLA	C1B-NB	-2.12	1.35	1.37
25	R	613	CLA	C1B-NB	-2.12	1.35	1.37
25	B	610	CLA	CHC-C4B	-2.12	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	612	CLA	MG-NB	-2.12	2.01	2.05
25	a	407	CLA	CMC-C2C	-2.12	1.46	1.50
25	r	613	CLA	C1B-NB	-2.12	1.35	1.37
25	2	614	CLA	CMC-C2C	-2.12	1.46	1.50
25	8	603	CLA	MG-NB	-2.12	2.01	2.05
25	7	603	CLA	C4B-NB	2.12	1.40	1.37
25	D	403	CLA	C1B-NB	-2.12	1.35	1.37
25	N	603	CLA	C1B-NB	-2.12	1.35	1.37
25	c	511	CLA	CMB-C2B	-2.12	1.46	1.50
27	2	1622	XAT	O4-C5	-2.12	1.43	1.46
25	y	610	CLA	C4B-NB	2.12	1.40	1.37
25	7	604	CLA	MG-ND	-2.12	2.01	2.05
25	C	504	CLA	CMD-C2D	-2.12	1.46	1.50
25	c	513	CLA	CMD-C2D	-2.12	1.46	1.50
24	S	608	CHL	CBD-CGD	-2.12	1.49	1.52
29	Y	2630	LHG	O8-C6	-2.11	1.40	1.45
24	g	609	CHL	CMC-C2C	2.11	1.49	1.44
34	b	623	SQD	O2-C2	-2.11	1.37	1.43
25	b	612	CLA	C4B-NB	2.11	1.40	1.37
28	2	1623	NEX	O24-C25	-2.11	1.43	1.46
25	r	609	CLA	MG-ND	-2.11	2.01	2.05
25	S	612	CLA	CMC-C2C	-2.11	1.46	1.50
25	G	613	CLA	C1B-NB	-2.11	1.35	1.37
25	4	611	CLA	MG-NB	-2.11	2.01	2.05
24	s	608	CHL	CBD-CGD	-2.11	1.49	1.52
25	7	604	CLA	MG-NB	-2.11	2.01	2.05
25	R	602	CLA	CMB-C2B	-2.11	1.46	1.50
25	Y	613	CLA	CMC-C2C	-2.11	1.46	1.50
25	3	611	CLA	CMC-C2C	-2.11	1.46	1.50
25	n	614	CLA	MG-NB	-2.11	2.01	2.05
25	c	504	CLA	C3B-C4B	2.11	1.48	1.42
25	C	510	CLA	CHC-C1C	2.11	1.42	1.38
25	R	603	CLA	C1B-NB	-2.11	1.35	1.37
25	S	611	CLA	CMB-C2B	-2.11	1.46	1.50
25	N	613	CLA	CMB-C2B	-2.11	1.46	1.50
25	N	604	CLA	C3B-C4B	2.11	1.48	1.42
26	6	1621	LUT	C22-C21	-2.11	1.52	1.54
34	B	623	SQD	O2-C2	-2.11	1.37	1.43
25	C	509	CLA	CMC-C2C	-2.10	1.46	1.50
25	c	504	CLA	CMD-C2D	-2.10	1.46	1.50
25	n	613	CLA	C1B-NB	-2.10	1.35	1.37
25	2	602	CLA	C3B-C4B	2.10	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	602	CLA	CMB-C2B	-2.10	1.46	1.50
25	G	603	CLA	C1B-NB	-2.10	1.35	1.37
25	s	612	CLA	CMC-C2C	-2.10	1.46	1.50
30	h	101	BCR	C1-C6	-2.10	1.51	1.53
37	C	519	DGD	O5D-C6D	-2.10	1.40	1.43
25	3	604	CLA	MG-NB	-2.10	2.01	2.05
25	c	510	CLA	CHC-C1C	2.10	1.42	1.38
25	1	602	CLA	C3B-C4B	2.10	1.48	1.42
25	5	602	CLA	C3B-C4B	2.10	1.48	1.42
25	C	502	CLA	CMC-C2C	-2.10	1.46	1.50
25	Y	613	CLA	CMD-C2D	-2.10	1.46	1.50
25	a	406	CLA	CMC-C2C	-2.10	1.46	1.50
25	N	614	CLA	MG-NB	-2.10	2.01	2.05
25	S	602	CLA	CMB-C2B	-2.10	1.46	1.50
25	s	604	CLA	CMB-C2B	-2.10	1.46	1.50
25	B	605	CLA	CAC-C3C	-2.10	1.45	1.51
25	5	604	CLA	CHC-C4B	-2.10	1.34	1.39
25	n	603	CLA	C1B-NB	-2.10	1.35	1.37
25	A	406	CLA	CMC-C2C	-2.10	1.46	1.50
34	B	623	SQD	O4-C4	-2.10	1.37	1.43
25	g	611	CLA	C3B-C4B	2.10	1.48	1.42
25	R	616	CLA	CHC-C4B	-2.10	1.34	1.39
25	3	604	CLA	MG-ND	-2.10	2.01	2.05
37	c	519	DGD	O5D-C6D	-2.10	1.40	1.43
25	1	603	CLA	C1B-NB	-2.10	1.35	1.37
33	A	409	PHO	CBD-CGD	-2.10	1.49	1.52
25	b	610	CLA	CHC-C4B	-2.10	1.34	1.39
25	s	610	CLA	CHC-C1C	2.09	1.42	1.38
25	4	602	CLA	CMD-C2D	-2.09	1.46	1.50
25	C	507	CLA	CMC-C2C	-2.09	1.46	1.50
25	5	611	CLA	O2A-CGA	2.09	1.37	1.30
25	s	602	CLA	CHC-C1C	2.09	1.42	1.38
25	S	610	CLA	CHC-C1C	2.09	1.42	1.38
34	b	623	SQD	O4-C4	-2.09	1.37	1.43
25	5	613	CLA	MG-NB	-2.09	2.01	2.05
24	5	605	CHL	CHA-CBD	-2.09	1.49	1.51
25	3	603	CLA	C1B-NB	-2.09	1.35	1.37
25	c	502	CLA	CMC-C2C	-2.09	1.46	1.50
25	n	613	CLA	CMB-C2B	-2.09	1.46	1.50
25	1	613	CLA	MG-NB	-2.09	2.01	2.05
25	b	605	CLA	CAC-C3C	-2.09	1.45	1.51
25	r	616	CLA	CHC-C4B	-2.09	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	603	CLA	C1B-NB	-2.09	1.35	1.37
25	7	611	CLA	C1B-C2B	2.09	1.48	1.43
25	R	611	CLA	CMC-C2C	-2.09	1.46	1.50
25	S	602	CLA	CHC-C1C	2.09	1.42	1.38
25	1	611	CLA	O2A-CGA	2.09	1.37	1.30
25	G	611	CLA	C3B-C4B	2.09	1.48	1.42
24	g	605	CHL	CBD-CGD	-2.09	1.49	1.52
25	S	613	CLA	C3B-C4B	2.09	1.48	1.42
25	y	613	CLA	CMD-C2D	-2.09	1.46	1.50
24	Y	606	CHL	MG-ND	-2.09	2.01	2.05
25	A	407	CLA	MG-NB	-2.09	2.01	2.05
30	D	404	BCR	C30-C25	-2.09	1.51	1.53
25	7	603	CLA	C1B-NB	-2.09	1.35	1.37
25	a	407	CLA	MG-NB	-2.09	2.01	2.05
25	g	602	CLA	C1B-NB	-2.09	1.35	1.37
25	N	602	CLA	C1B-NB	-2.08	1.35	1.37
25	R	610	CLA	C1B-C2B	2.08	1.48	1.43
25	r	610	CLA	C1B-C2B	2.08	1.48	1.43
28	y	1623	NEX	C22-C21	-2.08	1.51	1.54
25	c	507	CLA	CMB-C2B	-2.08	1.46	1.50
25	D	403	CLA	C4B-NB	2.08	1.40	1.37
25	C	503	CLA	CMB-C2B	-2.08	1.46	1.50
25	a	406	CLA	MG-NB	-2.08	2.01	2.05
34	A	418	SQD	O2-C2	-2.08	1.37	1.43
25	4	602	CLA	MG-ND	-2.08	2.01	2.05
25	A	406	CLA	MG-NB	-2.08	2.01	2.05
25	c	510	CLA	MG-NB	-2.08	2.01	2.05
25	r	613	CLA	MG-NB	-2.08	2.01	2.05
27	N	1622	XAT	O24-C25	-2.08	1.43	1.46
25	c	503	CLA	CMB-C2B	-2.08	1.46	1.50
25	c	509	CLA	CMC-C2C	-2.08	1.46	1.50
24	2	607	CHL	MG-ND	-2.08	2.01	2.05
28	S	1623	NEX	O24-C25	-2.08	1.43	1.46
30	d	404	BCR	C30-C25	-2.08	1.51	1.53
26	2	1621	LUT	C22-C21	-2.08	1.52	1.54
25	1	604	CLA	CHC-C4B	-2.08	1.34	1.39
25	B	608	CLA	CHC-C4B	-2.08	1.34	1.39
25	8	602	CLA	CMD-C2D	-2.08	1.46	1.50
25	c	509	CLA	MG-ND	-2.08	2.01	2.05
24	1	605	CHL	CHA-CBD	-2.08	1.49	1.51
25	c	511	CLA	CHC-C1C	2.08	1.42	1.38
25	d	403	CLA	C1B-NB	-2.08	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	611	CLA	C1B-C2B	2.08	1.48	1.43
25	A	405	CLA	CMB-C2B	-2.08	1.46	1.50
25	C	510	CLA	MG-NB	-2.08	2.01	2.05
25	B	605	CLA	C4B-NB	2.08	1.40	1.37
27	r	622	XAT	O24-C25	-2.08	1.43	1.46
24	6	607	CHL	MG-ND	-2.08	2.01	2.05
25	C	509	CLA	MG-ND	-2.08	2.01	2.05
25	N	603	CLA	MG-NB	-2.08	2.01	2.05
25	r	603	CLA	C1B-NB	-2.07	1.35	1.37
27	n	1622	XAT	O24-C25	-2.07	1.43	1.46
25	B	605	CLA	CAA-C2A	-2.07	1.50	1.54
34	a	418	SQD	O2-C2	-2.07	1.37	1.43
24	5	601	CHL	MG-ND	-2.07	2.01	2.05
25	5	602	CLA	C1B-NB	-2.07	1.35	1.37
25	R	613	CLA	MG-NB	-2.07	2.01	2.05
25	2	612	CLA	CMC-C2C	-2.07	1.46	1.50
25	S	610	CLA	CMC-C2C	-2.07	1.46	1.50
25	8	602	CLA	MG-ND	-2.07	2.01	2.05
25	S	613	CLA	CMC-C2C	-2.07	1.46	1.50
25	b	608	CLA	CHC-C4B	-2.07	1.34	1.39
25	g	613	CLA	C1B-NB	-2.07	1.35	1.37
28	s	1623	NEX	O24-C25	-2.07	1.43	1.46
28	Y	1623	NEX	C22-C21	-2.07	1.51	1.54
33	a	408	PHO	C3D-CAD	-2.07	1.43	1.47
25	r	602	CLA	CAC-C3C	-2.07	1.45	1.51
25	G	612	CLA	CMB-C2B	-2.07	1.46	1.50
25	B	610	CLA	C4B-NB	2.07	1.40	1.37
25	D	402	CLA	C1B-C2B	2.07	1.48	1.43
25	c	506	CLA	MG-ND	-2.07	2.01	2.05
25	b	605	CLA	C4B-NB	2.07	1.40	1.37
25	g	612	CLA	CMB-C2B	-2.07	1.46	1.50
25	2	603	CLA	MG-NB	-2.07	2.01	2.05
25	c	507	CLA	CMC-C2C	-2.07	1.46	1.50
25	N	613	CLA	C1B-NB	-2.07	1.35	1.37
25	r	611	CLA	CMC-C2C	-2.07	1.46	1.50
25	B	603	CLA	C1B-C2B	2.07	1.48	1.43
25	R	616	CLA	CAC-C3C	-2.07	1.45	1.51
25	6	603	CLA	MG-NB	-2.06	2.01	2.05
25	d	402	CLA	C1B-C2B	2.06	1.48	1.43
27	R	622	XAT	O24-C25	-2.06	1.43	1.46
25	r	616	CLA	CAC-C3C	-2.06	1.45	1.51
25	G	612	CLA	MG-NB	-2.06	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	603	CLA	MG-ND	-2.06	2.01	2.05
25	b	603	CLA	C1B-C2B	2.06	1.48	1.43
25	B	603	CLA	MG-ND	-2.06	2.01	2.05
25	c	508	CLA	MG-NB	-2.06	2.01	2.05
25	8	610	CLA	C1B-C2B	2.06	1.48	1.43
25	b	605	CLA	CAA-C2A	-2.06	1.50	1.54
30	H	101	BCR	C1-C6	-2.06	1.51	1.53
25	C	507	CLA	CMB-C2B	-2.06	1.46	1.50
25	a	405	CLA	CMB-C2B	-2.06	1.46	1.50
25	8	611	CLA	C3B-C4B	2.06	1.48	1.42
25	1	604	CLA	C1B-NB	-2.06	1.35	1.37
25	C	508	CLA	MG-NB	-2.06	2.01	2.05
25	d	403	CLA	C4B-NB	2.06	1.40	1.37
25	1	614	CLA	C3B-C4B	2.06	1.48	1.42
25	s	610	CLA	CMC-C2C	-2.06	1.46	1.50
25	s	613	CLA	C3B-C4B	2.06	1.48	1.42
25	R	602	CLA	CAC-C3C	-2.06	1.45	1.51
25	4	611	CLA	C3B-C4B	2.06	1.48	1.42
25	c	513	CLA	C3B-C4B	2.06	1.48	1.42
33	A	408	PHO	C3D-CAD	-2.06	1.43	1.47
25	Y	612	CLA	C1B-NB	-2.06	1.35	1.37
25	C	506	CLA	MG-ND	-2.06	2.01	2.05
25	b	607	CLA	MG-ND	-2.06	2.01	2.05
25	g	602	CLA	C3B-C4B	2.06	1.48	1.42
25	4	610	CLA	C1B-C2B	2.06	1.48	1.43
25	c	503	CLA	MG-NB	-2.06	2.01	2.05
25	4	611	CLA	CMC-C2C	-2.06	1.46	1.50
25	B	604	CLA	CHC-C4B	-2.05	1.34	1.39
25	B	616	CLA	C3B-C4B	2.05	1.48	1.42
25	5	611	CLA	C1B-NB	-2.05	1.35	1.37
25	C	513	CLA	C3B-C4B	2.05	1.48	1.42
25	n	613	CLA	CHC-C4B	-2.05	1.34	1.39
25	G	613	CLA	CMB-C2B	-2.05	1.46	1.50
25	G	611	CLA	CHC-C1C	2.05	1.42	1.38
25	g	611	CLA	CHC-C1C	2.05	1.42	1.38
25	b	605	CLA	CMA-C3A	-2.05	1.48	1.53
24	7	601	CHL	CAC-C3C	-2.05	1.48	1.51
25	b	616	CLA	MG-NB	-2.05	2.01	2.05
25	5	614	CLA	C3B-C4B	2.05	1.48	1.42
25	6	612	CLA	CMC-C2C	-2.05	1.46	1.50
24	3	601	CHL	CAC-C3C	-2.05	1.48	1.51
25	2	612	CLA	MG-NB	-2.05	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	511	CLA	CHC-C1C	2.05	1.42	1.38
25	r	610	CLA	C3B-C4B	2.05	1.48	1.42
25	R	601	CLA	CMC-C2C	-2.05	1.46	1.50
25	g	612	CLA	MG-NB	-2.05	2.01	2.05
25	n	603	CLA	MG-NB	-2.05	2.01	2.05
25	G	602	CLA	C1B-NB	-2.05	1.35	1.37
25	n	602	CLA	C1B-NB	-2.05	1.35	1.37
25	C	503	CLA	MG-NB	-2.05	2.01	2.05
24	G	605	CHL	CBD-CGD	-2.05	1.49	1.52
25	N	613	CLA	CMD-C2D	-2.05	1.46	1.50
25	s	613	CLA	CMC-C2C	-2.05	1.46	1.50
25	b	616	CLA	C3B-C4B	2.05	1.48	1.42
25	n	613	CLA	CMD-C2D	-2.05	1.46	1.50
25	b	604	CLA	CHC-C4B	-2.04	1.34	1.39
25	r	601	CLA	MG-NB	-2.04	2.01	2.05
25	G	602	CLA	C3B-C4B	2.04	1.48	1.42
25	B	605	CLA	CMA-C3A	-2.04	1.48	1.53
29	C	523	LHG	P-O6	2.04	1.67	1.59
25	B	607	CLA	MG-ND	-2.04	2.01	2.05
25	B	614	CLA	C4B-NB	2.04	1.40	1.37
25	D	402	CLA	C1B-NB	-2.04	1.35	1.37
25	a	405	CLA	C1B-NB	-2.04	1.35	1.37
24	2	608	CHL	CMC-C2C	2.04	1.49	1.44
24	1	601	CHL	MG-ND	-2.04	2.01	2.05
25	g	614	CLA	C3B-C4B	2.04	1.48	1.42
25	R	601	CLA	MG-NB	-2.04	2.01	2.05
25	s	610	CLA	CMD-C2D	-2.04	1.46	1.50
29	c	523	LHG	P-O6	2.04	1.67	1.59
25	R	610	CLA	C3B-C4B	2.04	1.48	1.42
25	B	616	CLA	MG-NB	-2.04	2.01	2.05
25	B	612	CLA	C1D-ND	2.04	1.40	1.37
25	S	604	CLA	CMD-C2D	-2.04	1.46	1.50
25	s	609	CLA	CMB-C2B	-2.04	1.46	1.50
25	c	507	CLA	MG-NB	-2.04	2.01	2.05
25	8	612	CLA	CMB-C2B	-2.03	1.46	1.50
33	A	409	PHO	C3D-CAD	-2.03	1.43	1.47
25	d	402	CLA	C1B-NB	-2.03	1.35	1.37
25	4	612	CLA	CMB-C2B	-2.03	1.46	1.50
25	c	512	CLA	CMC-C2C	-2.03	1.46	1.50
25	3	613	CLA	CAC-C3C	-2.03	1.45	1.51
25	N	613	CLA	CHC-C4B	-2.03	1.34	1.39
25	C	502	CLA	C3B-C4B	2.03	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	609	CHL	CMA-C3A	-2.03	1.49	1.53
25	r	601	CLA	CMC-C2C	-2.03	1.46	1.50
25	G	614	CLA	C3B-C4B	2.03	1.48	1.42
25	A	407	CLA	MG-ND	-2.03	2.01	2.05
24	S	607	CHL	CBD-CGD	-2.03	1.49	1.52
25	N	614	CLA	MG-ND	-2.03	2.01	2.05
25	7	613	CLA	CAC-C3C	-2.03	1.45	1.51
29	8	2630	LHG	O7-C5	-2.03	1.41	1.46
25	R	601	CLA	MG-ND	-2.03	2.01	2.05
25	c	510	CLA	MG-ND	-2.03	2.01	2.05
25	1	611	CLA	C1B-NB	-2.03	1.35	1.37
25	g	613	CLA	CMB-C2B	-2.03	1.46	1.50
25	6	612	CLA	MG-NB	-2.03	2.01	2.05
29	4	2630	LHG	O7-C5	-2.03	1.41	1.46
33	a	409	PHO	CBD-CGD	-2.02	1.50	1.52
24	3	609	CHL	CHA-CBD	-2.02	1.49	1.51
25	4	610	CLA	C3B-C4B	2.02	1.48	1.42
25	r	601	CLA	MG-ND	-2.02	2.01	2.05
25	4	604	CLA	C1B-C2B	2.02	1.47	1.43
25	A	405	CLA	C1B-NB	-2.02	1.35	1.37
25	8	604	CLA	C1B-C2B	2.02	1.47	1.43
25	g	604	CLA	CHC-C4B	-2.02	1.34	1.39
25	C	510	CLA	MG-ND	-2.02	2.01	2.05
25	b	610	CLA	C4B-NB	2.02	1.40	1.37
25	c	506	CLA	C3B-C4B	2.02	1.48	1.42
25	S	609	CLA	CMB-C2B	-2.02	1.46	1.50
24	s	607	CHL	CBD-CGD	-2.02	1.50	1.52
28	N	1623	NEX	C22-C21	-2.02	1.51	1.54
25	8	610	CLA	C3B-C4B	2.02	1.48	1.42
25	C	503	CLA	CMC-C2C	-2.02	1.46	1.50
25	C	507	CLA	CHC-C4B	-2.02	1.34	1.39
35	d	411	LMG	O1-C7	-2.02	1.40	1.43
34	A	412	SQD	O4-C4	-2.02	1.38	1.43
34	a	412	SQD	O4-C4	-2.02	1.38	1.43
25	b	614	CLA	C4B-NB	2.02	1.40	1.37
25	c	505	CLA	C3B-C4B	2.02	1.48	1.42
24	n	609	CHL	CMA-C3A	-2.02	1.49	1.53
25	5	604	CLA	C1B-NB	-2.02	1.35	1.37
25	c	507	CLA	CHC-C4B	-2.02	1.34	1.39
25	c	501	CLA	CHC-C1C	2.02	1.42	1.38
34	B	621	SQD	O2-C2	-2.02	1.38	1.43
25	C	505	CLA	C3B-C4B	2.02	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	f	101	HEM	C2A-C3A	-2.02	1.33	1.38
25	S	610	CLA	CMD-C2D	-2.01	1.46	1.50
25	8	611	CLA	CMC-C2C	-2.01	1.46	1.50
25	R	609	CLA	CHC-C4B	-2.01	1.34	1.39
25	n	614	CLA	MG-ND	-2.01	2.01	2.05
25	S	614	CLA	CMC-C2C	-2.01	1.46	1.50
25	c	503	CLA	CMC-C2C	-2.01	1.46	1.50
27	y	1622	XAT	C22-C21	-2.01	1.51	1.54
25	b	608	CLA	C3B-C4B	2.01	1.48	1.42
25	a	407	CLA	MG-ND	-2.01	2.01	2.05
25	3	610	CLA	C1B-NB	-2.01	1.35	1.37
25	a	405	CLA	C3B-C4B	2.01	1.48	1.42
28	n	1623	NEX	C22-C21	-2.01	1.51	1.54
25	C	509	CLA	C3B-C4B	2.01	1.48	1.42
25	R	604	CLA	C3B-C4B	2.01	1.48	1.42
25	c	509	CLA	C3B-C4B	2.01	1.48	1.42
25	c	503	CLA	CHC-C1C	2.01	1.42	1.38
25	7	613	CLA	C3B-C4B	2.01	1.48	1.42
25	C	507	CLA	MG-NB	-2.01	2.01	2.05
33	a	409	PHO	C3D-CAD	-2.01	1.43	1.47
25	1	610	CLA	C4B-NB	2.01	1.40	1.37
25	S	604	CLA	CMC-C2C	-2.01	1.46	1.50
24	6	608	CHL	CMC-C2C	2.01	1.49	1.44
25	C	501	CLA	CHC-C1C	2.01	1.42	1.38
25	b	613	CLA	C1B-C2B	2.01	1.47	1.43
24	8	601	CHL	CMC-C2C	2.01	1.49	1.44
34	A	412	SQD	O3-C3	-2.00	1.38	1.43
25	B	612	CLA	C1B-C2B	2.00	1.47	1.43
25	D	403	CLA	CHC-C4B	-2.00	1.34	1.39
25	S	604	CLA	CHC-C1C	2.00	1.42	1.38
25	1	612	CLA	C1B-NB	-2.00	1.35	1.37
25	B	613	CLA	C1B-C2B	2.00	1.47	1.43
25	C	512	CLA	CMC-C2C	-2.00	1.46	1.50
25	r	604	CLA	C3B-C4B	2.00	1.48	1.42
25	3	613	CLA	C3B-C4B	2.00	1.48	1.42
25	6	610	CLA	C3B-C4B	2.00	1.48	1.42
25	b	609	CLA	C1B-C2B	2.00	1.47	1.43
25	8	602	CLA	C1B-NB	-2.00	1.35	1.37
26	G	1620	LUT	C22-C21	-2.00	1.52	1.54
25	C	503	CLA	CHC-C1C	2.00	1.42	1.38
39	F	101	HEM	C2A-C3A	-2.00	1.33	1.38

All (5065) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	601	CHL	C1B-CHB-C4A	12.09	129.10	121.32
24	Y	601	CHL	C1B-CHB-C4A	12.06	129.08	121.32
24	y	606	CHL	C1B-CHB-C4A	10.80	128.27	121.32
24	Y	606	CHL	C1B-CHB-C4A	10.76	128.24	121.32
24	n	607	CHL	C1B-CHB-C4A	10.55	128.11	121.32
24	R	608	CHL	C1B-CHB-C4A	10.54	128.10	121.32
24	r	608	CHL	C1B-CHB-C4A	10.53	128.10	121.32
24	N	607	CHL	C1B-CHB-C4A	10.52	128.09	121.32
24	g	601	CHL	C1B-CHB-C4A	10.21	127.89	121.32
24	G	601	CHL	C1B-CHB-C4A	10.18	127.87	121.32
24	7	601	CHL	C1B-CHB-C4A	10.03	127.78	121.32
24	y	609	CHL	O2D-CGD-CBD	10.02	121.95	110.95
24	Y	609	CHL	O2D-CGD-CBD	10.01	121.95	110.95
24	3	601	CHL	C1B-CHB-C4A	9.99	127.75	121.32
24	3	609	CHL	O2D-CGD-CBD	9.87	121.79	110.95
24	1	606	CHL	C1B-CHB-C4A	9.85	127.66	121.32
24	5	606	CHL	C1B-CHB-C4A	9.83	127.65	121.32
24	7	609	CHL	O2D-CGD-CBD	9.82	121.74	110.95
24	n	608	CHL	C1B-CHB-C4A	9.71	127.57	121.32
24	8	606	CHL	C1B-CHB-C4A	9.69	127.56	121.32
24	4	606	CHL	C1B-CHB-C4A	9.68	127.55	121.32
24	N	608	CHL	C1B-CHB-C4A	9.68	127.55	121.32
24	s	607	CHL	C1B-CHB-C4A	9.63	127.52	121.32
24	S	607	CHL	C1B-CHB-C4A	9.63	127.52	121.32
24	Y	607	CHL	C1B-CHB-C4A	9.58	127.48	121.32
24	n	606	CHL	C1B-CHB-C4A	9.57	127.48	121.32
24	y	607	CHL	C1B-CHB-C4A	9.55	127.46	121.32
24	1	607	CHL	C1B-CHB-C4A	9.54	127.46	121.32
24	N	606	CHL	C1B-CHB-C4A	9.53	127.45	121.32
24	3	606	CHL	O2D-CGD-CBD	9.51	121.39	110.95
24	5	607	CHL	C1B-CHB-C4A	9.50	127.43	121.32
24	7	606	CHL	O2D-CGD-CBD	9.50	121.38	110.95
24	g	608	CHL	C1B-CHB-C4A	9.46	127.41	121.32
24	4	608	CHL	C1B-CHB-C4A	9.42	127.38	121.32
24	8	608	CHL	C1B-CHB-C4A	9.40	127.37	121.32
24	G	608	CHL	C1B-CHB-C4A	9.38	127.36	121.32
24	r	606	CHL	C1B-CHB-C4A	9.32	127.32	121.32
24	R	606	CHL	C1B-CHB-C4A	9.28	127.30	121.32
24	6	609	CHL	O2D-CGD-CBD	9.26	121.12	110.95
24	n	601	CHL	C1B-CHB-C4A	9.26	127.28	121.32
25	Y	613	CLA	C4A-NA-C1A	9.25	110.90	106.68
25	y	613	CLA	C4A-NA-C1A	9.23	110.89	106.68
24	2	609	CHL	O2D-CGD-CBD	9.23	121.09	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	601	CHL	C1B-CHB-C4A	9.21	127.25	121.32
24	n	601	CHL	O2D-CGD-CBD	9.12	120.96	110.95
24	N	601	CHL	O2D-CGD-CBD	9.07	120.92	110.95
24	3	601	CHL	O2D-CGD-CBD	9.01	120.85	110.95
24	S	601	CHL	C1B-CHB-C4A	8.97	127.09	121.32
24	7	601	CHL	O2D-CGD-CBD	8.95	120.78	110.95
24	s	601	CHL	C1B-CHB-C4A	8.95	127.08	121.32
24	n	608	CHL	O2D-CGD-CBD	8.89	120.72	110.95
24	N	608	CHL	O2D-CGD-CBD	8.89	120.71	110.95
24	N	605	CHL	O2D-CGD-CBD	8.87	120.69	110.95
24	n	605	CHL	O2D-CGD-CBD	8.84	120.66	110.95
24	g	606	CHL	C1B-CHB-C4A	8.81	126.99	121.32
24	5	609	CHL	O2D-CGD-CBD	8.77	120.59	110.95
24	G	606	CHL	C1B-CHB-C4A	8.77	126.96	121.32
24	1	609	CHL	O2D-CGD-CBD	8.77	120.58	110.95
24	2	608	CHL	C1B-CHB-C4A	8.76	126.96	121.32
24	1	608	CHL	C1B-CHB-C4A	8.76	126.95	121.32
24	y	608	CHL	C1B-CHB-C4A	8.72	126.93	121.32
24	5	608	CHL	C1B-CHB-C4A	8.72	126.93	121.32
24	Y	608	CHL	C1B-CHB-C4A	8.70	126.92	121.32
24	6	608	CHL	C1B-CHB-C4A	8.67	126.90	121.32
24	2	606	CHL	C1B-CHB-C4A	8.66	126.90	121.32
25	n	613	CLA	C4A-NA-C1A	8.65	110.63	106.68
24	6	606	CHL	C1B-CHB-C4A	8.65	126.89	121.32
24	G	605	CHL	C1B-CHB-C4A	8.62	126.87	121.32
25	N	613	CLA	C4A-NA-C1A	8.59	110.60	106.68
24	N	609	CHL	O2D-CGD-CBD	8.57	120.36	110.95
24	n	609	CHL	O2D-CGD-CBD	8.56	120.35	110.95
24	G	609	CHL	C1B-CHB-C4A	8.54	126.82	121.32
24	g	609	CHL	C1B-CHB-C4A	8.52	126.80	121.32
24	R	606	CHL	O2D-CGD-CBD	8.51	120.30	110.95
24	r	606	CHL	O2D-CGD-CBD	8.51	120.30	110.95
24	g	605	CHL	C1B-CHB-C4A	8.50	126.79	121.32
24	Y	601	CHL	O2D-CGD-CBD	8.43	120.21	110.95
24	y	601	CHL	O2D-CGD-CBD	8.43	120.20	110.95
24	2	605	CHL	O2D-CGD-CBD	8.35	120.12	110.95
24	S	606	CHL	O2D-CGD-CBD	8.34	120.11	110.95
24	s	606	CHL	O2D-CGD-CBD	8.33	120.10	110.95
27	5	1622	XAT	O24-C25-C24	8.31	121.28	113.49
27	1	1622	XAT	O24-C25-C24	8.31	121.28	113.49
24	6	605	CHL	O2D-CGD-CBD	8.31	120.07	110.95
24	8	609	CHL	C1B-CHB-C4A	8.30	126.67	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	609	CHL	O2D-CGD-CBD	8.29	120.06	110.95
24	g	609	CHL	O2D-CGD-CBD	8.27	120.04	110.95
24	4	609	CHL	C1B-CHB-C4A	8.25	126.63	121.32
24	7	608	CHL	C1B-CHB-C4A	8.25	126.63	121.32
24	3	608	CHL	C1B-CHB-C4A	8.23	126.62	121.32
24	r	607	CHL	O2D-CGD-CBD	8.19	119.94	110.95
24	1	606	CHL	O2D-CGD-CBD	8.19	119.94	110.95
24	g	601	CHL	O2D-CGD-CBD	8.18	119.94	110.95
24	5	606	CHL	O2D-CGD-CBD	8.17	119.93	110.95
24	N	606	CHL	O2D-CGD-CBD	8.17	119.93	110.95
24	n	606	CHL	O2D-CGD-CBD	8.17	119.93	110.95
24	G	601	CHL	O2D-CGD-CBD	8.17	119.92	110.95
24	g	605	CHL	O2D-CGD-CBD	8.16	119.91	110.95
24	R	607	CHL	O2D-CGD-CBD	8.16	119.91	110.95
24	G	605	CHL	O2D-CGD-CBD	8.14	119.89	110.95
24	4	609	CHL	O2D-CGD-CBD	8.06	119.80	110.95
24	8	607	CHL	O2D-CGD-CBD	8.02	119.76	110.95
24	4	607	CHL	O2D-CGD-CBD	8.02	119.76	110.95
24	8	609	CHL	O2D-CGD-CBD	8.02	119.76	110.95
24	r	608	CHL	O2D-CGD-CBD	8.01	119.74	110.95
24	R	608	CHL	O2D-CGD-CBD	8.00	119.74	110.95
24	y	605	CHL	C1B-CHB-C4A	8.00	126.47	121.32
24	2	601	CHL	C1B-CHB-C4A	7.98	126.45	121.32
24	Y	605	CHL	C1B-CHB-C4A	7.96	126.44	121.32
24	6	601	CHL	C1B-CHB-C4A	7.95	126.44	121.32
25	c	502	CLA	C4A-NA-C1A	7.93	110.30	106.68
24	s	601	CHL	O2D-CGD-CBD	7.92	119.65	110.95
25	C	502	CLA	C4A-NA-C1A	7.91	110.29	106.68
24	G	607	CHL	O2D-CGD-CBD	7.91	119.64	110.95
24	S	601	CHL	O2D-CGD-CBD	7.90	119.63	110.95
24	g	607	CHL	O2D-CGD-CBD	7.89	119.61	110.95
24	5	601	CHL	C1B-CHB-C4A	7.87	126.38	121.32
24	1	601	CHL	C1B-CHB-C4A	7.85	126.37	121.32
24	3	605	CHL	O2D-CGD-CBD	7.84	119.56	110.95
24	s	606	CHL	C1B-CHB-C4A	7.83	126.36	121.32
24	S	606	CHL	C1B-CHB-C4A	7.82	126.36	121.32
24	r	614	CHL	O2D-CGD-CBD	7.82	119.53	110.95
24	R	614	CHL	O2D-CGD-CBD	7.81	119.53	110.95
24	7	605	CHL	O2D-CGD-CBD	7.81	119.52	110.95
30	8	623	BCR	C24-C23-C22	-7.80	114.70	126.23
30	4	623	BCR	C24-C23-C22	-7.78	114.73	126.23
28	6	1623	NEX	O24-C25-C24	7.76	120.76	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	2	1622	XAT	O4-C5-C4	7.75	120.75	113.49
27	6	1622	XAT	O4-C5-C4	7.75	120.75	113.49
28	G	1623	NEX	O24-C25-C24	7.72	120.73	113.49
28	g	1623	NEX	O24-C25-C24	7.72	120.73	113.49
24	Y	605	CHL	O2D-CGD-CBD	7.71	119.42	110.95
24	y	605	CHL	O2D-CGD-CBD	7.70	119.41	110.95
28	2	1623	NEX	O24-C25-C24	7.68	120.69	113.49
24	1	605	CHL	O2D-CGD-CBD	7.68	119.39	110.95
24	5	605	CHL	O2D-CGD-CBD	7.67	119.38	110.95
27	N	1622	XAT	C15-C14-C13	-7.66	116.54	127.28
24	n	609	CHL	C1B-CHB-C4A	7.65	126.24	121.32
24	3	607	CHL	O2D-CGD-CBD	7.63	119.33	110.95
27	n	1622	XAT	C15-C14-C13	-7.63	116.58	127.28
24	N	609	CHL	C1B-CHB-C4A	7.61	126.22	121.32
24	7	607	CHL	O2D-CGD-CBD	7.61	119.30	110.95
24	n	605	CHL	C1B-CHB-C4A	7.58	126.20	121.32
24	2	606	CHL	O2D-CGD-CBD	7.58	119.28	110.95
24	6	606	CHL	O2D-CGD-CBD	7.57	119.26	110.95
24	N	605	CHL	C1B-CHB-C4A	7.56	126.19	121.32
33	a	409	PHO	C4D-CHA-CBD	-7.56	104.83	108.45
33	A	409	PHO	C4D-CHA-CBD	-7.56	104.83	108.45
28	5	1623	NEX	O24-C25-C24	7.55	120.57	113.49
24	g	607	CHL	C1B-CHB-C4A	7.52	126.16	121.32
28	1	1623	NEX	O24-C25-C24	7.51	120.53	113.49
24	G	607	CHL	C1B-CHB-C4A	7.50	126.15	121.32
24	1	601	CHL	O2D-CGD-CBD	7.49	119.17	110.95
24	y	606	CHL	O2D-CGD-CBD	7.49	119.17	110.95
24	5	601	CHL	O2D-CGD-CBD	7.48	119.17	110.95
24	G	608	CHL	O2D-CGD-CBD	7.47	119.16	110.95
24	Y	606	CHL	O2D-CGD-CBD	7.46	119.14	110.95
24	S	607	CHL	O2D-CGD-CBD	7.45	119.13	110.95
24	g	608	CHL	O2D-CGD-CBD	7.44	119.13	110.95
24	r	607	CHL	C1B-CHB-C4A	7.43	126.10	121.32
27	2	1622	XAT	O24-C25-C24	7.42	120.45	113.49
24	s	607	CHL	O2D-CGD-CBD	7.41	119.09	110.95
24	7	605	CHL	C1B-CHB-C4A	7.40	126.08	121.32
27	6	1622	XAT	O24-C25-C24	7.39	120.42	113.49
24	1	608	CHL	O2D-CGD-CBD	7.38	119.06	110.95
24	5	608	CHL	O2D-CGD-CBD	7.37	119.04	110.95
24	R	607	CHL	C1B-CHB-C4A	7.35	126.05	121.32
24	3	605	CHL	C1B-CHB-C4A	7.34	126.04	121.32
24	S	608	CHL	O2D-CGD-CBD	7.33	119.00	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	3	1623	NEX	O24-C25-C24	7.32	120.35	113.49
28	7	1623	NEX	O24-C25-C24	7.32	120.35	113.49
27	G	1622	XAT	O24-C25-C24	7.28	120.31	113.49
24	s	608	CHL	O2D-CGD-CBD	7.27	118.94	110.95
27	g	1622	XAT	O24-C25-C24	7.27	120.31	113.49
25	g	613	CLA	C4A-NA-C1A	7.26	109.99	106.68
25	G	613	CLA	C4A-NA-C1A	7.25	109.99	106.68
30	t	101	BCR	C24-C23-C22	-7.19	115.60	126.23
30	T	101	BCR	C24-C23-C22	-7.19	115.60	126.23
25	n	611	CLA	C4A-NA-C1A	7.18	109.95	106.68
25	N	611	CLA	C4A-NA-C1A	7.18	109.95	106.68
24	Y	601	CHL	C4D-ND-C1D	-7.17	99.77	105.22
25	B	613	CLA	C4A-NA-C1A	7.16	109.94	106.68
24	7	606	CHL	C1B-CHB-C4A	7.14	125.92	121.32
24	y	601	CHL	C4D-ND-C1D	-7.14	99.80	105.22
25	b	613	CLA	C4A-NA-C1A	7.14	109.94	106.68
27	Y	1622	XAT	C15-C14-C13	-7.13	117.28	127.28
27	y	1622	XAT	C15-C14-C13	-7.13	117.28	127.28
24	3	606	CHL	C1B-CHB-C4A	7.11	125.90	121.32
24	5	607	CHL	O2D-CGD-CBD	7.09	118.74	110.95
24	1	607	CHL	O2D-CGD-CBD	7.06	118.70	110.95
33	a	408	PHO	C4D-CHA-CBD	-7.03	105.08	108.45
24	y	608	CHL	C4D-ND-C1D	-7.02	99.90	105.22
24	3	608	CHL	O2D-CGD-CBD	7.01	118.65	110.95
24	Y	608	CHL	C4D-ND-C1D	-7.00	99.91	105.22
33	A	408	PHO	C4D-CHA-CBD	-6.98	105.11	108.45
24	7	608	CHL	O2D-CGD-CBD	6.97	118.60	110.95
24	n	607	CHL	O2D-CGD-CBD	6.95	118.59	110.95
27	3	1622	XAT	O4-C5-C4	6.94	120.00	113.49
24	4	606	CHL	O2D-CGD-CBD	6.93	118.56	110.95
24	6	607	CHL	O2D-CGD-CBD	6.93	118.56	110.95
27	7	1622	XAT	O4-C5-C4	6.93	119.98	113.49
24	2	607	CHL	O2D-CGD-CBD	6.93	118.56	110.95
24	N	607	CHL	O2D-CGD-CBD	6.91	118.54	110.95
24	8	606	CHL	O2D-CGD-CBD	6.90	118.53	110.95
24	Y	607	CHL	O2D-CGD-CBD	6.90	118.53	110.95
24	y	607	CHL	O2D-CGD-CBD	6.89	118.52	110.95
24	2	608	CHL	O2D-CGD-CBD	6.86	118.49	110.95
24	6	608	CHL	O2D-CGD-CBD	6.85	118.47	110.95
24	8	608	CHL	O2D-CGD-CBD	6.85	118.47	110.95
24	4	608	CHL	O2D-CGD-CBD	6.84	118.46	110.95
24	6	601	CHL	O2D-CGD-CBD	6.79	118.41	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	601	CHL	O2D-CGD-CBD	6.77	118.39	110.95
25	B	605	CLA	C4A-NA-C1A	6.75	109.76	106.68
25	b	614	CLA	C4A-NA-C1A	6.72	109.74	106.68
25	B	614	CLA	C4A-NA-C1A	6.71	109.74	106.68
25	b	605	CLA	C4A-NA-C1A	6.70	109.74	106.68
24	Y	608	CHL	O2D-CGD-CBD	6.68	118.29	110.95
25	C	507	CLA	C4A-NA-C1A	6.67	109.72	106.68
24	3	608	CHL	C4D-ND-C1D	-6.67	100.16	105.22
24	y	608	CHL	O2D-CGD-CBD	6.67	118.27	110.95
24	8	608	CHL	C4D-ND-C1D	-6.66	100.16	105.22
25	c	507	CLA	C4A-NA-C1A	6.65	109.71	106.68
24	7	608	CHL	C4D-ND-C1D	-6.62	100.19	105.22
28	n	1623	NEX	O24-C25-C24	6.62	119.70	113.49
28	N	1623	NEX	O24-C25-C24	6.62	119.69	113.49
30	t	101	BCR	C16-C17-C18	-6.61	118.00	127.28
30	T	101	BCR	C16-C17-C18	-6.61	118.01	127.28
24	4	608	CHL	C4D-ND-C1D	-6.60	100.21	105.22
25	B	612	CLA	C4A-NA-C1A	6.60	109.69	106.68
24	G	608	CHL	C4D-ND-C1D	-6.60	100.21	105.22
24	g	608	CHL	C4D-ND-C1D	-6.59	100.22	105.22
25	b	617	CLA	C4A-NA-C1A	6.58	109.68	106.68
25	b	612	CLA	C4A-NA-C1A	6.58	109.68	106.68
24	g	606	CHL	O2D-CGD-CBD	6.57	118.17	110.95
24	G	606	CHL	O2D-CGD-CBD	6.55	118.14	110.95
24	3	601	CHL	C4D-ND-C1D	-6.53	100.26	105.22
25	B	617	CLA	C4A-NA-C1A	6.52	109.65	106.68
30	T	101	BCR	C20-C21-C22	-6.52	118.13	127.28
30	t	101	BCR	C20-C21-C22	-6.52	118.14	127.28
27	n	1622	XAT	C31-C30-C29	-6.51	118.15	127.28
27	N	1622	XAT	C31-C30-C29	-6.51	118.16	127.28
24	s	601	CHL	C4D-ND-C1D	-6.50	100.28	105.22
24	7	601	CHL	C4D-ND-C1D	-6.48	100.30	105.22
27	G	1622	XAT	C15-C14-C13	-6.47	118.20	127.28
27	g	1622	XAT	C15-C14-C13	-6.47	118.21	127.28
24	S	601	CHL	C4D-ND-C1D	-6.45	100.32	105.22
25	5	611	CLA	C4A-NA-C1A	6.44	109.62	106.68
25	b	606	CLA	C4A-NA-C1A	6.44	109.62	106.68
24	N	601	CHL	C4D-ND-C1D	-6.43	100.34	105.22
24	n	608	CHL	C4D-ND-C1D	-6.43	100.34	105.22
24	n	601	CHL	C4D-ND-C1D	-6.41	100.35	105.22
24	N	608	CHL	C4D-ND-C1D	-6.41	100.36	105.22
27	Y	1622	XAT	O4-C5-C18	6.40	122.19	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	611	CLA	C4A-NA-C1A	6.39	109.59	106.68
27	y	1622	XAT	O4-C5-C18	6.39	122.19	115.05
25	B	606	CLA	C4A-NA-C1A	6.36	109.58	106.68
24	r	608	CHL	C4D-ND-C1D	-6.35	100.40	105.22
24	R	608	CHL	C4D-ND-C1D	-6.35	100.40	105.22
24	2	608	CHL	C4D-ND-C1D	-6.34	100.40	105.22
24	G	601	CHL	C4D-ND-C1D	-6.34	100.40	105.22
24	4	601	CHL	C1B-CHB-C4A	-6.33	117.25	121.32
24	8	601	CHL	C1B-CHB-C4A	-6.33	117.25	121.32
24	g	601	CHL	C4D-ND-C1D	-6.32	100.42	105.22
24	6	608	CHL	C4D-ND-C1D	-6.29	100.44	105.22
24	5	608	CHL	C4D-ND-C1D	-6.28	100.45	105.22
24	1	608	CHL	C4D-ND-C1D	-6.26	100.47	105.22
24	7	605	CHL	C4D-ND-C1D	-6.25	100.47	105.22
24	3	605	CHL	C4D-ND-C1D	-6.25	100.47	105.22
24	2	609	CHL	C1B-CHB-C4A	6.24	125.33	121.32
26	3	1620	LUT	C7-C8-C9	-6.23	117.02	126.23
26	7	1620	LUT	C7-C8-C9	-6.23	117.02	126.23
25	C	505	CLA	C4A-NA-C1A	6.23	109.52	106.68
24	6	609	CHL	C1B-CHB-C4A	6.22	125.32	121.32
25	c	505	CLA	C4A-NA-C1A	6.22	109.52	106.68
25	5	603	CLA	C4A-NA-C1A	6.20	109.51	106.68
24	2	601	CHL	C4D-ND-C1D	-6.20	100.51	105.22
25	g	611	CLA	C4A-NA-C1A	6.20	109.51	106.68
25	1	603	CLA	C4A-NA-C1A	6.20	109.51	106.68
24	6	601	CHL	C4D-ND-C1D	-6.19	100.52	105.22
25	A	410	CLA	C4A-NA-C1A	6.19	109.50	106.68
30	d	404	BCR	C7-C8-C9	-6.18	117.10	126.23
25	G	611	CLA	C4A-NA-C1A	6.17	109.49	106.68
25	a	410	CLA	C4A-NA-C1A	6.17	109.49	106.68
25	S	604	CLA	C4A-NA-C1A	6.16	109.49	106.68
25	s	604	CLA	C4A-NA-C1A	6.16	109.49	106.68
30	D	404	BCR	C7-C8-C9	-6.15	117.14	126.23
28	S	1623	NEX	O24-C25-C24	6.15	119.25	113.49
27	1	1622	XAT	O4-C5-C4	6.14	119.25	113.49
25	r	612	CLA	C4A-NA-C1A	6.14	109.48	106.68
25	R	612	CLA	C4A-NA-C1A	6.14	109.48	106.68
25	r	616	CLA	C4A-NA-C1A	6.14	109.48	106.68
25	R	616	CLA	C4A-NA-C1A	6.13	109.48	106.68
28	s	1623	NEX	O24-C25-C24	6.13	119.23	113.49
30	C	516	BCR	C24-C23-C22	-6.13	117.17	126.23
30	c	516	BCR	C24-C23-C22	-6.12	117.18	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	n	607	CHL	C4D-ND-C1D	-6.10	100.59	105.22
24	G	606	CHL	C4D-ND-C1D	-6.10	100.59	105.22
24	1	607	CHL	C4D-ND-C1D	-6.10	100.59	105.22
27	5	1622	XAT	O4-C5-C4	6.10	119.20	113.49
25	r	613	CLA	C4A-NA-C1A	6.10	109.46	106.68
25	A	406	CLA	C4A-NA-C1A	6.09	109.46	106.68
24	N	607	CHL	C4D-ND-C1D	-6.08	100.60	105.22
27	n	1622	XAT	O24-C25-C24	6.08	119.19	113.49
25	R	613	CLA	C4A-NA-C1A	6.07	109.45	106.68
24	5	607	CHL	C4D-ND-C1D	-6.06	100.62	105.22
24	7	601	CHL	CBC-CAC-C3C	-6.06	104.20	112.87
27	N	1622	XAT	O24-C25-C24	6.06	119.17	113.49
24	g	606	CHL	C4D-ND-C1D	-6.04	100.63	105.22
24	3	601	CHL	CBC-CAC-C3C	-6.03	104.24	112.87
24	5	601	CHL	C4D-ND-C1D	-6.00	100.66	105.22
24	y	601	CHL	CHA-C1A-C2A	-6.00	119.22	133.31
24	Y	601	CHL	CHA-C1A-C2A	-5.99	119.23	133.31
27	y	1622	XAT	C31-C30-C29	-5.98	118.90	127.28
24	1	601	CHL	C4D-ND-C1D	-5.98	100.68	105.22
27	R	622	XAT	O4-C5-C18	5.97	121.72	115.05
27	r	622	XAT	O4-C5-C18	5.97	121.72	115.05
25	a	406	CLA	C4A-NA-C1A	5.96	109.40	106.68
27	Y	1622	XAT	C31-C30-C29	-5.96	118.92	127.28
25	3	603	CLA	C4A-NA-C1A	5.95	109.39	106.68
24	4	606	CHL	C4D-ND-C1D	-5.93	100.72	105.22
24	g	607	CHL	C4D-ND-C1D	-5.93	100.72	105.22
27	7	1622	XAT	C31-C30-C29	-5.92	118.98	127.28
24	G	607	CHL	C4D-ND-C1D	-5.91	100.73	105.22
28	y	1623	NEX	C17-C1-C6	-5.91	105.18	110.47
25	B	605	CLA	CAA-C2A-C3A	-5.91	97.03	113.00
25	b	605	CLA	CAA-C2A-C3A	-5.91	97.04	113.00
28	Y	1623	NEX	C17-C1-C6	-5.91	105.19	110.47
27	Y	1622	XAT	C6-C7-C8	-5.89	113.53	125.99
24	8	609	CHL	C4D-ND-C1D	-5.89	100.75	105.22
24	Y	607	CHL	C4D-ND-C1D	-5.89	100.75	105.22
25	7	603	CLA	C4A-NA-C1A	5.88	109.36	106.68
27	3	1622	XAT	C31-C30-C29	-5.88	119.03	127.28
24	4	609	CHL	C4D-ND-C1D	-5.87	100.76	105.22
27	y	1622	XAT	C6-C7-C8	-5.87	113.58	125.99
24	8	606	CHL	C4D-ND-C1D	-5.87	100.76	105.22
30	c	517	BCR	C7-C8-C9	-5.87	117.55	126.23
30	C	517	BCR	C7-C8-C9	-5.86	117.57	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	607	CHL	C4D-ND-C1D	-5.85	100.78	105.22
27	8	622	XAT	C6-C7-C8	-5.85	113.62	125.99
24	s	601	CHL	CHA-C1A-C2A	-5.85	119.58	133.31
24	S	607	CHL	C4D-ND-C1D	-5.85	100.78	105.22
24	R	606	CHL	C4D-ND-C1D	-5.84	100.78	105.22
24	S	601	CHL	CHA-C1A-C2A	-5.84	119.59	133.31
27	4	622	XAT	C6-C7-C8	-5.84	113.65	125.99
24	n	605	CHL	C4D-ND-C1D	-5.83	100.79	105.22
24	Y	605	CHL	C4D-ND-C1D	-5.83	100.80	105.22
24	2	601	CHL	CHA-C1A-C2A	-5.83	119.63	133.31
24	y	605	CHL	C4D-ND-C1D	-5.83	100.80	105.22
24	1	605	CHL	C1B-CHB-C4A	5.82	125.06	121.32
24	6	601	CHL	CHA-C1A-C2A	-5.82	119.65	133.31
24	s	607	CHL	C4D-ND-C1D	-5.82	100.81	105.22
27	R	622	XAT	O24-C25-C24	5.81	118.94	113.49
24	r	606	CHL	C4D-ND-C1D	-5.81	100.81	105.22
25	B	609	CLA	C4A-NA-C1A	5.80	109.33	106.68
24	2	609	CHL	C4D-ND-C1D	-5.80	100.82	105.22
27	r	622	XAT	O24-C25-C24	5.79	118.91	113.49
24	R	614	CHL	C4D-ND-C1D	-5.78	100.83	105.22
24	r	607	CHL	C4D-ND-C1D	-5.77	100.84	105.22
26	R	620	LUT	C26-C27-C28	-5.77	115.60	124.58
24	5	605	CHL	C1B-CHB-C4A	5.77	125.03	121.32
24	N	605	CHL	C4D-ND-C1D	-5.77	100.84	105.22
30	4	623	BCR	C28-C27-C26	-5.76	103.78	114.06
26	r	620	LUT	C26-C27-C28	-5.76	115.61	124.58
24	6	609	CHL	C4D-ND-C1D	-5.75	100.85	105.22
30	8	623	BCR	C28-C27-C26	-5.75	103.80	114.06
25	b	609	CLA	C4A-NA-C1A	5.75	109.30	106.68
27	G	1622	XAT	C6-C7-C8	-5.74	113.85	125.99
24	R	607	CHL	C4D-ND-C1D	-5.74	100.86	105.22
27	g	1622	XAT	C6-C7-C8	-5.74	113.86	125.99
24	r	614	CHL	C4D-ND-C1D	-5.74	100.86	105.22
24	S	607	CHL	CBC-CAC-C3C	-5.74	104.66	112.87
24	s	607	CHL	CBC-CAC-C3C	-5.73	104.66	112.87
24	S	606	CHL	C4D-ND-C1D	-5.73	100.87	105.22
27	3	1622	XAT	C27-C28-C29	-5.73	116.64	125.53
27	8	622	XAT	C38-C25-C26	-5.72	112.88	122.30
27	n	1622	XAT	O4-C5-C4	5.72	118.85	113.49
25	3	611	CLA	C4A-NA-C1A	5.72	109.29	106.68
25	7	611	CLA	C4A-NA-C1A	5.72	109.29	106.68
27	7	1622	XAT	C27-C28-C29	-5.72	116.66	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	605	CHL	C4D-ND-C1D	-5.71	100.88	105.22
28	R	623	NEX	O24-C25-C24	5.71	118.84	113.49
24	2	605	CHL	C4D-ND-C1D	-5.71	100.89	105.22
24	7	606	CHL	CHA-C1A-C2A	-5.71	119.91	133.31
27	4	622	XAT	C38-C25-C26	-5.70	112.91	122.30
24	6	605	CHL	C4D-ND-C1D	-5.70	100.89	105.22
24	Y	609	CHL	CHA-C1A-C2A	-5.70	119.92	133.31
24	7	601	CHL	CHA-C1A-C2A	-5.70	119.92	133.31
24	n	601	CHL	CHA-C1A-C2A	-5.70	119.93	133.31
27	N	1622	XAT	O4-C5-C4	5.70	118.83	113.49
24	3	606	CHL	CHA-C1A-C2A	-5.69	119.94	133.31
24	s	606	CHL	C4D-ND-C1D	-5.69	100.90	105.22
24	3	601	CHL	CHA-C1A-C2A	-5.69	119.94	133.31
24	y	609	CHL	CHA-C1A-C2A	-5.69	119.95	133.31
24	N	601	CHL	CHA-C1A-C2A	-5.68	119.96	133.31
28	r	623	NEX	O24-C25-C24	5.68	118.81	113.49
30	H	101	BCR	C11-C10-C9	-5.68	119.32	127.28
24	G	605	CHL	C4D-ND-C1D	-5.67	100.91	105.22
24	G	601	CHL	CHA-C1A-C2A	-5.67	119.99	133.31
24	g	601	CHL	CHA-C1A-C2A	-5.67	120.00	133.31
30	h	101	BCR	C11-C10-C9	-5.67	119.33	127.28
27	R	622	XAT	C38-C25-C26	-5.65	113.01	122.30
25	c	509	CLA	C4A-NA-C1A	5.64	109.25	106.68
27	7	1622	XAT	C6-C7-C8	-5.64	114.07	125.99
28	1	1623	NEX	C27-C28-C29	-5.64	116.78	125.53
27	7	1622	XAT	C15-C14-C13	-5.64	119.37	127.28
24	G	606	CHL	CHA-C1A-C2A	-5.64	120.08	133.31
27	r	622	XAT	C38-C25-C26	-5.63	113.04	122.30
24	r	606	CHL	CHA-C1A-C2A	-5.63	120.10	133.31
24	g	606	CHL	CHA-C1A-C2A	-5.62	120.10	133.31
25	S	603	CLA	C4A-NA-C1A	5.62	109.25	106.68
24	1	608	CHL	CHA-C1A-C2A	-5.62	120.11	133.31
27	r	622	XAT	C6-C7-C8	-5.62	114.12	125.99
27	3	1622	XAT	C15-C14-C13	-5.62	119.40	127.28
27	3	1622	XAT	C6-C7-C8	-5.61	114.13	125.99
27	R	622	XAT	C26-C27-C28	-5.61	114.13	125.99
28	3	1623	NEX	C15-C14-C13	-5.61	119.41	127.28
28	5	1623	NEX	C27-C28-C29	-5.61	116.83	125.53
24	R	606	CHL	CHA-C1A-C2A	-5.61	120.14	133.31
28	y	1623	NEX	O24-C25-C38	5.61	121.32	115.05
25	N	612	CLA	C4A-NA-C1A	5.61	109.24	106.68
27	r	622	XAT	C26-C27-C28	-5.61	114.13	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	n	612	CLA	C4A-NA-C1A	5.61	109.24	106.68
28	7	1623	NEX	C15-C14-C13	-5.61	119.42	127.28
27	R	622	XAT	C6-C7-C8	-5.60	114.15	125.99
24	5	608	CHL	CHA-C1A-C2A	-5.60	120.16	133.31
26	n	1621	LUT	C26-C27-C28	-5.60	115.87	124.58
30	B	620	BCR	C7-C8-C9	-5.60	117.96	126.23
24	5	601	CHL	CHA-C1A-C2A	-5.59	120.17	133.31
28	Y	1623	NEX	O24-C25-C38	5.59	121.30	115.05
25	s	603	CLA	C4A-NA-C1A	5.59	109.23	106.68
30	b	620	BCR	C7-C8-C9	-5.59	117.97	126.23
24	6	608	CHL	CHA-C1A-C2A	-5.59	120.19	133.31
24	1	601	CHL	CHA-C1A-C2A	-5.58	120.20	133.31
24	2	608	CHL	CHA-C1A-C2A	-5.58	120.20	133.31
26	N	1621	LUT	C26-C27-C28	-5.57	115.91	124.58
25	C	509	CLA	C4A-NA-C1A	5.57	109.22	106.68
24	3	605	CHL	CHA-C1A-C2A	-5.57	120.22	133.31
24	S	608	CHL	C4D-ND-C1D	-5.57	100.99	105.22
24	7	605	CHL	CHA-C1A-C2A	-5.56	120.25	133.31
25	b	608	CLA	C4A-NA-C1A	5.56	109.22	106.68
38	D	401	BCT	O2-C-O1	5.56	133.89	119.68
24	3	608	CHL	CHA-C1A-C2A	-5.55	120.27	133.31
25	7	614	CLA	C4A-NA-C1A	5.55	109.21	106.68
28	6	1623	NEX	C27-C28-C29	-5.55	116.92	125.53
25	3	614	CLA	C4A-NA-C1A	5.55	109.21	106.68
24	7	608	CHL	CHA-C1A-C2A	-5.54	120.29	133.31
38	d	401	BCT	O2-C-O1	5.54	133.84	119.68
28	2	1623	NEX	C27-C28-C29	-5.53	116.94	125.53
24	8	608	CHL	CHA-C1A-C2A	-5.52	120.34	133.31
25	B	608	CLA	C4A-NA-C1A	5.52	109.20	106.68
25	8	603	CLA	C4A-NA-C1A	5.52	109.20	106.68
24	4	608	CHL	CHA-C1A-C2A	-5.51	120.36	133.31
24	g	608	CHL	CHA-C1A-C2A	-5.50	120.39	133.31
25	4	603	CLA	C4A-NA-C1A	5.50	109.19	106.68
25	b	610	CLA	C4A-NA-C1A	5.50	109.19	106.68
25	b	611	CLA	C4A-NA-C1A	5.50	109.19	106.68
24	s	608	CHL	C4D-ND-C1D	-5.50	101.05	105.22
24	N	609	CHL	CHA-C1A-C2A	-5.50	120.40	133.31
24	n	608	CHL	CHA-C1A-C2A	-5.49	120.41	133.31
28	Y	1623	NEX	C35-C34-C33	-5.49	119.58	127.28
36	a	414	PL9	C7-C3-C2	-5.49	116.92	123.39
24	G	608	CHL	CHA-C1A-C2A	-5.49	120.42	133.31
24	n	609	CHL	CHA-C1A-C2A	-5.49	120.42	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	608	CHL	CHA-C1A-C2A	-5.49	120.43	133.31
27	n	1622	XAT	C38-C25-C26	-5.48	113.28	122.30
25	B	611	CLA	C4A-NA-C1A	5.47	109.18	106.68
27	N	1622	XAT	C38-C25-C26	-5.47	113.30	122.30
24	2	606	CHL	CHA-C1A-C2A	-5.47	120.46	133.31
24	6	606	CHL	CHA-C1A-C2A	-5.47	120.47	133.31
24	N	606	CHL	CHA-C1A-C2A	-5.47	120.47	133.31
24	2	609	CHL	CHA-C1A-C2A	-5.46	120.48	133.31
30	C	517	BCR	C11-C10-C9	-5.46	119.62	127.28
24	n	606	CHL	CHA-C1A-C2A	-5.46	120.48	133.31
24	7	606	CHL	C4D-ND-C1D	-5.46	101.08	105.22
25	B	610	CLA	C4A-NA-C1A	5.46	109.17	106.68
28	y	1623	NEX	C35-C34-C33	-5.46	119.62	127.28
24	8	606	CHL	CHA-C1A-C2A	-5.46	120.49	133.31
24	1	605	CHL	CHA-C1A-C2A	-5.46	120.50	133.31
24	5	605	CHL	CHA-C1A-C2A	-5.45	120.51	133.31
30	c	517	BCR	C11-C10-C9	-5.45	119.63	127.28
36	A	414	PL9	C7-C3-C2	-5.45	116.97	123.39
24	6	609	CHL	CHA-C1A-C2A	-5.45	120.52	133.31
24	4	606	CHL	CHA-C1A-C2A	-5.44	120.52	133.31
25	r	603	CLA	C4A-NA-C1A	5.44	109.16	106.68
30	D	404	BCR	C24-C23-C22	-5.44	118.19	126.23
28	Y	1623	NEX	C38-C25-C26	-5.44	113.35	122.30
30	d	404	BCR	C24-C23-C22	-5.44	118.19	126.23
28	y	1623	NEX	C38-C25-C26	-5.43	113.36	122.30
25	R	603	CLA	C4A-NA-C1A	5.42	109.15	106.68
24	7	607	CHL	C4D-ND-C1D	-5.42	101.10	105.22
24	3	606	CHL	C4D-ND-C1D	-5.42	101.11	105.22
24	r	607	CHL	CHA-C1A-C2A	-5.41	120.59	133.31
24	R	607	CHL	CHA-C1A-C2A	-5.41	120.60	133.31
24	y	606	CHL	C4D-ND-C1D	-5.41	101.12	105.22
28	y	1623	NEX	C11-C10-C9	-5.40	119.70	127.28
27	8	622	XAT	C18-C5-C6	-5.40	113.42	122.30
27	4	622	XAT	C18-C5-C6	-5.38	113.44	122.30
28	Y	1623	NEX	C11-C10-C9	-5.38	119.73	127.28
24	y	608	CHL	CHA-C1A-C2A	-5.37	120.69	133.31
24	Y	608	CHL	CHA-C1A-C2A	-5.37	120.69	133.31
24	s	606	CHL	CHA-C1A-C2A	-5.36	120.72	133.31
27	r	622	XAT	C18-C5-C6	-5.36	113.48	122.30
24	3	607	CHL	C4D-ND-C1D	-5.36	101.15	105.22
24	5	606	CHL	CHA-C1A-C2A	-5.36	120.72	133.31
27	y	1622	XAT	O24-C25-C38	5.36	121.04	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	607	CHL	C4D-ND-C1D	-5.35	101.16	105.22
24	S	606	CHL	CHA-C1A-C2A	-5.35	120.74	133.31
27	R	622	XAT	C18-C5-C6	-5.34	113.50	122.30
26	4	620	LUT	C21-C26-C27	-5.34	106.68	112.83
24	1	606	CHL	CHA-C1A-C2A	-5.34	120.76	133.31
24	4	607	CHL	C4D-ND-C1D	-5.34	101.17	105.22
27	Y	1622	XAT	O24-C25-C38	5.34	121.02	115.05
24	Y	606	CHL	C4D-ND-C1D	-5.34	101.17	105.22
25	b	616	CLA	C4A-NA-C1A	5.34	109.11	106.68
27	y	1622	XAT	O24-C25-C24	5.34	118.49	113.49
25	2	611	CLA	C4A-NA-C1A	5.33	109.11	106.68
26	8	620	LUT	C21-C26-C27	-5.33	106.70	112.83
27	r	622	XAT	O4-C5-C4	5.33	118.48	113.49
24	Y	609	CHL	C1B-CHB-C4A	5.31	124.74	121.32
24	G	609	CHL	CHA-C1A-C2A	-5.30	120.85	133.31
24	g	609	CHL	CHA-C1A-C2A	-5.30	120.86	133.31
24	5	606	CHL	C4D-ND-C1D	-5.30	101.20	105.22
24	n	606	CHL	C4D-ND-C1D	-5.30	101.20	105.22
24	2	606	CHL	C4D-ND-C1D	-5.29	101.20	105.22
27	R	622	XAT	O4-C5-C4	5.29	118.45	113.49
24	8	609	CHL	CHA-C1A-C2A	-5.29	120.89	133.31
24	1	609	CHL	C4D-ND-C1D	-5.29	101.21	105.22
24	6	606	CHL	C4D-ND-C1D	-5.29	101.21	105.22
25	c	511	CLA	C4A-NA-C1A	5.28	109.09	106.68
24	y	609	CHL	C1B-CHB-C4A	5.28	124.72	121.32
27	Y	1622	XAT	O24-C25-C24	5.28	118.44	113.49
24	5	609	CHL	C4D-ND-C1D	-5.28	101.22	105.22
24	N	606	CHL	C4D-ND-C1D	-5.27	101.22	105.22
25	1	613	CLA	C4A-NA-C1A	5.27	109.08	106.68
28	G	1623	NEX	C27-C28-C29	-5.27	117.35	125.53
25	6	611	CLA	C4A-NA-C1A	5.27	109.08	106.68
24	4	609	CHL	CHA-C1A-C2A	-5.27	120.93	133.31
28	g	1623	NEX	C27-C28-C29	-5.27	117.36	125.53
25	B	616	CLA	C4A-NA-C1A	5.26	109.08	106.68
28	G	1623	NEX	C35-C34-C33	-5.25	119.91	127.28
27	Y	1622	XAT	C38-C25-C26	-5.25	113.66	122.30
24	5	607	CHL	CHA-C1A-C2A	-5.25	120.97	133.31
27	y	1622	XAT	C38-C25-C26	-5.25	113.66	122.30
24	1	607	CHL	CHA-C1A-C2A	-5.25	120.98	133.31
24	g	605	CHL	CHA-C1A-C2A	-5.25	120.99	133.31
24	G	605	CHL	CHA-C1A-C2A	-5.24	120.99	133.31
28	G	1623	NEX	C11-C10-C9	-5.24	119.92	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	R	623	NEX	C15-C14-C13	-5.24	119.93	127.28
24	3	607	CHL	C1B-CHB-C4A	5.23	124.69	121.32
24	Y	606	CHL	CHA-C1A-C2A	-5.23	121.02	133.31
24	1	609	CHL	CHA-C1A-C2A	-5.23	121.03	133.31
28	r	623	NEX	C38-C25-C26	-5.22	113.70	122.30
28	g	1623	NEX	C35-C34-C33	-5.22	119.95	127.28
24	y	606	CHL	CHA-C1A-C2A	-5.22	121.05	133.31
24	1	606	CHL	C4D-ND-C1D	-5.22	101.26	105.22
28	R	623	NEX	C38-C25-C26	-5.22	113.71	122.30
28	r	623	NEX	C15-C14-C13	-5.22	119.96	127.28
25	7	613	CLA	C4A-NA-C1A	5.22	109.06	106.68
28	g	1623	NEX	C11-C10-C9	-5.21	119.97	127.28
25	3	604	CLA	C4A-NA-C1A	5.21	109.06	106.68
25	C	511	CLA	C4A-NA-C1A	5.21	109.06	106.68
36	a	414	PL9	C7-C3-C4	5.21	123.65	117.88
36	A	414	PL9	C7-C3-C4	5.20	123.64	117.88
26	Y	1620	LUT	C26-C27-C28	-5.20	116.49	124.58
24	5	609	CHL	CHA-C1A-C2A	-5.20	121.10	133.31
24	7	607	CHL	C1B-CHB-C4A	5.20	124.67	121.32
26	5	1621	LUT	C26-C27-C28	-5.19	116.50	124.58
26	y	1620	LUT	C26-C27-C28	-5.19	116.50	124.58
25	c	506	CLA	C4A-NA-C1A	5.19	109.05	106.68
26	1	1621	LUT	C26-C27-C28	-5.18	116.51	124.58
25	6	603	CLA	C4A-NA-C1A	5.18	109.04	106.68
25	7	604	CLA	C4A-NA-C1A	5.18	109.04	106.68
25	5	613	CLA	C4A-NA-C1A	5.18	109.04	106.68
25	R	601	CLA	CAC-C3C-C4C	5.18	131.53	124.79
25	C	506	CLA	C4A-NA-C1A	5.18	109.04	106.68
24	r	608	CHL	CHA-C1A-C2A	-5.17	121.16	133.31
24	8	607	CHL	CHA-C1A-C2A	-5.17	121.16	133.31
24	4	607	CHL	CHA-C1A-C2A	-5.17	121.17	133.31
30	c	517	BCR	C24-C23-C22	-5.17	118.59	126.23
24	R	608	CHL	CHA-C1A-C2A	-5.16	121.19	133.31
27	4	622	XAT	C26-C27-C28	-5.16	115.08	125.99
25	N	614	CLA	C4A-NA-C1A	5.16	109.03	106.68
25	3	613	CLA	C4A-NA-C1A	5.15	109.03	106.68
25	r	601	CLA	CAC-C3C-C4C	5.15	131.49	124.79
27	8	622	XAT	C26-C27-C28	-5.15	115.11	125.99
30	C	517	BCR	C24-C23-C22	-5.14	118.64	126.23
25	2	603	CLA	C4A-NA-C1A	5.12	109.01	106.68
27	8	622	XAT	O4-C5-C4	5.12	118.29	113.49
28	3	1623	NEX	C38-C25-C26	-5.12	113.88	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	4	622	XAT	O4-C5-C4	5.11	118.28	113.49
30	C	516	BCR	C16-C17-C18	-5.11	120.12	127.28
28	7	1623	NEX	C38-C25-C26	-5.10	113.91	122.30
26	G	1620	LUT	C35-C34-C33	-5.10	120.13	127.28
24	Y	609	CHL	C4D-ND-C1D	-5.09	101.35	105.22
26	g	1620	LUT	C35-C34-C33	-5.09	120.13	127.28
27	N	1622	XAT	C6-C7-C8	-5.09	115.22	125.99
25	n	614	CLA	C4A-NA-C1A	5.09	109.00	106.68
24	5	605	CHL	C4D-ND-C1D	-5.09	101.36	105.22
27	n	1622	XAT	C6-C7-C8	-5.09	115.23	125.99
25	C	508	CLA	C4A-NA-C1A	5.09	109.00	106.68
30	c	516	BCR	C16-C17-C18	-5.08	120.15	127.28
25	c	508	CLA	C4A-NA-C1A	5.08	109.00	106.68
24	G	609	CHL	C4D-ND-C1D	-5.08	101.36	105.22
24	g	609	CHL	C4D-ND-C1D	-5.08	101.36	105.22
30	T	101	BCR	C7-C8-C9	-5.08	118.72	126.23
24	1	605	CHL	C4D-ND-C1D	-5.08	101.36	105.22
28	Y	1623	NEX	O24-C25-C24	5.08	118.25	113.49
24	y	609	CHL	C4D-ND-C1D	-5.08	101.37	105.22
27	6	1622	XAT	C38-C25-C26	-5.07	113.95	122.30
25	g	602	CLA	C4A-NA-C1A	5.07	108.99	106.68
30	t	101	BCR	C7-C8-C9	-5.07	118.73	126.23
27	7	1622	XAT	C38-C25-C26	-5.07	113.96	122.30
27	3	1622	XAT	C38-C25-C26	-5.07	113.96	122.30
25	G	602	CLA	C4A-NA-C1A	5.07	108.99	106.68
25	S	613	CLA	C4A-NA-C1A	5.07	108.99	106.68
27	2	1622	XAT	C38-C25-C26	-5.06	113.97	122.30
27	g	1622	XAT	O4-C5-C18	5.06	120.70	115.05
24	7	609	CHL	CHA-C1A-C2A	-5.06	121.43	133.31
25	y	614	CLA	C4A-NA-C1A	5.05	108.98	106.68
24	3	609	CHL	CHA-C1A-C2A	-5.05	121.45	133.31
26	2	1620	LUT	C26-C27-C28	-5.05	116.72	124.58
30	4	623	BCR	C11-C10-C9	-5.04	120.20	127.28
25	s	613	CLA	C4A-NA-C1A	5.04	108.98	106.68
30	8	623	BCR	C11-C10-C9	-5.04	120.21	127.28
28	y	1623	NEX	O24-C25-C24	5.04	118.21	113.49
28	r	623	NEX	C11-C10-C9	-5.03	120.22	127.28
26	6	1620	LUT	C26-C27-C28	-5.03	116.76	124.58
24	Y	605	CHL	CHA-C1A-C2A	-5.03	121.51	133.31
30	4	623	BCR	C15-C14-C13	-5.02	120.24	127.28
24	N	605	CHL	CHA-C1A-C2A	-5.02	121.52	133.31
24	y	605	CHL	CHA-C1A-C2A	-5.02	121.53	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	R	623	NEX	C11-C10-C9	-5.02	120.24	127.28
27	G	1622	XAT	O4-C5-C18	5.01	120.65	115.05
24	n	605	CHL	CHA-C1A-C2A	-5.00	121.56	133.31
26	3	1620	LUT	C26-C27-C28	-5.00	116.79	124.58
30	8	623	BCR	C15-C14-C13	-5.00	120.27	127.28
26	7	1620	LUT	C26-C27-C28	-4.98	116.82	124.58
25	Y	614	CLA	C4A-NA-C1A	4.97	108.94	106.68
27	g	1622	XAT	C31-C30-C29	-4.97	120.31	127.28
25	C	512	CLA	C4A-NA-C1A	4.96	108.94	106.68
27	G	1622	XAT	C31-C30-C29	-4.96	120.32	127.28
25	c	512	CLA	C4A-NA-C1A	4.96	108.94	106.68
27	8	622	XAT	O24-C25-C24	4.96	118.14	113.49
27	4	622	XAT	O24-C25-C24	4.95	118.13	113.49
27	2	1622	XAT	C15-C35-C34	-4.95	113.39	123.52
30	c	517	BCR	C15-C14-C13	-4.95	120.34	127.28
27	6	1622	XAT	C15-C35-C34	-4.95	113.40	123.52
30	C	517	BCR	C15-C14-C13	-4.94	120.35	127.28
27	N	1622	XAT	C27-C28-C29	-4.94	117.86	125.53
28	r	623	NEX	C27-C28-C29	-4.94	117.86	125.53
27	n	1622	XAT	C27-C28-C29	-4.94	117.86	125.53
24	g	607	CHL	CHA-C1A-C2A	-4.94	121.71	133.31
24	G	607	CHL	CHA-C1A-C2A	-4.93	121.73	133.31
24	s	607	CHL	CHA-C1A-C2A	-4.93	121.73	133.31
28	R	623	NEX	C27-C28-C29	-4.93	117.89	125.53
26	5	1620	LUT	C35-C34-C33	-4.92	120.37	127.28
24	S	607	CHL	CHA-C1A-C2A	-4.92	121.75	133.31
27	y	1622	XAT	C15-C35-C34	-4.91	113.48	123.52
26	1	1620	LUT	C35-C34-C33	-4.91	120.39	127.28
26	G	1621	LUT	C26-C27-C28	-4.90	116.95	124.58
27	Y	1622	XAT	C15-C35-C34	-4.90	113.50	123.52
26	S	1621	LUT	C26-C27-C28	-4.90	116.96	124.58
24	Y	607	CHL	CHA-C1A-C2A	-4.90	121.81	133.31
25	C	510	CLA	C4A-NA-C1A	4.89	108.91	106.68
27	2	1622	XAT	C31-C30-C29	-4.89	120.42	127.28
26	s	1621	LUT	C26-C27-C28	-4.89	116.98	124.58
27	5	1622	XAT	C15-C14-C13	-4.89	120.43	127.28
27	7	1622	XAT	C11-C10-C9	-4.88	120.43	127.28
28	N	1623	NEX	C38-C25-C26	-4.88	114.27	122.30
24	y	607	CHL	CHA-C1A-C2A	-4.88	121.84	133.31
27	6	1622	XAT	C31-C30-C29	-4.88	120.43	127.28
27	3	1622	XAT	C11-C10-C9	-4.88	120.43	127.28
25	a	407	CLA	C4A-NA-C1A	4.88	108.91	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	g	1621	LUT	C26-C27-C28	-4.88	116.98	124.58
28	n	1623	NEX	C38-C25-C26	-4.88	114.27	122.30
27	1	1622	XAT	C15-C14-C13	-4.88	120.44	127.28
26	4	620	LUT	C35-C34-C33	-4.88	120.44	127.28
30	b	618	BCR	C15-C14-C13	-4.88	120.44	127.28
27	7	1622	XAT	O24-C25-C38	4.87	120.49	115.05
27	y	1622	XAT	C18-C5-C6	-4.87	114.28	122.30
28	N	1623	NEX	C15-C14-C13	-4.87	120.45	127.28
30	c	515	BCR	C15-C14-C13	-4.87	120.45	127.28
25	B	602	CLA	C4A-NA-C1A	4.87	108.90	106.68
25	c	510	CLA	C4A-NA-C1A	4.87	108.90	106.68
25	y	612	CLA	C4A-NA-C1A	4.86	108.90	106.68
37	c	518	DGD	O3G-C3G-C2G	-4.86	99.00	110.82
25	Y	612	CLA	C4A-NA-C1A	4.86	108.89	106.68
30	B	618	BCR	C15-C14-C13	-4.86	120.47	127.28
30	C	515	BCR	C15-C14-C13	-4.86	120.47	127.28
27	3	1622	XAT	O24-C25-C38	4.85	120.47	115.05
28	n	1623	NEX	C15-C14-C13	-4.85	120.47	127.28
37	C	518	DGD	O3G-C3G-C2G	-4.85	99.02	110.82
25	S	611	CLA	C4A-NA-C1A	4.85	108.89	106.68
26	8	620	LUT	C35-C34-C33	-4.85	120.48	127.28
27	Y	1622	XAT	C18-C5-C6	-4.85	114.33	122.30
30	C	514	BCR	C15-C14-C13	-4.85	120.48	127.28
30	T	101	BCR	C11-C10-C9	-4.84	120.48	127.28
25	A	407	CLA	C4A-NA-C1A	4.84	108.89	106.68
30	t	101	BCR	C11-C10-C9	-4.83	120.50	127.28
30	c	514	BCR	C15-C14-C13	-4.82	120.51	127.28
25	A	405	CLA	C4A-NA-C1A	4.82	108.88	106.68
26	8	620	LUT	C7-C8-C9	-4.81	119.12	126.23
24	S	608	CHL	CHA-C1A-C2A	-4.81	122.02	133.31
28	6	1623	NEX	C15-C14-C13	-4.81	120.54	127.28
26	4	620	LUT	C7-C8-C9	-4.80	119.13	126.23
25	C	504	CLA	C4A-NA-C1A	4.80	108.87	106.68
25	g	612	CLA	C4A-NA-C1A	4.80	108.87	106.68
25	s	611	CLA	C4A-NA-C1A	4.79	108.87	106.68
25	c	504	CLA	C4A-NA-C1A	4.79	108.86	106.68
24	s	608	CHL	CHA-C1A-C2A	-4.79	122.06	133.31
28	2	1623	NEX	C15-C14-C13	-4.79	120.56	127.28
30	b	619	BCR	C15-C14-C13	-4.78	120.57	127.28
24	2	605	CHL	CHA-C1A-C2A	-4.77	122.10	133.31
25	b	602	CLA	C4A-NA-C1A	4.77	108.86	106.68
24	6	605	CHL	CHA-C1A-C2A	-4.77	122.11	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	8	622	XAT	O24-C25-C38	4.77	120.38	115.05
30	B	619	BCR	C15-C14-C13	-4.77	120.59	127.28
27	g	1622	XAT	C38-C25-C26	-4.77	114.45	122.30
27	y	1622	XAT	C11-C10-C9	-4.77	120.59	127.28
26	N	1621	LUT	C15-C14-C13	-4.77	120.59	127.28
25	C	513	CLA	C4A-NA-C1A	4.76	108.85	106.68
26	n	1621	LUT	C15-C14-C13	-4.76	120.60	127.28
27	4	622	XAT	O24-C25-C38	4.76	120.36	115.05
28	6	1623	NEX	C38-C25-C26	-4.76	114.47	122.30
27	G	1622	XAT	C38-C25-C26	-4.75	114.48	122.30
25	G	612	CLA	C4A-NA-C1A	4.75	108.85	106.68
28	y	1623	NEX	C27-C28-C29	-4.74	118.17	125.53
30	H	101	BCR	C16-C17-C18	-4.74	120.62	127.28
28	S	1623	NEX	C38-C25-C26	-4.74	114.49	122.30
26	4	620	LUT	C15-C14-C13	-4.74	120.63	127.28
28	s	1623	NEX	C27-C28-C29	-4.74	118.17	125.53
28	2	1623	NEX	C38-C25-C26	-4.74	114.50	122.30
27	1	1622	XAT	C27-C28-C29	-4.74	118.18	125.53
26	8	620	LUT	C15-C14-C13	-4.73	120.64	127.28
27	Y	1622	XAT	C11-C10-C9	-4.73	120.65	127.28
27	2	1622	XAT	C27-C28-C29	-4.73	118.20	125.53
28	S	1623	NEX	C27-C28-C29	-4.73	118.20	125.53
28	s	1623	NEX	C38-C25-C26	-4.72	114.53	122.30
24	N	609	CHL	C4D-ND-C1D	-4.72	101.64	105.22
28	S	1623	NEX	C15-C14-C13	-4.72	120.66	127.28
27	6	1622	XAT	C27-C28-C29	-4.72	118.21	125.53
24	n	609	CHL	C4D-ND-C1D	-4.72	101.64	105.22
24	3	607	CHL	CHA-C1A-C2A	-4.72	122.23	133.31
30	h	101	BCR	C16-C17-C18	-4.72	120.67	127.28
27	5	1622	XAT	C27-C28-C29	-4.72	118.21	125.53
25	S	614	CLA	C4A-NA-C1A	4.71	108.83	106.68
25	a	405	CLA	C4A-NA-C1A	4.71	108.83	106.68
25	c	513	CLA	C4A-NA-C1A	4.71	108.83	106.68
24	7	607	CHL	CHA-C1A-C2A	-4.71	122.25	133.31
28	N	1623	NEX	C35-C34-C33	-4.71	120.68	127.28
27	2	1622	XAT	C7-C8-C9	-4.70	118.24	125.53
25	C	503	CLA	C4A-NA-C1A	4.70	108.82	106.68
25	5	612	CLA	C4A-NA-C1A	4.70	108.82	106.68
29	D	408	LHG	O4-P-O5	4.69	134.28	112.44
28	s	1623	NEX	C15-C14-C13	-4.69	120.70	127.28
28	Y	1623	NEX	C27-C28-C29	-4.69	118.25	125.53
29	d	408	LHG	O4-P-O5	4.69	134.26	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	408	PHO	C2B-C1B-NB	-4.69	106.04	109.43
28	n	1623	NEX	C35-C34-C33	-4.69	120.71	127.28
27	6	1622	XAT	C7-C8-C9	-4.68	118.27	125.53
33	A	408	PHO	C2B-C1B-NB	-4.67	106.06	109.43
24	g	609	CHL	CBC-CAC-C3C	-4.66	106.20	112.87
30	c	515	BCR	C21-C20-C19	-4.66	109.71	123.20
28	G	1623	NEX	C15-C14-C13	-4.66	120.75	127.28
30	C	515	BCR	C21-C20-C19	-4.65	109.72	123.20
25	1	612	CLA	C4A-NA-C1A	4.64	108.80	106.68
30	A	411	BCR	C7-C8-C9	-4.64	119.37	126.23
28	1	1623	NEX	C35-C34-C33	-4.64	120.77	127.28
24	3	609	CHL	C4D-ND-C1D	-4.64	101.70	105.22
30	a	411	BCR	C7-C8-C9	-4.64	119.38	126.23
24	G	609	CHL	CBC-CAC-C3C	-4.63	106.24	112.87
28	5	1623	NEX	C35-C34-C33	-4.63	120.78	127.28
25	Y	604	CLA	CMB-C2B-C1B	-4.63	118.37	125.42
28	g	1623	NEX	C15-C14-C13	-4.63	120.78	127.28
24	N	607	CHL	CHA-C1A-C2A	-4.63	122.44	133.31
24	n	607	CHL	CHA-C1A-C2A	-4.63	122.44	133.31
26	S	1620	LUT	C35-C34-C33	-4.62	120.80	127.28
26	s	1620	LUT	C35-C34-C33	-4.62	120.80	127.28
24	6	607	CHL	CHA-C1A-C2A	-4.62	122.46	133.31
25	y	604	CLA	CMB-C2B-C1B	-4.62	118.39	125.42
24	2	607	CHL	CHA-C1A-C2A	-4.62	122.47	133.31
25	s	614	CLA	C4A-NA-C1A	4.61	108.78	106.68
25	d	403	CLA	C4A-NA-C1A	4.61	108.78	106.68
28	y	1623	NEX	C15-C14-C13	-4.61	120.82	127.28
25	Y	603	CLA	C4A-NA-C1A	4.60	108.78	106.68
27	n	1622	XAT	C18-C5-C6	-4.60	114.73	122.30
25	c	503	CLA	C4A-NA-C1A	4.60	108.78	106.68
27	N	1622	XAT	C18-C5-C6	-4.60	114.73	122.30
27	g	1622	XAT	C18-C5-C6	-4.60	114.73	122.30
25	D	403	CLA	C4A-NA-C1A	4.60	108.78	106.68
24	7	609	CHL	C4D-ND-C1D	-4.60	101.73	105.22
26	N	1620	LUT	C26-C27-C28	-4.59	117.43	124.58
27	G	1622	XAT	C18-C5-C6	-4.59	114.75	122.30
28	Y	1623	NEX	C15-C14-C13	-4.59	120.84	127.28
36	d	405	PL9	C7-C3-C4	4.59	120.69	116.91
26	S	1620	LUT	C26-C27-C28	-4.58	117.44	124.58
25	y	602	CLA	C4A-NA-C1A	4.58	108.77	106.68
28	G	1623	NEX	C38-C25-C26	-4.58	114.76	122.30
30	h	101	BCR	C15-C14-C13	-4.58	120.86	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	610	CLA	C4A-NA-C1A	4.58	108.77	106.68
36	D	405	PL9	C7-C3-C4	4.58	120.68	116.91
28	g	1623	NEX	C38-C25-C26	-4.58	114.77	122.30
25	B	607	CLA	C4A-NA-C1A	4.57	108.77	106.68
26	n	1620	LUT	C26-C27-C28	-4.57	117.46	124.58
24	N	609	CHL	CBC-CAC-C3C	-4.57	106.33	112.87
30	H	101	BCR	C15-C14-C13	-4.57	120.87	127.28
30	H	101	BCR	C24-C23-C22	-4.57	119.48	126.23
30	h	101	BCR	C24-C23-C22	-4.57	119.48	126.23
26	s	1620	LUT	C26-C27-C28	-4.57	117.47	124.58
25	y	603	CLA	C4A-NA-C1A	4.57	108.76	106.68
24	n	609	CHL	CBC-CAC-C3C	-4.56	106.34	112.87
30	4	623	BCR	C16-C17-C18	-4.56	120.89	127.28
29	l	101	LHG	O4-P-O5	4.56	133.64	112.44
30	8	623	BCR	C16-C17-C18	-4.55	120.89	127.28
25	r	610	CLA	C4A-NA-C1A	4.55	108.75	106.68
26	S	1621	LUT	C35-C34-C33	-4.55	120.90	127.28
29	L	101	LHG	O4-P-O5	4.55	133.60	112.44
28	5	1623	NEX	C38-C25-C26	-4.55	114.82	122.30
26	s	1621	LUT	C35-C34-C33	-4.54	120.91	127.28
29	4	2630	LHG	O4-P-O5	4.54	133.57	112.44
26	G	1621	LUT	C15-C14-C13	-4.54	120.92	127.28
29	8	2630	LHG	O4-P-O5	4.54	133.55	112.44
25	Y	602	CLA	C4A-NA-C1A	4.54	108.75	106.68
25	n	602	CLA	C4A-NA-C1A	4.53	108.75	106.68
26	g	1621	LUT	C15-C14-C13	-4.53	120.92	127.28
30	H	101	BCR	C7-C8-C9	-4.53	119.54	126.23
28	1	1623	NEX	C38-C25-C26	-4.53	114.85	122.30
26	1	1621	LUT	C15-C14-C13	-4.52	120.94	127.28
29	Y	2630	LHG	O4-P-O5	4.52	133.45	112.44
29	y	2630	LHG	O4-P-O5	4.52	133.45	112.44
25	4	602	CLA	O2D-CGD-O1D	-4.51	115.06	123.85
30	h	101	BCR	C7-C8-C9	-4.50	119.57	126.23
25	N	602	CLA	C4A-NA-C1A	4.50	108.73	106.68
25	b	607	CLA	C4A-NA-C1A	4.50	108.73	106.68
26	5	1621	LUT	C15-C14-C13	-4.50	120.97	127.28
25	R	609	CLA	C4A-NA-C1A	4.50	108.73	106.68
25	S	612	CLA	C4A-NA-C1A	4.50	108.73	106.68
25	s	612	CLA	C4A-NA-C1A	4.50	108.73	106.68
29	c	523	LHG	O4-P-O5	4.49	133.34	112.44
27	4	622	XAT	C35-C34-C33	-4.49	120.98	127.28
27	2	1622	XAT	C15-C14-C13	-4.49	120.98	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	523	LHG	O4-P-O5	4.48	133.31	112.44
25	8	602	CLA	O2D-CGD-O1D	-4.48	115.12	123.85
29	R	2630	LHG	O4-P-O5	4.48	133.28	112.44
29	d	410	LHG	O4-P-O5	4.48	133.28	112.44
37	C	520	DGD	O3G-C3G-C2G	-4.48	99.93	110.82
27	1	1622	XAT	C31-C30-C29	-4.48	121.00	127.28
29	D	410	LHG	O4-P-O5	4.48	133.26	112.44
37	c	520	DGD	O3G-C3G-C2G	-4.47	99.94	110.82
24	1	609	CHL	C1B-CHB-C4A	4.47	124.20	121.32
29	r	2630	LHG	O4-P-O5	4.47	133.26	112.44
27	6	1622	XAT	C15-C14-C13	-4.47	121.00	127.28
27	5	1622	XAT	C38-C25-C26	-4.47	114.94	122.30
25	8	604	CLA	C4A-NA-C1A	4.47	108.72	106.68
24	5	609	CHL	C1B-CHB-C4A	4.47	124.20	121.32
27	6	1622	XAT	O24-C25-C38	4.47	120.04	115.05
27	1	1622	XAT	C38-C25-C26	-4.46	114.96	122.30
25	4	604	CLA	C4A-NA-C1A	4.46	108.72	106.68
26	N	1620	LUT	C35-C34-C33	-4.46	121.03	127.28
25	R	602	CLA	C4A-NA-C1A	4.46	108.71	106.68
27	2	1622	XAT	O24-C25-C38	4.46	120.03	115.05
27	5	1622	XAT	C31-C30-C29	-4.45	121.03	127.28
26	n	1620	LUT	C35-C34-C33	-4.45	121.03	127.28
27	8	622	XAT	C35-C34-C33	-4.45	121.04	127.28
25	r	609	CLA	C4A-NA-C1A	4.45	108.71	106.68
29	d	409	LHG	O4-P-O5	4.44	133.12	112.44
29	D	409	LHG	O4-P-O5	4.44	133.12	112.44
29	s	2630	LHG	O4-P-O5	4.44	133.10	112.44
29	n	2630	LHG	O4-P-O5	4.44	133.09	112.44
29	N	2630	LHG	O4-P-O5	4.44	133.08	112.44
29	S	2630	LHG	O4-P-O5	4.43	133.07	112.44
30	c	515	BCR	C7-C8-C9	-4.43	119.67	126.23
29	C	522	LHG	O4-P-O5	4.43	133.04	112.44
29	6	2630	LHG	O4-P-O5	4.43	133.04	112.44
29	c	522	LHG	O4-P-O5	4.43	133.03	112.44
29	2	2630	LHG	O4-P-O5	4.42	133.02	112.44
30	C	515	BCR	C7-C8-C9	-4.42	119.70	126.23
25	D	402	CLA	C4A-NA-C1A	4.42	108.69	106.68
30	D	404	BCR	C11-C10-C9	-4.41	121.09	127.28
27	7	1622	XAT	O24-C25-C24	4.40	117.62	113.49
27	g	1622	XAT	C4-C3-C2	-4.40	102.56	110.79
26	Y	1621	LUT	C35-C34-C33	-4.39	121.12	127.28
34	B	621	SQD	O9-S-C6	4.39	113.31	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	y	1621	LUT	C35-C34-C33	-4.39	121.12	127.28
30	d	404	BCR	C11-C10-C9	-4.39	121.13	127.28
29	c	2630	LHG	O4-P-O5	4.39	132.84	112.44
27	3	1622	XAT	O24-C25-C24	4.38	117.60	113.49
25	n	603	CLA	C4A-NA-C1A	4.38	108.68	106.68
27	G	1622	XAT	C4-C3-C2	-4.38	102.60	110.79
30	t	101	BCR	C20-C19-C18	-4.38	114.36	126.36
29	1	2630	LHG	O4-P-O5	4.38	132.80	112.44
29	C	2630	LHG	O4-P-O5	4.38	132.80	112.44
29	5	2630	LHG	O4-P-O5	4.38	132.80	112.44
25	r	602	CLA	C4A-NA-C1A	4.38	108.67	106.68
24	8	608	CHL	CBC-CAC-C3C	-4.37	106.61	112.87
34	b	621	SQD	O9-S-C6	4.37	113.28	106.76
25	d	402	CLA	C4A-NA-C1A	4.37	108.67	106.68
30	T	101	BCR	C20-C19-C18	-4.37	114.38	126.36
29	B	2630	LHG	O4-P-O5	4.36	132.74	112.44
29	b	2630	LHG	O4-P-O5	4.36	132.72	112.44
26	3	1621	LUT	C10-C11-C12	-4.35	110.59	123.20
26	Y	1621	LUT	C15-C14-C13	-4.35	121.18	127.28
24	4	608	CHL	CBC-CAC-C3C	-4.35	106.65	112.87
26	y	1621	LUT	C15-C14-C13	-4.34	121.19	127.28
25	N	603	CLA	C4A-NA-C1A	4.34	108.66	106.68
27	1	1622	XAT	C18-C5-C6	-4.34	115.16	122.30
26	7	1621	LUT	C10-C11-C12	-4.34	110.63	123.20
26	5	1620	LUT	C26-C27-C28	-4.33	117.84	124.58
25	4	612	CLA	C4A-NA-C1A	4.33	108.65	106.68
29	B	2631	LHG	O4-P-O5	4.32	132.56	112.44
29	b	2631	LHG	O4-P-O5	4.32	132.55	112.44
26	1	1620	LUT	C26-C27-C28	-4.32	117.85	124.58
27	5	1622	XAT	C18-C5-C6	-4.32	115.19	122.30
25	8	612	CLA	C4A-NA-C1A	4.31	108.65	106.68
27	Y	1622	XAT	C4-C3-C2	-4.31	102.73	110.79
27	G	1622	XAT	O24-C25-C38	4.30	119.85	115.05
27	y	1622	XAT	C4-C3-C2	-4.29	102.76	110.79
27	7	1622	XAT	C4-C3-C2	-4.29	102.77	110.79
27	1	1622	XAT	C11-C10-C9	-4.28	121.27	127.28
27	3	1622	XAT	C4-C3-C2	-4.28	102.79	110.79
34	A	418	SQD	O7-S-C6	4.27	113.13	106.76
24	s	608	CHL	C1B-CHB-C4A	4.27	124.07	121.32
30	b	618	BCR	C16-C17-C18	-4.27	121.29	127.28
27	5	1622	XAT	C11-C10-C9	-4.26	121.30	127.28
27	n	1622	XAT	C11-C10-C9	-4.26	121.30	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	418	SQD	O7-S-C6	4.26	113.12	106.76
29	G	2630	LHG	O4-P-O5	4.26	132.27	112.44
29	g	2630	LHG	O4-P-O5	4.26	132.27	112.44
26	8	620	LUT	C26-C27-C28	-4.26	117.95	124.58
27	4	622	XAT	C15-C14-C13	-4.26	121.31	127.28
27	g	1622	XAT	O24-C25-C38	4.25	119.80	115.05
27	8	622	XAT	C15-C14-C13	-4.25	121.32	127.28
26	4	620	LUT	C26-C27-C28	-4.25	117.97	124.58
27	N	1622	XAT	C11-C10-C9	-4.25	121.32	127.28
24	2	607	CHL	C4D-ND-C1D	-4.24	102.00	105.22
24	6	607	CHL	C4D-ND-C1D	-4.24	102.00	105.22
30	B	618	BCR	C16-C17-C18	-4.24	121.34	127.28
25	r	604	CLA	CAA-C2A-C3A	-4.23	101.57	113.00
25	R	604	CLA	CAA-C2A-C3A	-4.23	101.57	113.00
29	7	2630	LHG	O4-P-O5	4.23	132.12	112.44
29	3	2630	LHG	O4-P-O5	4.22	132.09	112.44
24	S	608	CHL	C1B-CHB-C4A	4.22	124.04	121.32
24	8	607	CHL	C1B-CHB-C4A	4.22	124.04	121.32
25	B	611	CLA	CAA-C2A-C3A	-4.22	101.60	113.00
25	b	611	CLA	CAA-C2A-C3A	-4.21	101.63	113.00
25	8	602	CLA	C4A-NA-C1A	4.21	108.60	106.68
25	g	604	CLA	C4A-NA-C1A	4.21	108.60	106.68
26	g	1621	LUT	C35-C34-C33	-4.18	121.41	127.28
28	1	1623	NEX	C17-C1-C6	-4.18	106.73	110.47
27	G	1622	XAT	C27-C28-C29	-4.18	119.04	125.53
27	g	1622	XAT	C27-C28-C29	-4.18	119.04	125.53
30	c	514	BCR	C16-C17-C18	-4.18	121.42	127.28
25	G	604	CLA	C4A-NA-C1A	4.17	108.58	106.68
26	G	1620	LUT	C26-C27-C28	-4.17	118.09	124.58
30	A	411	BCR	C11-C10-C9	-4.17	121.43	127.28
27	2	1622	XAT	C18-C5-C6	-4.17	115.44	122.30
26	G	1621	LUT	C35-C34-C33	-4.17	121.43	127.28
30	c	516	BCR	C28-C27-C26	-4.17	106.62	114.06
30	C	516	BCR	C28-C27-C26	-4.17	106.62	114.06
24	2	609	CHL	CBC-CAC-C3C	-4.16	106.91	112.87
30	a	411	BCR	C11-C10-C9	-4.16	121.44	127.28
26	g	1620	LUT	C26-C27-C28	-4.16	118.10	124.58
27	6	1622	XAT	C18-C5-C6	-4.16	115.45	122.30
24	6	609	CHL	CBC-CAC-C3C	-4.16	106.92	112.87
28	5	1623	NEX	C17-C1-C6	-4.16	106.75	110.47
24	n	605	CHL	O2D-CGD-O1D	-4.16	115.75	123.85
30	C	514	BCR	C16-C17-C18	-4.15	121.45	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	609	CHL	CBC-CAC-C3C	-4.15	106.93	112.87
30	C	517	BCR	C20-C21-C22	-4.15	121.46	127.28
24	N	605	CHL	O2D-CGD-O1D	-4.14	115.78	123.85
25	4	602	CLA	C4A-NA-C1A	4.14	108.57	106.68
28	s	1623	NEX	O24-C25-C38	4.14	119.68	115.05
24	4	607	CHL	C1B-CHB-C4A	4.14	123.99	121.32
27	y	1622	XAT	C10-C11-C12	-4.14	111.20	123.20
24	Y	609	CHL	CBC-CAC-C3C	-4.14	106.94	112.87
30	c	517	BCR	C20-C21-C22	-4.14	121.47	127.28
26	2	1621	LUT	C35-C34-C33	-4.14	121.47	127.28
26	N	1621	LUT	C35-C34-C33	-4.14	121.48	127.28
26	n	1621	LUT	C35-C34-C33	-4.13	121.49	127.28
27	r	622	XAT	O24-C25-C38	4.13	119.66	115.05
27	Y	1622	XAT	C10-C11-C12	-4.13	111.25	123.20
27	r	622	XAT	C35-C34-C33	-4.12	121.49	127.28
27	4	622	XAT	C4-C3-C2	-4.12	103.08	110.79
30	T	101	BCR	C4-C5-C6	-4.12	117.14	122.70
30	b	618	BCR	C21-C20-C19	-4.12	111.27	123.20
27	R	622	XAT	O24-C25-C38	4.12	119.65	115.05
27	8	622	XAT	C4-C3-C2	-4.11	103.09	110.79
26	R	620	LUT	C10-C11-C12	-4.11	111.29	123.20
26	r	620	LUT	C10-C11-C12	-4.11	111.29	123.20
26	6	1621	LUT	C35-C34-C33	-4.11	121.51	127.28
25	B	605	CLA	CAA-CBA-CGA	-4.11	101.55	113.21
30	B	618	BCR	C21-C20-C19	-4.10	111.31	123.20
27	R	622	XAT	C35-C34-C33	-4.10	121.52	127.28
28	S	1623	NEX	O24-C25-C38	4.10	119.63	115.05
25	b	605	CLA	CAA-CBA-CGA	-4.10	101.56	113.21
30	t	101	BCR	C4-C5-C6	-4.10	117.17	122.70
37	c	519	DGD	O3G-C3G-C2G	-4.09	100.86	110.82
25	1	614	CLA	C4A-NA-C1A	4.09	108.55	106.68
26	6	1620	LUT	C15-C14-C13	-4.09	121.54	127.28
25	B	615	CLA	C4A-NA-C1A	4.09	108.54	106.68
27	3	1622	XAT	C18-C5-C6	-4.09	115.58	122.30
28	R	623	NEX	O24-C25-C38	4.08	119.61	115.05
25	R	604	CLA	C4A-NA-C1A	4.08	108.54	106.68
37	C	519	DGD	O3G-C3G-C2G	-4.08	100.89	110.82
26	2	1620	LUT	C15-C14-C13	-4.08	121.55	127.28
28	r	623	NEX	O24-C25-C38	4.08	119.61	115.05
30	C	517	BCR	C33-C5-C6	-4.08	120.04	124.48
30	B	620	BCR	C16-C17-C18	-4.07	121.57	127.28
25	b	615	CLA	C4A-NA-C1A	4.07	108.53	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	2	1621	LUT	C26-C27-C28	-4.07	118.25	124.58
26	6	1621	LUT	C26-C27-C28	-4.06	118.26	124.58
30	c	517	BCR	C33-C5-C6	-4.06	120.05	124.48
27	7	1622	XAT	C18-C5-C6	-4.06	115.62	122.30
28	R	623	NEX	C31-C30-C29	-4.06	121.58	127.28
26	y	1621	LUT	C26-C27-C28	-4.06	118.26	124.58
28	7	1623	NEX	O24-C25-C38	4.06	119.58	115.05
28	N	1623	NEX	C27-C28-C29	-4.05	119.24	125.53
28	3	1623	NEX	O24-C25-C38	4.05	119.58	115.05
25	4	611	CLA	C4A-NA-C1A	4.05	108.53	106.68
30	T	101	BCR	C33-C5-C4	4.05	122.23	113.60
26	Y	1621	LUT	C26-C27-C28	-4.05	118.28	124.58
30	b	620	BCR	C16-C17-C18	-4.05	121.60	127.28
34	a	412	SQD	O9-S-O7	-4.04	100.67	113.82
28	3	1623	NEX	C11-C10-C9	-4.04	121.61	127.28
28	7	1623	NEX	C11-C10-C9	-4.04	121.61	127.28
34	A	412	SQD	O9-S-O7	-4.04	100.69	113.82
25	5	614	CLA	C4A-NA-C1A	4.04	108.52	106.68
27	N	1622	XAT	C4-C3-C2	-4.04	103.24	110.79
28	n	1623	NEX	C27-C28-C29	-4.03	119.28	125.53
27	n	1622	XAT	C4-C3-C2	-4.03	103.25	110.79
30	t	101	BCR	C33-C5-C4	4.03	122.19	113.60
30	B	620	BCR	C28-C27-C26	-4.03	106.87	114.06
24	R	608	CHL	CBC-CAC-C3C	-4.03	107.11	112.87
24	r	608	CHL	CBC-CAC-C3C	-4.02	107.11	112.87
28	r	623	NEX	C31-C30-C29	-4.02	121.64	127.28
25	1	604	CLA	C4A-NA-C1A	4.02	108.51	106.68
30	b	620	BCR	C28-C27-C26	-4.02	106.89	114.06
26	r	620	LUT	C35-C34-C33	-4.02	121.64	127.28
26	R	620	LUT	C35-C34-C33	-4.02	121.65	127.28
34	b	623	SQD	O9-S-O7	-4.01	100.77	113.82
27	n	1622	XAT	C15-C35-C34	-4.01	115.31	123.52
25	N	604	CLA	CMB-C2B-C1B	-4.01	119.31	125.42
25	r	604	CLA	C4A-NA-C1A	4.01	108.51	106.68
30	T	101	BCR	C28-C27-C26	-4.01	106.91	114.06
25	n	604	CLA	CMB-C2B-C1B	-4.01	119.32	125.42
30	t	101	BCR	C28-C27-C26	-4.00	106.92	114.06
27	N	1622	XAT	C15-C35-C34	-4.00	115.33	123.52
34	B	623	SQD	O9-S-O7	-4.00	100.81	113.82
28	N	1623	NEX	O24-C25-C38	4.00	119.52	115.05
30	c	517	BCR	C16-C17-C18	-4.00	121.67	127.28
26	1	1621	LUT	C35-C34-C33	-3.99	121.68	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	n	1623	NEX	O24-C25-C38	3.99	119.51	115.05
25	5	604	CLA	C4A-NA-C1A	3.99	108.50	106.68
33	a	409	PHO	CMB-C2B-C3B	3.98	132.65	124.68
25	8	611	CLA	C4A-NA-C1A	3.98	108.50	106.68
30	C	517	BCR	C16-C17-C18	-3.98	121.70	127.28
26	5	1621	LUT	C35-C34-C33	-3.98	121.70	127.28
27	Y	1622	XAT	C27-C28-C29	-3.98	119.36	125.53
33	A	409	PHO	CMB-C2B-C3B	3.98	132.63	124.68
27	G	1622	XAT	O4-C5-C4	3.97	117.22	113.49
30	b	619	BCR	C11-C10-C9	-3.97	121.70	127.28
25	G	614	CLA	C4A-NA-C1A	3.97	108.49	106.68
30	b	618	BCR	C24-C23-C22	-3.97	120.36	126.23
26	1	1620	LUT	C10-C11-C12	-3.97	111.70	123.20
28	7	1623	NEX	C27-C28-C29	-3.96	119.38	125.53
26	5	1620	LUT	C10-C11-C12	-3.96	111.73	123.20
27	g	1622	XAT	O4-C5-C4	3.96	117.20	113.49
30	B	619	BCR	C11-C10-C9	-3.96	121.73	127.28
30	B	618	BCR	C24-C23-C22	-3.96	120.38	126.23
27	n	1622	XAT	O24-C25-C38	3.95	119.47	115.05
28	2	1623	NEX	O24-C25-C38	3.95	119.46	115.05
30	b	619	BCR	C16-C17-C18	-3.95	121.75	127.28
27	7	1622	XAT	C15-C35-C34	-3.95	115.45	123.52
27	y	1622	XAT	C27-C28-C29	-3.94	119.41	125.53
36	d	405	PL9	C7-C3-C2	-3.94	118.74	123.39
27	N	1622	XAT	O24-C25-C38	3.94	119.45	115.05
28	3	1623	NEX	C27-C28-C29	-3.94	119.42	125.53
36	D	405	PL9	C7-C3-C2	-3.94	118.75	123.39
25	S	602	CLA	C4A-NA-C1A	3.93	108.47	106.68
30	B	619	BCR	C16-C17-C18	-3.93	121.77	127.28
25	3	602	CLA	C4A-NA-C1A	3.93	108.47	106.68
28	6	1623	NEX	O24-C25-C38	3.92	119.43	115.05
34	b	623	SQD	O47-C7-C8	3.92	119.97	111.48
28	s	1623	NEX	C24-C23-C22	-3.92	103.45	110.79
27	3	1622	XAT	C15-C35-C34	-3.92	115.49	123.52
26	r	620	LUT	C15-C14-C13	-3.92	121.78	127.28
25	b	609	CLA	CMB-C2B-C1B	-3.92	119.46	125.42
26	R	620	LUT	C15-C14-C13	-3.92	121.79	127.28
30	h	101	BCR	C20-C21-C22	-3.92	121.79	127.28
34	B	623	SQD	O47-C7-C8	3.91	119.95	111.48
25	s	602	CLA	C4A-NA-C1A	3.91	108.47	106.68
25	2	604	CLA	C4A-NA-C1A	3.91	108.46	106.68
37	c	520	DGD	O6D-C1D-O3G	-3.91	100.81	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	1	1623	NEX	O24-C25-C38	3.91	119.42	115.05
26	y	1620	LUT	C10-C11-C12	-3.91	111.88	123.20
26	Y	1620	LUT	C10-C11-C12	-3.91	111.88	123.20
25	g	614	CLA	C4A-NA-C1A	3.91	108.46	106.68
25	B	609	CLA	CMB-C2B-C1B	-3.90	119.47	125.42
30	C	516	BCR	C20-C21-C22	-3.90	121.80	127.28
24	5	605	CHL	OMC-CMC-C2C	-3.90	118.34	125.12
30	C	515	BCR	C11-C10-C9	-3.90	121.81	127.28
28	S	1623	NEX	C24-C23-C22	-3.90	103.50	110.79
30	c	515	BCR	C11-C10-C9	-3.90	121.81	127.28
30	c	516	BCR	C20-C21-C22	-3.90	121.81	127.28
34	A	418	SQD	O9-S-O7	-3.89	101.16	113.82
37	C	520	DGD	O6D-C1D-O3G	-3.89	100.85	110.04
24	y	609	CHL	CMA-C3A-C4A	-3.89	106.23	114.61
30	H	101	BCR	C20-C21-C22	-3.89	121.83	127.28
25	r	601	CLA	CBC-CAC-C3C	3.89	122.96	112.42
34	a	418	SQD	O9-S-O7	-3.88	101.19	113.82
26	8	620	LUT	C27-C28-C29	-3.88	117.97	126.32
34	b	623	SQD	C1-O5-C5	3.88	121.30	113.72
25	R	601	CLA	CBC-CAC-C3C	3.88	122.94	112.42
28	r	623	NEX	C26-C27-C28	-3.88	117.79	125.99
24	Y	609	CHL	CMA-C3A-C4A	-3.88	106.25	114.61
25	G	603	CLA	C4A-NA-C1A	3.88	108.45	106.68
24	1	605	CHL	OMC-CMC-C2C	-3.88	118.39	125.12
30	C	516	BCR	C33-C5-C6	-3.88	120.25	124.48
30	c	516	BCR	C33-C5-C6	-3.88	120.25	124.48
27	4	622	XAT	O4-C5-C18	3.88	119.38	115.05
30	a	411	BCR	C24-C23-C22	-3.87	120.50	126.23
30	A	411	BCR	C24-C23-C22	-3.87	120.51	126.23
34	B	623	SQD	C1-O5-C5	3.87	121.28	113.72
25	7	602	CLA	C4A-NA-C1A	3.87	108.44	106.68
28	R	623	NEX	C26-C27-C28	-3.87	117.81	125.99
28	5	1623	NEX	O24-C25-C38	3.87	119.37	115.05
24	1	607	CHL	CMA-C3A-C4A	-3.87	106.28	114.61
26	4	620	LUT	C27-C28-C29	-3.87	118.01	126.32
30	H	101	BCR	C31-C1-C6	-3.86	104.18	110.24
24	5	607	CHL	CMA-C3A-C4A	-3.86	106.28	114.61
30	h	101	BCR	C31-C1-C6	-3.86	104.18	110.24
27	N	1622	XAT	O4-C5-C18	3.86	119.36	115.05
27	n	1622	XAT	O4-C5-C18	3.86	119.36	115.05
30	d	404	BCR	C38-C26-C25	-3.86	120.28	124.48
30	A	411	BCR	C15-C14-C13	-3.86	121.87	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	r	613	CLA	O2D-CGD-O1D	-3.86	116.34	123.85
30	D	404	BCR	C38-C26-C25	-3.85	120.28	124.48
27	8	622	XAT	O4-C5-C18	3.85	119.35	115.05
28	N	1623	NEX	C11-C10-C9	-3.85	121.88	127.28
28	Y	1623	NEX	C2-C1-C6	3.85	112.95	109.21
24	6	609	CHL	O1D-CGD-CBD	-3.85	118.89	124.72
26	Y	1620	LUT	C35-C34-C33	-3.85	121.88	127.28
30	a	411	BCR	C15-C14-C13	-3.85	121.88	127.28
26	g	1620	LUT	C30-C31-C32	-3.84	112.06	123.20
26	G	1620	LUT	C30-C31-C32	-3.84	112.07	123.20
26	y	1620	LUT	C35-C34-C33	-3.84	121.89	127.28
28	y	1623	NEX	C2-C1-C6	3.84	112.94	109.21
25	g	603	CLA	C4A-NA-C1A	3.84	108.43	106.68
30	A	411	BCR	C20-C21-C22	-3.83	121.90	127.28
25	R	613	CLA	O2D-CGD-O1D	-3.82	116.41	123.85
25	B	603	CLA	C4A-NA-C1A	3.82	108.42	106.68
24	1	607	CHL	OMC-CMC-C2C	-3.82	118.49	125.12
30	a	411	BCR	C20-C21-C22	-3.81	121.93	127.28
28	n	1623	NEX	C11-C10-C9	-3.81	121.93	127.28
25	2	612	CLA	C4A-NA-C1A	3.81	108.42	106.68
24	4	601	CHL	C4D-ND-C1D	-3.81	102.33	105.22
24	2	609	CHL	O1D-CGD-CBD	-3.81	118.95	124.72
24	5	607	CHL	OMC-CMC-C2C	-3.80	118.52	125.12
24	8	601	CHL	C4D-ND-C1D	-3.79	102.34	105.22
30	C	516	BCR	C16-C15-C14	-3.79	115.76	123.52
30	c	516	BCR	C16-C15-C14	-3.79	115.77	123.52
24	6	605	CHL	C1B-CHB-C4A	3.79	123.76	121.32
24	Y	605	CHL	CBC-CAC-C3C	-3.78	107.46	112.87
24	y	605	CHL	CBC-CAC-C3C	-3.78	107.46	112.87
25	6	612	CLA	C4A-NA-C1A	3.77	108.40	106.68
27	7	1622	XAT	C35-C34-C33	-3.77	122.00	127.28
25	6	604	CLA	C4A-NA-C1A	3.77	108.40	106.68
26	7	1620	LUT	C35-C34-C33	-3.76	122.00	127.28
30	B	620	BCR	C24-C23-C22	-3.76	120.67	126.23
30	b	620	BCR	C24-C23-C22	-3.76	120.67	126.23
26	3	1620	LUT	C35-C34-C33	-3.76	122.00	127.28
28	s	1623	NEX	C11-C10-C9	-3.76	122.00	127.28
34	A	412	SQD	O5-C5-C4	3.76	116.47	109.70
25	C	508	CLA	CMB-C2B-C1B	-3.76	119.70	125.42
26	3	1620	LUT	C21-C26-C27	-3.76	108.50	112.83
25	b	603	CLA	C4A-NA-C1A	3.76	108.39	106.68
25	c	508	CLA	CMB-C2B-C1B	-3.76	119.70	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	605	CHL	C1B-CHB-C4A	3.75	123.73	121.32
27	G	1622	XAT	C10-C11-C12	-3.74	112.35	123.20
26	1	1620	LUT	C35-C15-C14	-3.74	115.86	123.52
27	g	1622	XAT	C10-C11-C12	-3.74	112.36	123.20
26	s	1621	LUT	C10-C11-C12	-3.74	112.36	123.20
30	b	620	BCR	C11-C10-C9	-3.74	122.03	127.28
26	S	1621	LUT	C10-C11-C12	-3.74	112.37	123.20
34	a	412	SQD	O5-C5-C4	3.74	116.43	109.70
24	3	606	CHL	C1C-CHC-C4B	3.74	129.44	116.07
26	5	1620	LUT	C35-C15-C14	-3.74	115.87	123.52
26	7	1620	LUT	C21-C26-C27	-3.74	108.53	112.83
24	7	606	CHL	C1C-CHC-C4B	3.73	129.43	116.07
37	H	102	DGD	C3D-C4D-C5D	-3.73	103.46	110.23
27	3	1622	XAT	C35-C34-C33	-3.73	122.04	127.28
24	R	606	CHL	CBC-CAC-C3C	-3.73	107.54	112.87
37	h	102	DGD	C3D-C4D-C5D	-3.73	103.47	110.23
34	B	621	SQD	O9-S-O7	-3.73	101.71	113.82
28	S	1623	NEX	C11-C10-C9	-3.72	122.05	127.28
27	2	1622	XAT	C11-C10-C9	-3.72	122.06	127.28
28	s	1623	NEX	C35-C34-C33	-3.72	122.06	127.28
34	b	621	SQD	O9-S-O7	-3.72	101.74	113.82
25	6	602	CLA	C4A-NA-C1A	3.71	108.37	106.68
25	2	614	CLA	O2D-CGD-O1D	-3.71	116.63	123.85
27	8	622	XAT	C24-C23-C22	-3.71	103.86	110.79
26	1	1620	LUT	C15-C14-C13	-3.71	122.08	127.28
30	B	620	BCR	C11-C10-C9	-3.71	122.08	127.28
26	5	1620	LUT	C15-C14-C13	-3.71	122.08	127.28
30	C	514	BCR	C10-C11-C12	-3.70	112.47	123.20
27	6	1622	XAT	C11-C10-C9	-3.70	122.09	127.28
25	6	614	CLA	O2D-CGD-O1D	-3.70	116.64	123.85
27	1	1622	XAT	C6-C7-C8	-3.70	118.17	125.99
27	5	1622	XAT	C6-C7-C8	-3.70	118.18	125.99
30	c	514	BCR	C10-C11-C12	-3.70	112.49	123.20
26	n	1620	LUT	C21-C26-C27	-3.69	108.58	112.83
28	R	623	NEX	C15-C35-C34	-3.69	115.96	123.52
30	t	101	BCR	C1-C6-C7	3.69	125.66	115.65
27	1	1622	XAT	C4-C3-C2	-3.69	103.89	110.79
25	2	602	CLA	C4A-NA-C1A	3.69	108.36	106.68
24	r	606	CHL	CBC-CAC-C3C	-3.69	107.59	112.87
26	7	1620	LUT	C16-C1-C6	-3.69	104.46	110.24
27	5	1622	XAT	C4-C3-C2	-3.69	103.89	110.79
30	T	101	BCR	C1-C6-C7	3.69	125.65	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	612	CLA	CMB-C2B-C1B	-3.69	119.81	125.42
27	4	622	XAT	C24-C23-C22	-3.68	103.90	110.79
33	a	409	PHO	C2B-C1B-NB	-3.68	106.77	109.43
25	b	612	CLA	CMB-C2B-C1B	-3.68	119.81	125.42
26	N	1620	LUT	C21-C26-C27	-3.68	108.59	112.83
26	3	1620	LUT	C16-C1-C6	-3.68	104.48	110.24
34	b	621	SQD	O47-C7-C8	3.67	119.43	111.48
28	S	1623	NEX	C35-C34-C33	-3.67	122.12	127.28
37	c	518	DGD	O6D-C1D-O3G	-3.67	101.37	110.04
28	r	623	NEX	C15-C35-C34	-3.67	116.01	123.52
33	A	409	PHO	C2B-C1B-NB	-3.67	106.78	109.43
34	B	621	SQD	O47-C7-C8	3.67	119.42	111.48
26	N	1621	LUT	C10-C11-C12	-3.67	112.57	123.20
26	G	1621	LUT	C10-C11-C12	-3.67	112.58	123.20
27	7	1622	XAT	O4-C5-C18	3.67	119.14	115.05
30	A	411	BCR	C16-C17-C18	-3.66	122.14	127.28
24	4	609	CHL	OMC-CMC-C2C	-3.66	118.76	125.12
37	C	518	DGD	O6D-C1D-O3G	-3.66	101.39	110.04
30	B	618	BCR	C7-C8-C9	-3.66	120.82	126.23
34	a	412	SQD	C1-O5-C5	3.66	120.86	113.72
25	g	603	CLA	CBC-CAC-C3C	-3.66	102.51	112.42
24	8	609	CHL	OMC-CMC-C2C	-3.65	118.77	125.12
26	g	1621	LUT	C10-C11-C12	-3.65	112.61	123.20
30	a	411	BCR	C16-C17-C18	-3.65	122.15	127.28
27	3	1622	XAT	O4-C5-C18	3.65	119.13	115.05
26	n	1621	LUT	C10-C11-C12	-3.65	112.62	123.20
25	G	603	CLA	CBC-CAC-C3C	-3.65	102.52	112.42
25	g	610	CLA	C4A-NA-C1A	3.65	108.34	106.68
27	r	622	XAT	C15-C14-C13	-3.65	122.16	127.28
34	A	412	SQD	C1-O5-C5	3.63	120.82	113.72
30	b	619	BCR	C20-C21-C22	-3.63	122.19	127.28
27	5	1622	XAT	O4-C5-C18	3.63	119.10	115.05
26	8	620	LUT	C31-C30-C29	-3.63	122.19	127.28
25	r	611	CLA	C4A-NA-C1A	3.63	108.33	106.68
27	R	622	XAT	C15-C14-C13	-3.62	122.20	127.28
30	B	619	BCR	C20-C21-C22	-3.62	122.20	127.28
26	4	620	LUT	C31-C30-C29	-3.62	122.20	127.28
30	b	618	BCR	C7-C8-C9	-3.62	120.88	126.23
26	3	1621	LUT	C26-C27-C28	-3.61	118.96	124.58
24	y	609	CHL	O1D-CGD-CBD	-3.61	119.25	124.72
26	7	1621	LUT	C26-C27-C28	-3.61	118.96	124.58
24	Y	609	CHL	O1D-CGD-CBD	-3.61	119.25	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y	1620	LUT	C35-C15-C14	-3.61	116.14	123.52
24	3	609	CHL	O1D-CGD-CBD	-3.61	119.26	124.72
27	1	1622	XAT	O4-C5-C18	3.60	119.07	115.05
25	C	513	CLA	O2D-CGD-O1D	-3.60	116.84	123.85
37	H	102	DGD	C1D-C2D-C3D	-3.60	102.44	110.01
25	8	602	CLA	O2D-CGD-CBD	3.60	117.52	111.23
28	1	1623	NEX	C15-C35-C34	-3.60	116.16	123.52
28	5	1623	NEX	C15-C35-C34	-3.60	116.16	123.52
37	h	102	DGD	C1D-C2D-C3D	-3.60	102.44	110.01
25	4	602	CLA	O2D-CGD-CBD	3.60	117.52	111.23
27	Y	1622	XAT	C26-C27-C28	-3.60	118.39	125.99
30	b	620	BCR	C15-C14-C13	-3.60	122.23	127.28
26	5	1621	LUT	C19-C9-C8	3.60	123.58	118.09
26	y	1620	LUT	C35-C15-C14	-3.60	116.16	123.52
24	G	608	CHL	CBC-CAC-C3C	-3.59	107.73	112.87
25	c	513	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
30	B	619	BCR	C39-C30-C25	-3.59	104.61	110.24
26	1	1621	LUT	C19-C9-C8	3.59	123.57	118.09
30	d	404	BCR	C21-C20-C19	-3.58	112.81	123.20
30	b	619	BCR	C39-C30-C25	-3.58	104.62	110.24
24	g	608	CHL	CBC-CAC-C3C	-3.58	107.75	112.87
24	Y	608	CHL	CBC-CAC-C3C	-3.58	107.75	112.87
27	6	1622	XAT	O4-C5-C18	3.58	119.05	115.05
27	2	1622	XAT	O4-C5-C18	3.58	119.05	115.05
26	5	1620	LUT	C30-C31-C32	-3.57	112.84	123.20
26	1	1620	LUT	C30-C31-C32	-3.57	112.85	123.20
27	y	1622	XAT	C26-C27-C28	-3.57	118.44	125.99
24	7	609	CHL	O1D-CGD-CBD	-3.57	119.31	124.72
30	D	404	BCR	C21-C20-C19	-3.57	112.86	123.20
26	y	1621	LUT	C21-C26-C27	-3.57	108.72	112.83
27	N	1622	XAT	C10-C11-C12	-3.57	112.87	123.20
26	r	620	LUT	C30-C31-C32	-3.56	112.87	123.20
26	R	620	LUT	C30-C31-C32	-3.56	112.88	123.20
26	Y	1620	LUT	C15-C14-C13	-3.56	122.28	127.28
24	1	608	CHL	C1C-CHC-C4B	3.56	128.82	116.07
26	G	1620	LUT	C35-C15-C14	-3.56	116.23	123.52
24	y	608	CHL	CBC-CAC-C3C	-3.56	107.78	112.87
25	G	610	CLA	C4A-NA-C1A	3.56	108.30	106.68
30	B	620	BCR	C15-C14-C13	-3.56	122.29	127.28
27	n	1622	XAT	C10-C11-C12	-3.56	112.89	123.20
24	5	608	CHL	C1C-CHC-C4B	3.56	128.79	116.07
26	y	1621	LUT	C10-C11-C12	-3.55	112.90	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y	1621	LUT	C21-C26-C27	-3.55	108.74	112.83
26	y	1620	LUT	C15-C14-C13	-3.55	122.30	127.28
26	Y	1621	LUT	C10-C11-C12	-3.55	112.91	123.20
28	s	1623	NEX	C31-C30-C29	-3.54	122.31	127.28
30	T	101	BCR	C33-C5-C6	-3.54	120.62	124.48
26	g	1620	LUT	C35-C15-C14	-3.54	116.28	123.52
27	y	1622	XAT	O4-C5-C4	3.54	116.81	113.49
25	R	611	CLA	C4A-NA-C1A	3.54	108.29	106.68
28	S	1623	NEX	C31-C30-C29	-3.54	122.32	127.28
25	r	612	CLA	CAA-C2A-C3A	-3.53	103.46	113.00
26	G	1620	LUT	C15-C14-C13	-3.53	122.33	127.28
30	t	101	BCR	C33-C5-C6	-3.53	120.63	124.48
24	N	608	CHL	C1C-CHC-C4B	3.53	128.70	116.07
25	c	507	CLA	CAA-C2A-C3A	-3.53	103.47	113.00
25	7	612	CLA	O2D-CGD-O1D	-3.53	116.98	123.85
25	C	507	CLA	CAA-C2A-C3A	-3.52	103.49	113.00
25	R	612	CLA	CAA-C2A-C3A	-3.52	103.49	113.00
25	3	612	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
26	g	1620	LUT	C21-C26-C27	-3.52	108.78	112.83
24	3	601	CHL	O1D-CGD-CBD	-3.52	119.39	124.72
24	n	608	CHL	C1C-CHC-C4B	3.52	128.65	116.07
24	7	601	CHL	O1D-CGD-CBD	-3.52	119.39	124.72
24	2	605	CHL	O1D-CGD-CBD	-3.51	119.39	124.72
26	g	1620	LUT	C15-C14-C13	-3.51	122.35	127.28
37	b	626	DGD	C3G-C2G-C1G	-3.51	103.61	111.78
24	Y	608	CHL	C1C-CHC-C4B	3.51	128.62	116.07
24	y	608	CHL	C1C-CHC-C4B	3.51	128.61	116.07
27	7	1622	XAT	C35-C15-C14	-3.50	116.35	123.52
26	G	1620	LUT	C21-C26-C27	-3.50	108.80	112.83
24	6	605	CHL	O1D-CGD-CBD	-3.50	119.42	124.72
25	n	610	CLA	C4A-NA-C1A	3.50	108.27	106.68
24	y	606	CHL	OMC-CMC-C2C	-3.49	119.05	125.12
26	N	1620	LUT	C35-C15-C14	-3.49	116.37	123.52
27	3	1622	XAT	C35-C15-C14	-3.49	116.38	123.52
27	Y	1622	XAT	O4-C5-C4	3.49	116.76	113.49
28	2	1623	NEX	C11-C10-C9	-3.49	122.39	127.28
37	B	626	DGD	C3G-C2G-C1G	-3.49	103.65	111.78
24	Y	606	CHL	OMC-CMC-C2C	-3.49	119.06	125.12
33	a	408	PHO	O1D-CGD-CBD	3.48	130.00	124.72
26	n	1620	LUT	C35-C15-C14	-3.48	116.39	123.52
25	N	604	CLA	C4A-NA-C1A	3.48	108.27	106.68
25	b	611	CLA	C3B-C4B-NB	-3.47	107.43	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	A	412	SQD	O47-C7-C8	3.47	118.98	111.48
28	6	1623	NEX	C11-C10-C9	-3.47	122.42	127.28
34	a	412	SQD	O47-C7-C8	3.47	118.98	111.48
26	S	1620	LUT	C15-C14-C13	-3.47	122.42	127.28
33	A	408	PHO	O1D-CGD-CBD	3.47	129.98	124.72
27	1	1622	XAT	O24-C25-C38	3.46	118.92	115.05
26	n	1621	LUT	C7-C8-C9	-3.46	121.11	126.23
26	N	1621	LUT	C7-C8-C9	-3.46	121.11	126.23
24	S	601	CHL	C3D-C4D-ND	3.46	118.49	112.94
24	G	608	CHL	C1C-CHC-C4B	3.46	128.45	116.07
34	A	418	SQD	C45-O47-C7	3.46	126.07	117.80
26	n	1620	LUT	C10-C11-C12	-3.46	113.18	123.20
24	g	608	CHL	C1C-CHC-C4B	3.46	128.44	116.07
24	s	601	CHL	C3D-C4D-ND	3.46	118.49	112.94
24	Y	609	CHL	C1C-CHC-C4B	3.46	128.44	116.07
24	1	609	CHL	O1D-CGD-CBD	-3.46	119.48	124.72
25	G	603	CLA	CAA-C2A-C3A	-3.46	103.66	113.00
30	B	618	BCR	C29-C28-C27	-3.46	103.68	111.28
26	g	1620	LUT	C16-C1-C6	-3.46	104.82	110.24
24	y	609	CHL	C1C-CHC-C4B	3.46	128.43	116.07
27	5	1622	XAT	O24-C25-C38	3.45	118.91	115.05
26	6	1620	LUT	C35-C34-C33	-3.45	122.43	127.28
26	N	1620	LUT	C10-C11-C12	-3.45	113.19	123.20
25	g	603	CLA	CAA-C2A-C3A	-3.45	103.67	113.00
26	1	1621	LUT	C18-C5-C6	-3.45	120.72	124.48
25	r	610	CLA	CHB-C4A-NA	3.45	129.38	124.40
26	2	1620	LUT	C35-C34-C33	-3.45	122.44	127.28
30	b	618	BCR	C29-C28-C27	-3.45	103.69	111.28
34	a	418	SQD	C45-O47-C7	3.45	126.05	117.80
25	R	610	CLA	CHB-C4A-NA	3.45	129.38	124.40
26	3	1621	LUT	C7-C8-C9	-3.45	121.13	126.23
25	N	610	CLA	C4A-NA-C1A	3.45	108.25	106.68
24	5	609	CHL	O1D-CGD-CBD	-3.45	119.50	124.72
24	3	605	CHL	C3D-C4D-ND	3.45	118.47	112.94
24	7	605	CHL	C3D-C4D-ND	3.44	118.46	112.94
26	G	1620	LUT	C16-C1-C6	-3.44	104.85	110.24
33	a	408	PHO	C3B-C4B-NB	-3.44	105.22	107.46
27	7	1622	XAT	C30-C31-C32	-3.44	113.23	123.20
26	7	1621	LUT	C7-C8-C9	-3.44	121.15	126.23
26	s	1620	LUT	C15-C14-C13	-3.44	122.45	127.28
33	A	408	PHO	C3B-C4B-NB	-3.44	105.22	107.46
24	1	609	CHL	CMB-C2B-C3B	3.43	131.55	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	611	CLA	C3B-C4B-NB	-3.43	107.47	110.53
26	1	1621	LUT	C10-C11-C12	-3.43	113.25	123.20
26	5	1621	LUT	C18-C5-C6	-3.43	120.74	124.48
26	5	1621	LUT	C10-C11-C12	-3.43	113.26	123.20
27	Y	1622	XAT	C24-C23-C22	-3.43	104.38	110.79
25	B	617	CLA	CAA-C2A-C3A	-3.43	103.74	113.00
25	C	507	CLA	O2D-CGD-O1D	-3.43	117.18	123.85
24	r	607	CHL	C1C-CHC-C4B	3.42	128.32	116.07
24	5	609	CHL	CMB-C2B-C3B	3.42	131.52	124.68
26	3	1620	LUT	C11-C10-C9	-3.42	122.48	127.28
27	g	1622	XAT	C15-C35-C34	-3.42	116.52	123.52
25	b	617	CLA	CAA-C2A-C3A	-3.42	103.75	113.00
27	3	1622	XAT	C30-C31-C32	-3.42	113.29	123.20
27	y	1622	XAT	C24-C23-C22	-3.42	104.39	110.79
24	N	601	CHL	CBC-CAC-C3C	-3.42	107.98	112.87
25	n	604	CLA	C4A-NA-C1A	3.42	108.24	106.68
25	n	603	CLA	CAA-C2A-C3A	-3.42	103.76	113.00
27	G	1622	XAT	C15-C35-C34	-3.42	116.53	123.52
25	c	507	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
24	s	601	CHL	OMC-CMC-C2C	-3.41	119.19	125.12
24	R	607	CHL	C1C-CHC-C4B	3.41	128.29	116.07
24	n	601	CHL	CBC-CAC-C3C	-3.41	107.99	112.87
25	N	603	CLA	CAA-C2A-C3A	-3.41	103.78	113.00
30	B	618	BCR	C11-C10-C9	-3.41	122.50	127.28
25	2	612	CLA	CAA-C2A-C3A	-3.41	103.79	113.00
34	b	621	SQD	C1-O5-C5	3.41	120.37	113.72
28	5	1623	NEX	C11-C10-C9	-3.40	122.51	127.28
25	B	613	CLA	CHB-C4A-NA	3.40	129.31	124.40
26	7	1620	LUT	C11-C10-C9	-3.40	122.51	127.28
25	6	612	CLA	CAA-C2A-C3A	-3.40	103.81	113.00
30	4	623	BCR	C11-C12-C13	-3.40	117.05	126.36
28	6	1623	NEX	C24-C23-C22	-3.40	104.44	110.79
34	B	621	SQD	C1-O5-C5	3.40	120.35	113.72
26	7	1620	LUT	C30-C31-C32	-3.39	113.36	123.20
30	t	101	BCR	C1-C6-C5	-3.39	118.00	122.64
24	G	601	CHL	C1C-CHC-C4B	3.39	128.21	116.07
24	g	601	CHL	C1C-CHC-C4B	3.39	128.21	116.07
25	b	613	CLA	CHB-C4A-NA	3.39	129.29	124.40
28	1	1623	NEX	C11-C10-C9	-3.39	122.53	127.28
30	T	101	BCR	C1-C6-C5	-3.39	118.00	122.64
30	8	623	BCR	C11-C12-C13	-3.39	117.07	126.36
25	Y	611	CLA	C4A-NA-C1A	3.39	108.22	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	606	CHL	O1D-CGD-CBD	-3.38	119.59	124.72
24	R	614	CHL	CBC-CAC-C3C	-3.38	108.03	112.87
25	y	604	CLA	C4A-NA-C1A	3.38	108.22	106.68
28	2	1623	NEX	C24-C23-C22	-3.38	104.47	110.79
26	3	1620	LUT	C30-C31-C32	-3.38	113.41	123.20
24	S	601	CHL	OMC-CMC-C2C	-3.38	119.25	125.12
30	b	618	BCR	C11-C10-C9	-3.38	122.54	127.28
37	h	102	DGD	O2D-C2D-C3D	-3.38	102.41	110.38
24	7	606	CHL	C3D-C4D-ND	3.38	118.36	112.94
37	H	102	DGD	O2D-C2D-C3D	-3.38	102.42	110.38
24	r	607	CHL	O1D-CGD-CBD	-3.38	119.60	124.72
25	y	611	CLA	C4A-NA-C1A	3.38	108.22	106.68
24	7	606	CHL	O1D-CGD-CBD	-3.37	119.61	124.72
24	n	607	CHL	CAA-C2A-C3A	-3.37	103.88	113.00
24	3	601	CHL	C3D-C4D-ND	3.37	118.35	112.94
24	N	607	CHL	CAA-C2A-C3A	-3.37	103.88	113.00
34	B	621	SQD	O5-C5-C4	3.37	115.78	109.70
27	4	622	XAT	C10-C11-C12	-3.37	113.43	123.20
25	3	603	CLA	CHB-C4A-NA	3.37	129.26	124.40
28	1	1623	NEX	C24-C23-C22	-3.37	104.49	110.79
25	7	603	CLA	CHB-C4A-NA	3.37	129.26	124.40
28	5	1623	NEX	C24-C23-C22	-3.37	104.49	110.79
25	A	405	CLA	CMB-C2B-C1B	-3.37	120.29	125.42
34	b	621	SQD	O5-C5-C4	3.37	115.77	109.70
37	c	519	DGD	O6D-C1D-O3G	-3.37	102.09	110.04
24	3	606	CHL	C3D-C4D-ND	3.36	118.34	112.94
27	8	622	XAT	C10-C11-C12	-3.36	113.45	123.20
30	t	101	BCR	C15-C14-C13	-3.36	122.56	127.28
24	N	609	CHL	CMA-C3A-C4A	-3.36	107.37	114.61
30	T	101	BCR	C15-C14-C13	-3.36	122.56	127.28
37	C	519	DGD	O6D-C1D-O3G	-3.36	102.10	110.04
26	N	1620	LUT	C15-C14-C13	-3.36	122.57	127.28
24	n	609	CHL	CMA-C3A-C4A	-3.36	107.38	114.61
26	3	1621	LUT	C35-C34-C33	-3.35	122.57	127.28
26	Y	1620	LUT	C30-C31-C32	-3.35	113.48	123.20
25	a	405	CLA	CMB-C2B-C1B	-3.35	120.32	125.42
24	r	614	CHL	CBC-CAC-C3C	-3.35	108.08	112.87
25	b	604	CLA	C4A-NA-C1A	3.35	108.21	106.68
30	c	515	BCR	C16-C17-C18	-3.35	122.58	127.28
25	4	612	CLA	CAA-C2A-C3A	-3.35	103.95	113.00
24	4	609	CHL	O1D-CGD-CBD	-3.35	119.65	124.72
24	R	607	CHL	O1D-CGD-CBD	-3.35	119.65	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	y	1620	LUT	C30-C31-C32	-3.34	113.51	123.20
26	n	1620	LUT	C15-C14-C13	-3.34	122.59	127.28
24	1	606	CHL	O1D-CGD-CBD	-3.34	119.65	124.72
24	7	601	CHL	C3D-C4D-ND	3.34	118.30	112.94
25	3	610	CLA	C3B-C4B-NB	-3.34	107.55	110.53
30	C	515	BCR	C16-C17-C18	-3.34	122.59	127.28
24	R	614	CHL	C3D-C4D-ND	3.34	118.30	112.94
24	N	601	CHL	C1C-CHC-C4B	3.34	128.02	116.07
26	n	1620	LUT	C30-C31-C32	-3.34	113.53	123.20
24	7	601	CHL	CMA-C3A-C4A	-3.34	107.42	114.61
24	n	601	CHL	C1C-CHC-C4B	3.34	128.02	116.07
25	8	612	CLA	CAA-C2A-C3A	-3.34	103.98	113.00
24	N	601	CHL	O1D-CGD-CBD	-3.34	119.66	124.72
24	8	608	CHL	C1C-CHC-C4B	3.34	128.01	116.07
24	8	609	CHL	O1D-CGD-CBD	-3.34	119.66	124.72
24	n	601	CHL	O1D-CGD-CBD	-3.34	119.66	124.72
26	N	1620	LUT	C30-C31-C32	-3.34	113.54	123.20
30	c	515	BCR	C15-C16-C17	-3.33	116.70	123.52
24	4	608	CHL	C1C-CHC-C4B	3.33	127.99	116.07
25	R	601	CLA	C4A-NA-C1A	3.33	108.20	106.68
25	Y	604	CLA	C4A-NA-C1A	3.33	108.20	106.68
26	3	1620	LUT	C35-C15-C14	-3.33	116.71	123.52
30	b	618	BCR	C15-C16-C17	-3.33	116.71	123.52
30	B	618	BCR	C28-C27-C26	-3.33	108.12	114.06
26	7	1620	LUT	C35-C15-C14	-3.33	116.71	123.52
24	5	606	CHL	O1D-CGD-CBD	-3.33	119.68	124.72
24	4	601	CHL	CHA-C1A-C2A	-3.33	125.50	133.31
24	G	609	CHL	C1C-CHC-C4B	3.33	127.97	116.07
30	b	618	BCR	C28-C27-C26	-3.32	108.13	114.06
24	3	601	CHL	CMA-C3A-C4A	-3.32	107.45	114.61
27	g	1622	XAT	C24-C23-C22	-3.32	104.58	110.79
25	2	613	CLA	C4A-NA-C1A	3.32	108.19	106.68
26	7	1621	LUT	C35-C34-C33	-3.32	122.62	127.28
28	N	1623	NEX	C24-C23-C22	-3.32	104.59	110.79
30	C	515	BCR	C15-C16-C17	-3.32	116.73	123.52
24	s	608	CHL	C1C-CHC-C4B	3.32	127.94	116.07
24	g	609	CHL	C1C-CHC-C4B	3.32	127.94	116.07
24	r	614	CHL	C3D-C4D-ND	3.32	118.26	112.94
30	b	619	BCR	C24-C23-C22	-3.31	121.33	126.23
30	B	618	BCR	C15-C16-C17	-3.31	116.74	123.52
24	S	608	CHL	C1C-CHC-C4B	3.31	127.92	116.07
25	7	610	CLA	C3B-C4B-NB	-3.31	107.57	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	8	620	LUT	C11-C10-C9	-3.31	122.64	127.28
24	8	601	CHL	CHA-C1A-C2A	-3.31	125.53	133.31
30	C	514	BCR	C21-C20-C19	-3.31	113.61	123.20
28	n	1623	NEX	C24-C23-C22	-3.31	104.60	110.79
30	c	514	BCR	C21-C20-C19	-3.31	113.61	123.20
25	B	604	CLA	C4A-NA-C1A	3.31	108.19	106.68
25	6	613	CLA	C4A-NA-C1A	3.31	108.19	106.68
24	N	601	CHL	C3D-C4D-ND	3.30	118.24	112.94
24	Y	601	CHL	CBC-CAC-C3C	-3.30	108.15	112.87
25	3	603	CLA	CBC-CAC-C3C	-3.30	103.48	112.42
34	A	418	SQD	O6-C1-C2	3.30	113.28	108.27
25	Y	611	CLA	C3B-C4B-NB	-3.30	107.59	110.53
25	7	603	CLA	CBC-CAC-C3C	-3.30	103.49	112.42
36	a	414	PL9	O2-C1-C2	-3.30	116.74	121.43
26	4	620	LUT	C11-C10-C9	-3.29	122.66	127.28
24	n	601	CHL	C3D-C4D-ND	3.29	118.22	112.94
27	G	1622	XAT	C24-C23-C22	-3.29	104.63	110.79
24	Y	601	CHL	C1C-CHC-C4B	3.29	127.86	116.07
26	N	1620	LUT	C16-C1-C6	-3.29	105.08	110.24
25	R	602	CLA	CMB-C2B-C1B	-3.29	120.40	125.42
24	y	601	CHL	CBC-CAC-C3C	-3.29	108.16	112.87
26	n	1620	LUT	C16-C1-C6	-3.29	105.08	110.24
25	y	611	CLA	C3B-C4B-NB	-3.29	107.59	110.53
25	7	614	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
24	Y	601	CHL	C3D-C4D-ND	3.29	118.21	112.94
26	3	1620	LUT	C15-C14-C13	-3.29	122.67	127.28
24	y	601	CHL	C1C-CHC-C4B	3.29	127.83	116.07
26	7	1620	LUT	C15-C14-C13	-3.28	122.67	127.28
30	B	619	BCR	C24-C23-C22	-3.28	121.38	126.23
25	b	606	CLA	CHB-C4A-NA	3.28	129.13	124.40
24	N	609	CHL	C1C-CHC-C4B	3.28	127.81	116.07
24	n	609	CHL	C1C-CHC-C4B	3.28	127.81	116.07
24	N	606	CHL	OMC-CMC-C2C	-3.28	119.42	125.12
26	1	1621	LUT	C15-C35-C34	-3.28	116.81	123.52
24	n	606	CHL	OMC-CMC-C2C	-3.28	119.43	125.12
25	r	602	CLA	CMB-C2B-C1B	-3.28	120.43	125.42
30	B	619	BCR	C15-C16-C17	-3.28	116.82	123.52
30	b	619	BCR	C15-C16-C17	-3.28	116.82	123.52
24	6	601	CHL	C1C-CHC-C4B	3.27	127.79	116.07
24	y	601	CHL	C3D-C4D-ND	3.27	118.19	112.94
28	Y	1623	NEX	C24-C23-C22	-3.27	104.67	110.79
34	a	418	SQD	O6-C1-C2	3.27	113.24	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	607	CHL	C3D-C4D-ND	3.27	118.19	112.94
24	1	609	CHL	CMA-C3A-C4A	-3.27	107.56	114.61
26	5	1621	LUT	C15-C35-C34	-3.27	116.83	123.52
25	s	610	CLA	C4A-NA-C1A	3.27	108.17	106.68
24	g	606	CHL	CMB-C2B-C3B	3.27	131.22	124.68
26	y	1621	LUT	C7-C8-C9	-3.27	121.40	126.23
28	y	1623	NEX	C24-C23-C22	-3.27	104.68	110.79
24	5	607	CHL	C3D-C4D-ND	3.27	118.18	112.94
25	3	614	CLA	O2D-CGD-O1D	-3.26	117.49	123.85
24	2	601	CHL	C1C-CHC-C4B	3.26	127.75	116.07
25	S	610	CLA	C4A-NA-C1A	3.26	108.17	106.68
27	N	1622	XAT	C24-C23-C22	-3.26	104.69	110.79
30	A	411	BCR	C33-C5-C6	-3.26	120.92	124.48
35	d	411	LMG	C1-C2-C3	-3.26	103.15	110.01
35	D	411	LMG	C1-C2-C3	-3.26	103.15	110.01
24	5	609	CHL	CMA-C3A-C4A	-3.26	107.59	114.61
30	b	619	BCR	C8-C7-C6	-3.26	118.29	127.00
36	A	414	PL9	O2-C1-C2	-3.26	116.79	121.43
27	n	1622	XAT	C24-C23-C22	-3.26	104.70	110.79
24	G	606	CHL	C3D-C4D-ND	3.26	118.16	112.94
30	B	619	BCR	C8-C7-C6	-3.26	118.30	127.00
25	6	611	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
25	2	611	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
25	B	606	CLA	CHB-C4A-NA	3.26	129.10	124.40
24	G	601	CHL	C1-C2-C3	-3.25	120.86	126.20
24	G	606	CHL	CMB-C2B-C3B	3.25	131.19	124.68
26	Y	1621	LUT	C7-C8-C9	-3.25	121.43	126.23
24	R	607	CHL	O2A-CGA-CBA	3.25	121.74	111.83
30	c	517	BCR	C15-C16-C17	-3.25	116.87	123.52
30	C	517	BCR	C15-C16-C17	-3.25	116.88	123.52
30	a	411	BCR	C33-C5-C6	-3.25	120.94	124.48
24	3	608	CHL	C1C-CHC-C4B	3.25	127.68	116.07
24	r	607	CHL	O2A-CGA-CBA	3.24	121.73	111.83
24	7	608	CHL	C1C-CHC-C4B	3.24	127.67	116.07
24	g	605	CHL	C3D-C4D-ND	3.24	118.14	112.94
28	G	1623	NEX	O24-C25-C38	3.24	118.67	115.05
26	r	620	LUT	C39-C29-C28	3.24	123.04	118.09
25	C	501	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
25	B	605	CLA	C1-C2-C3	-3.24	120.89	126.20
25	c	501	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
26	1	1620	LUT	C31-C30-C29	-3.24	122.74	127.28
26	s	1621	LUT	C17-C1-C6	3.23	115.32	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	R	620	LUT	C39-C29-C28	3.23	123.03	118.09
25	b	605	CLA	C1-C2-C3	-3.23	120.90	126.20
24	5	601	CHL	O1D-CGD-CBD	-3.23	119.82	124.72
24	g	601	CHL	C1-C2-C3	-3.23	120.90	126.20
25	y	604	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
26	5	1620	LUT	C31-C30-C29	-3.23	122.75	127.28
26	6	1621	LUT	C10-C11-C12	-3.23	113.84	123.20
29	D	408	LHG	O8-C23-C24	3.23	121.68	111.83
24	g	606	CHL	C3D-C4D-ND	3.23	118.12	112.94
27	Y	1622	XAT	C35-C34-C33	-3.23	122.75	127.28
25	Y	604	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
25	s	602	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
26	2	1621	LUT	C10-C11-C12	-3.22	113.87	123.20
24	R	608	CHL	C1C-CHC-C4B	3.22	127.59	116.07
24	R	606	CHL	C3D-C4D-ND	3.22	118.10	112.94
25	S	602	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
26	r	620	LUT	C21-C26-C27	-3.22	109.13	112.83
24	7	607	CHL	C3D-C4D-ND	3.22	118.10	112.94
24	r	606	CHL	C3D-C4D-ND	3.22	118.10	112.94
26	S	1621	LUT	C17-C1-C6	3.22	115.28	110.24
25	C	513	CLA	CMB-C2B-C1B	-3.21	120.53	125.42
24	1	601	CHL	O1D-CGD-CBD	-3.21	119.85	124.72
30	c	515	BCR	C37-C22-C23	3.21	123.00	118.09
26	G	1621	LUT	C39-C29-C28	3.21	123.00	118.09
24	r	608	CHL	C1C-CHC-C4B	3.21	127.56	116.07
29	d	408	LHG	O8-C23-C24	3.21	121.63	111.83
27	y	1622	XAT	C35-C34-C33	-3.21	122.78	127.28
25	B	605	CLA	C6-C5-C3	-3.21	105.65	113.47
28	g	1623	NEX	O24-C25-C38	3.21	118.64	115.05
25	b	605	CLA	C6-C5-C3	-3.21	105.65	113.47
30	C	514	BCR	C15-C16-C17	-3.21	116.95	123.52
30	c	514	BCR	C15-C16-C17	-3.21	116.96	123.52
26	2	1621	LUT	C30-C31-C32	-3.21	113.91	123.20
25	Y	610	CLA	C4A-NA-C1A	3.20	108.14	106.68
24	6	609	CHL	C3D-C4D-ND	3.20	118.08	112.94
25	y	612	CLA	CAA-C2A-C3A	-3.20	104.34	113.00
28	5	1623	NEX	C15-C14-C13	-3.20	122.79	127.28
24	7	609	CHL	C1B-CHB-C4A	3.20	123.38	121.32
26	S	1620	LUT	C35-C15-C14	-3.20	116.97	123.52
30	C	515	BCR	C37-C22-C23	3.20	122.98	118.09
24	3	607	CHL	C3D-C4D-ND	3.20	118.07	112.94
24	2	609	CHL	C3D-C4D-ND	3.20	118.07	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	605	CHL	C3D-C4D-ND	3.20	118.07	112.94
26	S	1621	LUT	C30-C31-C32	-3.20	113.93	123.20
25	n	603	CLA	CBC-CAC-C3C	-3.20	103.75	112.42
26	s	1621	LUT	C30-C31-C32	-3.20	113.94	123.20
24	2	601	CHL	C3D-C4D-ND	3.20	118.07	112.94
37	b	626	DGD	O6D-C1D-O3G	-3.20	102.49	110.04
37	B	626	DGD	O6D-C1D-O3G	-3.20	102.49	110.04
26	6	1621	LUT	C30-C31-C32	-3.20	113.94	123.20
25	C	508	CLA	O2D-CGD-O1D	-3.20	117.63	123.85
25	Y	612	CLA	CAA-C2A-C3A	-3.20	104.36	113.00
24	S	606	CHL	C3D-C4D-ND	3.19	118.06	112.94
26	g	1621	LUT	C39-C29-C28	3.19	122.97	118.09
25	c	513	CLA	CMB-C2B-C1B	-3.19	120.56	125.42
24	6	601	CHL	C3D-C4D-ND	3.19	118.05	112.94
24	8	608	CHL	C3D-C4D-ND	3.19	118.05	112.94
24	1	608	CHL	O1D-CGD-CBD	-3.19	119.89	124.72
28	1	1623	NEX	C15-C14-C13	-3.19	122.81	127.28
25	N	603	CLA	CBC-CAC-C3C	-3.19	103.78	112.42
30	b	618	BCR	C20-C21-C22	-3.19	122.81	127.28
24	s	606	CHL	C3D-C4D-ND	3.19	118.05	112.94
25	g	602	CLA	CMB-C2B-C1B	-3.19	120.57	125.42
30	b	620	BCR	C4-C5-C6	-3.19	118.40	122.70
24	3	609	CHL	C1B-CHB-C4A	3.19	123.37	121.32
26	s	1620	LUT	C35-C15-C14	-3.18	117.00	123.52
25	G	604	CLA	CMB-C2B-C1B	-3.18	120.57	125.42
34	B	623	SQD	O9-S-C6	3.18	111.50	106.76
28	r	623	NEX	C24-C23-C22	-3.18	104.84	110.79
34	b	623	SQD	O9-S-C6	3.18	111.50	106.76
25	y	610	CLA	C4A-NA-C1A	3.18	108.13	106.68
24	N	605	CHL	C1C-CHC-C4B	3.18	127.44	116.07
26	R	620	LUT	C21-C26-C27	-3.18	109.17	112.83
24	G	601	CHL	C3D-C4D-ND	3.18	118.03	112.94
25	r	601	CLA	C4A-NA-C1A	3.18	108.13	106.68
25	R	610	CLA	O2D-CGD-O1D	-3.18	117.67	123.85
28	R	623	NEX	C24-C23-C22	-3.18	104.85	110.79
24	n	605	CHL	C1C-CHC-C4B	3.17	127.43	116.07
25	G	602	CLA	CMB-C2B-C1B	-3.17	120.59	125.42
26	4	620	LUT	C30-C31-C32	-3.17	114.02	123.20
24	R	607	CHL	C3D-C4D-ND	3.17	118.02	112.94
25	c	508	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
30	B	620	BCR	C1-C6-C5	-3.17	118.31	122.64
26	Y	1621	LUT	C30-C31-C32	-3.16	114.03	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	8	620	LUT	C30-C31-C32	-3.16	114.03	123.20
30	B	618	BCR	C20-C21-C22	-3.16	122.84	127.28
24	n	608	CHL	O1D-CGD-CBD	-3.16	119.93	124.72
25	g	604	CLA	CMB-C2B-C1B	-3.16	120.61	125.42
24	1	609	CHL	C3D-C4D-ND	3.16	118.01	112.94
25	1	612	CLA	CAA-C2A-C3A	-3.16	104.46	113.00
30	B	620	BCR	C4-C5-C6	-3.16	118.43	122.70
30	b	620	BCR	C1-C6-C5	-3.16	118.32	122.64
28	N	1623	NEX	C26-C27-C28	-3.16	119.31	125.99
24	r	607	CHL	C3D-C4D-ND	3.16	118.01	112.94
25	B	613	CLA	CMD-C2D-C1D	-3.16	119.16	124.73
25	5	612	CLA	CAA-C2A-C3A	-3.16	104.46	113.00
25	c	505	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
25	r	610	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
24	4	608	CHL	C3D-C4D-ND	3.16	118.00	112.94
25	3	612	CLA	CAA-C2A-C3A	-3.16	104.47	113.00
24	N	608	CHL	O1D-CGD-CBD	-3.16	119.94	124.72
25	7	612	CLA	CAA-C2A-C3A	-3.16	104.47	113.00
25	b	609	CLA	CMB-C2B-C3B	3.16	133.97	126.55
24	r	614	CHL	O2D-CGD-O1D	-3.16	117.70	123.85
24	s	606	CHL	OMC-CMC-C2C	-3.16	119.64	125.12
24	5	609	CHL	C3D-C4D-ND	3.16	118.00	112.94
28	n	1623	NEX	C26-C27-C28	-3.15	119.33	125.99
24	S	606	CHL	OMC-CMC-C2C	-3.15	119.64	125.12
24	5	608	CHL	O1D-CGD-CBD	-3.15	119.94	124.72
26	y	1621	LUT	C30-C31-C32	-3.15	114.07	123.20
24	2	605	CHL	C3D-C4D-ND	3.15	118.00	112.94
26	S	1620	LUT	C11-C10-C9	-3.15	122.86	127.28
26	r	620	LUT	C18-C5-C6	-3.15	121.05	124.48
24	6	605	CHL	C3D-C4D-ND	3.15	117.99	112.94
24	g	601	CHL	C3D-C4D-ND	3.15	117.99	112.94
25	C	505	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
24	R	614	CHL	O2D-CGD-O1D	-3.15	117.72	123.85
28	6	1623	NEX	C35-C34-C33	-3.15	122.87	127.28
24	G	608	CHL	C3D-C4D-ND	3.14	117.98	112.94
25	2	603	CLA	CHB-C4A-NA	3.14	128.94	124.40
28	n	1623	NEX	C16-C1-C6	3.14	113.28	110.47
24	y	605	CHL	C3D-C4D-ND	3.14	117.98	112.94
24	3	609	CHL	C1C-CHC-C4B	3.14	127.31	116.07
25	B	609	CLA	CMB-C2B-C3B	3.14	133.94	126.55
30	B	618	BCR	C3-C4-C5	-3.14	108.46	114.06
25	2	603	CLA	CAA-C2A-C3A	-3.14	104.53	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	603	CLA	CHB-C4A-NA	3.14	128.93	124.40
24	Y	606	CHL	O2A-CGA-CBA	3.14	121.39	111.83
24	8	608	CHL	O1D-CGD-CBD	-3.13	119.97	124.72
25	6	603	CLA	CAA-C2A-C3A	-3.13	104.53	113.00
24	5	605	CHL	C3D-C4D-ND	3.13	117.97	112.94
24	7	609	CHL	C1C-CHC-C4B	3.13	127.28	116.07
24	Y	605	CHL	C3D-C4D-ND	3.13	117.96	112.94
25	B	607	CLA	CAA-CBA-CGA	-3.13	104.31	113.21
30	b	618	BCR	C3-C4-C5	-3.13	108.47	114.06
25	b	613	CLA	CMD-C2D-C1D	-3.13	119.21	124.73
24	r	614	CHL	C1C-CHC-C4B	3.13	127.27	116.07
24	4	608	CHL	O1D-CGD-CBD	-3.13	119.97	124.72
24	g	608	CHL	C3D-C4D-ND	3.13	117.96	112.94
24	R	614	CHL	C1C-CHC-C4B	3.13	127.26	116.07
26	s	1620	LUT	C11-C10-C9	-3.13	122.89	127.28
30	D	404	BCR	C16-C17-C18	-3.13	122.89	127.28
28	N	1623	NEX	C16-C1-C6	3.13	113.27	110.47
24	n	601	CHL	C1-C2-C3	-3.13	121.08	126.20
26	S	1620	LUT	C10-C11-C12	-3.13	114.14	123.20
25	b	607	CLA	CAA-CBA-CGA	-3.13	104.33	113.21
25	S	609	CLA	O2D-CGD-O1D	-3.13	117.77	123.85
25	c	506	CLA	CMB-C2B-C1B	-3.12	120.66	125.42
25	b	613	CLA	CMB-C2B-C1B	-3.12	120.66	125.42
25	s	609	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
25	b	608	CLA	CMB-C2B-C1B	-3.12	120.66	125.42
27	g	1622	XAT	C18-C5-C4	3.12	117.75	114.24
26	g	1620	LUT	C10-C11-C12	-3.12	114.16	123.20
27	G	1622	XAT	C18-C5-C4	3.12	117.75	114.24
24	y	606	CHL	O2A-CGA-CBA	3.12	121.35	111.83
25	C	506	CLA	CMB-C2B-C1B	-3.12	120.67	125.42
24	1	605	CHL	C3D-C4D-ND	3.12	117.94	112.94
24	n	605	CHL	C3D-C4D-ND	3.12	117.94	112.94
24	N	601	CHL	C1-C2-C3	-3.12	121.09	126.20
24	G	607	CHL	C1C-CHC-C4B	3.12	127.23	116.07
30	d	404	BCR	C16-C17-C18	-3.12	122.90	127.28
25	C	512	CLA	CAA-C2A-C3A	-3.12	104.57	113.00
28	2	1623	NEX	C35-C34-C33	-3.12	122.91	127.28
26	s	1620	LUT	C10-C11-C12	-3.12	114.17	123.20
25	c	512	CLA	CAA-C2A-C3A	-3.11	104.58	113.00
25	B	608	CLA	CMB-C2B-C1B	-3.11	120.68	125.42
24	y	608	CHL	C1-C2-C3	-3.11	121.09	126.20
24	R	606	CHL	O1D-CGD-CBD	-3.11	120.00	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	S	614	CLA	CMB-C2B-C1B	-3.11	120.68	125.42
27	7	1622	XAT	C24-C23-C22	-3.11	104.97	110.79
27	1	1622	XAT	C35-C34-C33	-3.11	122.92	127.28
28	g	1623	NEX	C24-C23-C22	-3.11	104.97	110.79
24	8	607	CHL	C3D-C4D-ND	3.11	117.93	112.94
26	G	1620	LUT	C10-C11-C12	-3.11	114.20	123.20
24	g	607	CHL	C1C-CHC-C4B	3.11	127.19	116.07
26	g	1621	LUT	C7-C8-C9	-3.11	121.64	126.23
24	7	609	CHL	CBC-CAC-C3C	-3.11	108.43	112.87
28	3	1623	NEX	C11-C12-C13	-3.10	117.85	126.36
24	3	609	CHL	CBC-CAC-C3C	-3.10	108.43	112.87
37	H	102	DGD	O3E-C3E-C2E	-3.10	103.06	110.38
24	N	605	CHL	C3D-C4D-ND	3.10	117.92	112.94
24	N	605	CHL	O2A-CGA-CBA	3.10	121.30	111.83
28	G	1623	NEX	C24-C23-C22	-3.10	104.99	110.79
25	B	613	CLA	CMB-C2B-C1B	-3.10	120.70	125.42
26	r	620	LUT	C15-C35-C34	-3.10	117.17	123.52
24	s	606	CHL	C1C-CHC-C4B	3.10	127.16	116.07
26	R	620	LUT	C15-C35-C34	-3.10	117.18	123.52
24	Y	605	CHL	C1C-CHC-C4B	3.10	127.16	116.07
24	n	605	CHL	O2A-CGA-CBA	3.10	121.28	111.83
28	7	1623	NEX	C11-C12-C13	-3.10	117.87	126.36
26	3	1620	LUT	C10-C11-C12	-3.10	114.23	123.20
27	G	1622	XAT	C11-C10-C9	-3.10	122.94	127.28
27	7	1622	XAT	C40-C33-C32	3.10	122.82	118.09
24	r	606	CHL	O1D-CGD-CBD	-3.09	120.03	124.72
28	3	1623	NEX	C19-C9-C10	-3.09	117.80	122.82
24	y	605	CHL	C1C-CHC-C4B	3.09	127.14	116.07
37	h	102	DGD	O3E-C3E-C2E	-3.09	103.08	110.38
24	S	606	CHL	C1C-CHC-C4B	3.09	127.14	116.07
24	4	607	CHL	C3D-C4D-ND	3.09	117.90	112.94
25	s	609	CLA	C4A-NA-C1A	3.09	108.09	106.68
27	g	1622	XAT	C11-C10-C9	-3.09	122.94	127.28
24	4	606	CHL	C3D-C4D-ND	3.09	117.89	112.94
24	N	608	CHL	C1-C2-C3	-3.09	121.14	126.20
25	s	614	CLA	CMB-C2B-C1B	-3.09	120.72	125.42
24	Y	607	CHL	C1C-CHC-C4B	3.09	127.12	116.07
28	7	1623	NEX	C19-C9-C10	-3.09	117.81	122.82
26	R	620	LUT	C18-C5-C6	-3.09	121.12	124.48
24	4	609	CHL	C1C-CHC-C4B	3.09	127.11	116.07
27	3	1622	XAT	C24-C23-C22	-3.09	105.02	110.79
27	3	1622	XAT	C40-C33-C32	3.08	122.80	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	614	CLA	O2D-CGD-O1D	-3.08	117.84	123.85
26	7	1620	LUT	C10-C11-C12	-3.08	114.27	123.20
24	3	607	CHL	OMC-CMC-C2C	-3.08	119.77	125.12
24	8	609	CHL	C1C-CHC-C4B	3.08	127.10	116.07
24	Y	608	CHL	C1-C2-C3	-3.08	121.15	126.20
24	n	608	CHL	C1-C2-C3	-3.08	121.15	126.20
24	5	601	CHL	C3D-C4D-ND	3.08	117.88	112.94
24	y	607	CHL	C1C-CHC-C4B	3.08	127.08	116.07
24	1	607	CHL	C1C-CHC-C4B	3.08	127.08	116.07
26	G	1621	LUT	C7-C8-C9	-3.08	121.68	126.23
24	5	607	CHL	C1C-CHC-C4B	3.08	127.08	116.07
25	S	609	CLA	C4A-NA-C1A	3.08	108.08	106.68
27	r	622	XAT	C10-C11-C12	-3.08	114.29	123.20
27	5	1622	XAT	C35-C34-C33	-3.07	122.97	127.28
24	1	601	CHL	C3D-C4D-ND	3.07	117.87	112.94
25	C	513	CLA	CAA-C2A-C3A	-3.07	104.70	113.00
27	R	622	XAT	C10-C11-C12	-3.07	114.31	123.20
24	2	608	CHL	C3D-C4D-ND	3.07	117.86	112.94
27	5	1622	XAT	C7-C8-C9	-3.07	120.77	125.53
25	y	614	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
25	1	604	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
24	Y	601	CHL	C4-C3-C5	3.06	120.55	115.23
35	B	2633	LMG	O2-C2-C1	-3.06	102.77	110.08
24	y	601	CHL	C4-C3-C5	3.06	120.54	115.23
25	r	603	CLA	CAA-C2A-C3A	-3.06	104.72	113.00
24	8	606	CHL	C3D-C4D-ND	3.06	117.85	112.94
25	N	612	CLA	CHB-C4A-NA	3.06	128.81	124.40
25	n	614	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
25	c	513	CLA	CAA-C2A-C3A	-3.06	104.73	113.00
27	1	1622	XAT	C15-C35-C34	-3.06	117.26	123.52
25	R	603	CLA	CAA-C2A-C3A	-3.06	104.74	113.00
24	g	607	CHL	C3D-C4D-ND	3.06	117.84	112.94
26	8	620	LUT	C18-C5-C6	-3.06	121.15	124.48
25	R	604	CLA	O2D-CGD-CBD	3.06	116.57	111.23
34	a	418	SQD	C4-C3-C2	3.05	116.19	110.83
24	7	607	CHL	OMC-CMC-C2C	-3.05	119.82	125.12
25	b	616	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
25	5	604	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
24	8	609	CHL	C3D-C4D-ND	3.05	117.83	112.94
37	b	626	DGD	O3G-C3G-C2G	-3.05	103.40	110.82
35	b	2633	LMG	O2-C2-C1	-3.05	102.81	110.08
24	6	608	CHL	C3D-C4D-ND	3.05	117.83	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	608	CHL	OMC-CMC-C2C	-3.05	119.83	125.12
25	C	509	CLA	CHB-C4A-NA	3.05	128.80	124.40
25	b	614	CLA	CMB-C2B-C1B	-3.05	120.78	125.42
25	B	616	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
24	G	605	CHL	C1C-CHC-C4B	3.05	126.97	116.07
26	4	620	LUT	C18-C5-C6	-3.05	121.16	124.48
25	Y	614	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
28	y	1623	NEX	C26-C27-C28	-3.05	119.55	125.99
25	C	504	CLA	CMB-C2B-C1B	-3.04	120.78	125.42
24	g	605	CHL	C1C-CHC-C4B	3.04	126.96	116.07
27	1	1622	XAT	C7-C8-C9	-3.04	120.81	125.53
24	4	606	CHL	O1D-CGD-CBD	-3.04	120.11	124.72
25	c	509	CLA	CHB-C4A-NA	3.04	128.79	124.40
25	n	612	CLA	CHB-C4A-NA	3.04	128.79	124.40
35	A	413	LMG	O6-C1-O1	-3.04	102.86	110.04
25	r	604	CLA	O2D-CGD-CBD	3.04	116.55	111.23
35	a	413	LMG	O6-C1-O1	-3.04	102.86	110.04
24	2	608	CHL	C1C-CHC-C4B	3.04	126.95	116.07
24	3	608	CHL	C3D-C4D-ND	3.04	117.81	112.94
24	4	608	CHL	OMC-CMC-C2C	-3.04	119.84	125.12
26	6	1620	LUT	C21-C26-C27	-3.04	109.33	112.83
25	C	501	CLA	C3B-C4B-NB	-3.04	107.82	110.53
27	3	1622	XAT	C7-C8-C9	-3.04	120.81	125.53
25	c	504	CLA	CMB-C2B-C1B	-3.04	120.79	125.42
24	n	609	CHL	O1D-CGD-CBD	-3.04	120.12	124.72
34	A	418	SQD	C4-C3-C2	3.04	116.16	110.83
26	2	1620	LUT	C21-C26-C27	-3.03	109.34	112.83
26	6	1620	LUT	C30-C31-C32	-3.03	114.41	123.20
24	G	607	CHL	C3D-C4D-ND	3.03	117.80	112.94
28	r	623	NEX	C11-C12-C13	-3.03	118.05	126.36
25	4	604	CLA	CHB-C4A-NA	3.03	128.77	124.40
25	G	612	CLA	CAA-C2A-C3A	-3.03	104.81	113.00
37	B	626	DGD	O3G-C3G-C2G	-3.03	103.45	110.82
37	h	102	DGD	O3G-C3G-C2G	-3.03	103.45	110.82
27	7	1622	XAT	C7-C8-C9	-3.03	120.83	125.53
24	6	608	CHL	C1C-CHC-C4B	3.03	126.91	116.07
37	H	102	DGD	O3G-C3G-C2G	-3.03	103.45	110.82
26	2	1620	LUT	C30-C31-C32	-3.03	114.42	123.20
28	y	1623	NEX	C11-C12-C13	-3.03	118.06	126.36
28	R	623	NEX	C11-C12-C13	-3.03	118.06	126.36
24	8	606	CHL	O1D-CGD-CBD	-3.02	120.14	124.72
24	4	609	CHL	C3D-C4D-ND	3.02	117.79	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	A	408	PHO	CBC-CAC-C3C	3.02	117.20	112.87
24	R	606	CHL	C1C-CHC-C4B	3.02	126.89	116.07
24	r	606	CHL	C1C-CHC-C4B	3.02	126.88	116.07
24	3	607	CHL	CMA-C3A-C4A	-3.02	108.10	114.61
27	5	1622	XAT	C15-C35-C34	-3.02	117.34	123.52
28	Y	1623	NEX	C11-C12-C13	-3.02	118.08	126.36
24	7	608	CHL	C3D-C4D-ND	3.02	117.78	112.94
25	8	604	CLA	CHB-C4A-NA	3.02	128.76	124.40
24	G	607	CHL	O1D-CGD-CBD	-3.02	120.15	124.72
24	N	609	CHL	O1D-CGD-CBD	-3.02	120.15	124.72
28	Y	1623	NEX	C26-C27-C28	-3.02	119.62	125.99
25	B	614	CLA	CMB-C2B-C1B	-3.02	120.83	125.42
25	Y	603	CLA	CBC-CAC-C3C	-3.02	104.25	112.42
25	g	612	CLA	CAA-C2A-C3A	-3.01	104.85	113.00
26	2	1621	LUT	C15-C14-C13	-3.01	123.05	127.28
25	6	604	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
24	Y	601	CHL	C1-C2-C3	-3.01	121.26	126.20
37	H	102	DGD	CDB-CCB-CBB	-3.01	99.14	114.37
37	h	102	DGD	CDB-CCB-CBB	-3.01	99.14	114.37
24	7	607	CHL	CMA-C3A-C4A	-3.01	108.12	114.61
25	S	614	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
34	b	621	SQD	O7-S-C6	3.01	111.25	106.76
26	1	1620	LUT	C21-C26-C27	-3.01	109.36	112.83
25	c	501	CLA	C3B-C4B-NB	-3.01	107.84	110.53
24	y	608	CHL	C3D-C4D-ND	3.01	117.76	112.94
25	B	603	CLA	C3B-C4B-NB	-3.01	107.84	110.53
26	4	620	LUT	C15-C35-C34	-3.01	117.36	123.52
27	6	1622	XAT	C40-C33-C32	3.01	122.68	118.09
25	b	611	CLA	CAA-CBA-CGA	-3.01	104.67	113.21
25	B	609	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
25	s	614	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
24	N	608	CHL	C3D-C4D-ND	3.00	117.76	112.94
26	6	1621	LUT	C15-C14-C13	-3.00	123.07	127.28
33	a	408	PHO	CBC-CAC-C3C	3.00	117.17	112.87
30	C	514	BCR	C20-C21-C22	-3.00	123.07	127.28
24	g	607	CHL	O1D-CGD-CBD	-3.00	120.17	124.72
24	Y	608	CHL	C3D-C4D-ND	3.00	117.75	112.94
25	B	611	CLA	CAA-CBA-CGA	-3.00	104.69	113.21
30	b	620	BCR	C33-C5-C4	3.00	119.99	113.60
25	r	613	CLA	CHB-C4A-NA	3.00	128.73	124.40
24	y	601	CHL	C1-C2-C3	-3.00	121.29	126.20
26	5	1620	LUT	C21-C26-C27	-3.00	109.38	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	606	CHL	CMA-C3A-C4A	-2.99	108.16	114.61
25	d	403	CLA	CMB-C2B-C1B	-2.99	120.86	125.42
25	5	603	CLA	CHB-C4A-NA	2.99	128.72	124.40
25	C	501	CLA	C4A-NA-C1A	2.99	108.05	106.68
25	7	602	CLA	CMB-C2B-C1B	-2.99	120.86	125.42
25	y	603	CLA	CBC-CAC-C3C	-2.99	104.31	112.42
26	6	1620	LUT	C31-C30-C29	-2.99	123.08	127.28
24	n	608	CHL	C3D-C4D-ND	2.99	117.74	112.94
30	t	101	BCR	C16-C15-C14	-2.99	117.40	123.52
25	3	602	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
24	2	609	CHL	C1C-CHC-C4B	2.99	126.77	116.07
24	N	607	CHL	C1C-CHC-C4B	2.99	126.77	116.07
26	s	1620	LUT	C30-C31-C32	-2.99	114.54	123.20
25	c	501	CLA	C4A-NA-C1A	2.99	108.04	106.68
27	2	1622	XAT	C40-C33-C32	2.99	122.65	118.09
24	6	609	CHL	C1C-CHC-C4B	2.99	126.76	116.07
28	R	623	NEX	C30-C31-C32	-2.99	114.55	123.20
26	8	620	LUT	C15-C35-C34	-2.99	117.41	123.52
25	3	602	CLA	CMB-C2B-C1B	-2.98	120.88	125.42
24	G	608	CHL	C1-C2-C3	-2.98	121.31	126.20
26	S	1620	LUT	C30-C31-C32	-2.98	114.55	123.20
25	b	616	CLA	CHB-C4A-NA	2.98	128.71	124.40
34	A	412	SQD	O8-S-C6	2.98	111.73	105.97
34	B	621	SQD	O7-S-C6	2.98	111.21	106.76
30	c	515	BCR	C23-C22-C21	-2.98	114.32	119.01
34	b	621	SQD	C4-C3-C2	2.98	116.06	110.83
25	B	606	CLA	C6-C5-C3	-2.98	106.21	113.47
25	b	609	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
24	n	607	CHL	C1C-CHC-C4B	2.98	126.73	116.07
30	c	514	BCR	C20-C21-C22	-2.98	123.10	127.28
26	N	1620	LUT	C17-C1-C6	2.98	114.91	110.24
30	B	620	BCR	C33-C5-C4	2.98	119.95	113.60
24	g	605	CHL	O2D-CGD-O1D	-2.98	118.05	123.85
25	R	601	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
25	1	603	CLA	CHB-C4A-NA	2.98	128.70	124.40
30	D	404	BCR	C16-C15-C14	-2.98	117.43	123.52
25	2	604	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
24	g	608	CHL	C1-C2-C3	-2.98	121.32	126.20
25	R	613	CLA	CHB-C4A-NA	2.98	128.69	124.40
26	2	1620	LUT	C31-C30-C29	-2.98	123.11	127.28
25	b	606	CLA	C6-C5-C3	-2.98	106.22	113.47
24	5	606	CHL	CMA-C3A-C4A	-2.98	108.20	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	505	CLA	O2D-CGD-CBD	2.97	116.43	111.23
25	a	410	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
30	T	101	BCR	C16-C15-C14	-2.97	117.44	123.52
25	B	616	CLA	CHB-C4A-NA	2.97	128.69	124.40
24	2	606	CHL	C3D-C4D-ND	2.97	117.71	112.94
28	r	623	NEX	C30-C31-C32	-2.97	114.59	123.20
25	r	601	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
25	D	403	CLA	CMB-C2B-C1B	-2.97	120.89	125.42
25	c	505	CLA	O2D-CGD-CBD	2.97	116.42	111.23
24	g	601	CHL	O1D-CGD-CBD	-2.97	120.22	124.72
24	Y	607	CHL	CMB-C2B-C3B	2.97	130.62	124.68
34	a	412	SQD	O8-S-C6	2.97	111.70	105.97
25	n	612	CLA	CAA-C2A-C3A	-2.97	104.98	113.00
30	d	404	BCR	C16-C15-C14	-2.97	117.45	123.52
29	D	410	LHG	O8-C23-C24	2.97	120.88	111.83
24	6	606	CHL	C3D-C4D-ND	2.97	117.70	112.94
27	8	622	XAT	C31-C30-C29	-2.96	123.12	127.28
34	B	621	SQD	C4-C3-C2	2.96	116.03	110.83
25	C	511	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
25	S	610	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
25	7	602	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
24	8	606	CHL	C1C-CHC-C4B	2.96	126.67	116.07
24	G	605	CHL	O2D-CGD-O1D	-2.96	118.08	123.85
29	d	410	LHG	O8-C23-C24	2.96	120.87	111.83
30	4	623	BCR	C20-C21-C22	-2.96	123.12	127.28
27	4	622	XAT	C31-C30-C29	-2.96	123.13	127.28
30	8	623	BCR	C20-C21-C22	-2.96	123.13	127.28
24	5	609	CHL	C1C-CHC-C4B	2.96	126.66	116.07
24	G	601	CHL	O1D-CGD-CBD	-2.96	120.24	124.72
24	y	607	CHL	CMB-C2B-C3B	2.96	130.59	124.68
25	B	616	CLA	CAA-C2A-C3A	-2.96	105.01	113.00
25	b	616	CLA	CAA-C2A-C3A	-2.96	105.01	113.00
30	C	515	BCR	C23-C22-C21	-2.96	114.36	119.01
24	n	606	CHL	CMB-C2B-C3B	2.96	130.59	124.68
25	C	502	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
25	C	507	CLA	CHB-C4A-NA	2.96	128.66	124.40
25	b	603	CLA	C3B-C4B-NB	-2.96	107.89	110.53
25	A	410	CLA	O2D-CGD-O1D	-2.96	118.10	123.85
25	N	612	CLA	CAA-C2A-C3A	-2.95	105.01	113.00
25	g	611	CLA	CHB-C4A-NA	2.95	128.66	124.40
24	4	606	CHL	C1C-CHC-C4B	2.95	126.64	116.07
24	5	608	CHL	C3D-C4D-ND	2.95	117.68	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	1620	LUT	C10-C11-C12	-2.95	114.64	123.20
24	1	609	CHL	C1C-CHC-C4B	2.95	126.63	116.07
25	s	610	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
26	n	1620	LUT	C17-C1-C6	2.95	114.87	110.24
25	c	511	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
25	c	502	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
25	G	611	CLA	CHB-C4A-NA	2.95	128.66	124.40
27	R	622	XAT	C24-C23-C22	-2.95	105.28	110.79
25	g	602	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
24	Y	607	CHL	CAA-C2A-C3A	-2.95	105.04	113.00
25	c	507	CLA	CHB-C4A-NA	2.95	128.65	124.40
27	r	622	XAT	C24-C23-C22	-2.95	105.28	110.79
26	3	1621	LUT	C15-C14-C13	-2.94	123.15	127.28
28	N	1623	NEX	C39-C29-C30	-2.94	118.05	122.82
24	6	605	CHL	C1C-CHC-C4B	2.94	126.60	116.07
34	a	412	SQD	O9-S-C6	2.94	111.15	106.76
24	S	607	CHL	C1C-CHC-C4B	2.94	126.59	116.07
25	5	614	CLA	CHB-C4A-NA	2.94	128.64	124.40
25	C	503	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
24	n	608	CHL	OBD-CAD-C3D	-2.94	123.31	127.89
25	y	604	CLA	CHB-C1B-NB	2.94	128.46	124.05
24	N	606	CHL	CMB-C2B-C3B	2.94	130.56	124.68
26	2	1620	LUT	C10-C11-C12	-2.94	114.69	123.20
34	A	412	SQD	O9-S-C6	2.94	111.14	106.76
24	2	605	CHL	C1C-CHC-C4B	2.94	126.58	116.07
24	s	607	CHL	C1C-CHC-C4B	2.94	126.58	116.07
30	h	101	BCR	C38-C26-C25	-2.94	121.28	124.48
24	2	601	CHL	CMD-C2D-C3D	-2.94	118.81	124.68
24	y	607	CHL	CAA-C2A-C3A	-2.94	105.06	113.00
25	b	609	CLA	CHB-C4A-NA	2.94	128.64	124.40
24	g	606	CHL	O2A-CGA-CBA	2.94	120.79	111.83
24	S	607	CHL	C3D-C4D-ND	2.94	117.65	112.94
28	5	1623	NEX	C30-C31-C32	-2.93	114.70	123.20
26	7	1621	LUT	C15-C14-C13	-2.93	123.16	127.28
24	1	608	CHL	C3D-C4D-ND	2.93	117.64	112.94
28	n	1623	NEX	C39-C29-C30	-2.93	118.06	122.82
24	N	608	CHL	OBD-CAD-C3D	-2.93	123.32	127.89
25	Y	604	CLA	CHB-C1B-NB	2.93	128.45	124.05
25	G	602	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
29	b	2631	LHG	O8-C23-C24	2.93	120.77	111.83
26	4	620	LUT	C18-C5-C4	2.93	119.81	114.42
28	1	1623	NEX	C30-C31-C32	-2.93	114.71	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	2631	LHG	O8-C23-C24	2.93	120.77	111.83
25	1	614	CLA	CHB-C4A-NA	2.93	128.63	124.40
25	c	503	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
24	4	607	CHL	C1C-CHC-C4B	2.93	126.54	116.07
25	B	609	CLA	CHB-C4A-NA	2.92	128.62	124.40
24	6	601	CHL	CMD-C2D-C3D	-2.92	118.84	124.68
36	d	405	PL9	C7-C8-C9	-2.92	121.79	126.83
34	a	412	SQD	O7-S-C6	2.92	111.12	106.76
26	8	620	LUT	C18-C5-C4	2.92	119.79	114.42
24	8	607	CHL	C1C-CHC-C4B	2.92	126.52	116.07
36	A	414	PL9	C8-C7-C3	2.92	119.58	112.03
24	G	606	CHL	O2A-CGA-CBA	2.92	120.74	111.83
28	R	623	NEX	C17-C1-C6	-2.92	107.86	110.47
24	G	601	CHL	CBC-CAC-C3C	-2.92	108.69	112.87
28	1	1623	NEX	C26-C27-C28	-2.92	119.82	125.99
25	n	613	CLA	CMB-C2B-C1B	-2.92	120.98	125.42
24	G	606	CHL	CBC-CAC-C3C	-2.92	108.70	112.87
36	D	405	PL9	C7-C8-C9	-2.92	121.81	126.83
25	8	602	CLA	CHB-C4A-NA	2.92	128.61	124.40
24	1	609	CHL	O2A-CGA-CBA	2.91	120.72	111.83
25	N	613	CLA	CMB-C2B-C1B	-2.91	120.98	125.42
25	3	613	CLA	CHB-C4A-NA	2.91	128.60	124.40
25	G	603	CLA	C3B-C4B-NB	-2.91	107.93	110.53
24	Y	601	CHL	O1D-CGD-CBD	-2.91	120.31	124.72
25	G	611	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
24	N	608	CHL	O2A-CGA-CBA	2.91	120.70	111.83
24	S	607	CHL	CMA-C3A-C4A	-2.91	108.34	114.61
24	5	609	CHL	O2A-CGA-CBA	2.91	120.70	111.83
24	s	607	CHL	CMA-C3A-C4A	-2.91	108.35	114.61
24	s	607	CHL	C3D-C4D-ND	2.91	117.60	112.94
30	b	620	BCR	C29-C30-C25	2.91	114.66	110.44
34	A	412	SQD	O7-S-C6	2.91	111.09	106.76
24	n	608	CHL	O2A-CGA-CBA	2.91	120.69	111.83
25	C	510	CLA	CMB-C2B-C1B	-2.91	121.00	125.42
24	3	605	CHL	C1C-CHC-C4B	2.90	126.46	116.07
36	a	414	PL9	C8-C7-C3	2.90	119.54	112.03
25	4	602	CLA	CHB-C4A-NA	2.90	128.59	124.40
25	g	603	CLA	C3B-C4B-NB	-2.90	107.94	110.53
24	7	605	CHL	C1C-CHC-C4B	2.90	126.45	116.07
30	H	101	BCR	C38-C26-C25	-2.90	121.32	124.48
25	7	613	CLA	CHB-C4A-NA	2.90	128.58	124.40
36	D	405	PL9	C8-C7-C3	2.90	119.52	112.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	r	623	NEX	C17-C1-C6	-2.90	107.88	110.47
25	g	602	CLA	CAC-C3C-C4C	2.90	128.56	124.79
24	g	606	CHL	CBC-CAC-C3C	-2.90	108.72	112.87
30	c	515	BCR	C33-C5-C6	-2.90	121.32	124.48
34	b	623	SQD	O5-C1-C2	2.90	116.32	110.37
25	A	410	CLA	C3B-C4B-NB	-2.90	107.94	110.53
28	5	1623	NEX	C26-C27-C28	-2.90	119.87	125.99
24	1	605	CHL	CMA-C3A-C4A	-2.90	108.37	114.61
35	a	415	LMG	O6-C1-O1	-2.90	103.20	110.04
28	5	1623	NEX	C39-C29-C30	-2.89	118.13	122.82
25	R	609	CLA	CHB-C4A-NA	2.89	128.57	124.40
30	B	620	BCR	C29-C30-C25	2.89	114.64	110.44
25	b	614	CLA	C4-C3-C5	2.89	120.25	115.23
25	g	611	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
34	a	412	SQD	O48-C23-C24	2.89	120.65	111.83
36	d	405	PL9	C8-C7-C3	2.89	119.50	112.03
24	2	605	CHL	OMC-CMC-C2C	-2.89	120.10	125.12
25	G	602	CLA	CAC-C3C-C4C	2.89	128.55	124.79
34	B	623	SQD	O5-C1-C2	2.89	116.31	110.37
28	G	1623	NEX	C39-C29-C30	-2.89	118.14	122.82
24	g	601	CHL	CBC-CAC-C3C	-2.89	108.74	112.87
27	r	622	XAT	C35-C15-C14	-2.89	117.61	123.52
35	A	415	LMG	O6-C1-O1	-2.89	103.22	110.04
30	C	515	BCR	C33-C5-C6	-2.89	121.33	124.48
25	c	510	CLA	CMB-C2B-C1B	-2.89	121.03	125.42
25	Y	613	CLA	CHC-C4B-NB	2.89	128.38	124.05
24	5	605	CHL	CMA-C3A-C4A	-2.88	108.39	114.61
25	B	612	CLA	CAC-C3C-C4C	2.88	128.54	124.79
26	s	1620	LUT	C21-C26-C27	-2.88	109.51	112.83
26	S	1621	LUT	C15-C14-C13	-2.88	123.23	127.28
26	G	1621	LUT	C28-C29-C30	-2.88	114.47	119.01
25	r	609	CLA	CHB-C4A-NA	2.88	128.56	124.40
25	A	410	CLA	CAA-CBA-CGA	-2.88	105.03	113.21
34	A	412	SQD	O48-C23-C24	2.88	120.62	111.83
25	a	410	CLA	CAA-CBA-CGA	-2.88	105.03	113.21
28	R	623	NEX	C4-C3-C2	-2.88	105.40	110.79
26	S	1620	LUT	C21-C26-C27	-2.88	109.51	112.83
30	b	618	BCR	C10-C11-C12	-2.88	114.86	123.20
27	R	622	XAT	C35-C15-C14	-2.88	117.63	123.52
24	6	609	CHL	O2A-CGA-CBA	2.88	120.61	111.83
25	2	614	CLA	CHB-C4A-NA	2.88	128.55	124.40
28	1	1623	NEX	C39-C29-C30	-2.88	118.16	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	410	CLA	C3B-C4B-NB	-2.88	107.96	110.53
28	r	623	NEX	C4-C3-C2	-2.88	105.41	110.79
25	B	614	CLA	C4-C3-C5	2.88	120.22	115.23
34	a	418	SQD	O47-C7-C8	2.88	117.70	111.48
24	R	608	CHL	O2A-CGA-CBA	2.87	120.60	111.83
30	t	101	BCR	C35-C13-C12	2.87	122.48	118.09
25	S	603	CLA	CHB-C4A-NA	2.87	128.55	124.40
30	B	618	BCR	C10-C11-C12	-2.87	114.87	123.20
24	r	608	CHL	O2A-CGA-CBA	2.87	120.60	111.83
29	b	2630	LHG	O8-C23-C24	2.87	120.60	111.83
29	B	2630	LHG	O8-C23-C24	2.87	120.60	111.83
26	S	1621	LUT	C35-C15-C14	-2.87	117.64	123.52
27	3	1622	XAT	C38-C25-C24	2.87	117.47	114.24
27	7	1622	XAT	C10-C11-C12	-2.87	114.88	123.20
26	1	1620	LUT	C8-C9-C10	-2.87	114.49	119.01
37	c	520	DGD	C3G-C2G-C1G	-2.87	105.09	111.78
25	2	612	CLA	CHB-C4A-NA	2.87	128.54	124.40
25	6	612	CLA	CHB-C4A-NA	2.87	128.54	124.40
24	2	609	CHL	O2A-CGA-CBA	2.87	120.59	111.83
25	b	612	CLA	CAC-C3C-C4C	2.87	128.53	124.79
34	A	418	SQD	O47-C7-C8	2.87	117.69	111.48
27	3	1622	XAT	C10-C11-C12	-2.87	114.88	123.20
24	Y	606	CHL	CBC-CAC-C3C	-2.87	108.77	112.87
24	y	601	CHL	O1D-CGD-CBD	-2.87	120.37	124.72
28	R	623	NEX	C35-C34-C33	-2.87	123.26	127.28
26	s	1621	LUT	C15-C14-C13	-2.87	123.26	127.28
24	y	606	CHL	CBC-CAC-C3C	-2.87	108.77	112.87
30	T	101	BCR	C35-C13-C12	2.87	122.47	118.09
28	g	1623	NEX	C39-C29-C30	-2.87	118.17	122.82
24	s	606	CHL	O2D-CGD-O1D	-2.86	118.27	123.85
37	C	520	DGD	C3G-C2G-C1G	-2.86	105.11	111.78
29	d	409	LHG	C11-C10-C9	-2.86	99.91	114.37
24	6	605	CHL	OMC-CMC-C2C	-2.86	120.15	125.12
29	D	409	LHG	C11-C10-C9	-2.86	99.91	114.37
24	s	601	CHL	C1C-CHC-C4B	2.86	126.30	116.07
30	A	411	BCR	C21-C20-C19	-2.86	114.92	123.20
24	R	614	CHL	CAA-C2A-C3A	-2.86	109.67	116.23
25	B	615	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
25	y	613	CLA	CHC-C4B-NB	2.86	128.34	124.05
25	6	610	CLA	C3B-C4B-NB	-2.86	107.98	110.53
26	s	1621	LUT	C35-C15-C14	-2.86	117.67	123.52
25	8	603	CLA	CHB-C4A-NA	2.86	128.52	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	8	622	XAT	C18-C5-C4	2.86	117.45	114.24
26	5	1620	LUT	C8-C9-C10	-2.86	114.52	119.01
26	g	1621	LUT	C28-C29-C30	-2.86	114.52	119.01
25	b	615	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
24	S	606	CHL	O2D-CGD-O1D	-2.85	118.30	123.85
25	Y	612	CLA	CHB-C4A-NA	2.85	128.51	124.40
25	y	611	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
24	r	614	CHL	CAA-C2A-C3A	-2.85	109.70	116.23
24	S	601	CHL	C1C-CHC-C4B	2.85	126.26	116.07
30	a	411	BCR	C21-C20-C19	-2.85	114.95	123.20
26	r	620	LUT	C20-C13-C12	2.85	122.44	118.09
26	g	1621	LUT	C30-C31-C32	-2.85	114.95	123.20
26	6	1620	LUT	C15-C35-C34	-2.85	117.69	123.52
24	3	605	CHL	O1D-CGD-CBD	-2.85	120.41	124.72
24	8	601	CHL	CMA-C3A-C4A	-2.85	108.48	114.61
25	y	612	CLA	CHB-C4A-NA	2.85	128.51	124.40
24	4	601	CHL	CMA-C3A-C4A	-2.84	108.48	114.61
25	6	614	CLA	CHB-C4A-NA	2.84	128.50	124.40
25	s	603	CLA	CHB-C4A-NA	2.84	128.50	124.40
28	5	1623	NEX	C31-C30-C29	-2.84	123.29	127.28
24	8	606	CHL	CBC-CAC-C3C	-2.84	108.80	112.87
30	C	516	BCR	C10-C11-C12	-2.84	114.97	123.20
27	7	1622	XAT	C38-C25-C24	2.84	117.43	114.24
24	2	606	CHL	C1C-CHC-C4B	2.84	126.23	116.07
28	7	1623	NEX	C39-C29-C30	-2.84	118.21	122.82
28	r	623	NEX	C35-C34-C33	-2.84	123.29	127.28
24	4	606	CHL	CBC-CAC-C3C	-2.84	108.81	112.87
24	Y	607	CHL	CMA-C3A-C4A	-2.84	108.49	114.61
27	r	622	XAT	C19-C9-C8	2.84	122.42	118.09
24	N	606	CHL	O2A-CGA-CBA	2.84	120.49	111.83
25	2	604	CLA	CHB-C4A-NA	2.84	128.50	124.40
28	1	1623	NEX	C31-C30-C29	-2.84	123.30	127.28
25	2	613	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
24	3	606	CHL	CMD-C2D-C3D	-2.84	119.02	124.68
28	2	1623	NEX	C39-C29-C30	-2.83	118.22	122.82
25	n	602	CLA	CMB-C2B-C1B	-2.83	121.10	125.42
27	4	622	XAT	C18-C5-C4	2.83	117.42	114.24
24	S	608	CHL	C3D-C4D-ND	2.83	117.48	112.94
24	n	606	CHL	C3D-C4D-ND	2.83	117.48	112.94
25	C	504	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
27	R	622	XAT	C19-C9-C8	2.83	122.41	118.09
24	n	606	CHL	O2A-CGA-CBA	2.83	120.46	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	607	CHL	C3D-C4D-ND	2.83	117.48	112.94
29	c	2630	LHG	O8-C23-C24	2.83	120.46	111.83
24	6	606	CHL	C1C-CHC-C4B	2.83	126.19	116.07
26	R	620	LUT	C20-C13-C12	2.83	122.41	118.09
25	2	610	CLA	C3B-C4B-NB	-2.83	108.00	110.53
25	B	612	CLA	CMB-C2B-C3B	2.83	133.20	126.55
24	y	606	CHL	C1C-CHC-C4B	2.83	126.19	116.07
24	7	606	CHL	CMD-C2D-C3D	-2.83	119.03	124.68
27	2	1622	XAT	C35-C34-C33	-2.83	123.31	127.28
25	c	504	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
25	D	402	CLA	CAC-C3C-C4C	2.83	128.47	124.79
25	b	610	CLA	CMB-C2B-C1B	-2.83	121.12	125.42
28	3	1623	NEX	C39-C29-C30	-2.83	118.24	122.82
25	4	603	CLA	CHB-C4A-NA	2.83	128.48	124.40
25	Y	611	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
29	C	2630	LHG	O8-C23-C24	2.82	120.45	111.83
26	2	1620	LUT	C15-C35-C34	-2.82	117.74	123.52
24	y	607	CHL	CMA-C3A-C4A	-2.82	108.53	114.61
27	6	1622	XAT	C35-C34-C33	-2.82	123.32	127.28
24	6	607	CHL	C3D-C4D-ND	2.82	117.47	112.94
25	R	604	CLA	CHB-C4A-NA	2.82	128.47	124.40
24	Y	606	CHL	C1C-CHC-C4B	2.82	126.16	116.07
26	G	1621	LUT	C30-C31-C32	-2.82	115.03	123.20
25	6	613	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
25	5	612	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
24	7	605	CHL	CBC-CAC-C3C	-2.82	108.84	112.87
24	7	605	CHL	O1D-CGD-CBD	-2.82	120.45	124.72
24	N	606	CHL	C3D-C4D-ND	2.82	117.46	112.94
24	N	605	CHL	CMA-C3A-C4A	-2.82	108.54	114.61
28	1	1623	NEX	C11-C12-C13	-2.82	118.64	126.36
25	b	612	CLA	CMB-C2B-C3B	2.82	133.18	126.55
37	c	518	DGD	CDB-CCB-CBB	-2.82	100.13	114.37
25	6	604	CLA	CHB-C4A-NA	2.82	128.46	124.40
28	5	1623	NEX	C11-C12-C13	-2.82	118.64	126.36
37	C	518	DGD	CDB-CCB-CBB	-2.81	100.14	114.37
25	s	612	CLA	CHB-C4A-NA	2.81	128.46	124.40
30	c	516	BCR	C10-C11-C12	-2.81	115.05	123.20
25	B	610	CLA	CMB-C2B-C1B	-2.81	121.13	125.42
28	6	1623	NEX	C39-C29-C30	-2.81	118.26	122.82
25	s	611	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
25	y	610	CLA	C1D-ND-C4D	-2.81	104.34	106.31
25	B	607	CLA	CHB-C4A-NA	2.81	128.46	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	r	604	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
25	B	612	CLA	CHB-C4A-NA	2.81	128.46	124.40
25	D	403	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
25	B	608	CLA	CHB-C4A-NA	2.81	128.46	124.40
25	C	513	CLA	CMB-C2B-C3B	2.81	133.16	126.55
25	b	607	CLA	CHB-C4A-NA	2.81	128.46	124.40
25	b	612	CLA	CHB-C4A-NA	2.81	128.46	124.40
25	r	604	CLA	CHB-C4A-NA	2.81	128.46	124.40
24	n	605	CHL	CMA-C3A-C4A	-2.81	108.56	114.61
25	S	611	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
28	3	1623	NEX	C28-C29-C30	2.81	123.43	119.01
25	d	403	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
25	R	604	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
24	G	608	CHL	O2A-CGA-CBA	2.81	120.39	111.83
24	2	609	CHL	CMB-C2B-C3B	2.81	130.29	124.68
25	g	603	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
26	1	1620	LUT	C19-C9-C8	2.81	122.37	118.09
24	3	609	CHL	C3D-C4D-ND	2.80	117.44	112.94
25	N	602	CLA	CMB-C2B-C1B	-2.80	121.15	125.42
29	Y	2630	LHG	O8-C23-C24	2.80	120.39	111.83
24	6	601	CHL	O1D-CGD-CBD	-2.80	120.47	124.72
29	y	2630	LHG	O8-C23-C24	2.80	120.38	111.83
24	y	606	CHL	O1D-CGD-CBD	-2.80	120.47	124.72
24	s	608	CHL	C3D-C4D-ND	2.80	117.44	112.94
26	n	1621	LUT	C22-C23-C24	-2.80	107.02	111.18
25	r	601	CLA	C3B-C4B-NB	-2.80	108.03	110.53
24	g	608	CHL	O2A-CGA-CBA	2.80	120.37	111.83
25	C	502	CLA	CHB-C4A-NA	2.80	128.44	124.40
25	d	402	CLA	CAC-C3C-C4C	2.80	128.43	124.79
30	A	411	BCR	C16-C15-C14	-2.80	117.79	123.52
25	B	606	CLA	C1-C2-C3	-2.80	121.61	126.20
26	2	1621	LUT	C39-C29-C28	2.80	122.36	118.09
24	8	606	CHL	CMA-C3A-C4A	-2.80	108.59	114.61
25	G	614	CLA	C3B-C4B-NB	-2.80	108.03	110.53
24	s	601	CHL	O1D-CGD-CBD	-2.80	120.48	124.72
24	4	606	CHL	CMA-C3A-C4A	-2.79	108.59	114.61
25	c	513	CLA	CMB-C2B-C3B	2.79	133.12	126.55
37	B	626	DGD	CDB-CCB-CBB	-2.79	100.24	114.37
25	b	608	CLA	CHB-C4A-NA	2.79	128.43	124.40
25	G	603	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
28	7	1623	NEX	C28-C29-C30	2.79	123.40	119.01
24	n	607	CHL	O2A-CGA-CBA	2.79	120.35	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	601	CLA	C3B-C4B-NB	-2.79	108.04	110.53
24	g	609	CHL	C3D-C4D-ND	2.79	117.42	112.94
37	b	626	DGD	CDB-CCB-CBB	-2.79	100.25	114.37
25	Y	610	CLA	C1D-ND-C4D	-2.79	104.35	106.31
26	5	1620	LUT	C19-C9-C8	2.79	122.35	118.09
26	6	1621	LUT	C39-C29-C28	2.79	122.35	118.09
25	B	602	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
26	N	1621	LUT	C22-C23-C24	-2.79	107.04	111.18
24	5	605	CHL	O2D-CGD-O1D	-2.79	118.42	123.85
25	R	602	CLA	CMB-C2B-C3B	2.79	133.11	126.55
25	b	602	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
28	3	1623	NEX	C15-C35-C34	-2.79	117.81	123.52
25	c	510	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
24	3	605	CHL	CBC-CAC-C3C	-2.79	108.88	112.87
24	6	609	CHL	CMB-C2B-C3B	2.79	130.26	124.68
25	Y	614	CLA	C3B-C4B-NB	-2.79	108.04	110.53
25	S	612	CLA	CHB-C4A-NA	2.79	128.42	124.40
25	S	603	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
25	s	603	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
25	y	614	CLA	C3B-C4B-NB	-2.79	108.04	110.53
24	y	601	CHL	CMD-C2D-C3D	-2.79	119.11	124.68
24	S	601	CHL	O1D-CGD-CBD	-2.79	120.50	124.72
24	N	607	CHL	O2A-CGA-CBA	2.79	120.33	111.83
25	c	502	CLA	CHB-C4A-NA	2.79	128.42	124.40
25	1	612	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
25	g	614	CLA	C3B-C4B-NB	-2.78	108.04	110.53
30	C	517	BCR	C21-C20-C19	-2.78	115.13	123.20
29	c	523	LHG	O8-C23-C24	2.78	120.33	111.83
30	c	517	BCR	C21-C20-C19	-2.78	115.13	123.20
25	A	406	CLA	CHB-C4A-NA	2.78	128.42	124.40
24	6	606	CHL	CBC-CAC-C3C	-2.78	108.89	112.87
25	b	606	CLA	C1-C2-C3	-2.78	121.64	126.20
26	7	1621	LUT	C30-C31-C32	-2.78	115.14	123.20
25	B	608	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
24	5	606	CHL	C3D-C4D-ND	2.78	117.40	112.94
25	5	603	CLA	CBC-CAC-C3C	-2.78	104.88	112.42
26	Y	1620	LUT	C11-C10-C9	-2.78	123.38	127.28
25	1	603	CLA	CBC-CAC-C3C	-2.78	104.88	112.42
27	N	1622	XAT	C18-C5-C4	2.78	117.37	114.24
25	g	612	CLA	CHB-C4A-NA	2.78	128.41	124.40
30	a	411	BCR	C16-C15-C14	-2.78	117.83	123.52
25	N	604	CLA	C1-C2-C3	-2.78	122.26	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	510	CLA	CAA-C2A-C3A	-2.78	105.48	113.00
24	2	606	CHL	CBC-CAC-C3C	-2.78	108.89	112.87
29	n	2630	LHG	C11-C10-C9	-2.78	100.31	114.37
24	4	607	CHL	O1D-CGD-CBD	-2.78	120.51	124.72
25	r	602	CLA	CMB-C2B-C3B	2.78	133.09	126.55
25	c	510	CLA	CAA-C2A-C3A	-2.78	105.49	113.00
25	a	406	CLA	CHB-C4A-NA	2.78	128.41	124.40
29	N	2630	LHG	C11-C10-C9	-2.78	100.32	114.37
29	C	523	LHG	O8-C23-C24	2.78	120.31	111.83
28	3	1623	NEX	C24-C23-C22	-2.78	105.59	110.79
25	2	614	CLA	C4A-NA-C1A	2.78	107.95	106.68
24	G	609	CHL	C3D-C4D-ND	2.78	117.39	112.94
24	Y	606	CHL	O1D-CGD-CBD	-2.78	120.51	124.72
24	Y	609	CHL	C3D-C4D-ND	2.78	117.39	112.94
25	b	613	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
36	d	405	PL9	O1-C4-C3	-2.77	117.80	120.73
25	5	612	CLA	CHB-C4A-NA	2.77	128.40	124.40
25	d	403	CLA	CHB-C4A-NA	2.77	128.40	124.40
25	b	613	CLA	CMB-C2B-C3B	2.77	133.07	126.55
25	4	603	CLA	CAA-C2A-C3A	-2.77	105.50	113.00
25	s	612	CLA	CMB-C2B-C1B	-2.77	121.20	125.42
24	7	609	CHL	C3D-C4D-ND	2.77	117.39	112.94
28	7	1623	NEX	C24-C23-C22	-2.77	105.61	110.79
24	6	606	CHL	CMA-C3A-C4A	-2.77	108.64	114.61
24	1	605	CHL	O2D-CGD-O1D	-2.77	118.45	123.85
29	G	2630	LHG	O8-C23-C24	2.77	120.28	111.83
26	y	1620	LUT	C11-C10-C9	-2.77	123.39	127.28
24	y	601	CHL	C1C-C2C-CMC	2.77	131.79	126.80
24	1	606	CHL	C3D-C4D-ND	2.77	117.38	112.94
28	3	1623	NEX	C35-C34-C33	-2.77	123.39	127.28
24	Y	601	CHL	CMD-C2D-C3D	-2.77	119.15	124.68
25	n	604	CLA	C1-C2-C3	-2.77	122.28	126.76
25	D	403	CLA	CHB-C4A-NA	2.77	128.40	124.40
25	8	603	CLA	CAA-C2A-C3A	-2.77	105.52	113.00
25	G	612	CLA	CHB-C4A-NA	2.77	128.40	124.40
25	C	510	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
25	b	608	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
24	r	607	CHL	CBC-CAC-C3C	-2.77	108.91	112.87
26	3	1621	LUT	C30-C31-C32	-2.77	115.18	123.20
27	n	1622	XAT	C18-C5-C4	2.77	117.35	114.24
24	5	605	CHL	C1C-CHC-C4B	2.77	125.97	116.07
25	S	612	CLA	CMB-C2B-C1B	-2.77	121.21	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	602	CLA	C1-C2-C3	-2.77	121.67	126.20
26	6	1621	LUT	C22-C23-C24	-2.77	107.08	111.18
25	c	505	CLA	CHB-C4A-NA	2.77	128.39	124.40
26	5	1621	LUT	C31-C30-C29	-2.77	123.40	127.28
29	d	408	LHG	C11-C10-C9	-2.76	100.40	114.37
24	6	607	CHL	C1C-CHC-C4B	2.76	125.96	116.07
24	2	607	CHL	C1C-CHC-C4B	2.76	125.96	116.07
24	2	606	CHL	CMA-C3A-C4A	-2.76	108.66	114.61
29	D	408	LHG	C11-C10-C9	-2.76	100.41	114.37
25	B	610	CLA	C1-C2-C3	-2.76	121.67	126.20
29	g	2630	LHG	O8-C23-C24	2.76	120.26	111.83
25	A	405	CLA	CMB-C2B-C3B	2.76	133.04	126.55
26	3	1620	LUT	C22-C23-C24	2.76	115.28	111.18
25	B	613	CLA	CMB-C2B-C3B	2.76	133.04	126.55
24	G	609	CHL	CAA-C2A-C3A	-2.76	105.54	113.00
24	1	605	CHL	C1C-CHC-C4B	2.76	125.94	116.07
25	y	611	CLA	O2A-CGA-O1A	-2.76	116.72	123.63
25	n	602	CLA	C1-C2-C3	-2.76	121.67	126.20
28	7	1623	NEX	C15-C35-C34	-2.76	117.87	123.52
25	b	610	CLA	C1-C2-C3	-2.76	121.68	126.20
25	B	613	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
30	C	516	BCR	C7-C8-C9	-2.76	122.15	126.23
24	N	606	CHL	O1D-CGD-CBD	-2.76	120.54	124.72
24	y	609	CHL	C3D-C4D-ND	2.76	117.36	112.94
24	2	601	CHL	O1D-CGD-CBD	-2.76	120.55	124.72
24	Y	607	CHL	C3D-C4D-ND	2.75	117.36	112.94
25	C	505	CLA	CHB-C4A-NA	2.75	128.38	124.40
26	2	1621	LUT	C22-C23-C24	-2.75	107.09	111.18
24	8	607	CHL	O1D-CGD-CBD	-2.75	120.55	124.72
25	1	612	CLA	CHB-C4A-NA	2.75	128.37	124.40
24	n	607	CHL	C3D-C4D-ND	2.75	117.36	112.94
24	Y	601	CHL	C1C-C2C-CMC	2.75	131.76	126.80
26	n	1621	LUT	C30-C31-C32	-2.75	115.23	123.20
26	7	1620	LUT	C22-C23-C24	2.75	115.27	111.18
24	2	606	CHL	O1D-CGD-CBD	-2.75	120.55	124.72
36	D	405	PL9	O1-C4-C3	-2.75	117.83	120.73
24	2	607	CHL	CAA-C2A-C3A	-2.75	105.57	113.00
25	2	602	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
25	g	610	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
24	r	608	CHL	O1D-CGD-CBD	-2.75	120.56	124.72
26	N	1621	LUT	C30-C31-C32	-2.75	115.24	123.20
24	g	609	CHL	CAA-C2A-C3A	-2.75	105.57	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	n	606	CHL	O1D-CGD-CBD	-2.75	120.56	124.72
24	6	607	CHL	O1D-CGD-CBD	-2.75	120.56	124.72
25	G	610	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
26	Y	1620	LUT	C21-C26-C27	-2.75	109.67	112.83
25	Y	611	CLA	O2A-CGA-O1A	-2.75	116.76	123.63
29	c	522	LHG	O8-C23-C24	2.75	120.21	111.83
24	R	607	CHL	CBC-CAC-C3C	-2.74	108.94	112.87
24	6	607	CHL	CAA-C2A-C3A	-2.74	105.58	113.00
27	R	622	XAT	C4-C3-C2	-2.74	105.66	110.79
25	a	405	CLA	CMB-C2B-C3B	2.74	133.00	126.55
25	c	508	CLA	CHB-C4A-NA	2.74	128.36	124.40
25	N	611	CLA	CHB-C4A-NA	2.74	128.36	124.40
24	2	607	CHL	O1D-CGD-CBD	-2.74	120.56	124.72
24	5	601	CHL	CMD-C2D-C3D	-2.74	119.20	124.68
24	R	608	CHL	O1D-CGD-CBD	-2.74	120.57	124.72
24	1	601	CHL	C1C-CHC-C4B	2.74	125.87	116.07
25	6	602	CLA	CMB-C2B-C1B	-2.74	121.25	125.42
25	B	602	CLA	CHB-C4A-NA	2.74	128.35	124.40
30	b	620	BCR	C20-C21-C22	-2.74	123.44	127.28
25	C	508	CLA	CHB-C4A-NA	2.74	128.35	124.40
24	N	607	CHL	C3D-C4D-ND	2.74	117.33	112.94
26	g	1621	LUT	C11-C10-C9	-2.74	123.44	127.28
24	5	606	CHL	C1C-CHC-C4B	2.74	125.87	116.07
28	7	1623	NEX	C35-C34-C33	-2.74	123.44	127.28
25	B	611	CLA	CHB-C1B-NB	2.74	128.16	124.05
25	A	407	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
26	1	1621	LUT	C31-C30-C29	-2.74	123.44	127.28
25	n	611	CLA	CHB-C4A-NA	2.74	128.35	124.40
30	c	516	BCR	C7-C8-C9	-2.74	122.19	126.23
24	1	606	CHL	C1C-CHC-C4B	2.74	125.86	116.07
24	y	607	CHL	C3D-C4D-ND	2.74	117.33	112.94
25	B	605	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
26	G	1621	LUT	C11-C10-C9	-2.74	123.44	127.28
25	B	604	CLA	CMB-C2B-C1B	-2.73	121.25	125.42
25	2	602	CLA	C1-C2-C3	-2.73	121.72	126.20
25	n	603	CLA	CHB-C4A-NA	2.73	128.34	124.40
25	Y	604	CLA	CMB-C2B-C3B	2.73	132.98	126.55
25	6	602	CLA	C1-C2-C3	-2.73	121.72	126.20
24	5	607	CHL	O2A-CGA-CBA	2.73	120.17	111.83
25	S	602	CLA	CMB-C2B-C1B	-2.73	121.26	125.42
24	y	605	CHL	CMA-C3A-C4A	-2.73	108.72	114.61
28	G	1623	NEX	C31-C30-C29	-2.73	123.45	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	601	CHL	CMD-C2D-C3D	-2.73	119.22	124.68
29	C	522	LHG	O8-C23-C24	2.73	120.16	111.83
24	5	609	CHL	C4-C3-C5	2.73	119.97	115.23
26	r	620	LUT	C37-C21-C22	-2.73	104.31	109.41
25	2	610	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
25	B	604	CLA	CHB-C1B-NB	2.73	128.15	124.05
30	4	623	BCR	C1-C6-C5	-2.73	118.90	122.64
24	R	606	CHL	O2A-CGA-CBA	2.73	120.16	111.83
24	5	601	CHL	C1C-CHC-C4B	2.73	125.84	116.07
25	6	610	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
24	Y	605	CHL	CMA-C3A-C4A	-2.73	108.73	114.61
26	y	1620	LUT	C21-C26-C27	-2.73	109.69	112.83
25	y	604	CLA	CMB-C2B-C3B	2.73	132.97	126.55
25	c	509	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
35	D	411	LMG	O6-C1-O1	-2.73	103.60	110.04
24	3	609	CHL	O2A-CGA-CBA	2.73	120.15	111.83
24	7	609	CHL	O2A-CGA-CBA	2.73	120.15	111.83
26	4	620	LUT	C35-C15-C14	-2.73	117.94	123.52
25	1	613	CLA	CHB-C4A-NA	2.73	128.33	124.40
25	D	402	CLA	CMB-C2B-C1B	-2.72	121.27	125.42
27	r	622	XAT	C4-C3-C2	-2.72	105.70	110.79
24	1	609	CHL	C4-C3-C5	2.72	119.95	115.23
25	b	604	CLA	CHB-C1B-NB	2.72	128.13	124.05
25	C	509	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
25	8	612	CLA	CMB-C2B-C1B	-2.72	121.28	125.42
25	b	605	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
24	1	607	CHL	O2A-CGA-CBA	2.72	120.13	111.83
35	d	411	LMG	O6-C1-O1	-2.72	103.62	110.04
25	6	614	CLA	C4A-NA-C1A	2.72	107.92	106.68
24	6	606	CHL	O1D-CGD-CBD	-2.72	120.60	124.72
25	b	604	CLA	CMB-C2B-C1B	-2.72	121.28	125.42
25	N	603	CLA	CHB-C4A-NA	2.72	128.32	124.40
24	4	601	CHL	CBC-CAC-C3C	-2.72	108.98	112.87
25	b	602	CLA	CHB-C4A-NA	2.72	128.32	124.40
24	5	607	CHL	CAA-C2A-C3A	-2.72	105.66	113.00
26	8	620	LUT	C35-C15-C14	-2.71	117.96	123.52
26	g	1620	LUT	C39-C29-C28	2.71	122.23	118.09
25	s	602	CLA	CMB-C2B-C1B	-2.71	121.29	125.42
25	a	407	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
27	y	1622	XAT	C31-C32-C33	-2.71	118.92	126.36
26	R	620	LUT	C37-C21-C22	-2.71	104.35	109.41
24	r	606	CHL	O2A-CGA-CBA	2.71	120.11	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	L	101	LHG	O8-C23-C24	2.71	120.10	111.83
25	C	512	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
27	N	1622	XAT	C35-C34-C33	-2.71	123.48	127.28
25	D	402	CLA	CBA-CAA-C2A	-2.71	105.73	113.79
26	5	1621	LUT	C30-C31-C32	-2.71	115.35	123.20
25	c	506	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
29	l	101	LHG	O8-C23-C24	2.71	120.09	111.83
24	6	608	CHL	O1D-CGD-CBD	-2.71	120.62	124.72
30	8	623	BCR	C1-C6-C5	-2.71	118.94	122.64
28	g	1623	NEX	C31-C30-C29	-2.71	123.48	127.28
25	D	402	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
25	d	402	CLA	CBA-CAA-C2A	-2.71	105.74	113.79
25	d	402	CLA	CMB-C2B-C1B	-2.71	121.30	125.42
25	G	611	CLA	C3B-C4B-NB	-2.71	108.11	110.53
30	b	620	BCR	C33-C5-C6	-2.71	121.53	124.48
30	B	620	BCR	C20-C21-C22	-2.71	123.48	127.28
25	5	611	CLA	CHB-C4A-NA	2.71	128.31	124.40
27	Y	1622	XAT	C31-C32-C33	-2.71	118.94	126.36
26	1	1621	LUT	C30-C31-C32	-2.70	115.36	123.20
25	C	506	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
25	c	512	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
25	s	604	CLA	CMB-C2B-C1B	-2.70	121.30	125.42
25	A	410	CLA	CHB-C4A-NA	2.70	128.30	124.40
25	b	611	CLA	CHB-C1B-NB	2.70	128.10	124.05
25	d	402	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
30	A	411	BCR	C38-C26-C25	-2.70	121.54	124.48
25	c	511	CLA	CHB-C4A-NA	2.70	128.30	124.40
25	R	612	CLA	CHB-C4A-NA	2.70	128.30	124.40
24	8	601	CHL	CBC-CAC-C3C	-2.70	109.01	112.87
27	4	622	XAT	C15-C35-C34	-2.70	118.00	123.52
26	R	620	LUT	C28-C29-C30	-2.70	114.76	119.01
27	n	1622	XAT	C35-C34-C33	-2.70	123.49	127.28
25	g	611	CLA	C3B-C4B-NB	-2.70	108.12	110.53
25	g	602	CLA	C1-C2-C3	-2.70	121.78	126.20
30	B	620	BCR	C33-C5-C6	-2.70	121.54	124.48
24	Y	606	CHL	C3D-C4D-ND	2.70	117.27	112.94
24	y	606	CHL	C3D-C4D-ND	2.70	117.27	112.94
24	2	608	CHL	O1D-CGD-CBD	-2.70	120.63	124.72
24	Y	607	CHL	O1D-CGD-CBD	-2.70	120.63	124.72
24	1	606	CHL	CBC-CAC-C3C	-2.70	109.01	112.87
26	r	620	LUT	C28-C29-C30	-2.70	114.77	119.01
35	b	622	LMG	O6-C1-O1	-2.70	103.67	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	3	603	CLA	CAA-C2A-C3A	-2.69	105.72	113.00
25	G	602	CLA	C1-C2-C3	-2.69	121.78	126.20
37	c	519	DGD	CDB-CCB-CBB	-2.69	100.75	114.37
25	5	613	CLA	CHB-C4A-NA	2.69	128.29	124.40
25	r	604	CLA	CMB-C2B-C1B	-2.69	121.32	125.42
37	C	519	DGD	CDB-CCB-CBB	-2.69	100.75	114.37
24	2	606	CHL	CMB-C2B-C3B	2.69	130.06	124.68
24	g	606	CHL	C1C-CHC-C4B	2.69	125.70	116.07
24	1	607	CHL	CAA-C2A-C3A	-2.69	105.73	113.00
25	4	612	CLA	CMB-C2B-C1B	-2.69	121.32	125.42
25	1	611	CLA	CHB-C4A-NA	2.69	128.28	124.40
24	8	601	CHL	C1C-CHC-C4B	2.69	125.69	116.07
24	N	607	CHL	CMB-C2B-C3B	2.69	130.06	124.68
25	c	508	CLA	CMB-C2B-C3B	2.69	132.88	126.55
24	3	608	CHL	O1D-CGD-CBD	-2.69	120.64	124.72
30	b	618	BCR	C16-C15-C14	-2.69	118.02	123.52
25	c	504	CLA	CHB-C4A-NA	2.69	128.28	124.40
24	3	607	CHL	C1C-CHC-C4B	2.69	125.68	116.07
25	n	604	CLA	CHB-C1B-NB	2.69	128.08	124.05
24	4	606	CHL	CMB-C2B-C3B	2.69	130.05	124.68
25	7	603	CLA	CAA-C2A-C3A	-2.69	105.74	113.00
25	S	614	CLA	CMB-C2B-C3B	2.68	132.87	126.55
24	6	606	CHL	CMB-C2B-C3B	2.68	130.05	124.68
25	R	604	CLA	CMB-C2B-C1B	-2.68	121.33	125.42
24	n	607	CHL	CMB-C2B-C3B	2.68	130.05	124.68
25	r	612	CLA	CHB-C4A-NA	2.68	128.27	124.40
24	4	601	CHL	C1C-CHC-C4B	2.68	125.67	116.07
34	B	623	SQD	O7-S-C6	2.68	110.76	106.76
24	7	607	CHL	C1C-CHC-C4B	2.68	125.66	116.07
35	B	622	LMG	O6-C1-O1	-2.68	103.71	110.04
25	6	603	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
24	G	606	CHL	C1C-CHC-C4B	2.68	125.66	116.07
24	5	606	CHL	CBC-CAC-C3C	-2.68	109.03	112.87
25	7	612	CLA	CHB-C4A-NA	2.68	128.27	124.40
25	5	602	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
24	R	614	CHL	C1B-CHB-C4A	2.68	123.05	121.32
29	d	409	LHG	O8-C23-C24	2.68	120.00	111.83
25	1	612	CLA	C2A-C1A-CHA	2.68	128.52	123.87
26	Y	1620	LUT	C19-C9-C8	2.68	122.18	118.09
24	3	606	CHL	CMA-C3A-C4A	-2.68	108.84	114.61
24	n	609	CHL	C3D-C4D-ND	2.68	117.24	112.94
26	N	1621	LUT	C31-C30-C29	-2.68	123.52	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	n	1621	LUT	C31-C30-C29	-2.68	123.52	127.28
25	B	615	CLA	CMB-C2B-C1B	-2.68	121.34	125.42
25	1	602	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
36	D	405	PL9	C22-C23-C24	-2.68	121.49	127.62
24	N	609	CHL	C3D-C4D-ND	2.68	117.23	112.94
25	G	604	CLA	CHB-C1B-NB	2.68	128.06	124.05
25	N	604	CLA	CHB-C1B-NB	2.68	128.06	124.05
24	r	614	CHL	C1B-CHB-C4A	2.68	123.05	121.32
25	a	410	CLA	CHB-C4A-NA	2.68	128.26	124.40
25	R	601	CLA	CAC-C3C-C2C	-2.68	122.64	127.56
28	s	1623	NEX	C11-C12-C13	-2.68	119.03	126.36
34	b	623	SQD	O7-S-C6	2.67	110.75	106.76
24	8	606	CHL	CMB-C2B-C3B	2.67	130.03	124.68
26	G	1620	LUT	C39-C29-C28	2.67	122.17	118.09
33	A	409	PHO	O1D-CGD-CBD	2.67	128.78	124.72
25	C	508	CLA	CMB-C2B-C3B	2.67	132.84	126.55
30	a	411	BCR	C38-C26-C25	-2.67	121.57	124.48
25	8	610	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
25	C	511	CLA	CHB-C4A-NA	2.67	128.26	124.40
29	D	409	LHG	O8-C23-C24	2.67	119.99	111.83
25	b	615	CLA	CMB-C2B-C1B	-2.67	121.35	125.42
25	1	603	CLA	CAA-C2A-C3A	-2.67	105.78	113.00
24	7	607	CHL	O2A-CGA-CBA	2.67	119.98	111.83
30	B	618	BCR	C16-C15-C14	-2.67	118.05	123.52
25	N	614	CLA	CHB-C4A-NA	2.67	128.26	124.40
26	2	1621	LUT	C21-C26-C27	-2.67	109.75	112.83
24	n	609	CHL	CAA-C2A-C3A	-2.67	105.78	113.00
25	C	504	CLA	CHB-C4A-NA	2.67	128.25	124.40
25	4	604	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
25	6	602	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
27	8	622	XAT	C15-C35-C34	-2.67	118.06	123.52
25	6	612	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
25	5	603	CLA	CAA-C2A-C3A	-2.67	105.79	113.00
25	S	604	CLA	CMB-C2B-C1B	-2.67	121.36	125.42
24	7	608	CHL	O1D-CGD-CBD	-2.67	120.68	124.72
25	g	604	CLA	CHB-C1B-NB	2.67	128.05	124.05
24	7	606	CHL	CMA-C3A-C4A	-2.67	108.87	114.61
24	N	609	CHL	CAA-C2A-C3A	-2.67	105.79	113.00
25	s	614	CLA	CMB-C2B-C3B	2.67	132.82	126.55
28	g	1623	NEX	C11-C12-C13	-2.67	119.05	126.36
30	4	623	BCR	C7-C8-C9	-2.67	122.29	126.23
25	3	612	CLA	CHB-C4A-NA	2.66	128.25	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	612	CLA	C2A-C1A-CHA	2.66	128.49	123.87
25	n	614	CLA	CHB-C4A-NA	2.66	128.25	124.40
30	8	623	BCR	C7-C8-C9	-2.66	122.30	126.23
25	B	607	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
24	g	601	CHL	CMA-C3A-C4A	-2.66	108.87	114.61
28	G	1623	NEX	C11-C12-C13	-2.66	119.06	126.36
26	y	1620	LUT	C19-C9-C8	2.66	122.16	118.09
36	d	405	PL9	C22-C23-C24	-2.66	121.53	127.62
25	C	510	CLA	CMB-C2B-C3B	2.66	132.81	126.55
25	y	614	CLA	CHB-C4A-NA	2.66	128.24	124.40
24	7	606	CHL	CMB-C2B-C3B	2.66	130.00	124.68
33	a	409	PHO	O1D-CGD-CBD	2.66	128.76	124.72
25	2	603	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
24	1	608	CHL	CBC-CAC-C3C	-2.66	109.06	112.87
25	4	610	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
25	r	601	CLA	CAC-C3C-C2C	-2.66	122.67	127.56
24	G	601	CHL	C1C-C2C-CMC	2.66	131.60	126.80
24	3	607	CHL	O2A-CGA-CBA	2.66	119.94	111.83
25	2	602	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
25	B	605	CLA	CHB-C4A-NA	2.66	128.24	124.40
28	y	1623	NEX	C35-C15-C14	-2.66	118.08	123.52
35	b	622	LMG	C38-C37-C36	-2.66	100.94	114.37
24	n	608	CHL	CBC-CAC-C3C	-2.66	109.07	112.87
24	y	607	CHL	O1D-CGD-CBD	-2.66	120.69	124.72
35	B	622	LMG	C38-C37-C36	-2.66	100.94	114.37
28	1	1623	NEX	C16-C1-C6	2.65	112.85	110.47
26	6	1621	LUT	C21-C26-C27	-2.65	109.77	112.83
24	G	601	CHL	CMA-C3A-C4A	-2.65	108.89	114.61
25	s	604	CLA	CHB-C4A-NA	2.65	128.23	124.40
30	B	619	BCR	C29-C30-C25	2.65	114.29	110.44
28	S	1623	NEX	C11-C12-C13	-2.65	119.09	126.36
25	8	604	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
24	5	607	CHL	O1D-CGD-CBD	-2.65	120.70	124.72
24	1	607	CHL	O1D-CGD-CBD	-2.65	120.70	124.72
24	N	608	CHL	CBC-CAC-C3C	-2.65	109.08	112.87
25	c	510	CLA	CMB-C2B-C3B	2.65	132.78	126.55
24	5	608	CHL	CBC-CAC-C3C	-2.65	109.08	112.87
30	b	619	BCR	C29-C30-C25	2.65	114.29	110.44
25	S	604	CLA	CHB-C4A-NA	2.65	128.22	124.40
25	B	604	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
25	R	601	CLA	CHB-C4A-NA	2.65	128.22	124.40
25	8	602	CLA	CMB-C2B-C1B	-2.65	121.39	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	607	CHL	O2A-CGA-CBA	2.65	119.90	111.83
25	Y	611	CLA	CHB-C1B-NB	2.65	128.02	124.05
25	Y	614	CLA	CHB-C4A-NA	2.65	128.22	124.40
28	Y	1623	NEX	C35-C15-C14	-2.65	118.11	123.52
25	2	612	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
25	N	613	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
26	1	1621	LUT	C8-C7-C6	-2.64	119.94	127.00
28	2	1623	NEX	C16-C1-C6	2.64	112.84	110.47
25	a	406	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
25	b	607	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
24	3	606	CHL	CMB-C2B-C3B	2.64	129.96	124.68
25	R	611	CLA	C3B-C4B-NB	-2.64	108.17	110.53
24	g	601	CHL	C1C-C2C-CMC	2.64	131.56	126.80
29	6	2630	LHG	O8-C23-C24	2.64	119.89	111.83
25	B	613	CLA	CMD-C2D-C3D	2.64	133.74	127.69
24	2	609	CHL	C1-C2-C3	-2.64	121.87	126.20
26	5	1621	LUT	C8-C7-C6	-2.64	119.95	127.00
25	B	617	CLA	CHB-C4A-NA	2.64	128.21	124.40
25	y	611	CLA	CHB-C1B-NB	2.64	128.01	124.05
29	2	2630	LHG	O8-C23-C24	2.64	119.87	111.83
25	b	604	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
29	c	522	LHG	C11-C10-C9	-2.64	101.05	114.37
25	g	602	CLA	CMB-C2B-C3B	2.64	132.75	126.55
25	r	602	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
25	r	611	CLA	C3B-C4B-NB	-2.63	108.18	110.53
25	b	617	CLA	CHB-C4A-NA	2.63	128.20	124.40
28	s	1623	NEX	C15-C35-C34	-2.63	118.13	123.52
25	b	605	CLA	CHB-C4A-NA	2.63	128.20	124.40
24	6	607	CHL	O2A-CGA-CBA	2.63	119.86	111.83
25	S	613	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
29	C	522	LHG	C11-C10-C9	-2.63	101.06	114.37
25	n	610	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
25	n	602	CLA	CAC-C3C-C4C	2.63	128.21	124.79
25	N	604	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
24	N	606	CHL	CMA-C3A-C4A	-2.63	108.94	114.61
25	G	603	CLA	CHB-C4A-NA	2.63	128.19	124.40
24	n	606	CHL	CMA-C3A-C4A	-2.63	108.95	114.61
24	7	609	CHL	CMA-C3A-C4A	-2.63	108.95	114.61
25	r	601	CLA	CHB-C4A-NA	2.63	128.19	124.40
25	3	611	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
27	3	1622	XAT	C19-C9-C8	2.63	122.10	118.09
28	6	1623	NEX	C16-C1-C6	2.62	112.82	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	611	CLA	O2D-CGD-CBD	2.62	115.82	111.23
25	b	613	CLA	CMD-C2D-C3D	2.62	133.71	127.69
25	A	406	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
25	G	602	CLA	CMB-C2B-C3B	2.62	132.72	126.55
24	n	609	CHL	CMB-C2B-C3B	2.62	129.92	124.68
25	n	613	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
35	z	101	LMG	C1-O6-C5	-2.62	108.60	113.72
24	3	609	CHL	CMA-C3A-C4A	-2.62	108.96	114.61
25	4	602	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
25	S	614	CLA	CHB-C4A-NA	2.62	128.18	124.40
25	R	602	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
25	C	513	CLA	CHB-C4A-NA	2.62	128.18	124.40
24	g	606	CHL	CMA-C3A-C4A	-2.62	108.97	114.61
35	Z	101	LMG	C1-O6-C5	-2.62	108.60	113.72
25	7	611	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
28	S	1623	NEX	C15-C35-C34	-2.62	118.16	123.52
24	G	606	CHL	CMA-C3A-C4A	-2.62	108.97	114.61
25	y	602	CLA	CAA-CBA-CGA	-2.62	105.77	113.21
28	Y	1623	NEX	C30-C31-C32	-2.62	115.61	123.20
25	Y	603	CLA	CHB-C4A-NA	2.62	128.18	124.40
24	g	609	CHL	O2D-CGD-O1D	-2.62	118.75	123.85
25	y	603	CLA	CHB-C4A-NA	2.62	128.18	124.40
25	s	613	CLA	CMB-C2B-C1B	-2.62	121.44	125.42
30	b	619	BCR	C21-C20-C19	-2.61	115.62	123.20
25	c	513	CLA	CHB-C4A-NA	2.61	128.17	124.40
26	Y	1621	LUT	C15-C35-C34	-2.61	118.17	123.52
25	Y	602	CLA	CAA-CBA-CGA	-2.61	105.79	113.21
34	A	418	SQD	O5-C5-C4	2.61	114.41	109.70
24	6	609	CHL	C1-C2-C3	-2.61	121.92	126.20
29	g	2630	LHG	C20-C19-C18	-2.61	101.16	114.37
30	8	623	BCR	C27-C26-C25	-2.61	119.17	122.70
24	y	609	CHL	C4-C3-C5	2.61	119.76	115.23
24	6	607	CHL	CED-O2D-CGD	2.61	121.84	115.92
30	c	515	BCR	C33-C5-C4	2.61	119.16	113.60
28	5	1623	NEX	C16-C1-C6	2.61	112.81	110.47
30	B	619	BCR	C21-C20-C19	-2.61	115.64	123.20
28	y	1623	NEX	C30-C31-C32	-2.61	115.64	123.20
24	N	609	CHL	CMB-C2B-C3B	2.61	129.90	124.68
25	Y	602	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
25	N	610	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
25	n	604	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
25	g	603	CLA	CHB-C4A-NA	2.61	128.16	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	s	613	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
25	S	613	CLA	CMB-C2B-C1B	-2.61	121.45	125.42
24	2	607	CHL	CED-O2D-CGD	2.61	121.83	115.92
24	6	607	CHL	CBA-CAA-C2A	-2.60	106.11	113.78
25	B	610	CLA	CHB-C4A-NA	2.60	128.16	124.40
24	G	609	CHL	O2D-CGD-O1D	-2.60	118.78	123.85
24	R	607	CHL	C4-C3-C5	2.60	119.75	115.23
25	y	603	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
29	G	2630	LHG	C20-C19-C18	-2.60	101.21	114.37
27	r	622	XAT	C38-C25-C24	2.60	117.17	114.24
25	5	610	CLA	C3B-C4B-NB	-2.60	108.21	110.53
24	8	601	CHL	OMC-CMC-C2C	-2.60	120.60	125.12
24	n	609	CHL	CAC-C3C-C4C	2.60	130.72	124.03
24	4	601	CHL	OMC-CMC-C2C	-2.60	120.60	125.12
25	b	610	CLA	CHB-C4A-NA	2.60	128.15	124.40
24	Y	609	CHL	C4-C3-C5	2.60	119.74	115.23
26	g	1621	LUT	C31-C30-C29	-2.60	123.63	127.28
27	7	1622	XAT	C19-C9-C8	2.60	122.06	118.09
35	B	622	LMG	C40-C39-C38	-2.60	101.23	114.37
26	y	1621	LUT	C39-C29-C28	2.60	122.06	118.09
35	b	622	LMG	C40-C39-C38	-2.60	101.24	114.37
25	C	509	CLA	CMB-C2B-C1B	-2.60	121.47	125.42
24	4	609	CHL	CMA-C3A-C4A	-2.60	109.02	114.61
30	C	515	BCR	C33-C5-C4	2.60	119.13	113.60
35	A	413	LMG	O3-C3-C2	-2.60	104.26	110.38
24	7	607	CHL	O1D-CGD-CBD	-2.60	120.79	124.72
26	y	1621	LUT	C8-C9-C10	-2.60	114.93	119.01
25	s	614	CLA	CHB-C4A-NA	2.60	128.15	124.40
25	S	610	CLA	CHB-C4A-NA	2.60	128.15	124.40
29	l	101	LHG	C11-C10-C9	-2.59	101.25	114.37
26	Y	1621	LUT	C39-C29-C28	2.59	122.05	118.09
25	2	611	CLA	O2D-CGD-CBD	2.59	115.77	111.23
30	B	619	BCR	C10-C11-C12	-2.59	115.68	123.20
30	B	619	BCR	C28-C27-C26	-2.59	109.43	114.06
24	y	609	CHL	O2D-CGD-O1D	-2.59	118.80	123.85
24	r	607	CHL	C4-C3-C5	2.59	119.73	115.23
24	N	609	CHL	CAC-C3C-C4C	2.59	130.69	124.03
25	c	513	CLA	CBA-CAA-C2A	2.59	121.51	113.79
25	1	610	CLA	C3B-C4B-NB	-2.59	108.22	110.53
25	s	610	CLA	C3B-C4B-NB	-2.59	108.22	110.53
24	n	605	CHL	OMC-CMC-C2C	-2.59	120.62	125.12
27	2	1622	XAT	C6-C7-C8	-2.59	120.51	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	L	101	LHG	C11-C10-C9	-2.59	101.27	114.37
26	y	1621	LUT	C15-C35-C34	-2.59	118.22	123.52
24	2	607	CHL	CBA-CAA-C2A	-2.59	106.14	113.78
34	a	418	SQD	O5-C5-C4	2.59	114.37	109.70
25	g	602	CLA	CHB-C4A-NA	2.59	128.14	124.40
24	Y	609	CHL	O2D-CGD-O1D	-2.59	118.80	123.85
26	G	1621	LUT	C31-C30-C29	-2.59	123.64	127.28
25	Y	603	CLA	C3B-C4B-NB	-2.59	108.22	110.53
25	a	407	CLA	CHB-C4A-NA	2.59	128.14	124.40
24	2	609	CHL	C4-C3-C5	2.59	119.72	115.23
27	2	1622	XAT	C10-C11-C12	-2.59	115.69	123.20
26	2	1620	LUT	C8-C7-C6	-2.59	120.08	127.00
25	y	602	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
26	4	620	LUT	C8-C7-C6	-2.59	120.08	127.00
25	r	602	CLA	CAA-CBA-CGA	-2.59	105.86	113.21
30	b	619	BCR	C10-C11-C12	-2.59	115.70	123.20
24	6	609	CHL	CMA-C3A-C4A	-2.59	109.03	114.61
26	Y	1620	LUT	C15-C35-C34	-2.59	118.22	123.52
35	a	413	LMG	O3-C3-C2	-2.59	104.28	110.38
25	s	610	CLA	CHB-C4A-NA	2.59	128.13	124.40
27	6	1622	XAT	C10-C11-C12	-2.59	115.70	123.20
27	R	622	XAT	C38-C25-C24	2.59	117.15	114.24
27	6	1622	XAT	C6-C7-C8	-2.59	120.52	125.99
24	3	607	CHL	O1D-CGD-CBD	-2.59	120.80	124.72
25	B	610	CLA	C7-C6-C5	-2.59	106.37	113.26
30	B	620	BCR	C16-C15-C14	-2.59	118.23	123.52
28	y	1623	NEX	C39-C29-C30	-2.59	118.63	122.82
25	A	407	CLA	CHB-C4A-NA	2.59	128.13	124.40
24	N	605	CHL	OMC-CMC-C2C	-2.59	120.63	125.12
25	D	402	CLA	C3B-C4B-NB	-2.59	108.22	110.53
24	2	609	CHL	CMA-C3A-C4A	-2.59	109.04	114.61
24	G	601	CHL	O2A-CGA-CBA	2.59	119.72	111.83
24	6	607	CHL	C1-C2-C3	-2.58	121.96	126.20
25	4	611	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
36	D	405	PL9	C27-C28-C29	-2.58	121.71	127.62
25	6	613	CLA	CHB-C4A-NA	2.58	128.13	124.40
30	b	620	BCR	C16-C15-C14	-2.58	118.23	123.52
26	6	1620	LUT	C8-C7-C6	-2.58	120.10	127.00
25	Y	613	CLA	CAC-C3C-C4C	2.58	128.15	124.79
25	D	403	CLA	CMB-C2B-C3B	2.58	132.63	126.55
25	Y	603	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
24	g	601	CHL	O2A-CGA-CBA	2.58	119.71	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	607	CHL	C1-C2-C3	-2.58	121.97	126.20
25	Y	612	CLA	C1-C2-C3	-2.58	121.97	126.20
29	g	2630	LHG	C11-C10-C9	-2.58	101.32	114.37
26	G	1620	LUT	C19-C9-C8	2.58	122.03	118.09
25	2	613	CLA	CHB-C4A-NA	2.58	128.12	124.40
25	G	613	CLA	CHC-C4B-NB	2.58	127.92	124.05
36	d	405	PL9	C27-C28-C29	-2.58	121.72	127.62
26	8	620	LUT	C8-C7-C6	-2.58	120.11	127.00
25	d	402	CLA	C3B-C4B-NB	-2.58	108.23	110.53
25	R	602	CLA	CAA-CBA-CGA	-2.58	105.88	113.21
30	4	623	BCR	C27-C26-C25	-2.58	119.22	122.70
24	Y	608	CHL	O2A-CGA-CBA	2.58	119.70	111.83
30	b	619	BCR	C28-C27-C26	-2.58	109.46	114.06
26	s	1620	LUT	C16-C1-C6	-2.58	106.20	110.24
25	y	612	CLA	C1-C2-C3	-2.58	121.97	126.20
25	N	602	CLA	CAC-C3C-C4C	2.58	128.14	124.79
25	R	612	CLA	C3B-C4B-NB	-2.58	108.23	110.53
25	r	612	CLA	C3B-C4B-NB	-2.58	108.23	110.53
25	3	604	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
24	s	607	CHL	OMC-CMC-C2C	-2.58	120.64	125.12
25	d	403	CLA	CMB-C2B-C3B	2.58	132.61	126.55
26	y	1620	LUT	C15-C35-C34	-2.58	118.25	123.52
25	c	509	CLA	CMB-C2B-C1B	-2.58	121.50	125.42
26	g	1620	LUT	C19-C9-C8	2.58	122.02	118.09
29	1	2630	LHG	O8-C23-C24	2.57	119.69	111.83
25	b	610	CLA	C7-C6-C5	-2.57	106.40	113.26
25	N	603	CLA	C3B-C4B-NB	-2.57	108.23	110.53
25	C	513	CLA	CBA-CAA-C2A	2.57	121.45	113.79
25	3	611	CLA	CHB-C4A-NA	2.57	128.11	124.40
24	r	608	CHL	OBD-CAD-C3D	-2.57	123.88	127.89
24	5	601	CHL	CMA-C3A-C4A	-2.57	109.07	114.61
24	g	601	CHL	CAC-C3C-C4C	2.57	130.64	124.03
29	C	2630	LHG	C11-C10-C9	-2.57	101.36	114.37
29	G	2630	LHG	C11-C10-C9	-2.57	101.37	114.37
30	C	517	BCR	C33-C5-C4	2.57	119.08	113.60
29	d	410	LHG	C11-C10-C9	-2.57	101.37	114.37
26	Y	1621	LUT	C8-C9-C10	-2.57	114.96	119.01
36	d	405	PL9	C40-C39-C41	2.57	119.69	115.23
24	8	609	CHL	CMA-C3A-C4A	-2.57	109.07	114.61
25	7	604	CLA	CHB-C4A-NA	2.57	128.11	124.40
24	3	608	CHL	CMB-C2B-C3B	2.57	129.82	124.68
29	c	2630	LHG	C11-C10-C9	-2.57	101.38	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	D	410	LHG	C11-C10-C9	-2.57	101.38	114.37
25	7	612	CLA	C4A-NA-C1A	2.57	107.85	106.68
24	6	609	CHL	C4-C3-C5	2.57	119.69	115.23
30	C	517	BCR	C38-C26-C25	-2.57	121.68	124.48
35	C	521	LMG	O6-C1-O1	-2.57	103.98	110.04
24	G	601	CHL	C4-C3-C5	2.57	119.68	115.23
26	S	1620	LUT	C31-C30-C29	-2.57	123.68	127.28
26	7	1620	LUT	C37-C21-C22	-2.57	104.62	109.41
29	5	2630	LHG	O8-C23-C24	2.57	119.66	111.83
24	3	605	CHL	OMC-CMC-C2C	-2.57	120.66	125.12
35	c	521	LMG	O6-C1-O1	-2.57	103.98	110.04
26	6	1620	LUT	C19-C9-C8	2.57	122.01	118.09
30	c	517	BCR	C33-C5-C4	2.57	119.07	113.60
25	7	604	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
26	7	1620	LUT	C31-C30-C29	-2.57	123.68	127.28
26	r	620	LUT	C35-C15-C14	-2.57	118.27	123.52
25	8	611	CLA	O2D-CGD-O1D	-2.57	118.86	123.85
24	S	607	CHL	OMC-CMC-C2C	-2.56	120.67	125.12
26	S	1620	LUT	C16-C1-C6	-2.56	106.22	110.24
30	b	620	BCR	C10-C11-C12	-2.56	115.77	123.20
25	G	602	CLA	CHB-C4A-NA	2.56	128.10	124.40
24	y	608	CHL	O2A-CGA-CBA	2.56	119.65	111.83
26	S	1620	LUT	C39-C29-C28	2.56	122.00	118.09
24	g	606	CHL	OMC-CMC-C2C	-2.56	120.67	125.12
30	C	516	BCR	C11-C10-C9	-2.56	123.68	127.28
25	7	611	CLA	CHB-C4A-NA	2.56	128.10	124.40
26	R	620	LUT	C35-C15-C14	-2.56	118.28	123.52
24	3	607	CHL	C4-C3-C5	2.56	119.67	115.23
26	3	1620	LUT	C31-C30-C29	-2.56	123.69	127.28
24	n	605	CHL	CBC-CAC-C3C	-2.56	109.21	112.87
24	7	605	CHL	OMC-CMC-C2C	-2.56	120.67	125.12
26	2	1620	LUT	C19-C9-C8	2.56	122.00	118.09
28	Y	1623	NEX	C39-C29-C30	-2.56	118.67	122.82
24	G	601	CHL	CAC-C3C-C4C	2.56	130.61	124.03
24	7	607	CHL	C4-C3-C5	2.56	119.67	115.23
30	t	101	BCR	C8-C9-C10	2.56	123.03	119.01
24	G	606	CHL	OMC-CMC-C2C	-2.56	120.68	125.12
27	y	1622	XAT	C7-C8-C9	-2.56	121.56	125.53
25	y	603	CLA	C1-C2-C3	-2.56	122.00	126.20
25	g	613	CLA	CHC-C4B-NB	2.56	127.89	124.05
26	5	1620	LUT	C39-C29-C28	2.56	122.00	118.09
25	y	603	CLA	C3B-C4B-NB	-2.56	108.25	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	Y	1622	XAT	C7-C8-C9	-2.56	121.56	125.53
25	b	613	CLA	C3B-C4B-NB	-2.56	108.25	110.53
25	1	604	CLA	CHB-C4A-NA	2.56	128.09	124.40
26	3	1620	LUT	C37-C21-C22	-2.56	104.64	109.41
34	b	621	SQD	C44-O6-C1	2.56	119.28	113.80
24	1	601	CHL	CMA-C3A-C4A	-2.56	109.10	114.61
24	7	608	CHL	CMB-C2B-C3B	2.56	129.79	124.68
24	g	601	CHL	C4-C3-C5	2.56	119.66	115.23
24	G	601	CHL	OBD-CAD-C3D	-2.56	123.91	127.89
25	b	614	CLA	CAA-C2A-C3A	-2.56	106.09	113.00
24	R	607	CHL	C1-C2-C3	-2.55	122.01	126.20
30	c	517	BCR	C38-C26-C25	-2.55	121.70	124.48
34	B	621	SQD	C44-O6-C1	2.55	119.27	113.80
24	Y	608	CHL	OBD-CAD-C3D	-2.55	123.91	127.89
25	7	614	CLA	CHB-C4A-NA	2.55	128.09	124.40
36	D	405	PL9	C40-C39-C41	2.55	119.66	115.23
24	4	607	CHL	OMC-CMC-C2C	-2.55	120.69	125.12
28	S	1623	NEX	C39-C29-C30	-2.55	118.68	122.82
28	s	1623	NEX	C39-C29-C30	-2.55	118.68	122.82
25	G	612	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
25	B	614	CLA	CAA-C2A-C3A	-2.55	106.11	113.00
25	y	603	CLA	CAA-C2A-C3A	-2.55	106.11	113.00
30	T	101	BCR	C8-C9-C10	2.55	123.02	119.01
24	R	608	CHL	OBD-CAD-C3D	-2.55	123.92	127.89
24	8	607	CHL	OMC-CMC-C2C	-2.55	120.69	125.12
25	g	612	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
24	R	607	CHL	CMA-C3A-C4A	-2.55	109.12	114.61
26	s	1620	LUT	C39-C29-C28	2.55	121.98	118.09
25	Y	603	CLA	CAA-C2A-C3A	-2.55	106.11	113.00
26	n	1620	LUT	C39-C29-C28	2.55	121.98	118.09
24	r	606	CHL	C1-C2-C3	-2.55	122.02	126.20
30	B	620	BCR	C10-C11-C12	-2.55	115.82	123.20
25	4	603	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
25	Y	603	CLA	C1-C2-C3	-2.55	122.02	126.20
26	y	1621	LUT	C28-C29-C30	-2.55	115.00	119.01
25	3	614	CLA	CHB-C4A-NA	2.55	128.07	124.40
24	1	601	CHL	CBC-CAC-C3C	-2.55	109.23	112.87
29	3	2630	LHG	C11-C10-C9	-2.55	101.50	114.37
25	7	614	CLA	C3B-C4B-NB	-2.55	108.26	110.53
24	r	607	CHL	CMA-C3A-C4A	-2.55	109.12	114.61
25	y	613	CLA	CAC-C3C-C4C	2.55	128.10	124.79
25	3	612	CLA	C4A-NA-C1A	2.54	107.84	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	613	CLA	CHB-C4A-NA	2.54	128.07	124.40
26	s	1620	LUT	C31-C30-C29	-2.54	123.71	127.28
26	g	1621	LUT	C19-C9-C8	2.54	121.97	118.09
25	B	613	CLA	CAA-CBA-CGA	-2.54	105.99	113.21
25	3	604	CLA	CHB-C4A-NA	2.54	128.07	124.40
24	N	605	CHL	CBC-CAC-C3C	-2.54	109.24	112.87
29	7	2630	LHG	C11-C10-C9	-2.54	101.53	114.37
25	R	603	CLA	CHB-C4A-NA	2.54	128.06	124.40
25	y	613	CLA	CHB-C4A-NA	2.54	128.06	124.40
30	h	101	BCR	C3-C4-C5	-2.54	109.53	114.06
25	S	610	CLA	C3B-C4B-NB	-2.54	108.26	110.53
25	4	612	CLA	CHB-C4A-NA	2.54	128.06	124.40
25	4	610	CLA	C4A-NA-C1A	2.54	107.84	106.68
24	g	601	CHL	OBD-CAD-C3D	-2.54	123.93	127.89
26	1	1620	LUT	C39-C29-C28	2.54	121.97	118.09
26	Y	1621	LUT	C28-C29-C30	-2.54	115.02	119.01
25	B	613	CLA	C3B-C4B-NB	-2.54	108.27	110.53
28	y	1623	NEX	C31-C30-C29	-2.54	123.72	127.28
25	5	604	CLA	CHB-C4A-NA	2.54	128.06	124.40
25	4	612	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
29	S	2630	LHG	O8-C23-C24	2.54	119.56	111.83
25	b	613	CLA	CAA-CBA-CGA	-2.53	106.01	113.21
25	8	612	CLA	CHB-C4A-NA	2.53	128.06	124.40
24	y	608	CHL	OBD-CAD-C3D	-2.53	123.94	127.89
24	g	609	CHL	C4-C3-C5	2.53	119.62	115.23
37	h	102	DGD	O2D-C2D-C1D	-2.53	104.04	110.08
24	r	607	CHL	C1-C2-C3	-2.53	122.05	126.20
25	8	603	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
37	H	102	DGD	O2D-C2D-C1D	-2.53	104.04	110.08
29	D	409	LHG	C20-C19-C18	-2.53	101.57	114.37
25	a	406	CLA	O2D-CGD-CBD	2.53	115.66	111.23
24	R	606	CHL	C1-C2-C3	-2.53	122.05	126.20
24	N	606	CHL	CBC-CAC-C3C	-2.53	109.25	112.87
24	5	601	CHL	CBC-CAC-C3C	-2.53	109.25	112.87
29	s	2630	LHG	O8-C23-C24	2.53	119.55	111.83
25	r	603	CLA	CHB-C4A-NA	2.53	128.05	124.40
25	S	612	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
29	c	2630	LHG	C20-C19-C18	-2.53	101.58	114.37
29	C	2630	LHG	C20-C19-C18	-2.53	101.58	114.37
28	Y	1623	NEX	C31-C30-C29	-2.53	123.73	127.28
25	3	614	CLA	C3B-C4B-NB	-2.53	108.27	110.53
26	N	1620	LUT	C39-C29-C28	2.53	121.95	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	n	1621	LUT	C19-C9-C8	2.53	121.95	118.09
30	H	101	BCR	C3-C4-C5	-2.53	109.55	114.06
24	n	606	CHL	CBC-CAC-C3C	-2.53	109.26	112.87
29	d	409	LHG	C20-C19-C18	-2.53	101.60	114.37
35	Z	101	LMG	O8-C28-O10	-2.53	117.31	123.63
30	T	101	BCR	C29-C30-C25	2.53	114.11	110.44
25	n	603	CLA	C3B-C4B-NB	-2.52	108.28	110.53
25	y	612	CLA	C3B-C4B-NB	-2.52	108.28	110.53
25	R	612	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
25	d	402	CLA	CAA-CBA-CGA	-2.52	106.05	113.21
25	n	602	CLA	CAA-CBA-CGA	-2.52	106.05	113.21
25	g	604	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
24	G	609	CHL	C4-C3-C5	2.52	119.61	115.23
25	A	406	CLA	O2D-CGD-CBD	2.52	115.64	111.23
25	s	604	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
25	N	602	CLA	CAA-CBA-CGA	-2.52	106.05	113.21
28	S	1623	NEX	C19-C9-C10	-2.52	118.73	122.82
25	N	612	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
26	S	1621	LUT	C19-C9-C8	2.52	121.93	118.09
25	N	611	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
24	3	609	CHL	O2D-CGD-O1D	-2.52	118.95	123.85
33	A	409	PHO	O2D-CGD-O1D	-2.52	118.95	123.85
24	n	606	CHL	C1C-CHC-C4B	2.52	125.07	116.07
25	D	402	CLA	CAA-CBA-CGA	-2.51	106.07	113.21
24	N	606	CHL	C1C-CHC-C4B	2.51	125.07	116.07
26	G	1621	LUT	C19-C9-C8	2.51	121.93	118.09
24	7	609	CHL	O2D-CGD-O1D	-2.51	118.95	123.85
25	s	612	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
25	n	612	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
24	3	609	CHL	CMB-C2B-C3B	2.51	129.71	124.68
25	g	602	CLA	C6-C7-C8	-2.51	107.62	115.97
29	d	409	LHG	C18-C17-C16	-2.51	101.68	114.37
29	D	409	LHG	C18-C17-C16	-2.51	101.68	114.37
24	Y	601	CHL	O2A-CGA-CBA	2.51	119.49	111.83
26	N	1621	LUT	C19-C9-C8	2.51	121.92	118.09
25	1	602	CLA	C3B-C4B-NB	-2.51	108.29	110.53
25	Y	612	CLA	C3B-C4B-NB	-2.51	108.29	110.53
35	z	101	LMG	O8-C28-O10	-2.51	117.35	123.63
25	r	612	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
34	b	623	SQD	O48-C23-C24	2.51	119.48	111.83
35	a	413	LMG	C40-C39-C38	-2.51	101.70	114.37
25	r	610	CLA	O2A-CGA-O1A	-2.51	117.36	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	509	CLA	CAA-C2A-C3A	-2.51	106.23	113.00
24	7	609	CHL	CMB-C2B-C3B	2.51	129.69	124.68
24	R	608	CHL	C3D-C4D-ND	2.51	116.96	112.94
25	c	509	CLA	CAA-C2A-C3A	-2.51	106.23	113.00
26	r	620	LUT	C19-C9-C8	2.51	121.92	118.09
26	8	620	LUT	C1-C6-C5	-2.50	119.21	122.64
25	g	603	CLA	CHB-C1B-NB	2.50	127.81	124.05
25	G	604	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
25	8	612	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
24	y	601	CHL	O2A-CGA-CBA	2.50	119.47	111.83
25	8	610	CLA	C4A-NA-C1A	2.50	107.82	106.68
25	S	604	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
25	4	610	CLA	C3B-C4B-NB	-2.50	108.30	110.53
25	B	615	CLA	CHB-C4A-NA	2.50	128.01	124.40
30	c	516	BCR	C11-C10-C9	-2.50	123.77	127.28
35	A	413	LMG	C40-C39-C38	-2.50	101.72	114.37
24	n	606	CHL	CAC-C3C-C4C	2.50	130.46	124.03
25	R	610	CLA	O2A-CGA-O1A	-2.50	117.37	123.63
30	t	101	BCR	C29-C30-C25	2.50	114.07	110.44
24	S	607	CHL	O2A-CGA-CBA	2.50	119.45	111.83
25	B	605	CLA	C2D-C1D-ND	-2.50	107.65	110.13
25	b	615	CLA	CHB-C4A-NA	2.50	128.00	124.40
24	S	607	CHL	O1D-CGD-CBD	-2.50	120.94	124.72
25	r	609	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
25	G	602	CLA	C6-C7-C8	-2.50	107.66	115.97
24	s	607	CHL	O1D-CGD-CBD	-2.50	120.94	124.72
26	4	620	LUT	C1-C6-C5	-2.50	119.22	122.64
24	N	606	CHL	CAC-C3C-C4C	2.50	130.45	124.03
34	B	623	SQD	O48-C23-C24	2.50	119.44	111.83
25	n	611	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
24	r	608	CHL	C3D-C4D-ND	2.50	116.94	112.94
26	6	1621	LUT	C8-C7-C6	-2.50	120.33	127.00
26	2	1621	LUT	C35-C15-C14	-2.49	118.41	123.52
30	C	517	BCR	C11-C12-C13	-2.49	119.52	126.36
28	s	1623	NEX	C19-C9-C10	-2.49	118.78	122.82
27	5	1622	XAT	C24-C23-C22	-2.49	106.13	110.79
26	s	1621	LUT	C19-C9-C8	2.49	121.90	118.09
25	6	611	CLA	C3B-C4B-NB	-2.49	108.31	110.53
25	1	613	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
29	r	2630	LHG	C11-C10-C9	-2.49	101.77	114.37
30	4	623	BCR	C29-C30-C25	2.49	114.06	110.44
25	g	610	CLA	CHB-C4A-NA	2.49	127.99	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	603	CLA	CHB-C1B-NB	2.49	127.78	124.05
25	2	604	CLA	O2A-CGA-O1A	-2.49	116.93	123.33
27	1	1622	XAT	C24-C23-C22	-2.49	106.13	110.79
33	a	409	PHO	O2D-CGD-O1D	-2.49	119.00	123.85
29	R	2630	LHG	C11-C10-C9	-2.49	101.79	114.37
26	6	1621	LUT	C35-C15-C14	-2.49	118.43	123.52
25	6	604	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
25	5	613	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
26	R	620	LUT	C19-C9-C8	2.49	121.89	118.09
25	8	610	CLA	C3B-C4B-NB	-2.49	108.31	110.53
24	7	606	CHL	O2D-CGD-O1D	-2.49	119.01	123.85
24	3	606	CHL	O2D-CGD-O1D	-2.48	119.01	123.85
24	s	607	CHL	O2A-CGA-CBA	2.48	119.41	111.83
24	G	608	CHL	CMB-C2B-C3B	2.48	129.65	124.68
25	6	604	CLA	O2A-CGA-O1A	-2.48	116.94	123.33
25	R	609	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
25	G	610	CLA	CHB-C4A-NA	2.48	127.98	124.40
25	A	406	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
25	7	602	CLA	CMB-C2B-C3B	2.48	132.39	126.55
26	6	1620	LUT	C35-C15-C14	-2.48	118.44	123.52
26	S	1620	LUT	C19-C9-C8	2.48	121.88	118.09
30	c	517	BCR	C11-C12-C13	-2.48	119.56	126.36
26	Y	1620	LUT	C8-C9-C10	-2.48	115.11	119.01
26	2	1621	LUT	C8-C7-C6	-2.48	120.37	127.00
25	1	611	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
25	R	611	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
24	n	607	CHL	O1D-CGD-CBD	-2.48	120.96	124.72
25	R	616	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
24	s	607	CHL	C4-C3-C5	2.48	119.53	115.23
24	8	601	CHL	O2D-CGD-CBD	2.48	119.98	113.90
24	3	601	CHL	C1C-CHC-C4B	2.48	124.94	116.07
24	S	607	CHL	C4-C3-C5	2.48	119.53	115.23
26	S	1620	LUT	C7-C8-C9	-2.48	122.57	126.23
24	G	607	CHL	O2A-CGA-CBA	2.48	119.39	111.83
25	R	602	CLA	CHB-C4A-NA	2.48	127.97	124.40
37	C	518	DGD	C3G-C2G-C1G	-2.48	106.01	111.78
24	5	607	CHL	CMB-C2B-C3B	2.48	129.63	124.68
25	r	613	CLA	C1-C2-C3	-2.48	122.14	126.20
30	8	623	BCR	C29-C30-C25	2.48	114.03	110.44
24	g	607	CHL	O2A-CGA-CBA	2.47	119.38	111.83
24	r	606	CHL	CMB-C2B-C3B	2.47	129.63	124.68
24	7	601	CHL	C1C-CHC-C4B	2.47	124.92	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	s	1620	LUT	C19-C9-C8	2.47	121.87	118.09
26	N	1621	LUT	C15-C35-C34	-2.47	118.46	123.52
25	N	610	CLA	CMB-C2B-C1B	-2.47	121.65	125.42
39	F	101	HEM	CMC-C2C-C1C	-2.47	120.37	124.73
25	S	611	CLA	C3B-C4B-NB	-2.47	108.32	110.53
33	a	408	PHO	O2A-CGA-O1A	-2.47	117.44	123.63
24	N	601	CHL	C1C-C2C-CMC	2.47	131.26	126.80
37	c	518	DGD	C3G-C2G-C1G	-2.47	106.02	111.78
25	b	605	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
28	n	1623	NEX	C30-C31-C32	-2.47	116.04	123.20
37	C	520	DGD	O5D-C6D-C5D	-2.47	103.85	109.42
26	N	1620	LUT	C19-C9-C8	2.47	121.86	118.09
24	4	601	CHL	O2D-CGD-CBD	2.47	119.96	113.90
25	5	602	CLA	C3B-C4B-NB	-2.47	108.33	110.53
25	a	406	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
25	S	604	CLA	C1-C2-C3	-2.47	122.77	126.76
26	y	1620	LUT	C38-C25-C24	-2.47	117.52	123.36
24	g	608	CHL	CMB-C2B-C3B	2.47	129.62	124.68
26	2	1620	LUT	C35-C15-C14	-2.47	118.47	123.52
25	r	602	CLA	CHB-C4A-NA	2.47	127.96	124.40
35	b	2633	LMG	C40-C39-C38	-2.47	101.89	114.37
25	b	605	CLA	C2D-C1D-ND	-2.47	107.68	110.13
25	R	613	CLA	C1-C2-C3	-2.47	122.15	126.20
25	3	602	CLA	CMB-C2B-C3B	2.47	132.35	126.55
25	r	616	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
25	2	604	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
35	B	2633	LMG	C40-C39-C38	-2.47	101.90	114.37
28	N	1623	NEX	C30-C31-C32	-2.47	116.05	123.20
26	Y	1621	LUT	C16-C1-C6	-2.47	106.37	110.24
25	7	603	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
25	R	603	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
26	y	1620	LUT	C8-C9-C10	-2.47	115.13	119.01
25	r	611	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
25	s	604	CLA	C1-C2-C3	-2.47	122.77	126.76
25	n	610	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
25	5	611	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
25	3	610	CLA	C1-C2-C3	-2.47	122.16	126.20
25	b	611	CLA	CHB-C4A-NA	2.47	127.96	124.40
25	2	602	CLA	CAA-CBA-CGA	-2.47	106.21	113.21
24	2	606	CHL	CAA-C2A-C3A	-2.47	106.34	113.00
24	6	606	CHL	CAA-C2A-C3A	-2.46	106.34	113.00
29	D	408	LHG	O8-C23-O10	-2.46	117.46	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	611	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
26	n	1621	LUT	C15-C35-C34	-2.46	118.48	123.52
25	2	610	CLA	CHB-C4A-NA	2.46	127.95	124.40
26	g	1620	LUT	C38-C25-C24	-2.46	117.53	123.36
25	y	611	CLA	CAA-CBA-CGA	-2.46	106.22	113.21
29	N	2630	LHG	C20-C19-C18	-2.46	101.92	114.37
25	B	614	CLA	C3B-C4B-NB	-2.46	108.33	110.53
25	B	605	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
25	r	603	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
36	D	405	PL9	C50-C49-C48	-2.46	115.27	122.66
37	c	518	DGD	C1E-O6E-C5E	2.46	118.53	113.72
29	n	2630	LHG	C20-C19-C18	-2.46	101.93	114.37
24	n	601	CHL	C1C-C2C-CMC	2.46	131.24	126.80
27	R	622	XAT	C8-C9-C10	-2.46	115.14	119.01
24	5	605	CHL	CMB-C2B-C3B	2.46	129.60	124.68
24	N	607	CHL	O1D-CGD-CBD	-2.46	120.99	124.72
24	R	614	CHL	CMA-C3A-C4A	-2.46	109.31	114.61
24	r	614	CHL	CMA-C3A-C4A	-2.46	109.31	114.61
26	Y	1620	LUT	C38-C25-C24	-2.46	117.54	123.36
25	5	604	CLA	C3B-C4B-NB	-2.46	108.33	110.53
25	c	503	CLA	CHB-C4A-NA	2.46	127.95	124.40
25	n	602	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
34	B	621	SQD	O48-C23-C24	2.46	119.33	111.83
24	1	605	CHL	CMB-C2B-C3B	2.46	129.60	124.68
24	8	607	CHL	CMB-C2B-C3B	2.46	129.60	124.68
25	b	614	CLA	C3B-C4B-NB	-2.46	108.33	110.53
26	n	1620	LUT	C19-C9-C8	2.46	121.84	118.09
27	r	622	XAT	C8-C9-C10	-2.46	115.14	119.01
37	C	518	DGD	C1E-O6E-C5E	2.46	118.52	113.72
25	7	610	CLA	C1-C2-C3	-2.46	122.17	126.20
25	B	611	CLA	CHB-C4A-NA	2.46	127.95	124.40
34	a	418	SQD	O47-C45-C44	2.46	117.16	108.34
26	3	1621	LUT	C15-C35-C34	-2.46	118.49	123.52
33	A	408	PHO	O2A-CGA-O1A	-2.46	117.48	123.63
25	3	603	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
25	N	602	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
24	s	601	CHL	CMB-C2B-C3B	2.46	129.59	124.68
25	C	503	CLA	CHB-C4A-NA	2.46	127.94	124.40
25	s	611	CLA	CHB-C4A-NA	2.46	127.94	124.40
36	d	405	PL9	C50-C49-C48	-2.46	115.28	122.66
26	s	1620	LUT	C7-C8-C9	-2.46	122.60	126.23
29	d	408	LHG	O8-C23-O10	-2.46	117.49	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	601	CLA	CAA-C2A-C3A	-2.45	106.36	113.00
25	n	610	CLA	CMB-C2B-C3B	2.45	132.32	126.55
27	5	1622	XAT	C31-C32-C33	-2.45	119.63	126.36
24	1	607	CHL	CMB-C2B-C3B	2.45	129.59	124.68
29	1	2630	LHG	C18-C17-C16	-2.45	101.96	114.37
26	7	1620	LUT	C20-C13-C12	2.45	121.84	118.09
24	4	607	CHL	CMB-C2B-C3B	2.45	129.59	124.68
29	5	2630	LHG	C18-C17-C16	-2.45	101.97	114.37
27	1	1622	XAT	C31-C32-C33	-2.45	119.64	126.36
34	A	418	SQD	O8-S-C6	2.45	110.70	105.97
24	2	607	CHL	CMB-C2B-C3B	2.45	129.58	124.68
26	r	620	LUT	C12-C13-C14	-2.45	115.15	119.01
34	b	621	SQD	O48-C23-C24	2.45	119.31	111.83
25	Y	610	CLA	CHB-C4A-NA	2.45	127.94	124.40
25	6	602	CLA	CAA-CBA-CGA	-2.45	106.25	113.21
35	d	411	LMG	C6-C5-C4	-2.45	107.00	113.02
25	3	612	CLA	CMD-C2D-C1D	-2.45	120.41	124.73
25	Y	602	CLA	CHB-C4A-NA	2.45	127.94	124.40
25	6	610	CLA	CHB-C4A-NA	2.45	127.94	124.40
25	y	602	CLA	CHB-C4A-NA	2.45	127.94	124.40
25	8	612	CLA	CMB-C2B-C3B	2.45	132.31	126.55
26	Y	1620	LUT	C39-C29-C28	2.45	121.83	118.09
25	1	604	CLA	C3B-C4B-NB	-2.45	108.34	110.53
25	B	612	CLA	CHC-C1C-NC	2.45	128.00	124.31
26	7	1621	LUT	C15-C35-C34	-2.45	118.51	123.52
29	3	2630	LHG	O8-C6-C5	-2.45	101.34	108.40
24	8	606	CHL	OMC-CMC-C2C	-2.45	120.87	125.12
26	R	620	LUT	C12-C13-C14	-2.45	115.16	119.01
24	S	601	CHL	CMB-C2B-C3B	2.45	129.57	124.68
34	a	418	SQD	O8-S-C6	2.45	110.70	105.97
39	f	101	HEM	CMC-C2C-C1C	-2.45	120.42	124.73
35	D	411	LMG	C6-C5-C4	-2.45	107.01	113.02
24	S	601	CHL	CMA-C3A-C4A	-2.45	109.34	114.61
25	S	611	CLA	CHB-C4A-NA	2.45	127.93	124.40
25	Y	611	CLA	CAA-CBA-CGA	-2.45	106.26	113.21
24	R	606	CHL	CMB-C2B-C3B	2.45	129.57	124.68
34	A	418	SQD	O47-C45-C44	2.45	117.12	108.34
29	7	2630	LHG	O8-C6-C5	-2.45	101.35	108.40
37	c	520	DGD	O5D-C6D-C5D	-2.45	103.91	109.42
25	r	601	CLA	CAA-C2A-C3A	-2.44	106.39	113.00
26	y	1621	LUT	C16-C1-C6	-2.44	106.41	110.24
25	s	612	CLA	CMB-C2B-C3B	2.44	132.30	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	603	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
25	5	610	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	B	611	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
25	N	610	CLA	CMB-C2B-C3B	2.44	132.29	126.55
25	8	602	CLA	CMB-C2B-C3B	2.44	132.29	126.55
25	1	610	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
26	3	1620	LUT	C20-C13-C12	2.44	121.81	118.09
25	b	617	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
25	n	610	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	S	612	CLA	CAA-C2A-C3A	-2.44	106.41	113.00
26	G	1620	LUT	C38-C25-C24	-2.44	117.59	123.36
25	Y	610	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
37	c	518	DGD	O3E-C3E-C2E	-2.44	104.63	110.38
25	A	410	CLA	C1-C2-C3	-2.44	122.20	126.20
24	3	609	CHL	OMC-CMC-C2C	-2.44	120.89	125.12
25	4	602	CLA	CMB-C2B-C3B	2.44	132.28	126.55
24	6	607	CHL	CMB-C2B-C3B	2.44	129.55	124.68
33	A	409	PHO	C2D-C1D-ND	-2.44	107.67	109.43
25	S	612	CLA	CMB-C2B-C3B	2.44	132.28	126.55
25	7	612	CLA	CMD-C2D-C1D	-2.44	120.44	124.73
26	2	1621	LUT	C31-C30-C29	-2.44	123.86	127.28
25	n	613	CLA	CAC-C3C-C4C	2.44	127.96	124.79
24	4	606	CHL	OMC-CMC-C2C	-2.43	120.89	125.12
25	1	610	CLA	CHB-C4A-NA	2.43	127.91	124.40
25	a	410	CLA	C1-C2-C3	-2.43	122.21	126.20
26	n	1621	LUT	C16-C1-C6	-2.43	106.43	110.24
24	s	601	CHL	CMA-C3A-C4A	-2.43	109.37	114.61
24	7	609	CHL	OMC-CMC-C2C	-2.43	120.89	125.12
25	R	603	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
26	y	1620	LUT	C39-C29-C28	2.43	121.80	118.09
24	s	608	CHL	CMB-C2B-C3B	2.43	129.54	124.68
29	L	101	LHG	C20-C19-C18	-2.43	102.08	114.37
25	n	603	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
25	4	611	CLA	C3B-C4B-NB	-2.43	108.36	110.53
25	4	612	CLA	CMB-C2B-C3B	2.43	132.27	126.55
25	1	604	CLA	CHB-C1B-NB	2.43	127.69	124.05
26	N	1620	LUT	C38-C25-C24	-2.43	117.61	123.36
29	y	2630	LHG	C20-C19-C18	-2.43	102.09	114.37
25	N	610	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
25	7	610	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
25	N	613	CLA	CAC-C3C-C4C	2.43	127.95	124.79
25	2	611	CLA	C3B-C4B-NB	-2.43	108.36	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	617	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
29	Y	2630	LHG	C20-C19-C18	-2.43	102.09	114.37
25	y	610	CLA	CHB-C4A-NA	2.43	127.90	124.40
24	S	608	CHL	CMB-C2B-C3B	2.43	129.53	124.68
37	C	518	DGD	O3E-C3E-C2E	-2.43	104.65	110.38
25	n	610	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
26	6	1621	LUT	C7-C8-C9	-2.43	122.64	126.23
25	s	612	CLA	CAA-C2A-C3A	-2.43	106.44	113.00
26	n	1621	LUT	C8-C9-C10	-2.43	115.19	119.01
26	n	1620	LUT	C38-C25-C24	-2.43	117.62	123.36
26	y	1620	LUT	C37-C21-C22	-2.43	104.88	109.41
25	y	610	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
26	s	1621	LUT	C21-C26-C27	-2.42	110.04	112.83
28	r	623	NEX	C38-C25-C24	2.42	116.96	114.24
26	N	1621	LUT	C16-C1-C6	-2.42	106.44	110.24
30	t	101	BCR	C39-C30-C25	-2.42	106.44	110.24
25	4	602	CLA	C3B-C4B-NB	-2.42	108.37	110.53
25	Y	610	CLA	C3B-C4B-NB	-2.42	108.37	110.53
25	B	614	CLA	CMB-C2B-C3B	2.42	132.25	126.55
26	Y	1620	LUT	C37-C21-C22	-2.42	104.89	109.41
25	5	602	CLA	C1-C2-C3	-2.42	122.23	126.20
25	2	602	CLA	C3B-C4B-NB	-2.42	108.37	110.53
25	5	610	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
25	1	614	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
28	1	1623	NEX	C2-C1-C6	2.42	111.56	109.21
29	l	101	LHG	C20-C19-C18	-2.42	102.13	114.37
26	S	1621	LUT	C21-C26-C27	-2.42	110.04	112.83
27	8	622	XAT	C19-C9-C8	2.42	121.79	118.09
25	N	610	CLA	CHB-C4A-NA	2.42	127.89	124.40
24	S	601	CHL	CBC-CAC-C3C	-2.42	109.41	112.87
33	a	409	PHO	C2D-C1D-ND	-2.42	107.68	109.43
25	2	610	CLA	C4A-NA-C1A	2.42	107.78	106.68
25	g	614	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
25	b	614	CLA	CMB-C2B-C3B	2.42	132.24	126.55
26	7	1620	LUT	C39-C29-C28	2.42	121.78	118.09
25	Y	611	CLA	CHB-C4A-NA	2.42	127.89	124.40
25	6	602	CLA	C3B-C4B-NB	-2.42	108.37	110.53
25	y	610	CLA	C3B-C4B-NB	-2.42	108.37	110.53
30	C	516	BCR	C29-C30-C25	2.42	113.95	110.44
25	r	603	CLA	O2D-CGD-O1D	-2.42	119.15	123.85
24	R	607	CHL	CMB-C2B-C3B	2.42	129.51	124.68
24	3	605	CHL	CAA-C2A-C3A	-2.41	106.47	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	n	2630	LHG	C27-C26-C25	-2.41	102.16	114.37
25	3	603	CLA	C2A-C1A-CHA	2.41	128.06	123.87
25	5	614	CLA	CMB-C2B-C1B	-2.41	121.74	125.42
37	c	520	DGD	O3G-C1D-C2D	-2.41	104.61	108.27
25	6	610	CLA	C4A-NA-C1A	2.41	107.78	106.68
24	g	605	CHL	OMC-CMC-C2C	-2.41	120.93	125.12
25	5	604	CLA	CHB-C1B-NB	2.41	127.67	124.05
30	c	516	BCR	C29-C30-C25	2.41	113.94	110.44
37	C	520	DGD	O3G-C1D-C2D	-2.41	104.61	108.27
24	7	605	CHL	CAA-C2A-C3A	-2.41	106.48	113.00
25	1	602	CLA	C1-C2-C3	-2.41	122.25	126.20
25	b	604	CLA	O2D-CGD-CBD	2.41	115.45	111.23
29	B	2631	LHG	C11-C10-C9	-2.41	102.18	114.37
26	3	1620	LUT	C39-C29-C28	2.41	121.77	118.09
29	N	2630	LHG	C27-C26-C25	-2.41	102.18	114.37
25	2	602	CLA	CMB-C2B-C3B	2.41	132.22	126.55
26	N	1621	LUT	C8-C9-C10	-2.41	115.22	119.01
26	Y	1620	LUT	C8-C7-C6	-2.41	120.56	127.00
28	2	1623	NEX	C8-C7-C6	-2.41	174.82	177.66
27	4	622	XAT	C19-C9-C8	2.41	121.77	118.09
29	n	2630	LHG	C18-C17-C16	-2.41	102.19	114.37
30	T	101	BCR	C39-C30-C25	-2.41	106.47	110.24
25	B	615	CLA	C3B-C4B-NB	-2.41	108.38	110.53
29	N	2630	LHG	C18-C17-C16	-2.41	102.20	114.37
25	N	613	CLA	CHB-C4A-NA	2.41	127.88	124.40
25	G	614	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
26	6	1621	LUT	C31-C30-C29	-2.41	123.90	127.28
25	b	615	CLA	C3B-C4B-NB	-2.41	108.38	110.53
24	4	601	CHL	CMB-C2B-C3B	2.41	129.49	124.68
25	C	510	CLA	CHB-C4A-NA	2.41	127.87	124.40
25	n	613	CLA	CHB-C4A-NA	2.41	127.87	124.40
26	5	1621	LUT	C7-C8-C9	-2.41	122.68	126.23
27	5	1622	XAT	C18-C5-C4	2.41	116.94	114.24
25	6	602	CLA	CMB-C2B-C3B	2.41	132.21	126.55
25	8	602	CLA	C3B-C4B-NB	-2.41	108.38	110.53
24	1	606	CHL	CMB-C2B-C3B	2.41	129.49	124.68
24	Y	606	CHL	CMA-C3A-C4A	-2.40	109.43	114.61
25	c	512	CLA	CHB-C4A-NA	2.40	127.87	124.40
25	1	604	CLA	C1-C2-C3	-2.40	122.87	126.76
26	g	1620	LUT	C28-C29-C30	-2.40	115.23	119.01
34	a	418	SQD	O9-S-C6	2.40	110.34	106.76
25	b	612	CLA	CHC-C1C-NC	2.40	127.93	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	r	608	CHL	CMB-C2B-C3B	2.40	129.49	124.68
29	5	2630	LHG	C20-C19-C18	-2.40	102.22	114.37
25	c	510	CLA	CHB-C4A-NA	2.40	127.87	124.40
24	G	605	CHL	OMC-CMC-C2C	-2.40	120.95	125.12
24	8	601	CHL	CMB-C2B-C3B	2.40	129.48	124.68
26	2	1621	LUT	C7-C8-C9	-2.40	122.68	126.23
28	n	1623	NEX	C11-C12-C13	-2.40	119.78	126.36
25	3	610	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
25	y	604	CLA	C1-C2-C3	-2.40	122.88	126.76
26	y	1620	LUT	C8-C7-C6	-2.40	120.58	127.00
24	s	601	CHL	CBC-CAC-C3C	-2.40	109.44	112.87
28	5	1623	NEX	C2-C1-C6	2.40	111.54	109.21
30	C	514	BCR	C34-C9-C8	2.40	121.75	118.09
28	N	1623	NEX	C11-C12-C13	-2.40	119.78	126.36
25	y	610	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
24	5	606	CHL	CMB-C2B-C3B	2.40	129.48	124.68
29	b	2631	LHG	C11-C10-C9	-2.40	102.24	114.37
26	1	1621	LUT	C7-C8-C9	-2.40	122.69	126.23
24	8	607	CHL	CMA-C3A-C4A	-2.40	109.44	114.61
26	2	1621	LUT	C27-C28-C29	-2.40	121.16	126.32
27	1	1622	XAT	C18-C5-C4	2.40	116.94	114.24
30	c	514	BCR	C34-C9-C8	2.40	121.75	118.09
25	B	604	CLA	O2D-CGD-CBD	2.40	115.42	111.23
30	d	404	BCR	C38-C26-C27	2.40	118.71	113.60
29	S	2630	LHG	C11-C10-C9	-2.40	102.24	114.37
29	s	2630	LHG	C11-C10-C9	-2.40	102.24	114.37
24	y	606	CHL	CMA-C3A-C4A	-2.40	109.44	114.61
29	1	2630	LHG	C20-C19-C18	-2.40	102.25	114.37
26	6	1621	LUT	C27-C28-C29	-2.40	121.17	126.32
26	1	1621	LUT	O3-C3-C2	-2.40	104.85	109.75
24	4	607	CHL	CMA-C3A-C4A	-2.40	109.45	114.61
25	Y	610	CLA	O2A-CGA-O1A	-2.40	117.64	123.63
24	g	607	CHL	CAA-C2A-C3A	-2.39	106.53	113.00
28	7	1623	NEX	C12-C13-C14	2.39	122.78	119.01
25	y	611	CLA	CHB-C4A-NA	2.39	127.86	124.40
24	r	608	CHL	C1C-C2C-CMC	2.39	131.12	126.80
24	7	606	CHL	CAC-C3C-C4C	2.39	130.18	124.03
24	R	608	CHL	CMB-C2B-C3B	2.39	129.46	124.68
24	r	607	CHL	CMB-C2B-C3B	2.39	129.46	124.68
25	s	611	CLA	C3B-C4B-NB	-2.39	108.39	110.53
25	C	512	CLA	CHB-C4A-NA	2.39	127.85	124.40
25	C	504	CLA	CMB-C2B-C3B	2.39	132.17	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	516	BCR	C15-C14-C13	-2.39	123.93	127.28
37	c	519	DGD	O5D-C6D-C5D	-2.39	104.03	109.42
25	7	603	CLA	C2A-C1A-CHA	2.39	128.01	123.87
26	G	1620	LUT	C28-C29-C30	-2.39	115.25	119.01
26	S	1621	LUT	C7-C8-C9	-2.39	122.70	126.23
29	c	2630	LHG	C18-C17-C16	-2.39	102.30	114.37
30	D	404	BCR	C38-C26-C27	2.39	118.69	113.60
29	C	2630	LHG	C18-C17-C16	-2.39	102.30	114.37
24	G	607	CHL	CAA-C2A-C3A	-2.39	106.55	113.00
24	R	608	CHL	C1C-C2C-CMC	2.39	131.10	126.80
35	D	411	LMG	O1-C7-C8	-2.39	105.01	110.82
28	R	623	NEX	C39-C29-C30	-2.38	118.95	122.82
37	h	102	DGD	O6D-C1D-O3G	-2.38	104.41	110.04
26	5	1621	LUT	O3-C3-C2	-2.38	104.87	109.75
26	8	620	LUT	C10-C11-C12	-2.38	116.29	123.20
26	R	620	LUT	C1-C2-C3	2.38	118.82	113.59
24	Y	605	CHL	CMB-C2B-C3B	2.38	129.44	124.68
25	5	604	CLA	C1-C2-C3	-2.38	122.91	126.76
27	2	1622	XAT	C4-C3-C2	-2.38	106.33	110.79
34	A	418	SQD	O9-S-C6	2.38	110.31	106.76
24	3	601	CHL	CMD-C2D-C3D	-2.38	119.93	124.68
26	4	620	LUT	C10-C11-C12	-2.38	116.31	123.20
25	c	504	CLA	CMB-C2B-C3B	2.38	132.15	126.55
25	c	502	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
26	r	620	LUT	C1-C2-C3	2.38	118.81	113.59
34	b	623	SQD	O6-C44-C45	-2.38	105.03	110.82
28	R	623	NEX	C38-C25-C24	2.38	116.91	114.24
24	Y	609	CHL	O2A-CGA-CBA	2.38	119.08	111.83
28	3	1623	NEX	C12-C13-C14	2.38	122.75	119.01
25	n	612	CLA	CHC-C4B-NB	2.38	127.61	124.05
26	6	1620	LUT	C39-C29-C28	2.38	121.72	118.09
35	d	411	LMG	O1-C7-C8	-2.38	105.04	110.82
26	7	1620	LUT	C18-C5-C6	-2.38	121.89	124.48
25	Y	604	CLA	C1-C2-C3	-2.38	122.92	126.76
25	N	612	CLA	CHC-C4B-NB	2.38	127.61	124.05
25	G	613	CLA	CHB-C4A-NA	2.38	127.83	124.40
24	3	606	CHL	CAC-C3C-C4C	2.37	130.13	124.03
25	b	615	CLA	CMB-C2B-C3B	2.37	132.13	126.55
30	C	516	BCR	C15-C14-C13	-2.37	123.95	127.28
25	S	603	CLA	C2A-C1A-CHA	2.37	127.98	123.87
25	s	603	CLA	C2A-C1A-CHA	2.37	127.98	123.87
26	7	1621	LUT	C1-C2-C3	2.37	118.80	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	g	604	CLA	C1-C2-C3	-2.37	122.92	126.76
25	Y	602	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
26	s	1621	LUT	C7-C8-C9	-2.37	122.73	126.23
30	c	515	BCR	C4-C5-C6	-2.37	119.50	122.70
25	C	505	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
25	1	604	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
25	C	503	CLA	C3B-C4B-NB	-2.37	108.41	110.53
25	g	613	CLA	CHB-C4A-NA	2.37	127.82	124.40
27	6	1622	XAT	C4-C3-C2	-2.37	106.36	110.79
29	6	2630	LHG	C11-C10-C9	-2.37	102.38	114.37
25	5	604	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
26	1	1620	LUT	C40-C33-C32	2.37	121.71	118.09
37	C	519	DGD	O5D-C6D-C5D	-2.37	104.08	109.42
24	y	609	CHL	O2A-CGA-CBA	2.37	119.06	111.83
28	2	1623	NEX	C28-C29-C30	2.37	122.74	119.01
24	y	605	CHL	CMB-C2B-C3B	2.37	129.42	124.68
25	G	604	CLA	C1-C2-C3	-2.37	122.93	126.76
26	n	1620	LUT	C28-C29-C30	-2.37	115.28	119.01
25	1	613	CLA	CHC-C4B-NB	2.37	127.60	124.05
25	5	613	CLA	CHC-C4B-NB	2.37	127.60	124.05
26	S	1620	LUT	C20-C13-C12	2.37	121.70	118.09
25	b	605	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
28	6	1623	NEX	C8-C7-C6	-2.37	174.87	177.66
25	c	510	CLA	C1-C2-C3	-2.37	122.32	126.20
37	H	102	DGD	O6D-C1D-O3G	-2.37	104.45	110.04
25	r	603	CLA	C3B-C4B-NB	-2.37	108.42	110.53
28	r	623	NEX	C39-C29-C30	-2.37	118.98	122.82
36	D	405	PL9	O2-C1-C6	2.37	124.24	120.48
25	c	505	CLA	CMB-C2B-C1B	-2.36	121.82	125.42
25	r	613	CLA	O1D-CGD-CBD	2.36	129.18	124.52
26	2	1620	LUT	C39-C29-C28	2.36	121.70	118.09
25	R	603	CLA	C3B-C4B-NB	-2.36	108.42	110.53
26	Y	1620	LUT	C1-C2-C3	2.36	118.78	113.59
25	8	611	CLA	C3B-C4B-NB	-2.36	108.42	110.53
29	2	2630	LHG	C11-C10-C9	-2.36	102.43	114.37
26	S	1621	LUT	C39-C29-C28	2.36	121.70	118.09
26	3	1621	LUT	C18-C5-C6	-2.36	121.91	124.48
25	B	615	CLA	CMB-C2B-C3B	2.36	132.10	126.55
25	2	602	CLA	CHB-C4A-NA	2.36	127.81	124.40
27	7	1622	XAT	C32-C33-C34	-2.36	115.30	119.01
30	C	515	BCR	C4-C5-C6	-2.36	119.52	122.70
26	G	1621	LUT	C18-C5-C6	-2.36	121.91	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	7	1621	LUT	C18-C5-C6	-2.36	121.91	124.48
25	6	602	CLA	CHB-C4A-NA	2.36	127.80	124.40
29	c	523	LHG	C20-C19-C18	-2.36	102.45	114.37
34	B	623	SQD	O6-C44-C45	-2.36	105.08	110.82
27	8	622	XAT	C38-C25-C24	2.36	116.89	114.24
26	s	1621	LUT	C39-C29-C28	2.36	121.69	118.09
26	s	1620	LUT	C20-C13-C12	2.36	121.69	118.09
26	3	1621	LUT	C1-C2-C3	2.36	118.76	113.59
26	y	1620	LUT	C1-C2-C3	2.36	118.76	113.59
26	3	1620	LUT	C18-C5-C6	-2.36	121.91	124.48
25	N	614	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
24	6	609	CHL	C6-C5-C3	-2.36	107.73	113.47
27	N	1622	XAT	C40-C33-C32	2.36	121.69	118.09
25	2	612	CLA	C2A-C1A-CHA	2.36	127.95	123.87
24	7	601	CHL	CMD-C2D-C3D	-2.35	119.98	124.68
25	R	613	CLA	O1D-CGD-CBD	2.35	129.16	124.52
24	2	609	CHL	C6-C5-C3	-2.35	107.73	113.47
24	g	609	CHL	CMB-C2B-C3B	2.35	129.39	124.68
26	5	1620	LUT	C40-C33-C32	2.35	121.68	118.09
25	8	604	CLA	O2A-CGA-O1A	-2.35	117.28	123.33
29	C	523	LHG	C20-C19-C18	-2.35	102.48	114.37
25	y	602	CLA	CMB-C2B-C1B	-2.35	121.84	125.42
37	C	519	DGD	C3G-C2G-C1G	-2.35	106.30	111.78
29	d	408	LHG	C27-C26-C25	-2.35	102.48	114.37
26	5	1621	LUT	C8-C9-C10	-2.35	115.31	119.01
26	1	1621	LUT	C8-C9-C10	-2.35	115.31	119.01
30	B	620	BCR	C21-C20-C19	-2.35	116.39	123.20
26	R	620	LUT	C7-C8-C9	-2.35	122.76	126.23
25	B	605	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
24	G	609	CHL	C1-C2-C3	-2.35	122.35	126.20
30	b	620	BCR	C21-C20-C19	-2.35	116.39	123.20
25	C	502	CLA	CMB-C2B-C1B	-2.35	121.84	125.42
24	n	601	CHL	OBD-CAD-C3D	-2.35	124.23	127.89
29	D	408	LHG	C27-C26-C25	-2.35	102.50	114.37
26	N	1620	LUT	C28-C29-C30	-2.35	115.32	119.01
36	d	405	PL9	O2-C1-C6	2.35	124.21	120.48
29	R	2630	LHG	O8-C23-C24	2.35	118.99	111.83
26	S	1621	LUT	C8-C9-C10	-2.35	115.32	119.01
24	N	607	CHL	CMA-C3A-C4A	-2.35	109.56	114.61
24	n	607	CHL	CMA-C3A-C4A	-2.35	109.56	114.61
24	G	609	CHL	O1D-CGD-CBD	-2.35	121.17	124.72
25	n	614	CLA	CMB-C2B-C1B	-2.35	121.85	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	604	CLA	O2A-CGA-O1A	-2.35	117.30	123.33
27	4	622	XAT	C38-C25-C24	2.34	116.88	114.24
25	2	614	CLA	C3B-C4B-NB	-2.34	108.44	110.53
25	b	611	CLA	C3A-C2A-C1A	2.34	104.85	101.34
30	H	101	BCR	C2-C3-C4	-2.34	106.12	111.28
25	6	612	CLA	C2A-C1A-CHA	2.34	127.93	123.87
26	y	1621	LUT	C19-C9-C8	2.34	121.67	118.09
25	B	611	CLA	C3A-C2A-C1A	2.34	104.85	101.34
29	r	2630	LHG	O8-C23-C24	2.34	118.97	111.83
25	r	604	CLA	CBA-CAA-C2A	2.34	120.76	113.79
24	8	601	CHL	C3D-C4D-ND	2.34	116.69	112.94
25	b	610	CLA	CMB-C2B-C3B	2.34	132.06	126.55
26	y	1620	LUT	C16-C1-C6	-2.34	106.57	110.24
24	Y	605	CHL	O2D-CGD-O1D	-2.34	119.29	123.85
28	6	1623	NEX	C28-C29-C30	2.34	122.69	119.01
25	b	605	CLA	C2A-C1A-CHA	2.34	127.93	123.87
37	c	519	DGD	C3G-C2G-C1G	-2.34	106.33	111.78
25	B	605	CLA	C2A-C1A-CHA	2.34	127.93	123.87
25	1	612	CLA	CHA-C1A-NA	-2.34	121.09	126.39
24	G	609	CHL	CMB-C2B-C3B	2.34	129.35	124.68
27	3	1622	XAT	C32-C33-C34	-2.34	115.33	119.01
25	C	510	CLA	C1-C2-C3	-2.34	122.37	126.20
24	4	601	CHL	C3D-C4D-ND	2.34	116.69	112.94
26	Y	1621	LUT	C19-C9-C8	2.34	121.66	118.09
30	C	515	BCR	C23-C24-C25	-2.33	120.76	127.00
25	6	611	CLA	CHB-C4A-NA	2.33	127.77	124.40
25	B	610	CLA	CMB-C2B-C3B	2.33	132.04	126.55
26	s	1621	LUT	C8-C9-C10	-2.33	115.34	119.01
30	t	101	BCR	C11-C12-C13	-2.33	119.96	126.36
35	c	521	LMG	C40-C39-C38	-2.33	102.57	114.37
24	S	606	CHL	CAC-C3C-C4C	2.33	130.03	124.03
25	1	610	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
25	S	602	CLA	O1D-CGD-CBD	2.33	129.12	124.52
35	C	521	LMG	C40-C39-C38	-2.33	102.57	114.37
25	2	611	CLA	CHB-C4A-NA	2.33	127.77	124.40
26	r	620	LUT	C7-C8-C9	-2.33	122.78	126.23
24	g	605	CHL	CMB-C2B-C3B	2.33	129.34	124.68
27	R	622	XAT	C20-C13-C12	2.33	121.65	118.09
27	n	1622	XAT	C40-C33-C32	2.33	121.65	118.09
24	g	609	CHL	C1-C2-C3	-2.33	122.38	126.20
25	3	613	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
30	h	101	BCR	C2-C3-C4	-2.33	106.15	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	604	CLA	CBA-CAA-C2A	2.33	120.73	113.79
30	T	101	BCR	C11-C12-C13	-2.33	119.97	126.36
29	R	2630	LHG	C20-C19-C18	-2.33	102.59	114.37
24	N	601	CHL	OBD-CAD-C3D	-2.33	124.26	127.89
24	s	606	CHL	CAC-C3C-C4C	2.33	130.02	124.03
25	6	614	CLA	C3B-C4B-NB	-2.33	108.45	110.53
29	1	2630	LHG	C11-C10-C9	-2.33	102.60	114.37
24	N	608	CHL	O2D-CGD-O1D	-2.33	119.32	123.85
25	5	612	CLA	CHA-C1A-NA	-2.33	121.12	126.39
26	g	1621	LUT	C18-C5-C6	-2.33	121.94	124.48
26	Y	1620	LUT	C28-C29-C30	-2.33	115.35	119.01
24	G	605	CHL	CMB-C2B-C3B	2.33	129.33	124.68
24	6	601	CHL	O2A-CGA-CBA	2.33	121.35	114.00
25	c	503	CLA	C3B-C4B-NB	-2.33	108.45	110.53
24	Y	606	CHL	CAC-C3C-C4C	2.33	130.01	124.03
24	5	607	CHL	CMD-C2D-C3D	-2.33	120.03	124.68
25	7	613	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
25	5	612	CLA	CHC-C4B-NB	2.33	127.54	124.05
24	s	607	CHL	CMB-C2B-C3B	2.32	129.33	124.68
25	B	608	CLA	CHB-C1B-NB	2.32	127.54	124.05
24	7	606	CHL	CBC-CAC-C3C	-2.32	109.55	112.87
24	n	608	CHL	O2D-CGD-O1D	-2.32	119.32	123.85
25	N	604	CLA	CMB-C2B-C3B	2.32	132.02	126.55
24	G	608	CHL	O1D-CGD-CBD	-2.32	121.20	124.72
35	A	415	LMG	C40-C39-C38	-2.32	102.62	114.37
25	Y	612	CLA	CHB-C1B-NB	2.32	127.53	124.05
25	C	505	CLA	C1-C2-C3	-2.32	122.39	126.20
29	r	2630	LHG	C20-C19-C18	-2.32	102.63	114.37
24	G	601	CHL	C4C-CHD-C1D	2.32	124.38	116.07
24	2	601	CHL	O2A-CGA-CBA	2.32	121.34	114.00
29	5	2630	LHG	C11-C10-C9	-2.32	102.63	114.37
26	y	1621	LUT	C27-C28-C29	-2.32	121.33	126.32
25	R	611	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
27	r	622	XAT	C20-C13-C12	2.32	121.63	118.09
24	1	607	CHL	CMD-C2D-C3D	-2.32	120.05	124.68
30	A	411	BCR	C10-C11-C12	-2.32	116.47	123.20
24	y	605	CHL	O2D-CGD-O1D	-2.32	119.33	123.85
24	g	609	CHL	O1D-CGD-CBD	-2.32	121.20	124.72
24	y	608	CHL	CMA-C3A-C4A	-2.32	109.61	114.61
26	Y	1620	LUT	C16-C1-C6	-2.32	106.61	110.24
35	b	2633	LMG	C38-C37-C36	-2.32	102.65	114.37
24	S	607	CHL	CMB-C2B-C3B	2.32	129.32	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	515	BCR	C23-C24-C25	-2.32	120.80	127.00
35	a	415	LMG	C40-C39-C38	-2.32	102.65	114.37
25	s	602	CLA	O1D-CGD-CBD	2.32	129.09	124.52
24	y	606	CHL	CAC-C3C-C4C	2.32	129.99	124.03
25	s	609	CLA	O2D-CGD-CBD	2.32	115.28	111.23
35	B	2633	LMG	C38-C37-C36	-2.32	102.65	114.37
30	a	411	BCR	C10-C11-C12	-2.32	116.48	123.20
25	5	610	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
25	b	608	CLA	CHB-C1B-NB	2.32	127.53	124.05
24	Y	609	CHL	CAC-C3C-C4C	2.32	129.99	124.03
25	A	407	CLA	C1-C2-C3	-2.32	123.01	126.76
27	n	1622	XAT	C26-C27-C28	-2.32	121.09	125.99
24	3	606	CHL	CBC-CAC-C3C	-2.32	109.56	112.87
25	b	612	CLA	CGD-CBD-CAD	-2.32	103.35	110.85
24	Y	608	CHL	CMA-C3A-C4A	-2.32	109.62	114.61
24	g	608	CHL	O1D-CGD-CBD	-2.32	121.21	124.72
24	g	601	CHL	C4C-CHD-C1D	2.32	124.35	116.07
24	n	605	CHL	CMB-C2B-C3B	2.31	129.31	124.68
27	N	1622	XAT	C38-C25-C24	2.31	116.84	114.24
25	y	612	CLA	O2D-CGD-O1D	-2.31	119.34	123.85
24	G	601	CHL	C1-O2A-CGA	2.31	122.25	116.65
26	Y	1621	LUT	C27-C28-C29	-2.31	121.35	126.32
29	C	523	LHG	C11-C10-C9	-2.31	102.67	114.37
29	c	523	LHG	C11-C10-C9	-2.31	102.67	114.37
33	a	408	PHO	CMB-C2B-C3B	2.31	129.31	124.68
25	y	612	CLA	CHB-C1B-NB	2.31	127.52	124.05
25	n	604	CLA	CMB-C2B-C3B	2.31	131.99	126.55
25	s	604	CLA	CMB-C2B-C3B	2.31	131.99	126.55
25	B	613	CLA	C16-C15-C13	-2.31	108.28	115.97
25	S	609	CLA	O2D-CGD-CBD	2.31	115.27	111.23
24	y	607	CHL	O2A-CGA-CBA	2.31	118.88	111.83
25	b	613	CLA	C16-C15-C13	-2.31	108.28	115.97
25	a	407	CLA	C1-C2-C3	-2.31	123.02	126.76
24	y	609	CHL	CAC-C3C-C4C	2.31	129.97	124.03
25	r	611	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
25	S	604	CLA	CMB-C2B-C3B	2.31	131.99	126.55
25	R	616	CLA	CHB-C4A-NA	2.31	127.73	124.40
33	A	408	PHO	CMB-C2B-C3B	2.31	129.30	124.68
24	N	601	CHL	O2A-CGA-CBA	2.31	118.88	111.83
37	C	518	DGD	O6E-C5E-C4E	2.31	113.86	109.70
24	g	601	CHL	C1-O2A-CGA	2.31	122.24	116.65
25	B	612	CLA	CGD-CBD-CAD	-2.31	103.37	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	410	CLA	O2D-CGD-CBD	2.31	115.26	111.23
24	Y	607	CHL	O2A-CGA-CBA	2.31	118.87	111.83
24	R	606	CHL	CAA-C2A-C3A	-2.31	106.77	113.00
25	4	610	CLA	CHB-C4A-NA	2.31	127.73	124.40
25	S	602	CLA	C3B-C4B-NB	-2.31	108.47	110.53
27	3	1622	XAT	C26-C27-C28	-2.30	121.12	125.99
25	B	616	CLA	C3A-C2A-C1A	2.30	104.79	101.34
24	y	605	CHL	O2A-CGA-CBA	2.30	118.86	111.83
27	N	1622	XAT	C26-C27-C28	-2.30	121.12	125.99
27	6	1622	XAT	C24-C23-C22	-2.30	106.48	110.79
35	A	413	LMG	C38-C37-C36	-2.30	102.73	114.37
35	D	411	LMG	O3-C3-C2	-2.30	104.95	110.38
25	1	612	CLA	CHC-C4B-NB	2.30	127.50	124.05
24	7	601	CHL	CMB-C2B-C3B	2.30	129.28	124.68
29	b	2631	LHG	C27-C26-C25	-2.30	102.73	114.37
35	b	622	LMG	O1-C7-C8	-2.30	105.22	110.82
25	Y	612	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
35	a	413	LMG	C38-C37-C36	-2.30	102.73	114.37
25	8	612	CLA	C3B-C4B-NB	-2.30	108.47	110.53
25	r	616	CLA	CHB-C4A-NA	2.30	127.72	124.40
38	D	401	BCT	O3-C-O1	-2.30	113.79	119.68
24	r	606	CHL	CAA-C2A-C3A	-2.30	106.78	113.00
25	1	614	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
29	B	2631	LHG	C27-C26-C25	-2.30	102.73	114.37
35	d	411	LMG	O3-C3-C2	-2.30	104.95	110.38
25	5	610	CLA	CMB-C2B-C3B	2.30	131.96	126.55
24	n	601	CHL	O2D-CGD-O1D	-2.30	119.37	123.85
25	s	609	CLA	C3B-C4B-NB	-2.30	108.48	110.53
27	2	1622	XAT	C24-C23-C22	-2.30	106.49	110.79
25	8	610	CLA	CHB-C4A-NA	2.30	127.72	124.40
28	s	1623	NEX	C26-C27-C28	-2.30	121.13	125.99
25	c	505	CLA	C1-C2-C3	-2.30	122.43	126.20
25	S	609	CLA	C3B-C4B-NB	-2.30	108.48	110.53
25	B	611	CLA	C2A-C1A-CHA	2.30	127.86	123.87
24	s	608	CHL	OBD-CAD-C3D	-2.30	124.31	127.89
27	n	1622	XAT	C38-C25-C24	2.30	116.82	114.24
24	N	601	CHL	C4C-CHD-C1D	2.30	124.30	116.07
25	y	614	CLA	CHC-C4B-NB	2.30	127.50	124.05
26	y	1620	LUT	C28-C29-C30	-2.30	115.39	119.01
28	S	1623	NEX	C26-C27-C28	-2.30	121.14	125.99
24	y	601	CHL	O2D-CGD-O1D	-2.30	119.38	123.85
24	Y	605	CHL	O2A-CGA-CBA	2.30	118.84	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	515	BCR	C8-C7-C6	-2.30	120.87	127.00
24	n	601	CHL	O2A-CGA-CBA	2.30	118.83	111.83
25	4	610	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
29	r	2630	LHG	C18-C17-C16	-2.29	102.77	114.37
27	7	1622	XAT	C26-C27-C28	-2.29	121.14	125.99
24	y	605	CHL	O1D-CGD-CBD	-2.29	121.24	124.72
37	c	518	DGD	O6E-C5E-C4E	2.29	113.83	109.70
24	7	605	CHL	CMB-C2B-C3B	2.29	129.26	124.68
35	B	622	LMG	O1-C7-C8	-2.29	105.24	110.82
24	n	601	CHL	C4C-CHD-C1D	2.29	124.27	116.07
25	N	611	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
25	B	605	CLA	C1-O2A-CGA	-2.29	111.10	116.65
30	C	516	BCR	C8-C7-C6	-2.29	120.88	127.00
25	b	605	CLA	C1-O2A-CGA	-2.29	111.11	116.65
25	n	611	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
25	B	614	CLA	CHB-C4A-NA	2.29	127.70	124.40
24	N	605	CHL	CMB-C2B-C3B	2.29	129.26	124.68
24	S	608	CHL	O1D-CGD-CBD	-2.29	121.25	124.72
24	Y	609	CHL	CMB-C2B-C3B	2.29	129.26	124.68
24	S	607	CHL	CED-O2D-CGD	2.29	121.11	115.92
30	C	515	BCR	C1-C6-C5	-2.29	119.51	122.64
25	4	612	CLA	C3B-C4B-NB	-2.29	108.49	110.53
24	g	607	CHL	CMA-C3A-C4A	-2.29	109.68	114.61
24	3	605	CHL	CMB-C2B-C3B	2.29	129.26	124.68
24	8	607	CHL	CAC-C3C-C4C	2.29	129.91	124.03
24	r	608	CHL	C4-C3-C5	2.29	119.20	115.23
25	5	614	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
38	d	401	BCT	O3-C-O1	-2.29	113.82	119.68
24	4	607	CHL	CAC-C3C-C4C	2.29	129.91	124.03
24	3	601	CHL	CMB-C2B-C3B	2.29	129.25	124.68
26	1	1620	LUT	C8-C7-C6	-2.29	120.89	127.00
30	C	515	BCR	C8-C7-C6	-2.29	120.89	127.00
25	7	611	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
24	6	605	CHL	CMB-C2B-C3B	2.29	129.25	124.68
29	B	2630	LHG	C20-C19-C18	-2.29	102.81	114.37
29	R	2630	LHG	C18-C17-C16	-2.29	102.81	114.37
24	g	607	CHL	CAC-C3C-C4C	2.29	129.91	124.03
25	r	616	CLA	CHC-C4B-NB	2.29	127.48	124.05
25	B	617	CLA	CHC-C1C-NC	2.29	127.75	124.31
25	7	602	CLA	C1-C2-C3	-2.29	122.45	126.20
25	B	610	CLA	O2A-CGA-O1A	-2.28	117.91	123.63
24	g	607	CHL	C6-C7-C8	-2.28	108.37	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	609	CHL	C1-C2-C3	-2.28	122.45	126.20
25	5	610	CLA	CHB-C1B-NB	2.28	127.48	124.05
25	1	610	CLA	CMB-C2B-C3B	2.28	131.92	126.55
30	c	516	BCR	C8-C7-C6	-2.28	120.90	127.00
30	t	101	BCR	C7-C6-C5	-2.28	116.29	121.56
25	b	614	CLA	CHB-C4A-NA	2.28	127.69	124.40
30	T	101	BCR	C7-C6-C5	-2.28	116.30	121.56
37	c	519	DGD	CBB-CAB-C9B	-2.28	102.83	114.37
25	b	611	CLA	C2A-C1A-CHA	2.28	127.83	123.87
25	Y	610	CLA	CHB-C1B-NB	2.28	127.47	124.05
25	b	610	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
24	G	607	CHL	CMA-C3A-C4A	-2.28	109.70	114.61
24	Y	605	CHL	O1D-CGD-CBD	-2.28	121.27	124.72
29	y	2630	LHG	C27-C26-C25	-2.28	102.84	114.37
25	n	602	CLA	CMB-C2B-C3B	2.28	131.91	126.55
25	3	611	CLA	CAA-CBA-CGA	2.28	119.68	113.21
29	b	2630	LHG	C20-C19-C18	-2.28	102.84	114.37
26	5	1620	LUT	C8-C7-C6	-2.28	120.91	127.00
24	y	609	CHL	CMB-C2B-C3B	2.28	129.24	124.68
24	5	608	CHL	OBD-CAD-C3D	-2.28	124.34	127.89
30	c	515	BCR	C1-C6-C5	-2.28	119.52	122.64
37	C	520	DGD	C3D-C4D-C5D	-2.28	106.10	110.23
24	Y	601	CHL	CMA-C3A-C4A	-2.28	109.70	114.61
25	R	616	CLA	CHC-C4B-NB	2.28	127.47	124.05
25	Y	614	CLA	CHC-C4B-NB	2.28	127.47	124.05
25	r	611	CLA	CHA-C1A-NA	-2.28	121.23	126.39
24	N	601	CHL	O2D-CGD-O1D	-2.28	119.42	123.85
24	s	608	CHL	O1D-CGD-CBD	-2.28	121.27	124.72
25	N	602	CLA	CMB-C2B-C3B	2.28	131.90	126.55
25	N	611	CLA	CAA-CBA-CGA	-2.28	106.75	113.21
25	A	410	CLA	O2D-CGD-CBD	2.28	115.21	111.23
25	C	506	CLA	C1-C2-C3	-2.28	122.47	126.20
25	3	611	CLA	CAA-C2A-C3A	-2.28	106.85	113.00
37	C	519	DGD	CBB-CAB-C9B	-2.28	102.87	114.37
24	n	609	CHL	O2A-CGA-CBA	2.27	118.77	111.83
25	y	610	CLA	CHB-C1B-NB	2.27	127.46	124.05
24	S	608	CHL	OBD-CAD-C3D	-2.27	124.34	127.89
26	2	1621	LUT	C36-C21-C26	2.27	112.99	109.55
24	s	607	CHL	CED-O2D-CGD	2.27	121.07	115.92
24	G	607	CHL	C6-C7-C8	-2.27	108.41	115.97
24	2	605	CHL	CMB-C2B-C3B	2.27	129.22	124.68
30	t	101	BCR	C31-C1-C6	-2.27	106.68	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	g	2630	LHG	C27-C26-C25	-2.27	102.88	114.37
25	R	611	CLA	CHA-C1A-NA	-2.27	121.25	126.39
25	b	617	CLA	CHC-C1C-NC	2.27	127.73	124.31
29	Y	2630	LHG	C27-C26-C25	-2.27	102.88	114.37
24	G	607	CHL	CAC-C3C-C4C	2.27	129.87	124.03
25	5	603	CLA	C2A-C1A-CHA	2.27	127.81	123.87
24	4	607	CHL	CBC-CAC-C3C	-2.27	109.62	112.87
25	5	612	CLA	O2D-CGD-CBD	2.27	115.20	111.23
24	N	608	CHL	C1C-C2C-CMC	2.27	130.90	126.80
25	b	616	CLA	C3A-C2A-C1A	2.27	104.74	101.34
25	n	611	CLA	CAA-CBA-CGA	-2.27	106.76	113.21
29	L	101	LHG	C18-C17-C16	-2.27	102.89	114.37
25	B	602	CLA	CHB-C1B-NB	2.27	127.45	124.05
37	c	520	DGD	C3D-C4D-C5D	-2.27	106.12	110.23
24	1	609	CHL	CBC-CAC-C3C	-2.27	109.62	112.87
25	2	613	CLA	CHB-C1B-NB	2.27	127.45	124.05
25	7	611	CLA	CAA-CBA-CGA	2.27	119.65	113.21
25	7	610	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
29	l	101	LHG	C18-C17-C16	-2.27	102.90	114.37
25	1	612	CLA	O2D-CGD-CBD	2.27	115.20	111.23
25	s	602	CLA	C3B-C4B-NB	-2.27	108.50	110.53
24	Y	606	CHL	O2A-CGA-O1A	-2.27	117.95	123.63
24	Y	601	CHL	O2D-CGD-O1D	-2.27	119.43	123.85
25	1	603	CLA	C2A-C1A-CHA	2.27	127.80	123.87
24	4	609	CHL	CMD-C2D-C3D	-2.27	120.15	124.68
24	R	608	CHL	C4-C3-C5	2.27	119.16	115.23
25	b	602	CLA	CHB-C1B-NB	2.27	127.45	124.05
35	Z	101	LMG	C38-C37-C36	-2.27	102.92	114.37
30	T	101	BCR	C31-C1-C6	-2.27	106.69	110.24
25	c	506	CLA	C1-C2-C3	-2.27	122.49	126.20
25	n	602	CLA	C6-C7-C8	-2.26	108.44	115.97
25	B	604	CLA	C3B-C4B-NB	-2.26	108.51	110.53
25	1	613	CLA	CHB-C1B-NB	2.26	127.44	124.05
25	6	613	CLA	CHB-C1B-NB	2.26	127.44	124.05
30	D	404	BCR	C3-C4-C5	-2.26	110.02	114.06
29	G	2630	LHG	C27-C26-C25	-2.26	102.93	114.37
30	B	619	BCR	C33-C5-C6	-2.26	122.02	124.48
24	N	609	CHL	O2A-CGA-CBA	2.26	118.73	111.83
26	N	1621	LUT	C28-C29-C30	-2.26	115.45	119.01
30	8	623	BCR	C21-C20-C19	-2.26	116.64	123.20
26	n	1621	LUT	C28-C29-C30	-2.26	115.45	119.01
26	7	1620	LUT	C27-C28-C29	-2.26	121.46	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	7	1623	NEX	C30-C31-C32	-2.26	116.65	123.20
26	R	620	LUT	C38-C25-C24	-2.26	118.01	123.36
24	y	601	CHL	CMA-C3A-C4A	-2.26	109.74	114.61
35	z	101	LMG	C38-C37-C36	-2.26	102.94	114.37
24	n	608	CHL	C1C-C2C-CMC	2.26	130.87	126.80
26	3	1620	LUT	C27-C28-C29	-2.26	121.47	126.32
24	S	606	CHL	CMB-C2B-C3B	2.26	129.19	124.68
25	C	501	CLA	CHB-C1B-NB	2.26	127.44	124.05
25	N	602	CLA	C6-C7-C8	-2.26	108.46	115.97
24	s	606	CHL	CMB-C2B-C3B	2.26	129.19	124.68
24	5	609	CHL	CBC-CAC-C3C	-2.26	109.64	112.87
35	b	2633	LMG	C42-C41-C40	-2.26	102.96	114.37
25	5	613	CLA	CHB-C1B-NB	2.26	127.43	124.05
30	B	619	BCR	C40-C30-C25	2.26	113.78	110.24
25	Y	604	CLA	C3B-C4B-NB	-2.26	108.52	110.53
25	G	613	CLA	CHB-C1B-NB	2.26	127.43	124.05
30	4	623	BCR	C21-C20-C19	-2.26	116.66	123.20
24	Y	601	CHL	C4C-CHD-C1D	2.26	124.14	116.07
30	b	619	BCR	C40-C30-C25	2.26	113.78	110.24
35	B	2633	LMG	C42-C41-C40	-2.26	102.97	114.37
25	8	610	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
26	6	1621	LUT	C36-C21-C26	2.26	112.96	109.55
25	s	610	CLA	CMB-C2B-C3B	2.25	131.85	126.55
24	y	601	CHL	C4C-CHD-C1D	2.25	124.13	116.07
25	3	602	CLA	C1-C2-C3	-2.25	122.51	126.20
25	D	402	CLA	O2D-CGD-CBD	2.25	115.17	111.23
25	d	402	CLA	O2D-CGD-CBD	2.25	115.17	111.23
25	S	602	CLA	CMB-C2B-C3B	2.25	131.85	126.55
27	8	622	XAT	C8-C9-C10	-2.25	115.47	119.01
24	y	609	CHL	C1-C2-C3	-2.25	122.51	126.20
24	2	608	CHL	CMB-C2B-C3B	2.25	129.18	124.68
24	3	601	CHL	C4-C3-C5	2.25	119.14	115.23
25	r	611	CLA	CHB-C4A-NA	2.25	127.65	124.40
25	r	602	CLA	O2D-CGD-CBD	2.25	115.16	111.23
25	C	505	CLA	CMB-C2B-C3B	2.25	131.84	126.55
27	g	1622	XAT	C26-C27-C28	-2.25	121.24	125.99
24	1	601	CHL	C1C-C2C-CMC	2.25	130.86	126.80
25	n	604	CLA	O1D-CGD-CBD	2.25	128.96	124.52
24	1	608	CHL	OBD-CAD-C3D	-2.25	124.38	127.89
28	3	1623	NEX	C30-C31-C32	-2.25	116.68	123.20
25	s	602	CLA	CMB-C2B-C3B	2.25	131.84	126.55
25	N	604	CLA	O1D-CGD-CBD	2.25	128.95	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	609	CHL	CMD-C2D-C3D	-2.25	120.19	124.68
30	b	619	BCR	C33-C5-C6	-2.25	122.03	124.48
30	A	411	BCR	C15-C16-C17	-2.25	118.92	123.52
26	G	1620	LUT	C8-C9-C10	-2.25	115.47	119.01
27	4	622	XAT	C8-C9-C10	-2.25	115.47	119.01
24	N	601	CHL	C1-O2A-CGA	2.25	122.09	116.65
30	c	514	BCR	C3-C4-C5	-2.25	110.05	114.06
24	8	607	CHL	CBC-CAC-C3C	-2.25	109.66	112.87
28	6	1623	NEX	C30-C31-C32	-2.25	116.69	123.20
25	S	610	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
30	C	514	BCR	C3-C4-C5	-2.24	110.05	114.06
34	A	418	SQD	O48-C23-C24	2.24	118.68	111.83
24	n	601	CHL	C1-O2A-CGA	2.24	122.08	116.65
25	3	610	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
24	r	614	CHL	CMB-C2B-C3B	2.24	129.17	124.68
26	r	620	LUT	C38-C25-C24	-2.24	118.05	123.36
27	G	1622	XAT	C26-C27-C28	-2.24	121.25	125.99
28	N	1623	NEX	C28-C29-C30	2.24	122.54	119.01
28	2	1623	NEX	C30-C31-C32	-2.24	116.70	123.20
25	c	501	CLA	CHB-C1B-NB	2.24	127.41	124.05
24	g	606	CHL	O2A-CGA-O1A	-2.24	118.02	123.63
24	G	608	CHL	OBD-CAD-C3D	-2.24	124.39	127.89
24	g	608	CHL	OBD-CAD-C3D	-2.24	124.39	127.89
24	7	601	CHL	C4-C3-C5	2.24	119.12	115.23
25	B	617	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
29	d	409	LHG	C27-C26-C25	-2.24	103.04	114.37
25	1	610	CLA	CHB-C1B-NB	2.24	127.41	124.05
24	2	601	CHL	CED-O2D-CGD	2.24	121.00	115.92
26	n	1621	LUT	C37-C21-C22	-2.24	105.23	109.41
25	g	613	CLA	CHB-C1B-NB	2.24	127.41	124.05
24	5	601	CHL	C1C-C2C-CMC	2.24	130.84	126.80
30	d	404	BCR	C3-C4-C5	-2.24	110.06	114.06
24	8	609	CHL	CMB-C2B-C3B	2.24	129.16	124.68
25	g	602	CLA	CAA-CBA-CGA	-2.24	106.85	113.21
25	D	402	CLA	CMB-C2B-C3B	2.24	131.82	126.55
25	4	611	CLA	CHB-C4A-NA	2.24	127.63	124.40
24	N	609	CHL	O2D-CGD-O1D	-2.24	119.49	123.85
24	r	607	CHL	CED-O2D-CGD	2.24	120.99	115.92
25	n	613	CLA	CMB-C2B-C3B	2.24	131.82	126.55
25	r	610	CLA	C1-C2-C3	-2.24	122.53	126.20
24	8	601	CHL	C3D-C4D-CHA	2.24	111.94	108.54
29	n	2630	LHG	O8-C23-C24	2.24	118.66	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	608	CHL	CMA-C3A-C4A	-2.24	109.79	114.61
24	R	607	CHL	CED-O2D-CGD	2.24	120.99	115.92
30	C	515	BCR	C10-C11-C12	-2.24	116.72	123.20
25	S	610	CLA	CMB-C2B-C3B	2.24	131.81	126.55
27	R	622	XAT	O24-C25-C26	-2.24	57.16	58.93
24	7	607	CHL	CAC-C3C-C4C	2.24	129.78	124.03
24	6	607	CHL	C4-C3-C5	2.24	119.11	115.23
30	c	515	BCR	C10-C11-C12	-2.24	116.72	123.20
24	y	606	CHL	O2A-CGA-O1A	-2.24	118.03	123.63
24	g	605	CHL	CMA-C3A-C4A	-2.24	109.80	114.61
26	3	1620	LUT	C17-C1-C6	2.24	113.75	110.24
24	N	601	CHL	CAC-C3C-C4C	2.24	129.78	124.03
29	D	409	LHG	C27-C26-C25	-2.23	103.07	114.37
34	a	418	SQD	O48-C23-C24	2.23	118.65	111.83
30	D	404	BCR	C33-C5-C6	-2.23	122.05	124.48
25	b	617	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
29	N	2630	LHG	O8-C23-C24	2.23	118.65	111.83
26	g	1620	LUT	C8-C9-C10	-2.23	115.50	119.01
29	d	410	LHG	C27-C26-C25	-2.23	103.08	114.37
25	N	613	CLA	CMB-C2B-C3B	2.23	131.80	126.55
25	y	604	CLA	C3B-C4B-NB	-2.23	108.54	110.53
24	g	601	CHL	CMD-C2D-C3D	-2.23	120.22	124.68
28	n	1623	NEX	C28-C29-C30	2.23	122.52	119.01
25	c	502	CLA	CBC-CAC-C3C	-2.23	106.37	112.42
25	B	602	CLA	C3B-C4B-NB	-2.23	108.54	110.53
24	G	605	CHL	CMA-C3A-C4A	-2.23	109.80	114.61
24	G	601	CHL	CMD-C2D-C3D	-2.23	120.22	124.68
27	r	622	XAT	O24-C25-C26	-2.23	57.16	58.93
25	b	604	CLA	C3B-C4B-NB	-2.23	108.54	110.53
24	n	601	CHL	CAC-C3C-C4C	2.23	129.76	124.03
30	a	411	BCR	C15-C16-C17	-2.23	118.95	123.52
25	c	505	CLA	CMB-C2B-C3B	2.23	131.80	126.55
25	C	511	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
29	D	410	LHG	C27-C26-C25	-2.23	103.09	114.37
24	4	601	CHL	C3D-C4D-CHA	2.23	111.93	108.54
25	b	616	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
29	y	2630	LHG	C18-C17-C16	-2.23	103.10	114.37
24	Y	601	CHL	OBD-CAD-C3D	-2.23	124.42	127.89
24	s	608	CHL	CBC-CAC-C3C	-2.23	109.68	112.87
26	s	1620	LUT	C38-C25-C24	-2.23	118.09	123.36
24	6	608	CHL	CMB-C2B-C3B	2.23	129.14	124.68
29	Y	2630	LHG	C18-C17-C16	-2.23	103.10	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	608	CHL	O2A-CGA-CBA	2.23	121.04	114.00
25	B	616	CLA	O2D-CGD-CBD	2.23	115.12	111.23
25	G	602	CLA	CAA-CBA-CGA	-2.23	106.89	113.21
30	D	404	BCR	C10-C11-C12	-2.23	116.75	123.20
24	4	608	CHL	O2A-CGA-CBA	2.23	121.03	114.00
25	6	604	CLA	O1A-CGA-CBA	2.23	130.15	123.09
24	n	606	CHL	O2D-CGD-O1D	-2.22	119.52	123.85
25	2	604	CLA	O1A-CGA-CBA	2.22	130.15	123.09
26	7	1620	LUT	C17-C1-C6	2.22	113.73	110.24
35	C	521	LMG	C38-C37-C36	-2.22	103.12	114.37
24	4	606	CHL	O2A-CGA-CBA	2.22	121.03	114.00
24	6	601	CHL	CED-O2D-CGD	2.22	120.96	115.92
28	r	623	NEX	C2-C1-C6	2.22	111.37	109.21
35	c	521	LMG	C38-C37-C36	-2.22	103.13	114.37
25	s	610	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
35	A	415	LMG	O3-C3-C2	-2.22	105.14	110.38
28	G	1623	NEX	C35-C15-C14	-2.22	118.97	123.52
24	7	608	CHL	CMA-C3A-C4A	-2.22	109.82	114.61
24	2	607	CHL	C4-C3-C5	2.22	119.09	115.23
35	B	2633	LMG	C6-C5-C4	-2.22	107.56	113.02
25	C	502	CLA	CBC-CAC-C3C	-2.22	106.40	112.42
24	R	606	CHL	CMA-C3A-C4A	-2.22	109.82	114.61
35	b	2633	LMG	C6-C5-C4	-2.22	107.56	113.02
25	Y	613	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
24	8	606	CHL	O2A-CGA-CBA	2.22	121.02	114.00
25	R	602	CLA	O2D-CGD-CBD	2.22	115.11	111.23
24	3	607	CHL	CAC-C3C-C4C	2.22	129.74	124.03
25	d	402	CLA	CMB-C2B-C3B	2.22	131.77	126.55
28	g	1623	NEX	C35-C15-C14	-2.22	118.97	123.52
25	R	610	CLA	C1-C2-C3	-2.22	122.56	126.20
30	h	101	BCR	C2-C1-C6	2.22	113.66	110.44
24	n	609	CHL	O2D-CGD-O1D	-2.22	119.53	123.85
24	Y	601	CHL	CAC-C3C-C4C	2.22	129.73	124.03
26	S	1620	LUT	C38-C25-C24	-2.22	118.11	123.36
30	d	404	BCR	C10-C11-C12	-2.22	116.77	123.20
25	8	611	CLA	O2A-CGA-O1A	-2.22	117.63	123.33
24	4	609	CHL	CMB-C2B-C3B	2.22	129.12	124.68
24	G	606	CHL	O2A-CGA-O1A	-2.22	118.08	123.63
24	y	601	CHL	CAC-C3C-C4C	2.22	129.73	124.03
24	7	601	CHL	O2A-CGA-CBA	2.22	118.59	111.83
28	g	1623	NEX	C16-C1-C6	2.22	112.46	110.47
24	N	606	CHL	O2D-CGD-O1D	-2.22	119.53	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	611	CLA	CHB-C4A-NA	2.22	127.60	124.40
30	H	101	BCR	C16-C15-C14	-2.22	118.98	123.52
24	R	614	CHL	CMB-C2B-C3B	2.22	129.11	124.68
24	R	607	CHL	CAA-CBA-CGA	-2.22	106.92	113.21
36	D	405	PL9	O2-C1-C2	-2.22	116.79	121.83
25	4	603	CLA	CMB-C2B-C1B	-2.22	122.05	125.42
25	B	616	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
25	G	614	CLA	CHB-C4A-NA	2.21	127.60	124.40
25	b	602	CLA	C3B-C4B-NB	-2.21	108.55	110.53
24	8	608	CHL	CMA-C3A-C2A	-2.21	105.58	114.13
25	c	513	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
25	5	613	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
25	8	603	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
25	r	609	CLA	CHB-C1B-NB	2.21	127.37	124.05
26	2	1621	LUT	C16-C1-C6	-2.21	106.77	110.24
25	3	602	CLA	CHB-C4A-NA	2.21	127.59	124.40
37	c	520	DGD	CAB-C9B-C8B	-2.21	103.18	114.37
25	8	611	CLA	CHB-C4A-NA	2.21	127.59	124.40
25	C	506	CLA	CHB-C1B-NB	2.21	127.37	124.05
24	7	608	CHL	O2A-CGA-CBA	2.21	120.99	114.00
25	b	606	CLA	CHC-C1C-NC	2.21	127.64	124.31
25	b	616	CLA	O2D-CGD-CBD	2.21	115.09	111.23
25	S	609	CLA	CHB-C4A-NA	2.21	127.59	124.40
24	4	608	CHL	CMA-C3A-C2A	-2.21	105.59	114.13
25	R	609	CLA	CHB-C1B-NB	2.21	127.36	124.05
25	y	613	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
37	C	520	DGD	CAB-C9B-C8B	-2.21	103.20	114.37
25	s	609	CLA	CHB-C4A-NA	2.21	127.59	124.40
36	D	405	PL9	C20-C19-C21	2.21	119.06	115.23
35	a	415	LMG	O3-C3-C2	-2.21	105.17	110.38
25	1	613	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
24	r	607	CHL	CAA-CBA-CGA	-2.21	106.94	113.21
25	b	607	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
25	c	506	CLA	CHB-C1B-NB	2.21	127.36	124.05
39	F	101	HEM	CMB-C2B-C1B	-2.21	121.58	125.03
35	c	521	LMG	C1-C2-C3	-2.21	105.37	110.01
30	H	101	BCR	C2-C1-C6	2.21	113.64	110.44
30	h	101	BCR	C16-C15-C14	-2.21	119.00	123.52
29	G	2630	LHG	C18-C17-C16	-2.21	103.22	114.37
36	d	405	PL9	C20-C19-C21	2.21	119.06	115.23
25	A	410	CLA	CHC-C4B-NB	2.21	127.36	124.05
26	G	1621	LUT	C37-C21-C22	-2.21	105.29	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	N	1621	LUT	C37-C21-C22	-2.21	105.29	109.41
24	r	606	CHL	CMA-C3A-C4A	-2.21	109.86	114.61
26	N	1620	LUT	C36-C21-C26	2.20	112.89	109.55
26	R	620	LUT	C31-C30-C29	-2.20	124.19	127.28
26	5	1620	LUT	C20-C13-C12	2.20	121.45	118.09
24	3	601	CHL	O2A-CGA-CBA	2.20	118.55	111.83
26	r	620	LUT	C31-C30-C29	-2.20	124.19	127.28
29	C	522	LHG	C27-C26-C25	-2.20	103.23	114.37
35	C	521	LMG	C1-C2-C3	-2.20	105.38	110.01
28	R	623	NEX	C2-C1-C6	2.20	111.35	109.21
25	B	613	CLA	C1-C2-C3	-2.20	122.59	126.20
25	b	613	CLA	C1-C2-C3	-2.20	122.59	126.20
26	1	1620	LUT	C20-C13-C12	2.20	121.45	118.09
25	b	605	CLA	CHA-C1A-NA	-2.20	121.41	126.39
25	c	501	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
29	g	2630	LHG	C18-C17-C16	-2.20	103.25	114.37
25	7	602	CLA	CHB-C4A-NA	2.20	127.58	124.40
30	C	516	BCR	C35-C13-C12	2.20	121.45	118.09
37	C	518	DGD	CBB-CAB-C9B	-2.20	103.25	114.37
25	B	605	CLA	C1D-ND-C4D	2.20	107.86	106.31
24	3	608	CHL	O2A-CGA-CBA	2.20	120.95	114.00
29	c	522	LHG	C27-C26-C25	-2.20	103.25	114.37
30	c	516	BCR	C35-C13-C12	2.20	121.45	118.09
29	Y	2630	LHG	C11-C10-C9	-2.20	103.26	114.37
37	c	518	DGD	O6D-C5D-C6D	-2.20	102.34	106.69
25	4	611	CLA	O2A-CGA-O1A	-2.20	117.68	123.33
24	S	608	CHL	CBC-CAC-C3C	-2.20	109.73	112.87
25	a	410	CLA	CHC-C4B-NB	2.20	127.35	124.05
25	3	612	CLA	CMD-C2D-C3D	2.20	132.73	127.69
29	y	2630	LHG	C11-C10-C9	-2.20	103.26	114.37
36	d	405	PL9	O2-C1-C2	-2.20	116.83	121.83
25	n	610	CLA	C2A-C1A-CHA	2.20	127.68	123.87
37	c	518	DGD	CBB-CAB-C9B	-2.20	103.26	114.37
26	7	1621	LUT	C38-C25-C24	-2.20	118.16	123.36
30	d	404	BCR	C33-C5-C6	-2.20	122.09	124.48
25	B	605	CLA	CHA-C1A-NA	-2.20	121.42	126.39
24	5	608	CHL	CMB-C2B-C3B	2.20	129.07	124.68
25	7	613	CLA	C1-C2-C3	-2.20	122.60	126.20
25	C	513	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
25	n	614	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
26	6	1621	LUT	C16-C1-C6	-2.20	106.80	110.24
25	3	613	CLA	C1-C2-C3	-2.19	122.60	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	402	CLA	CHC-C4B-NB	2.19	127.34	124.05
30	H	101	BCR	C15-C16-C17	-2.19	119.03	123.52
24	R	607	CHL	CAC-C3C-C4C	2.19	129.67	124.03
25	g	610	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
29	7	2630	LHG	C18-C17-C16	-2.19	103.28	114.37
25	G	604	CLA	CHB-C4A-NA	2.19	127.56	124.40
25	C	513	CLA	O2D-CGD-CBD	2.19	115.06	111.23
24	7	607	CHL	CMB-C2B-C3B	2.19	129.06	124.68
25	B	608	CLA	CMB-C2B-C3B	2.19	131.71	126.55
29	3	2630	LHG	C18-C17-C16	-2.19	103.29	114.37
25	c	511	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
24	y	601	CHL	OBD-CAD-C3D	-2.19	124.47	127.89
25	2	604	CLA	CHB-C1B-NB	2.19	127.34	124.05
26	n	1620	LUT	C36-C21-C26	2.19	112.86	109.55
29	c	523	LHG	C18-C17-C16	-2.19	103.29	114.37
24	N	609	CHL	C4-C3-C5	2.19	119.03	115.23
25	C	501	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
26	Y	1620	LUT	C31-C30-C29	-2.19	124.21	127.28
39	f	101	HEM	CMB-C2B-C1B	-2.19	121.61	125.03
25	3	610	CLA	CHB-C1B-NB	2.19	127.33	124.05
25	6	604	CLA	CHB-C1B-NB	2.19	127.33	124.05
30	c	515	BCR	C36-C18-C19	2.19	121.43	118.09
24	n	609	CHL	C4-C3-C5	2.19	119.03	115.23
25	B	606	CLA	CHC-C1C-NC	2.19	127.61	124.31
28	G	1623	NEX	C16-C1-C6	2.19	112.43	110.47
26	g	1621	LUT	C37-C21-C22	-2.19	105.33	109.41
25	N	614	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
25	1	603	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
25	N	604	CLA	CHB-C4A-NA	2.19	127.56	124.40
24	R	614	CHL	CMD-C2D-C3D	-2.19	120.31	124.68
24	6	606	CHL	CED-O2D-CGD	2.19	120.88	115.92
25	c	513	CLA	O2D-CGD-CBD	2.19	115.05	111.23
37	C	518	DGD	O6D-C5D-C6D	-2.19	102.36	106.69
28	y	1623	NEX	C4-C3-C2	-2.19	106.70	110.79
25	D	402	CLA	CHC-C4B-NB	2.19	127.33	124.05
26	6	1620	LUT	C8-C9-C10	-2.19	115.57	119.01
25	g	603	CLA	CHB-C1B-C2B	-2.18	121.08	127.43
25	b	608	CLA	CMB-C2B-C3B	2.18	131.69	126.55
29	C	523	LHG	C18-C17-C16	-2.18	103.32	114.37
28	Y	1623	NEX	C4-C3-C2	-2.18	106.70	110.79
25	n	604	CLA	CHB-C4A-NA	2.18	127.55	124.40
25	c	507	CLA	C2A-C1A-CHA	2.18	127.66	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	3	1621	LUT	C38-C25-C24	-2.18	118.19	123.36
24	3	607	CHL	CMB-C2B-C3B	2.18	129.04	124.68
25	B	607	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
24	1	608	CHL	CMB-C2B-C3B	2.18	129.04	124.68
34	B	623	SQD	C44-O6-C1	2.18	118.47	113.80
25	C	507	CLA	C2A-C1A-CHA	2.18	127.65	123.87
24	8	608	CHL	CMA-C3A-C4A	-2.18	109.91	114.61
24	2	606	CHL	CED-O2D-CGD	2.18	120.86	115.92
24	4	608	CHL	CMA-C3A-C4A	-2.18	109.91	114.61
28	r	623	NEX	C40-C33-C32	2.18	121.42	118.09
25	g	614	CLA	CHB-C4A-NA	2.18	127.55	124.40
24	r	607	CHL	CAC-C3C-C4C	2.18	129.63	124.03
24	3	609	CHL	C4-C3-C5	2.18	119.01	115.23
26	g	1621	LUT	C1-C2-C3	2.18	118.37	113.59
25	A	405	CLA	CHB-C4A-NA	2.18	127.54	124.40
25	1	602	CLA	CHA-C1A-NA	-2.18	121.46	126.39
35	B	622	LMG	O2-C2-C1	-2.18	104.89	110.08
30	8	623	BCR	C4-C5-C6	-2.18	119.76	122.70
25	B	609	CLA	CAC-C3C-C4C	2.18	127.62	124.79
25	N	610	CLA	C2A-C1A-CHA	2.18	127.65	123.87
26	7	1620	LUT	C15-C35-C34	-2.18	119.06	123.52
24	8	609	CHL	O2A-CGA-CBA	2.18	120.88	114.00
24	4	609	CHL	O2A-CGA-CBA	2.18	120.88	114.00
35	A	415	LMG	O2-C2-C1	-2.18	104.89	110.08
25	b	615	CLA	CHB-C1B-NB	2.18	127.31	124.05
35	b	622	LMG	O2-C2-C1	-2.18	104.89	110.08
25	G	610	CLA	CMB-C2B-C1B	-2.18	122.11	125.42
25	n	610	CLA	C1-C2-C3	-2.18	122.63	126.20
25	C	507	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
35	B	2633	LMG	O6-C1-O1	-2.17	104.91	110.04
24	7	609	CHL	C4-C3-C5	2.17	119.00	115.23
25	5	602	CLA	CHA-C1A-NA	-2.17	121.47	126.39
26	r	620	LUT	C4-C5-C6	2.17	125.22	120.76
26	3	1620	LUT	C15-C35-C34	-2.17	119.07	123.52
29	l	101	LHG	C27-C26-C25	-2.17	103.38	114.37
30	C	515	BCR	C36-C18-C19	2.17	121.41	118.09
25	g	604	CLA	CHB-C4A-NA	2.17	127.54	124.40
25	b	603	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
25	7	612	CLA	CMD-C2D-C3D	2.17	132.67	127.69
24	7	601	CHL	C1C-C2C-CMC	2.17	130.72	126.80
27	n	1622	XAT	C28-C29-C30	2.17	122.43	119.01
25	b	612	CLA	C11-C12-C13	-2.17	108.75	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	S	2630	LHG	C18-C17-C16	-2.17	103.39	114.37
26	g	1620	LUT	C27-C28-C29	-2.17	121.65	126.32
25	B	603	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
25	y	602	CLA	CAC-C3C-C4C	2.17	127.61	124.79
30	h	101	BCR	C15-C16-C17	-2.17	119.08	123.52
25	N	610	CLA	C1-C2-C3	-2.17	122.64	126.20
25	r	603	CLA	C1-C2-C3	-2.17	122.64	126.20
24	r	614	CHL	CMD-C2D-C3D	-2.17	120.34	124.68
24	6	601	CHL	CMB-C2B-C3B	2.17	129.02	124.68
24	G	606	CHL	CAC-C3C-C4C	2.17	129.61	124.03
25	5	614	CLA	CMB-C2B-C3B	2.17	131.66	126.55
29	L	101	LHG	C27-C26-C25	-2.17	103.40	114.37
30	c	514	BCR	C7-C8-C9	-2.17	123.03	126.23
25	R	603	CLA	C1-C2-C3	-2.17	122.64	126.20
25	G	603	CLA	CHB-C1B-C2B	-2.17	121.13	127.43
26	Y	1621	LUT	C35-C15-C14	-2.17	119.08	123.52
25	5	614	CLA	C3B-C4B-NB	-2.17	108.59	110.53
24	5	601	CHL	C4C-CHD-C1D	2.17	123.83	116.07
30	b	619	BCR	C37-C22-C23	2.17	121.40	118.09
26	G	1621	LUT	C1-C2-C3	2.17	118.35	113.59
27	G	1622	XAT	O24-C25-C26	-2.17	57.21	58.93
25	B	615	CLA	CHB-C1B-NB	2.17	127.30	124.05
37	C	518	DGD	O3G-C1D-C2D	-2.17	104.98	108.27
25	y	610	CLA	CHB-C1B-C2B	-2.17	121.14	127.43
37	c	518	DGD	O3G-C1D-C2D	-2.17	104.98	108.27
25	B	612	CLA	C11-C12-C13	-2.17	108.77	115.97
24	5	607	CHL	C1-C2-C3	-2.17	122.65	126.20
25	7	603	CLA	CHA-C1A-NA	-2.17	121.49	126.39
29	s	2630	LHG	C18-C17-C16	-2.17	103.42	114.37
37	H	102	DGD	O1G-C1A-O1A	-2.17	118.21	123.63
25	C	509	CLA	CMB-C2B-C3B	2.17	131.64	126.55
29	s	2630	LHG	C5-O7-C7	-2.17	112.61	117.80
25	3	603	CLA	CHA-C1A-NA	-2.17	121.49	126.39
24	G	608	CHL	O2D-CGD-O1D	-2.17	119.63	123.85
30	4	623	BCR	C3-C4-C5	-2.16	110.19	114.06
30	8	623	BCR	C3-C4-C5	-2.16	110.19	114.06
28	R	623	NEX	C40-C33-C32	2.16	121.39	118.09
26	R	620	LUT	C4-C5-C6	2.16	125.20	120.76
24	Y	608	CHL	O1D-CGD-CBD	-2.16	121.44	124.72
26	2	1620	LUT	C8-C9-C10	-2.16	115.61	119.01
27	1	1622	XAT	C10-C11-C12	-2.16	116.93	123.20
30	C	514	BCR	C7-C8-C9	-2.16	123.03	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	507	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
25	1	614	CLA	CMB-C2B-C3B	2.16	131.64	126.55
35	a	415	LMG	O2-C2-C1	-2.16	104.92	110.08
30	D	404	BCR	C36-C18-C19	2.16	121.39	118.09
26	G	1620	LUT	C27-C28-C29	-2.16	121.67	126.32
24	6	609	CHL	CAC-C3C-C4C	2.16	129.59	124.03
34	b	623	SQD	C44-O6-C1	2.16	118.43	113.80
35	c	521	LMG	O1-C7-C8	-2.16	105.56	110.82
35	b	2633	LMG	O6-C1-O1	-2.16	104.94	110.04
27	g	1622	XAT	O24-C25-C26	-2.16	57.22	58.93
25	Y	602	CLA	CMB-C2B-C3B	2.16	131.63	126.55
25	B	612	CLA	C1-C2-C3	-2.16	122.66	126.20
24	7	601	CHL	C4C-CHD-C1D	2.16	123.80	116.07
25	c	507	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
25	5	603	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
26	y	1620	LUT	C31-C30-C29	-2.16	124.25	127.28
25	c	509	CLA	CMB-C2B-C3B	2.16	131.63	126.55
24	3	601	CHL	C4C-CHD-C1D	2.16	123.80	116.07
25	b	605	CLA	C1D-ND-C4D	2.16	107.83	106.31
29	S	2630	LHG	C5-O7-C7	-2.16	112.63	117.80
25	n	602	CLA	CHB-C4A-NA	2.16	127.52	124.40
35	a	415	LMG	C38-C37-C36	-2.16	103.45	114.37
24	2	609	CHL	CAC-C3C-C4C	2.16	129.58	124.03
26	s	1621	LUT	C38-C25-C24	-2.16	118.25	123.36
25	n	613	CLA	CHC-C4B-NB	2.16	127.29	124.05
25	b	609	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
35	A	415	LMG	C38-C37-C36	-2.16	103.46	114.37
26	y	1621	LUT	C31-C30-C29	-2.16	124.25	127.28
24	1	607	CHL	C1-C2-C3	-2.16	122.66	126.20
37	B	626	DGD	C3D-C4D-C5D	-2.16	106.32	110.23
27	2	1622	XAT	C16-C1-C2	-2.16	105.18	108.97
25	3	614	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
35	C	521	LMG	O1-C7-C8	-2.16	105.57	110.82
34	b	623	SQD	O5-C5-C4	2.16	113.59	109.70
24	3	601	CHL	C1C-C2C-CMC	2.16	130.69	126.80
25	b	612	CLA	C1-C2-C3	-2.16	122.66	126.20
25	Y	610	CLA	CHB-C1B-C2B	-2.16	121.17	127.43
25	g	610	CLA	C2A-C1A-CHA	2.16	127.61	123.87
24	4	609	CHL	CAC-C3C-C4C	2.16	129.57	124.03
30	4	623	BCR	C4-C5-C6	-2.16	119.79	122.70
25	g	603	CLA	C3C-C4C-NC	-2.16	107.67	110.43
34	B	623	SQD	O5-C5-C4	2.16	113.58	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	608	CHL	O2D-CGD-O1D	-2.16	119.65	123.85
24	g	606	CHL	CAC-C3C-C4C	2.16	129.57	124.03
26	7	1620	LUT	C38-C25-C24	-2.16	118.26	123.36
24	2	601	CHL	CMB-C2B-C3B	2.16	128.99	124.68
27	5	1622	XAT	C10-C11-C12	-2.15	116.96	123.20
24	Y	601	CHL	CGD-CBD-CAD	-2.15	103.87	110.85
26	y	1620	LUT	C36-C21-C26	2.15	112.81	109.55
24	1	601	CHL	C4C-CHD-C1D	2.15	123.78	116.07
29	2	2630	LHG	C27-C26-C25	-2.15	103.48	114.37
24	y	601	CHL	CGD-CBD-CAD	-2.15	103.87	110.85
29	C	2630	LHG	C27-C26-C25	-2.15	103.48	114.37
25	7	610	CLA	CHB-C1B-NB	2.15	127.28	124.05
26	Y	1621	LUT	C31-C30-C29	-2.15	124.26	127.28
25	b	607	CLA	C6-C7-C8	-2.15	108.81	115.97
25	7	614	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
27	N	1622	XAT	C28-C29-C30	2.15	122.39	119.01
37	h	102	DGD	O1G-C1A-O1A	-2.15	118.25	123.63
25	B	609	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
27	8	622	XAT	C30-C31-C32	-2.15	116.97	123.20
24	N	601	CHL	CMB-C2B-C3B	2.15	128.98	124.68
25	B	607	CLA	C6-C7-C8	-2.15	108.81	115.97
29	6	2630	LHG	C27-C26-C25	-2.15	103.50	114.37
25	Y	602	CLA	CAC-C3C-C4C	2.15	127.59	124.79
25	y	602	CLA	CMB-C2B-C3B	2.15	131.61	126.55
25	b	609	CLA	CAC-C3C-C4C	2.15	127.59	124.79
25	G	603	CLA	C3C-C4C-NC	-2.15	107.68	110.43
25	g	610	CLA	CMB-C2B-C3B	2.15	131.61	126.55
24	n	607	CHL	CAA-CBA-CGA	-2.15	107.11	113.21
25	4	610	CLA	CMB-C2B-C3B	2.15	131.60	126.55
24	3	608	CHL	C4C-CHD-C1D	2.15	123.76	116.07
30	B	619	BCR	C37-C22-C23	2.15	121.37	118.09
29	c	2630	LHG	C27-C26-C25	-2.15	103.51	114.37
24	y	608	CHL	O1D-CGD-CBD	-2.15	121.47	124.72
24	r	606	CHL	C6-C5-C3	-2.15	108.23	113.47
24	N	607	CHL	CAA-CBA-CGA	-2.15	107.11	113.21
26	y	1621	LUT	C35-C15-C14	-2.15	119.12	123.52
30	d	404	BCR	C36-C18-C19	2.15	121.37	118.09
25	C	507	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
28	G	1623	NEX	C30-C31-C32	-2.15	116.98	123.20
26	3	1621	LUT	C39-C29-C28	2.15	121.37	118.09
24	5	609	CHL	C1-C2-C3	-2.15	122.68	126.20
25	R	601	CLA	CMB-C2B-C3B	2.15	131.60	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	7	608	CHL	C4C-CHD-C1D	2.15	123.75	116.07
27	4	622	XAT	C30-C31-C32	-2.15	116.98	123.20
26	6	1621	LUT	C11-C10-C9	-2.15	124.27	127.28
24	8	606	CHL	C4C-CHD-C1D	2.15	123.75	116.07
25	2	603	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
37	b	626	DGD	C3D-C4D-C5D	-2.15	106.34	110.23
24	r	606	CHL	O2D-CGD-O1D	-2.15	119.67	123.85
24	n	605	CHL	OBD-CAD-C3D	-2.15	124.55	127.89
25	G	610	CLA	C2A-C1A-CHA	2.14	127.59	123.87
26	7	1621	LUT	C39-C29-C28	2.14	121.36	118.09
24	8	608	CHL	O2A-CGA-O1A	-2.14	117.82	123.33
26	S	1621	LUT	C38-C25-C24	-2.14	118.29	123.36
24	4	608	CHL	O2A-CGA-O1A	-2.14	117.82	123.33
24	s	607	CHL	CAC-C3C-C4C	2.14	129.54	124.03
29	B	2630	LHG	C27-C26-C25	-2.14	103.53	114.37
29	5	2630	LHG	C27-C26-C25	-2.14	103.53	114.37
29	b	2630	LHG	C27-C26-C25	-2.14	103.53	114.37
24	y	606	CHL	CMB-C2B-C3B	2.14	128.97	124.68
26	3	1620	LUT	C38-C25-C24	-2.14	118.29	123.36
24	8	609	CHL	CAC-C3C-C4C	2.14	129.54	124.03
28	g	1623	NEX	C30-C31-C32	-2.14	116.99	123.20
24	4	606	CHL	C4C-CHD-C1D	2.14	123.73	116.07
25	r	604	CLA	CMB-C2B-C3B	2.14	131.59	126.55
25	s	602	CLA	CHB-C4A-NA	2.14	127.49	124.40
26	1	1621	LUT	C31-C32-C33	-2.14	120.49	126.36
25	n	611	CLA	C3B-C4B-NB	-2.14	108.62	110.53
25	B	604	CLA	CHC-C4B-NB	2.14	127.26	124.05
24	n	601	CHL	CMB-C2B-C3B	2.14	128.96	124.68
26	Y	1620	LUT	C36-C21-C26	2.14	112.79	109.55
37	C	518	DGD	CAB-C9B-C8B	-2.14	103.55	114.37
27	6	1622	XAT	C16-C1-C2	-2.14	105.21	108.97
25	N	602	CLA	CHB-C4A-NA	2.14	127.49	124.40
25	r	601	CLA	CMB-C2B-C3B	2.14	131.58	126.55
24	2	601	CHL	CMA-C3A-C4A	-2.14	110.00	114.61
24	8	607	CHL	O2D-CGD-O1D	-2.14	119.68	123.85
24	1	606	CHL	O2A-CGA-CBA	2.14	120.76	114.00
25	8	610	CLA	CMB-C2B-C3B	2.14	131.58	126.55
25	6	603	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
25	1	602	CLA	CHB-C4A-NA	2.14	127.48	124.40
25	C	506	CLA	CHB-C4A-NA	2.14	127.48	124.40
24	S	607	CHL	CAC-C3C-C4C	2.14	129.53	124.03
25	G	610	CLA	CMB-C2B-C3B	2.14	131.58	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	614	CLA	CHC-C4B-NB	2.14	127.25	124.05
25	n	603	CLA	CHB-C1B-NB	2.14	127.25	124.05
25	b	604	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
24	R	607	CHL	CMD-C2D-C3D	-2.14	120.41	124.68
29	1	2630	LHG	C27-C26-C25	-2.14	103.57	114.37
25	Y	612	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
24	r	607	CHL	CMD-C2D-C3D	-2.14	120.41	124.68
25	N	611	CLA	C3B-C4B-NB	-2.14	108.62	110.53
24	N	605	CHL	OBD-CAD-C3D	-2.14	124.56	127.89
24	R	608	CHL	O2D-CGD-O1D	-2.14	119.69	123.85
25	Y	610	CLA	CMB-C2B-C1B	-2.14	122.17	125.42
24	1	609	CHL	C1-C2-C3	-2.14	122.70	126.20
24	g	606	CHL	O2D-CGD-O1D	-2.13	119.69	123.85
24	2	601	CHL	C4C-CHD-C1D	2.13	123.71	116.07
25	n	604	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
24	Y	606	CHL	CMB-C2B-C3B	2.13	128.95	124.68
26	5	1621	LUT	C31-C32-C33	-2.13	120.51	126.36
37	c	518	DGD	CAB-C9B-C8B	-2.13	103.58	114.37
37	c	520	DGD	CBB-CAB-C9B	-2.13	103.58	114.37
26	2	1621	LUT	C11-C10-C9	-2.13	124.28	127.28
30	b	619	BCR	C34-C9-C8	2.13	121.35	118.09
25	B	604	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
29	c	522	LHG	C18-C17-C16	-2.13	103.58	114.37
25	a	405	CLA	CHB-C4A-NA	2.13	127.48	124.40
24	R	606	CHL	O2D-CGD-O1D	-2.13	119.69	123.85
24	6	601	CHL	C4C-CHD-C1D	2.13	123.70	116.07
29	b	2630	LHG	C11-C10-C9	-2.13	103.58	114.37
24	y	609	CHL	C11-C12-C13	-2.13	108.87	115.97
24	r	608	CHL	O2D-CGD-O1D	-2.13	119.70	123.85
24	R	606	CHL	C6-C5-C3	-2.13	108.27	113.47
24	s	606	CHL	CMA-C3A-C4A	-2.13	110.02	114.61
25	N	613	CLA	CHC-C4B-NB	2.13	127.25	124.05
29	B	2630	LHG	C11-C10-C9	-2.13	103.59	114.37
24	7	601	CHL	C1-O2A-CGA	2.13	121.81	116.65
25	s	610	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
25	4	610	CLA	CHB-C1B-NB	2.13	127.25	124.05
25	S	602	CLA	CHB-C4A-NA	2.13	127.48	124.40
26	y	1621	LUT	C37-C21-C22	-2.13	105.43	109.41
37	C	520	DGD	CBB-CAB-C9B	-2.13	103.59	114.37
24	4	601	CHL	CAC-C3C-C4C	2.13	129.51	124.03
27	g	1622	XAT	C35-C34-C33	-2.13	124.29	127.28
24	8	607	CHL	CAA-CBA-CGA	-2.13	106.81	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	7	1622	XAT	C11-C12-C13	-2.13	120.52	126.36
30	C	515	BCR	C3-C4-C5	-2.13	110.26	114.06
25	R	604	CLA	CMB-C2B-C3B	2.13	131.56	126.55
24	8	601	CHL	CAC-C3C-C4C	2.13	129.50	124.03
25	S	610	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
30	c	515	BCR	C3-C4-C5	-2.13	110.26	114.06
24	4	607	CHL	CAA-CBA-CGA	-2.13	106.81	112.49
25	c	506	CLA	CHB-C4A-NA	2.13	127.47	124.40
24	Y	607	CHL	CAC-C3C-C4C	2.13	129.50	124.03
25	2	604	CLA	CMB-C2B-C3B	2.13	131.56	126.55
25	5	602	CLA	CHB-C4A-NA	2.13	127.47	124.40
24	5	606	CHL	O2A-CGA-CBA	2.13	120.72	114.00
36	D	405	PL9	C41-C39-C38	-2.13	116.39	121.17
24	5	607	CHL	CAC-C3C-C4C	2.13	129.50	124.03
29	C	522	LHG	C18-C17-C16	-2.13	103.62	114.37
37	c	519	DGD	CAB-C9B-C8B	-2.13	103.62	114.37
24	G	608	CHL	CMA-C3A-C4A	-2.13	110.03	114.61
25	b	610	CLA	CAA-CBA-CGA	-2.13	107.17	113.21
24	3	601	CHL	C1-O2A-CGA	2.13	121.80	116.65
28	g	1623	NEX	O4-C5-C18	-2.13	105.18	109.22
24	1	607	CHL	CAC-C3C-C4C	2.13	129.50	124.03
24	G	606	CHL	O2D-CGD-O1D	-2.13	119.71	123.85
36	d	405	PL9	C41-C39-C38	-2.13	116.40	121.17
39	f	101	HEM	CHC-C1C-NC	2.13	126.77	124.45
25	8	610	CLA	CHB-C1B-NB	2.13	127.24	124.05
25	1	614	CLA	C3B-C4B-NB	-2.13	108.63	110.53
24	5	607	CHL	CBA-CAA-C2A	-2.12	107.52	113.78
30	c	517	BCR	C36-C18-C19	2.12	121.33	118.09
27	G	1622	XAT	C35-C34-C33	-2.12	124.30	127.28
25	6	604	CLA	CMB-C2B-C3B	2.12	131.54	126.55
24	S	606	CHL	CMA-C3A-C4A	-2.12	110.04	114.61
25	S	610	CLA	O2D-CGD-CBD	2.12	114.94	111.23
24	y	607	CHL	CAC-C3C-C4C	2.12	129.49	124.03
25	B	610	CLA	CAA-CBA-CGA	-2.12	107.18	113.21
24	2	609	CHL	OMC-CMC-C2C	-2.12	121.44	125.12
25	1	603	CLA	CHA-C1A-NA	-2.12	121.59	126.39
25	D	403	CLA	CHA-C1A-NA	-2.12	121.59	126.39
30	c	514	BCR	C37-C22-C23	2.12	121.33	118.09
26	4	620	LUT	C20-C13-C12	2.12	121.33	118.09
30	C	517	BCR	C36-C18-C19	2.12	121.33	118.09
24	G	607	CHL	CMB-C2B-C3B	2.12	128.92	124.68
24	g	608	CHL	CMA-C3A-C4A	-2.12	110.04	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	S	2630	LHG	C27-C26-C25	-2.12	103.65	114.37
24	Y	609	CHL	C11-C12-C13	-2.12	108.92	115.97
27	3	1622	XAT	C11-C12-C13	-2.12	120.55	126.36
25	5	603	CLA	CHA-C1A-NA	-2.12	121.59	126.39
25	y	612	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
25	b	612	CLA	CAA-CBA-CGA	-2.12	107.19	113.21
24	1	607	CHL	CBA-CAA-C2A	-2.12	107.54	113.78
29	B	2631	LHG	C20-C19-C18	-2.12	103.66	114.37
25	B	615	CLA	O1D-CGD-CBD	2.12	128.70	124.52
26	Y	1621	LUT	C37-C21-C22	-2.12	105.46	109.41
37	h	102	DGD	CBB-CAB-C9B	-2.12	103.66	114.37
39	F	101	HEM	CHC-C1C-NC	2.12	126.76	124.45
25	c	502	CLA	O1D-CGD-CBD	2.12	128.69	124.52
24	6	601	CHL	CMA-C3A-C4A	-2.12	110.05	114.61
25	N	604	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
24	g	609	CHL	C1-O2A-CGA	2.12	121.78	116.65
26	6	1621	LUT	C3-C4-C5	-2.12	106.91	112.18
24	1	601	CHL	CAC-C3C-C4C	2.12	129.47	124.03
24	6	605	CHL	CMA-C3A-C4A	-2.12	110.05	114.61
37	H	102	DGD	CBB-CAB-C9B	-2.12	103.67	114.37
28	G	1623	NEX	O4-C5-C18	-2.12	105.19	109.22
26	g	1621	LUT	C15-C35-C34	-2.12	119.19	123.52
24	4	607	CHL	O2D-CGD-O1D	-2.12	119.73	123.85
25	C	512	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
25	y	614	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
29	r	2630	LHG	C27-C26-C25	-2.12	103.67	114.37
37	C	519	DGD	CAB-C9B-C8B	-2.12	103.67	114.37
25	s	610	CLA	O2D-CGD-CBD	2.12	114.93	111.23
25	B	612	CLA	CAA-CBA-CGA	-2.12	107.20	113.21
25	n	614	CLA	CHC-C4B-NB	2.12	127.22	124.05
28	n	1623	NEX	C19-C9-C10	-2.11	119.39	122.82
26	8	620	LUT	C20-C13-C12	2.11	121.32	118.09
25	B	613	CLA	C9-C8-C10	-2.11	103.74	111.27
29	s	2630	LHG	C27-C26-C25	-2.11	103.68	114.37
25	Y	613	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
25	y	613	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
24	6	607	CHL	CAC-C3C-C4C	2.11	129.46	124.03
24	G	609	CHL	C1-O2A-CGA	2.11	121.77	116.65
29	R	2630	LHG	C27-C26-C25	-2.11	103.68	114.37
26	2	1621	LUT	C3-C4-C5	-2.11	106.92	112.18
24	S	608	CHL	O2D-CGD-O1D	-2.11	119.74	123.85
25	Y	614	CLA	O2A-CGA-O1A	-2.11	118.34	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	r	623	NEX	O24-C25-C26	-2.11	57.26	58.93
24	g	607	CHL	CMB-C2B-C3B	2.11	128.90	124.68
24	2	607	CHL	CAC-C3C-C4C	2.11	129.46	124.03
24	5	601	CHL	CAC-C3C-C4C	2.11	129.46	124.03
25	2	613	CLA	O1D-CGD-CBD	2.11	128.68	124.52
25	b	611	CLA	O1D-CGD-CBD	2.11	128.68	124.52
29	b	2631	LHG	C20-C19-C18	-2.11	103.70	114.37
25	C	501	CLA	CHB-C4A-NA	2.11	127.44	124.40
26	N	1620	LUT	C20-C13-C12	2.11	121.31	118.09
26	n	1620	LUT	C20-C13-C12	2.11	121.31	118.09
26	S	1621	LUT	C16-C1-C6	-2.11	106.94	110.24
35	d	411	LMG	O7-C10-O9	-2.11	118.78	123.70
24	6	609	CHL	OMC-CMC-C2C	-2.11	121.46	125.12
25	c	512	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
25	a	405	CLA	C16-C15-C13	-2.11	108.96	115.97
24	s	601	CHL	C4C-CHD-C1D	2.11	123.61	116.07
24	1	601	CHL	CMB-C2B-C3B	2.11	128.90	124.68
25	8	604	CLA	C3B-C4B-NB	-2.11	108.65	110.53
25	b	615	CLA	O1D-CGD-CBD	2.11	128.68	124.52
24	4	608	CHL	OBD-CAD-C3D	-2.11	124.60	127.89
25	S	603	CLA	CHA-C1A-NA	-2.11	121.62	126.39
24	S	601	CHL	C4C-CHD-C1D	2.11	123.61	116.07
25	6	613	CLA	O1D-CGD-CBD	2.11	128.68	124.52
25	B	614	CLA	O2D-CGD-O1D	-2.11	119.75	123.85
30	B	619	BCR	C34-C9-C8	2.11	121.31	118.09
35	D	411	LMG	O7-C10-O9	-2.11	118.78	123.70
25	y	610	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
24	8	608	CHL	OBD-CAD-C3D	-2.11	124.61	127.89
30	C	514	BCR	C37-C22-C23	2.11	121.31	118.09
30	C	514	BCR	C24-C23-C22	-2.11	123.12	126.23
25	A	405	CLA	C16-C15-C13	-2.11	108.97	115.97
24	2	605	CHL	CMA-C3A-C4A	-2.11	110.07	114.61
25	b	613	CLA	C9-C8-C10	-2.11	103.77	111.27
28	G	1623	NEX	O24-C25-C26	-2.11	57.26	58.93
25	1	602	CLA	CMB-C2B-C3B	2.11	131.50	126.55
24	R	607	CHL	CGD-CBD-CAD	-2.10	104.03	110.85
24	s	606	CHL	C4C-CHD-C1D	2.10	123.60	116.07
25	d	403	CLA	CHA-C1A-NA	-2.10	121.63	126.39
26	n	1620	LUT	C8-C9-C10	-2.10	115.70	119.01
24	g	606	CHL	C4C-CHD-C1D	2.10	123.59	116.07
24	S	606	CHL	C4C-CHD-C1D	2.10	123.59	116.07
37	c	520	DGD	O2D-C2D-C1D	-2.10	105.06	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	605	CHL	O2A-CGA-O1A	-2.10	118.37	123.63
24	3	601	CHL	O2D-CGD-O1D	-2.10	119.75	123.85
25	y	604	CLA	O1D-CGD-CBD	2.10	128.66	124.52
25	g	610	CLA	CAA-C2A-C1A	2.10	118.86	111.97
26	G	1621	LUT	C15-C35-C34	-2.10	119.22	123.52
25	S	613	CLA	CHB-C4A-NA	2.10	127.43	124.40
26	s	1621	LUT	C16-C1-C6	-2.10	106.95	110.24
25	s	603	CLA	CHA-C1A-NA	-2.10	121.63	126.39
35	c	521	LMG	O3-C3-C2	-2.10	105.42	110.38
26	S	1621	LUT	C20-C13-C12	2.10	121.30	118.09
25	N	603	CLA	CHB-C1B-NB	2.10	127.20	124.05
25	c	501	CLA	CHB-C4A-NA	2.10	127.43	124.40
25	C	502	CLA	O1D-CGD-CBD	2.10	128.66	124.52
28	g	1623	NEX	O24-C25-C26	-2.10	57.26	58.93
30	c	514	BCR	C24-C23-C22	-2.10	123.13	126.23
25	5	602	CLA	CMB-C2B-C3B	2.10	131.49	126.55
24	n	605	CHL	O2A-CGA-O1A	-2.10	118.38	123.63
25	C	507	CLA	CHC-C4B-NB	2.10	127.20	124.05
25	5	610	CLA	CHB-C1B-C2B	-2.10	121.33	127.43
30	4	623	BCR	C15-C16-C17	-2.10	119.23	123.52
25	N	612	CLA	C2A-C1A-CHA	2.10	127.51	123.87
25	n	612	CLA	C2A-C1A-CHA	2.10	127.51	123.87
25	Y	604	CLA	O1D-CGD-CBD	2.10	128.66	124.52
29	C	522	LHG	C20-C19-C18	-2.10	103.76	114.37
25	B	603	CLA	CHB-C1B-NB	2.10	127.20	124.05
25	c	507	CLA	CHC-C4B-NB	2.10	127.20	124.05
25	n	614	CLA	CMB-C2B-C3B	2.10	131.48	126.55
24	5	601	CHL	CMB-C2B-C3B	2.10	128.87	124.68
25	G	610	CLA	CAA-C2A-C1A	2.10	118.85	111.97
37	B	626	DGD	C1D-C2D-C3D	-2.10	105.60	110.01
25	1	610	CLA	C4A-NA-C1A	2.10	107.64	106.68
30	b	619	BCR	C16-C15-C14	-2.10	119.23	123.52
24	1	607	CHL	C1C-C2C-CMC	-2.09	123.03	126.80
25	C	507	CLA	O2D-CGD-CBD	2.09	114.89	111.23
30	B	619	BCR	C16-C15-C14	-2.09	119.23	123.52
25	D	403	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
25	3	610	CLA	CHB-C4A-NA	2.09	127.42	124.40
25	C	502	CLA	C1-C2-C3	-2.09	122.77	126.20
24	r	607	CHL	CGD-CBD-CAD	-2.09	104.07	110.85
25	b	604	CLA	CHC-C4B-NB	2.09	127.19	124.05
25	G	610	CLA	CHA-C1A-NA	-2.09	121.65	126.39
25	g	610	CLA	CHA-C1A-NA	-2.09	121.65	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	606	CHL	C4C-CHD-C1D	2.09	123.56	116.07
24	n	609	CHL	C4C-CHD-C1D	2.09	123.56	116.07
37	C	519	DGD	C5B-C4B-C3B	-2.09	103.79	114.37
29	c	522	LHG	C20-C19-C18	-2.09	103.79	114.37
28	y	1623	NEX	O24-C25-C26	-2.09	57.27	58.93
24	3	605	CHL	C4C-CHD-C1D	2.09	123.56	116.07
24	s	608	CHL	O2D-CGD-O1D	-2.09	119.78	123.85
24	S	606	CHL	O1D-CGD-CBD	-2.09	121.55	124.72
25	2	612	CLA	CHB-C1B-C2B	-2.09	121.35	127.43
24	N	609	CHL	C4C-CHD-C1D	2.09	123.55	116.07
25	G	612	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
37	c	519	DGD	C5B-C4B-C3B	-2.09	103.80	114.37
25	6	604	CLA	CHC-C4B-NB	2.09	127.19	124.05
35	C	521	LMG	O3-C3-C2	-2.09	105.45	110.38
25	5	614	CLA	O2A-CGA-O1A	-2.09	117.95	123.33
24	5	607	CHL	C1C-C2C-CMC	-2.09	123.03	126.80
25	N	614	CLA	CMB-C2B-C3B	2.09	131.47	126.55
25	d	403	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
25	B	611	CLA	O1D-CGD-CBD	2.09	128.64	124.52
28	N	1623	NEX	C19-C9-C10	-2.09	119.43	122.82
37	b	626	DGD	C1D-C2D-C3D	-2.09	105.62	110.01
25	6	603	CLA	C2A-C1A-CHA	2.09	127.49	123.87
26	N	1620	LUT	C8-C9-C10	-2.09	115.73	119.01
25	6	604	CLA	CAC-C3C-C4C	2.09	127.50	124.79
25	1	614	CLA	O2A-CGA-O1A	-2.09	117.97	123.33
25	6	612	CLA	CHB-C1B-NB	2.09	127.18	124.05
24	7	605	CHL	C4C-CHD-C1D	2.09	123.53	116.07
25	c	507	CLA	O2D-CGD-CBD	2.09	114.88	111.23
37	C	520	DGD	O2D-C2D-C1D	-2.09	105.10	110.08
25	s	613	CLA	CHB-C4A-NA	2.09	127.41	124.40
25	b	615	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
25	1	610	CLA	CHB-C1B-C2B	-2.09	121.37	127.43
29	S	2630	LHG	C20-C19-C18	-2.08	103.83	114.37
24	3	601	CHL	C1-C2-C3	-2.08	122.78	126.20
25	b	605	CLA	CMB-C2B-C3B	2.08	131.45	126.55
25	2	612	CLA	CHB-C1B-NB	2.08	127.17	124.05
25	y	602	CLA	C1-C2-C3	-2.08	122.78	126.20
25	b	603	CLA	CHB-C1B-NB	2.08	127.17	124.05
25	c	508	CLA	CHC-C1C-NC	2.08	127.45	124.31
25	b	614	CLA	O2D-CGD-O1D	-2.08	119.79	123.85
28	Y	1623	NEX	O24-C25-C26	-2.08	57.28	58.93
25	B	615	CLA	O2A-CGA-O1A	-2.08	118.42	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	n	1622	XAT	C39-C29-C30	-2.08	119.44	122.82
25	R	616	CLA	O2D-CGD-CBD	2.08	114.87	111.23
25	A	406	CLA	CMB-C2B-C3B	2.08	131.44	126.55
35	Z	101	LMG	O5-C6-C5	-2.08	104.25	111.33
25	7	603	CLA	CHC-C4B-NB	2.08	127.17	124.05
25	3	602	CLA	O1D-CGD-CBD	2.08	128.62	124.52
25	6	612	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
25	B	610	CLA	O2D-CGD-O1D	-2.08	119.80	123.85
25	B	616	CLA	C2A-C1A-CHA	2.08	127.47	123.87
27	6	1622	XAT	O24-C25-C26	-2.08	57.28	58.93
25	C	508	CLA	CHC-C1C-NC	2.08	127.44	124.31
29	s	2630	LHG	C20-C19-C18	-2.08	103.86	114.37
25	Y	603	CLA	C11-C10-C8	-2.08	109.06	115.97
24	1	607	CHL	CAA-CBA-CGA	-2.08	107.31	113.21
27	N	1622	XAT	C39-C29-C30	-2.08	119.45	122.82
27	5	1622	XAT	O24-C25-C26	-2.08	57.28	58.93
37	C	518	DGD	C5B-C4B-C3B	-2.08	103.86	114.37
24	7	608	CHL	OBD-CAD-C3D	-2.08	124.65	127.89
26	7	1621	LUT	C31-C30-C29	-2.08	124.37	127.28
25	S	602	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
26	s	1621	LUT	C20-C13-C12	2.08	121.26	118.09
30	8	623	BCR	C15-C16-C17	-2.08	119.27	123.52
27	2	1622	XAT	O24-C25-C26	-2.08	57.28	58.93
29	D	409	LHG	O8-C6-C5	-2.08	102.41	108.40
25	s	602	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
25	3	603	CLA	CHC-C4B-NB	2.08	127.16	124.05
24	R	607	CHL	O2A-CGA-O1A	-2.07	118.44	123.63
29	d	409	LHG	O8-C6-C5	-2.07	102.42	108.40
25	y	610	CLA	CMB-C2B-C3B	2.07	131.43	126.55
37	c	520	DGD	O6E-C1E-O5D	-2.07	105.14	110.04
24	5	607	CHL	CAA-CBA-CGA	-2.07	107.32	113.21
25	b	607	CLA	C3B-C4B-NB	-2.07	108.68	110.53
35	z	101	LMG	O5-C6-C5	-2.07	104.27	111.33
25	C	503	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
25	g	612	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
25	S	610	CLA	CHB-C1B-C2B	-2.07	121.41	127.43
25	7	614	CLA	O2D-CGD-CBD	2.07	114.85	111.23
25	y	603	CLA	C11-C10-C8	-2.07	109.08	115.97
25	s	610	CLA	CHB-C1B-C2B	-2.07	121.41	127.43
25	7	610	CLA	CHB-C4A-NA	2.07	127.39	124.40
27	g	1622	XAT	C7-C8-C9	-2.07	122.31	125.53
37	c	518	DGD	C5B-C4B-C3B	-2.07	103.90	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	605	CHL	CBC-CAC-C3C	-2.07	109.91	112.87
25	y	613	CLA	C1-C2-C3	-2.07	122.80	126.20
24	3	607	CHL	O2D-CGD-O1D	-2.07	119.82	123.85
25	B	605	CLA	CMB-C2B-C3B	2.07	131.42	126.55
25	R	603	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
25	B	602	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
25	c	502	CLA	C1-C2-C3	-2.07	122.81	126.20
25	6	612	CLA	CHA-C1A-NA	-2.07	121.70	126.39
25	r	616	CLA	O2D-CGD-CBD	2.07	114.85	111.23
27	N	1622	XAT	C7-C8-C9	-2.07	122.32	125.53
24	r	607	CHL	O2A-CGA-O1A	-2.07	118.45	123.63
25	Y	610	CLA	CMB-C2B-C3B	2.07	131.42	126.55
25	a	406	CLA	CMB-C2B-C3B	2.07	131.42	126.55
25	2	604	CLA	CHC-C4B-NB	2.07	127.15	124.05
25	2	603	CLA	C2A-C1A-CHA	2.07	127.46	123.87
25	s	610	CLA	CHB-C1B-NB	2.07	127.15	124.05
24	7	601	CHL	O2D-CGD-O1D	-2.07	119.82	123.85
24	2	601	CHL	C1C-C2C-CMC	2.07	130.53	126.80
25	5	610	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
24	N	609	CHL	CED-O2D-CGD	2.07	120.61	115.92
25	2	612	CLA	CHA-C1A-NA	-2.07	121.71	126.39
25	B	612	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
29	C	523	LHG	C27-C26-C25	-2.07	103.92	114.37
25	C	507	CLA	CMB-C2B-C3B	2.07	131.41	126.55
25	Y	602	CLA	C1-C2-C3	-2.07	122.81	126.20
25	4	611	CLA	CHC-C4B-NB	2.07	127.15	124.05
25	2	604	CLA	CAC-C3C-C4C	2.07	127.48	124.79
24	2	606	CHL	O2A-CGA-CBA	2.07	120.53	114.00
24	3	608	CHL	OBD-CAD-C3D	-2.07	124.67	127.89
24	g	605	CHL	CBC-CAC-C3C	-2.07	109.91	112.87
24	s	606	CHL	O1D-CGD-CBD	-2.07	121.59	124.72
24	2	605	CHL	CAA-C2A-C3A	-2.07	107.42	113.00
24	6	606	CHL	O2A-CGA-CBA	2.07	120.53	114.00
27	y	1622	XAT	O24-C25-C26	-2.07	57.29	58.93
25	s	613	CLA	CMB-C2B-C3B	2.07	131.41	126.55
25	b	602	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
25	4	604	CLA	C3B-C4B-NB	-2.07	108.69	110.53
27	8	622	XAT	C39-C29-C28	2.07	121.24	118.09
24	s	606	CHL	CBC-CAC-C3C	-2.07	109.92	112.87
33	a	409	PHO	C3B-C4B-NB	-2.07	106.12	107.46
24	r	606	CHL	C4-C3-C5	2.06	118.81	115.23
29	c	523	LHG	C27-C26-C25	-2.06	103.93	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	602	CLA	O1D-CGD-CBD	2.06	128.59	124.52
25	S	610	CLA	CHB-C1B-NB	2.06	127.15	124.05
29	4	2630	LHG	C5-O7-C7	-2.06	114.20	117.85
25	B	611	CLA	CAA-C2A-C1A	-2.06	105.21	111.97
24	1	607	CHL	C4-C3-C5	2.06	118.81	115.23
25	Y	613	CLA	O2D-CGD-CBD	2.06	114.84	111.23
27	n	1622	XAT	C7-C8-C9	-2.06	122.33	125.53
30	T	101	BCR	C38-C26-C25	-2.06	122.23	124.48
25	r	603	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
37	C	520	DGD	O6E-C1E-O5D	-2.06	105.17	110.04
28	n	1623	NEX	O24-C25-C26	-2.06	57.29	58.93
28	S	1623	NEX	C30-C31-C32	-2.06	117.22	123.20
25	1	610	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
25	y	604	CLA	CHB-C4A-NA	2.06	127.38	124.40
29	8	2630	LHG	C5-O7-C7	-2.06	114.21	117.85
25	B	617	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
25	g	610	CLA	C1-C2-C3	-2.06	122.82	126.20
24	6	601	CHL	C1C-C2C-CMC	2.06	130.52	126.80
27	G	1622	XAT	C7-C8-C9	-2.06	122.33	125.53
25	b	612	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
24	s	607	CHL	CAA-C2A-C3A	-2.06	107.43	113.00
25	2	614	CLA	O2D-CGD-CBD	2.06	114.83	111.23
28	6	1623	NEX	C15-C35-C34	-2.06	119.31	123.52
24	G	601	CHL	O2D-CGD-O1D	-2.06	119.84	123.85
25	B	614	CLA	C3A-C2A-C1A	2.06	104.42	101.34
25	c	507	CLA	CMB-C2B-C3B	2.06	131.39	126.55
25	c	511	CLA	C3B-C4B-NB	-2.06	108.69	110.53
24	7	607	CHL	C1-C2-C3	-2.06	122.82	126.20
25	b	610	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
25	8	611	CLA	CHC-C4B-NB	2.06	127.14	124.05
24	R	606	CHL	C4-C3-C5	2.06	118.80	115.23
25	g	612	CLA	C2A-C1A-CHA	2.06	127.44	123.87
24	y	609	CHL	CMD-C2D-C3D	-2.06	120.57	124.68
27	1	1622	XAT	O24-C25-C26	-2.06	57.30	58.93
25	y	603	CLA	CHA-C1A-NA	-2.06	121.73	126.39
25	b	608	CLA	CHC-C1C-NC	2.06	127.41	124.31
24	g	601	CHL	O2D-CGD-O1D	-2.06	119.84	123.85
30	t	101	BCR	C38-C26-C25	-2.06	122.24	124.48
24	n	609	CHL	CED-O2D-CGD	2.06	120.58	115.92
24	S	607	CHL	CAA-C2A-C3A	-2.06	107.44	113.00
24	7	609	CHL	CMD-C2D-C3D	-2.06	120.57	124.68
24	6	605	CHL	CAA-C2A-C3A	-2.06	107.44	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	613	CLA	CHB-C1B-C2B	-2.06	121.46	127.43
24	R	606	CHL	CMD-C2D-C3D	-2.06	120.57	124.68
26	y	1620	LUT	O3-C3-C4	-2.06	105.08	109.71
25	6	614	CLA	CMB-C2B-C1B	-2.06	122.29	125.42
27	4	622	XAT	C39-C29-C28	2.06	121.23	118.09
26	n	1620	LUT	C11-C10-C9	-2.05	124.40	127.28
25	N	603	CLA	CHB-C1B-C2B	-2.05	121.46	127.43
25	s	609	CLA	O2A-CGA-O1A	-2.05	118.05	123.33
25	b	611	CLA	CAA-C2A-C1A	-2.05	105.24	111.97
26	g	1621	LUT	C8-C9-C10	-2.05	115.78	119.01
24	Y	609	CHL	CMD-C2D-C3D	-2.05	120.58	124.68
25	2	611	CLA	CHB-C1B-NB	2.05	127.13	124.05
30	D	404	BCR	C15-C14-C13	-2.05	124.40	127.28
30	d	404	BCR	C15-C14-C13	-2.05	124.40	127.28
25	y	613	CLA	O2D-CGD-CBD	2.05	114.82	111.23
25	6	613	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
34	B	621	SQD	C3-C4-C5	2.05	113.95	110.23
25	b	617	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
25	3	610	CLA	C7-C6-C5	-2.05	107.79	113.26
28	s	1623	NEX	C30-C31-C32	-2.05	117.25	123.20
25	5	612	CLA	CHC-C1C-NC	2.05	127.40	124.31
24	g	609	CHL	CAC-C3C-C4C	2.05	129.31	124.03
25	Y	613	CLA	C1-C2-C3	-2.05	122.83	126.20
26	N	1621	LUT	C39-C29-C28	2.05	121.22	118.09
25	y	603	CLA	CHB-C1B-NB	2.05	127.13	124.05
25	n	603	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
27	Y	1622	XAT	O24-C25-C26	-2.05	57.30	58.93
24	r	614	CHL	C1C-C2C-CMC	2.05	130.50	126.80
25	7	610	CLA	C7-C6-C5	-2.05	107.80	113.26
25	s	604	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
25	G	612	CLA	C2A-C1A-CHA	2.05	127.43	123.87
24	3	607	CHL	C1-C2-C3	-2.05	122.84	126.20
25	S	604	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
24	3	609	CHL	CMD-C2D-C3D	-2.05	120.59	124.68
24	7	607	CHL	O2D-CGD-O1D	-2.05	119.86	123.85
25	b	616	CLA	C2A-C1A-CHA	2.05	127.42	123.87
25	G	610	CLA	C1-C2-C3	-2.05	122.84	126.20
25	3	614	CLA	O2D-CGD-CBD	2.05	114.81	111.23
24	2	601	CHL	CBC-CAC-C3C	-2.05	109.94	112.87
25	Y	604	CLA	CHB-C4A-NA	2.05	127.36	124.40
29	N	2630	LHG	C29-C28-C27	-2.05	104.01	114.37
25	6	614	CLA	O2D-CGD-CBD	2.05	114.81	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	A	409	PHO	C3B-C4B-NB	-2.05	106.13	107.46
25	3	611	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
25	n	603	CLA	C3C-C4C-NC	-2.05	107.81	110.43
24	y	608	CHL	C7-C6-C5	2.05	118.72	113.26
25	C	511	CLA	CMB-C2B-C3B	2.05	131.37	126.55
25	S	613	CLA	CMB-C2B-C3B	2.05	131.37	126.55
28	R	623	NEX	O24-C25-C26	-2.05	57.31	58.93
26	6	1620	LUT	C11-C10-C9	-2.05	124.41	127.28
25	Y	603	CLA	CHA-C1A-NA	-2.05	121.76	126.39
24	G	609	CHL	CAC-C3C-C4C	2.05	129.29	124.03
25	3	611	CLA	CHC-C4B-NB	2.05	127.12	124.05
27	2	1622	XAT	C20-C13-C12	2.05	121.21	118.09
24	s	601	CHL	O2D-CGD-O1D	-2.05	119.86	123.85
28	Y	1623	NEX	O4-C5-C18	-2.05	105.33	109.22
24	R	614	CHL	C1C-C2C-CMC	2.05	130.49	126.80
24	n	608	CHL	C7-C6-C5	2.05	118.72	113.26
26	Y	1620	LUT	O3-C3-C4	-2.05	105.10	109.71
24	2	605	CHL	CBC-CAC-C3C	-2.05	109.94	112.87
27	y	1622	XAT	O4-C5-C6	-2.05	57.31	58.93
29	n	2630	LHG	C29-C28-C27	-2.05	104.03	114.37
33	A	409	PHO	CMA-C3A-C4A	-2.05	110.20	114.61
33	a	409	PHO	CMA-C3A-C4A	-2.05	110.20	114.61
25	b	607	CLA	C1-C2-C3	-2.05	122.85	126.20
27	6	1622	XAT	C31-C32-C33	-2.05	120.75	126.36
25	c	503	CLA	CMB-C2B-C1B	-2.05	122.31	125.42
24	7	601	CHL	C1-C2-C3	-2.04	122.85	126.20
26	7	1620	LUT	C36-C21-C26	2.04	112.64	109.55
24	N	609	CHL	CMD-C2D-C3D	-2.04	120.60	124.68
24	S	601	CHL	O2D-CGD-O1D	-2.04	119.87	123.85
28	S	1623	NEX	C38-C25-C24	2.04	116.54	114.24
27	Y	1622	XAT	O4-C5-C6	-2.04	57.31	58.93
30	D	404	BCR	C28-C27-C26	-2.04	110.41	114.06
24	n	609	CHL	CMD-C2D-C3D	-2.04	120.60	124.68
25	s	614	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
33	A	408	PHO	C2D-C1D-ND	-2.04	107.95	109.43
33	a	408	PHO	C2D-C1D-ND	-2.04	107.95	109.43
27	6	1622	XAT	C39-C29-C30	-2.04	119.51	122.82
30	d	404	BCR	C20-C21-C22	-2.04	124.41	127.28
25	6	611	CLA	CHB-C1B-NB	2.04	127.11	124.05
37	c	519	DGD	O3E-C3E-C2E	-2.04	105.56	110.38
25	G	612	CLA	CHA-C1A-NA	-2.04	121.77	126.39
27	3	1622	XAT	C39-C29-C30	-2.04	119.51	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	601	CHL	CMB-C2B-C3B	2.04	128.76	124.68
24	6	608	CHL	C4C-CHD-C1D	2.04	123.37	116.07
26	N	1620	LUT	C11-C10-C9	-2.04	124.42	127.28
25	S	609	CLA	O2A-CGA-O1A	-2.04	118.08	123.33
25	r	602	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
28	3	1623	NEX	C20-C13-C14	-2.04	119.51	122.82
25	6	614	CLA	O1D-CGD-CBD	2.04	128.54	124.52
25	B	607	CLA	C3B-C4B-NB	-2.04	108.71	110.53
24	6	605	CHL	CBC-CAC-C3C	-2.04	109.95	112.87
35	B	622	LMG	O3-C3-C2	-2.04	105.57	110.38
28	s	1623	NEX	C38-C25-C24	2.04	116.53	114.24
25	S	614	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
25	7	611	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
26	n	1621	LUT	C39-C29-C28	2.04	121.20	118.09
27	6	1622	XAT	C20-C13-C12	2.04	121.20	118.09
35	a	415	LMG	O1-C7-C8	-2.04	105.86	110.82
25	2	614	CLA	O1D-CGD-CBD	2.04	128.54	124.52
25	B	608	CLA	CHC-C1C-NC	2.04	127.38	124.31
24	3	605	CHL	CGD-CBD-CAD	-2.04	104.24	110.85
25	R	602	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
25	b	612	CLA	C1C-C2C-C3C	2.04	109.12	106.98
35	Z	101	LMG	O3-C3-C2	-2.04	105.57	110.38
28	1	1623	NEX	C19-C9-C10	-2.04	119.51	122.82
25	1	613	CLA	CHB-C1B-C2B	-2.04	121.51	127.43
24	y	608	CHL	CMB-C2B-C3B	2.04	128.75	124.68
35	z	101	LMG	O3-C3-C2	-2.04	105.57	110.38
25	B	607	CLA	C1-C2-C3	-2.04	122.86	126.20
24	6	601	CHL	CBC-CAC-C3C	-2.04	109.96	112.87
24	4	609	CHL	CED-O2D-CGD	2.04	120.53	115.92
24	7	605	CHL	CGD-CBD-CAD	-2.04	104.25	110.85
25	Y	603	CLA	CHB-C1B-NB	2.04	127.10	124.05
25	R	603	CLA	CMB-C2B-C3B	2.04	131.34	126.55
24	r	606	CHL	CMD-C2D-C3D	-2.04	120.61	124.68
24	y	606	CHL	CAA-C2A-C3A	-2.04	107.50	113.00
25	B	611	CLA	CHB-C1B-C2B	-2.04	121.52	127.43
24	n	609	CHL	C1-O2A-CGA	2.04	121.58	116.65
28	2	1623	NEX	C15-C35-C34	-2.04	119.35	123.52
25	5	613	CLA	CHB-C1B-C2B	-2.04	121.52	127.43
27	2	1622	XAT	C31-C32-C33	-2.04	120.78	126.36
24	s	607	CHL	C4C-CHD-C1D	2.03	123.35	116.07
24	Y	608	CHL	CMB-C2B-C3B	2.03	128.75	124.68
24	2	608	CHL	C4C-CHD-C1D	2.03	123.35	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	601	CHL	CMB-C2B-C3B	2.03	128.75	124.68
25	1	602	CLA	C4A-NA-C1A	2.03	107.61	106.68
25	C	508	CLA	CMC-C2C-C1C	-2.03	121.86	125.03
24	1	608	CHL	O2A-CGA-CBA	2.03	120.42	114.00
25	N	603	CLA	C3C-C4C-NC	-2.03	107.83	110.43
24	R	606	CHL	C4C-CHD-C1D	2.03	123.34	116.07
33	a	408	PHO	O2D-CGD-O1D	-2.03	119.89	123.85
29	b	2631	LHG	C5-O7-C7	-2.03	112.93	117.80
24	Y	608	CHL	C7-C6-C5	2.03	118.68	113.26
25	8	604	CLA	O1A-CGA-CBA	2.03	129.54	123.09
30	d	404	BCR	C35-C13-C12	2.03	121.19	118.09
35	b	622	LMG	O3-C3-C2	-2.03	105.58	110.38
24	S	606	CHL	CBC-CAC-C3C	-2.03	109.96	112.87
25	B	605	CLA	CHC-C1C-NC	2.03	127.37	124.31
24	N	606	CHL	C4C-CHD-C1D	2.03	123.34	116.07
26	3	1621	LUT	C31-C30-C29	-2.03	124.43	127.28
30	d	404	BCR	C28-C27-C26	-2.03	110.43	114.06
25	r	603	CLA	CMB-C2B-C3B	2.03	131.33	126.55
24	n	606	CHL	C4C-CHD-C1D	2.03	123.34	116.07
28	5	1623	NEX	C19-C9-C10	-2.03	119.53	122.82
25	c	511	CLA	CMB-C2B-C3B	2.03	131.33	126.55
30	c	516	BCR	C34-C9-C8	2.03	121.19	118.09
35	A	415	LMG	O1-C7-C8	-2.03	105.88	110.82
25	B	612	CLA	C1C-C2C-C3C	2.03	109.12	106.98
34	A	412	SQD	O47-C7-O49	-2.03	118.96	123.70
24	5	607	CHL	C4-C3-C5	2.03	118.75	115.23
24	N	608	CHL	C7-C6-C5	2.03	118.67	113.26
37	c	519	DGD	O2D-C2D-C1D	-2.03	105.24	110.08
25	B	612	CLA	C4D-CHA-C1A	2.03	123.67	121.24
24	8	608	CHL	CED-O2D-CGD	2.03	120.52	115.92
24	Y	606	CHL	CAA-C2A-C3A	-2.03	107.52	113.00
26	2	1621	LUT	C18-C5-C6	-2.03	122.27	124.48
25	1	612	CLA	CHC-C1C-NC	2.03	127.37	124.31
27	7	1622	XAT	C39-C29-C30	-2.03	119.53	122.82
25	7	611	CLA	CHC-C4B-NB	2.03	127.09	124.05
37	C	519	DGD	O3E-C3E-C2E	-2.03	105.59	110.38
24	r	606	CHL	C4C-CHD-C1D	2.03	123.33	116.07
24	5	608	CHL	O2A-CGA-CBA	2.03	120.41	114.00
25	c	511	CLA	CAA-C2A-C1A	2.03	118.62	111.97
34	b	623	SQD	O8-S-C6	2.03	109.89	105.97
28	y	1623	NEX	O4-C5-C18	-2.03	105.36	109.22
24	N	601	CHL	CMD-C2D-C3D	-2.03	120.63	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	605	CLA	CHC-C1C-NC	2.03	127.36	124.31
27	2	1622	XAT	C39-C29-C30	-2.03	119.53	122.82
28	S	1623	NEX	C16-C1-C6	2.03	112.29	110.47
25	3	611	CLA	CHB-C1B-NB	2.03	127.09	124.05
24	S	607	CHL	C4C-CHD-C1D	2.03	123.32	116.07
25	r	610	CLA	C3B-C4B-NB	-2.03	108.72	110.53
28	7	1623	NEX	C20-C13-C14	-2.03	119.53	122.82
25	S	611	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
25	2	614	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
25	C	511	CLA	CAA-C2A-C1A	2.03	118.61	111.97
25	y	604	CLA	CHB-C1B-C2B	-2.03	121.55	127.43
25	g	612	CLA	CHA-C1A-NA	-2.03	121.80	126.39
25	B	602	CLA	CAC-C3C-C4C	2.03	127.42	124.79
25	A	406	CLA	CHD-C4C-NC	2.03	127.37	124.23
30	C	516	BCR	C34-C9-C8	2.03	121.18	118.09
25	R	610	CLA	C3B-C4B-NB	-2.03	108.72	110.53
25	5	610	CLA	C4A-NA-C1A	2.03	107.60	106.68
24	S	607	CHL	O2D-CGD-O1D	-2.03	119.91	123.85
24	5	609	CHL	O2D-CGD-O1D	-2.03	119.91	123.85
25	1	611	CLA	O2A-CGA-O1A	-2.02	118.12	123.33
24	g	605	CHL	O2A-CGA-CBA	2.02	120.40	114.00
26	G	1621	LUT	C8-C9-C10	-2.02	115.82	119.01
25	r	610	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
25	3	604	CLA	O1A-CGA-CBA	2.02	129.51	123.09
24	N	609	CHL	C1-C2-C3	-2.02	122.88	126.20
25	7	611	CLA	CHB-C1B-NB	2.02	127.08	124.05
25	C	510	CLA	C3B-C4B-NB	-2.02	108.72	110.53
34	B	623	SQD	O8-S-C6	2.02	109.88	105.97
24	S	601	CHL	CAC-C3C-C4C	2.02	129.23	124.03
24	s	601	CHL	CAC-C3C-C4C	2.02	129.23	124.03
26	6	1621	LUT	C18-C5-C6	-2.02	122.28	124.48
25	b	602	CLA	CAC-C3C-C4C	2.02	127.42	124.79
30	D	404	BCR	C35-C13-C12	2.02	121.18	118.09
25	1	613	CLA	O2D-CGD-CBD	2.02	114.77	111.23
24	G	609	CHL	C4C-CHD-C1D	2.02	123.30	116.07
25	b	611	CLA	CHB-C1B-C2B	-2.02	121.56	127.43
24	n	601	CHL	CMD-C2D-C3D	-2.02	120.64	124.68
25	b	604	CLA	CHA-C1A-NA	-2.02	121.81	126.39
30	c	514	BCR	C40-C30-C25	-2.02	107.07	110.24
26	3	1620	LUT	C36-C21-C26	2.02	112.61	109.55
25	5	611	CLA	O2A-CGA-O1A	-2.02	118.13	123.33
33	A	409	PHO	C1-C2-C3	-2.02	122.89	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	608	CHL	O2A-CGA-CBA	2.02	120.38	114.00
25	Y	602	CLA	C4-C3-C5	2.02	118.73	115.23
26	S	1620	LUT	C15-C35-C34	-2.02	119.39	123.52
35	z	101	LMG	O2-C2-C1	-2.02	105.26	110.08
35	A	413	LMG	O7-C10-O9	-2.02	118.98	123.70
25	C	511	CLA	C3B-C4B-NB	-2.02	108.73	110.53
35	Z	101	LMG	O2-C2-C1	-2.02	105.26	110.08
24	G	605	CHL	O2A-CGA-CBA	2.02	120.38	114.00
34	b	621	SQD	C3-C4-C5	2.02	113.89	110.23
25	c	509	CLA	C11-C12-C13	-2.02	109.25	115.97
25	b	606	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
25	c	510	CLA	C3B-C4B-NB	-2.02	108.73	110.53
25	B	606	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
25	y	612	CLA	CHB-C1B-C2B	-2.02	121.57	127.43
25	c	510	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
25	N	610	CLA	CAA-C2A-C3A	-2.02	107.55	113.00
24	6	607	CHL	C1B-CHB-C4A	2.02	122.62	121.32
25	b	614	CLA	C3A-C2A-C1A	2.02	104.36	101.34
28	N	1623	NEX	O24-C25-C26	-2.02	57.33	58.93
26	s	1620	LUT	C15-C35-C34	-2.02	119.39	123.52
28	Y	1623	NEX	C5-C6-C1	2.02	121.70	119.70
26	2	1620	LUT	C11-C10-C9	-2.02	124.45	127.28
25	6	611	CLA	CHC-C4B-NB	2.02	127.08	124.05
24	N	609	CHL	C1-O2A-CGA	2.02	121.53	116.65
24	8	609	CHL	CED-O2D-CGD	2.02	120.49	115.92
37	C	519	DGD	O2D-C2D-C1D	-2.02	105.27	110.08
25	B	604	CLA	CHA-C1A-NA	-2.02	121.83	126.39
25	C	505	CLA	CHC-C4B-NB	2.02	127.07	124.05
25	c	505	CLA	CHC-C4B-NB	2.02	127.07	124.05
25	a	406	CLA	CHD-C4C-NC	2.02	127.36	124.23
25	7	604	CLA	O1A-CGA-CBA	2.02	129.49	123.09
25	Y	604	CLA	CHB-C1B-C2B	-2.02	121.58	127.43
25	N	603	CLA	O1D-CGD-CBD	2.02	128.49	124.52
24	1	609	CHL	O2D-CGD-O1D	-2.01	119.93	123.85
25	b	611	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
25	c	502	CLA	CMB-C2B-C3B	2.01	131.29	126.55
24	g	609	CHL	C4C-CHD-C1D	2.01	123.28	116.07
24	6	601	CHL	CAC-C3C-C4C	2.01	129.21	124.03
25	A	406	CLA	C1-C2-C3	-2.01	122.90	126.20
25	C	510	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
24	2	608	CHL	O2A-CGA-CBA	2.01	120.36	114.00
24	2	601	CHL	CAC-C3C-C4C	2.01	129.21	124.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	n	605	CHL	C4C-CHD-C1D	2.01	123.27	116.07
25	4	604	CLA	O1A-CGA-CBA	2.01	129.48	123.09
24	4	608	CHL	CED-O2D-CGD	2.01	120.48	115.92
25	C	509	CLA	C11-C12-C13	-2.01	109.27	115.97
26	5	1621	LUT	C36-C21-C26	2.01	112.59	109.55
24	3	608	CHL	CAC-C3C-C4C	2.01	129.20	124.03
25	y	602	CLA	C6-C7-C8	-2.01	109.28	115.97
25	B	612	CLA	C7-C6-C5	-2.01	107.90	113.26
34	A	418	SQD	C3-C4-C5	2.01	113.88	110.23
29	B	2631	LHG	C5-O7-C7	-2.01	112.98	117.80
25	R	604	CLA	C2A-C1A-CHA	2.01	127.36	123.87
24	2	609	CHL	O2D-CGD-O1D	-2.01	119.93	123.85
25	5	613	CLA	O2D-CGD-CBD	2.01	114.75	111.23
24	S	601	CHL	CED-O2D-CGD	2.01	120.48	115.92
30	c	514	BCR	C36-C18-C19	2.01	121.16	118.09
25	G	614	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
25	2	611	CLA	CHC-C4B-NB	2.01	127.06	124.05
25	c	508	CLA	CMC-C2C-C1C	-2.01	121.89	125.03
28	y	1623	NEX	C5-C6-C1	2.01	121.69	119.70
25	s	611	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
24	R	608	CHL	CAC-C3C-C4C	2.01	129.19	124.03
24	7	608	CHL	CAC-C3C-C4C	2.01	129.19	124.03
25	g	614	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
30	D	404	BCR	C20-C21-C22	-2.01	124.46	127.28
24	s	601	CHL	CED-O2D-CGD	2.01	120.47	115.92
25	r	604	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
25	b	605	CLA	CAA-C2A-C1A	2.01	118.55	111.97
37	c	519	DGD	O6E-C1E-O5D	-2.01	105.30	110.04
27	N	1622	XAT	O24-C25-C26	-2.01	57.34	58.93
25	n	610	CLA	CAA-C2A-C3A	-2.01	107.58	113.00
26	1	1621	LUT	C36-C21-C26	2.01	112.58	109.55
26	R	620	LUT	C40-C33-C32	2.01	121.15	118.09
25	C	501	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
24	N	605	CHL	C4C-CHD-C1D	2.01	123.24	116.07
34	a	412	SQD	O47-C7-O49	-2.01	119.02	123.70
33	A	408	PHO	O2D-CGD-O1D	-2.01	119.94	123.85
25	Y	612	CLA	CHB-C1B-C2B	-2.00	121.61	127.43
25	Y	602	CLA	C6-C7-C8	-2.00	109.30	115.97
25	b	604	CLA	CAA-CBA-CGA	-2.00	107.52	113.21
36	D	405	PL9	C12-C13-C14	-2.00	123.04	127.62
24	s	607	CHL	O2D-CGD-O1D	-2.00	119.95	123.85
30	C	514	BCR	C40-C30-C25	-2.00	107.10	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	602	CLA	C4-C3-C5	2.00	118.70	115.23
25	R	604	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
25	2	613	CLA	CHC-C4B-NB	2.00	127.05	124.05
25	b	609	CLA	CHB-C1B-NB	2.00	127.05	124.05
26	g	1621	LUT	C31-C32-C33	-2.00	120.87	126.36
30	c	514	BCR	C2-C3-C4	-2.00	106.88	111.28
28	5	1623	NEX	C35-C15-C14	-2.00	119.42	123.52
25	r	604	CLA	C2A-C1A-CHA	2.00	127.34	123.87
26	r	620	LUT	C40-C33-C32	2.00	121.15	118.09
30	C	514	BCR	C36-C18-C19	2.00	121.15	118.09
24	N	608	CHL	CAC-C3C-C4C	2.00	129.18	124.03
25	B	603	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
24	6	609	CHL	O2D-CGD-O1D	-2.00	119.95	123.85
25	c	513	CLA	CHA-C1A-NA	-2.00	121.86	126.39
25	B	611	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
25	R	610	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
24	1	608	CHL	C4C-CHD-C1D	2.00	123.23	116.07
25	B	605	CLA	CAA-C2A-C1A	2.00	118.53	111.97
25	N	603	CLA	C2D-C1D-ND	-2.00	108.15	110.13
25	B	609	CLA	C16-C15-C13	-2.00	109.32	115.97
37	C	519	DGD	O6E-C1E-O5D	-2.00	105.32	110.04
25	c	501	CLA	CHB-C1B-C2B	-2.00	121.62	127.43
25	R	612	CLA	CAA-CBA-CGA	-2.00	107.53	113.21
25	r	612	CLA	CAA-CBA-CGA	-2.00	107.53	113.21

All (526) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	1	601	CHL	NA
24	1	601	CHL	ND
24	1	601	CHL	NC
24	1	605	CHL	NA
24	1	605	CHL	ND
24	1	605	CHL	NC
24	1	606	CHL	NA
24	1	606	CHL	ND
24	1	606	CHL	NC
24	1	607	CHL	C8
24	1	607	CHL	NA
24	1	607	CHL	ND
24	1	607	CHL	NC
24	1	608	CHL	NA

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Mol	Chain	Res	Type	Atom
24	1	608	CHL	ND
24	1	608	CHL	NC
24	1	609	CHL	C8
24	1	609	CHL	NA
24	1	609	CHL	ND
24	1	609	CHL	NC
24	2	601	CHL	NA
24	2	601	CHL	ND
24	2	601	CHL	NC
24	2	605	CHL	NA
24	2	605	CHL	ND
24	2	605	CHL	NC
24	2	606	CHL	NA
24	2	606	CHL	ND
24	2	606	CHL	NC
24	2	607	CHL	C8
24	2	607	CHL	NA
24	2	607	CHL	ND
24	2	607	CHL	NC
24	2	608	CHL	NA
24	2	608	CHL	ND
24	2	608	CHL	NC
24	2	609	CHL	C8
24	2	609	CHL	NA
24	2	609	CHL	ND
24	2	609	CHL	NC
24	3	601	CHL	C8
24	3	601	CHL	NA
24	3	601	CHL	ND
24	3	601	CHL	NC
24	3	605	CHL	NA
24	3	605	CHL	ND
24	3	605	CHL	NC
24	3	606	CHL	NA
24	3	606	CHL	ND
24	3	606	CHL	NC
24	3	607	CHL	NA
24	3	607	CHL	ND
24	3	607	CHL	NC
24	3	608	CHL	NA
24	3	608	CHL	ND
24	3	608	CHL	NC

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Mol	Chain	Res	Type	Atom
24	3	609	CHL	C8
24	3	609	CHL	NA
24	3	609	CHL	ND
24	3	609	CHL	NC
24	4	601	CHL	NA
24	4	601	CHL	ND
24	4	601	CHL	NC
24	4	606	CHL	NA
24	4	606	CHL	ND
24	4	606	CHL	NC
24	4	607	CHL	NA
24	4	607	CHL	ND
24	4	607	CHL	NC
24	4	608	CHL	NA
24	4	608	CHL	ND
24	4	608	CHL	NC
24	4	609	CHL	NA
24	4	609	CHL	ND
24	4	609	CHL	NC
24	G	601	CHL	C8
24	G	601	CHL	NA
24	G	601	CHL	ND
24	G	601	CHL	NC
24	G	605	CHL	NA
24	G	605	CHL	ND
24	G	605	CHL	NC
24	G	606	CHL	NA
24	G	606	CHL	ND
24	G	606	CHL	NC
24	G	607	CHL	C8
24	G	607	CHL	NA
24	G	607	CHL	ND
24	G	607	CHL	NC
24	G	608	CHL	C8
24	G	608	CHL	NA
24	G	608	CHL	ND
24	G	608	CHL	NC
24	G	609	CHL	C8
24	G	609	CHL	NA
24	G	609	CHL	ND
24	G	609	CHL	NC
24	N	601	CHL	C8

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

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Mol	Chain	Res	Type	Atom
24	S	607	CHL	C8
24	S	607	CHL	NA
24	S	607	CHL	ND
24	S	607	CHL	NC
24	S	608	CHL	NA
24	S	608	CHL	ND
24	S	608	CHL	NC
24	Y	601	CHL	C8
24	Y	601	CHL	NA
24	Y	601	CHL	ND
24	Y	601	CHL	NC
24	Y	605	CHL	NA
24	Y	605	CHL	ND
24	Y	605	CHL	NC
24	Y	606	CHL	NA
24	Y	606	CHL	ND
24	Y	606	CHL	NC
24	Y	607	CHL	C8
24	Y	607	CHL	NA
24	Y	607	CHL	ND
24	Y	607	CHL	NC
24	Y	608	CHL	C8
24	Y	608	CHL	NA
24	Y	608	CHL	ND
24	Y	608	CHL	NC
24	Y	609	CHL	C8
24	Y	609	CHL	NA
24	Y	609	CHL	ND
24	Y	609	CHL	NC
24	5	601	CHL	NA
24	5	601	CHL	ND
24	5	601	CHL	NC
24	5	605	CHL	NA
24	5	605	CHL	ND
24	5	605	CHL	NC
24	5	606	CHL	NA
24	5	606	CHL	ND
24	5	606	CHL	NC
24	5	607	CHL	C8
24	5	607	CHL	NA
24	5	607	CHL	ND
24	5	607	CHL	NC

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Mol	Chain	Res	Type	Atom
24	5	608	CHL	NA
24	5	608	CHL	ND
24	5	608	CHL	NC
24	5	609	CHL	C8
24	5	609	CHL	NA
24	5	609	CHL	ND
24	5	609	CHL	NC
24	6	601	CHL	NA
24	6	601	CHL	ND
24	6	601	CHL	NC
24	6	605	CHL	NA
24	6	605	CHL	ND
24	6	605	CHL	NC
24	6	606	CHL	NA
24	6	606	CHL	ND
24	6	606	CHL	NC
24	6	607	CHL	C8
24	6	607	CHL	NA
24	6	607	CHL	ND
24	6	607	CHL	NC
24	6	608	CHL	NA
24	6	608	CHL	ND
24	6	608	CHL	NC
24	6	609	CHL	C8
24	6	609	CHL	NA
24	6	609	CHL	ND
24	6	609	CHL	NC
24	7	601	CHL	C8
24	7	601	CHL	NA
24	7	601	CHL	ND
24	7	601	CHL	NC
24	7	605	CHL	NA
24	7	605	CHL	ND
24	7	605	CHL	NC
24	7	606	CHL	NA
24	7	606	CHL	ND
24	7	606	CHL	NC
24	7	607	CHL	NA
24	7	607	CHL	ND
24	7	607	CHL	NC
24	7	608	CHL	NA
24	7	608	CHL	ND

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Mol	Chain	Res	Type	Atom
24	7	608	CHL	NC
24	7	609	CHL	C8
24	7	609	CHL	NA
24	7	609	CHL	ND
24	7	609	CHL	NC
24	8	601	CHL	NA
24	8	601	CHL	ND
24	8	601	CHL	NC
24	8	606	CHL	NA
24	8	606	CHL	ND
24	8	606	CHL	NC
24	8	607	CHL	NA
24	8	607	CHL	ND
24	8	607	CHL	NC
24	8	608	CHL	NA
24	8	608	CHL	ND
24	8	608	CHL	NC
24	8	609	CHL	NA
24	8	609	CHL	ND
24	8	609	CHL	NC
24	g	601	CHL	C8
24	g	601	CHL	NA
24	g	601	CHL	ND
24	g	601	CHL	NC
24	g	605	CHL	NA
24	g	605	CHL	ND
24	g	605	CHL	NC
24	g	606	CHL	NA
24	g	606	CHL	ND
24	g	606	CHL	NC
24	g	607	CHL	C8
24	g	607	CHL	NA
24	g	607	CHL	ND
24	g	607	CHL	NC
24	g	608	CHL	C8
24	g	608	CHL	NA
24	g	608	CHL	ND
24	g	608	CHL	NC
24	g	609	CHL	C8
24	g	609	CHL	NA
24	g	609	CHL	ND
24	g	609	CHL	NC

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

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Mol	Chain	Res	Type	Atom
24	s	606	CHL	NC
24	s	607	CHL	C8
24	s	607	CHL	NA
24	s	607	CHL	ND
24	s	607	CHL	NC
24	s	608	CHL	NA
24	s	608	CHL	ND
24	s	608	CHL	NC
24	y	601	CHL	C8
24	y	601	CHL	NA
24	y	601	CHL	ND
24	y	601	CHL	NC
24	y	605	CHL	NA
24	y	605	CHL	ND
24	y	605	CHL	NC
24	y	606	CHL	NA
24	y	606	CHL	ND
24	y	606	CHL	NC
24	y	607	CHL	C8
24	y	607	CHL	NA
24	y	607	CHL	ND
24	y	607	CHL	NC
24	y	608	CHL	C8
24	y	608	CHL	NA
24	y	608	CHL	ND
24	y	608	CHL	NC
24	y	609	CHL	C8
24	y	609	CHL	NA
24	y	609	CHL	ND
24	y	609	CHL	NC
25	1	602	CLA	ND
25	1	603	CLA	ND
25	1	604	CLA	ND
25	1	610	CLA	ND
25	1	611	CLA	ND
25	1	612	CLA	ND
25	1	614	CLA	ND
25	2	602	CLA	ND
25	2	603	CLA	ND
25	2	610	CLA	ND
25	2	611	CLA	ND
25	2	612	CLA	ND

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Mol	Chain	Res	Type	Atom
25	3	602	CLA	ND
25	3	603	CLA	ND
25	3	604	CLA	ND
25	3	610	CLA	ND
25	3	611	CLA	ND
25	3	612	CLA	ND
25	3	613	CLA	ND
25	3	614	CLA	ND
25	4	602	CLA	ND
25	4	603	CLA	ND
25	4	610	CLA	ND
25	4	611	CLA	ND
25	4	612	CLA	ND
25	A	405	CLA	ND
25	A	406	CLA	ND
25	A	407	CLA	ND
25	A	410	CLA	ND
25	B	602	CLA	ND
25	B	603	CLA	ND
25	B	604	CLA	ND
25	B	605	CLA	ND
25	B	606	CLA	ND
25	B	607	CLA	ND
25	B	608	CLA	ND
25	B	609	CLA	ND
25	B	611	CLA	ND
25	B	612	CLA	ND
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	B	616	CLA	ND
25	B	617	CLA	ND
25	C	501	CLA	ND
25	C	502	CLA	ND
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	507	CLA	ND
25	C	508	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	512	CLA	ND
25	D	402	CLA	ND

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Mol	Chain	Res	Type	Atom
25	G	602	CLA	ND
25	G	603	CLA	ND
25	G	610	CLA	ND
25	G	611	CLA	ND
25	G	612	CLA	ND
25	G	614	CLA	ND
25	N	602	CLA	ND
25	N	603	CLA	ND
25	N	604	CLA	ND
25	N	610	CLA	ND
25	N	611	CLA	ND
25	N	612	CLA	ND
25	N	613	CLA	ND
25	N	614	CLA	ND
25	R	601	CLA	ND
25	R	602	CLA	ND
25	R	603	CLA	ND
25	R	604	CLA	ND
25	R	609	CLA	ND
25	R	610	CLA	ND
25	R	611	CLA	ND
25	R	612	CLA	ND
25	R	613	CLA	ND
25	S	602	CLA	ND
25	S	603	CLA	ND
25	S	604	CLA	ND
25	S	609	CLA	ND
25	S	610	CLA	ND
25	S	611	CLA	ND
25	S	612	CLA	ND
25	S	613	CLA	ND
25	S	614	CLA	ND
25	Y	602	CLA	ND
25	Y	603	CLA	ND
25	Y	604	CLA	ND
25	Y	610	CLA	ND
25	Y	611	CLA	ND
25	Y	612	CLA	ND
25	Y	613	CLA	ND
25	Y	614	CLA	ND
25	5	602	CLA	ND
25	5	603	CLA	ND

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Mol	Chain	Res	Type	Atom
25	5	604	CLA	ND
25	5	610	CLA	ND
25	5	611	CLA	ND
25	5	612	CLA	ND
25	5	614	CLA	ND
25	6	602	CLA	ND
25	6	603	CLA	ND
25	6	610	CLA	ND
25	6	611	CLA	ND
25	6	612	CLA	ND
25	7	602	CLA	ND
25	7	603	CLA	ND
25	7	604	CLA	ND
25	7	610	CLA	ND
25	7	611	CLA	ND
25	7	612	CLA	ND
25	7	613	CLA	ND
25	7	614	CLA	ND
25	8	602	CLA	ND
25	8	603	CLA	ND
25	8	610	CLA	ND
25	8	611	CLA	ND
25	8	612	CLA	ND
25	a	405	CLA	ND
25	a	406	CLA	ND
25	a	407	CLA	ND
25	a	410	CLA	ND
25	b	602	CLA	ND
25	b	603	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	609	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	b	617	CLA	ND

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Mol	Chain	Res	Type	Atom
25	c	501	CLA	ND
25	c	502	CLA	ND
25	c	503	CLA	ND
25	c	504	CLA	ND
25	c	507	CLA	ND
25	c	508	CLA	ND
25	c	509	CLA	ND
25	c	510	CLA	ND
25	c	512	CLA	ND
25	d	402	CLA	ND
25	g	602	CLA	ND
25	g	603	CLA	ND
25	g	610	CLA	ND
25	g	611	CLA	ND
25	g	612	CLA	ND
25	g	614	CLA	ND
25	n	602	CLA	ND
25	n	603	CLA	ND
25	n	604	CLA	ND
25	n	610	CLA	ND
25	n	611	CLA	ND
25	n	612	CLA	ND
25	n	613	CLA	ND
25	n	614	CLA	ND
25	r	601	CLA	ND
25	r	602	CLA	ND
25	r	603	CLA	ND
25	r	604	CLA	ND
25	r	609	CLA	ND
25	r	610	CLA	ND
25	r	611	CLA	ND
25	r	612	CLA	ND
25	r	613	CLA	ND
25	s	602	CLA	ND
25	s	603	CLA	ND
25	s	604	CLA	ND
25	s	609	CLA	ND
25	s	610	CLA	ND
25	s	611	CLA	ND
25	s	612	CLA	ND
25	s	613	CLA	ND
25	s	614	CLA	ND

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Mol	Chain	Res	Type	Atom
25	y	602	CLA	ND
25	y	603	CLA	ND
25	y	604	CLA	ND
25	y	610	CLA	ND
25	y	611	CLA	ND
25	y	612	CLA	ND
25	y	613	CLA	ND
25	y	614	CLA	ND

All (4801) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	1	605	CHL	C1A-C2A-CAA-CBA
24	1	605	CHL	C1C-C2C-CMC-OMC
24	1	605	CHL	C3C-C2C-CMC-OMC
24	1	606	CHL	C3C-C2C-CMC-OMC
24	1	606	CHL	CBD-CGD-O2D-CED
24	1	607	CHL	C1C-C2C-CMC-OMC
24	1	607	CHL	C3C-C2C-CMC-OMC
24	1	607	CHL	C4C-C3C-CAC-CBC
24	1	608	CHL	C1A-C2A-CAA-CBA
24	1	609	CHL	C1C-C2C-CMC-OMC
24	1	609	CHL	C3C-C2C-CMC-OMC
24	1	609	CHL	C4C-C3C-CAC-CBC
24	1	609	CHL	CHA-CBD-CGD-O1D
24	2	601	CHL	C3A-C2A-CAA-CBA
24	2	605	CHL	C1A-C2A-CAA-CBA
24	2	605	CHL	C1C-C2C-CMC-OMC
24	2	605	CHL	C3C-C2C-CMC-OMC
24	2	606	CHL	C3C-C2C-CMC-OMC
24	2	607	CHL	C1C-C2C-CMC-OMC
24	2	607	CHL	C3C-C2C-CMC-OMC
24	2	607	CHL	C4C-C3C-CAC-CBC
24	2	607	CHL	CHA-CBD-CGD-O1D
24	2	607	CHL	CHA-CBD-CGD-O2D
24	2	608	CHL	C1C-C2C-CMC-OMC
24	2	608	CHL	C3C-C2C-CMC-OMC
24	2	608	CHL	C4C-C3C-CAC-CBC
24	2	609	CHL	C1C-C2C-CMC-OMC
24	2	609	CHL	C3C-C2C-CMC-OMC
24	3	605	CHL	C1A-C2A-CAA-CBA
24	3	605	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	3	605	CHL	C3C-C2C-CMC-OMC
24	3	606	CHL	C3A-C2A-CAA-CBA
24	3	607	CHL	C1C-C2C-CMC-OMC
24	3	607	CHL	C3C-C2C-CMC-OMC
24	3	609	CHL	C1C-C2C-CMC-OMC
24	3	609	CHL	C3C-C2C-CMC-OMC
24	3	609	CHL	C4C-C3C-CAC-CBC
24	4	601	CHL	C1C-C2C-CMC-OMC
24	4	601	CHL	C3C-C2C-CMC-OMC
24	4	606	CHL	C3A-C2A-CAA-CBA
24	4	606	CHL	C1C-C2C-CMC-OMC
24	4	607	CHL	C1C-C2C-CMC-OMC
24	4	607	CHL	C3C-C2C-CMC-OMC
24	4	608	CHL	C1A-C2A-CAA-CBA
24	4	608	CHL	C1C-C2C-CMC-OMC
24	4	608	CHL	C3C-C2C-CMC-OMC
24	4	608	CHL	CHA-CBD-CGD-O1D
24	4	608	CHL	CHA-CBD-CGD-O2D
24	4	608	CHL	CBD-CGD-O2D-CED
24	4	609	CHL	C1C-C2C-CMC-OMC
24	4	609	CHL	C3C-C2C-CMC-OMC
24	4	609	CHL	C4C-C3C-CAC-CBC
24	G	605	CHL	C1C-C2C-CMC-OMC
24	G	605	CHL	C3C-C2C-CMC-OMC
24	G	605	CHL	CAD-CBD-CGD-O1D
24	G	605	CHL	CAD-CBD-CGD-O2D
24	G	605	CHL	CBD-CGD-O2D-CED
24	G	606	CHL	C1C-C2C-CMC-OMC
24	G	607	CHL	C1C-C2C-CMC-OMC
24	G	607	CHL	C3C-C2C-CMC-OMC
24	G	608	CHL	C1A-C2A-CAA-CBA
24	G	608	CHL	C1C-C2C-CMC-OMC
24	G	608	CHL	C3C-C2C-CMC-OMC
24	G	608	CHL	CBD-CGD-O2D-CED
24	G	609	CHL	C1C-C2C-CMC-OMC
24	G	609	CHL	C3C-C2C-CMC-OMC
24	N	605	CHL	C1A-C2A-CAA-CBA
24	N	605	CHL	C1C-C2C-CMC-OMC
24	N	605	CHL	C3C-C2C-CMC-OMC
24	N	605	CHL	CAD-CBD-CGD-O1D
24	N	605	CHL	CAD-CBD-CGD-O2D
24	N	606	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	N	606	CHL	C3C-C2C-CMC-OMC
24	N	606	CHL	CHA-CBD-CGD-O1D
24	N	606	CHL	CHA-CBD-CGD-O2D
24	N	607	CHL	C1C-C2C-CMC-OMC
24	N	607	CHL	C3C-C2C-CMC-OMC
24	N	608	CHL	C1A-C2A-CAA-CBA
24	N	608	CHL	CBD-CGD-O2D-CED
24	N	609	CHL	C1C-C2C-CMC-OMC
24	N	609	CHL	C3C-C2C-CMC-OMC
24	R	606	CHL	C1A-C2A-CAA-CBA
24	R	608	CHL	CBD-CGD-O2D-CED
24	R	614	CHL	CAD-CBD-CGD-O1D
24	R	614	CHL	CAD-CBD-CGD-O2D
24	R	614	CHL	CBD-CGD-O2D-CED
24	S	601	CHL	C1C-C2C-CMC-OMC
24	S	601	CHL	C3C-C2C-CMC-OMC
24	S	606	CHL	C1C-C2C-CMC-OMC
24	S	606	CHL	C3C-C2C-CMC-OMC
24	S	606	CHL	CAD-CBD-CGD-O1D
24	S	606	CHL	CAD-CBD-CGD-O2D
24	S	607	CHL	C1C-C2C-CMC-OMC
24	S	607	CHL	C3C-C2C-CMC-OMC
24	S	608	CHL	C1A-C2A-CAA-CBA
24	Y	605	CHL	C1A-C2A-CAA-CBA
24	Y	605	CHL	C1C-C2C-CMC-OMC
24	Y	605	CHL	C3C-C2C-CMC-OMC
24	Y	606	CHL	C1C-C2C-CMC-OMC
24	Y	606	CHL	C3C-C2C-CMC-OMC
24	Y	607	CHL	C1C-C2C-CMC-OMC
24	Y	607	CHL	C3C-C2C-CMC-OMC
24	Y	608	CHL	C1A-C2A-CAA-CBA
24	Y	608	CHL	CBD-CGD-O2D-CED
24	Y	609	CHL	C1C-C2C-CMC-OMC
24	Y	609	CHL	C3C-C2C-CMC-OMC
24	5	605	CHL	C1A-C2A-CAA-CBA
24	5	605	CHL	C1C-C2C-CMC-OMC
24	5	605	CHL	C3C-C2C-CMC-OMC
24	5	606	CHL	C3C-C2C-CMC-OMC
24	5	606	CHL	CBD-CGD-O2D-CED
24	5	607	CHL	C1C-C2C-CMC-OMC
24	5	607	CHL	C3C-C2C-CMC-OMC
24	5	607	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
24	5	608	CHL	C1A-C2A-CAA-CBA
24	5	609	CHL	C1C-C2C-CMC-OMC
24	5	609	CHL	C3C-C2C-CMC-OMC
24	5	609	CHL	C4C-C3C-CAC-CBC
24	5	609	CHL	CHA-CBD-CGD-O1D
24	6	601	CHL	C3A-C2A-CAA-CBA
24	6	605	CHL	C1A-C2A-CAA-CBA
24	6	605	CHL	C1C-C2C-CMC-OMC
24	6	605	CHL	C3C-C2C-CMC-OMC
24	6	606	CHL	C3C-C2C-CMC-OMC
24	6	607	CHL	C1C-C2C-CMC-OMC
24	6	607	CHL	C3C-C2C-CMC-OMC
24	6	607	CHL	C4C-C3C-CAC-CBC
24	6	607	CHL	CHA-CBD-CGD-O1D
24	6	607	CHL	CHA-CBD-CGD-O2D
24	6	608	CHL	C1C-C2C-CMC-OMC
24	6	608	CHL	C3C-C2C-CMC-OMC
24	6	608	CHL	C4C-C3C-CAC-CBC
24	6	609	CHL	C1C-C2C-CMC-OMC
24	6	609	CHL	C3C-C2C-CMC-OMC
24	7	605	CHL	C1A-C2A-CAA-CBA
24	7	605	CHL	C1C-C2C-CMC-OMC
24	7	605	CHL	C3C-C2C-CMC-OMC
24	7	606	CHL	C3A-C2A-CAA-CBA
24	7	607	CHL	C1C-C2C-CMC-OMC
24	7	607	CHL	C3C-C2C-CMC-OMC
24	7	609	CHL	C1C-C2C-CMC-OMC
24	7	609	CHL	C3C-C2C-CMC-OMC
24	7	609	CHL	C4C-C3C-CAC-CBC
24	8	601	CHL	C1C-C2C-CMC-OMC
24	8	601	CHL	C3C-C2C-CMC-OMC
24	8	606	CHL	C3A-C2A-CAA-CBA
24	8	606	CHL	C1C-C2C-CMC-OMC
24	8	607	CHL	C1C-C2C-CMC-OMC
24	8	607	CHL	C3C-C2C-CMC-OMC
24	8	608	CHL	C1A-C2A-CAA-CBA
24	8	608	CHL	C1C-C2C-CMC-OMC
24	8	608	CHL	C3C-C2C-CMC-OMC
24	8	608	CHL	CHA-CBD-CGD-O1D
24	8	608	CHL	CHA-CBD-CGD-O2D
24	8	608	CHL	CBD-CGD-O2D-CED
24	8	609	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	8	609	CHL	C3C-C2C-CMC-OMC
24	8	609	CHL	C4C-C3C-CAC-CBC
24	g	605	CHL	C1C-C2C-CMC-OMC
24	g	605	CHL	C3C-C2C-CMC-OMC
24	g	605	CHL	CAD-CBD-CGD-O1D
24	g	605	CHL	CAD-CBD-CGD-O2D
24	g	605	CHL	CBD-CGD-O2D-CED
24	g	606	CHL	C1C-C2C-CMC-OMC
24	g	607	CHL	C1C-C2C-CMC-OMC
24	g	607	CHL	C3C-C2C-CMC-OMC
24	g	608	CHL	C1A-C2A-CAA-CBA
24	g	608	CHL	C1C-C2C-CMC-OMC
24	g	608	CHL	C3C-C2C-CMC-OMC
24	g	608	CHL	CBD-CGD-O2D-CED
24	g	609	CHL	C1C-C2C-CMC-OMC
24	g	609	CHL	C3C-C2C-CMC-OMC
24	n	605	CHL	C1A-C2A-CAA-CBA
24	n	605	CHL	C1C-C2C-CMC-OMC
24	n	605	CHL	C3C-C2C-CMC-OMC
24	n	605	CHL	CAD-CBD-CGD-O1D
24	n	605	CHL	CAD-CBD-CGD-O2D
24	n	606	CHL	C1C-C2C-CMC-OMC
24	n	606	CHL	C3C-C2C-CMC-OMC
24	n	606	CHL	CHA-CBD-CGD-O1D
24	n	606	CHL	CHA-CBD-CGD-O2D
24	n	607	CHL	C1C-C2C-CMC-OMC
24	n	607	CHL	C3C-C2C-CMC-OMC
24	n	608	CHL	C1A-C2A-CAA-CBA
24	n	608	CHL	CBD-CGD-O2D-CED
24	n	609	CHL	C1C-C2C-CMC-OMC
24	n	609	CHL	C3C-C2C-CMC-OMC
24	r	606	CHL	C1A-C2A-CAA-CBA
24	r	608	CHL	CBD-CGD-O2D-CED
24	r	614	CHL	CAD-CBD-CGD-O1D
24	r	614	CHL	CAD-CBD-CGD-O2D
24	r	614	CHL	CBD-CGD-O2D-CED
24	s	601	CHL	C1C-C2C-CMC-OMC
24	s	601	CHL	C3C-C2C-CMC-OMC
24	s	606	CHL	C1C-C2C-CMC-OMC
24	s	606	CHL	C3C-C2C-CMC-OMC
24	s	606	CHL	CAD-CBD-CGD-O1D
24	s	606	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	s	607	CHL	C1C-C2C-CMC-OMC
24	s	607	CHL	C3C-C2C-CMC-OMC
24	s	608	CHL	C1A-C2A-CAA-CBA
24	y	605	CHL	C1A-C2A-CAA-CBA
24	y	605	CHL	C1C-C2C-CMC-OMC
24	y	605	CHL	C3C-C2C-CMC-OMC
24	y	606	CHL	C1C-C2C-CMC-OMC
24	y	606	CHL	C3C-C2C-CMC-OMC
24	y	607	CHL	C1C-C2C-CMC-OMC
24	y	607	CHL	C3C-C2C-CMC-OMC
24	y	608	CHL	C1A-C2A-CAA-CBA
24	y	608	CHL	CBD-CGD-O2D-CED
24	y	609	CHL	C1C-C2C-CMC-OMC
24	y	609	CHL	C3C-C2C-CMC-OMC
25	1	603	CLA	C4B-C3B-CAB-CBB
25	1	603	CLA	CBD-CGD-O2D-CED
25	1	604	CLA	CAD-CBD-CGD-O1D
25	1	604	CLA	CAD-CBD-CGD-O2D
25	1	611	CLA	C2B-C3B-CAB-CBB
25	1	611	CLA	C4B-C3B-CAB-CBB
25	1	612	CLA	CHA-CBD-CGD-O1D
25	1	612	CLA	CHA-CBD-CGD-O2D
25	1	613	CLA	CBD-CGD-O2D-CED
25	1	614	CLA	CBD-CGD-O2D-CED
25	2	603	CLA	C2B-C3B-CAB-CBB
25	2	603	CLA	C4B-C3B-CAB-CBB
25	2	603	CLA	CBD-CGD-O2D-CED
25	2	604	CLA	C1A-C2A-CAA-CBA
25	2	604	CLA	C3A-C2A-CAA-CBA
25	2	604	CLA	CAD-CBD-CGD-O1D
25	2	604	CLA	CAD-CBD-CGD-O2D
25	2	604	CLA	CBD-CGD-O2D-CED
25	2	610	CLA	C2B-C3B-CAB-CBB
25	2	610	CLA	C4B-C3B-CAB-CBB
25	2	611	CLA	C2B-C3B-CAB-CBB
25	2	611	CLA	C4B-C3B-CAB-CBB
25	2	612	CLA	CHA-CBD-CGD-O1D
25	2	612	CLA	CHA-CBD-CGD-O2D
25	2	613	CLA	CBD-CGD-O2D-CED
25	2	614	CLA	C1A-C2A-CAA-CBA
25	2	614	CLA	C3A-C2A-CAA-CBA
25	3	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	3	603	CLA	O1A-CGA-O2A-C1
25	3	603	CLA	C4B-C3B-CAB-CBB
25	3	610	CLA	C4B-C3B-CAB-CBB
25	3	611	CLA	C1A-C2A-CAA-CBA
25	3	611	CLA	C4B-C3B-CAB-CBB
25	3	612	CLA	C2B-C3B-CAB-CBB
25	3	612	CLA	C4B-C3B-CAB-CBB
25	3	612	CLA	CAD-CBD-CGD-O1D
25	3	612	CLA	CAD-CBD-CGD-O2D
25	3	613	CLA	C2B-C3B-CAB-CBB
25	3	613	CLA	C4B-C3B-CAB-CBB
25	3	614	CLA	CAD-CBD-CGD-O1D
25	3	614	CLA	CAD-CBD-CGD-O2D
25	3	614	CLA	CBD-CGD-O2D-CED
25	4	602	CLA	CBD-CGD-O2D-CED
25	4	604	CLA	C1A-C2A-CAA-CBA
25	4	610	CLA	C1A-C2A-CAA-CBA
25	4	611	CLA	C2B-C3B-CAB-CBB
25	4	611	CLA	C4B-C3B-CAB-CBB
25	4	611	CLA	CBD-CGD-O2D-CED
25	A	405	CLA	CBD-CGD-O2D-CED
25	A	405	CLA	O1D-CGD-O2D-CED
25	A	407	CLA	C4B-C3B-CAB-CBB
25	B	602	CLA	CAD-CBD-CGD-O1D
25	B	602	CLA	CAD-CBD-CGD-O2D
25	B	603	CLA	C2-C3-C5-C6
25	B	603	CLA	C4-C3-C5-C6
25	B	604	CLA	C2-C3-C5-C6
25	B	604	CLA	C4-C3-C5-C6
25	B	607	CLA	C4B-C3B-CAB-CBB
25	B	608	CLA	CBD-CGD-O2D-CED
25	B	610	CLA	C1A-C2A-CAA-CBA
25	B	613	CLA	C1A-C2A-CAA-CBA
25	B	613	CLA	C3A-C2A-CAA-CBA
25	B	616	CLA	C4B-C3B-CAB-CBB
25	B	616	CLA	C11-C10-C8-C9
25	B	617	CLA	CHA-CBD-CGD-O2D
25	C	502	CLA	C6-C7-C8-C9
25	C	507	CLA	C1A-C2A-CAA-CBA
25	C	507	CLA	C3A-C2A-CAA-CBA
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	C	507	CLA	C11-C10-C8-C9
25	G	610	CLA	C1A-C2A-CAA-CBA
25	G	610	CLA	C3A-C2A-CAA-CBA
25	G	611	CLA	C1A-C2A-CAA-CBA
25	G	611	CLA	C3A-C2A-CAA-CBA
25	G	611	CLA	C2B-C3B-CAB-CBB
25	G	611	CLA	C4B-C3B-CAB-CBB
25	N	610	CLA	C1A-C2A-CAA-CBA
25	N	610	CLA	C3A-C2A-CAA-CBA
25	N	611	CLA	C2B-C3B-CAB-CBB
25	N	611	CLA	C4B-C3B-CAB-CBB
25	N	612	CLA	CBD-CGD-O2D-CED
25	N	614	CLA	CBD-CGD-O2D-CED
25	R	601	CLA	C2B-C3B-CAB-CBB
25	R	601	CLA	C4B-C3B-CAB-CBB
25	R	601	CLA	CBD-CGD-O2D-CED
25	R	604	CLA	CHA-CBD-CGD-O1D
25	R	604	CLA	CHA-CBD-CGD-O2D
25	R	611	CLA	C1A-C2A-CAA-CBA
25	R	611	CLA	C3A-C2A-CAA-CBA
25	R	611	CLA	CBA-CGA-O2A-C1
25	R	612	CLA	CBD-CGD-O2D-CED
25	R	613	CLA	C2B-C3B-CAB-CBB
25	R	613	CLA	C4B-C3B-CAB-CBB
25	R	616	CLA	C1A-C2A-CAA-CBA
25	R	616	CLA	C4B-C3B-CAB-CBB
25	S	602	CLA	C1A-C2A-CAA-CBA
25	S	604	CLA	C1A-C2A-CAA-CBA
25	S	609	CLA	C2B-C3B-CAB-CBB
25	S	609	CLA	C4B-C3B-CAB-CBB
25	S	611	CLA	C2B-C3B-CAB-CBB
25	S	611	CLA	C4B-C3B-CAB-CBB
25	S	612	CLA	CBD-CGD-O2D-CED
25	Y	612	CLA	C6-C7-C8-C10
25	Y	614	CLA	C2B-C3B-CAB-CBB
25	Y	614	CLA	C4B-C3B-CAB-CBB
25	5	603	CLA	C4B-C3B-CAB-CBB
25	5	603	CLA	CBD-CGD-O2D-CED
25	5	604	CLA	CAD-CBD-CGD-O1D
25	5	604	CLA	CAD-CBD-CGD-O2D
25	5	611	CLA	C2B-C3B-CAB-CBB
25	5	611	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	5	612	CLA	CHA-CBD-CGD-O1D
25	5	612	CLA	CHA-CBD-CGD-O2D
25	5	613	CLA	CBD-CGD-O2D-CED
25	5	614	CLA	CBD-CGD-O2D-CED
25	6	603	CLA	C2B-C3B-CAB-CBB
25	6	603	CLA	C4B-C3B-CAB-CBB
25	6	603	CLA	CBD-CGD-O2D-CED
25	6	604	CLA	C1A-C2A-CAA-CBA
25	6	604	CLA	C3A-C2A-CAA-CBA
25	6	604	CLA	CAD-CBD-CGD-O1D
25	6	604	CLA	CAD-CBD-CGD-O2D
25	6	604	CLA	CBD-CGD-O2D-CED
25	6	610	CLA	C2B-C3B-CAB-CBB
25	6	610	CLA	C4B-C3B-CAB-CBB
25	6	611	CLA	C2B-C3B-CAB-CBB
25	6	611	CLA	C4B-C3B-CAB-CBB
25	6	612	CLA	CHA-CBD-CGD-O1D
25	6	612	CLA	CHA-CBD-CGD-O2D
25	6	613	CLA	CBD-CGD-O2D-CED
25	6	614	CLA	C1A-C2A-CAA-CBA
25	6	614	CLA	C3A-C2A-CAA-CBA
25	7	602	CLA	CHA-CBD-CGD-O2D
25	7	603	CLA	O1A-CGA-O2A-C1
25	7	603	CLA	C4B-C3B-CAB-CBB
25	7	610	CLA	C4B-C3B-CAB-CBB
25	7	611	CLA	C1A-C2A-CAA-CBA
25	7	611	CLA	C4B-C3B-CAB-CBB
25	7	612	CLA	C2B-C3B-CAB-CBB
25	7	612	CLA	C4B-C3B-CAB-CBB
25	7	612	CLA	CAD-CBD-CGD-O1D
25	7	612	CLA	CAD-CBD-CGD-O2D
25	7	613	CLA	C2B-C3B-CAB-CBB
25	7	613	CLA	C4B-C3B-CAB-CBB
25	7	614	CLA	CAD-CBD-CGD-O1D
25	7	614	CLA	CAD-CBD-CGD-O2D
25	7	614	CLA	CBD-CGD-O2D-CED
25	8	602	CLA	CBD-CGD-O2D-CED
25	8	604	CLA	C1A-C2A-CAA-CBA
25	8	610	CLA	C1A-C2A-CAA-CBA
25	8	611	CLA	C2B-C3B-CAB-CBB
25	8	611	CLA	C4B-C3B-CAB-CBB
25	8	611	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	a	405	CLA	CBD-CGD-O2D-CED
25	a	405	CLA	O1D-CGD-O2D-CED
25	a	407	CLA	C4B-C3B-CAB-CBB
25	b	602	CLA	CAD-CBD-CGD-O1D
25	b	602	CLA	CAD-CBD-CGD-O2D
25	b	603	CLA	C2-C3-C5-C6
25	b	603	CLA	C4-C3-C5-C6
25	b	604	CLA	C2-C3-C5-C6
25	b	604	CLA	C4-C3-C5-C6
25	b	607	CLA	C4B-C3B-CAB-CBB
25	b	608	CLA	CBD-CGD-O2D-CED
25	b	610	CLA	C1A-C2A-CAA-CBA
25	b	613	CLA	C1A-C2A-CAA-CBA
25	b	613	CLA	C3A-C2A-CAA-CBA
25	b	616	CLA	C4B-C3B-CAB-CBB
25	b	616	CLA	C11-C10-C8-C9
25	b	617	CLA	CHA-CBD-CGD-O2D
25	c	502	CLA	C6-C7-C8-C9
25	c	507	CLA	C1A-C2A-CAA-CBA
25	c	507	CLA	C3A-C2A-CAA-CBA
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	507	CLA	C11-C10-C8-C9
25	g	610	CLA	C1A-C2A-CAA-CBA
25	g	610	CLA	C3A-C2A-CAA-CBA
25	g	611	CLA	C1A-C2A-CAA-CBA
25	g	611	CLA	C3A-C2A-CAA-CBA
25	g	611	CLA	C2B-C3B-CAB-CBB
25	g	611	CLA	C4B-C3B-CAB-CBB
25	n	610	CLA	C1A-C2A-CAA-CBA
25	n	610	CLA	C3A-C2A-CAA-CBA
25	n	611	CLA	C2B-C3B-CAB-CBB
25	n	611	CLA	C4B-C3B-CAB-CBB
25	n	612	CLA	CBD-CGD-O2D-CED
25	n	614	CLA	CBD-CGD-O2D-CED
25	r	601	CLA	C2B-C3B-CAB-CBB
25	r	601	CLA	C4B-C3B-CAB-CBB
25	r	601	CLA	CBD-CGD-O2D-CED
25	r	604	CLA	CHA-CBD-CGD-O1D
25	r	604	CLA	CHA-CBD-CGD-O2D
25	r	611	CLA	C1A-C2A-CAA-CBA
25	r	611	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	r	611	CLA	CBA-CGA-O2A-C1
25	r	612	CLA	CBD-CGD-O2D-CED
25	r	613	CLA	C2B-C3B-CAB-CBB
25	r	613	CLA	C4B-C3B-CAB-CBB
25	r	616	CLA	C1A-C2A-CAA-CBA
25	r	616	CLA	C4B-C3B-CAB-CBB
25	s	602	CLA	C1A-C2A-CAA-CBA
25	s	604	CLA	C1A-C2A-CAA-CBA
25	s	609	CLA	C2B-C3B-CAB-CBB
25	s	609	CLA	C4B-C3B-CAB-CBB
25	s	611	CLA	C2B-C3B-CAB-CBB
25	s	611	CLA	C4B-C3B-CAB-CBB
25	s	612	CLA	CBD-CGD-O2D-CED
25	y	612	CLA	C6-C7-C8-C10
25	y	614	CLA	C2B-C3B-CAB-CBB
25	y	614	CLA	C4B-C3B-CAB-CBB
26	4	620	LUT	C11-C12-C13-C14
26	4	620	LUT	C11-C12-C13-C20
26	8	620	LUT	C11-C12-C13-C14
26	8	620	LUT	C11-C12-C13-C20
27	1	1622	XAT	C31-C32-C33-C34
27	1	1622	XAT	C31-C32-C33-C40
27	2	1622	XAT	O4-C6-C7-C8
27	2	1622	XAT	C31-C32-C33-C34
27	G	1622	XAT	C11-C12-C13-C14
27	N	1622	XAT	C11-C12-C13-C14
27	N	1622	XAT	C11-C12-C13-C20
27	5	1622	XAT	C31-C32-C33-C34
27	5	1622	XAT	C31-C32-C33-C40
27	6	1622	XAT	O4-C6-C7-C8
27	6	1622	XAT	C31-C32-C33-C34
27	g	1622	XAT	C11-C12-C13-C14
27	n	1622	XAT	C11-C12-C13-C14
27	n	1622	XAT	C11-C12-C13-C20
28	1	1623	NEX	C11-C12-C13-C14
28	1	1623	NEX	C11-C12-C13-C20
28	N	1623	NEX	C31-C32-C33-C34
28	S	1623	NEX	C7-C8-C9-C19
28	5	1623	NEX	C11-C12-C13-C14
28	5	1623	NEX	C11-C12-C13-C20
28	n	1623	NEX	C31-C32-C33-C34
28	s	1623	NEX	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
29	2	2630	LHG	C4-O6-P-O5
29	3	2630	LHG	O1-C1-C2-C3
29	3	2630	LHG	C4-O6-P-O3
29	3	2630	LHG	C4-O6-P-O5
29	4	2630	LHG	O1-C1-C2-O2
29	4	2630	LHG	C3-O3-P-O5
29	4	2630	LHG	C3-O3-P-O6
29	B	2630	LHG	C1-C2-C3-O3
29	B	2630	LHG	C3-O3-P-O5
29	B	2630	LHG	C4-O6-P-O3
29	B	2631	LHG	O1-C1-C2-O2
29	B	2631	LHG	O1-C1-C2-C3
29	B	2631	LHG	O2-C2-C3-O3
29	C	2630	LHG	O1-C1-C2-O2
29	C	2630	LHG	O1-C1-C2-C3
29	C	522	LHG	C3-O3-P-O4
29	C	522	LHG	C3-O3-P-O6
29	C	523	LHG	C3-O3-P-O5
29	C	523	LHG	C4-O6-P-O4
29	C	523	LHG	C8-C7-O7-C5
29	D	409	LHG	C4-O6-P-O3
29	D	409	LHG	C4-O6-P-O4
29	D	409	LHG	C4-O6-P-O5
29	D	410	LHG	C4-O6-P-O3
29	G	2630	LHG	C4-O6-P-O3
29	G	2630	LHG	C4-O6-P-O5
29	L	101	LHG	C3-O3-P-O5
29	L	101	LHG	C3-O3-P-O6
29	N	2630	LHG	C3-O3-P-O6
29	N	2630	LHG	C4-O6-P-O5
29	R	2630	LHG	O1-C1-C2-C3
29	S	2630	LHG	O1-C1-C2-C3
29	S	2630	LHG	C4-O6-P-O5
29	Y	2630	LHG	O1-C1-C2-C3
29	Y	2630	LHG	C4-O6-P-O5
29	6	2630	LHG	C4-O6-P-O5
29	7	2630	LHG	O1-C1-C2-C3
29	7	2630	LHG	C4-O6-P-O3
29	7	2630	LHG	C4-O6-P-O5
29	8	2630	LHG	O1-C1-C2-O2
29	8	2630	LHG	C3-O3-P-O5
29	8	2630	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
29	b	2630	LHG	C1-C2-C3-O3
29	b	2630	LHG	C3-O3-P-O5
29	b	2630	LHG	C4-O6-P-O3
29	b	2631	LHG	O1-C1-C2-O2
29	b	2631	LHG	O1-C1-C2-C3
29	b	2631	LHG	O2-C2-C3-O3
29	c	2630	LHG	O1-C1-C2-O2
29	c	2630	LHG	O1-C1-C2-C3
29	c	522	LHG	C3-O3-P-O4
29	c	522	LHG	C3-O3-P-O6
29	c	523	LHG	C3-O3-P-O5
29	c	523	LHG	C4-O6-P-O4
29	c	523	LHG	C8-C7-O7-C5
29	d	409	LHG	C4-O6-P-O3
29	d	409	LHG	C4-O6-P-O4
29	d	409	LHG	C4-O6-P-O5
29	d	410	LHG	C4-O6-P-O3
29	g	2630	LHG	C4-O6-P-O3
29	g	2630	LHG	C4-O6-P-O5
29	l	101	LHG	C3-O3-P-O5
29	l	101	LHG	C3-O3-P-O6
29	n	2630	LHG	C3-O3-P-O6
29	n	2630	LHG	C4-O6-P-O5
29	r	2630	LHG	O1-C1-C2-C3
29	s	2630	LHG	O1-C1-C2-C3
29	s	2630	LHG	C4-O6-P-O5
29	y	2630	LHG	O1-C1-C2-C3
29	y	2630	LHG	C4-O6-P-O5
30	4	623	BCR	C11-C12-C13-C14
30	4	623	BCR	C11-C12-C13-C35
30	4	623	BCR	C21-C22-C23-C24
30	4	623	BCR	C37-C22-C23-C24
30	B	620	BCR	C7-C8-C9-C10
30	C	516	BCR	C7-C8-C9-C10
30	C	516	BCR	C7-C8-C9-C34
30	C	516	BCR	C21-C22-C23-C24
30	C	516	BCR	C37-C22-C23-C24
30	C	517	BCR	C7-C8-C9-C10
30	C	517	BCR	C7-C8-C9-C34
30	D	404	BCR	C7-C8-C9-C10
30	H	101	BCR	C7-C8-C9-C10
30	H	101	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
30	T	101	BCR	C1-C6-C7-C8
30	T	101	BCR	C5-C6-C7-C8
30	T	101	BCR	C7-C8-C9-C10
30	T	101	BCR	C7-C8-C9-C34
30	T	101	BCR	C17-C18-C19-C20
30	T	101	BCR	C36-C18-C19-C20
30	T	101	BCR	C21-C22-C23-C24
30	8	623	BCR	C11-C12-C13-C14
30	8	623	BCR	C11-C12-C13-C35
30	8	623	BCR	C21-C22-C23-C24
30	8	623	BCR	C37-C22-C23-C24
30	b	620	BCR	C7-C8-C9-C10
30	c	516	BCR	C7-C8-C9-C10
30	c	516	BCR	C7-C8-C9-C34
30	c	516	BCR	C21-C22-C23-C24
30	c	516	BCR	C37-C22-C23-C24
30	c	517	BCR	C7-C8-C9-C10
30	c	517	BCR	C7-C8-C9-C34
30	d	404	BCR	C7-C8-C9-C10
30	h	101	BCR	C7-C8-C9-C10
30	h	101	BCR	C7-C8-C9-C34
30	t	101	BCR	C1-C6-C7-C8
30	t	101	BCR	C5-C6-C7-C8
30	t	101	BCR	C7-C8-C9-C10
30	t	101	BCR	C7-C8-C9-C34
30	t	101	BCR	C17-C18-C19-C20
30	t	101	BCR	C36-C18-C19-C20
30	t	101	BCR	C21-C22-C23-C24
34	A	412	SQD	O49-C7-O47-C45
34	A	412	SQD	C8-C7-O47-C45
34	A	412	SQD	O5-C5-C6-S
34	A	418	SQD	C2-C1-O6-C44
34	A	418	SQD	O5-C5-C6-S
34	B	621	SQD	C2-C1-O6-C44
34	B	621	SQD	O5-C1-O6-C44
34	B	621	SQD	C46-C45-O47-C7
34	B	621	SQD	C8-C7-O47-C45
34	B	621	SQD	O5-C5-C6-S
34	B	623	SQD	O47-C45-C46-O48
34	B	623	SQD	C8-C7-O47-C45
34	B	623	SQD	C5-C6-S-O7
34	a	412	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
34	a	412	SQD	C8-C7-O47-C45
34	a	412	SQD	O5-C5-C6-S
34	a	418	SQD	C2-C1-O6-C44
34	a	418	SQD	O5-C5-C6-S
34	b	621	SQD	C2-C1-O6-C44
34	b	621	SQD	O5-C1-O6-C44
34	b	621	SQD	C46-C45-O47-C7
34	b	621	SQD	C8-C7-O47-C45
34	b	621	SQD	O5-C5-C6-S
34	b	623	SQD	O47-C45-C46-O48
34	b	623	SQD	C8-C7-O47-C45
34	b	623	SQD	C5-C6-S-O7
35	B	2633	LMG	O9-C10-O7-C8
35	C	521	LMG	C2-C1-O1-C7
35	Z	101	LMG	O10-C28-O8-C9
35	b	2633	LMG	O9-C10-O7-C8
35	c	521	LMG	C2-C1-O1-C7
35	z	101	LMG	O10-C28-O8-C9
37	B	626	DGD	O1A-C1A-O1G-C1G
37	B	626	DGD	C2B-C1B-O2G-C2G
37	C	519	DGD	O1G-C1G-C2G-O2G
37	b	626	DGD	O1A-C1A-O1G-C1G
37	b	626	DGD	C2B-C1B-O2G-C2G
37	c	519	DGD	O1G-C1G-C2G-O2G
39	F	101	HEM	C3D-CAD-CBD-CGD
39	f	101	HEM	C3D-CAD-CBD-CGD
25	2	612	CLA	O1D-CGD-O2D-CED
25	4	604	CLA	O1D-CGD-O2D-CED
25	6	612	CLA	O1D-CGD-O2D-CED
25	8	604	CLA	O1D-CGD-O2D-CED
24	1	608	CHL	O1D-CGD-O2D-CED
24	5	608	CHL	O1D-CGD-O2D-CED
25	2	613	CLA	O1D-CGD-O2D-CED
25	4	611	CLA	O1D-CGD-O2D-CED
25	G	613	CLA	O1D-CGD-O2D-CED
25	R	612	CLA	O1D-CGD-O2D-CED
25	6	613	CLA	O1D-CGD-O2D-CED
25	8	611	CLA	O1D-CGD-O2D-CED
25	g	613	CLA	O1D-CGD-O2D-CED
25	r	612	CLA	O1D-CGD-O2D-CED
29	4	2630	LHG	C24-C23-O8-C6
29	8	2630	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
24	1	608	CHL	CBD-CGD-O2D-CED
24	2	606	CHL	CBD-CGD-O2D-CED
24	2	608	CHL	CBD-CGD-O2D-CED
24	3	607	CHL	CBD-CGD-O2D-CED
24	3	608	CHL	CBD-CGD-O2D-CED
24	4	606	CHL	CBD-CGD-O2D-CED
24	G	606	CHL	CBD-CGD-O2D-CED
24	G	609	CHL	CBD-CGD-O2D-CED
24	N	605	CHL	CBD-CGD-O2D-CED
24	S	608	CHL	CBD-CGD-O2D-CED
24	5	608	CHL	CBD-CGD-O2D-CED
24	6	606	CHL	CBD-CGD-O2D-CED
24	6	608	CHL	CBD-CGD-O2D-CED
24	7	607	CHL	CBD-CGD-O2D-CED
24	7	608	CHL	CBD-CGD-O2D-CED
24	8	606	CHL	CBD-CGD-O2D-CED
24	g	606	CHL	CBD-CGD-O2D-CED
24	g	609	CHL	CBD-CGD-O2D-CED
24	n	605	CHL	CBD-CGD-O2D-CED
24	s	608	CHL	CBD-CGD-O2D-CED
25	2	602	CLA	CBD-CGD-O2D-CED
25	2	612	CLA	CBD-CGD-O2D-CED
25	2	614	CLA	CBD-CGD-O2D-CED
25	3	603	CLA	CBD-CGD-O2D-CED
25	3	612	CLA	CBD-CGD-O2D-CED
25	3	613	CLA	CBD-CGD-O2D-CED
25	4	604	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	CBD-CGD-O2D-CED
25	B	615	CLA	CBD-CGD-O2D-CED
25	C	503	CLA	CBD-CGD-O2D-CED
25	C	508	CLA	CBD-CGD-O2D-CED
25	D	403	CLA	CBD-CGD-O2D-CED
25	G	612	CLA	CBD-CGD-O2D-CED
25	G	613	CLA	CBD-CGD-O2D-CED
25	S	602	CLA	CBD-CGD-O2D-CED
25	Y	604	CLA	CBD-CGD-O2D-CED
25	6	602	CLA	CBD-CGD-O2D-CED
25	6	612	CLA	CBD-CGD-O2D-CED
25	6	614	CLA	CBD-CGD-O2D-CED
25	7	603	CLA	CBD-CGD-O2D-CED
25	7	612	CLA	CBD-CGD-O2D-CED
25	7	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	8	604	CLA	CBD-CGD-O2D-CED
25	b	606	CLA	CBD-CGD-O2D-CED
25	b	615	CLA	CBD-CGD-O2D-CED
25	c	503	CLA	CBD-CGD-O2D-CED
25	c	508	CLA	CBD-CGD-O2D-CED
25	d	403	CLA	CBD-CGD-O2D-CED
25	g	612	CLA	CBD-CGD-O2D-CED
25	g	613	CLA	CBD-CGD-O2D-CED
25	s	602	CLA	CBD-CGD-O2D-CED
25	y	604	CLA	CBD-CGD-O2D-CED
25	N	611	CLA	O1A-CGA-O2A-C1
25	R	611	CLA	O1A-CGA-O2A-C1
25	Y	611	CLA	O1A-CGA-O2A-C1
25	n	611	CLA	O1A-CGA-O2A-C1
25	r	611	CLA	O1A-CGA-O2A-C1
25	y	611	CLA	O1A-CGA-O2A-C1
25	R	601	CLA	C2C-C3C-CAC-CBC
25	r	601	CLA	C2C-C3C-CAC-CBC
25	R	601	CLA	O1D-CGD-O2D-CED
25	r	601	CLA	O1D-CGD-O2D-CED
24	Y	608	CHL	C3-C5-C6-C7
24	y	608	CHL	C3-C5-C6-C7
24	3	608	CHL	O1D-CGD-O2D-CED
24	4	606	CHL	O1D-CGD-O2D-CED
24	G	606	CHL	O1D-CGD-O2D-CED
24	S	608	CHL	O1D-CGD-O2D-CED
24	7	608	CHL	O1D-CGD-O2D-CED
24	8	606	CHL	O1D-CGD-O2D-CED
24	g	606	CHL	O1D-CGD-O2D-CED
24	s	608	CHL	O1D-CGD-O2D-CED
25	3	613	CLA	O1D-CGD-O2D-CED
25	C	503	CLA	O1D-CGD-O2D-CED
25	7	613	CLA	O1D-CGD-O2D-CED
25	c	503	CLA	O1D-CGD-O2D-CED
25	3	603	CLA	CBA-CGA-O2A-C1
25	Y	611	CLA	CBA-CGA-O2A-C1
25	7	603	CLA	CBA-CGA-O2A-C1
25	y	611	CLA	CBA-CGA-O2A-C1
35	Z	101	LMG	C29-C28-O8-C9
35	z	101	LMG	C29-C28-O8-C9
37	B	626	DGD	C2A-C1A-O1G-C1G
37	b	626	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
25	B	617	CLA	O1A-CGA-O2A-C1
25	C	510	CLA	O1A-CGA-O2A-C1
25	b	617	CLA	O1A-CGA-O2A-C1
25	c	510	CLA	O1A-CGA-O2A-C1
29	S	2630	LHG	O10-C23-O8-C6
29	s	2630	LHG	O10-C23-O8-C6
33	A	408	PHO	O1A-CGA-O2A-C1
33	a	408	PHO	O1A-CGA-O2A-C1
24	1	606	CHL	O1D-CGD-O2D-CED
24	G	608	CHL	O1D-CGD-O2D-CED
24	5	606	CHL	O1D-CGD-O2D-CED
24	g	608	CHL	O1D-CGD-O2D-CED
25	1	613	CLA	O1D-CGD-O2D-CED
25	2	603	CLA	O1D-CGD-O2D-CED
25	4	602	CLA	O1D-CGD-O2D-CED
25	N	612	CLA	O1D-CGD-O2D-CED
25	S	612	CLA	O1D-CGD-O2D-CED
25	5	613	CLA	O1D-CGD-O2D-CED
25	6	603	CLA	O1D-CGD-O2D-CED
25	8	602	CLA	O1D-CGD-O2D-CED
25	n	612	CLA	O1D-CGD-O2D-CED
25	s	612	CLA	O1D-CGD-O2D-CED
24	4	608	CHL	O1D-CGD-O2D-CED
24	N	605	CHL	O1D-CGD-O2D-CED
24	R	608	CHL	O1D-CGD-O2D-CED
24	Y	608	CHL	O1D-CGD-O2D-CED
24	8	608	CHL	O1D-CGD-O2D-CED
24	n	605	CHL	O1D-CGD-O2D-CED
24	r	608	CHL	O1D-CGD-O2D-CED
24	y	608	CHL	O1D-CGD-O2D-CED
25	1	614	CLA	O1D-CGD-O2D-CED
25	2	604	CLA	O1D-CGD-O2D-CED
25	3	614	CLA	O1D-CGD-O2D-CED
25	B	608	CLA	O1D-CGD-O2D-CED
25	5	614	CLA	O1D-CGD-O2D-CED
25	6	604	CLA	O1D-CGD-O2D-CED
25	7	614	CLA	O1D-CGD-O2D-CED
25	b	608	CLA	O1D-CGD-O2D-CED
25	S	603	CLA	CBD-CGD-O2D-CED
25	7	604	CLA	CBD-CGD-O2D-CED
25	s	603	CLA	CBD-CGD-O2D-CED
25	S	611	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	s	611	CLA	O1A-CGA-O2A-C1
29	C	523	LHG	O9-C7-O7-C5
29	c	523	LHG	O9-C7-O7-C5
34	A	418	SQD	O49-C7-O47-C45
34	B	621	SQD	O49-C7-O47-C45
34	B	623	SQD	O49-C7-O47-C45
34	a	418	SQD	O49-C7-O47-C45
34	b	621	SQD	O49-C7-O47-C45
34	b	623	SQD	O49-C7-O47-C45
24	1	607	CHL	C3-C5-C6-C7
24	1	609	CHL	C3-C5-C6-C7
24	2	607	CHL	C3-C5-C6-C7
24	3	601	CHL	C3-C5-C6-C7
24	Y	607	CHL	C3-C5-C6-C7
24	5	607	CHL	C3-C5-C6-C7
24	5	609	CHL	C3-C5-C6-C7
24	6	607	CHL	C3-C5-C6-C7
24	7	601	CHL	C3-C5-C6-C7
24	y	607	CHL	C3-C5-C6-C7
25	1	603	CLA	C3-C5-C6-C7
25	B	608	CLA	C3-C5-C6-C7
25	B	615	CLA	C3-C5-C6-C7
25	B	617	CLA	C3-C5-C6-C7
25	C	513	CLA	C3-C5-C6-C7
25	R	603	CLA	C3-C5-C6-C7
25	R	613	CLA	C3-C5-C6-C7
25	S	611	CLA	C3-C5-C6-C7
25	S	613	CLA	C3-C5-C6-C7
25	Y	613	CLA	C3-C5-C6-C7
25	5	603	CLA	C3-C5-C6-C7
25	b	608	CLA	C3-C5-C6-C7
25	b	615	CLA	C3-C5-C6-C7
25	b	617	CLA	C3-C5-C6-C7
25	c	513	CLA	C3-C5-C6-C7
25	r	603	CLA	C3-C5-C6-C7
25	r	613	CLA	C3-C5-C6-C7
25	s	611	CLA	C3-C5-C6-C7
25	s	613	CLA	C3-C5-C6-C7
25	y	613	CLA	C3-C5-C6-C7
24	G	605	CHL	O1D-CGD-O2D-CED
24	g	605	CHL	O1D-CGD-O2D-CED
25	N	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	N	611	CLA	CBA-CGA-O2A-C1
25	n	603	CLA	CBA-CGA-O2A-C1
25	n	611	CLA	CBA-CGA-O2A-C1
33	A	408	PHO	CBA-CGA-O2A-C1
33	a	408	PHO	CBA-CGA-O2A-C1
24	2	601	CHL	CBD-CGD-O2D-CED
24	2	605	CHL	CBD-CGD-O2D-CED
24	2	609	CHL	CBD-CGD-O2D-CED
24	3	605	CHL	CBD-CGD-O2D-CED
24	R	607	CHL	CBD-CGD-O2D-CED
24	S	601	CHL	CBD-CGD-O2D-CED
24	S	606	CHL	CBD-CGD-O2D-CED
24	6	601	CHL	CBD-CGD-O2D-CED
24	6	605	CHL	CBD-CGD-O2D-CED
24	6	609	CHL	CBD-CGD-O2D-CED
24	7	605	CHL	CBD-CGD-O2D-CED
24	r	607	CHL	CBD-CGD-O2D-CED
24	s	601	CHL	CBD-CGD-O2D-CED
24	s	606	CHL	CBD-CGD-O2D-CED
25	1	604	CLA	CBD-CGD-O2D-CED
25	3	604	CLA	CBD-CGD-O2D-CED
25	4	612	CLA	CBD-CGD-O2D-CED
25	C	506	CLA	CBD-CGD-O2D-CED
25	C	510	CLA	CBD-CGD-O2D-CED
25	C	511	CLA	CBD-CGD-O2D-CED
25	N	613	CLA	CBD-CGD-O2D-CED
25	R	602	CLA	CBD-CGD-O2D-CED
25	R	603	CLA	CBD-CGD-O2D-CED
25	R	611	CLA	CBD-CGD-O2D-CED
25	5	604	CLA	CBD-CGD-O2D-CED
25	8	612	CLA	CBD-CGD-O2D-CED
25	c	506	CLA	CBD-CGD-O2D-CED
25	c	510	CLA	CBD-CGD-O2D-CED
25	c	511	CLA	CBD-CGD-O2D-CED
25	n	613	CLA	CBD-CGD-O2D-CED
25	r	602	CLA	CBD-CGD-O2D-CED
25	r	603	CLA	CBD-CGD-O2D-CED
25	r	611	CLA	CBD-CGD-O2D-CED
35	B	2633	LMG	C11-C10-O7-C8
35	b	2633	LMG	C11-C10-O7-C8
24	2	606	CHL	O1D-CGD-O2D-CED
24	N	608	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	R	614	CHL	O1D-CGD-O2D-CED
24	6	606	CHL	O1D-CGD-O2D-CED
24	n	608	CHL	O1D-CGD-O2D-CED
24	r	614	CHL	O1D-CGD-O2D-CED
25	1	603	CLA	O1D-CGD-O2D-CED
25	2	602	CLA	O1D-CGD-O2D-CED
25	3	612	CLA	O1D-CGD-O2D-CED
25	G	612	CLA	O1D-CGD-O2D-CED
25	N	614	CLA	O1D-CGD-O2D-CED
25	5	603	CLA	O1D-CGD-O2D-CED
25	6	602	CLA	O1D-CGD-O2D-CED
25	7	612	CLA	O1D-CGD-O2D-CED
25	g	612	CLA	O1D-CGD-O2D-CED
25	n	614	CLA	O1D-CGD-O2D-CED
24	G	601	CHL	C4-C3-C5-C6
24	g	601	CHL	C4-C3-C5-C6
25	G	610	CLA	C4-C3-C5-C6
25	G	611	CLA	C4-C3-C5-C6
25	S	610	CLA	C4-C3-C5-C6
25	g	610	CLA	C4-C3-C5-C6
25	g	611	CLA	C4-C3-C5-C6
25	s	610	CLA	C4-C3-C5-C6
25	S	610	CLA	C2-C3-C5-C6
25	s	610	CLA	C2-C3-C5-C6
25	Y	612	CLA	CBD-CGD-O2D-CED
25	y	612	CLA	CBD-CGD-O2D-CED
24	N	601	CHL	C2A-CAA-CBA-CGA
24	n	601	CHL	C2A-CAA-CBA-CGA
25	B	607	CLA	C2A-CAA-CBA-CGA
25	C	507	CLA	C2A-CAA-CBA-CGA
25	R	604	CLA	C2A-CAA-CBA-CGA
25	b	607	CLA	C2A-CAA-CBA-CGA
25	c	507	CLA	C2A-CAA-CBA-CGA
25	r	604	CLA	C2A-CAA-CBA-CGA
24	G	607	CHL	C3-C5-C6-C7
24	N	607	CHL	C3-C5-C6-C7
24	R	606	CHL	C3-C5-C6-C7
24	g	607	CHL	C3-C5-C6-C7
24	n	607	CHL	C3-C5-C6-C7
24	r	606	CHL	C3-C5-C6-C7
25	1	613	CLA	C3-C5-C6-C7
25	C	512	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	N	613	CLA	C3-C5-C6-C7
25	5	613	CLA	C3-C5-C6-C7
25	c	512	CLA	C3-C5-C6-C7
25	n	613	CLA	C3-C5-C6-C7
33	A	408	PHO	C3-C5-C6-C7
33	a	408	PHO	C3-C5-C6-C7
24	G	601	CHL	CBA-CGA-O2A-C1
24	S	607	CHL	CBA-CGA-O2A-C1
24	g	601	CHL	CBA-CGA-O2A-C1
24	s	607	CHL	CBA-CGA-O2A-C1
25	B	617	CLA	CBA-CGA-O2A-C1
25	C	510	CLA	CBA-CGA-O2A-C1
25	G	603	CLA	CBA-CGA-O2A-C1
25	S	611	CLA	CBA-CGA-O2A-C1
25	Y	612	CLA	CBA-CGA-O2A-C1
25	b	617	CLA	CBA-CGA-O2A-C1
25	c	510	CLA	CBA-CGA-O2A-C1
25	g	603	CLA	CBA-CGA-O2A-C1
25	s	611	CLA	CBA-CGA-O2A-C1
25	y	612	CLA	CBA-CGA-O2A-C1
29	B	2631	LHG	C24-C23-O8-C6
29	S	2630	LHG	C24-C23-O8-C6
29	b	2631	LHG	C24-C23-O8-C6
29	s	2630	LHG	C24-C23-O8-C6
37	C	520	DGD	C2A-C1A-O1G-C1G
37	c	520	DGD	C2A-C1A-O1G-C1G
29	4	2630	LHG	O10-C23-O8-C6
29	8	2630	LHG	O10-C23-O8-C6
36	D	405	PL9	C7-C8-C9-C10
36	d	405	PL9	C7-C8-C9-C10
30	4	623	BCR	C19-C20-C21-C22
30	8	623	BCR	C19-C20-C21-C22
24	Y	601	CHL	O1A-CGA-O2A-C1
24	y	601	CHL	O1A-CGA-O2A-C1
25	2	603	CLA	O1A-CGA-O2A-C1
25	G	603	CLA	O1A-CGA-O2A-C1
25	6	603	CLA	O1A-CGA-O2A-C1
25	g	603	CLA	O1A-CGA-O2A-C1
29	B	2631	LHG	O10-C23-O8-C6
29	b	2631	LHG	O10-C23-O8-C6
25	B	606	CLA	O1D-CGD-O2D-CED
25	D	403	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	b	606	CLA	O1D-CGD-O2D-CED
25	d	403	CLA	O1D-CGD-O2D-CED
25	2	602	CLA	C3-C5-C6-C7
25	2	603	CLA	C3-C5-C6-C7
25	B	614	CLA	C3-C5-C6-C7
25	C	510	CLA	C3-C5-C6-C7
25	6	602	CLA	C3-C5-C6-C7
25	6	603	CLA	C3-C5-C6-C7
25	b	614	CLA	C3-C5-C6-C7
25	c	510	CLA	C3-C5-C6-C7
24	g	601	CHL	CBD-CGD-O2D-CED
25	B	612	CLA	CBD-CGD-O2D-CED
25	C	502	CLA	CBD-CGD-O2D-CED
25	Y	614	CLA	CBD-CGD-O2D-CED
25	b	612	CLA	CBD-CGD-O2D-CED
25	c	502	CLA	CBD-CGD-O2D-CED
25	y	614	CLA	CBD-CGD-O2D-CED
29	2	2630	LHG	O2-C2-C3-O3
29	B	2630	LHG	O2-C2-C3-O3
29	D	410	LHG	O2-C2-C3-O3
29	6	2630	LHG	O2-C2-C3-O3
29	b	2630	LHG	O2-C2-C3-O3
29	d	410	LHG	O2-C2-C3-O3
24	2	608	CHL	O1D-CGD-O2D-CED
24	6	608	CHL	O1D-CGD-O2D-CED
25	2	614	CLA	O1D-CGD-O2D-CED
25	6	614	CLA	O1D-CGD-O2D-CED
24	Y	601	CHL	CBA-CGA-O2A-C1
24	y	601	CHL	CBA-CGA-O2A-C1
25	S	604	CLA	CBA-CGA-O2A-C1
25	s	604	CLA	CBA-CGA-O2A-C1
37	C	520	DGD	O6E-C5E-C6E-O5E
37	c	520	DGD	O6E-C5E-C6E-O5E
24	G	601	CHL	O1A-CGA-O2A-C1
24	g	601	CHL	O1A-CGA-O2A-C1
25	N	603	CLA	O1A-CGA-O2A-C1
25	n	603	CLA	O1A-CGA-O2A-C1
37	B	626	DGD	C4E-C5E-C6E-O5E
37	b	626	DGD	C4E-C5E-C6E-O5E
24	G	609	CHL	O1D-CGD-O2D-CED
25	3	603	CLA	O1D-CGD-O2D-CED
25	7	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
37	C	520	DGD	C4E-C5E-C6E-O5E
37	c	520	DGD	C4E-C5E-C6E-O5E
24	G	601	CHL	CBD-CGD-O2D-CED
24	g	609	CHL	O1D-CGD-O2D-CED
37	C	520	DGD	O1A-C1A-O1G-C1G
37	c	520	DGD	O1A-C1A-O1G-C1G
25	B	615	CLA	O1D-CGD-O2D-CED
25	C	508	CLA	O1D-CGD-O2D-CED
25	c	508	CLA	O1D-CGD-O2D-CED
24	R	608	CHL	C3-C5-C6-C7
24	r	608	CHL	C3-C5-C6-C7
25	R	609	CLA	CBD-CGD-O2D-CED
25	r	609	CLA	CBD-CGD-O2D-CED
24	3	607	CHL	O1D-CGD-O2D-CED
24	7	607	CHL	O1D-CGD-O2D-CED
25	b	615	CLA	O1D-CGD-O2D-CED
25	2	603	CLA	CBA-CGA-O2A-C1
25	6	603	CLA	CBA-CGA-O2A-C1
25	B	614	CLA	C4-C3-C5-C6
25	Y	602	CLA	C4-C3-C5-C6
25	b	614	CLA	C4-C3-C5-C6
25	y	602	CLA	C4-C3-C5-C6
33	A	409	PHO	C4-C3-C5-C6
33	a	409	PHO	C4-C3-C5-C6
24	Y	601	CHL	C2-C3-C5-C6
24	y	601	CHL	C2-C3-C5-C6
25	B	614	CLA	C2-C3-C5-C6
25	G	611	CLA	C2-C3-C5-C6
25	b	614	CLA	C2-C3-C5-C6
25	g	611	CLA	C2-C3-C5-C6
33	A	409	PHO	C2-C3-C5-C6
33	a	409	PHO	C2-C3-C5-C6
24	S	607	CHL	O1A-CGA-O2A-C1
24	s	607	CHL	O1A-CGA-O2A-C1
25	R	601	CLA	C4C-C3C-CAC-CBC
25	r	601	CLA	C4C-C3C-CAC-CBC
37	C	520	DGD	O1B-C1B-O2G-C2G
37	c	520	DGD	O1B-C1B-O2G-C2G
25	Y	603	CLA	CBD-CGD-O2D-CED
25	y	603	CLA	CBD-CGD-O2D-CED
25	y	604	CLA	O1D-CGD-O2D-CED
24	R	608	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	r	608	CHL	C2A-CAA-CBA-CGA
25	1	611	CLA	C2A-CAA-CBA-CGA
25	B	602	CLA	C2A-CAA-CBA-CGA
25	5	611	CLA	C2A-CAA-CBA-CGA
25	b	602	CLA	C2A-CAA-CBA-CGA
25	Y	604	CLA	O1D-CGD-O2D-CED
25	S	604	CLA	O1A-CGA-O2A-C1
25	Y	612	CLA	O1A-CGA-O2A-C1
25	s	604	CLA	O1A-CGA-O2A-C1
25	y	612	CLA	O1A-CGA-O2A-C1
24	N	608	CHL	C3-C5-C6-C7
24	n	608	CHL	C3-C5-C6-C7
34	A	418	SQD	O5-C1-O6-C44
34	a	418	SQD	O5-C1-O6-C44
35	A	413	LMG	O6-C1-O1-C7
35	C	521	LMG	O6-C1-O1-C7
35	a	413	LMG	O6-C1-O1-C7
35	c	521	LMG	O6-C1-O1-C7
37	B	626	DGD	O6D-C1D-O3G-C3G
37	b	626	DGD	O6D-C1D-O3G-C3G
37	H	102	DGD	O6E-C5E-C6E-O5E
37	h	102	DGD	O6E-C5E-C6E-O5E
24	R	608	CHL	CBA-CGA-O2A-C1
24	r	608	CHL	CBA-CGA-O2A-C1
25	N	614	CLA	CBA-CGA-O2A-C1
25	R	612	CLA	CBA-CGA-O2A-C1
25	n	614	CLA	CBA-CGA-O2A-C1
25	r	612	CLA	CBA-CGA-O2A-C1
34	B	623	SQD	C24-C23-O48-C46
34	b	623	SQD	C24-C23-O48-C46
24	1	605	CHL	CBD-CGD-O2D-CED
24	3	601	CHL	CBD-CGD-O2D-CED
24	4	607	CHL	CBD-CGD-O2D-CED
24	N	601	CHL	CBD-CGD-O2D-CED
24	R	606	CHL	CBD-CGD-O2D-CED
24	Y	609	CHL	CBD-CGD-O2D-CED
24	5	605	CHL	CBD-CGD-O2D-CED
24	7	601	CHL	CBD-CGD-O2D-CED
24	8	607	CHL	CBD-CGD-O2D-CED
24	n	601	CHL	CBD-CGD-O2D-CED
24	r	606	CHL	CBD-CGD-O2D-CED
24	y	609	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	611	CLA	CBD-CGD-O2D-CED
25	C	507	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	CBD-CGD-O2D-CED
25	C	513	CLA	CBD-CGD-O2D-CED
25	N	602	CLA	CBD-CGD-O2D-CED
25	S	609	CLA	CBD-CGD-O2D-CED
25	b	611	CLA	CBD-CGD-O2D-CED
25	c	507	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	CBD-CGD-O2D-CED
25	n	602	CLA	CBD-CGD-O2D-CED
25	s	609	CLA	CBD-CGD-O2D-CED
35	D	411	LMG	O6-C5-C6-O5
35	d	411	LMG	O6-C5-C6-O5
37	B	626	DGD	O6E-C5E-C6E-O5E
37	b	626	DGD	O6E-C5E-C6E-O5E
24	R	607	CHL	O1D-CGD-O2D-CED
24	r	607	CHL	O1D-CGD-O2D-CED
25	S	602	CLA	O1D-CGD-O2D-CED
25	s	602	CLA	O1D-CGD-O2D-CED
24	N	609	CHL	CBD-CGD-O2D-CED
24	n	609	CHL	CBD-CGD-O2D-CED
24	R	608	CHL	O1A-CGA-O2A-C1
24	r	608	CHL	O1A-CGA-O2A-C1
29	B	2630	LHG	O9-C7-O7-C5
29	C	2630	LHG	O9-C7-O7-C5
29	b	2630	LHG	O9-C7-O7-C5
29	c	2630	LHG	O9-C7-O7-C5
29	2	2630	LHG	C1-C2-C3-O3
29	N	2630	LHG	C1-C2-C3-O3
29	6	2630	LHG	C1-C2-C3-O3
29	n	2630	LHG	C1-C2-C3-O3
25	S	603	CLA	O1D-CGD-O2D-CED
25	s	603	CLA	O1D-CGD-O2D-CED
25	D	403	CLA	CBA-CGA-O2A-C1
25	R	601	CLA	CBA-CGA-O2A-C1
25	d	403	CLA	CBA-CGA-O2A-C1
25	r	601	CLA	CBA-CGA-O2A-C1
34	B	621	SQD	C24-C23-O48-C46
34	b	621	SQD	C24-C23-O48-C46
35	B	622	LMG	C29-C28-O8-C9
35	b	622	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
37	C	519	DGD	C2A-C1A-O1G-C1G
37	c	519	DGD	C2A-C1A-O1G-C1G
25	C	501	CLA	CBD-CGD-O2D-CED
25	G	604	CLA	CBD-CGD-O2D-CED
25	c	501	CLA	CBD-CGD-O2D-CED
25	g	604	CLA	CBD-CGD-O2D-CED
35	D	411	LMG	C4-C5-C6-O5
35	d	411	LMG	C4-C5-C6-O5
25	3	604	CLA	O1D-CGD-O2D-CED
25	4	612	CLA	O1D-CGD-O2D-CED
25	7	604	CLA	O1D-CGD-O2D-CED
25	8	612	CLA	O1D-CGD-O2D-CED
24	Y	601	CHL	C4-C3-C5-C6
24	y	601	CHL	C4-C3-C5-C6
24	G	601	CHL	C2-C3-C5-C6
24	g	601	CHL	C2-C3-C5-C6
25	G	610	CLA	C2-C3-C5-C6
25	Y	602	CLA	C2-C3-C5-C6
25	g	610	CLA	C2-C3-C5-C6
25	y	602	CLA	C2-C3-C5-C6
25	R	602	CLA	C3-C5-C6-C7
25	r	602	CLA	C3-C5-C6-C7
25	A	407	CLA	CBD-CGD-O2D-CED
25	a	407	CLA	CBD-CGD-O2D-CED
24	G	608	CHL	C14-C13-C15-C16
24	N	601	CHL	C11-C10-C8-C9
24	N	608	CHL	C14-C13-C15-C16
24	R	606	CHL	C11-C10-C8-C9
24	Y	608	CHL	C14-C13-C15-C16
24	Y	609	CHL	C14-C13-C15-C16
24	g	608	CHL	C14-C13-C15-C16
24	n	601	CHL	C11-C10-C8-C9
24	n	608	CHL	C14-C13-C15-C16
24	r	606	CHL	C11-C10-C8-C9
24	y	608	CHL	C14-C13-C15-C16
24	y	609	CHL	C14-C13-C15-C16
25	B	602	CLA	C14-C13-C15-C16
25	B	606	CLA	C6-C7-C8-C9
25	C	506	CLA	C11-C12-C13-C14
25	C	509	CLA	C6-C7-C8-C9
25	N	612	CLA	C6-C7-C8-C9
25	R	610	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	Y	611	CLA	C6-C7-C8-C9
25	b	602	CLA	C14-C13-C15-C16
25	b	606	CLA	C6-C7-C8-C9
25	c	506	CLA	C11-C12-C13-C14
25	c	509	CLA	C6-C7-C8-C9
25	n	612	CLA	C6-C7-C8-C9
25	r	610	CLA	C11-C12-C13-C14
25	y	611	CLA	C6-C7-C8-C9
33	A	409	PHO	C6-C7-C8-C9
33	a	409	PHO	C6-C7-C8-C9
35	Z	101	LMG	O6-C5-C6-O5
35	z	101	LMG	O6-C5-C6-O5
37	H	102	DGD	C4E-C5E-C6E-O5E
37	h	102	DGD	C4E-C5E-C6E-O5E
24	2	605	CHL	O1D-CGD-O2D-CED
24	3	605	CHL	O1D-CGD-O2D-CED
24	6	605	CHL	O1D-CGD-O2D-CED
24	7	605	CHL	O1D-CGD-O2D-CED
35	A	413	LMG	C2-C1-O1-C7
35	a	413	LMG	C2-C1-O1-C7
37	B	626	DGD	C2D-C1D-O3G-C3G
37	b	626	DGD	C2D-C1D-O3G-C3G
29	D	408	LHG	C23-C24-C25-C26
29	d	408	LHG	C23-C24-C25-C26
25	N	613	CLA	O1D-CGD-O2D-CED
25	n	613	CLA	O1D-CGD-O2D-CED
24	2	601	CHL	O1D-CGD-O2D-CED
24	6	601	CHL	O1D-CGD-O2D-CED
27	2	1622	XAT	C31-C32-C33-C40
27	G	1622	XAT	C11-C12-C13-C20
27	Y	1622	XAT	C11-C12-C13-C20
27	6	1622	XAT	C31-C32-C33-C40
27	g	1622	XAT	C11-C12-C13-C20
27	y	1622	XAT	C11-C12-C13-C20
28	N	1623	NEX	C31-C32-C33-C40
28	n	1623	NEX	C31-C32-C33-C40
30	B	619	BCR	C7-C8-C9-C34
30	B	620	BCR	C7-C8-C9-C34
30	D	404	BCR	C7-C8-C9-C34
30	T	101	BCR	C11-C12-C13-C35
30	T	101	BCR	C37-C22-C23-C24
30	b	619	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
30	b	620	BCR	C7-C8-C9-C34
30	d	404	BCR	C7-C8-C9-C34
30	t	101	BCR	C11-C12-C13-C35
30	t	101	BCR	C37-C22-C23-C24
30	4	623	BCR	C7-C8-C9-C10
30	T	101	BCR	C11-C12-C13-C14
30	8	623	BCR	C7-C8-C9-C10
30	t	101	BCR	C11-C12-C13-C14
25	B	611	CLA	C2A-CAA-CBA-CGA
25	b	611	CLA	C2A-CAA-CBA-CGA
37	H	102	DGD	C1A-C2A-C3A-C4A
37	h	102	DGD	C1A-C2A-C3A-C4A
25	R	601	CLA	O1A-CGA-O2A-C1
25	r	601	CLA	O1A-CGA-O2A-C1
25	A	410	CLA	C3-C5-C6-C7
25	a	410	CLA	C3-C5-C6-C7
37	H	102	DGD	C4D-C5D-C6D-O5D
37	h	102	DGD	C4D-C5D-C6D-O5D
37	C	520	DGD	O1G-C1G-C2G-O2G
37	c	520	DGD	O1G-C1G-C2G-O2G
25	C	511	CLA	O1D-CGD-O2D-CED
25	c	511	CLA	O1D-CGD-O2D-CED
24	N	601	CHL	CBA-CGA-O2A-C1
24	n	601	CHL	CBA-CGA-O2A-C1
25	B	602	CLA	CBA-CGA-O2A-C1
25	B	613	CLA	CBA-CGA-O2A-C1
25	G	614	CLA	CBA-CGA-O2A-C1
25	b	602	CLA	CBA-CGA-O2A-C1
25	b	613	CLA	CBA-CGA-O2A-C1
25	g	614	CLA	CBA-CGA-O2A-C1
29	R	2630	LHG	C24-C23-O8-C6
29	r	2630	LHG	C24-C23-O8-C6
25	N	612	CLA	C5-C6-C7-C8
25	n	612	CLA	C5-C6-C7-C8
24	S	601	CHL	O1D-CGD-O2D-CED
24	S	606	CHL	O1D-CGD-O2D-CED
24	s	601	CHL	O1D-CGD-O2D-CED
24	s	606	CHL	O1D-CGD-O2D-CED
25	C	506	CLA	O1D-CGD-O2D-CED
25	R	603	CLA	O1D-CGD-O2D-CED
25	c	506	CLA	O1D-CGD-O2D-CED
25	r	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	N	609	CHL	C15-C16-C17-C18
24	n	609	CHL	C15-C16-C17-C18
25	B	603	CLA	C5-C6-C7-C8
25	B	607	CLA	C13-C15-C16-C17
25	B	608	CLA	C13-C15-C16-C17
25	N	602	CLA	C10-C11-C12-C13
25	N	610	CLA	C5-C6-C7-C8
25	b	603	CLA	C5-C6-C7-C8
25	b	607	CLA	C13-C15-C16-C17
25	b	608	CLA	C13-C15-C16-C17
25	n	602	CLA	C10-C11-C12-C13
25	n	610	CLA	C5-C6-C7-C8
25	3	613	CLA	C3-C5-C6-C7
25	7	613	CLA	C3-C5-C6-C7
35	Z	101	LMG	C10-C11-C12-C13
35	z	101	LMG	C10-C11-C12-C13
24	3	601	CHL	C5-C6-C7-C8
24	7	601	CHL	C5-C6-C7-C8
25	B	614	CLA	C8-C10-C11-C12
25	B	617	CLA	C5-C6-C7-C8
25	N	612	CLA	C10-C11-C12-C13
25	b	614	CLA	C8-C10-C11-C12
25	b	617	CLA	C5-C6-C7-C8
25	n	612	CLA	C10-C11-C12-C13
25	r	613	CLA	CBD-CGD-O2D-CED
24	Y	601	CHL	C6-C7-C8-C10
24	y	601	CHL	C6-C7-C8-C10
25	B	612	CLA	C12-C13-C15-C16
25	b	612	CLA	C12-C13-C15-C16
25	1	602	CLA	C10-C11-C12-C13
25	B	615	CLA	C15-C16-C17-C18
25	5	602	CLA	C10-C11-C12-C13
25	b	615	CLA	C15-C16-C17-C18
25	y	612	CLA	O1D-CGD-O2D-CED
29	G	2630	LHG	C23-C24-C25-C26
27	3	1622	XAT	C29-C30-C31-C32
27	7	1622	XAT	C29-C30-C31-C32
24	2	609	CHL	O1D-CGD-O2D-CED
24	6	609	CHL	O1D-CGD-O2D-CED
25	R	611	CLA	O1D-CGD-O2D-CED
25	Y	612	CLA	O1D-CGD-O2D-CED
25	c	510	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	r	611	CLA	O1D-CGD-O2D-CED
25	B	608	CLA	C8-C10-C11-C12
25	B	609	CLA	C8-C10-C11-C12
25	b	608	CLA	C8-C10-C11-C12
25	b	609	CLA	C8-C10-C11-C12
25	C	510	CLA	O1D-CGD-O2D-CED
29	g	2630	LHG	C23-C24-C25-C26
35	C	521	LMG	C28-C29-C30-C31
35	c	521	LMG	C28-C29-C30-C31
24	N	601	CHL	O1A-CGA-O2A-C1
24	n	601	CHL	O1A-CGA-O2A-C1
25	D	403	CLA	O1A-CGA-O2A-C1
25	d	403	CLA	O1A-CGA-O2A-C1
24	3	609	CHL	CBD-CGD-O2D-CED
25	R	613	CLA	CBD-CGD-O2D-CED
25	1	604	CLA	O1D-CGD-O2D-CED
25	5	604	CLA	O1D-CGD-O2D-CED
24	2	607	CHL	C10-C11-C12-C13
24	Y	601	CHL	C8-C10-C11-C12
24	6	607	CHL	C10-C11-C12-C13
24	y	601	CHL	C8-C10-C11-C12
25	C	503	CLA	C5-C6-C7-C8
25	c	503	CLA	C5-C6-C7-C8
24	2	605	CHL	C2A-CAA-CBA-CGA
24	3	606	CHL	C2A-CAA-CBA-CGA
24	G	605	CHL	C2A-CAA-CBA-CGA
24	N	607	CHL	C2A-CAA-CBA-CGA
24	S	607	CHL	C2A-CAA-CBA-CGA
24	Y	607	CHL	C2A-CAA-CBA-CGA
24	6	605	CHL	C2A-CAA-CBA-CGA
24	7	606	CHL	C2A-CAA-CBA-CGA
24	g	605	CHL	C2A-CAA-CBA-CGA
24	n	607	CHL	C2A-CAA-CBA-CGA
24	s	607	CHL	C2A-CAA-CBA-CGA
24	y	607	CHL	C2A-CAA-CBA-CGA
25	3	603	CLA	C2A-CAA-CBA-CGA
25	3	604	CLA	C2A-CAA-CBA-CGA
25	3	611	CLA	C2A-CAA-CBA-CGA
25	4	604	CLA	C2A-CAA-CBA-CGA
25	B	605	CLA	C2A-CAA-CBA-CGA
25	N	610	CLA	C2A-CAA-CBA-CGA
25	R	611	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	7	603	CLA	C2A-CAA-CBA-CGA
25	7	604	CLA	C2A-CAA-CBA-CGA
25	7	611	CLA	C2A-CAA-CBA-CGA
25	8	604	CLA	C2A-CAA-CBA-CGA
25	b	605	CLA	C2A-CAA-CBA-CGA
25	n	610	CLA	C2A-CAA-CBA-CGA
25	r	611	CLA	C2A-CAA-CBA-CGA
24	3	601	CHL	C10-C11-C12-C13
24	N	601	CHL	C8-C10-C11-C12
24	R	606	CHL	C8-C10-C11-C12
24	Y	608	CHL	C15-C16-C17-C18
24	7	601	CHL	C10-C11-C12-C13
24	n	601	CHL	C8-C10-C11-C12
24	r	606	CHL	C8-C10-C11-C12
24	y	608	CHL	C15-C16-C17-C18
25	B	604	CLA	C15-C16-C17-C18
25	D	403	CLA	C8-C10-C11-C12
25	N	611	CLA	C5-C6-C7-C8
25	N	611	CLA	C8-C10-C11-C12
25	Y	602	CLA	C10-C11-C12-C13
25	Y	610	CLA	C5-C6-C7-C8
25	b	604	CLA	C15-C16-C17-C18
25	d	403	CLA	C8-C10-C11-C12
25	n	611	CLA	C5-C6-C7-C8
25	n	611	CLA	C8-C10-C11-C12
25	y	602	CLA	C10-C11-C12-C13
25	y	610	CLA	C5-C6-C7-C8
29	1	2630	LHG	C23-C24-C25-C26
29	N	2630	LHG	C23-C24-C25-C26
29	5	2630	LHG	C23-C24-C25-C26
29	n	2630	LHG	C23-C24-C25-C26
34	B	621	SQD	C7-C8-C9-C10
34	b	621	SQD	C7-C8-C9-C10
24	S	607	CHL	C3-C5-C6-C7
25	G	613	CLA	C3-C5-C6-C7
25	g	613	CLA	C3-C5-C6-C7
24	7	609	CHL	CBD-CGD-O2D-CED
25	1	602	CLA	CBD-CGD-O2D-CED
25	2	610	CLA	CBD-CGD-O2D-CED
25	5	602	CLA	CBD-CGD-O2D-CED
25	6	610	CLA	CBD-CGD-O2D-CED
35	B	2633	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
35	b	2633	LMG	O6-C1-O1-C7
37	C	519	DGD	O6E-C1E-O5D-C6D
37	c	519	DGD	O6E-C1E-O5D-C6D
29	B	2630	LHG	C32-C33-C34-C35
29	b	2630	LHG	C32-C33-C34-C35
24	2	607	CHL	C8-C10-C11-C12
24	3	601	CHL	C8-C10-C11-C12
24	3	601	CHL	C13-C15-C16-C17
24	R	608	CHL	C10-C11-C12-C13
24	S	607	CHL	C5-C6-C7-C8
24	Y	601	CHL	C13-C15-C16-C17
24	Y	609	CHL	C13-C15-C16-C17
24	6	607	CHL	C8-C10-C11-C12
24	7	601	CHL	C8-C10-C11-C12
24	7	601	CHL	C13-C15-C16-C17
24	r	608	CHL	C10-C11-C12-C13
24	s	607	CHL	C5-C6-C7-C8
24	y	601	CHL	C13-C15-C16-C17
24	y	609	CHL	C13-C15-C16-C17
25	A	410	CLA	C5-C6-C7-C8
25	A	410	CLA	C8-C10-C11-C12
25	B	614	CLA	C10-C11-C12-C13
25	B	616	CLA	C8-C10-C11-C12
25	C	503	CLA	C15-C16-C17-C18
25	G	603	CLA	C15-C16-C17-C18
25	a	410	CLA	C5-C6-C7-C8
25	a	410	CLA	C8-C10-C11-C12
25	b	614	CLA	C10-C11-C12-C13
25	b	616	CLA	C8-C10-C11-C12
25	c	503	CLA	C15-C16-C17-C18
25	g	603	CLA	C15-C16-C17-C18
29	C	2630	LHG	O2-C2-C3-O3
29	D	408	LHG	O2-C2-C3-O3
29	N	2630	LHG	O2-C2-C3-O3
29	c	2630	LHG	O2-C2-C3-O3
29	d	408	LHG	O2-C2-C3-O3
29	n	2630	LHG	O2-C2-C3-O3
25	R	612	CLA	O1A-CGA-O2A-C1
25	r	612	CLA	O1A-CGA-O2A-C1
25	2	602	CLA	C10-C11-C12-C13
25	C	512	CLA	C8-C10-C11-C12
25	D	402	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	G	603	CLA	C13-C15-C16-C17
25	6	602	CLA	C10-C11-C12-C13
25	c	512	CLA	C8-C10-C11-C12
25	d	402	CLA	C15-C16-C17-C18
25	g	603	CLA	C13-C15-C16-C17
24	s	607	CHL	C3-C5-C6-C7
24	N	601	CHL	C13-C15-C16-C17
24	N	607	CHL	C5-C6-C7-C8
24	Y	601	CHL	C10-C11-C12-C13
24	n	601	CHL	C13-C15-C16-C17
24	n	607	CHL	C5-C6-C7-C8
24	y	601	CHL	C10-C11-C12-C13
25	B	605	CLA	C8-C10-C11-C12
25	B	617	CLA	C13-C15-C16-C17
25	C	508	CLA	C5-C6-C7-C8
25	G	602	CLA	C8-C10-C11-C12
25	G	602	CLA	C10-C11-C12-C13
25	b	605	CLA	C8-C10-C11-C12
25	b	617	CLA	C13-C15-C16-C17
25	c	508	CLA	C5-C6-C7-C8
25	g	602	CLA	C8-C10-C11-C12
25	g	602	CLA	C10-C11-C12-C13
33	a	408	PHO	C13-C15-C16-C17
25	3	602	CLA	CBD-CGD-O2D-CED
25	B	602	CLA	O1A-CGA-O2A-C1
25	b	602	CLA	O1A-CGA-O2A-C1
34	A	418	SQD	C23-C24-C25-C26
34	a	418	SQD	C23-C24-C25-C26
25	C	502	CLA	O1D-CGD-O2D-CED
25	R	602	CLA	O1D-CGD-O2D-CED
25	c	502	CLA	O1D-CGD-O2D-CED
25	r	602	CLA	O1D-CGD-O2D-CED
24	1	607	CHL	C5-C6-C7-C8
24	3	609	CHL	C10-C11-C12-C13
24	G	601	CHL	C10-C11-C12-C13
24	R	606	CHL	C15-C16-C17-C18
24	Y	601	CHL	C5-C6-C7-C8
24	5	607	CHL	C5-C6-C7-C8
24	7	609	CHL	C10-C11-C12-C13
24	g	601	CHL	C10-C11-C12-C13
24	r	606	CHL	C15-C16-C17-C18
24	y	601	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	3	611	CLA	C5-C6-C7-C8
25	B	604	CLA	C5-C6-C7-C8
25	B	608	CLA	C5-C6-C7-C8
25	B	615	CLA	C13-C15-C16-C17
25	C	507	CLA	C15-C16-C17-C18
25	G	610	CLA	C5-C6-C7-C8
25	7	611	CLA	C5-C6-C7-C8
25	b	604	CLA	C5-C6-C7-C8
25	b	615	CLA	C13-C15-C16-C17
25	c	507	CLA	C15-C16-C17-C18
25	g	610	CLA	C5-C6-C7-C8
33	A	408	PHO	C13-C15-C16-C17
24	Y	609	CHL	CBA-CGA-O2A-C1
25	C	501	CLA	CBA-CGA-O2A-C1
25	C	505	CLA	CBA-CGA-O2A-C1
25	c	501	CLA	CBA-CGA-O2A-C1
25	c	505	CLA	CBA-CGA-O2A-C1
29	C	522	LHG	C24-C23-O8-C6
29	c	522	LHG	C24-C23-O8-C6
25	7	602	CLA	CBD-CGD-O2D-CED
34	A	418	SQD	C8-C7-O47-C45
34	a	418	SQD	C8-C7-O47-C45
25	N	614	CLA	O1A-CGA-O2A-C1
25	n	614	CLA	O1A-CGA-O2A-C1
24	G	601	CHL	O1D-CGD-O2D-CED
24	g	601	CHL	O1D-CGD-O2D-CED
25	R	609	CLA	O1D-CGD-O2D-CED
25	r	609	CLA	O1D-CGD-O2D-CED
25	b	608	CLA	C5-C6-C7-C8
25	3	611	CLA	C3-C5-C6-C7
25	7	611	CLA	C3-C5-C6-C7
24	y	607	CHL	C15-C16-C17-C18
25	Y	613	CLA	C8-C10-C11-C12
25	y	613	CLA	C8-C10-C11-C12
29	D	408	LHG	C7-C8-C9-C10
29	d	408	LHG	C7-C8-C9-C10
34	A	418	SQD	C7-C8-C9-C10
34	a	418	SQD	C7-C8-C9-C10
29	S	2630	LHG	O9-C7-O7-C5
29	s	2630	LHG	O9-C7-O7-C5
29	B	2631	LHG	C1-C2-C3-O3
29	C	2630	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
29	D	408	LHG	C1-C2-C3-O3
29	b	2631	LHG	C1-C2-C3-O3
29	c	2630	LHG	C1-C2-C3-O3
29	d	408	LHG	C1-C2-C3-O3
24	1	607	CHL	C2A-CAA-CBA-CGA
24	2	607	CHL	C2A-CAA-CBA-CGA
24	N	606	CHL	C2A-CAA-CBA-CGA
24	5	607	CHL	C2A-CAA-CBA-CGA
24	6	607	CHL	C2A-CAA-CBA-CGA
24	n	606	CHL	C2A-CAA-CBA-CGA
25	2	604	CLA	C2A-CAA-CBA-CGA
25	2	613	CLA	C2A-CAA-CBA-CGA
25	6	604	CLA	C2A-CAA-CBA-CGA
24	y	609	CHL	CBA-CGA-O2A-C1
25	3	611	CLA	CBA-CGA-O2A-C1
25	B	611	CLA	CBA-CGA-O2A-C1
25	S	614	CLA	CBA-CGA-O2A-C1
25	Y	603	CLA	CBA-CGA-O2A-C1
25	7	611	CLA	CBA-CGA-O2A-C1
25	b	611	CLA	CBA-CGA-O2A-C1
25	s	614	CLA	CBA-CGA-O2A-C1
25	y	603	CLA	CBA-CGA-O2A-C1
24	2	609	CHL	C8-C10-C11-C12
24	Y	607	CHL	C15-C16-C17-C18
24	6	609	CHL	C8-C10-C11-C12
25	3	610	CLA	C10-C11-C12-C13
25	B	610	CLA	C15-C16-C17-C18
25	B	611	CLA	C13-C15-C16-C17
25	B	615	CLA	C5-C6-C7-C8
25	C	507	CLA	C13-C15-C16-C17
25	C	510	CLA	C13-C15-C16-C17
25	R	603	CLA	C10-C11-C12-C13
25	7	610	CLA	C10-C11-C12-C13
25	b	610	CLA	C15-C16-C17-C18
25	b	611	CLA	C13-C15-C16-C17
25	b	615	CLA	C5-C6-C7-C8
25	c	507	CLA	C13-C15-C16-C17
25	c	510	CLA	C13-C15-C16-C17
25	r	603	CLA	C10-C11-C12-C13
25	G	614	CLA	O1A-CGA-O2A-C1
25	Y	614	CLA	O1D-CGD-O2D-CED
25	y	614	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	B	2630	LHG	C23-C24-C25-C26
29	b	2630	LHG	C23-C24-C25-C26
24	G	608	CHL	C8-C10-C11-C12
24	N	607	CHL	C15-C16-C17-C18
24	Y	608	CHL	C5-C6-C7-C8
24	g	608	CHL	C8-C10-C11-C12
24	n	607	CHL	C15-C16-C17-C18
24	y	608	CHL	C5-C6-C7-C8
25	B	606	CLA	C15-C16-C17-C18
25	Y	612	CLA	C10-C11-C12-C13
25	b	606	CLA	C15-C16-C17-C18
25	y	612	CLA	C10-C11-C12-C13
24	3	609	CHL	C8-C10-C11-C12
24	N	608	CHL	C15-C16-C17-C18
24	7	609	CHL	C8-C10-C11-C12
24	n	608	CHL	C15-C16-C17-C18
25	B	607	CLA	C8-C10-C11-C12
25	C	506	CLA	C13-C15-C16-C17
25	C	506	CLA	C15-C16-C17-C18
25	b	607	CLA	C8-C10-C11-C12
25	b	614	CLA	C13-C15-C16-C17
25	c	506	CLA	C13-C15-C16-C17
25	c	506	CLA	C15-C16-C17-C18
25	g	614	CLA	O1A-CGA-O2A-C1
25	R	603	CLA	CBA-CGA-O2A-C1
25	r	603	CLA	CBA-CGA-O2A-C1
24	1	607	CHL	C13-C15-C16-C17
24	5	607	CHL	C13-C15-C16-C17
29	C	2630	LHG	C23-C24-C25-C26
29	C	523	LHG	C23-C24-C25-C26
29	c	2630	LHG	C23-C24-C25-C26
25	C	507	CLA	C4-C3-C5-C6
25	c	507	CLA	C4-C3-C5-C6
25	b	612	CLA	O1D-CGD-O2D-CED
24	G	601	CHL	C13-C15-C16-C17
24	g	601	CHL	C13-C15-C16-C17
25	B	612	CLA	O1D-CGD-O2D-CED
25	y	603	CLA	O1D-CGD-O2D-CED
35	B	2633	LMG	C2-C1-O1-C7
35	b	2633	LMG	C2-C1-O1-C7
37	C	519	DGD	C2E-C1E-O5D-C6D
37	c	519	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
24	N	608	CHL	C13-C15-C16-C17
24	n	608	CHL	C13-C15-C16-C17
25	B	614	CLA	C13-C15-C16-C17
37	C	519	DGD	O6E-C5E-C6E-O5E
29	c	523	LHG	C23-C24-C25-C26
25	Y	603	CLA	O1D-CGD-O2D-CED
24	G	609	CHL	CBA-CGA-O2A-C1
24	N	609	CHL	CBA-CGA-O2A-C1
24	Y	605	CHL	CBA-CGA-O2A-C1
24	g	609	CHL	CBA-CGA-O2A-C1
24	n	609	CHL	CBA-CGA-O2A-C1
24	y	605	CHL	CBA-CGA-O2A-C1
25	C	511	CLA	CBA-CGA-O2A-C1
25	c	511	CLA	CBA-CGA-O2A-C1
37	c	519	DGD	O6E-C5E-C6E-O5E
24	Y	607	CHL	C16-C17-C18-C19
24	y	607	CHL	C16-C17-C18-C19
25	C	502	CLA	C16-C17-C18-C20
25	C	508	CLA	C16-C17-C18-C19
25	R	613	CLA	C11-C12-C13-C14
25	c	502	CLA	C16-C17-C18-C20
25	c	508	CLA	C16-C17-C18-C19
25	r	613	CLA	C11-C12-C13-C14
27	R	622	XAT	C27-C28-C29-C39
27	r	622	XAT	C27-C28-C29-C39
28	G	1623	NEX	C31-C32-C33-C40
28	g	1623	NEX	C31-C32-C33-C40
30	4	623	BCR	C7-C8-C9-C34
30	B	618	BCR	C36-C18-C19-C20
30	B	620	BCR	C37-C22-C23-C24
30	8	623	BCR	C7-C8-C9-C34
30	b	618	BCR	C36-C18-C19-C20
25	C	501	CLA	O1A-CGA-O2A-C1
25	c	501	CLA	O1A-CGA-O2A-C1
24	3	605	CHL	C2A-CAA-CBA-CGA
24	4	601	CHL	C2A-CAA-CBA-CGA
24	R	607	CHL	C2A-CAA-CBA-CGA
24	Y	601	CHL	C2A-CAA-CBA-CGA
24	7	605	CHL	C2A-CAA-CBA-CGA
24	8	601	CHL	C2A-CAA-CBA-CGA
24	g	607	CHL	C2A-CAA-CBA-CGA
24	r	607	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	y	601	CHL	C2A-CAA-CBA-CGA
25	B	608	CLA	C2A-CAA-CBA-CGA
25	B	613	CLA	C2A-CAA-CBA-CGA
25	C	501	CLA	C2A-CAA-CBA-CGA
25	C	503	CLA	C2A-CAA-CBA-CGA
25	S	602	CLA	C2A-CAA-CBA-CGA
25	6	613	CLA	C2A-CAA-CBA-CGA
25	b	608	CLA	C2A-CAA-CBA-CGA
25	b	613	CLA	C2A-CAA-CBA-CGA
25	c	501	CLA	C2A-CAA-CBA-CGA
25	c	503	CLA	C2A-CAA-CBA-CGA
25	s	602	CLA	C2A-CAA-CBA-CGA
25	B	607	CLA	C15-C16-C17-C18
25	C	508	CLA	C15-C16-C17-C18
25	C	510	CLA	C15-C16-C17-C18
25	b	607	CLA	C15-C16-C17-C18
25	c	508	CLA	C15-C16-C17-C18
25	c	510	CLA	C15-C16-C17-C18
29	2	2630	LHG	O1-C1-C2-C3
29	4	2630	LHG	O1-C1-C2-C3
29	B	2630	LHG	O1-C1-C2-C3
29	D	410	LHG	O1-C1-C2-C3
29	6	2630	LHG	O1-C1-C2-C3
29	8	2630	LHG	O1-C1-C2-C3
29	b	2630	LHG	O1-C1-C2-C3
29	d	410	LHG	O1-C1-C2-C3
34	A	418	SQD	C44-C45-O47-C7
34	a	418	SQD	C44-C45-O47-C7
25	B	613	CLA	O1A-CGA-O2A-C1
25	C	505	CLA	O1A-CGA-O2A-C1
25	b	613	CLA	O1A-CGA-O2A-C1
25	c	505	CLA	O1A-CGA-O2A-C1
24	1	607	CHL	C2C-C3C-CAC-CBC
24	5	607	CHL	C2C-C3C-CAC-CBC
24	Y	609	CHL	C10-C11-C12-C13
24	y	609	CHL	C10-C11-C12-C13
37	h	102	DGD	C1B-C2B-C3B-C4B
25	A	410	CLA	C10-C11-C12-C13
25	B	602	CLA	C5-C6-C7-C8
25	a	410	CLA	C10-C11-C12-C13
25	b	602	CLA	C5-C6-C7-C8
24	R	606	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	r	606	CHL	O1D-CGD-O2D-CED
29	S	2630	LHG	O7-C5-C6-O8
29	s	2630	LHG	O7-C5-C6-O8
34	A	412	SQD	O6-C44-C45-O47
34	a	412	SQD	O6-C44-C45-O47
24	G	608	CHL	C13-C15-C16-C17
24	g	608	CHL	C13-C15-C16-C17
37	H	102	DGD	C1B-C2B-C3B-C4B
35	Z	101	LMG	C4-C5-C6-O5
35	z	101	LMG	C4-C5-C6-O5
24	R	608	CHL	C2-C1-O2A-CGA
24	r	608	CHL	C2-C1-O2A-CGA
24	2	609	CHL	C11-C12-C13-C15
24	N	608	CHL	C16-C17-C18-C20
24	N	609	CHL	C16-C17-C18-C20
24	6	609	CHL	C11-C12-C13-C15
24	n	608	CHL	C16-C17-C18-C20
24	n	609	CHL	C16-C17-C18-C20
25	C	502	CLA	C16-C17-C18-C19
25	c	502	CLA	C16-C17-C18-C19
34	B	623	SQD	O10-C23-O48-C46
34	b	623	SQD	O10-C23-O48-C46
25	B	613	CLA	C13-C15-C16-C17
25	N	603	CLA	C5-C6-C7-C8
25	b	613	CLA	C13-C15-C16-C17
25	n	603	CLA	C5-C6-C7-C8
24	3	601	CHL	O1D-CGD-O2D-CED
24	5	605	CHL	O1D-CGD-O2D-CED
24	7	601	CHL	O1D-CGD-O2D-CED
29	B	2630	LHG	C27-C28-C29-C30
34	A	412	SQD	C18-C19-C20-C21
34	a	412	SQD	C18-C19-C20-C21
37	C	519	DGD	C4A-C5A-C6A-C7A
37	c	519	DGD	C4A-C5A-C6A-C7A
29	C	2630	LHG	C31-C32-C33-C34
29	G	2630	LHG	C25-C26-C27-C28
29	b	2630	LHG	C27-C28-C29-C30
29	c	2630	LHG	C31-C32-C33-C34
29	g	2630	LHG	C25-C26-C27-C28
35	B	2633	LMG	C30-C31-C32-C33
35	b	2633	LMG	C30-C31-C32-C33
24	1	605	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	D	410	LHG	C13-C14-C15-C16
29	d	410	LHG	C13-C14-C15-C16
35	B	622	LMG	C19-C20-C21-C22
35	C	521	LMG	C12-C13-C14-C15
35	C	521	LMG	C32-C33-C34-C35
35	Z	101	LMG	C18-C19-C20-C21
35	b	622	LMG	C19-C20-C21-C22
35	c	521	LMG	C12-C13-C14-C15
35	c	521	LMG	C32-C33-C34-C35
35	z	101	LMG	C18-C19-C20-C21
25	B	611	CLA	O1A-CGA-O2A-C1
25	b	611	CLA	O1A-CGA-O2A-C1
24	1	609	CHL	CBA-CGA-O2A-C1
24	5	609	CHL	CBA-CGA-O2A-C1
29	1	2630	LHG	C12-C13-C14-C15
29	C	522	LHG	C11-C10-C9-C8
29	Y	2630	LHG	C16-C17-C18-C19
29	5	2630	LHG	C12-C13-C14-C15
29	c	522	LHG	C11-C10-C9-C8
29	y	2630	LHG	C16-C17-C18-C19
35	A	415	LMG	C35-C36-C37-C38
35	B	622	LMG	C37-C38-C39-C40
35	B	2633	LMG	C32-C33-C34-C35
35	a	415	LMG	C35-C36-C37-C38
35	b	622	LMG	C37-C38-C39-C40
35	b	2633	LMG	C32-C33-C34-C35
37	B	626	DGD	O1B-C1B-O2G-C2G
37	b	626	DGD	O1B-C1B-O2G-C2G
29	R	2630	LHG	O1-C1-C2-O2
29	Y	2630	LHG	O1-C1-C2-O2
29	r	2630	LHG	O1-C1-C2-O2
29	y	2630	LHG	O1-C1-C2-O2
29	N	2630	LHG	C25-C26-C27-C28
29	n	2630	LHG	C25-C26-C27-C28
24	4	607	CHL	O1D-CGD-O2D-CED
24	Y	609	CHL	O1D-CGD-O2D-CED
24	8	607	CHL	O1D-CGD-O2D-CED
24	y	609	CHL	O1D-CGD-O2D-CED
25	B	613	CLA	C10-C11-C12-C13
25	b	613	CLA	C10-C11-C12-C13
25	1	604	CLA	C4B-C3B-CAB-CBB
25	2	613	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	2	614	CLA	C4B-C3B-CAB-CBB
25	3	604	CLA	C4B-C3B-CAB-CBB
25	4	603	CLA	C4B-C3B-CAB-CBB
25	B	604	CLA	C4B-C3B-CAB-CBB
25	B	606	CLA	C4B-C3B-CAB-CBB
25	R	610	CLA	C4B-C3B-CAB-CBB
25	S	603	CLA	C4B-C3B-CAB-CBB
25	S	610	CLA	C4B-C3B-CAB-CBB
25	5	604	CLA	C4B-C3B-CAB-CBB
25	6	613	CLA	C4B-C3B-CAB-CBB
25	6	614	CLA	C4B-C3B-CAB-CBB
25	7	604	CLA	C4B-C3B-CAB-CBB
25	8	603	CLA	C4B-C3B-CAB-CBB
25	b	604	CLA	C4B-C3B-CAB-CBB
25	b	606	CLA	C4B-C3B-CAB-CBB
25	r	610	CLA	C4B-C3B-CAB-CBB
25	s	603	CLA	C4B-C3B-CAB-CBB
25	s	610	CLA	C4B-C3B-CAB-CBB
29	3	2630	LHG	C23-C24-C25-C26
29	7	2630	LHG	C23-C24-C25-C26
35	B	2633	LMG	C16-C17-C18-C19
35	b	2633	LMG	C16-C17-C18-C19
24	2	609	CHL	C11-C12-C13-C14
24	6	609	CHL	C11-C12-C13-C14
25	B	605	CLA	C16-C17-C18-C19
25	B	605	CLA	C16-C17-C18-C20
25	b	605	CLA	C16-C17-C18-C19
25	b	605	CLA	C16-C17-C18-C20
25	r	603	CLA	C11-C12-C13-C14
25	C	513	CLA	O1D-CGD-O2D-CED
25	c	513	CLA	O1D-CGD-O2D-CED
24	3	608	CHL	C2A-CAA-CBA-CGA
24	G	607	CHL	C2A-CAA-CBA-CGA
24	7	608	CHL	C2A-CAA-CBA-CGA
25	G	610	CLA	C2A-CAA-CBA-CGA
25	g	610	CLA	C2A-CAA-CBA-CGA
37	C	520	DGD	C4B-C5B-C6B-C7B
37	c	520	DGD	C4B-C5B-C6B-C7B
29	D	409	LHG	C30-C31-C32-C33
29	d	409	LHG	C30-C31-C32-C33
37	B	626	DGD	C5B-C6B-C7B-C8B
37	b	626	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
25	B	613	CLA	C6-C7-C8-C10
25	Y	612	CLA	C11-C10-C8-C7
25	b	613	CLA	C6-C7-C8-C10
25	y	612	CLA	C11-C10-C8-C7
29	C	523	LHG	C15-C16-C17-C18
29	L	101	LHG	C25-C26-C27-C28
29	c	523	LHG	C15-C16-C17-C18
29	l	101	LHG	C25-C26-C27-C28
29	2	2630	LHG	C23-C24-C25-C26
29	Y	2630	LHG	C23-C24-C25-C26
29	6	2630	LHG	C23-C24-C25-C26
29	y	2630	LHG	C23-C24-C25-C26
24	G	601	CHL	C8-C10-C11-C12
24	g	601	CHL	C8-C10-C11-C12
29	D	408	LHG	C28-C29-C30-C31
29	Y	2630	LHG	C26-C27-C28-C29
29	d	408	LHG	C28-C29-C30-C31
29	y	2630	LHG	C26-C27-C28-C29
34	A	412	SQD	C10-C11-C12-C13
34	a	412	SQD	C10-C11-C12-C13
35	A	415	LMG	C30-C31-C32-C33
35	C	521	LMG	C11-C12-C13-C14
25	3	611	CLA	O1A-CGA-O2A-C1
25	S	614	CLA	O1A-CGA-O2A-C1
25	7	611	CLA	O1A-CGA-O2A-C1
25	s	614	CLA	O1A-CGA-O2A-C1
37	C	519	DGD	C4E-C5E-C6E-O5E
37	c	519	DGD	C4E-C5E-C6E-O5E
24	1	605	CHL	C3A-C2A-CAA-CBA
24	1	607	CHL	C3A-C2A-CAA-CBA
24	2	605	CHL	C3A-C2A-CAA-CBA
24	2	607	CHL	C3A-C2A-CAA-CBA
24	3	605	CHL	C3A-C2A-CAA-CBA
24	4	608	CHL	C3A-C2A-CAA-CBA
24	R	606	CHL	C3A-C2A-CAA-CBA
24	5	605	CHL	C3A-C2A-CAA-CBA
24	5	607	CHL	C3A-C2A-CAA-CBA
24	6	605	CHL	C3A-C2A-CAA-CBA
24	6	607	CHL	C3A-C2A-CAA-CBA
24	7	605	CHL	C3A-C2A-CAA-CBA
24	8	608	CHL	C3A-C2A-CAA-CBA
24	r	606	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	y	605	CHL	C3A-C2A-CAA-CBA
25	1	611	CLA	C3A-C2A-CAA-CBA
25	R	616	CLA	C3A-C2A-CAA-CBA
25	S	602	CLA	C3A-C2A-CAA-CBA
25	S	609	CLA	C3A-C2A-CAA-CBA
25	5	611	CLA	C3A-C2A-CAA-CBA
25	r	616	CLA	C3A-C2A-CAA-CBA
25	s	602	CLA	C3A-C2A-CAA-CBA
25	s	609	CLA	C3A-C2A-CAA-CBA
29	3	2630	LHG	C28-C29-C30-C31
29	7	2630	LHG	C28-C29-C30-C31
35	C	521	LMG	C17-C18-C19-C20
35	a	415	LMG	C30-C31-C32-C33
35	c	521	LMG	C11-C12-C13-C14
35	c	521	LMG	C17-C18-C19-C20
37	C	520	DGD	C6A-C7A-C8A-C9A
37	c	520	DGD	C6A-C7A-C8A-C9A
24	Y	607	CHL	C13-C15-C16-C17
24	y	607	CHL	C13-C15-C16-C17
25	B	606	CLA	C5-C6-C7-C8
25	Y	602	CLA	C8-C10-C11-C12
25	b	606	CLA	C5-C6-C7-C8
25	b	606	CLA	C8-C10-C11-C12
25	y	602	CLA	C8-C10-C11-C12
25	C	512	CLA	O1D-CGD-O2D-CED
25	s	609	CLA	O1D-CGD-O2D-CED
24	R	606	CHL	C16-C17-C18-C19
24	r	606	CHL	C16-C17-C18-C19
25	R	603	CLA	C11-C12-C13-C14
24	Y	609	CHL	O1A-CGA-O2A-C1
24	y	609	CHL	O1A-CGA-O2A-C1
25	R	603	CLA	O1A-CGA-O2A-C1
25	r	603	CLA	O1A-CGA-O2A-C1
25	B	611	CLA	O1D-CGD-O2D-CED
29	C	2630	LHG	C14-C15-C16-C17
37	B	626	DGD	CCB-CDB-CEB-CFB
24	G	607	CHL	C8-C10-C11-C12
24	g	607	CHL	C8-C10-C11-C12
25	B	606	CLA	C8-C10-C11-C12
25	G	602	CLA	CBD-CGD-O2D-CED
25	g	602	CLA	CBD-CGD-O2D-CED
25	n	611	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	B	2630	LHG	C11-C10-C9-C8
29	b	2630	LHG	C11-C10-C9-C8
29	c	2630	LHG	C14-C15-C16-C17
34	A	412	SQD	C12-C13-C14-C15
34	a	412	SQD	C12-C13-C14-C15
35	Z	101	LMG	C30-C31-C32-C33
35	z	101	LMG	C30-C31-C32-C33
37	b	626	DGD	CCB-CDB-CEB-CFB
29	D	410	LHG	C1-C2-C3-O3
29	d	410	LHG	C1-C2-C3-O3
25	c	512	CLA	O1D-CGD-O2D-CED
24	2	609	CHL	CBA-CGA-O2A-C1
24	G	606	CHL	CBA-CGA-O2A-C1
24	6	609	CHL	CBA-CGA-O2A-C1
24	g	606	CHL	CBA-CGA-O2A-C1
25	B	605	CLA	CBA-CGA-O2A-C1
25	b	605	CLA	CBA-CGA-O2A-C1
29	B	2630	LHG	C29-C30-C31-C32
29	G	2630	LHG	C18-C19-C20-C21
29	b	2630	LHG	C29-C30-C31-C32
29	g	2630	LHG	C18-C19-C20-C21
35	B	2633	LMG	C31-C32-C33-C34
35	C	521	LMG	C35-C36-C37-C38
35	c	521	LMG	C35-C36-C37-C38
37	B	626	DGD	C4B-C5B-C6B-C7B
37	b	626	DGD	C4B-C5B-C6B-C7B
29	B	2631	LHG	C23-C24-C25-C26
29	L	101	LHG	C7-C8-C9-C10
29	b	2631	LHG	C23-C24-C25-C26
29	l	101	LHG	C7-C8-C9-C10
37	C	520	DGD	C1A-C2A-C3A-C4A
37	c	520	DGD	C1A-C2A-C3A-C4A
25	S	609	CLA	O1D-CGD-O2D-CED
25	b	611	CLA	O1D-CGD-O2D-CED
29	3	2630	LHG	C14-C15-C16-C17
29	C	522	LHG	C28-C29-C30-C31
29	L	101	LHG	C30-C31-C32-C33
29	7	2630	LHG	C14-C15-C16-C17
29	c	522	LHG	C28-C29-C30-C31
29	l	101	LHG	C30-C31-C32-C33
35	b	2633	LMG	C31-C32-C33-C34
37	C	519	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
37	C	520	DGD	C7A-C8A-C9A-CAA
37	c	519	DGD	C4B-C5B-C6B-C7B
37	c	520	DGD	C7A-C8A-C9A-CAA
25	Y	603	CLA	O1A-CGA-O2A-C1
25	y	603	CLA	O1A-CGA-O2A-C1
29	C	523	LHG	C33-C34-C35-C36
29	D	410	LHG	C15-C16-C17-C18
29	D	410	LHG	C27-C28-C29-C30
29	S	2630	LHG	C32-C33-C34-C35
29	Y	2630	LHG	C12-C13-C14-C15
29	c	523	LHG	C33-C34-C35-C36
29	d	410	LHG	C15-C16-C17-C18
29	d	410	LHG	C27-C28-C29-C30
29	s	2630	LHG	C32-C33-C34-C35
29	y	2630	LHG	C12-C13-C14-C15
35	B	622	LMG	C35-C36-C37-C38
35	b	622	LMG	C35-C36-C37-C38
35	A	413	LMG	C37-C38-C39-C40
35	a	413	LMG	C37-C38-C39-C40
24	n	601	CHL	C5-C6-C7-C8
25	b	612	CLA	C15-C16-C17-C18
29	B	2630	LHG	C12-C13-C14-C15
29	L	101	LHG	C13-C14-C15-C16
29	b	2630	LHG	C12-C13-C14-C15
29	l	101	LHG	C13-C14-C15-C16
37	C	518	DGD	C4A-C5A-C6A-C7A
37	C	520	DGD	C2A-C3A-C4A-C5A
37	c	518	DGD	C4A-C5A-C6A-C7A
37	c	520	DGD	C2A-C3A-C4A-C5A
34	B	623	SQD	C23-C24-C25-C26
34	b	623	SQD	C23-C24-C25-C26
24	N	609	CHL	O1A-CGA-O2A-C1
24	Y	605	CHL	O1A-CGA-O2A-C1
24	n	609	CHL	O1A-CGA-O2A-C1
24	y	605	CHL	O1A-CGA-O2A-C1
25	C	511	CLA	O1A-CGA-O2A-C1
25	c	511	CLA	O1A-CGA-O2A-C1
25	1	603	CLA	C2B-C3B-CAB-CBB
25	3	611	CLA	C2B-C3B-CAB-CBB
25	4	603	CLA	C2B-C3B-CAB-CBB
25	A	407	CLA	C2B-C3B-CAB-CBB
25	B	607	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	B	616	CLA	C2B-C3B-CAB-CBB
25	R	616	CLA	C2B-C3B-CAB-CBB
25	5	603	CLA	C2B-C3B-CAB-CBB
25	7	611	CLA	C2B-C3B-CAB-CBB
25	8	603	CLA	C2B-C3B-CAB-CBB
25	a	407	CLA	C2B-C3B-CAB-CBB
25	b	607	CLA	C2B-C3B-CAB-CBB
25	b	616	CLA	C2B-C3B-CAB-CBB
25	r	616	CLA	C2B-C3B-CAB-CBB
26	1	1620	LUT	C1-C6-C7-C8
26	1	1620	LUT	C5-C6-C7-C8
26	2	1620	LUT	C1-C6-C7-C8
26	2	1620	LUT	C5-C6-C7-C8
26	R	620	LUT	C1-C6-C7-C8
26	R	620	LUT	C5-C6-C7-C8
26	5	1620	LUT	C1-C6-C7-C8
26	5	1620	LUT	C5-C6-C7-C8
26	6	1620	LUT	C1-C6-C7-C8
26	6	1620	LUT	C5-C6-C7-C8
26	r	620	LUT	C1-C6-C7-C8
26	r	620	LUT	C5-C6-C7-C8
30	B	618	BCR	C1-C6-C7-C8
30	B	618	BCR	C5-C6-C7-C8
30	b	618	BCR	C1-C6-C7-C8
30	b	618	BCR	C5-C6-C7-C8
25	N	611	CLA	CBD-CGD-O2D-CED
24	R	607	CHL	CBA-CGA-O2A-C1
24	r	607	CHL	CBA-CGA-O2A-C1
25	B	606	CLA	CBA-CGA-O2A-C1
25	b	606	CLA	CBA-CGA-O2A-C1
24	N	601	CHL	C5-C6-C7-C8
25	B	612	CLA	C15-C16-C17-C18
25	C	504	CLA	C13-C15-C16-C17
25	D	402	CLA	C10-C11-C12-C13
25	c	504	CLA	C13-C15-C16-C17
25	d	402	CLA	C10-C11-C12-C13
29	C	522	LHG	C27-C28-C29-C30
29	D	408	LHG	C26-C27-C28-C29
29	c	522	LHG	C27-C28-C29-C30
29	d	408	LHG	C26-C27-C28-C29
29	d	408	LHG	C27-C28-C29-C30
24	N	601	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	n	601	CHL	O1D-CGD-O2D-CED
25	N	602	CLA	O1D-CGD-O2D-CED
29	D	408	LHG	C27-C28-C29-C30
29	L	101	LHG	C32-C33-C34-C35
29	l	101	LHG	C32-C33-C34-C35
24	3	607	CHL	C2A-CAA-CBA-CGA
24	7	607	CHL	C2A-CAA-CBA-CGA
25	S	611	CLA	C2A-CAA-CBA-CGA
25	s	611	CLA	C2A-CAA-CBA-CGA
25	G	613	CLA	C8-C10-C11-C12
25	g	613	CLA	C8-C10-C11-C12
29	D	409	LHG	C34-C35-C36-C37
24	G	609	CHL	O1A-CGA-O2A-C1
24	g	609	CHL	O1A-CGA-O2A-C1
35	B	2633	LMG	O10-C28-O8-C9
35	b	2633	LMG	O10-C28-O8-C9
29	d	409	LHG	C34-C35-C36-C37
25	C	501	CLA	C4-C3-C5-C6
25	C	504	CLA	C4-C3-C5-C6
25	c	501	CLA	C4-C3-C5-C6
25	c	504	CLA	C4-C3-C5-C6
25	n	602	CLA	O1D-CGD-O2D-CED
29	2	2630	LHG	C12-C13-C14-C15
29	C	2630	LHG	C32-C33-C34-C35
29	R	2630	LHG	C12-C13-C14-C15
29	6	2630	LHG	C12-C13-C14-C15
29	c	2630	LHG	C32-C33-C34-C35
29	r	2630	LHG	C12-C13-C14-C15
34	A	412	SQD	C9-C10-C11-C12
34	a	412	SQD	C9-C10-C11-C12
24	1	607	CHL	C8-C10-C11-C12
24	Y	609	CHL	C15-C16-C17-C18
24	5	607	CHL	C8-C10-C11-C12
24	y	609	CHL	C15-C16-C17-C18
25	C	504	CLA	C2-C3-C5-C6
25	C	507	CLA	C2-C3-C5-C6
25	c	507	CLA	C2-C3-C5-C6
24	N	607	CHL	C16-C17-C18-C19
24	Y	607	CHL	C16-C17-C18-C20
24	n	607	CHL	C16-C17-C18-C19
24	y	607	CHL	C16-C17-C18-C20
29	3	2630	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	C	523	LHG	C24-C25-C26-C27
29	D	409	LHG	C33-C34-C35-C36
29	7	2630	LHG	C10-C11-C12-C13
29	d	409	LHG	C33-C34-C35-C36
29	l	101	LHG	C28-C29-C30-C31
34	A	412	SQD	C29-C30-C31-C32
34	B	621	SQD	C34-C35-C36-C37
34	a	412	SQD	C29-C30-C31-C32
34	b	621	SQD	C34-C35-C36-C37
35	A	413	LMG	C17-C18-C19-C20
35	a	413	LMG	C17-C18-C19-C20
37	B	626	DGD	C2A-C3A-C4A-C5A
37	b	626	DGD	C2A-C3A-C4A-C5A
25	B	608	CLA	CBA-CGA-O2A-C1
25	C	513	CLA	CBA-CGA-O2A-C1
25	b	608	CLA	CBA-CGA-O2A-C1
25	c	513	CLA	CBA-CGA-O2A-C1
24	1	609	CHL	C11-C10-C8-C9
25	D	403	CLA	C14-C13-C15-C16
25	Y	603	CLA	C6-C7-C8-C9
25	d	403	CLA	C14-C13-C15-C16
25	y	603	CLA	C6-C7-C8-C9
33	A	408	PHO	C14-C13-C15-C16
33	a	408	PHO	C14-C13-C15-C16
29	D	408	LHG	C30-C31-C32-C33
29	D	409	LHG	C12-C13-C14-C15
29	L	101	LHG	C10-C11-C12-C13
29	L	101	LHG	C28-C29-C30-C31
29	S	2630	LHG	C34-C35-C36-C37
29	c	523	LHG	C24-C25-C26-C27
29	d	408	LHG	C30-C31-C32-C33
29	d	409	LHG	C12-C13-C14-C15
29	s	2630	LHG	C34-C35-C36-C37
35	A	415	LMG	C36-C37-C38-C39
35	a	415	LMG	C36-C37-C38-C39
25	C	505	CLA	C5-C6-C7-C8
25	c	505	CLA	C5-C6-C7-C8
29	C	522	LHG	C32-C33-C34-C35
29	l	101	LHG	C10-C11-C12-C13
34	A	412	SQD	C13-C14-C15-C16
34	A	412	SQD	C17-C18-C19-C20
34	A	418	SQD	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
34	a	412	SQD	C13-C14-C15-C16
34	a	412	SQD	C17-C18-C19-C20
34	a	418	SQD	C32-C33-C34-C35
37	C	520	DGD	O6D-C1D-O3G-C3G
37	C	520	DGD	O6E-C1E-O5D-C6D
37	H	102	DGD	O6E-C1E-O5D-C6D
37	c	520	DGD	O6D-C1D-O3G-C3G
37	c	520	DGD	O6E-C1E-O5D-C6D
37	h	102	DGD	O6E-C1E-O5D-C6D
29	N	2630	LHG	C11-C10-C9-C8
29	c	522	LHG	C32-C33-C34-C35
37	H	102	DGD	C2E-C1E-O5D-C6D
37	h	102	DGD	C2E-C1E-O5D-C6D
25	B	617	CLA	C10-C11-C12-C13
25	B	617	CLA	C15-C16-C17-C18
25	b	617	CLA	C10-C11-C12-C13
25	b	617	CLA	C15-C16-C17-C18
29	C	2630	LHG	C24-C25-C26-C27
29	G	2630	LHG	C27-C28-C29-C30
29	L	101	LHG	C16-C17-C18-C19
29	g	2630	LHG	C27-C28-C29-C30
29	l	101	LHG	C16-C17-C18-C19
29	n	2630	LHG	C11-C10-C9-C8
35	B	2633	LMG	C15-C16-C17-C18
35	b	2633	LMG	C15-C16-C17-C18
29	L	101	LHG	C11-C10-C9-C8
29	N	2630	LHG	C27-C28-C29-C30
29	c	2630	LHG	C24-C25-C26-C27
29	l	101	LHG	C11-C10-C9-C8
29	n	2630	LHG	C27-C28-C29-C30
35	C	521	LMG	C16-C17-C18-C19
35	c	521	LMG	C16-C17-C18-C19
37	C	519	DGD	C5B-C6B-C7B-C8B
37	c	519	DGD	C5B-C6B-C7B-C8B
29	1	2630	LHG	C9-C10-C11-C12
29	S	2630	LHG	C24-C25-C26-C27
29	5	2630	LHG	C9-C10-C11-C12
29	s	2630	LHG	C24-C25-C26-C27
34	B	621	SQD	C9-C10-C11-C12
34	B	623	SQD	C9-C10-C11-C12
34	b	621	SQD	C9-C10-C11-C12
34	b	623	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
35	B	622	LMG	C13-C14-C15-C16
35	b	622	LMG	C13-C14-C15-C16
26	1	1621	LUT	C29-C30-C31-C32
26	N	1621	LUT	C29-C30-C31-C32
26	5	1621	LUT	C29-C30-C31-C32
26	n	1621	LUT	C29-C30-C31-C32
27	R	622	XAT	C29-C30-C31-C32
27	r	622	XAT	C29-C30-C31-C32
28	G	1623	NEX	C33-C34-C35-C15
28	g	1623	NEX	C33-C34-C35-C15
24	N	608	CHL	C16-C17-C18-C19
25	B	602	CLA	C16-C17-C18-C20
25	C	505	CLA	C16-C17-C18-C20
25	C	508	CLA	C16-C17-C18-C20
25	b	602	CLA	C16-C17-C18-C20
25	c	505	CLA	C16-C17-C18-C20
25	c	508	CLA	C16-C17-C18-C20
29	B	2630	LHG	C8-C7-O7-C5
29	C	2630	LHG	C8-C7-O7-C5
29	S	2630	LHG	C8-C7-O7-C5
29	b	2630	LHG	C8-C7-O7-C5
29	c	2630	LHG	C8-C7-O7-C5
29	s	2630	LHG	C8-C7-O7-C5
35	C	521	LMG	C11-C10-O7-C8
35	c	521	LMG	C11-C10-O7-C8
37	C	520	DGD	C2B-C1B-O2G-C2G
37	c	520	DGD	C2B-C1B-O2G-C2G
25	A	406	CLA	C10-C11-C12-C13
25	a	406	CLA	C10-C11-C12-C13
35	D	411	LMG	O9-C10-O7-C8
35	d	411	LMG	O9-C10-O7-C8
29	b	2630	LHG	C11-C12-C13-C14
35	c	521	LMG	C31-C32-C33-C34
37	C	519	DGD	C3B-C4B-C5B-C6B
37	c	519	DGD	C3B-C4B-C5B-C6B
29	B	2630	LHG	C11-C12-C13-C14
35	C	521	LMG	C31-C32-C33-C34
24	3	609	CHL	C2C-C3C-CAC-CBC
24	R	608	CHL	C8-C10-C11-C12
24	r	608	CHL	C8-C10-C11-C12
30	b	620	BCR	C37-C22-C23-C24
29	B	2631	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
35	D	411	LMG	C32-C33-C34-C35
37	C	520	DGD	CCA-CDA-CEA-CFA
37	c	520	DGD	CCA-CDA-CEA-CFA
29	B	2631	LHG	C27-C28-C29-C30
29	b	2631	LHG	C27-C28-C29-C30
29	b	2631	LHG	C32-C33-C34-C35
29	y	2630	LHG	C32-C33-C34-C35
34	B	621	SQD	C11-C12-C13-C14
34	b	621	SQD	C11-C12-C13-C14
35	d	411	LMG	C32-C33-C34-C35
25	G	611	CLA	C2A-CAA-CBA-CGA
25	g	611	CLA	C2A-CAA-CBA-CGA
24	7	609	CHL	C2C-C3C-CAC-CBC
24	R	606	CHL	C16-C17-C18-C20
24	n	608	CHL	C16-C17-C18-C19
24	r	606	CHL	C16-C17-C18-C20
25	3	602	CLA	C11-C12-C13-C14
25	3	602	CLA	C11-C12-C13-C15
25	B	602	CLA	C16-C17-C18-C19
25	N	603	CLA	C16-C17-C18-C19
25	R	603	CLA	C11-C12-C13-C15
25	7	602	CLA	C11-C12-C13-C14
25	7	602	CLA	C11-C12-C13-C15
25	b	602	CLA	C16-C17-C18-C19
25	n	603	CLA	C16-C17-C18-C19
25	r	603	CLA	C11-C12-C13-C15
29	Y	2630	LHG	C32-C33-C34-C35
24	2	607	CHL	C4-C3-C5-C6
24	6	607	CHL	C4-C3-C5-C6
37	c	519	DGD	O1A-C1A-O1G-C1G
25	c	504	CLA	C2-C3-C5-C6
37	c	519	DGD	C3A-C4A-C5A-C6A
24	N	607	CHL	C13-C15-C16-C17
24	n	607	CHL	C13-C15-C16-C17
37	C	519	DGD	C3A-C4A-C5A-C6A
37	C	518	DGD	C4B-C5B-C6B-C7B
37	c	518	DGD	C4B-C5B-C6B-C7B
24	1	609	CHL	O1A-CGA-O2A-C1
24	5	609	CHL	O1A-CGA-O2A-C1
37	C	519	DGD	O1A-C1A-O1G-C1G
24	1	609	CHL	C2C-C3C-CAC-CBC
24	5	609	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
25	G	604	CLA	CBA-CGA-O2A-C1
25	g	604	CLA	CBA-CGA-O2A-C1
35	Z	101	LMG	C28-C29-C30-C31
35	z	101	LMG	C28-C29-C30-C31
29	R	2630	LHG	C13-C14-C15-C16
29	r	2630	LHG	C13-C14-C15-C16
35	C	521	LMG	C29-C30-C31-C32
35	c	521	LMG	C29-C30-C31-C32
25	G	602	CLA	C15-C16-C17-C18
25	N	603	CLA	C10-C11-C12-C13
25	g	602	CLA	C15-C16-C17-C18
25	n	603	CLA	C10-C11-C12-C13
24	R	607	CHL	C6-C7-C8-C9
24	r	607	CHL	C6-C7-C8-C9
25	R	613	CLA	C11-C12-C13-C15
25	r	613	CLA	C11-C12-C13-C15
35	B	622	LMG	C18-C19-C20-C21
35	b	622	LMG	C18-C19-C20-C21
25	C	507	CLA	O1D-CGD-O2D-CED
25	c	507	CLA	O1D-CGD-O2D-CED
29	2	2630	LHG	C11-C12-C13-C14
25	R	602	CLA	C8-C10-C11-C12
25	r	602	CLA	C8-C10-C11-C12
29	6	2630	LHG	C11-C12-C13-C14
29	d	408	LHG	C29-C30-C31-C32
29	3	2630	LHG	O7-C5-C6-O8
29	4	2630	LHG	O7-C5-C6-O8
29	B	2631	LHG	O7-C5-C6-O8
29	7	2630	LHG	O7-C5-C6-O8
29	8	2630	LHG	O7-C5-C6-O8
29	b	2631	LHG	O7-C5-C6-O8
35	A	415	LMG	O7-C8-C9-O8
35	a	415	LMG	O7-C8-C9-O8
37	C	520	DGD	C5A-C6A-C7A-C8A
37	H	102	DGD	C9A-CAA-CBA-CCA
37	c	520	DGD	C5A-C6A-C7A-C8A
37	h	102	DGD	C9A-CAA-CBA-CCA
24	N	609	CHL	O1D-CGD-O2D-CED
24	n	609	CHL	O1D-CGD-O2D-CED
29	D	408	LHG	C29-C30-C31-C32
35	B	622	LMG	C21-C22-C23-C24
35	b	622	LMG	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
37	C	519	DGD	C6B-C7B-C8B-C9B
37	c	519	DGD	C6B-C7B-C8B-C9B
29	R	2630	LHG	C23-C24-C25-C26
29	2	2630	LHG	C24-C25-C26-C27
29	S	2630	LHG	C26-C27-C28-C29
29	s	2630	LHG	C26-C27-C28-C29
34	A	418	SQD	C11-C10-C9-C8
34	a	418	SQD	C11-C10-C9-C8
29	D	408	LHG	C25-C26-C27-C28
29	L	101	LHG	C29-C30-C31-C32
29	6	2630	LHG	C24-C25-C26-C27
29	d	408	LHG	C25-C26-C27-C28
29	l	101	LHG	C29-C30-C31-C32
35	B	622	LMG	C29-C30-C31-C32
35	b	622	LMG	C29-C30-C31-C32
35	z	101	LMG	C32-C33-C34-C35
37	B	626	DGD	C5A-C6A-C7A-C8A
37	b	626	DGD	C5A-C6A-C7A-C8A
24	1	609	CHL	C8-C10-C11-C12
24	5	609	CHL	C8-C10-C11-C12
35	B	2633	LMG	C34-C35-C36-C37
35	Z	101	LMG	C32-C33-C34-C35
35	b	2633	LMG	C34-C35-C36-C37
37	H	102	DGD	C7A-C8A-C9A-CAA
37	h	102	DGD	C7A-C8A-C9A-CAA
25	A	405	CLA	C3-C5-C6-C7
25	a	405	CLA	C3-C5-C6-C7
29	r	2630	LHG	C23-C24-C25-C26
24	2	607	CHL	C2-C3-C5-C6
24	6	607	CHL	C2-C3-C5-C6
36	D	405	PL9	C13-C14-C16-C17
36	d	405	PL9	C13-C14-C16-C17
25	N	602	CLA	C8-C10-C11-C12
25	n	602	CLA	C8-C10-C11-C12
29	B	2630	LHG	C25-C26-C27-C28
29	D	409	LHG	C24-C25-C26-C27
29	L	101	LHG	C24-C25-C26-C27
29	S	2630	LHG	C11-C12-C13-C14
29	b	2630	LHG	C25-C26-C27-C28
29	d	409	LHG	C24-C25-C26-C27
29	l	101	LHG	C24-C25-C26-C27
29	s	2630	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	C	505	CLA	C2A-CAA-CBA-CGA
25	G	602	CLA	C2A-CAA-CBA-CGA
25	Y	602	CLA	C2A-CAA-CBA-CGA
25	c	505	CLA	C2A-CAA-CBA-CGA
25	g	602	CLA	C2A-CAA-CBA-CGA
25	y	602	CLA	C2A-CAA-CBA-CGA
25	B	605	CLA	CBD-CGD-O2D-CED
25	R	610	CLA	CBD-CGD-O2D-CED
25	b	605	CLA	CBD-CGD-O2D-CED
25	r	610	CLA	CBD-CGD-O2D-CED
25	1	604	CLA	CBA-CGA-O2A-C1
25	R	613	CLA	CBA-CGA-O2A-C1
25	5	604	CLA	CBA-CGA-O2A-C1
25	r	613	CLA	CBA-CGA-O2A-C1
35	A	413	LMG	O6-C5-C6-O5
35	a	413	LMG	O6-C5-C6-O5
29	3	2630	LHG	C33-C34-C35-C36
29	B	2630	LHG	C26-C27-C28-C29
29	N	2630	LHG	C24-C25-C26-C27
29	N	2630	LHG	C30-C31-C32-C33
29	7	2630	LHG	C33-C34-C35-C36
29	b	2630	LHG	C26-C27-C28-C29
29	n	2630	LHG	C24-C25-C26-C27
29	n	2630	LHG	C30-C31-C32-C33
34	A	418	SQD	C13-C14-C15-C16
34	a	418	SQD	C13-C14-C15-C16
37	H	102	DGD	C5B-C6B-C7B-C8B
37	h	102	DGD	C5B-C6B-C7B-C8B
25	C	505	CLA	C15-C16-C17-C18
25	c	505	CLA	C15-C16-C17-C18
29	B	2631	LHG	C28-C29-C30-C31
29	b	2631	LHG	C28-C29-C30-C31
29	B	2631	LHG	C14-C15-C16-C17
29	b	2631	LHG	C14-C15-C16-C17
37	C	518	DGD	C5B-C6B-C7B-C8B
37	c	518	DGD	C5B-C6B-C7B-C8B
25	G	604	CLA	O1D-CGD-O2D-CED
25	g	604	CLA	O1D-CGD-O2D-CED
29	2	2630	LHG	O1-C1-C2-O2
29	3	2630	LHG	O1-C1-C2-O2
29	S	2630	LHG	O1-C1-C2-O2
29	6	2630	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
29	7	2630	LHG	O1-C1-C2-O2
29	s	2630	LHG	O1-C1-C2-O2
24	2	609	CHL	O1A-CGA-O2A-C1
24	G	606	CHL	O1A-CGA-O2A-C1
24	R	607	CHL	O1A-CGA-O2A-C1
24	6	609	CHL	O1A-CGA-O2A-C1
24	g	606	CHL	O1A-CGA-O2A-C1
24	r	607	CHL	O1A-CGA-O2A-C1
25	B	605	CLA	O1A-CGA-O2A-C1
25	B	606	CLA	O1A-CGA-O2A-C1
25	B	608	CLA	O1A-CGA-O2A-C1
25	b	605	CLA	O1A-CGA-O2A-C1
25	b	606	CLA	O1A-CGA-O2A-C1
25	b	608	CLA	O1A-CGA-O2A-C1
34	B	621	SQD	O10-C23-O48-C46
34	b	621	SQD	O10-C23-O48-C46
34	A	412	SQD	C11-C10-C9-C8
34	a	412	SQD	C11-C10-C9-C8
25	1	604	CLA	C1A-C2A-CAA-CBA
25	1	610	CLA	C1A-C2A-CAA-CBA
25	1	611	CLA	C1A-C2A-CAA-CBA
25	2	602	CLA	C1A-C2A-CAA-CBA
25	2	610	CLA	C1A-C2A-CAA-CBA
25	3	604	CLA	C1A-C2A-CAA-CBA
25	3	610	CLA	C1A-C2A-CAA-CBA
25	4	611	CLA	C1A-C2A-CAA-CBA
25	A	406	CLA	C1A-C2A-CAA-CBA
25	A	407	CLA	C1A-C2A-CAA-CBA
25	B	612	CLA	C1A-C2A-CAA-CBA
25	C	501	CLA	C1A-C2A-CAA-CBA
25	C	506	CLA	C1A-C2A-CAA-CBA
25	G	602	CLA	C1A-C2A-CAA-CBA
25	G	614	CLA	C1A-C2A-CAA-CBA
25	N	602	CLA	C1A-C2A-CAA-CBA
25	N	604	CLA	C1A-C2A-CAA-CBA
25	N	614	CLA	C1A-C2A-CAA-CBA
25	R	610	CLA	C1A-C2A-CAA-CBA
25	Y	602	CLA	C1A-C2A-CAA-CBA
25	Y	604	CLA	C1A-C2A-CAA-CBA
25	Y	610	CLA	C1A-C2A-CAA-CBA
25	5	604	CLA	C1A-C2A-CAA-CBA
25	5	610	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	5	611	CLA	C1A-C2A-CAA-CBA
25	6	602	CLA	C1A-C2A-CAA-CBA
25	6	610	CLA	C1A-C2A-CAA-CBA
25	7	604	CLA	C1A-C2A-CAA-CBA
25	7	610	CLA	C1A-C2A-CAA-CBA
25	8	611	CLA	C1A-C2A-CAA-CBA
25	a	406	CLA	C1A-C2A-CAA-CBA
25	a	407	CLA	C1A-C2A-CAA-CBA
25	b	612	CLA	C1A-C2A-CAA-CBA
25	c	501	CLA	C1A-C2A-CAA-CBA
25	c	506	CLA	C1A-C2A-CAA-CBA
25	g	602	CLA	C1A-C2A-CAA-CBA
25	g	614	CLA	C1A-C2A-CAA-CBA
25	n	602	CLA	C1A-C2A-CAA-CBA
25	n	604	CLA	C1A-C2A-CAA-CBA
25	n	614	CLA	C1A-C2A-CAA-CBA
25	r	610	CLA	C1A-C2A-CAA-CBA
25	y	602	CLA	C1A-C2A-CAA-CBA
25	y	604	CLA	C1A-C2A-CAA-CBA
25	y	610	CLA	C1A-C2A-CAA-CBA
25	4	603	CLA	CBD-CGD-O2D-CED
25	8	603	CLA	CBD-CGD-O2D-CED
35	B	622	LMG	C17-C18-C19-C20
35	b	622	LMG	C17-C18-C19-C20
37	H	102	DGD	CCA-CDA-CEA-CFA
25	C	513	CLA	O1A-CGA-O2A-C1
25	c	513	CLA	O1A-CGA-O2A-C1
37	C	519	DGD	C9A-CAA-CBA-CCA
37	c	519	DGD	C9A-CAA-CBA-CCA
37	h	102	DGD	CCA-CDA-CEA-CFA
25	b	614	CLA	C5-C6-C7-C8
34	A	418	SQD	C25-C26-C27-C28
34	a	418	SQD	C25-C26-C27-C28
35	D	411	LMG	C18-C19-C20-C21
35	d	411	LMG	C18-C19-C20-C21
24	G	608	CHL	C12-C13-C15-C16
24	g	608	CHL	C12-C13-C15-C16
25	3	602	CLA	C6-C7-C8-C10
25	B	616	CLA	C12-C13-C15-C16
25	C	502	CLA	C12-C13-C15-C16
25	C	504	CLA	C11-C10-C8-C7
25	C	510	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	G	603	CLA	C11-C10-C8-C7
25	G	610	CLA	C11-C12-C13-C15
25	N	602	CLA	C6-C7-C8-C10
25	N	612	CLA	C6-C7-C8-C10
25	R	610	CLA	C11-C12-C13-C15
25	7	602	CLA	C6-C7-C8-C10
25	b	616	CLA	C12-C13-C15-C16
25	c	502	CLA	C12-C13-C15-C16
25	c	504	CLA	C11-C10-C8-C7
25	c	510	CLA	C12-C13-C15-C16
25	g	603	CLA	C11-C10-C8-C7
25	g	610	CLA	C11-C12-C13-C15
25	n	602	CLA	C6-C7-C8-C10
25	n	612	CLA	C6-C7-C8-C10
25	r	610	CLA	C11-C12-C13-C15
29	C	523	LHG	C12-C13-C14-C15
29	c	523	LHG	C12-C13-C14-C15
25	B	614	CLA	C5-C6-C7-C8
34	A	418	SQD	C10-C11-C12-C13
34	a	418	SQD	C10-C11-C12-C13
24	1	607	CHL	C2-C3-C5-C6
24	3	607	CHL	C2-C3-C5-C6
24	7	607	CHL	C2-C3-C5-C6
24	Y	601	CHL	C15-C16-C17-C18
24	y	601	CHL	C15-C16-C17-C18
25	C	504	CLA	C10-C11-C12-C13
25	c	504	CLA	C10-C11-C12-C13
24	Y	606	CHL	C2A-CAA-CBA-CGA
24	y	606	CHL	C2A-CAA-CBA-CGA
25	3	602	CLA	C2A-CAA-CBA-CGA
25	N	602	CLA	C2A-CAA-CBA-CGA
25	7	602	CLA	C2A-CAA-CBA-CGA
25	n	602	CLA	C2A-CAA-CBA-CGA
24	G	607	CHL	C14-C13-C15-C16
24	5	609	CHL	C11-C10-C8-C9
24	g	607	CHL	C14-C13-C15-C16
25	B	612	CLA	C14-C13-C15-C16
25	B	615	CLA	C6-C7-C8-C9
25	B	616	CLA	C14-C13-C15-C16
25	C	502	CLA	C14-C13-C15-C16
25	C	512	CLA	C14-C13-C15-C16
25	R	610	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	Y	602	CLA	C6-C7-C8-C9
25	Y	613	CLA	C14-C13-C15-C16
25	b	612	CLA	C14-C13-C15-C16
25	b	615	CLA	C6-C7-C8-C9
25	b	616	CLA	C14-C13-C15-C16
25	c	502	CLA	C14-C13-C15-C16
25	c	512	CLA	C14-C13-C15-C16
25	r	610	CLA	C11-C10-C8-C9
25	y	602	CLA	C6-C7-C8-C9
25	y	613	CLA	C14-C13-C15-C16
29	G	2630	LHG	C28-C29-C30-C31
29	g	2630	LHG	C28-C29-C30-C31
35	A	415	LMG	C37-C38-C39-C40
35	a	415	LMG	C37-C38-C39-C40
35	b	2633	LMG	C17-C18-C19-C20
37	H	102	DGD	CBA-CCA-CDA-CEA
28	2	1623	NEX	C9-C10-C11-C12
28	6	1623	NEX	C9-C10-C11-C12
35	B	2633	LMG	C17-C18-C19-C20
37	h	102	DGD	CBA-CCA-CDA-CEA
25	c	501	CLA	O1D-CGD-O2D-CED
25	A	407	CLA	O1D-CGD-O2D-CED
25	C	501	CLA	O1D-CGD-O2D-CED
25	a	407	CLA	O1D-CGD-O2D-CED
37	C	520	DGD	C2E-C1E-O5D-C6D
37	c	520	DGD	C2E-C1E-O5D-C6D
25	D	402	CLA	C13-C15-C16-C17
25	d	402	CLA	C13-C15-C16-C17
35	a	415	LMG	C32-C33-C34-C35
37	C	518	DGD	O6E-C5E-C6E-O5E
37	c	518	DGD	O6E-C5E-C6E-O5E
25	S	602	CLA	C14-C13-C15-C16
25	s	602	CLA	C14-C13-C15-C16
29	2	2630	LHG	C4-C5-C6-O8
29	3	2630	LHG	C4-C5-C6-O8
29	C	522	LHG	C4-C5-C6-O8
29	Y	2630	LHG	C4-C5-C6-O8
29	6	2630	LHG	C4-C5-C6-O8
29	7	2630	LHG	C4-C5-C6-O8
29	c	522	LHG	C4-C5-C6-O8
29	y	2630	LHG	C4-C5-C6-O8
34	A	412	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
34	A	418	SQD	C44-C45-C46-O48
34	B	623	SQD	C44-C45-C46-O48
34	a	412	SQD	O6-C44-C45-C46
34	a	418	SQD	C44-C45-C46-O48
34	b	623	SQD	C44-C45-C46-O48
35	D	411	LMG	O1-C7-C8-C9
35	Z	101	LMG	O1-C7-C8-C9
35	d	411	LMG	O1-C7-C8-C9
35	z	101	LMG	O1-C7-C8-C9
37	C	519	DGD	O1G-C1G-C2G-C3G
37	c	519	DGD	O1G-C1G-C2G-C3G
35	A	415	LMG	C32-C33-C34-C35
29	b	2630	LHG	C10-C11-C12-C13
29	S	2630	LHG	O2-C2-C3-O3
29	s	2630	LHG	O2-C2-C3-O3
29	B	2630	LHG	C10-C11-C12-C13
29	D	410	LHG	C25-C26-C27-C28
29	S	2630	LHG	C29-C30-C31-C32
29	d	410	LHG	C25-C26-C27-C28
29	s	2630	LHG	C29-C30-C31-C32
25	N	604	CLA	CBA-CGA-O2A-C1
25	n	604	CLA	CBA-CGA-O2A-C1
29	C	523	LHG	C11-C10-C9-C8
29	c	523	LHG	C11-C10-C9-C8
29	y	2630	LHG	C18-C19-C20-C21
34	A	412	SQD	C14-C15-C16-C17
34	a	412	SQD	C14-C15-C16-C17
29	C	523	LHG	C13-C14-C15-C16
29	Y	2630	LHG	C18-C19-C20-C21
29	c	523	LHG	C13-C14-C15-C16
37	C	519	DGD	C2B-C3B-C4B-C5B
37	c	519	DGD	C2B-C3B-C4B-C5B
25	1	602	CLA	O1D-CGD-O2D-CED
25	5	602	CLA	O1D-CGD-O2D-CED
24	1	609	CHL	CHA-CBD-CGD-O2D
24	3	608	CHL	CHA-CBD-CGD-O1D
24	N	609	CHL	CHA-CBD-CGD-O1D
24	S	608	CHL	CHA-CBD-CGD-O1D
24	S	608	CHL	CHA-CBD-CGD-O2D
24	5	609	CHL	CHA-CBD-CGD-O2D
24	7	608	CHL	CHA-CBD-CGD-O1D
24	n	609	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	s	608	CHL	CHA-CBD-CGD-O1D
24	s	608	CHL	CHA-CBD-CGD-O2D
24	R	606	CHL	C13-C15-C16-C17
24	Y	607	CHL	C5-C6-C7-C8
24	r	606	CHL	C13-C15-C16-C17
24	y	607	CHL	C5-C6-C7-C8
24	1	607	CHL	C4-C3-C5-C6
24	3	607	CHL	C4-C3-C5-C6
24	5	607	CHL	C4-C3-C5-C6
24	7	607	CHL	C4-C3-C5-C6
24	5	607	CHL	C2-C3-C5-C6
25	C	501	CLA	C2-C3-C5-C6
25	c	501	CLA	C2-C3-C5-C6
29	C	2630	LHG	C28-C29-C30-C31
24	Y	608	CHL	C13-C15-C16-C17
24	g	607	CHL	C10-C11-C12-C13
24	y	608	CHL	C13-C15-C16-C17
35	B	2633	LMG	O6-C5-C6-O5
35	b	2633	LMG	O6-C5-C6-O5
24	G	607	CHL	C10-C11-C12-C13
24	Y	608	CHL	C8-C10-C11-C12
24	y	608	CHL	C8-C10-C11-C12
25	G	612	CLA	C8-C10-C11-C12
29	C	522	LHG	C33-C34-C35-C36
29	c	2630	LHG	C28-C29-C30-C31
29	c	522	LHG	C33-C34-C35-C36
37	C	518	DGD	C4D-C5D-C6D-O5D
37	c	518	DGD	C4D-C5D-C6D-O5D
25	g	612	CLA	C8-C10-C11-C12
29	L	101	LHG	C27-C28-C29-C30
34	B	623	SQD	C25-C26-C27-C28
34	b	623	SQD	C25-C26-C27-C28
37	C	520	DGD	C3B-C4B-C5B-C6B
35	B	622	LMG	C28-C29-C30-C31
35	b	622	LMG	C28-C29-C30-C31
25	G	604	CLA	O1A-CGA-O2A-C1
29	C	2630	LHG	C26-C27-C28-C29
29	c	2630	LHG	C26-C27-C28-C29
29	l	101	LHG	C27-C28-C29-C30
35	a	413	LMG	C32-C33-C34-C35
37	c	520	DGD	C3B-C4B-C5B-C6B
25	6	610	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	1	603	CLA	CBA-CGA-O2A-C1
25	B	615	CLA	CBA-CGA-O2A-C1
25	5	603	CLA	CBA-CGA-O2A-C1
25	b	615	CLA	CBA-CGA-O2A-C1
29	R	2630	LHG	C18-C19-C20-C21
29	r	2630	LHG	C18-C19-C20-C21
35	A	413	LMG	C32-C33-C34-C35
24	2	607	CHL	C5-C6-C7-C8
24	6	607	CHL	C5-C6-C7-C8
25	G	611	CLA	C5-C6-C7-C8
25	g	611	CLA	C5-C6-C7-C8
29	S	2630	LHG	C27-C28-C29-C30
29	s	2630	LHG	C27-C28-C29-C30
35	C	521	LMG	C37-C38-C39-C40
35	c	521	LMG	C37-C38-C39-C40
24	3	606	CHL	C3C-C2C-CMC-OMC
24	4	606	CHL	C3C-C2C-CMC-OMC
24	G	606	CHL	C3C-C2C-CMC-OMC
24	Y	608	CHL	C3C-C2C-CMC-OMC
24	7	606	CHL	C3C-C2C-CMC-OMC
24	8	606	CHL	C3C-C2C-CMC-OMC
24	g	606	CHL	C3C-C2C-CMC-OMC
24	y	608	CHL	C3C-C2C-CMC-OMC
30	T	101	BCR	C19-C20-C21-C22
30	t	101	BCR	C19-C20-C21-C22
25	1	604	CLA	O1A-CGA-O2A-C1
25	g	604	CLA	O1A-CGA-O2A-C1
29	g	2630	LHG	C12-C13-C14-C15
25	2	610	CLA	O1D-CGD-O2D-CED
29	G	2630	LHG	C12-C13-C14-C15
29	S	2630	LHG	C13-C14-C15-C16
29	D	410	LHG	O6-C4-C5-O7
29	d	410	LHG	O6-C4-C5-O7
29	g	2630	LHG	C13-C14-C15-C16
29	s	2630	LHG	C13-C14-C15-C16
37	B	626	DGD	C6A-C7A-C8A-C9A
37	b	626	DGD	C6A-C7A-C8A-C9A
25	C	503	CLA	CBA-CGA-O2A-C1
25	G	613	CLA	CBA-CGA-O2A-C1
25	c	503	CLA	CBA-CGA-O2A-C1
25	g	613	CLA	CBA-CGA-O2A-C1
25	5	604	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	G	2630	LHG	C13-C14-C15-C16
24	R	608	CHL	C2-C3-C5-C6
24	r	608	CHL	C2-C3-C5-C6
25	Y	603	CLA	C2-C3-C5-C6
25	y	603	CLA	C2-C3-C5-C6
29	C	522	LHG	C24-C25-C26-C27
29	D	408	LHG	C11-C12-C13-C14
29	L	101	LHG	C34-C35-C36-C37
29	N	2630	LHG	C13-C14-C15-C16
29	c	522	LHG	C24-C25-C26-C27
29	l	101	LHG	C34-C35-C36-C37
29	n	2630	LHG	C13-C14-C15-C16
35	C	521	LMG	C36-C37-C38-C39
35	c	521	LMG	C36-C37-C38-C39
37	C	520	DGD	C3A-C4A-C5A-C6A
29	1	2630	LHG	C26-C27-C28-C29
29	D	409	LHG	C32-C33-C34-C35
29	S	2630	LHG	C9-C10-C11-C12
29	d	408	LHG	C11-C12-C13-C14
29	s	2630	LHG	C9-C10-C11-C12
37	c	520	DGD	C3A-C4A-C5A-C6A
37	c	520	DGD	C6B-C7B-C8B-C9B
29	1	2630	LHG	C27-C28-C29-C30
29	5	2630	LHG	C27-C28-C29-C30
29	C	2630	LHG	C27-C28-C29-C30
29	D	409	LHG	C28-C29-C30-C31
29	5	2630	LHG	C26-C27-C28-C29
29	c	2630	LHG	C27-C28-C29-C30
29	d	409	LHG	C28-C29-C30-C31
29	d	409	LHG	C32-C33-C34-C35
37	C	520	DGD	C6B-C7B-C8B-C9B
29	Y	2630	LHG	O7-C5-C6-O8
29	y	2630	LHG	O7-C5-C6-O8
35	A	413	LMG	C19-C20-C21-C22
35	a	413	LMG	C19-C20-C21-C22
29	7	2630	LHG	C16-C17-C18-C19
29	y	2630	LHG	C34-C35-C36-C37
37	C	519	DGD	C2A-C3A-C4A-C5A
37	c	519	DGD	C2A-C3A-C4A-C5A
24	2	607	CHL	C2C-C3C-CAC-CBC
24	6	607	CHL	C2C-C3C-CAC-CBC
29	3	2630	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	B	2630	LHG	C13-C14-C15-C16
29	Y	2630	LHG	C34-C35-C36-C37
29	b	2630	LHG	C13-C14-C15-C16
34	B	623	SQD	C27-C28-C29-C30
34	b	623	SQD	C27-C28-C29-C30
25	A	405	CLA	C2A-CAA-CBA-CGA
25	a	405	CLA	C2A-CAA-CBA-CGA
35	b	622	LMG	C16-C17-C18-C19
37	C	518	DGD	O6D-C5D-C6D-O5D
37	c	518	DGD	O6D-C5D-C6D-O5D
24	G	607	CHL	C15-C16-C17-C18
24	g	607	CHL	C15-C16-C17-C18
35	B	622	LMG	C16-C17-C18-C19
29	D	408	LHG	C16-C17-C18-C19
29	d	408	LHG	C16-C17-C18-C19
37	B	626	DGD	CDB-CEB-CFB-CGB
37	b	626	DGD	CDB-CEB-CFB-CGB
29	B	2630	LHG	C19-C20-C21-C22
29	b	2630	LHG	C19-C20-C21-C22
35	B	622	LMG	C30-C31-C32-C33
35	b	622	LMG	C30-C31-C32-C33
37	C	518	DGD	CAB-CBB-CCB-CDB
37	c	518	DGD	CAB-CBB-CCB-CDB
25	R	613	CLA	O1D-CGD-O2D-CED
25	r	613	CLA	O1D-CGD-O2D-CED
25	3	610	CLA	CBA-CGA-O2A-C1
25	C	502	CLA	CBA-CGA-O2A-C1
25	7	610	CLA	CBA-CGA-O2A-C1
25	c	502	CLA	CBA-CGA-O2A-C1
35	C	521	LMG	C4-C5-C6-O5
35	c	521	LMG	C4-C5-C6-O5
24	1	606	CHL	C1C-C2C-CMC-OMC
24	2	606	CHL	C1C-C2C-CMC-OMC
24	3	606	CHL	C1C-C2C-CMC-OMC
24	5	606	CHL	C1C-C2C-CMC-OMC
24	6	606	CHL	C1C-C2C-CMC-OMC
24	7	606	CHL	C1C-C2C-CMC-OMC
35	B	622	LMG	C11-C10-O7-C8
35	b	622	LMG	C11-C10-O7-C8
29	3	2630	LHG	C35-C36-C37-C38
29	7	2630	LHG	C35-C36-C37-C38
29	Y	2630	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	y	2630	LHG	C14-C15-C16-C17
25	D	402	CLA	C8-C10-C11-C12
25	d	402	CLA	C8-C10-C11-C12
34	B	623	SQD	C11-C10-C9-C8
34	b	623	SQD	C11-C10-C9-C8
25	3	602	CLA	O1D-CGD-O2D-CED
25	7	602	CLA	O1D-CGD-O2D-CED
25	1	613	CLA	C6-C7-C8-C10
25	5	613	CLA	C6-C7-C8-C10
25	1	603	CLA	C4-C3-C5-C6
25	5	603	CLA	C4-C3-C5-C6
24	3	609	CHL	CBA-CGA-O2A-C1
24	7	609	CHL	CBA-CGA-O2A-C1
25	C	512	CLA	CBA-CGA-O2A-C1
25	G	612	CLA	CBA-CGA-O2A-C1
25	Y	613	CLA	CBA-CGA-O2A-C1
25	c	512	CLA	CBA-CGA-O2A-C1
25	g	612	CLA	CBA-CGA-O2A-C1
25	y	613	CLA	CBA-CGA-O2A-C1
29	G	2630	LHG	C17-C18-C19-C20
29	G	2630	LHG	C29-C30-C31-C32
29	g	2630	LHG	C17-C18-C19-C20
29	g	2630	LHG	C29-C30-C31-C32
35	D	411	LMG	C11-C12-C13-C14
29	D	410	LHG	O1-C1-C2-O2
29	d	410	LHG	O1-C1-C2-O2
24	1	607	CHL	C6-C7-C8-C9
24	3	601	CHL	C14-C13-C15-C16
24	5	607	CHL	C6-C7-C8-C9
24	7	601	CHL	C14-C13-C15-C16
25	3	602	CLA	C6-C7-C8-C9
25	B	603	CLA	C6-C7-C8-C9
25	B	609	CLA	C14-C13-C15-C16
25	C	502	CLA	C11-C10-C8-C9
25	C	507	CLA	C14-C13-C15-C16
25	C	510	CLA	C14-C13-C15-C16
25	G	603	CLA	C11-C10-C8-C9
25	G	610	CLA	C11-C12-C13-C14
25	G	610	CLA	C14-C13-C15-C16
25	G	612	CLA	C11-C10-C8-C9
25	G	613	CLA	C11-C12-C13-C14
25	N	602	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	Y	611	CLA	C11-C10-C8-C9
25	Y	612	CLA	C11-C10-C8-C9
25	7	602	CLA	C6-C7-C8-C9
25	b	603	CLA	C6-C7-C8-C9
25	b	609	CLA	C14-C13-C15-C16
25	c	502	CLA	C11-C10-C8-C9
25	c	507	CLA	C14-C13-C15-C16
25	c	510	CLA	C14-C13-C15-C16
25	g	603	CLA	C11-C10-C8-C9
25	g	610	CLA	C11-C12-C13-C14
25	g	610	CLA	C14-C13-C15-C16
25	g	612	CLA	C11-C10-C8-C9
25	g	613	CLA	C11-C12-C13-C14
25	n	602	CLA	C6-C7-C8-C9
25	y	611	CLA	C11-C10-C8-C9
25	y	612	CLA	C11-C10-C8-C9
35	d	411	LMG	C11-C12-C13-C14
24	G	608	CHL	C15-C16-C17-C18
24	g	608	CHL	C15-C16-C17-C18
25	N	603	CLA	C15-C16-C17-C18
25	1	610	CLA	C4B-C3B-CAB-CBB
25	1	612	CLA	C4B-C3B-CAB-CBB
25	1	614	CLA	C4B-C3B-CAB-CBB
25	4	604	CLA	C4B-C3B-CAB-CBB
25	4	610	CLA	C4B-C3B-CAB-CBB
25	A	410	CLA	C4B-C3B-CAB-CBB
25	B	602	CLA	C4B-C3B-CAB-CBB
25	B	603	CLA	C4B-C3B-CAB-CBB
25	B	611	CLA	C4B-C3B-CAB-CBB
25	G	614	CLA	C4B-C3B-CAB-CBB
25	R	603	CLA	C4B-C3B-CAB-CBB
25	Y	610	CLA	C4B-C3B-CAB-CBB
25	5	610	CLA	C4B-C3B-CAB-CBB
25	5	612	CLA	C4B-C3B-CAB-CBB
25	5	614	CLA	C4B-C3B-CAB-CBB
25	8	604	CLA	C4B-C3B-CAB-CBB
25	8	610	CLA	C4B-C3B-CAB-CBB
25	a	410	CLA	C4B-C3B-CAB-CBB
25	b	602	CLA	C4B-C3B-CAB-CBB
25	b	603	CLA	C4B-C3B-CAB-CBB
25	b	611	CLA	C4B-C3B-CAB-CBB
25	g	614	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	r	603	CLA	C4B-C3B-CAB-CBB
25	y	610	CLA	C4B-C3B-CAB-CBB
29	L	101	LHG	C33-C34-C35-C36
29	l	101	LHG	C33-C34-C35-C36
34	A	418	SQD	C18-C19-C20-C21
34	a	418	SQD	C18-C19-C20-C21
24	N	601	CHL	C10-C11-C12-C13
24	n	601	CHL	C10-C11-C12-C13
25	B	602	CLA	C13-C15-C16-C17
25	b	602	CLA	C13-C15-C16-C17
25	n	603	CLA	C15-C16-C17-C18
24	N	609	CHL	C16-C17-C18-C19
24	n	609	CHL	C16-C17-C18-C19
25	R	602	CLA	C2A-CAA-CBA-CGA
25	r	602	CLA	C2A-CAA-CBA-CGA
34	a	418	SQD	C17-C18-C19-C20
35	Z	101	LMG	C15-C16-C17-C18
35	z	101	LMG	C15-C16-C17-C18
24	S	607	CHL	C8-C10-C11-C12
24	s	607	CHL	C8-C10-C11-C12
34	A	418	SQD	C17-C18-C19-C20
35	D	411	LMG	C16-C17-C18-C19
35	d	411	LMG	C16-C17-C18-C19
29	D	409	LHG	O6-C4-C5-C6
29	d	409	LHG	O6-C4-C5-C6
24	1	607	CHL	C6-C7-C8-C10
24	2	607	CHL	C6-C7-C8-C10
24	G	607	CHL	C12-C13-C15-C16
24	Y	609	CHL	C12-C13-C15-C16
24	5	607	CHL	C6-C7-C8-C10
24	6	607	CHL	C6-C7-C8-C10
24	g	607	CHL	C12-C13-C15-C16
24	y	609	CHL	C12-C13-C15-C16
25	B	609	CLA	C12-C13-C15-C16
25	B	616	CLA	C11-C10-C8-C7
25	B	616	CLA	C11-C12-C13-C15
25	C	502	CLA	C6-C7-C8-C10
25	C	502	CLA	C11-C10-C8-C7
25	C	506	CLA	C11-C12-C13-C15
25	C	507	CLA	C11-C10-C8-C7
25	C	507	CLA	C12-C13-C15-C16
25	C	509	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	C	512	CLA	C12-C13-C15-C16
25	D	403	CLA	C11-C12-C13-C15
25	G	612	CLA	C11-C10-C8-C7
25	G	613	CLA	C11-C12-C13-C15
25	R	610	CLA	C11-C10-C8-C7
25	Y	602	CLA	C6-C7-C8-C10
25	Y	613	CLA	C12-C13-C15-C16
25	b	609	CLA	C12-C13-C15-C16
25	b	616	CLA	C11-C10-C8-C7
25	b	616	CLA	C11-C12-C13-C15
25	c	502	CLA	C6-C7-C8-C10
25	c	502	CLA	C11-C10-C8-C7
25	c	506	CLA	C11-C12-C13-C15
25	c	507	CLA	C11-C10-C8-C7
25	c	507	CLA	C12-C13-C15-C16
25	c	509	CLA	C6-C7-C8-C10
25	c	512	CLA	C12-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C15
25	g	612	CLA	C11-C10-C8-C7
25	g	613	CLA	C11-C12-C13-C15
25	r	610	CLA	C11-C10-C8-C7
25	y	602	CLA	C6-C7-C8-C10
25	y	613	CLA	C12-C13-C15-C16
24	R	607	CHL	C5-C6-C7-C8
24	r	607	CHL	C5-C6-C7-C8
25	B	616	CLA	C16-C17-C18-C19
25	b	616	CLA	C16-C17-C18-C19
37	C	520	DGD	C4D-C5D-C6D-O5D
24	3	609	CHL	O1D-CGD-O2D-CED
24	7	609	CHL	O1D-CGD-O2D-CED
34	b	623	SQD	C13-C14-C15-C16
24	R	608	CHL	C3A-C2A-CAA-CBA
24	Y	605	CHL	C3A-C2A-CAA-CBA
24	r	608	CHL	C3A-C2A-CAA-CBA
25	B	610	CLA	C3A-C2A-CAA-CBA
25	C	510	CLA	C4-C3-C5-C6
25	S	604	CLA	C3A-C2A-CAA-CBA
25	b	610	CLA	C3A-C2A-CAA-CBA
25	c	510	CLA	C4-C3-C5-C6
25	s	604	CLA	C3A-C2A-CAA-CBA
36	D	405	PL9	C45-C44-C46-C47
36	d	405	PL9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
29	3	2630	LHG	O8-C23-C24-C25
29	7	2630	LHG	O8-C23-C24-C25
36	D	405	PL9	C43-C44-C46-C47
36	d	405	PL9	C43-C44-C46-C47
34	B	623	SQD	C13-C14-C15-C16
37	H	102	DGD	C6A-C7A-C8A-C9A
37	h	102	DGD	C6A-C7A-C8A-C9A
25	N	604	CLA	O1A-CGA-O2A-C1
25	n	604	CLA	O1A-CGA-O2A-C1
37	c	520	DGD	C4D-C5D-C6D-O5D
29	Y	2630	LHG	C25-C26-C27-C28
29	y	2630	LHG	C25-C26-C27-C28
26	G	1621	LUT	C29-C30-C31-C32
26	Y	1621	LUT	C29-C30-C31-C32
26	g	1621	LUT	C29-C30-C31-C32
26	y	1621	LUT	C29-C30-C31-C32
30	H	101	BCR	C9-C10-C11-C12
30	h	101	BCR	C9-C10-C11-C12
29	R	2630	LHG	O10-C23-O8-C6
29	r	2630	LHG	O10-C23-O8-C6
29	n	2630	LHG	C34-C35-C36-C37
24	R	608	CHL	C5-C6-C7-C8
24	r	608	CHL	C5-C6-C7-C8
25	3	602	CLA	C8-C10-C11-C12
25	7	602	CLA	C8-C10-C11-C12
30	B	619	BCR	C7-C8-C9-C10
30	b	619	BCR	C7-C8-C9-C10
29	N	2630	LHG	C34-C35-C36-C37
29	5	2630	LHG	C11-C12-C13-C14
29	1	2630	LHG	C11-C12-C13-C14
29	B	2631	LHG	C31-C32-C33-C34
29	D	409	LHG	C15-C16-C17-C18
29	d	409	LHG	C15-C16-C17-C18
25	Y	611	CLA	C5-C6-C7-C8
25	y	611	CLA	C5-C6-C7-C8
29	B	2631	LHG	C4-C5-C6-O8
29	G	2630	LHG	C4-C5-C6-O8
29	R	2630	LHG	C4-C5-C6-O8
29	S	2630	LHG	C4-C5-C6-O8
29	b	2631	LHG	C4-C5-C6-O8
29	g	2630	LHG	C4-C5-C6-O8
29	r	2630	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
29	s	2630	LHG	C4-C5-C6-O8
34	B	621	SQD	C44-C45-C46-O48
34	b	621	SQD	C44-C45-C46-O48
35	A	415	LMG	C7-C8-C9-O8
35	B	2633	LMG	C7-C8-C9-O8
35	C	521	LMG	C7-C8-C9-O8
35	a	415	LMG	C7-C8-C9-O8
35	b	2633	LMG	C7-C8-C9-O8
35	c	521	LMG	C7-C8-C9-O8
37	C	520	DGD	O1G-C1G-C2G-C3G
37	c	520	DGD	O1G-C1G-C2G-C3G
29	b	2631	LHG	C31-C32-C33-C34
35	b	622	LMG	O10-C28-O8-C9
29	Y	2630	LHG	C35-C36-C37-C38
29	y	2630	LHG	C35-C36-C37-C38
24	2	601	CHL	C1A-C2A-CAA-CBA
24	2	607	CHL	C1A-C2A-CAA-CBA
24	2	608	CHL	C1A-C2A-CAA-CBA
24	3	606	CHL	C1A-C2A-CAA-CBA
24	3	608	CHL	C1A-C2A-CAA-CBA
24	4	606	CHL	C1A-C2A-CAA-CBA
24	6	601	CHL	C1A-C2A-CAA-CBA
24	6	607	CHL	C1A-C2A-CAA-CBA
24	6	608	CHL	C1A-C2A-CAA-CBA
24	7	606	CHL	C1A-C2A-CAA-CBA
24	7	608	CHL	C1A-C2A-CAA-CBA
24	8	606	CHL	C1A-C2A-CAA-CBA
24	G	601	CHL	C15-C16-C17-C18
24	g	601	CHL	C15-C16-C17-C18
29	C	2630	LHG	C30-C31-C32-C33
29	C	523	LHG	C27-C28-C29-C30
29	c	2630	LHG	C30-C31-C32-C33
29	c	523	LHG	C27-C28-C29-C30
24	R	608	CHL	C4-C3-C5-C6
24	r	608	CHL	C4-C3-C5-C6
25	B	616	CLA	C4-C3-C5-C6
25	Y	603	CLA	C4-C3-C5-C6
25	b	616	CLA	C4-C3-C5-C6
25	y	603	CLA	C4-C3-C5-C6
36	D	405	PL9	C15-C14-C16-C17
36	D	405	PL9	C30-C29-C31-C32
36	d	405	PL9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
36	d	405	PL9	C30-C29-C31-C32
35	B	622	LMG	C40-C41-C42-C43
35	b	622	LMG	C40-C41-C42-C43
25	B	616	CLA	C2-C3-C5-C6
25	5	603	CLA	C2-C3-C5-C6
25	b	616	CLA	C2-C3-C5-C6
35	B	622	LMG	O10-C28-O8-C9
29	Y	2630	LHG	C11-C12-C13-C14
29	Y	2630	LHG	C28-C29-C30-C31
29	y	2630	LHG	C11-C12-C13-C14
29	y	2630	LHG	C28-C29-C30-C31
25	N	610	CLA	C16-C17-C18-C19
25	n	610	CLA	C16-C17-C18-C19
25	3	610	CLA	C2B-C3B-CAB-CBB
25	7	610	CLA	C2B-C3B-CAB-CBB
26	1	1621	LUT	C1-C6-C7-C8
26	Y	1620	LUT	C1-C6-C7-C8
26	5	1621	LUT	C1-C6-C7-C8
26	y	1620	LUT	C1-C6-C7-C8
30	4	623	BCR	C1-C6-C7-C8
30	A	411	BCR	C23-C24-C25-C30
30	B	620	BCR	C23-C24-C25-C26
30	B	620	BCR	C23-C24-C25-C30
30	C	514	BCR	C1-C6-C7-C8
30	C	515	BCR	C23-C24-C25-C30
30	D	404	BCR	C1-C6-C7-C8
30	8	623	BCR	C1-C6-C7-C8
30	a	411	BCR	C23-C24-C25-C30
30	b	620	BCR	C23-C24-C25-C26
30	b	620	BCR	C23-C24-C25-C30
30	c	514	BCR	C1-C6-C7-C8
30	c	515	BCR	C23-C24-C25-C30
30	d	404	BCR	C1-C6-C7-C8
25	R	603	CLA	C5-C6-C7-C8
25	r	603	CLA	C5-C6-C7-C8
29	C	2630	LHG	C34-C35-C36-C37
25	Y	603	CLA	C5-C6-C7-C8
25	g	602	CLA	O1D-CGD-O2D-CED
29	c	2630	LHG	C34-C35-C36-C37
37	c	520	DGD	C5B-C6B-C7B-C8B
25	G	602	CLA	O1D-CGD-O2D-CED
24	G	609	CHL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	g	609	CHL	C10-C11-C12-C13
25	y	603	CLA	C5-C6-C7-C8
29	2	2630	LHG	O7-C5-C6-O8
29	G	2630	LHG	O7-C5-C6-O8
29	R	2630	LHG	O7-C5-C6-O8
29	6	2630	LHG	O7-C5-C6-O8
29	g	2630	LHG	O7-C5-C6-O8
29	r	2630	LHG	O7-C5-C6-O8
34	B	621	SQD	O6-C44-C45-O47
34	B	623	SQD	O6-C44-C45-O47
34	b	621	SQD	O6-C44-C45-O47
34	b	623	SQD	O6-C44-C45-O47
35	A	413	LMG	O1-C7-C8-O7
35	a	413	LMG	O1-C7-C8-O7
37	C	520	DGD	C5B-C6B-C7B-C8B
25	C	506	CLA	C3-C5-C6-C7
25	c	506	CLA	C3-C5-C6-C7
25	S	602	CLA	C12-C13-C15-C16
25	s	602	CLA	C12-C13-C15-C16
25	1	603	CLA	O1A-CGA-O2A-C1
25	B	615	CLA	O1A-CGA-O2A-C1
25	5	603	CLA	O1A-CGA-O2A-C1
25	b	615	CLA	O1A-CGA-O2A-C1
29	C	523	LHG	C30-C31-C32-C33
29	c	523	LHG	C30-C31-C32-C33
25	1	610	CLA	C5-C6-C7-C8
25	C	505	CLA	C10-C11-C12-C13
25	5	610	CLA	C5-C6-C7-C8
25	c	505	CLA	C10-C11-C12-C13
25	1	603	CLA	C2-C3-C5-C6
25	C	510	CLA	C2-C3-C5-C6
25	c	510	CLA	C2-C3-C5-C6
29	C	523	LHG	C16-C17-C18-C19
29	c	523	LHG	C16-C17-C18-C19
25	1	613	CLA	C6-C7-C8-C9
25	5	613	CLA	C6-C7-C8-C9
25	C	502	CLA	C3-C5-C6-C7
25	c	502	CLA	C3-C5-C6-C7
29	d	410	LHG	C32-C33-C34-C35
24	2	607	CHL	C6-C7-C8-C9
24	R	606	CHL	C14-C13-C15-C16
24	6	607	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	r	606	CHL	C14-C13-C15-C16
25	B	602	CLA	C6-C7-C8-C9
25	B	613	CLA	C11-C10-C8-C9
25	B	616	CLA	C11-C12-C13-C14
25	Y	612	CLA	C6-C7-C8-C9
25	b	602	CLA	C6-C7-C8-C9
25	b	613	CLA	C11-C10-C8-C9
25	b	616	CLA	C11-C12-C13-C14
25	c	504	CLA	C11-C10-C8-C9
25	y	612	CLA	C6-C7-C8-C9
29	3	2630	LHG	C24-C25-C26-C27
29	7	2630	LHG	C24-C25-C26-C27
29	D	410	LHG	C32-C33-C34-C35
25	N	611	CLA	O1D-CGD-O2D-CED
25	n	611	CLA	O1D-CGD-O2D-CED
25	C	503	CLA	O1A-CGA-O2A-C1
25	c	503	CLA	O1A-CGA-O2A-C1
24	N	607	CHL	C16-C17-C18-C20
24	n	607	CHL	C16-C17-C18-C20
25	C	505	CLA	C16-C17-C18-C19
25	N	610	CLA	C16-C17-C18-C20
25	c	505	CLA	C16-C17-C18-C19
25	n	610	CLA	C16-C17-C18-C20
24	N	601	CHL	C3-C5-C6-C7
24	n	601	CHL	C3-C5-C6-C7
29	Y	2630	LHG	C27-C28-C29-C30
29	y	2630	LHG	C27-C28-C29-C30
25	R	612	CLA	O2A-C1-C2-C3
25	r	612	CLA	O2A-C1-C2-C3
24	y	609	CHL	C8-C10-C11-C12
25	B	612	CLA	C8-C10-C11-C12
37	C	520	DGD	O6D-C5D-C6D-O5D
37	c	520	DGD	O6D-C5D-C6D-O5D
35	A	413	LMG	C11-C12-C13-C14
35	a	413	LMG	C11-C12-C13-C14
29	c	522	LHG	O2-C2-C3-O3
24	Y	609	CHL	C8-C10-C11-C12
25	B	611	CLA	C15-C16-C17-C18
25	b	611	CLA	C15-C16-C17-C18
25	b	612	CLA	C8-C10-C11-C12
25	N	612	CLA	C4-C3-C5-C6
25	n	612	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	N	1623	NEX	C33-C34-C35-C15
28	n	1623	NEX	C33-C34-C35-C15
29	S	2630	LHG	C35-C36-C37-C38
29	s	2630	LHG	C35-C36-C37-C38
24	r	608	CHL	C11-C12-C13-C15
29	L	101	LHG	C31-C32-C33-C34
29	l	101	LHG	C31-C32-C33-C34
25	C	513	CLA	C15-C16-C17-C18
25	c	513	CLA	C15-C16-C17-C18
29	R	2630	LHG	C15-C16-C17-C18
29	r	2630	LHG	C15-C16-C17-C18
25	G	613	CLA	O1A-CGA-O2A-C1
25	R	613	CLA	O1A-CGA-O2A-C1
25	g	613	CLA	O1A-CGA-O2A-C1
25	r	613	CLA	O1A-CGA-O2A-C1
29	Y	2630	LHG	O10-C23-O8-C6
29	y	2630	LHG	O10-C23-O8-C6
24	3	601	CHL	C15-C16-C17-C18
24	7	601	CHL	C15-C16-C17-C18
29	N	2630	LHG	C11-C12-C13-C14
29	n	2630	LHG	C11-C12-C13-C14
25	N	613	CLA	C8-C10-C11-C12
25	n	613	CLA	C8-C10-C11-C12
29	B	2630	LHG	C28-C29-C30-C31
29	b	2630	LHG	C28-C29-C30-C31
29	C	523	LHG	O6-C4-C5-C6
29	c	523	LHG	O6-C4-C5-C6
24	R	608	CHL	C11-C12-C13-C14
24	R	608	CHL	C11-C12-C13-C15
24	r	608	CHL	C11-C12-C13-C14
25	B	616	CLA	C16-C17-C18-C20
25	N	602	CLA	C16-C17-C18-C19
25	b	616	CLA	C16-C17-C18-C20
25	n	602	CLA	C16-C17-C18-C19
24	R	606	CHL	C5-C6-C7-C8
24	r	606	CHL	C5-C6-C7-C8
25	a	405	CLA	C5-C6-C7-C8
24	3	601	CHL	C11-C10-C8-C7
24	N	601	CHL	C11-C10-C8-C7
24	N	607	CHL	C12-C13-C15-C16
24	R	606	CHL	C6-C7-C8-C10
24	R	606	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	Y	607	CHL	C12-C13-C15-C16
24	7	601	CHL	C11-C10-C8-C7
24	n	601	CHL	C11-C10-C8-C7
24	n	607	CHL	C12-C13-C15-C16
24	r	606	CHL	C6-C7-C8-C10
24	r	606	CHL	C12-C13-C15-C16
24	y	607	CHL	C12-C13-C15-C16
25	1	602	CLA	C6-C7-C8-C10
25	B	613	CLA	C11-C10-C8-C7
25	C	507	CLA	C6-C7-C8-C10
25	C	509	CLA	C11-C10-C8-C7
25	C	510	CLA	C11-C10-C8-C7
25	N	603	CLA	C12-C13-C15-C16
25	S	611	CLA	C6-C7-C8-C10
25	Y	603	CLA	C12-C13-C15-C16
25	5	602	CLA	C6-C7-C8-C10
25	b	613	CLA	C11-C10-C8-C7
25	c	507	CLA	C6-C7-C8-C10
25	c	509	CLA	C11-C10-C8-C7
25	c	510	CLA	C11-C10-C8-C7
25	n	603	CLA	C12-C13-C15-C16
25	s	611	CLA	C6-C7-C8-C10
25	y	603	CLA	C12-C13-C15-C16
29	D	410	LHG	C28-C29-C30-C31
29	d	410	LHG	C28-C29-C30-C31
29	g	2630	LHG	C24-C25-C26-C27
35	D	411	LMG	C17-C18-C19-C20
35	d	411	LMG	C17-C18-C19-C20
24	G	607	CHL	C13-C15-C16-C17
25	A	405	CLA	C5-C6-C7-C8
26	4	620	LUT	C27-C28-C29-C30
26	8	620	LUT	C27-C28-C29-C30
27	Y	1622	XAT	C11-C12-C13-C14
27	y	1622	XAT	C11-C12-C13-C14
30	B	620	BCR	C21-C22-C23-C24
30	b	620	BCR	C21-C22-C23-C24
35	A	413	LMG	C29-C28-O8-C9
35	a	413	LMG	C29-C28-O8-C9
29	G	2630	LHG	C24-C25-C26-C27
24	7	609	CHL	O1A-CGA-O2A-C1
25	3	610	CLA	O1A-CGA-O2A-C1
25	C	512	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	7	610	CLA	O1A-CGA-O2A-C1
25	c	512	CLA	O1A-CGA-O2A-C1
34	B	623	SQD	C5-C6-S-O8
34	b	623	SQD	C5-C6-S-O8
24	G	609	CHL	C8-C10-C11-C12
24	g	607	CHL	C13-C15-C16-C17
25	D	403	CLA	C10-C11-C12-C13
25	d	403	CLA	C10-C11-C12-C13
25	2	602	CLA	C2A-CAA-CBA-CGA
25	G	603	CLA	C2A-CAA-CBA-CGA
25	S	614	CLA	C2A-CAA-CBA-CGA
25	6	602	CLA	C2A-CAA-CBA-CGA
25	g	603	CLA	C2A-CAA-CBA-CGA
25	s	614	CLA	C2A-CAA-CBA-CGA
24	3	609	CHL	O1A-CGA-O2A-C1
25	c	502	CLA	O1A-CGA-O2A-C1
37	h	102	DGD	O6D-C5D-C6D-O5D
24	g	609	CHL	C8-C10-C11-C12
25	G	603	CLA	C5-C6-C7-C8
25	g	603	CLA	C5-C6-C7-C8
25	y	610	CLA	C10-C11-C12-C13
25	C	502	CLA	O1A-CGA-O2A-C1
25	Y	613	CLA	O1A-CGA-O2A-C1
25	y	613	CLA	O1A-CGA-O2A-C1
29	c	522	LHG	O10-C23-O8-C6
35	C	521	LMG	C40-C41-C42-C43
35	c	521	LMG	C40-C41-C42-C43
37	h	102	DGD	CCB-CDB-CEB-CFB
25	B	614	CLA	C15-C16-C17-C18
25	Y	610	CLA	C10-C11-C12-C13
25	b	614	CLA	C15-C16-C17-C18
35	D	411	LMG	C33-C34-C35-C36
37	H	102	DGD	CCB-CDB-CEB-CFB
37	c	519	DGD	C8B-C9B-CAB-CBB
24	R	607	CHL	C6-C7-C8-C10
24	r	607	CHL	C6-C7-C8-C10
29	D	410	LHG	C16-C17-C18-C19
35	d	411	LMG	C33-C34-C35-C36
37	C	519	DGD	C8B-C9B-CAB-CBB
29	d	410	LHG	C16-C17-C18-C19
25	G	612	CLA	O1A-CGA-O2A-C1
25	g	612	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	C	522	LHG	O10-C23-O8-C6
29	C	522	LHG	O2-C2-C3-O3
25	b	613	CLA	C15-C16-C17-C18
25	c	501	CLA	C15-C16-C17-C18
25	G	610	CLA	C15-C16-C17-C18
25	g	610	CLA	C15-C16-C17-C18
24	N	607	CHL	C10-C11-C12-C13
24	n	607	CHL	C10-C11-C12-C13
25	B	613	CLA	C15-C16-C17-C18
25	C	501	CLA	C15-C16-C17-C18
29	D	409	LHG	O6-C4-C5-O7
29	d	409	LHG	O6-C4-C5-O7
29	1	2630	LHG	C15-C16-C17-C18
29	c	2630	LHG	C13-C14-C15-C16
37	H	102	DGD	C8A-C9A-CAA-CBA
37	h	102	DGD	C8A-C9A-CAA-CBA
37	H	102	DGD	O6D-C5D-C6D-O5D
29	C	2630	LHG	C13-C14-C15-C16
29	5	2630	LHG	C15-C16-C17-C18
29	4	2630	LHG	C4-C5-C6-O8
29	C	2630	LHG	C4-C5-C6-O8
29	8	2630	LHG	C4-C5-C6-O8
29	c	2630	LHG	C4-C5-C6-O8
34	B	621	SQD	O6-C44-C45-C46
34	b	621	SQD	O6-C44-C45-C46
36	D	405	PL9	C39-C41-C42-C43
36	d	405	PL9	C39-C41-C42-C43
25	B	604	CLA	C16-C17-C18-C19
25	N	603	CLA	C16-C17-C18-C20
25	b	604	CLA	C16-C17-C18-C19
25	n	603	CLA	C16-C17-C18-C20
25	B	612	CLA	C4-C3-C5-C6
25	Y	612	CLA	C4-C3-C5-C6
25	b	612	CLA	C4-C3-C5-C6
25	y	612	CLA	C4-C3-C5-C6
25	n	612	CLA	C2-C3-C5-C6
25	r	610	CLA	O1D-CGD-O2D-CED
29	C	522	LHG	O7-C5-C6-O8
29	c	522	LHG	O7-C5-C6-O8
34	A	418	SQD	O47-C45-C46-O48
34	a	418	SQD	O47-C45-C46-O48
35	B	2633	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
35	C	521	LMG	O7-C8-C9-O8
35	D	411	LMG	O1-C7-C8-O7
35	b	2633	LMG	O7-C8-C9-O8
35	c	521	LMG	O7-C8-C9-O8
35	d	411	LMG	O1-C7-C8-O7
24	n	609	CHL	C8-C10-C11-C12
25	c	511	CLA	C8-C10-C11-C12
24	N	607	CHL	C14-C13-C15-C16
24	n	607	CHL	C14-C13-C15-C16
25	1	602	CLA	C6-C7-C8-C9
25	C	504	CLA	C11-C10-C8-C9
25	C	507	CLA	C11-C12-C13-C14
25	G	611	CLA	C6-C7-C8-C9
25	5	602	CLA	C6-C7-C8-C9
25	c	507	CLA	C11-C12-C13-C14
25	g	611	CLA	C6-C7-C8-C9
29	D	410	LHG	C29-C30-C31-C32
29	d	410	LHG	C29-C30-C31-C32
29	N	2630	LHG	C14-C15-C16-C17
35	A	415	LMG	C29-C30-C31-C32
24	N	609	CHL	C8-C10-C11-C12
25	C	511	CLA	C8-C10-C11-C12
35	a	415	LMG	C29-C30-C31-C32
25	G	612	CLA	C3-C5-C6-C7
25	g	612	CLA	C3-C5-C6-C7
29	n	2630	LHG	C14-C15-C16-C17
24	G	608	CHL	C16-C17-C18-C20
24	g	608	CHL	C16-C17-C18-C20
25	Y	610	CLA	C11-C12-C13-C15
25	y	610	CLA	C11-C12-C13-C15
25	N	610	CLA	C13-C15-C16-C17
25	n	610	CLA	C13-C15-C16-C17
29	L	101	LHG	C9-C10-C11-C12
29	l	101	LHG	C9-C10-C11-C12
25	R	610	CLA	O1D-CGD-O2D-CED
25	4	603	CLA	O1D-CGD-O2D-CED
25	8	603	CLA	O1D-CGD-O2D-CED
25	N	612	CLA	C2-C3-C5-C6
25	Y	612	CLA	C2-C3-C5-C6
25	y	612	CLA	C2-C3-C5-C6
24	N	607	CHL	C8-C10-C11-C12
24	n	607	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	B	606	CLA	C2A-CAA-CBA-CGA
25	b	606	CLA	C2A-CAA-CBA-CGA
25	C	506	CLA	CBA-CGA-O2A-C1
34	A	418	SQD	C28-C29-C30-C31
34	a	418	SQD	C28-C29-C30-C31
35	Z	101	LMG	C11-C12-C13-C14
35	z	101	LMG	C11-C12-C13-C14
29	C	2630	LHG	C7-C8-C9-C10
29	c	2630	LHG	C7-C8-C9-C10
29	3	2630	LHG	O10-C23-O8-C6
29	7	2630	LHG	O10-C23-O8-C6
29	D	409	LHG	C25-C26-C27-C28
29	d	409	LHG	C25-C26-C27-C28
24	G	609	CHL	C4C-C3C-CAC-CBC
24	N	607	CHL	C4C-C3C-CAC-CBC
24	Y	607	CHL	C4C-C3C-CAC-CBC
24	Y	609	CHL	C4C-C3C-CAC-CBC
24	g	609	CHL	C4C-C3C-CAC-CBC
24	n	607	CHL	C4C-C3C-CAC-CBC
24	y	607	CHL	C4C-C3C-CAC-CBC
24	y	609	CHL	C4C-C3C-CAC-CBC
29	B	2631	LHG	C12-C13-C14-C15
29	b	2631	LHG	C12-C13-C14-C15
25	c	506	CLA	CBA-CGA-O2A-C1
25	N	602	CLA	C16-C17-C18-C20
25	n	602	CLA	C16-C17-C18-C20
25	1	614	CLA	C1A-C2A-CAA-CBA
25	2	612	CLA	C4B-C3B-CAB-CBB
25	3	602	CLA	C1A-C2A-CAA-CBA
25	C	513	CLA	C1A-C2A-CAA-CBA
25	R	611	CLA	C4B-C3B-CAB-CBB
25	Y	612	CLA	C4B-C3B-CAB-CBB
25	Y	614	CLA	C1A-C2A-CAA-CBA
25	5	614	CLA	C1A-C2A-CAA-CBA
25	6	612	CLA	C4B-C3B-CAB-CBB
25	7	602	CLA	C1A-C2A-CAA-CBA
25	c	513	CLA	C1A-C2A-CAA-CBA
25	r	611	CLA	C4B-C3B-CAB-CBB
25	y	612	CLA	C4B-C3B-CAB-CBB
25	y	614	CLA	C1A-C2A-CAA-CBA
29	D	408	LHG	C24-C23-O8-C6
29	d	408	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
24	G	608	CHL	C4-C3-C5-C6
24	g	608	CHL	C4-C3-C5-C6
25	2	603	CLA	C4-C3-C5-C6
25	6	603	CLA	C4-C3-C5-C6
28	G	1623	NEX	C31-C32-C33-C34
28	g	1623	NEX	C31-C32-C33-C34
30	C	517	BCR	C9-C10-C11-C12
30	c	517	BCR	C9-C10-C11-C12
29	G	2630	LHG	C9-C10-C11-C12
29	g	2630	LHG	C9-C10-C11-C12
37	H	102	DGD	C3A-C4A-C5A-C6A
37	h	102	DGD	C3A-C4A-C5A-C6A
29	2	2630	LHG	O10-C23-O8-C6
29	6	2630	LHG	O10-C23-O8-C6
25	G	613	CLA	C2A-CAA-CBA-CGA
25	N	603	CLA	C2A-CAA-CBA-CGA
25	Y	613	CLA	C2A-CAA-CBA-CGA
25	g	613	CLA	C2A-CAA-CBA-CGA
25	n	603	CLA	C2A-CAA-CBA-CGA
25	y	613	CLA	C2A-CAA-CBA-CGA
33	A	409	PHO	C5-C6-C7-C8
33	a	409	PHO	C5-C6-C7-C8
29	B	2630	LHG	O6-C4-C5-C6
29	b	2630	LHG	O6-C4-C5-C6
35	B	622	LMG	C33-C34-C35-C36
35	b	622	LMG	C33-C34-C35-C36
24	G	601	CHL	C12-C13-C15-C16
24	G	608	CHL	C11-C10-C8-C7
24	N	601	CHL	C12-C13-C15-C16
24	g	601	CHL	C12-C13-C15-C16
24	g	608	CHL	C11-C10-C8-C7
24	n	601	CHL	C12-C13-C15-C16
25	2	602	CLA	C11-C12-C13-C15
25	B	606	CLA	C6-C7-C8-C10
25	B	607	CLA	C11-C10-C8-C7
25	B	617	CLA	C6-C7-C8-C10
25	G	610	CLA	C12-C13-C15-C16
25	G	613	CLA	C12-C13-C15-C16
25	Y	613	CLA	C11-C12-C13-C15
25	6	602	CLA	C11-C12-C13-C15
25	b	606	CLA	C6-C7-C8-C10
25	b	607	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	b	617	CLA	C6-C7-C8-C10
25	g	610	CLA	C12-C13-C15-C16
25	g	613	CLA	C12-C13-C15-C16
25	y	613	CLA	C11-C12-C13-C15
25	B	603	CLA	C16-C17-C18-C19
25	b	603	CLA	C16-C17-C18-C19
35	A	413	LMG	C12-C13-C14-C15
35	a	413	LMG	C12-C13-C14-C15
37	H	102	DGD	CAB-CBB-CCB-CDB
37	h	102	DGD	CAB-CBB-CCB-CDB
29	C	523	LHG	O2-C2-C3-O3
29	c	523	LHG	O2-C2-C3-O3
29	N	2630	LHG	C29-C30-C31-C32
29	n	2630	LHG	C29-C30-C31-C32
34	A	412	SQD	C16-C17-C18-C19
34	a	412	SQD	C16-C17-C18-C19
37	c	520	DGD	C2B-C3B-C4B-C5B
34	a	412	SQD	C28-C29-C30-C31
25	c	511	CLA	C3-C5-C6-C7
34	A	412	SQD	C28-C29-C30-C31
37	C	520	DGD	C2B-C3B-C4B-C5B
25	C	513	CLA	C3A-C2A-CAA-CBA
25	c	513	CLA	C3A-C2A-CAA-CBA
29	C	523	LHG	C19-C20-C21-C22
29	c	523	LHG	C19-C20-C21-C22
24	N	601	CHL	C15-C16-C17-C18
29	g	2630	LHG	O9-C7-O7-C5
36	A	414	PL9	C2-C3-C7-C8
36	a	414	PL9	C2-C3-C7-C8
29	B	2630	LHG	O6-C4-C5-O7
29	C	522	LHG	O6-C4-C5-O7
29	C	523	LHG	O6-C4-C5-O7
29	b	2630	LHG	O6-C4-C5-O7
29	c	522	LHG	O6-C4-C5-O7
29	c	523	LHG	O6-C4-C5-O7
25	C	511	CLA	C3-C5-C6-C7
25	Y	602	CLA	C3-C5-C6-C7
25	y	602	CLA	C3-C5-C6-C7
24	3	601	CHL	C11-C10-C8-C9
24	R	606	CHL	C6-C7-C8-C9
24	Y	607	CHL	C14-C13-C15-C16
24	7	601	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	r	606	CHL	C6-C7-C8-C9
24	y	607	CHL	C14-C13-C15-C16
25	C	507	CLA	C6-C7-C8-C9
25	N	603	CLA	C14-C13-C15-C16
25	R	610	CLA	C14-C13-C15-C16
25	S	611	CLA	C6-C7-C8-C9
25	Y	603	CLA	C14-C13-C15-C16
25	Y	613	CLA	C11-C12-C13-C14
25	c	507	CLA	C6-C7-C8-C9
25	n	603	CLA	C14-C13-C15-C16
25	r	610	CLA	C14-C13-C15-C16
25	s	611	CLA	C6-C7-C8-C9
25	y	603	CLA	C14-C13-C15-C16
25	y	613	CLA	C11-C12-C13-C14
25	c	506	CLA	O1A-CGA-O2A-C1
37	c	518	DGD	CBB-CCB-CDB-CEB
24	1	607	CHL	C10-C11-C12-C13
24	5	607	CHL	C10-C11-C12-C13
24	n	601	CHL	C15-C16-C17-C18
24	4	609	CHL	C2C-C3C-CAC-CBC
37	C	518	DGD	CBB-CCB-CDB-CEB
28	1	1623	NEX	C33-C34-C35-C15
28	5	1623	NEX	C33-C34-C35-C15
30	D	404	BCR	C9-C10-C11-C12
30	d	404	BCR	C9-C10-C11-C12
25	C	502	CLA	C8-C10-C11-C12
25	G	612	CLA	C10-C11-C12-C13
25	c	502	CLA	C8-C10-C11-C12
25	g	612	CLA	C10-C11-C12-C13
35	B	2633	LMG	C21-C22-C23-C24
24	G	606	CHL	C1-C2-C3-C4
24	N	606	CHL	C1-C2-C3-C4
24	Y	606	CHL	C1-C2-C3-C4
24	g	606	CHL	C1-C2-C3-C4
24	n	606	CHL	C1-C2-C3-C4
24	y	606	CHL	C1-C2-C3-C4
25	R	601	CLA	C1-C2-C3-C4
25	R	611	CLA	C1-C2-C3-C4
25	R	612	CLA	C1-C2-C3-C4
25	S	612	CLA	C1-C2-C3-C4
25	r	601	CLA	C1-C2-C3-C4
25	r	611	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
25	r	612	CLA	C1-C2-C3-C4
25	s	612	CLA	C1-C2-C3-C4
28	S	1623	NEX	C7-C8-C9-C10
28	s	1623	NEX	C7-C8-C9-C10
35	b	2633	LMG	C21-C22-C23-C24
25	N	602	CLA	C3-C5-C6-C7
25	n	602	CLA	C3-C5-C6-C7
24	8	609	CHL	C2C-C3C-CAC-CBC
25	C	506	CLA	O1A-CGA-O2A-C1
29	G	2630	LHG	O9-C7-O7-C5
34	B	621	SQD	O47-C45-C46-O48
34	b	621	SQD	O47-C45-C46-O48
35	Z	101	LMG	O1-C7-C8-O7
35	z	101	LMG	O1-C7-C8-O7
29	B	2631	LHG	C33-C34-C35-C36
29	b	2631	LHG	C33-C34-C35-C36
25	G	614	CLA	O2A-C1-C2-C3
25	g	614	CLA	O2A-C1-C2-C3
24	N	608	CHL	C10-C11-C12-C13
24	n	608	CHL	C10-C11-C12-C13
29	B	2630	LHG	C4-C5-C6-O8
29	b	2630	LHG	C4-C5-C6-O8
34	B	623	SQD	O6-C44-C45-C46
34	b	623	SQD	O6-C44-C45-C46
29	S	2630	LHG	C19-C20-C21-C22
29	s	2630	LHG	C19-C20-C21-C22
25	1	603	CLA	CAD-CBD-CGD-O2D
25	2	603	CLA	CAD-CBD-CGD-O2D
25	3	603	CLA	CAD-CBD-CGD-O2D
25	3	604	CLA	CAD-CBD-CGD-O2D
25	B	605	CLA	CAD-CBD-CGD-O2D
25	B	606	CLA	CAD-CBD-CGD-O2D
25	B	613	CLA	CAD-CBD-CGD-O2D
25	B	615	CLA	CAD-CBD-CGD-O2D
25	C	502	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	CAD-CBD-CGD-O2D
25	C	513	CLA	CAD-CBD-CGD-O2D
25	5	603	CLA	CAD-CBD-CGD-O2D
25	6	603	CLA	CAD-CBD-CGD-O2D
25	7	603	CLA	CAD-CBD-CGD-O2D
25	7	604	CLA	CAD-CBD-CGD-O2D
25	b	605	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	b	606	CLA	CAD-CBD-CGD-O2D
25	b	613	CLA	CAD-CBD-CGD-O2D
25	b	615	CLA	CAD-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O2D
25	c	513	CLA	CAD-CBD-CGD-O2D
24	n	609	CHL	C10-C11-C12-C13
24	N	609	CHL	C10-C11-C12-C13
29	b	2631	LHG	C13-C14-C15-C16
29	B	2631	LHG	C13-C14-C15-C16
24	G	601	CHL	C2A-CAA-CBA-CGA
24	g	601	CHL	C2A-CAA-CBA-CGA
25	1	602	CLA	C2A-CAA-CBA-CGA
25	4	602	CLA	C2A-CAA-CBA-CGA
25	5	602	CLA	C2A-CAA-CBA-CGA
25	8	602	CLA	C2A-CAA-CBA-CGA
37	H	102	DGD	C3B-C4B-C5B-C6B
37	h	102	DGD	CAA-CBA-CCA-CDA
24	2	608	CHL	C2C-C3C-CAC-CBC
37	H	102	DGD	CAA-CBA-CCA-CDA
24	1	607	CHL	CHA-CBD-CGD-O2D
24	2	606	CHL	CHA-CBD-CGD-O2D
24	3	607	CHL	CHA-CBD-CGD-O1D
24	3	607	CHL	CHA-CBD-CGD-O2D
24	3	608	CHL	CHA-CBD-CGD-O2D
24	N	601	CHL	CHA-CBD-CGD-O1D
24	N	601	CHL	CHA-CBD-CGD-O2D
24	N	609	CHL	CHA-CBD-CGD-O2D
24	Y	601	CHL	CHA-CBD-CGD-O2D
24	5	607	CHL	CHA-CBD-CGD-O2D
24	6	606	CHL	CHA-CBD-CGD-O2D
24	7	607	CHL	CHA-CBD-CGD-O1D
24	7	607	CHL	CHA-CBD-CGD-O2D
24	7	608	CHL	CHA-CBD-CGD-O2D
24	n	601	CHL	CHA-CBD-CGD-O1D
24	n	601	CHL	CHA-CBD-CGD-O2D
24	n	609	CHL	CHA-CBD-CGD-O2D
24	y	601	CHL	CHA-CBD-CGD-O2D
25	1	603	CLA	CAD-CBD-CGD-O1D
25	2	603	CLA	CAD-CBD-CGD-O1D
25	3	602	CLA	CHA-CBD-CGD-O1D
25	3	603	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	3	604	CLA	CAD-CBD-CGD-O1D
25	4	612	CLA	CHA-CBD-CGD-O1D
25	4	612	CLA	CHA-CBD-CGD-O2D
25	B	605	CLA	CAD-CBD-CGD-O1D
25	B	606	CLA	CAD-CBD-CGD-O1D
25	B	613	CLA	CAD-CBD-CGD-O1D
25	B	615	CLA	CAD-CBD-CGD-O1D
25	B	617	CLA	CHA-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O1D
25	C	513	CLA	CAD-CBD-CGD-O1D
25	G	612	CLA	CHA-CBD-CGD-O2D
25	N	613	CLA	CHA-CBD-CGD-O1D
25	S	603	CLA	CHA-CBD-CGD-O1D
25	S	603	CLA	CHA-CBD-CGD-O2D
25	S	614	CLA	CHA-CBD-CGD-O1D
25	Y	602	CLA	CHA-CBD-CGD-O1D
25	Y	602	CLA	CHA-CBD-CGD-O2D
25	5	603	CLA	CAD-CBD-CGD-O1D
25	6	603	CLA	CAD-CBD-CGD-O1D
25	7	602	CLA	CHA-CBD-CGD-O1D
25	7	603	CLA	CAD-CBD-CGD-O1D
25	7	604	CLA	CAD-CBD-CGD-O1D
25	8	612	CLA	CHA-CBD-CGD-O1D
25	8	612	CLA	CHA-CBD-CGD-O2D
25	b	605	CLA	CAD-CBD-CGD-O1D
25	b	606	CLA	CAD-CBD-CGD-O1D
25	b	613	CLA	CAD-CBD-CGD-O1D
25	b	615	CLA	CAD-CBD-CGD-O1D
25	b	617	CLA	CHA-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CAD-CBD-CGD-O1D
25	c	513	CLA	CAD-CBD-CGD-O1D
25	g	612	CLA	CHA-CBD-CGD-O2D
25	n	613	CLA	CHA-CBD-CGD-O1D
25	s	603	CLA	CHA-CBD-CGD-O1D
25	s	603	CLA	CHA-CBD-CGD-O2D
25	s	614	CLA	CHA-CBD-CGD-O1D
25	y	602	CLA	CHA-CBD-CGD-O1D
25	y	602	CLA	CHA-CBD-CGD-O2D
28	3	1623	NEX	C9-C10-C11-C12
28	7	1623	NEX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	3	2630	LHG	C4-O6-P-O4
29	B	2630	LHG	C4-O6-P-O5
29	B	2631	LHG	C4-O6-P-O5
29	C	523	LHG	C4-O6-P-O3
29	D	409	LHG	C3-O3-P-O5
29	D	410	LHG	C4-O6-P-O5
29	G	2630	LHG	C4-O6-P-O4
29	N	2630	LHG	C3-O3-P-O5
29	N	2630	LHG	C4-O6-P-O3
29	R	2630	LHG	C3-O3-P-O5
29	7	2630	LHG	C4-O6-P-O4
29	b	2630	LHG	C4-O6-P-O5
29	b	2631	LHG	C4-O6-P-O5
29	c	523	LHG	C4-O6-P-O3
29	d	409	LHG	C3-O3-P-O5
29	d	410	LHG	C4-O6-P-O5
29	g	2630	LHG	C4-O6-P-O4
29	n	2630	LHG	C3-O3-P-O5
29	n	2630	LHG	C4-O6-P-O3
29	r	2630	LHG	C3-O3-P-O5
30	C	515	BCR	C9-C10-C11-C12
30	C	516	BCR	C19-C20-C21-C22
30	C	517	BCR	C19-C20-C21-C22
30	c	515	BCR	C9-C10-C11-C12
30	c	516	BCR	C19-C20-C21-C22
30	c	517	BCR	C19-C20-C21-C22
33	A	409	PHO	CHA-CBD-CGD-O2D
33	a	409	PHO	CHA-CBD-CGD-O2D
37	h	102	DGD	C3B-C4B-C5B-C6B
25	B	615	CLA	C16-C17-C18-C20
25	1	604	CLA	C2B-C3B-CAB-CBB
25	1	610	CLA	C2B-C3B-CAB-CBB
25	1	612	CLA	C2B-C3B-CAB-CBB
25	2	613	CLA	C2B-C3B-CAB-CBB
25	2	614	CLA	C2B-C3B-CAB-CBB
25	3	603	CLA	C2B-C3B-CAB-CBB
25	3	604	CLA	C2B-C3B-CAB-CBB
25	4	604	CLA	C2B-C3B-CAB-CBB
25	A	410	CLA	C2B-C3B-CAB-CBB
25	B	602	CLA	C2B-C3B-CAB-CBB
25	B	604	CLA	C2B-C3B-CAB-CBB
25	B	606	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	B	611	CLA	C2B-C3B-CAB-CBB
25	R	610	CLA	C2B-C3B-CAB-CBB
25	S	603	CLA	C2B-C3B-CAB-CBB
25	S	610	CLA	C2B-C3B-CAB-CBB
25	5	604	CLA	C2B-C3B-CAB-CBB
25	5	610	CLA	C2B-C3B-CAB-CBB
25	5	612	CLA	C2B-C3B-CAB-CBB
25	6	613	CLA	C2B-C3B-CAB-CBB
25	6	614	CLA	C2B-C3B-CAB-CBB
25	7	603	CLA	C2B-C3B-CAB-CBB
25	7	604	CLA	C2B-C3B-CAB-CBB
25	8	604	CLA	C2B-C3B-CAB-CBB
25	a	410	CLA	C2B-C3B-CAB-CBB
25	b	602	CLA	C2B-C3B-CAB-CBB
25	b	604	CLA	C2B-C3B-CAB-CBB
25	b	606	CLA	C2B-C3B-CAB-CBB
25	b	611	CLA	C2B-C3B-CAB-CBB
25	r	610	CLA	C2B-C3B-CAB-CBB
25	s	603	CLA	C2B-C3B-CAB-CBB
25	s	610	CLA	C2B-C3B-CAB-CBB
26	N	1620	LUT	C1-C6-C7-C8
26	n	1620	LUT	C1-C6-C7-C8
30	A	411	BCR	C23-C24-C25-C26
30	a	411	BCR	C23-C24-C25-C26
25	B	612	CLA	C2-C3-C5-C6
25	b	612	CLA	C2-C3-C5-C6
29	3	2630	LHG	C27-C28-C29-C30
26	4	620	LUT	C27-C28-C29-C39
26	8	620	LUT	C27-C28-C29-C39
30	4	623	BCR	C36-C18-C19-C20
30	C	515	BCR	C36-C18-C19-C20
30	8	623	BCR	C36-C18-C19-C20
30	c	515	BCR	C36-C18-C19-C20
29	g	2630	LHG	C14-C15-C16-C17
35	b	622	LMG	C38-C39-C40-C41
24	6	608	CHL	C2C-C3C-CAC-CBC
35	B	622	LMG	C38-C39-C40-C41
29	G	2630	LHG	C14-C15-C16-C17
25	B	617	CLA	C16-C17-C18-C20
25	b	615	CLA	C16-C17-C18-C20
25	b	617	CLA	C16-C17-C18-C20
29	7	2630	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
29	D	408	LHG	O1-C1-C2-O2
29	d	408	LHG	O1-C1-C2-O2
25	G	611	CLA	O1A-CGA-O2A-C1
25	g	611	CLA	O1A-CGA-O2A-C1
29	G	2630	LHG	O10-C23-O8-C6
29	g	2630	LHG	O10-C23-O8-C6
25	S	614	CLA	O2A-C1-C2-C3
25	s	614	CLA	O2A-C1-C2-C3
29	1	2630	LHG	C14-C15-C16-C17
29	5	2630	LHG	C14-C15-C16-C17
29	c	522	LHG	C17-C18-C19-C20
26	4	620	LUT	C29-C30-C31-C32
26	8	620	LUT	C29-C30-C31-C32
25	B	604	CLA	C16-C17-C18-C20
25	b	604	CLA	C16-C17-C18-C20
24	Y	607	CHL	C8-C10-C11-C12
24	y	607	CHL	C8-C10-C11-C12
29	C	522	LHG	C17-C18-C19-C20
37	H	102	DGD	CDB-CEB-CFB-CGB
37	h	102	DGD	CDB-CEB-CFB-CGB
24	Y	607	CHL	C11-C12-C13-C14
24	y	607	CHL	C11-C12-C13-C14
25	3	602	CLA	C11-C10-C8-C9
25	B	606	CLA	C14-C13-C15-C16
25	C	509	CLA	C11-C10-C8-C9
25	C	513	CLA	C11-C12-C13-C14
25	7	602	CLA	C11-C10-C8-C9
25	b	606	CLA	C14-C13-C15-C16
25	c	509	CLA	C11-C10-C8-C9
25	c	513	CLA	C11-C12-C13-C14
24	G	601	CHL	C6-C7-C8-C10
24	g	601	CHL	C6-C7-C8-C10
29	C	2630	LHG	C17-C18-C19-C20
29	S	2630	LHG	C33-C34-C35-C36
29	c	2630	LHG	C17-C18-C19-C20
29	s	2630	LHG	C33-C34-C35-C36
35	B	2633	LMG	C35-C36-C37-C38
25	3	603	CLA	C5-C6-C7-C8
25	7	603	CLA	C5-C6-C7-C8
34	A	418	SQD	O47-C7-C8-C9
34	a	418	SQD	O47-C7-C8-C9
35	b	2633	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
37	C	520	DGD	C2D-C1D-O3G-C3G
37	c	520	DGD	C2D-C1D-O3G-C3G
29	C	522	LHG	O9-C7-O7-C5
29	c	522	LHG	O9-C7-O7-C5
35	C	521	LMG	O9-C10-O7-C8
35	c	521	LMG	O9-C10-O7-C8
25	R	610	CLA	C5-C6-C7-C8
25	r	610	CLA	C5-C6-C7-C8
37	c	518	DGD	CCB-CDB-CEB-CFB
37	C	518	DGD	CCB-CDB-CEB-CFB
26	3	1621	LUT	C29-C30-C31-C32
30	4	623	BCR	C9-C10-C11-C12
30	8	623	BCR	C9-C10-C11-C12
35	D	411	LMG	C14-C15-C16-C17
24	G	608	CHL	C16-C17-C18-C19
24	g	608	CHL	C16-C17-C18-C19
37	c	519	DGD	CBA-CCA-CDA-CEA
37	C	519	DGD	C1B-C2B-C3B-C4B
37	c	519	DGD	C1B-C2B-C3B-C4B
24	1	606	CHL	C2A-CAA-CBA-CGA
24	5	606	CHL	C2A-CAA-CBA-CGA
35	d	411	LMG	C14-C15-C16-C17
37	C	519	DGD	CBA-CCA-CDA-CEA
37	H	102	DGD	O2G-C1B-C2B-C3B
37	h	102	DGD	O2G-C1B-C2B-C3B
29	d	408	LHG	C33-C34-C35-C36
29	D	408	LHG	C33-C34-C35-C36
28	1	1623	NEX	C31-C32-C33-C40
28	5	1623	NEX	C31-C32-C33-C40
25	Y	602	CLA	C16-C17-C18-C19
25	y	602	CLA	C16-C17-C18-C19
24	Y	608	CHL	C1C-C2C-CMC-OMC
24	y	608	CHL	C1C-C2C-CMC-OMC
35	Z	101	LMG	C8-C7-O1-C1
35	z	101	LMG	C8-C7-O1-C1
37	C	518	DGD	C5D-C6D-O5D-C1E
37	c	518	DGD	C5D-C6D-O5D-C1E
25	B	604	CLA	C2A-CAA-CBA-CGA
25	b	604	CLA	C2A-CAA-CBA-CGA
26	7	1621	LUT	C29-C30-C31-C32
27	N	1622	XAT	C29-C30-C31-C32
27	n	1622	XAT	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
30	C	515	BCR	C19-C20-C21-C22
30	c	515	BCR	C19-C20-C21-C22
25	b	603	CLA	C16-C17-C18-C20
24	3	609	CHL	C4-C3-C5-C6
24	7	609	CHL	C4-C3-C5-C6
25	c	509	CLA	C13-C15-C16-C17
25	N	614	CLA	O2A-C1-C2-C3
25	n	614	CLA	O2A-C1-C2-C3
25	2	603	CLA	C2-C3-C5-C6
25	6	603	CLA	C2-C3-C5-C6
29	C	522	LHG	C29-C30-C31-C32
25	C	509	CLA	C13-C15-C16-C17
24	y	601	CHL	O1D-CGD-O2D-CED
29	c	522	LHG	C29-C30-C31-C32
25	B	603	CLA	C16-C17-C18-C20
24	G	601	CHL	C14-C13-C15-C16
24	G	608	CHL	C11-C10-C8-C9
24	g	601	CHL	C14-C13-C15-C16
24	g	608	CHL	C11-C10-C8-C9
25	D	403	CLA	C11-C12-C13-C14
25	d	403	CLA	C11-C12-C13-C14
24	Y	601	CHL	O1D-CGD-O2D-CED
25	G	611	CLA	CBA-CGA-O2A-C1
25	g	611	CLA	CBA-CGA-O2A-C1
35	B	2633	LMG	C29-C28-O8-C9
35	b	2633	LMG	C29-C28-O8-C9
29	G	2630	LHG	C5-C4-O6-P
29	g	2630	LHG	C5-C4-O6-P
25	C	503	CLA	C4B-C3B-CAB-CBB
25	G	613	CLA	C4B-C3B-CAB-CBB
25	c	503	CLA	C4B-C3B-CAB-CBB
25	g	613	CLA	C4B-C3B-CAB-CBB
25	3	602	CLA	C10-C11-C12-C13
25	B	615	CLA	C16-C17-C18-C19
25	b	615	CLA	C16-C17-C18-C19
24	N	608	CHL	C5-C6-C7-C8
24	n	608	CHL	C5-C6-C7-C8
25	7	602	CLA	C10-C11-C12-C13
25	R	613	CLA	C2A-CAA-CBA-CGA
25	S	613	CLA	C2A-CAA-CBA-CGA
25	r	613	CLA	C2A-CAA-CBA-CGA
25	s	613	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	2	602	CLA	C4-C3-C5-C6
25	6	602	CLA	C4-C3-C5-C6
28	1	1623	NEX	C29-C30-C31-C32
28	5	1623	NEX	C29-C30-C31-C32
29	D	410	LHG	C10-C11-C12-C13
29	d	410	LHG	C10-C11-C12-C13
25	C	511	CLA	C6-C7-C8-C10
25	R	610	CLA	C12-C13-C15-C16
25	S	602	CLA	C6-C7-C8-C10
25	c	511	CLA	C6-C7-C8-C10
25	r	610	CLA	C12-C13-C15-C16
25	s	602	CLA	C6-C7-C8-C10
35	a	413	LMG	C36-C37-C38-C39
29	D	409	LHG	O2-C2-C3-O3
29	d	409	LHG	O2-C2-C3-O3
35	A	413	LMG	C36-C37-C38-C39
35	B	622	LMG	C32-C33-C34-C35
35	b	622	LMG	C32-C33-C34-C35
29	D	410	LHG	C9-C10-C11-C12
29	N	2630	LHG	C26-C27-C28-C29
24	S	607	CHL	C4-C3-C5-C6
24	s	607	CHL	C4-C3-C5-C6
25	4	610	CLA	C3A-C2A-CAA-CBA
25	R	604	CLA	C3A-C2A-CAA-CBA
25	8	610	CLA	C3A-C2A-CAA-CBA
25	r	604	CLA	C3A-C2A-CAA-CBA
29	d	410	LHG	C9-C10-C11-C12
29	n	2630	LHG	C26-C27-C28-C29
28	1	1623	NEX	C39-C29-C30-C31
28	2	1623	NEX	C39-C29-C30-C31
28	3	1623	NEX	C39-C29-C30-C31
28	G	1623	NEX	C39-C29-C30-C31
28	N	1623	NEX	C39-C29-C30-C31
28	R	623	NEX	C39-C29-C30-C31
28	S	1623	NEX	C39-C29-C30-C31
28	Y	1623	NEX	C39-C29-C30-C31
28	5	1623	NEX	C39-C29-C30-C31
28	6	1623	NEX	C39-C29-C30-C31
28	7	1623	NEX	C39-C29-C30-C31
28	g	1623	NEX	C39-C29-C30-C31
28	n	1623	NEX	C39-C29-C30-C31
28	r	623	NEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
28	s	1623	NEX	C39-C29-C30-C31
28	y	1623	NEX	C39-C29-C30-C31
37	H	102	DGD	O1B-C1B-C2B-C3B
37	h	102	DGD	O1B-C1B-C2B-C3B
24	2	609	CHL	C5-C6-C7-C8
24	6	609	CHL	C5-C6-C7-C8
25	b	617	CLA	O1D-CGD-O2D-CED
25	G	603	CLA	C2-C1-O2A-CGA
25	g	603	CLA	C2-C1-O2A-CGA
29	7	2630	LHG	C15-C16-C17-C18
29	N	2630	LHG	C35-C36-C37-C38
29	n	2630	LHG	C35-C36-C37-C38
29	3	2630	LHG	C15-C16-C17-C18
25	Y	611	CLA	C8-C10-C11-C12
25	y	611	CLA	C8-C10-C11-C12
24	G	609	CHL	C2C-C3C-CAC-CBC
29	7	2630	LHG	C29-C30-C31-C32
35	b	622	LMG	C31-C32-C33-C34
37	B	626	DGD	C7A-C8A-C9A-CAA
24	g	609	CHL	C2C-C3C-CAC-CBC
25	B	617	CLA	O1D-CGD-O2D-CED
25	5	612	CLA	CAA-CBA-CGA-O2A
37	b	626	DGD	C7A-C8A-C9A-CAA
29	3	2630	LHG	C29-C30-C31-C32
24	G	608	CHL	C2-C3-C5-C6
24	g	608	CHL	C2-C3-C5-C6
34	A	418	SQD	C11-C12-C13-C14
35	B	622	LMG	C31-C32-C33-C34
25	Y	610	CLA	C8-C10-C11-C12
25	y	610	CLA	C8-C10-C11-C12
34	A	418	SQD	C14-C15-C16-C17
34	a	418	SQD	C14-C15-C16-C17
34	b	621	SQD	C12-C13-C14-C15
25	1	612	CLA	CAA-CBA-CGA-O1A
25	5	612	CLA	CAA-CBA-CGA-O1A
24	2	609	CHL	C6-C7-C8-C9
24	N	601	CHL	C14-C13-C15-C16
24	N	609	CHL	C14-C13-C15-C16
24	6	609	CHL	C6-C7-C8-C9
24	n	601	CHL	C14-C13-C15-C16
24	n	609	CHL	C14-C13-C15-C16
25	A	410	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	B	603	CLA	C11-C10-C8-C9
25	B	608	CLA	C6-C7-C8-C9
25	N	603	CLA	C6-C7-C8-C9
25	N	610	CLA	C11-C12-C13-C14
25	S	602	CLA	C6-C7-C8-C9
25	a	410	CLA	C6-C7-C8-C9
25	b	603	CLA	C11-C10-C8-C9
25	b	608	CLA	C6-C7-C8-C9
25	n	603	CLA	C6-C7-C8-C9
25	n	610	CLA	C11-C12-C13-C14
25	s	602	CLA	C6-C7-C8-C9
34	a	418	SQD	C11-C12-C13-C14
29	D	408	LHG	O1-C1-C2-C3
29	d	408	LHG	O1-C1-C2-C3
29	D	410	LHG	C14-C15-C16-C17
29	d	410	LHG	C14-C15-C16-C17
34	B	621	SQD	C12-C13-C14-C15
35	Z	101	LMG	C33-C34-C35-C36
35	z	101	LMG	C33-C34-C35-C36
37	C	518	DGD	C5A-C6A-C7A-C8A
37	c	518	DGD	C5A-C6A-C7A-C8A
25	1	612	CLA	CAA-CBA-CGA-O2A
25	2	614	CLA	CAA-CBA-CGA-O2A
25	6	614	CLA	CAA-CBA-CGA-O2A
24	1	607	CHL	C1A-C2A-CAA-CBA
24	1	609	CHL	C1A-C2A-CAA-CBA
24	3	609	CHL	C1A-C2A-CAA-CBA
24	4	607	CHL	C1A-C2A-CAA-CBA
24	G	609	CHL	C1A-C2A-CAA-CBA
24	N	609	CHL	C1A-C2A-CAA-CBA
24	5	607	CHL	C1A-C2A-CAA-CBA
24	5	609	CHL	C1A-C2A-CAA-CBA
24	7	609	CHL	C1A-C2A-CAA-CBA
24	8	607	CHL	C1A-C2A-CAA-CBA
24	g	609	CHL	C1A-C2A-CAA-CBA
24	n	609	CHL	C1A-C2A-CAA-CBA
27	R	622	XAT	C9-C10-C11-C12
27	r	622	XAT	C9-C10-C11-C12
24	S	601	CHL	CAA-CBA-CGA-O2A
24	s	601	CHL	CAA-CBA-CGA-O2A
37	C	520	DGD	C9B-CAB-CBB-CCB
24	N	609	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	n	609	CHL	C4-C3-C5-C6
25	Y	611	CLA	C4-C3-C5-C6
25	y	611	CLA	C4-C3-C5-C6
37	c	520	DGD	C9B-CAB-CBB-CCB
24	4	607	CHL	CAA-CBA-CGA-O1A
24	8	607	CHL	CAA-CBA-CGA-O1A
25	2	614	CLA	CAA-CBA-CGA-O1A
25	6	614	CLA	CAA-CBA-CGA-O1A
25	8	603	CLA	CAA-CBA-CGA-O1A
25	B	615	CLA	C2A-CAA-CBA-CGA
25	b	615	CLA	C2A-CAA-CBA-CGA
35	C	521	LMG	O6-C5-C6-O5
29	G	2630	LHG	C11-C12-C13-C14
29	g	2630	LHG	C11-C12-C13-C14
25	C	508	CLA	C1A-C2A-CAA-CBA
25	C	511	CLA	C1A-C2A-CAA-CBA
25	G	604	CLA	C1A-C2A-CAA-CBA
25	R	602	CLA	C1A-C2A-CAA-CBA
25	S	609	CLA	C1A-C2A-CAA-CBA
25	S	610	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
25	c	511	CLA	C1A-C2A-CAA-CBA
25	g	604	CLA	C1A-C2A-CAA-CBA
25	r	602	CLA	C1A-C2A-CAA-CBA
25	s	609	CLA	C1A-C2A-CAA-CBA
25	s	610	CLA	C1A-C2A-CAA-CBA
28	1	1623	NEX	C28-C29-C30-C31
28	2	1623	NEX	C28-C29-C30-C31
28	3	1623	NEX	C28-C29-C30-C31
28	G	1623	NEX	C28-C29-C30-C31
28	N	1623	NEX	C28-C29-C30-C31
28	R	623	NEX	C28-C29-C30-C31
28	S	1623	NEX	C28-C29-C30-C31
28	Y	1623	NEX	C28-C29-C30-C31
28	5	1623	NEX	C28-C29-C30-C31
28	6	1623	NEX	C28-C29-C30-C31
28	7	1623	NEX	C28-C29-C30-C31
28	g	1623	NEX	C28-C29-C30-C31
28	n	1623	NEX	C28-C29-C30-C31
28	r	623	NEX	C28-C29-C30-C31
28	s	1623	NEX	C28-C29-C30-C31
28	y	1623	NEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
37	H	102	DGD	CBB-CCB-CDB-CEB
25	3	604	CLA	CAA-CBA-CGA-O2A
25	4	603	CLA	CAA-CBA-CGA-O1A
25	7	604	CLA	CAA-CBA-CGA-O2A
37	h	102	DGD	CBB-CCB-CDB-CEB
35	c	521	LMG	O6-C5-C6-O5
25	1	613	CLA	C2B-C3B-CAB-CBB
25	2	612	CLA	C2B-C3B-CAB-CBB
25	B	603	CLA	C2B-C3B-CAB-CBB
25	G	604	CLA	C2B-C3B-CAB-CBB
25	G	614	CLA	C2B-C3B-CAB-CBB
25	R	603	CLA	C2B-C3B-CAB-CBB
25	R	611	CLA	C2B-C3B-CAB-CBB
25	Y	610	CLA	C2B-C3B-CAB-CBB
25	5	613	CLA	C2B-C3B-CAB-CBB
25	6	612	CLA	C2B-C3B-CAB-CBB
25	b	603	CLA	C2B-C3B-CAB-CBB
25	g	604	CLA	C2B-C3B-CAB-CBB
25	g	614	CLA	C2B-C3B-CAB-CBB
25	r	603	CLA	C2B-C3B-CAB-CBB
25	r	611	CLA	C2B-C3B-CAB-CBB
25	y	610	CLA	C2B-C3B-CAB-CBB
26	1	1621	LUT	C5-C6-C7-C8
26	3	1621	LUT	C1-C6-C7-C8
26	N	1620	LUT	C5-C6-C7-C8
26	S	1621	LUT	C1-C6-C7-C8
26	Y	1620	LUT	C5-C6-C7-C8
26	5	1621	LUT	C5-C6-C7-C8
26	7	1621	LUT	C1-C6-C7-C8
26	n	1620	LUT	C5-C6-C7-C8
26	s	1621	LUT	C1-C6-C7-C8
26	y	1620	LUT	C5-C6-C7-C8
30	4	623	BCR	C5-C6-C7-C8
30	C	514	BCR	C5-C6-C7-C8
30	C	515	BCR	C23-C24-C25-C26
30	C	516	BCR	C1-C6-C7-C8
30	D	404	BCR	C5-C6-C7-C8
30	T	101	BCR	C23-C24-C25-C26
30	T	101	BCR	C23-C24-C25-C30
30	8	623	BCR	C5-C6-C7-C8
30	c	514	BCR	C5-C6-C7-C8
30	c	515	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
30	c	516	BCR	C1-C6-C7-C8
30	d	404	BCR	C5-C6-C7-C8
30	t	101	BCR	C23-C24-C25-C26
30	t	101	BCR	C23-C24-C25-C30
24	s	601	CHL	CAA-CBA-CGA-O1A
24	N	607	CHL	C2C-C3C-CAC-CBC
25	C	509	CLA	C8-C10-C11-C12
25	c	509	CLA	C8-C10-C11-C12
29	D	410	LHG	C2-C3-O3-P
29	d	410	LHG	C2-C3-O3-P
24	n	607	CHL	C2C-C3C-CAC-CBC
24	S	601	CHL	CAA-CBA-CGA-O1A
24	3	609	CHL	C2-C3-C5-C6
24	S	607	CHL	C2-C3-C5-C6
24	7	609	CHL	C2-C3-C5-C6
24	s	607	CHL	C2-C3-C5-C6
24	Y	606	CHL	O2A-C1-C2-C3
24	y	606	CHL	O2A-C1-C2-C3
25	8	612	CLA	CAA-CBA-CGA-O2A
25	b	609	CLA	C15-C16-C17-C18
24	N	608	CHL	C12-C13-C15-C16
24	R	606	CHL	C11-C10-C8-C7
24	Y	608	CHL	C12-C13-C15-C16
24	n	608	CHL	C12-C13-C15-C16
24	r	606	CHL	C11-C10-C8-C7
24	y	608	CHL	C12-C13-C15-C16
25	A	410	CLA	C6-C7-C8-C10
25	B	614	CLA	C11-C12-C13-C15
25	C	513	CLA	C11-C12-C13-C15
25	a	410	CLA	C6-C7-C8-C10
25	b	614	CLA	C11-C12-C13-C15
25	c	513	CLA	C11-C12-C13-C15
25	C	501	CLA	C16-C17-C18-C20
25	c	501	CLA	C16-C17-C18-C20
25	1	613	CLA	C2A-CAA-CBA-CGA
25	B	617	CLA	C2A-CAA-CBA-CGA
25	5	613	CLA	C2A-CAA-CBA-CGA
25	b	617	CLA	C2A-CAA-CBA-CGA
29	r	2630	LHG	C7-C8-C9-C10
25	B	616	CLA	C15-C16-C17-C18
25	b	616	CLA	C15-C16-C17-C18
29	B	2630	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
29	C	2630	LHG	O7-C5-C6-O8
29	b	2630	LHG	O7-C5-C6-O8
29	c	2630	LHG	O7-C5-C6-O8
24	4	609	CHL	CAA-CBA-CGA-O1A
24	4	609	CHL	CAA-CBA-CGA-O2A
25	4	612	CLA	CAA-CBA-CGA-O2A
29	R	2630	LHG	C14-C15-C16-C17
29	r	2630	LHG	C14-C15-C16-C17
25	B	609	CLA	C15-C16-C17-C18
37	c	518	DGD	C6A-C7A-C8A-C9A
29	R	2630	LHG	C7-C8-C9-C10
37	C	518	DGD	C6A-C7A-C8A-C9A
24	8	609	CHL	CAA-CBA-CGA-O1A
24	8	609	CHL	CAA-CBA-CGA-O2A
25	R	616	CLA	CAA-CBA-CGA-O1A
25	r	616	CLA	CAA-CBA-CGA-O1A
25	B	607	CLA	C10-C11-C12-C13
25	b	607	CLA	C10-C11-C12-C13
27	4	622	XAT	C27-C28-C29-C39
27	8	622	XAT	C27-C28-C29-C39
30	C	516	BCR	C36-C18-C19-C20
30	c	516	BCR	C36-C18-C19-C20
35	B	622	LMG	C22-C23-C24-C25
35	b	622	LMG	C22-C23-C24-C25
24	3	608	CHL	CAA-CBA-CGA-O2A
24	7	608	CHL	CAA-CBA-CGA-O2A
24	8	607	CHL	CAA-CBA-CGA-O2A
25	4	603	CLA	CAA-CBA-CGA-O2A
25	8	603	CLA	CAA-CBA-CGA-O2A
25	8	604	CLA	CAA-CBA-CGA-O2A
24	G	609	CHL	C4-C3-C5-C6
24	g	609	CHL	C4-C3-C5-C6
25	A	405	CLA	C4-C3-C5-C6
25	C	506	CLA	C4-C3-C5-C6
25	a	405	CLA	C4-C3-C5-C6
25	c	506	CLA	C4-C3-C5-C6
37	C	518	DGD	C6B-C7B-C8B-C9B
25	Y	611	CLA	C2-C3-C5-C6
25	y	611	CLA	C2-C3-C5-C6
37	h	102	DGD	CDA-CEA-CFA-CGA
37	H	102	DGD	CDA-CEA-CFA-CGA
29	S	2630	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
37	c	518	DGD	C6B-C7B-C8B-C9B
24	4	607	CHL	CAA-CBA-CGA-O2A
25	4	604	CLA	CAA-CBA-CGA-O2A
25	4	612	CLA	CAA-CBA-CGA-O1A
25	8	612	CLA	CAA-CBA-CGA-O1A
29	s	2630	LHG	C12-C13-C14-C15
35	B	2633	LMG	C39-C40-C41-C42
35	b	2633	LMG	C39-C40-C41-C42
25	C	511	CLA	C6-C7-C8-C9
25	c	511	CLA	C6-C7-C8-C9
35	B	2633	LMG	C8-C9-O8-C28
35	b	2633	LMG	C8-C9-O8-C28
29	d	410	LHG	C31-C32-C33-C34
27	Y	1622	XAT	C29-C30-C31-C32
27	y	1622	XAT	C29-C30-C31-C32
29	D	410	LHG	C31-C32-C33-C34
29	D	408	LHG	C14-C15-C16-C17
29	d	408	LHG	C14-C15-C16-C17
24	1	605	CHL	CAA-CBA-CGA-O2A
24	5	605	CHL	CAA-CBA-CGA-O2A
25	3	604	CLA	CAA-CBA-CGA-O1A
25	7	604	CLA	CAA-CBA-CGA-O1A
35	A	415	LMG	C29-C28-O8-C9
35	a	415	LMG	C29-C28-O8-C9
25	C	509	CLA	C10-C11-C12-C13
25	c	509	CLA	C10-C11-C12-C13
24	N	608	CHL	C4-C3-C5-C6
24	n	608	CHL	C4-C3-C5-C6
25	B	607	CLA	C4-C3-C5-C6
25	b	607	CLA	C4-C3-C5-C6
29	3	2630	LHG	C5-C4-O6-P
29	7	2630	LHG	C5-C4-O6-P
29	b	2630	LHG	C18-C19-C20-C21
25	B	612	CLA	C13-C15-C16-C17
25	b	612	CLA	C13-C15-C16-C17
25	3	614	CLA	O2A-C1-C2-C3
33	A	409	PHO	O1A-CGA-O2A-C1
33	a	409	PHO	O1A-CGA-O2A-C1
29	B	2630	LHG	C18-C19-C20-C21
35	A	413	LMG	O1-C7-C8-C9
35	a	413	LMG	O1-C7-C8-C9
24	S	606	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	s	606	CHL	CAA-CBA-CGA-O2A
25	N	613	CLA	C2A-CAA-CBA-CGA
25	n	613	CLA	C2A-CAA-CBA-CGA
29	B	2630	LHG	C17-C18-C19-C20
29	b	2630	LHG	C17-C18-C19-C20
35	a	413	LMG	C33-C34-C35-C36
24	3	605	CHL	CAA-CBA-CGA-O2A
24	7	605	CHL	CAA-CBA-CGA-O2A
25	4	611	CLA	CAA-CBA-CGA-O2A
25	8	611	CLA	CAA-CBA-CGA-O2A
25	B	614	CLA	O1A-CGA-O2A-C1
25	b	614	CLA	O1A-CGA-O2A-C1
35	A	413	LMG	C33-C34-C35-C36
35	B	622	LMG	O9-C10-O7-C8
35	b	622	LMG	O9-C10-O7-C8
25	C	503	CLA	C13-C15-C16-C17
25	c	503	CLA	C13-C15-C16-C17
25	D	403	CLA	C4-C3-C5-C6
25	d	403	CLA	C4-C3-C5-C6
29	s	2630	LHG	C31-C32-C33-C34
29	S	2630	LHG	C31-C32-C33-C34
25	4	602	CLA	C4B-C3B-CAB-CBB
25	8	602	CLA	C4B-C3B-CAB-CBB
24	R	606	CHL	O1A-CGA-O2A-C1
24	r	606	CHL	O1A-CGA-O2A-C1
25	R	616	CLA	CAA-CBA-CGA-O2A
25	r	616	CLA	CAA-CBA-CGA-O2A
37	B	626	DGD	O6D-C5D-C6D-O5D
37	b	626	DGD	O6D-C5D-C6D-O5D
25	7	614	CLA	O2A-C1-C2-C3
25	B	602	CLA	CAA-CBA-CGA-O2A
25	b	602	CLA	CAA-CBA-CGA-O2A
24	1	605	CHL	CAA-CBA-CGA-O1A
24	5	605	CHL	CAA-CBA-CGA-O1A
24	1	601	CHL	CHA-CBD-CGD-O1D
24	1	601	CHL	CHA-CBD-CGD-O2D
24	1	607	CHL	CHA-CBD-CGD-O1D
24	G	601	CHL	CHA-CBD-CGD-O1D
24	G	601	CHL	CHA-CBD-CGD-O2D
24	S	607	CHL	CHA-CBD-CGD-O1D
24	S	607	CHL	CHA-CBD-CGD-O2D
24	Y	601	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	5	601	CHL	CHA-CBD-CGD-O1D
24	5	601	CHL	CHA-CBD-CGD-O2D
24	5	607	CHL	CHA-CBD-CGD-O1D
24	g	601	CHL	CHA-CBD-CGD-O1D
24	g	601	CHL	CHA-CBD-CGD-O2D
24	s	607	CHL	CHA-CBD-CGD-O1D
24	s	607	CHL	CHA-CBD-CGD-O2D
24	y	601	CHL	CHA-CBD-CGD-O1D
37	c	518	DGD	O1A-C1A-O1G-C1G
25	G	610	CLA	C10-C11-C12-C13
24	N	606	CHL	CBA-CGA-O2A-C1
24	1	601	CHL	CAA-CBA-CGA-O2A
24	5	601	CHL	CAA-CBA-CGA-O2A
25	S	609	CLA	CAA-CBA-CGA-O2A
29	d	409	LHG	C13-C14-C15-C16
29	D	409	LHG	C13-C14-C15-C16
29	D	410	LHG	O6-C4-C5-C6
29	d	410	LHG	O6-C4-C5-C6
24	2	609	CHL	C4-C3-C5-C6
24	6	609	CHL	C4-C3-C5-C6
25	g	610	CLA	C10-C11-C12-C13
25	s	609	CLA	CAA-CBA-CGA-O2A
29	N	2630	LHG	C28-C29-C30-C31
29	n	2630	LHG	C28-C29-C30-C31
24	n	606	CHL	CBA-CGA-O2A-C1
29	n	2630	LHG	C12-C13-C14-C15
24	Y	608	CHL	C11-C10-C8-C7
24	y	608	CHL	C11-C10-C8-C7
25	B	604	CLA	C6-C7-C8-C10
25	N	610	CLA	C11-C12-C13-C15
25	b	604	CLA	C6-C7-C8-C10
25	n	610	CLA	C11-C12-C13-C15
29	N	2630	LHG	C12-C13-C14-C15
25	g	603	CLA	C10-C11-C12-C13
26	S	1621	LUT	C29-C30-C31-C32
26	s	1621	LUT	C29-C30-C31-C32
37	C	518	DGD	O1A-C1A-O1G-C1G
25	A	405	CLA	C4C-C3C-CAC-CBC
25	a	405	CLA	C4C-C3C-CAC-CBC
24	1	606	CHL	CAA-CBA-CGA-O2A
24	5	606	CHL	CAA-CBA-CGA-O2A
25	B	604	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	B	617	CLA	C6-C7-C8-C9
25	B	617	CLA	C14-C13-C15-C16
25	C	504	CLA	C11-C12-C13-C14
25	C	505	CLA	C14-C13-C15-C16
25	G	602	CLA	C6-C7-C8-C9
25	G	613	CLA	C14-C13-C15-C16
25	N	603	CLA	C11-C10-C8-C9
25	S	602	CLA	C11-C12-C13-C14
25	b	604	CLA	C6-C7-C8-C9
25	b	617	CLA	C6-C7-C8-C9
25	b	617	CLA	C14-C13-C15-C16
25	c	504	CLA	C11-C12-C13-C14
25	c	505	CLA	C14-C13-C15-C16
25	g	602	CLA	C6-C7-C8-C9
25	g	613	CLA	C14-C13-C15-C16
25	n	603	CLA	C11-C10-C8-C9
25	s	602	CLA	C11-C12-C13-C14
35	A	413	LMG	C31-C32-C33-C34
35	a	413	LMG	C31-C32-C33-C34
24	Y	607	CHL	C2C-C3C-CAC-CBC
24	y	607	CHL	C2C-C3C-CAC-CBC
29	C	523	LHG	C11-C12-C13-C14
29	c	523	LHG	C11-C12-C13-C14
25	4	604	CLA	CAA-CBA-CGA-O1A
25	8	604	CLA	CAA-CBA-CGA-O1A
24	G	606	CHL	C2-C1-O2A-CGA
24	R	606	CHL	C2-C1-O2A-CGA
24	Y	608	CHL	C2-C1-O2A-CGA
24	g	606	CHL	C2-C1-O2A-CGA
24	r	606	CHL	C2-C1-O2A-CGA
24	y	608	CHL	C2-C1-O2A-CGA
25	B	603	CLA	C2-C1-O2A-CGA
25	C	506	CLA	C2-C1-O2A-CGA
25	D	402	CLA	C2-C1-O2A-CGA
25	S	602	CLA	C2-C1-O2A-CGA
25	b	603	CLA	C2-C1-O2A-CGA
25	c	506	CLA	C2-C1-O2A-CGA
25	d	402	CLA	C2-C1-O2A-CGA
25	s	602	CLA	C2-C1-O2A-CGA
25	G	603	CLA	C10-C11-C12-C13
24	R	606	CHL	CBA-CGA-O2A-C1
24	r	606	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	B	2630	LHG	C31-C32-C33-C34
24	3	607	CHL	C3A-C2A-CAA-CBA
24	N	605	CHL	C3A-C2A-CAA-CBA
24	Y	608	CHL	C3A-C2A-CAA-CBA
24	7	607	CHL	C3A-C2A-CAA-CBA
24	n	605	CHL	C3A-C2A-CAA-CBA
24	y	608	CHL	C3A-C2A-CAA-CBA
24	3	608	CHL	CAA-CBA-CGA-O1A
29	b	2630	LHG	C31-C32-C33-C34
37	C	519	DGD	CBB-CCB-CDB-CEB
25	B	607	CLA	C2-C3-C5-C6
25	b	607	CLA	C2-C3-C5-C6
25	B	605	CLA	C10-C11-C12-C13
25	b	605	CLA	C10-C11-C12-C13
24	4	608	CHL	CAA-CBA-CGA-O2A
24	7	608	CHL	CAA-CBA-CGA-O1A
24	8	608	CHL	CAA-CBA-CGA-O2A
37	c	519	DGD	CBB-CCB-CDB-CEB
25	C	503	CLA	C16-C17-C18-C19
25	c	503	CLA	C16-C17-C18-C19
24	7	605	CHL	CAA-CBA-CGA-O1A
25	4	610	CLA	CAA-CBA-CGA-O2A
25	4	611	CLA	CAA-CBA-CGA-O1A
25	8	610	CLA	CAA-CBA-CGA-O2A
25	8	611	CLA	CAA-CBA-CGA-O1A
29	C	2630	LHG	C25-C26-C27-C28
29	c	2630	LHG	C25-C26-C27-C28
24	1	601	CHL	C3C-C2C-CMC-OMC
24	5	601	CHL	C3C-C2C-CMC-OMC
25	Y	610	CLA	C11-C12-C13-C14
25	y	610	CLA	C11-C12-C13-C14
24	5	606	CHL	CAA-CBA-CGA-O1A
24	s	606	CHL	CAA-CBA-CGA-O1A
37	B	626	DGD	C8B-C9B-CAB-CBB
37	b	626	DGD	C8B-C9B-CAB-CBB
24	R	606	CHL	C2A-CAA-CBA-CGA
24	r	606	CHL	C2A-CAA-CBA-CGA
29	5	2630	LHG	C18-C19-C20-C21
29	B	2630	LHG	C33-C34-C35-C36
29	1	2630	LHG	C18-C19-C20-C21
24	1	606	CHL	CAA-CBA-CGA-O1A
24	3	605	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	1	611	CLA	CAA-CBA-CGA-O2A
35	Z	101	LMG	C17-C18-C19-C20
35	z	101	LMG	C17-C18-C19-C20
25	C	504	CLA	CBA-CGA-O2A-C1
25	c	504	CLA	CBA-CGA-O2A-C1
33	A	409	PHO	CBA-CGA-O2A-C1
33	a	409	PHO	CBA-CGA-O2A-C1
29	b	2630	LHG	C33-C34-C35-C36
25	B	607	CLA	C16-C17-C18-C20
25	b	607	CLA	C16-C17-C18-C20
27	4	622	XAT	O4-C6-C7-C8
27	8	622	XAT	O4-C6-C7-C8
28	1	1623	NEX	O24-C26-C27-C28
28	2	1623	NEX	O24-C26-C27-C28
28	3	1623	NEX	O24-C26-C27-C28
28	R	623	NEX	O24-C26-C27-C28
28	S	1623	NEX	O24-C26-C27-C28
28	Y	1623	NEX	O24-C26-C27-C28
28	5	1623	NEX	O24-C26-C27-C28
28	6	1623	NEX	O24-C26-C27-C28
28	7	1623	NEX	O24-C26-C27-C28
28	g	1623	NEX	O24-C26-C27-C28
28	r	623	NEX	O24-C26-C27-C28
28	s	1623	NEX	O24-C26-C27-C28
28	y	1623	NEX	O24-C26-C27-C28
35	C	521	LMG	C14-C15-C16-C17
37	C	519	DGD	C6A-C7A-C8A-C9A
24	S	606	CHL	CAA-CBA-CGA-O1A
25	4	610	CLA	CAA-CBA-CGA-O1A
25	5	611	CLA	CAA-CBA-CGA-O2A
25	8	610	CLA	CAA-CBA-CGA-O1A
35	c	521	LMG	C14-C15-C16-C17
25	R	611	CLA	O2A-C1-C2-C3
25	r	611	CLA	O2A-C1-C2-C3
37	c	519	DGD	C6A-C7A-C8A-C9A
35	A	413	LMG	C15-C16-C17-C18
25	b	605	CLA	O1D-CGD-O2D-CED
35	a	413	LMG	C15-C16-C17-C18
35	Z	101	LMG	C7-C8-C9-O8
35	z	101	LMG	C7-C8-C9-O8
25	R	602	CLA	C4-C3-C5-C6
25	r	602	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	4	607	CHL	C2A-CAA-CBA-CGA
24	8	607	CHL	C2A-CAA-CBA-CGA
24	4	608	CHL	CAA-CBA-CGA-O1A
26	1	1621	LUT	C9-C10-C11-C12
26	5	1621	LUT	C9-C10-C11-C12
25	C	504	CLA	O1A-CGA-O2A-C1
25	n	613	CLA	C5-C6-C7-C8
25	b	617	CLA	CBD-CGD-O2D-CED
35	Z	101	LMG	C19-C20-C21-C22
24	8	608	CHL	CAA-CBA-CGA-O1A
25	1	611	CLA	CAA-CBA-CGA-O1A
25	5	611	CLA	CAA-CBA-CGA-O1A
25	c	504	CLA	O1A-CGA-O2A-C1
35	z	101	LMG	C19-C20-C21-C22
29	c	522	LHG	C30-C31-C32-C33
29	C	522	LHG	C30-C31-C32-C33
37	b	626	DGD	C7B-C8B-C9B-CAB
25	B	617	CLA	CBD-CGD-O2D-CED
25	B	605	CLA	C13-C15-C16-C17
25	N	613	CLA	C5-C6-C7-C8
25	b	605	CLA	C13-C15-C16-C17
25	2	602	CLA	C11-C12-C13-C14
25	B	607	CLA	C11-C10-C8-C9
25	C	510	CLA	C11-C10-C8-C9
25	6	602	CLA	C11-C12-C13-C14
25	b	607	CLA	C11-C10-C8-C9
25	c	510	CLA	C11-C10-C8-C9
37	B	626	DGD	C7B-C8B-C9B-CAB
25	S	604	CLA	CAA-CBA-CGA-O2A
25	s	604	CLA	CAA-CBA-CGA-O2A
24	2	601	CHL	CAA-CBA-CGA-O1A
27	R	622	XAT	C27-C28-C29-C30
27	r	622	XAT	C27-C28-C29-C30
24	G	607	CHL	C5-C6-C7-C8
24	g	607	CHL	C5-C6-C7-C8
25	B	605	CLA	O1D-CGD-O2D-CED
25	2	603	CLA	CAA-CBA-CGA-O2A
25	3	611	CLA	CAA-CBA-CGA-O2A
25	6	603	CLA	CAA-CBA-CGA-O2A
25	7	611	CLA	CAA-CBA-CGA-O2A
35	A	415	LMG	O7-C10-C11-C12
24	5	601	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	6	601	CHL	CAA-CBA-CGA-O1A
25	S	609	CLA	CAA-CBA-CGA-O1A
25	s	609	CLA	CAA-CBA-CGA-O1A
25	S	609	CLA	C2A-CAA-CBA-CGA
25	s	609	CLA	C2A-CAA-CBA-CGA
24	3	601	CHL	C11-C12-C13-C15
24	7	601	CHL	C11-C12-C13-C15
25	3	613	CLA	C6-C7-C8-C10
25	B	614	CLA	C6-C7-C8-C10
25	B	617	CLA	C12-C13-C15-C16
25	C	502	CLA	C11-C12-C13-C15
25	C	506	CLA	C6-C7-C8-C10
25	D	403	CLA	C12-C13-C15-C16
25	G	602	CLA	C6-C7-C8-C10
25	N	603	CLA	C11-C10-C8-C7
25	S	602	CLA	C11-C12-C13-C15
25	7	613	CLA	C6-C7-C8-C10
25	b	614	CLA	C6-C7-C8-C10
25	b	617	CLA	C12-C13-C15-C16
25	c	502	CLA	C11-C12-C13-C15
25	c	506	CLA	C6-C7-C8-C10
25	d	403	CLA	C12-C13-C15-C16
25	g	602	CLA	C6-C7-C8-C10
25	n	603	CLA	C11-C10-C8-C7
25	s	602	CLA	C11-C12-C13-C15
24	1	601	CHL	CAA-CBA-CGA-O1A
25	2	611	CLA	CAA-CBA-CGA-O2A
25	6	611	CLA	CAA-CBA-CGA-O2A
25	1	602	CLA	C2B-C3B-CAB-CBB
25	1	614	CLA	C2B-C3B-CAB-CBB
25	4	610	CLA	C2B-C3B-CAB-CBB
25	C	503	CLA	C2B-C3B-CAB-CBB
25	G	613	CLA	C2B-C3B-CAB-CBB
25	N	612	CLA	C2B-C3B-CAB-CBB
25	S	602	CLA	C2B-C3B-CAB-CBB
25	5	602	CLA	C2B-C3B-CAB-CBB
25	5	614	CLA	C2B-C3B-CAB-CBB
25	8	610	CLA	C2B-C3B-CAB-CBB
25	c	503	CLA	C2B-C3B-CAB-CBB
25	g	613	CLA	C2B-C3B-CAB-CBB
25	n	612	CLA	C2B-C3B-CAB-CBB
25	s	602	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	3	1620	LUT	C5-C6-C7-C8
26	3	1621	LUT	C5-C6-C7-C8
26	G	1620	LUT	C1-C6-C7-C8
26	G	1620	LUT	C5-C6-C7-C8
26	S	1620	LUT	C1-C6-C7-C8
26	S	1620	LUT	C5-C6-C7-C8
26	S	1621	LUT	C5-C6-C7-C8
26	7	1620	LUT	C5-C6-C7-C8
26	7	1621	LUT	C5-C6-C7-C8
26	g	1620	LUT	C1-C6-C7-C8
26	g	1620	LUT	C5-C6-C7-C8
26	s	1620	LUT	C1-C6-C7-C8
26	s	1620	LUT	C5-C6-C7-C8
26	s	1621	LUT	C5-C6-C7-C8
30	C	516	BCR	C5-C6-C7-C8
30	c	516	BCR	C5-C6-C7-C8
35	a	415	LMG	O7-C10-C11-C12
35	Z	101	LMG	O9-C10-O7-C8
35	z	101	LMG	O9-C10-O7-C8
29	R	2630	LHG	C24-C25-C26-C27
29	r	2630	LHG	C24-C25-C26-C27
24	N	608	CHL	C2-C1-O2A-CGA
24	N	609	CHL	C2-C1-O2A-CGA
24	n	608	CHL	C2-C1-O2A-CGA
24	n	609	CHL	C2-C1-O2A-CGA
25	1	604	CLA	C2-C1-O2A-CGA
25	A	405	CLA	C2-C1-O2A-CGA
25	B	605	CLA	C2-C1-O2A-CGA
25	C	511	CLA	C2-C1-O2A-CGA
25	5	604	CLA	C2-C1-O2A-CGA
25	a	405	CLA	C2-C1-O2A-CGA
25	b	605	CLA	C2-C1-O2A-CGA
25	c	511	CLA	C2-C1-O2A-CGA
37	B	626	DGD	C6B-C7B-C8B-C9B
37	b	626	DGD	C6B-C7B-C8B-C9B
25	Y	612	CLA	CAA-CBA-CGA-O2A
25	y	612	CLA	CAA-CBA-CGA-O2A
35	Z	101	LMG	O8-C28-C29-C30
35	z	101	LMG	O8-C28-C29-C30
37	c	518	DGD	O2G-C1B-C2B-C3B
25	B	610	CLA	CBD-CGD-O2D-CED
35	Z	101	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
25	C	502	CLA	C13-C15-C16-C17
25	c	502	CLA	C13-C15-C16-C17
37	B	626	DGD	C4D-C5D-C6D-O5D
37	b	626	DGD	C4D-C5D-C6D-O5D
35	z	101	LMG	C20-C21-C22-C23
25	b	610	CLA	CBD-CGD-O2D-CED
37	C	518	DGD	O2G-C1B-C2B-C3B
37	C	519	DGD	O1G-C1A-C2A-C3A
37	c	519	DGD	O1G-C1A-C2A-C3A
25	A	405	CLA	O1A-CGA-O2A-C1
29	d	409	LHG	C29-C30-C31-C32
29	2	2630	LHG	C13-C14-C15-C16
29	D	409	LHG	C29-C30-C31-C32
29	6	2630	LHG	C13-C14-C15-C16
25	a	405	CLA	O1A-CGA-O2A-C1
25	c	501	CLA	CAA-CBA-CGA-O2A
24	N	606	CHL	O1A-CGA-O2A-C1
34	A	412	SQD	C4-C5-C6-S
34	B	621	SQD	C4-C5-C6-S
34	a	412	SQD	C4-C5-C6-S
34	b	621	SQD	C4-C5-C6-S
35	B	622	LMG	C39-C40-C41-C42
25	C	501	CLA	CAA-CBA-CGA-O2A
29	C	2630	LHG	O8-C23-C24-C25
29	c	2630	LHG	O8-C23-C24-C25
29	C	2630	LHG	O10-C23-O8-C6
25	2	602	CLA	C2-C3-C5-C6
25	6	602	CLA	C2-C3-C5-C6
35	d	411	LMG	C11-C10-O7-C8
35	b	622	LMG	C39-C40-C41-C42
24	n	606	CHL	O1A-CGA-O2A-C1
29	c	2630	LHG	O10-C23-O8-C6
24	1	601	CHL	C2A-CAA-CBA-CGA
24	5	601	CHL	C2A-CAA-CBA-CGA
25	B	606	CLA	C13-C15-C16-C17
25	b	606	CLA	C13-C15-C16-C17
24	Y	608	CHL	C11-C10-C8-C9
24	y	608	CHL	C11-C10-C8-C9
25	B	614	CLA	C11-C12-C13-C14
25	b	614	CLA	C11-C12-C13-C14
35	D	411	LMG	C15-C16-C17-C18
24	N	601	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	n	601	CHL	CAA-CBA-CGA-O2A
25	B	617	CLA	CAA-CBA-CGA-O2A
25	7	602	CLA	CAA-CBA-CGA-O2A
25	b	617	CLA	CAA-CBA-CGA-O2A
35	d	411	LMG	C15-C16-C17-C18
25	B	611	CLA	C16-C17-C18-C19
25	b	611	CLA	C16-C17-C18-C19
25	C	507	CLA	C5-C6-C7-C8
25	c	507	CLA	C5-C6-C7-C8
25	2	612	CLA	C1A-C2A-CAA-CBA
25	4	612	CLA	C1A-C2A-CAA-CBA
25	G	604	CLA	C4B-C3B-CAB-CBB
25	S	602	CLA	C4B-C3B-CAB-CBB
25	6	612	CLA	C1A-C2A-CAA-CBA
25	8	612	CLA	C1A-C2A-CAA-CBA
25	g	604	CLA	C4B-C3B-CAB-CBB
25	s	602	CLA	C4B-C3B-CAB-CBB
25	A	405	CLA	CBA-CGA-O2A-C1
25	a	405	CLA	CBA-CGA-O2A-C1
25	R	613	CLA	C4-C3-C5-C6
25	r	613	CLA	C4-C3-C5-C6
35	D	411	LMG	C11-C10-O7-C8
37	C	518	DGD	O6E-C1E-O5D-C6D
37	c	518	DGD	O6E-C1E-O5D-C6D
24	1	607	CHL	CAA-CBA-CGA-O2A
24	2	607	CHL	CAA-CBA-CGA-O2A
24	3	607	CHL	CAA-CBA-CGA-O2A
24	5	607	CHL	CAA-CBA-CGA-O2A
24	6	607	CHL	CAA-CBA-CGA-O2A
25	1	602	CLA	CAA-CBA-CGA-O2A
25	C	507	CLA	CAA-CBA-CGA-O2A
25	G	612	CLA	CAA-CBA-CGA-O2A
25	5	602	CLA	CAA-CBA-CGA-O2A
25	6	602	CLA	CAA-CBA-CGA-O2A
25	c	507	CLA	CAA-CBA-CGA-O2A
25	g	612	CLA	CAA-CBA-CGA-O2A
29	D	410	LHG	O8-C23-C24-C25
29	d	410	LHG	O8-C23-C24-C25
36	D	405	PL9	C46-C47-C48-C49
36	d	405	PL9	C46-C47-C48-C49
26	1	1621	LUT	C7-C8-C9-C10
26	5	1621	LUT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
30	B	618	BCR	C17-C18-C19-C20
30	C	516	BCR	C17-C18-C19-C20
30	b	618	BCR	C17-C18-C19-C20
30	c	516	BCR	C17-C18-C19-C20
27	2	1622	XAT	C13-C14-C15-C35
27	6	1622	XAT	C13-C14-C15-C35
25	S	611	CLA	C5-C6-C7-C8
25	s	611	CLA	C5-C6-C7-C8
29	G	2630	LHG	C30-C31-C32-C33
29	g	2630	LHG	C30-C31-C32-C33
25	2	602	CLA	CAA-CBA-CGA-O2A
25	3	602	CLA	CAA-CBA-CGA-O2A
25	G	611	CLA	CAA-CBA-CGA-O2A
25	R	603	CLA	CAA-CBA-CGA-O2A
34	A	412	SQD	O47-C7-C8-C9
34	a	412	SQD	O47-C7-C8-C9
29	C	2630	LHG	C12-C13-C14-C15
29	c	2630	LHG	C12-C13-C14-C15
25	3	613	CLA	C2A-CAA-CBA-CGA
25	7	613	CLA	C2A-CAA-CBA-CGA
25	b	610	CLA	O1D-CGD-O2D-CED
25	g	611	CLA	CAA-CBA-CGA-O2A
25	r	603	CLA	CAA-CBA-CGA-O2A
34	B	623	SQD	C5-C6-S-O9
34	b	623	SQD	C5-C6-S-O9
25	B	610	CLA	O1D-CGD-O2D-CED
25	A	410	CLA	C4-C3-C5-C6
25	a	410	CLA	C4-C3-C5-C6
24	2	609	CHL	C2-C1-O2A-CGA
24	G	608	CHL	C2-C1-O2A-CGA
24	6	609	CHL	C2-C1-O2A-CGA
24	g	608	CHL	C2-C1-O2A-CGA
25	B	609	CLA	C2-C1-O2A-CGA
25	b	609	CLA	C2-C1-O2A-CGA
24	7	607	CHL	CAA-CBA-CGA-O2A
29	G	2630	LHG	O8-C23-C24-C25
29	g	2630	LHG	O8-C23-C24-C25
24	2	607	CHL	C11-C10-C8-C7
24	G	607	CHL	C11-C10-C8-C7
24	Y	609	CHL	C11-C12-C13-C15
24	6	607	CHL	C11-C10-C8-C7
24	g	607	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	y	609	CHL	C11-C12-C13-C15
25	2	602	CLA	C6-C7-C8-C10
25	B	602	CLA	C12-C13-C15-C16
25	B	603	CLA	C6-C7-C8-C10
25	B	608	CLA	C12-C13-C15-C16
25	C	505	CLA	C12-C13-C15-C16
25	G	602	CLA	C11-C12-C13-C15
25	6	602	CLA	C6-C7-C8-C10
25	b	602	CLA	C12-C13-C15-C16
25	b	603	CLA	C6-C7-C8-C10
25	b	608	CLA	C12-C13-C15-C16
25	c	505	CLA	C12-C13-C15-C16
25	g	602	CLA	C11-C12-C13-C15
25	B	614	CLA	CBA-CGA-O2A-C1
25	b	614	CLA	CBA-CGA-O2A-C1
25	2	603	CLA	C5-C6-C7-C8
25	6	603	CLA	C5-C6-C7-C8
29	D	409	LHG	C10-C11-C12-C13
29	d	409	LHG	C10-C11-C12-C13
35	B	2633	LMG	C7-C8-O7-C10
35	b	2633	LMG	C7-C8-O7-C10
35	D	411	LMG	C13-C14-C15-C16
35	d	411	LMG	C13-C14-C15-C16
25	C	510	CLA	CAA-CBA-CGA-O2A
25	c	510	CLA	CAA-CBA-CGA-O2A
29	L	101	LHG	O7-C7-C8-C9
29	l	101	LHG	O7-C7-C8-C9
24	1	609	CHL	C5-C6-C7-C8
24	5	609	CHL	C5-C6-C7-C8
25	C	506	CLA	C5-C6-C7-C8
25	c	506	CLA	C5-C6-C7-C8
25	C	513	CLA	C2A-CAA-CBA-CGA
25	R	610	CLA	C2A-CAA-CBA-CGA
25	Y	604	CLA	C2A-CAA-CBA-CGA
25	c	513	CLA	C2A-CAA-CBA-CGA
25	r	610	CLA	C2A-CAA-CBA-CGA
24	G	608	CHL	C3A-C2A-CAA-CBA
24	S	608	CHL	C3A-C2A-CAA-CBA
24	g	608	CHL	C3A-C2A-CAA-CBA
24	s	608	CHL	C3A-C2A-CAA-CBA
25	2	612	CLA	C3A-C2A-CAA-CBA
25	3	611	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	4	604	CLA	C3A-C2A-CAA-CBA
25	4	612	CLA	C3A-C2A-CAA-CBA
25	C	508	CLA	C4-C3-C5-C6
25	C	512	CLA	C3A-C2A-CAA-CBA
25	6	612	CLA	C3A-C2A-CAA-CBA
25	7	611	CLA	C3A-C2A-CAA-CBA
25	8	604	CLA	C3A-C2A-CAA-CBA
25	8	612	CLA	C3A-C2A-CAA-CBA
25	c	508	CLA	C4-C3-C5-C6
25	c	512	CLA	C3A-C2A-CAA-CBA
25	2	611	CLA	CAA-CBA-CGA-O1A
25	6	611	CLA	CAA-CBA-CGA-O1A
29	C	2630	LHG	O9-C7-C8-C9
29	c	2630	LHG	O9-C7-C8-C9
29	3	2630	LHG	C9-C10-C11-C12
29	7	2630	LHG	C9-C10-C11-C12
37	b	626	DGD	C3B-C4B-C5B-C6B
35	A	415	LMG	O8-C28-C29-C30
35	a	415	LMG	O8-C28-C29-C30
25	s	602	CLA	O1A-CGA-O2A-C1
29	G	2630	LHG	O10-C23-C24-C25
29	L	101	LHG	O9-C7-C8-C9
29	l	101	LHG	O9-C7-C8-C9
37	B	626	DGD	C3B-C4B-C5B-C6B
25	Y	610	CLA	C2A-CAA-CBA-CGA
25	y	604	CLA	C2A-CAA-CBA-CGA
25	y	610	CLA	C2A-CAA-CBA-CGA
24	2	601	CHL	CAA-CBA-CGA-O2A
24	6	601	CHL	CAA-CBA-CGA-O2A
25	3	613	CLA	C6-C7-C8-C9
25	B	608	CLA	C14-C13-C15-C16
25	B	613	CLA	C6-C7-C8-C9
25	C	506	CLA	C6-C7-C8-C9
25	G	602	CLA	C11-C12-C13-C14
25	7	613	CLA	C6-C7-C8-C9
25	b	608	CLA	C14-C13-C15-C16
25	b	613	CLA	C6-C7-C8-C9
25	c	506	CLA	C6-C7-C8-C9
25	g	602	CLA	C11-C12-C13-C14
25	6	603	CLA	CAA-CBA-CGA-O1A
25	y	612	CLA	CAA-CBA-CGA-O1A
29	C	2630	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
29	C	522	LHG	O9-C7-C8-C9
29	c	522	LHG	O9-C7-C8-C9
29	g	2630	LHG	O10-C23-C24-C25
25	S	602	CLA	O1A-CGA-O2A-C1
25	2	603	CLA	CAA-CBA-CGA-O1A
25	Y	612	CLA	CAA-CBA-CGA-O1A
29	c	2630	LHG	O10-C23-C24-C25
25	C	506	CLA	C2-C3-C5-C6
25	c	506	CLA	C2-C3-C5-C6
37	C	519	DGD	C7A-C8A-C9A-CAA
25	G	612	CLA	CAA-CBA-CGA-O1A
25	S	604	CLA	CAA-CBA-CGA-O1A
25	g	612	CLA	CAA-CBA-CGA-O1A
25	s	604	CLA	CAA-CBA-CGA-O1A
37	c	519	DGD	C7A-C8A-C9A-CAA
29	B	2630	LHG	O1-C1-C2-O2
29	b	2630	LHG	O1-C1-C2-O2
29	C	522	LHG	O7-C7-C8-C9
29	c	522	LHG	O7-C7-C8-C9
33	a	408	PHO	C2C-C3C-CAC-CBC
25	N	611	CLA	C10-C11-C12-C13
25	n	611	CLA	C10-C11-C12-C13
27	R	622	XAT	C11-C12-C13-C14
27	r	622	XAT	C11-C12-C13-C14
28	R	623	NEX	C11-C12-C13-C14
28	r	623	NEX	C11-C12-C13-C14
30	C	515	BCR	C17-C18-C19-C20
30	c	515	BCR	C17-C18-C19-C20
24	3	607	CHL	CAA-CBA-CGA-O1A
24	7	607	CHL	CAA-CBA-CGA-O1A
25	3	611	CLA	CAA-CBA-CGA-O1A
25	C	507	CLA	CAA-CBA-CGA-O1A
25	R	603	CLA	CAA-CBA-CGA-O1A
25	c	507	CLA	CAA-CBA-CGA-O1A
25	r	603	CLA	CAA-CBA-CGA-O1A
29	D	410	LHG	O10-C23-C24-C25
29	d	410	LHG	O10-C23-C24-C25
34	B	623	SQD	O49-C7-C8-C9
25	N	610	CLA	C8-C10-C11-C12
25	n	610	CLA	C8-C10-C11-C12
25	s	610	CLA	C5-C6-C7-C8
35	A	413	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
35	B	622	LMG	C8-C7-O1-C1
35	a	413	LMG	C8-C7-O1-C1
35	b	622	LMG	C8-C7-O1-C1
37	C	519	DGD	C2G-C3G-O3G-C1D
37	C	520	DGD	C5D-C6D-O5D-C1E
37	c	519	DGD	C2G-C3G-O3G-C1D
37	c	520	DGD	C5D-C6D-O5D-C1E
35	Z	101	LMG	O7-C8-C9-O8
35	z	101	LMG	O7-C8-C9-O8
29	b	2631	LHG	C11-C12-C13-C14
25	7	611	CLA	CAA-CBA-CGA-O1A
34	b	623	SQD	O49-C7-C8-C9
37	C	519	DGD	O1B-C1B-C2B-C3B
37	c	519	DGD	O1B-C1B-C2B-C3B
25	S	610	CLA	C5-C6-C7-C8
25	g	610	CLA	C16-C17-C18-C19
25	Y	603	CLA	C2A-CAA-CBA-CGA
25	y	603	CLA	C2A-CAA-CBA-CGA
29	B	2631	LHG	C11-C12-C13-C14
25	B	610	CLA	C16-C17-C18-C19
25	G	610	CLA	C16-C17-C18-C19
24	g	605	CHL	CAA-CBA-CGA-O2A
25	2	602	CLA	CAA-CBA-CGA-O1A
25	C	510	CLA	CAA-CBA-CGA-O1A
25	6	602	CLA	CAA-CBA-CGA-O1A
25	c	510	CLA	CAA-CBA-CGA-O1A
37	C	520	DGD	O1B-C1B-C2B-C3B
37	c	520	DGD	O1B-C1B-C2B-C3B
29	6	2630	LHG	C10-C11-C12-C13
25	B	603	CLA	C8-C10-C11-C12
25	R	610	CLA	C10-C11-C12-C13
25	b	603	CLA	C8-C10-C11-C12
25	c	510	CLA	C10-C11-C12-C13
25	r	610	CLA	C10-C11-C12-C13
29	N	2630	LHG	C5-C4-O6-P
29	n	2630	LHG	C5-C4-O6-P
33	A	408	PHO	C2C-C3C-CAC-CBC
24	2	607	CHL	CAA-CBA-CGA-O1A
25	3	602	CLA	CAA-CBA-CGA-O1A
25	7	602	CLA	CAA-CBA-CGA-O1A
25	b	617	CLA	CAA-CBA-CGA-O1A
29	N	2630	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
29	2	2630	LHG	C10-C11-C12-C13
29	3	2630	LHG	C17-C18-C19-C20
29	7	2630	LHG	C17-C18-C19-C20
25	b	610	CLA	C16-C17-C18-C19
24	R	606	CHL	CAD-CBD-CGD-O2D
24	r	606	CHL	CAD-CBD-CGD-O2D
25	1	602	CLA	CAD-CBD-CGD-O2D
25	4	611	CLA	CAD-CBD-CGD-O2D
25	D	403	CLA	CAD-CBD-CGD-O2D
25	G	614	CLA	CAD-CBD-CGD-O2D
25	N	602	CLA	CAD-CBD-CGD-O2D
25	N	610	CLA	CAD-CBD-CGD-O2D
25	5	602	CLA	CAD-CBD-CGD-O2D
25	8	611	CLA	CAD-CBD-CGD-O2D
25	d	403	CLA	CAD-CBD-CGD-O2D
25	g	614	CLA	CAD-CBD-CGD-O2D
25	n	602	CLA	CAD-CBD-CGD-O2D
25	n	610	CLA	CAD-CBD-CGD-O2D
25	C	510	CLA	C10-C11-C12-C13
24	Y	601	CHL	CAA-CBA-CGA-O2A
24	y	601	CHL	CAA-CBA-CGA-O2A
24	G	605	CHL	CAA-CBA-CGA-O2A
24	6	607	CHL	CAA-CBA-CGA-O1A
25	B	617	CLA	CAA-CBA-CGA-O1A
25	C	501	CLA	CAA-CBA-CGA-O1A
29	n	2630	LHG	O10-C23-C24-C25
33	A	409	PHO	C8-C10-C11-C12
33	a	409	PHO	C8-C10-C11-C12
24	3	609	CHL	C2-C1-O2A-CGA
24	7	609	CHL	C2-C1-O2A-CGA
25	C	502	CLA	C2-C1-O2A-CGA
25	D	403	CLA	C2-C1-O2A-CGA
25	c	502	CLA	C2-C1-O2A-CGA
25	d	403	CLA	C2-C1-O2A-CGA
25	c	501	CLA	CAA-CBA-CGA-O1A
25	N	612	CLA	CAA-CBA-CGA-O2A
25	n	612	CLA	CAA-CBA-CGA-O2A
24	3	607	CHL	C1A-C2A-CAA-CBA
24	7	607	CHL	C1A-C2A-CAA-CBA
35	a	413	LMG	O10-C28-C29-C30
25	Y	613	CLA	C5-C6-C7-C8
25	y	613	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	G	601	CHL	CAA-CBA-CGA-O2A
24	S	607	CHL	CAA-CBA-CGA-O2A
24	g	601	CHL	CAA-CBA-CGA-O2A
24	s	607	CHL	CAA-CBA-CGA-O2A
24	2	605	CHL	CAA-CBA-CGA-O2A
24	6	605	CHL	CAA-CBA-CGA-O2A
29	G	2630	LHG	C8-C7-O7-C5
29	g	2630	LHG	C8-C7-O7-C5
25	5	602	CLA	CAA-CBA-CGA-O1A
35	A	413	LMG	O10-C28-C29-C30
25	Y	602	CLA	C5-C6-C7-C8
29	N	2630	LHG	C16-C17-C18-C19
29	n	2630	LHG	C16-C17-C18-C19
25	1	613	CLA	CAA-CBA-CGA-O2A
25	Y	602	CLA	CAA-CBA-CGA-O2A
25	5	613	CLA	CAA-CBA-CGA-O2A
25	n	602	CLA	CAA-CBA-CGA-O2A
25	y	602	CLA	CAA-CBA-CGA-O2A
29	D	410	LHG	C23-C24-C25-C26
29	d	410	LHG	C23-C24-C25-C26
24	1	607	CHL	CAA-CBA-CGA-O1A
24	N	601	CHL	CAA-CBA-CGA-O1A
24	5	607	CHL	CAA-CBA-CGA-O1A
24	n	601	CHL	CAA-CBA-CGA-O1A
25	1	602	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

429 monomers are involved in 1087 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	Y	605	CHL	1	0
25	C	511	CLA	9	0
24	3	601	CHL	2	0
29	d	408	LHG	5	0
24	G	601	CHL	4	0
25	5	612	CLA	2	0
28	7	1623	NEX	2	0
25	a	406	CLA	2	0
25	3	610	CLA	2	0
25	2	613	CLA	2	0
24	s	607	CHL	3	0
26	y	1620	LUT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	5	602	CLA	4	0
24	7	606	CHL	4	0
30	C	515	BCR	2	0
25	B	617	CLA	1	0
34	a	418	SQD	6	0
24	Y	608	CHL	3	0
29	Y	2630	LHG	3	0
28	G	1623	NEX	3	0
24	g	608	CHL	4	0
24	R	606	CHL	1	0
25	6	611	CLA	1	0
25	b	607	CLA	3	0
25	c	507	CLA	5	0
25	b	614	CLA	4	0
24	3	607	CHL	6	0
25	2	614	CLA	1	0
38	D	401	BCT	1	0
24	3	606	CHL	4	0
25	C	510	CLA	5	0
25	r	609	CLA	3	0
26	n	1621	LUT	4	0
25	y	612	CLA	2	0
27	2	1622	XAT	6	0
25	g	611	CLA	1	0
27	N	1622	XAT	6	0
30	C	517	BCR	9	0
34	A	412	SQD	2	0
24	r	606	CHL	1	0
24	2	609	CHL	4	0
25	n	611	CLA	2	0
27	6	1622	XAT	5	0
28	r	623	NEX	2	0
24	5	605	CHL	1	0
24	g	607	CHL	4	0
29	D	410	LHG	4	0
24	r	607	CHL	1	0
25	N	603	CLA	4	0
24	n	601	CHL	1	0
25	s	603	CLA	1	0
24	n	607	CHL	3	0
29	C	523	LHG	1	0
25	S	610	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	7	613	CLA	2	0
25	4	610	CLA	1	0
24	2	608	CHL	2	0
25	B	605	CLA	7	0
26	3	1621	LUT	4	0
25	5	603	CLA	1	0
25	a	405	CLA	5	0
24	G	608	CHL	4	0
25	c	508	CLA	2	0
35	D	411	LMG	2	0
29	7	2630	LHG	4	0
25	R	602	CLA	4	0
25	2	610	CLA	3	0
26	1	1620	LUT	6	0
30	B	620	BCR	3	0
27	R	622	XAT	5	0
25	R	613	CLA	2	0
29	B	2630	LHG	2	0
26	6	1620	LUT	4	0
25	S	609	CLA	1	0
25	B	604	CLA	4	0
25	y	603	CLA	6	0
30	8	623	BCR	3	0
29	R	2630	LHG	3	0
25	r	616	CLA	2	0
28	Y	1623	NEX	1	0
28	1	1623	NEX	3	0
29	4	2630	LHG	1	0
38	d	401	BCT	1	0
30	b	619	BCR	5	0
24	N	609	CHL	5	0
37	b	626	DGD	1	0
30	c	516	BCR	2	0
29	c	523	LHG	1	0
37	C	519	DGD	3	0
24	y	607	CHL	2	0
25	Y	603	CLA	7	0
25	n	603	CLA	4	0
24	S	607	CHL	3	0
24	3	608	CHL	2	0
25	n	604	CLA	1	0
35	C	521	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	1	610	CLA	2	0
27	g	1622	XAT	4	0
24	N	607	CHL	4	0
25	y	610	CLA	1	0
26	n	1620	LUT	5	0
29	N	2630	LHG	4	0
25	g	614	CLA	2	0
27	G	1622	XAT	4	0
36	D	405	PL9	6	0
29	D	409	LHG	11	0
24	4	601	CHL	1	0
28	n	1623	NEX	5	0
30	T	101	BCR	3	0
25	Y	610	CLA	2	0
25	7	611	CLA	2	0
25	A	410	CLA	6	0
29	d	410	LHG	4	0
30	t	101	BCR	7	0
29	L	101	LHG	8	0
25	C	506	CLA	2	0
25	3	603	CLA	1	0
25	R	604	CLA	1	0
24	7	609	CHL	4	0
29	G	2630	LHG	2	0
28	3	1623	NEX	2	0
25	2	612	CLA	2	0
24	7	607	CHL	6	0
30	C	514	BCR	2	0
35	b	622	LMG	4	0
26	S	1621	LUT	4	0
26	5	1620	LUT	7	0
27	8	622	XAT	7	0
29	b	2631	LHG	5	0
30	d	404	BCR	7	0
24	y	606	CHL	1	0
25	D	402	CLA	7	0
30	D	404	BCR	4	0
34	a	412	SQD	2	0
24	1	609	CHL	4	0
25	c	501	CLA	4	0
26	S	1620	LUT	3	0
25	B	614	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	6	605	CHL	1	0
28	5	1623	NEX	3	0
25	2	602	CLA	3	0
24	6	609	CHL	5	0
29	y	2630	LHG	4	0
28	S	1623	NEX	1	0
24	4	606	CHL	1	0
26	R	620	LUT	4	0
27	y	1622	XAT	5	0
25	Y	611	CLA	2	0
37	c	519	DGD	3	0
25	s	604	CLA	1	0
24	7	608	CHL	3	0
24	r	608	CHL	1	0
29	D	408	LHG	4	0
26	4	620	LUT	4	0
26	y	1621	LUT	3	0
24	4	608	CHL	1	0
25	C	505	CLA	1	0
35	A	413	LMG	2	0
24	3	605	CHL	1	0
24	5	607	CHL	4	0
24	8	606	CHL	1	0
25	5	610	CLA	2	0
25	s	609	CLA	1	0
25	7	610	CLA	3	0
26	Y	1621	LUT	5	0
24	Y	607	CHL	3	0
25	s	610	CLA	1	0
25	r	602	CLA	5	0
26	1	1621	LUT	4	0
25	b	612	CLA	5	0
25	R	611	CLA	3	0
30	c	517	BCR	10	0
27	n	1622	XAT	7	0
25	g	604	CLA	2	0
24	3	609	CHL	3	0
29	b	2630	LHG	2	0
25	S	603	CLA	2	0
25	y	613	CLA	2	0
30	H	101	BCR	6	0
24	n	609	CHL	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	g	609	CHL	3	0
25	b	613	CLA	6	0
25	r	612	CLA	2	0
33	a	408	PHO	7	0
25	b	610	CLA	2	0
25	Y	612	CLA	3	0
25	c	512	CLA	1	0
24	5	606	CHL	2	0
25	1	613	CLA	1	0
26	s	1621	LUT	3	0
25	r	610	CLA	1	0
25	N	612	CLA	4	0
25	g	602	CLA	3	0
25	s	611	CLA	1	0
33	A	409	PHO	4	0
25	G	610	CLA	6	0
26	5	1621	LUT	4	0
25	R	609	CLA	4	0
37	C	518	DGD	3	0
25	d	402	CLA	5	0
27	r	622	XAT	5	0
25	4	611	CLA	1	0
25	c	511	CLA	9	0
25	C	503	CLA	2	0
25	B	606	CLA	4	0
24	6	606	CHL	3	0
25	B	611	CLA	5	0
25	g	610	CLA	6	0
24	1	608	CHL	1	0
35	Z	101	LMG	6	0
24	y	608	CHL	3	0
25	6	612	CLA	2	0
25	y	604	CLA	2	0
26	2	1621	LUT	3	0
24	2	607	CHL	2	0
25	b	616	CLA	4	0
24	G	609	CHL	2	0
25	B	616	CLA	4	0
29	6	2630	LHG	2	0
29	3	2630	LHG	3	0
25	Y	604	CLA	2	0
29	B	2631	LHG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	G	607	CHL	4	0
24	1	607	CHL	4	0
26	Y	1620	LUT	4	0
25	6	604	CLA	2	0
26	s	1620	LUT	2	0
25	3	613	CLA	3	0
25	b	602	CLA	4	0
24	S	606	CHL	2	0
25	b	604	CLA	3	0
25	4	612	CLA	2	0
24	S	608	CHL	1	0
25	B	603	CLA	8	0
29	S	2630	LHG	2	0
35	c	521	LMG	1	0
25	N	613	CLA	4	0
25	7	603	CLA	2	0
25	r	603	CLA	2	0
25	s	613	CLA	1	0
25	S	613	CLA	1	0
30	b	620	BCR	2	0
25	6	614	CLA	1	0
24	N	606	CHL	3	0
34	b	621	SQD	4	0
35	b	2633	LMG	2	0
25	g	612	CLA	2	0
25	6	613	CLA	2	0
25	8	612	CLA	2	0
25	B	612	CLA	3	0
29	d	409	LHG	11	0
25	C	512	CLA	1	0
24	G	605	CHL	1	0
24	y	601	CHL	8	0
29	8	2630	LHG	1	0
26	G	1620	LUT	8	0
25	B	602	CLA	4	0
30	a	411	BCR	3	0
25	R	616	CLA	4	0
25	G	611	CLA	1	0
25	N	602	CLA	8	0
25	2	603	CLA	2	0
24	Y	601	CHL	7	0
25	C	513	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	c	514	BCR	2	0
25	B	610	CLA	1	0
24	5	608	CHL	1	0
26	g	1620	LUT	8	0
24	g	601	CHL	4	0
25	A	406	CLA	3	0
37	H	102	DGD	6	0
24	y	605	CHL	1	0
26	g	1621	LUT	6	0
30	B	619	BCR	4	0
25	8	604	CLA	1	0
26	2	1620	LUT	4	0
30	A	411	BCR	2	0
25	G	603	CLA	3	0
28	2	1623	NEX	2	0
25	y	611	CLA	4	0
24	y	609	CHL	2	0
24	s	606	CHL	2	0
24	6	607	CHL	2	0
25	B	608	CLA	3	0
24	6	608	CHL	2	0
27	1	1622	XAT	4	0
25	c	506	CLA	3	0
28	s	1623	NEX	1	0
25	6	610	CLA	3	0
24	1	606	CHL	2	0
24	s	608	CHL	1	0
31	A	401	OEX	2	0
25	c	505	CLA	1	0
29	c	522	LHG	3	0
25	D	403	CLA	2	0
26	8	620	LUT	3	0
25	1	603	CLA	2	0
25	S	604	CLA	1	0
29	C	2630	LHG	4	0
25	b	615	CLA	5	0
35	d	411	LMG	3	0
25	b	611	CLA	4	0
34	b	623	SQD	5	0
25	c	510	CLA	4	0
25	N	611	CLA	2	0
34	B	621	SQD	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	l	101	LHG	8	0
29	r	2630	LHG	3	0
25	7	602	CLA	4	0
30	h	101	BCR	5	0
25	G	612	CLA	1	0
25	b	608	CLA	2	0
25	d	403	CLA	2	0
27	Y	1622	XAT	5	0
36	d	405	PL9	6	0
30	c	515	BCR	2	0
28	y	1623	NEX	4	0
29	C	522	LHG	2	0
25	C	502	CLA	1	0
33	a	409	PHO	4	0
24	g	605	CHL	1	0
25	1	612	CLA	2	0
25	A	407	CLA	1	0
25	G	614	CLA	2	0
25	3	611	CLA	2	0
25	G	613	CLA	5	0
24	8	608	CHL	1	0
25	b	605	CLA	8	0
24	g	606	CHL	2	0
25	B	615	CLA	5	0
29	s	2630	LHG	2	0
24	2	605	CHL	1	0
25	n	610	CLA	4	0
24	8	607	CHL	1	0
24	R	608	CHL	2	0
25	C	507	CLA	5	0
25	b	606	CLA	5	0
37	C	520	DGD	2	0
24	n	606	CHL	2	0
26	N	1620	LUT	2	0
25	A	405	CLA	5	0
26	N	1621	LUT	4	0
25	c	513	CLA	3	0
24	R	607	CHL	1	0
27	5	1622	XAT	4	0
37	c	518	DGD	3	0
35	a	413	LMG	2	0
25	8	611	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	3	1620	LUT	7	0
25	c	503	CLA	2	0
26	6	1621	LUT	3	0
25	G	602	CLA	3	0
24	n	608	CHL	3	0
37	h	102	DGD	6	0
24	5	609	CHL	6	0
25	r	613	CLA	2	0
28	N	1623	NEX	3	0
25	S	611	CLA	1	0
30	b	618	BCR	5	0
33	A	408	PHO	7	0
25	R	612	CLA	2	0
24	N	601	CHL	1	0
25	N	604	CLA	1	0
28	R	623	NEX	4	0
24	G	606	CHL	1	0
25	1	602	CLA	4	0
24	2	606	CHL	3	0
35	B	622	LMG	4	0
25	N	610	CLA	4	0
25	8	610	CLA	1	0
25	y	602	CLA	3	0
25	r	604	CLA	1	0
25	6	602	CLA	3	0
26	7	1620	LUT	6	0
25	R	610	CLA	1	0
25	b	603	CLA	9	0
25	G	604	CLA	2	0
25	1	604	CLA	1	0
30	C	516	BCR	2	0
24	7	601	CHL	2	0
34	B	623	SQD	5	0
25	Y	613	CLA	2	0
26	7	1621	LUT	3	0
25	n	613	CLA	4	0
25	g	613	CLA	5	0
24	Y	609	CHL	2	0
25	c	502	CLA	1	0
37	c	520	DGD	2	0
25	4	603	CLA	1	0
29	n	2630	LHG	4	0

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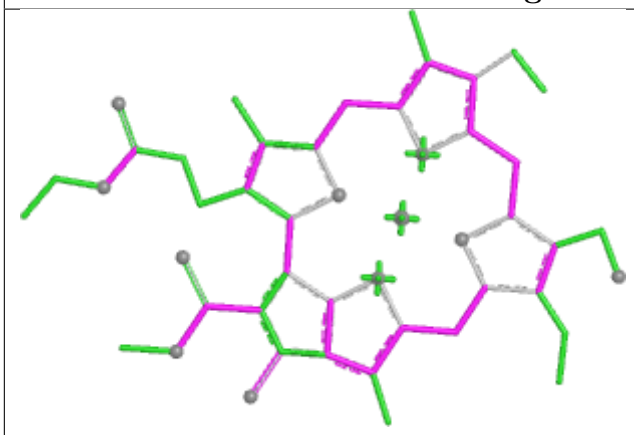
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	n	612	CLA	4	0
25	a	410	CLA	7	0
24	N	608	CHL	2	0
25	Y	602	CLA	5	0
34	A	418	SQD	6	0
29	2	2630	LHG	2	0
25	5	613	CLA	1	0
35	B	2633	LMG	2	0
25	2	604	CLA	1	0
25	B	613	CLA	7	0
25	8	603	CLA	1	0
27	3	1622	XAT	4	0
25	C	508	CLA	2	0
35	z	101	LMG	5	0
26	G	1621	LUT	6	0
25	6	603	CLA	1	0
27	4	622	XAT	5	0
25	c	504	CLA	1	0
25	C	501	CLA	4	0
25	R	603	CLA	2	0
31	a	401	OEX	2	0
26	r	620	LUT	4	0
25	s	614	CLA	1	0
37	B	626	DGD	1	0
28	g	1623	NEX	2	0
25	5	604	CLA	1	0
25	n	602	CLA	8	0
29	g	2630	LHG	4	0
25	g	603	CLA	4	0
27	7	1622	XAT	7	0
30	4	623	BCR	3	0
25	r	611	CLA	3	0
29	c	2630	LHG	5	0
24	7	605	CHL	1	0
25	3	602	CLA	3	0
25	C	504	CLA	1	0
25	a	407	CLA	1	0
30	B	618	BCR	6	0
25	B	607	CLA	4	0

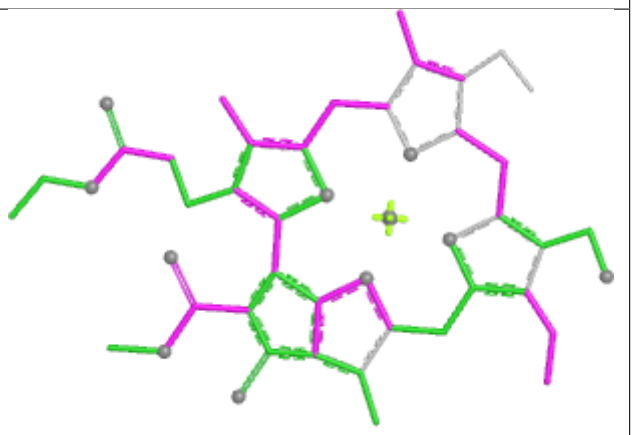
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

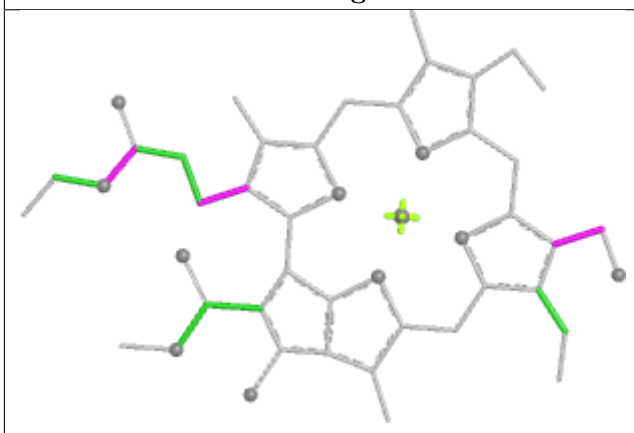
Ligand CHL Y 605



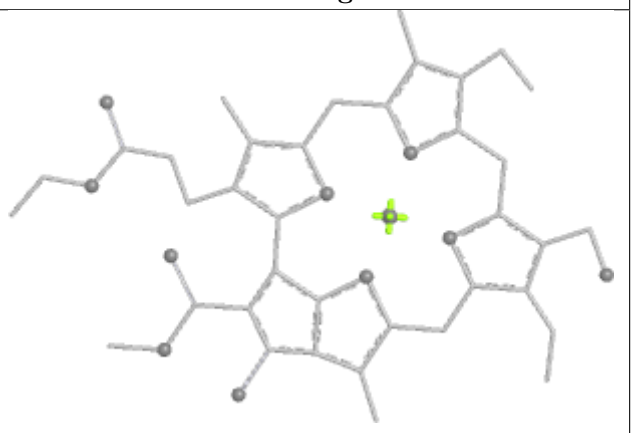
Bond lengths



Bond angles

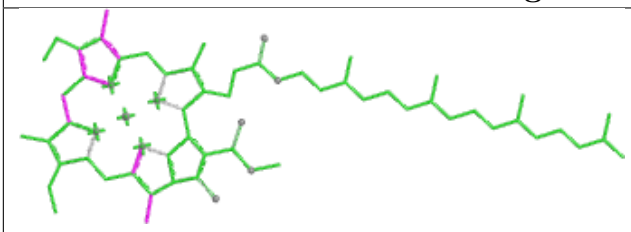


Torsions

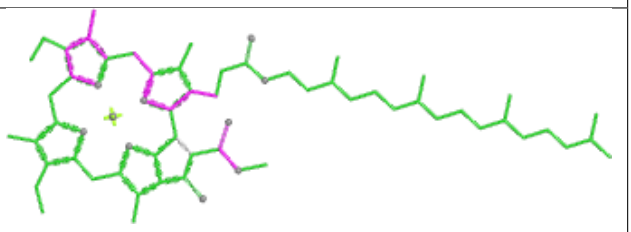


Rings

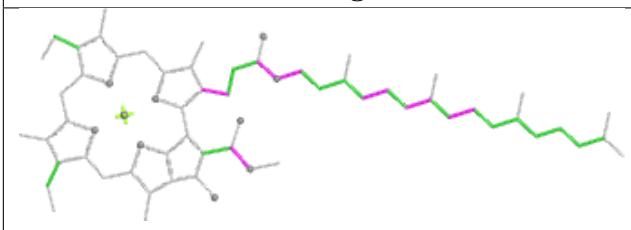
Ligand CLA C 511



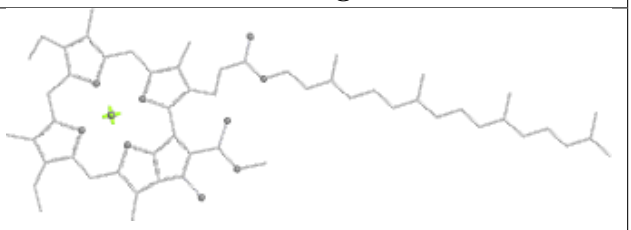
Bond lengths



Bond angles

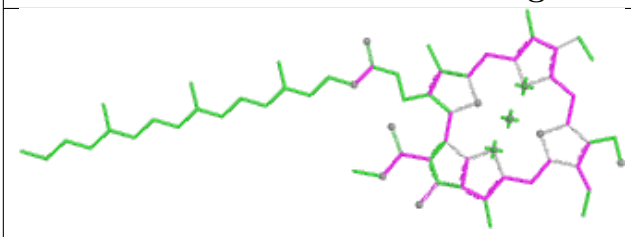


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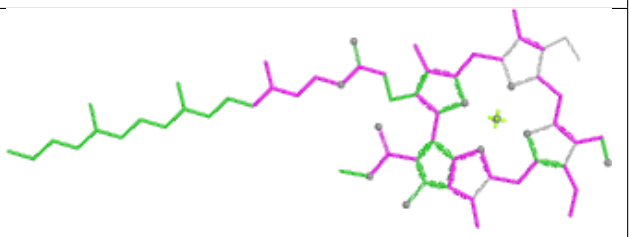


Rings

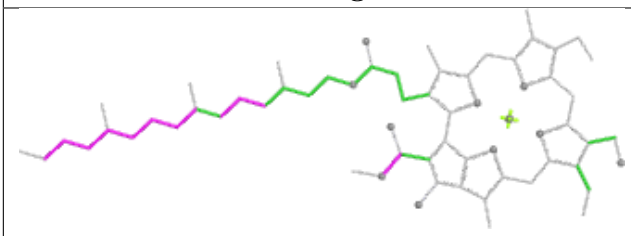
Ligand CHL 3 601



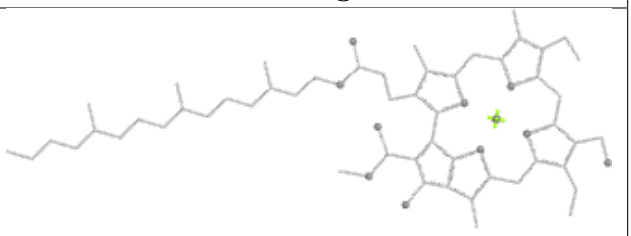
Bond lengths



Bond angles

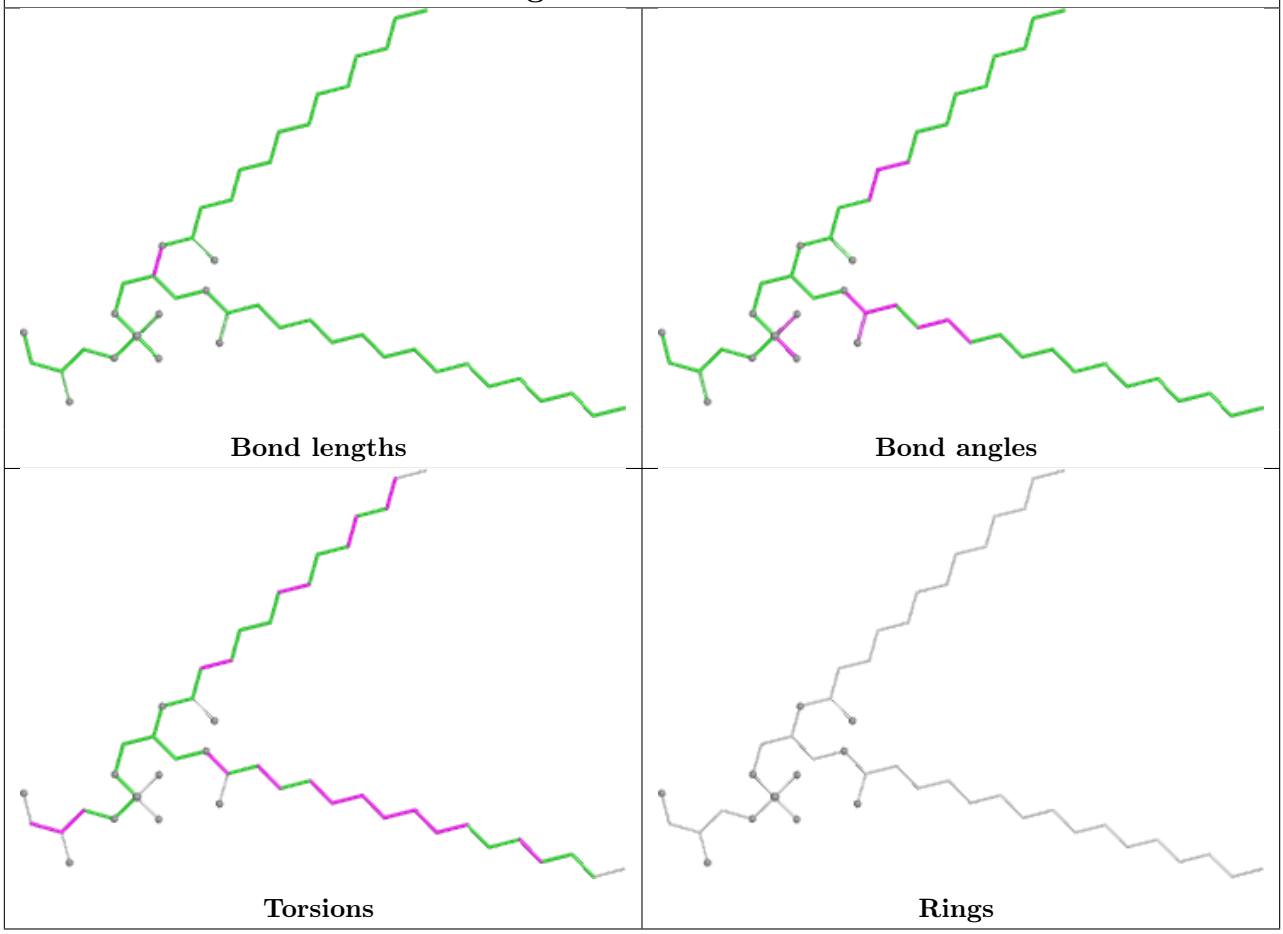


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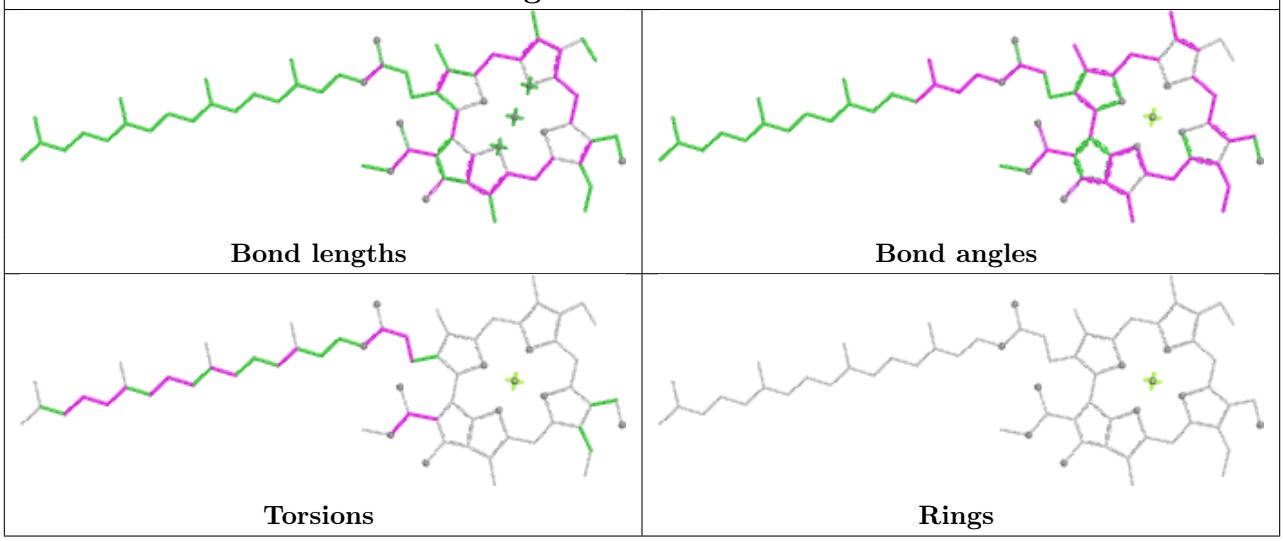


Rings

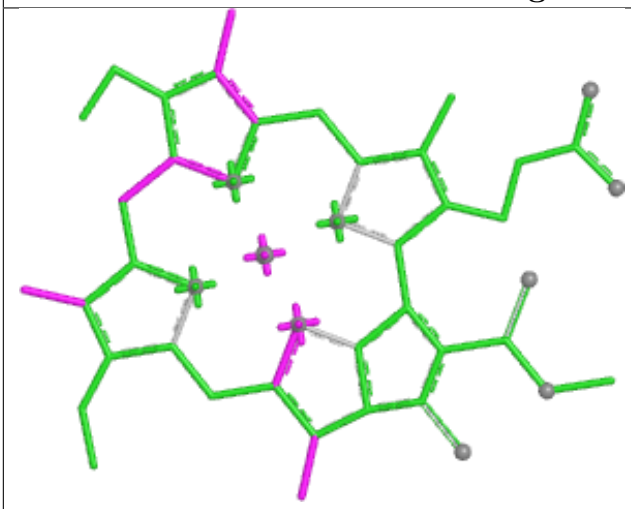
Ligand LHG d 408



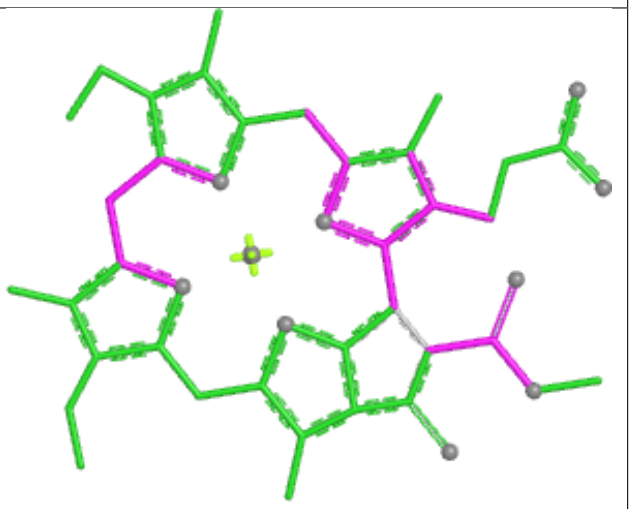
Ligand CHL G 601



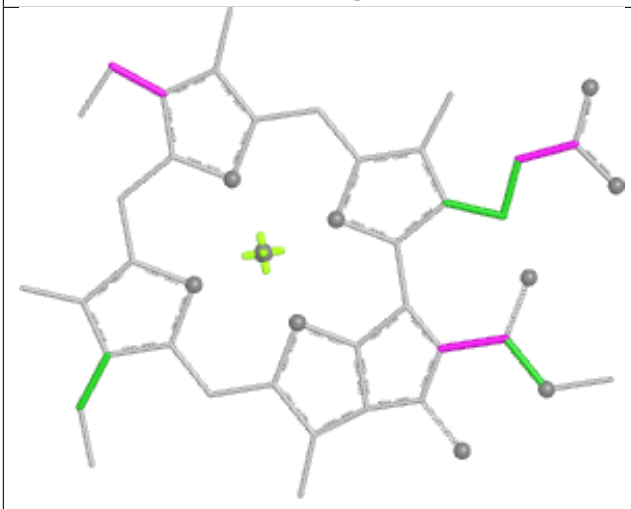
Ligand CLA 5 612



Bond lengths



Bond angles

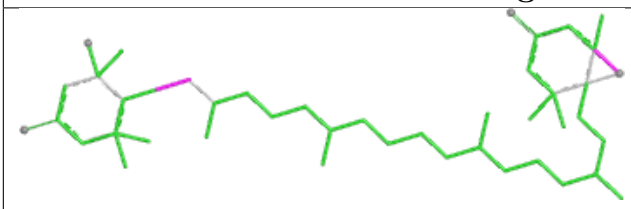


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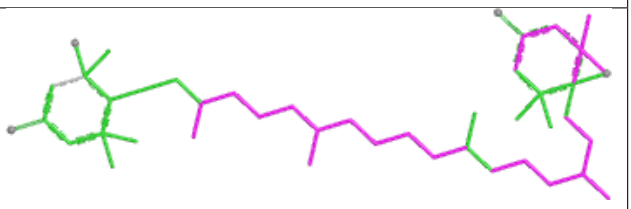


Rings

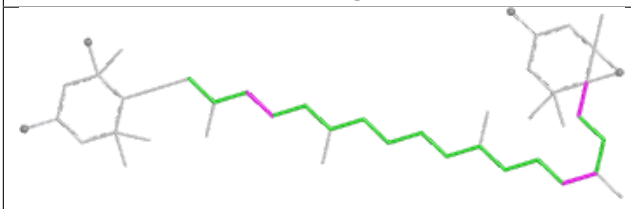
Ligand NEX 7 1623



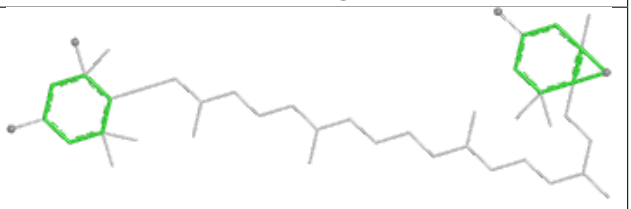
Bond lengths



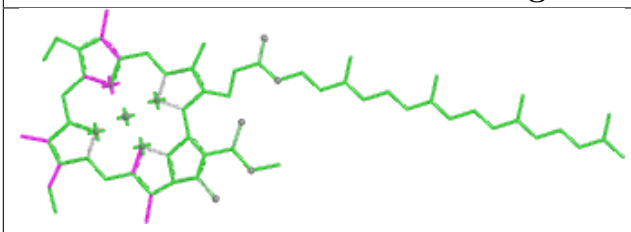
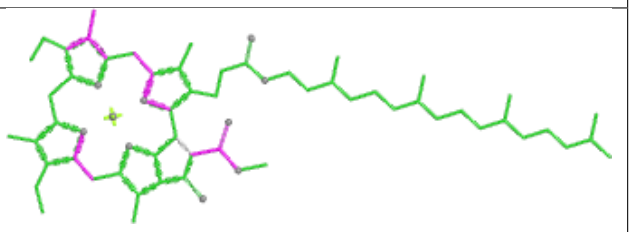
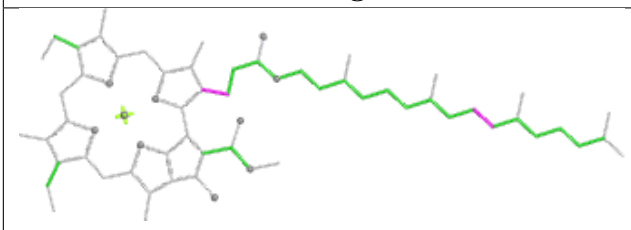
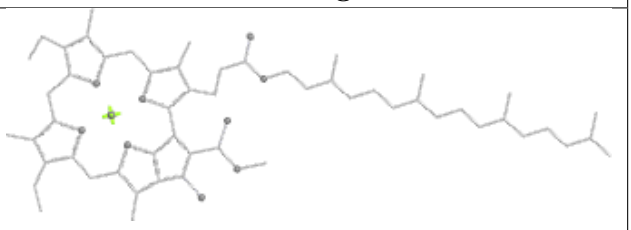
Bond angles

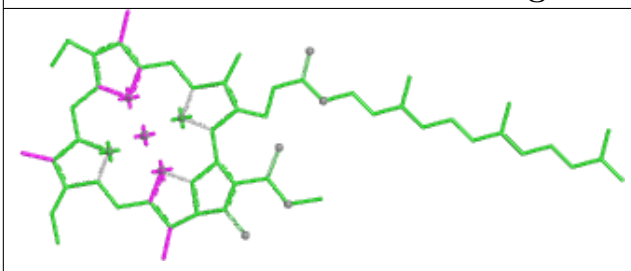
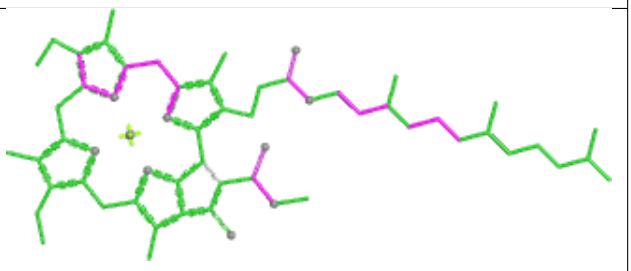
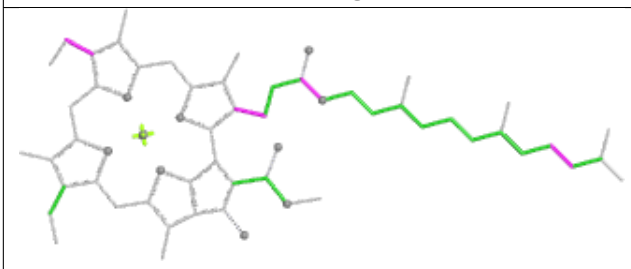
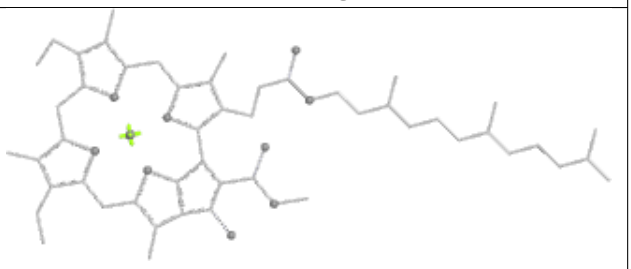


Torsions

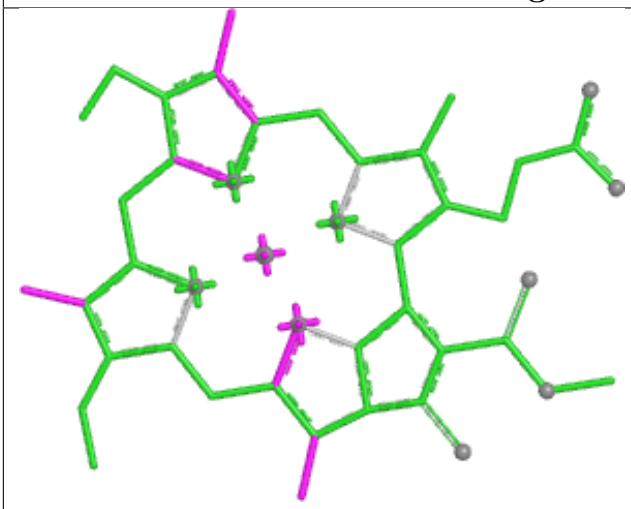


Rings

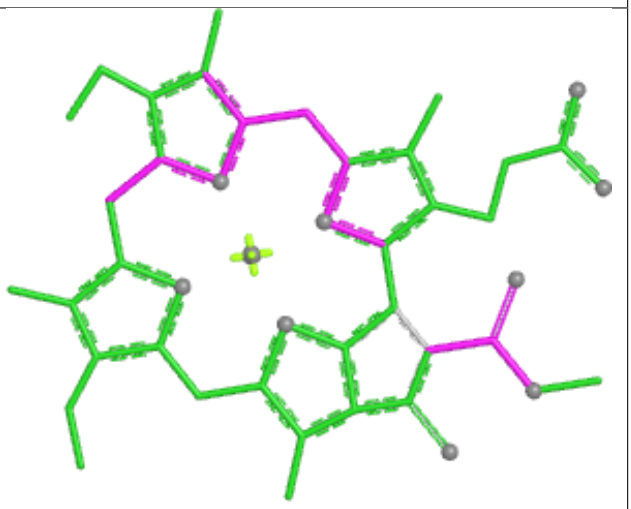
Ligand CLA a 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

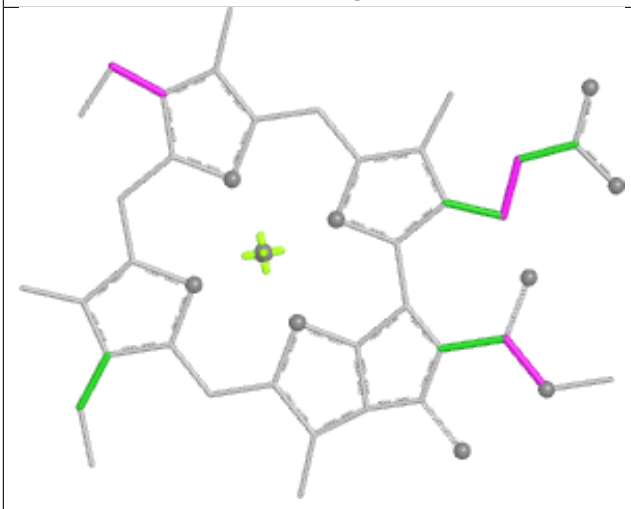
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Bond lengths



Bond angles

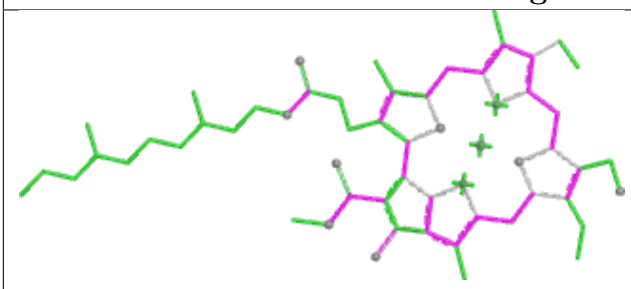


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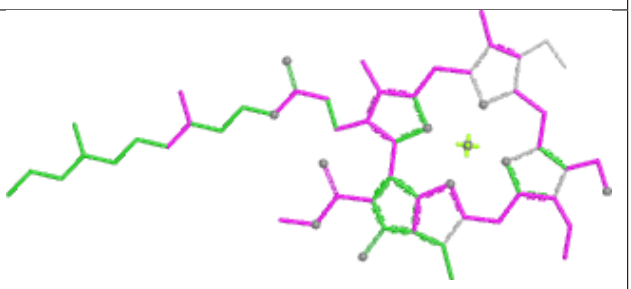


Rings

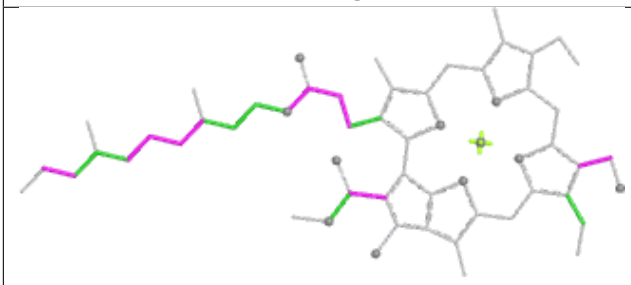
Ligand CHL s 607



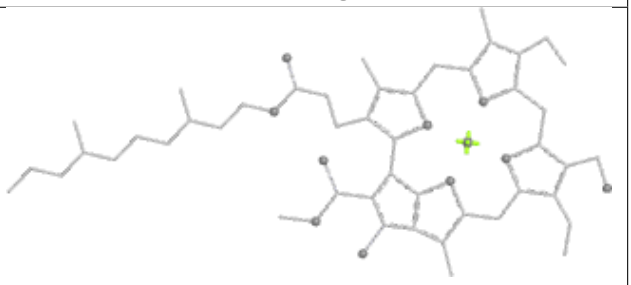
Bond lengths



Bond angles



Torsions

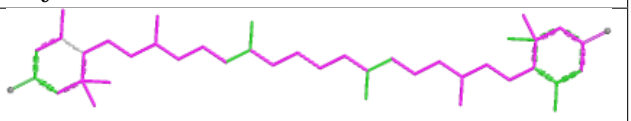


Rings

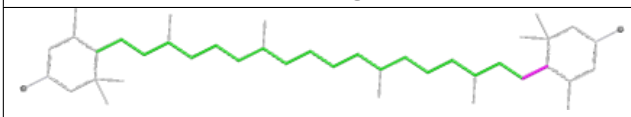
Ligand LUT y 1620



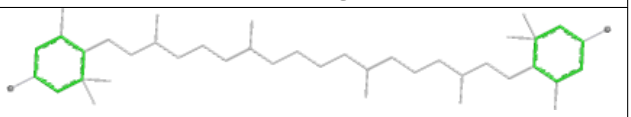
Bond lengths



Bond angles

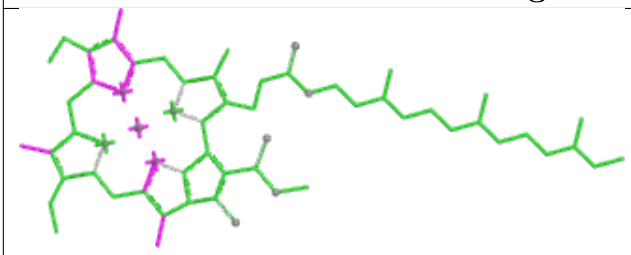


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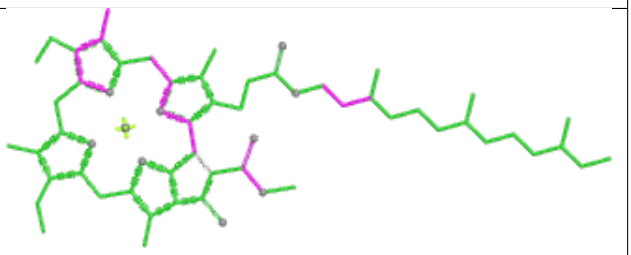


Rings

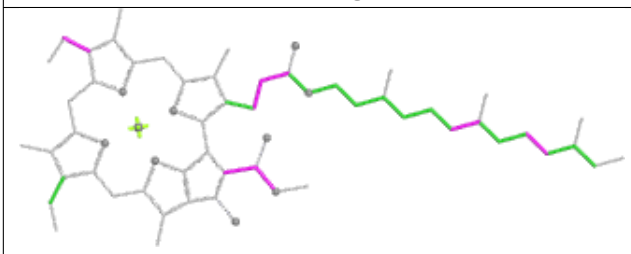
Ligand CLA 5 602



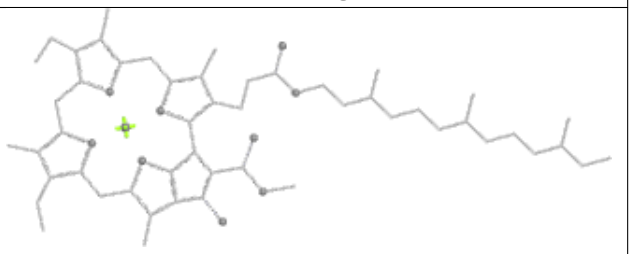
Bond lengths



Bond angles

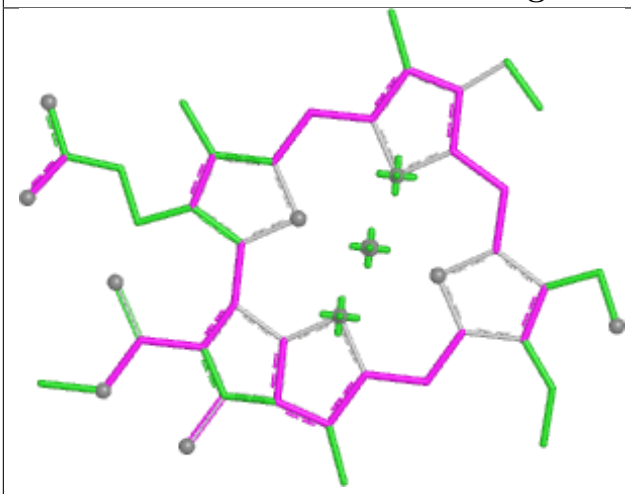


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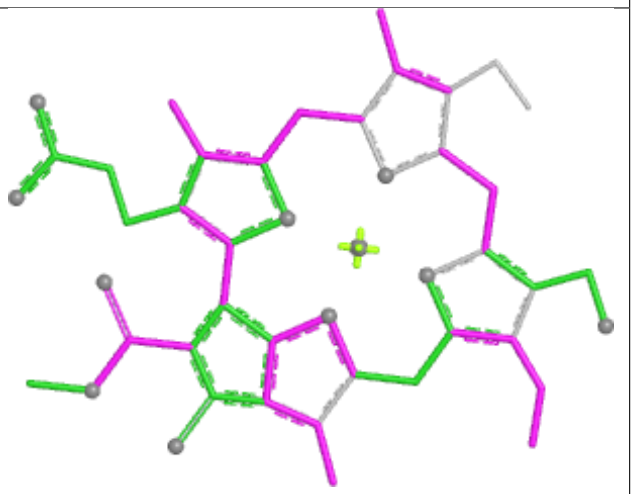


Rings

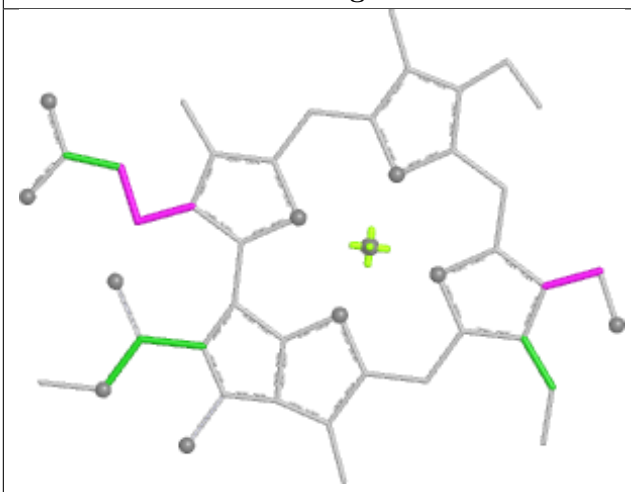
Ligand CHL 7 606



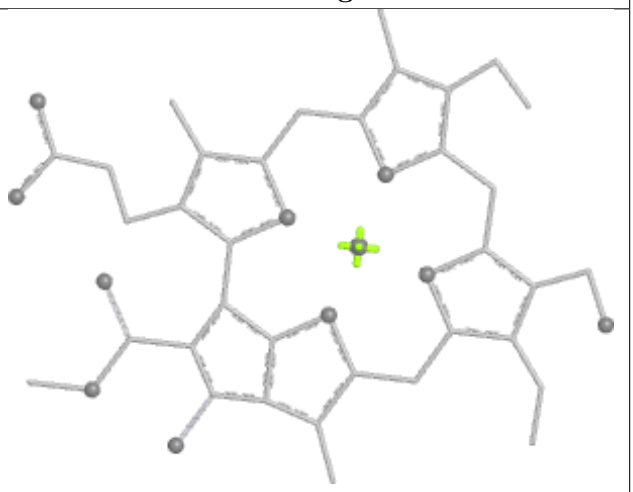
Bond lengths



Bond angles



Torsions



Rings

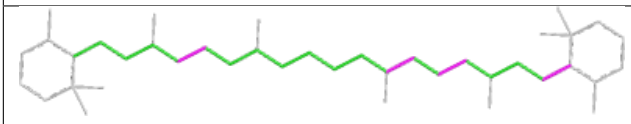
Ligand BCR C 515



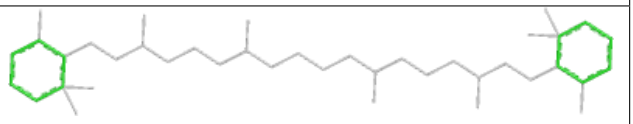
Bond lengths



Bond angles

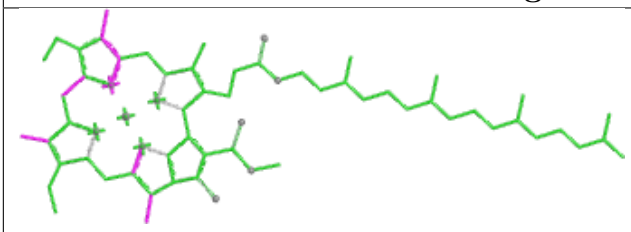


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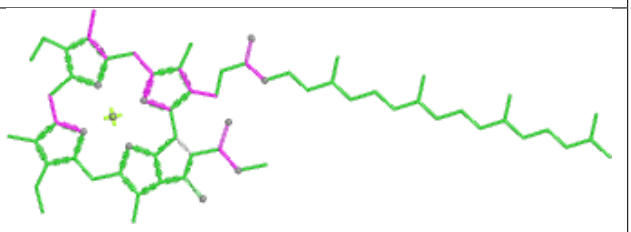


Rings

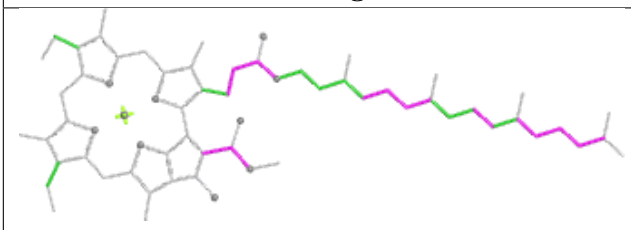
Ligand CLA B 617



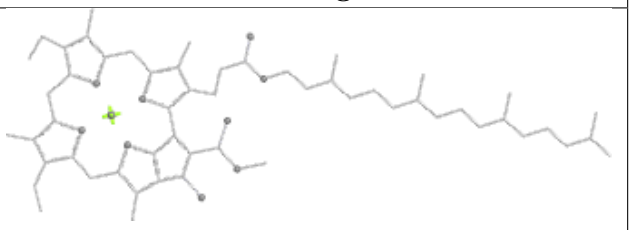
Bond lengths



Bond angles

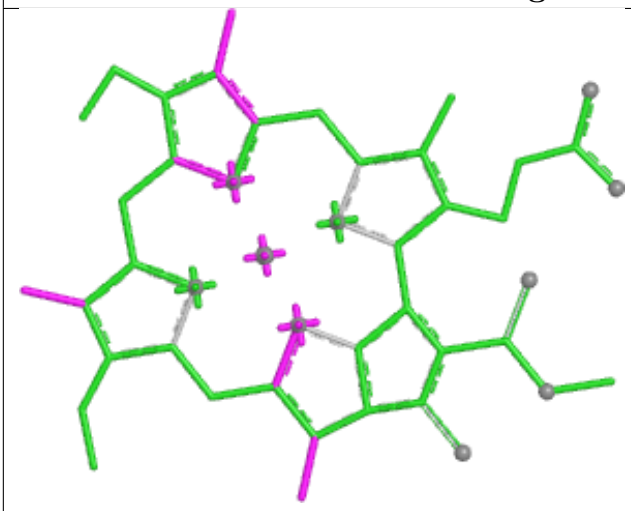


Torsions

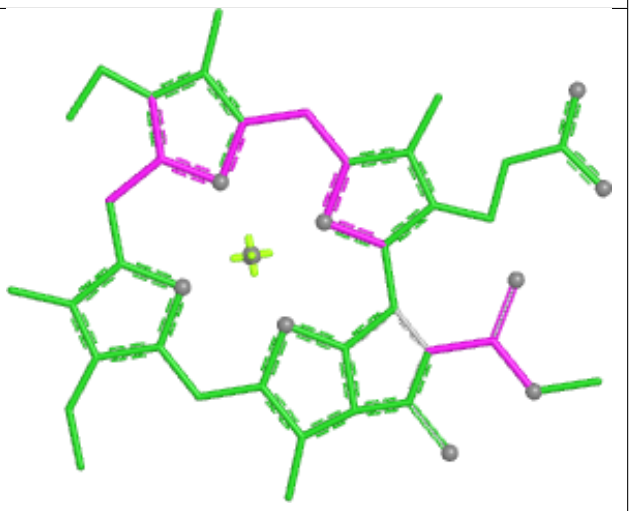


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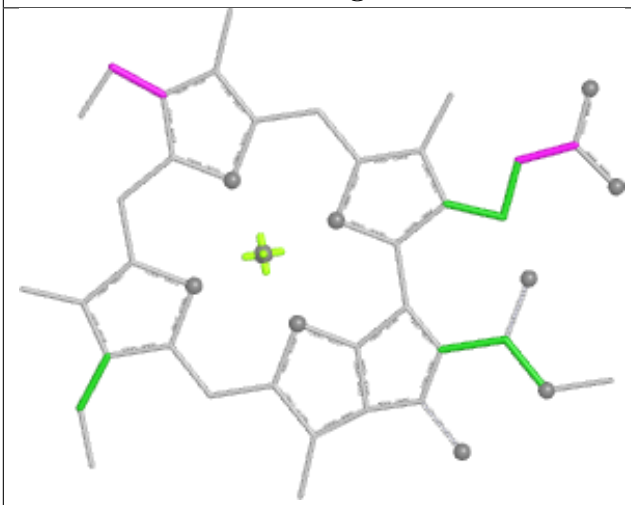
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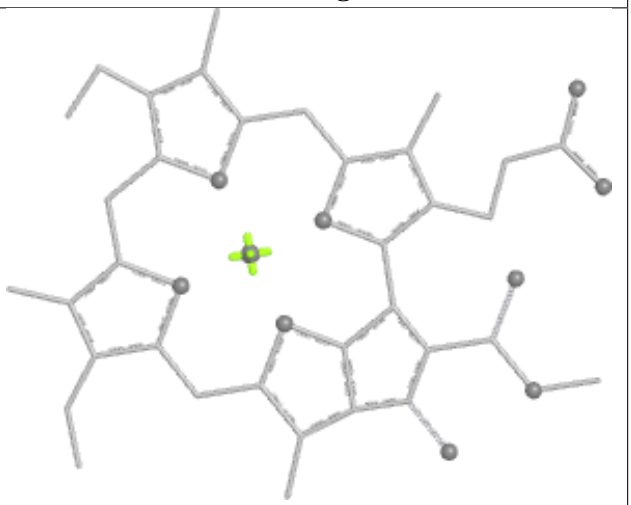
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Bond angles

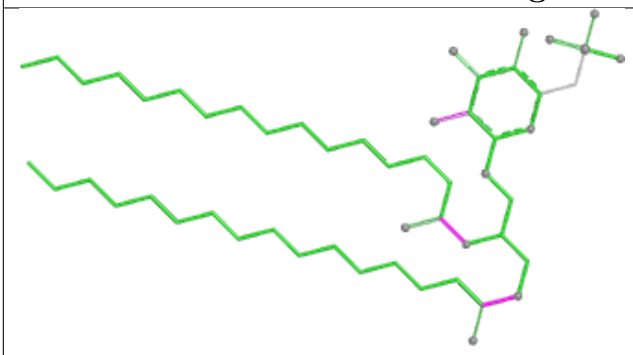


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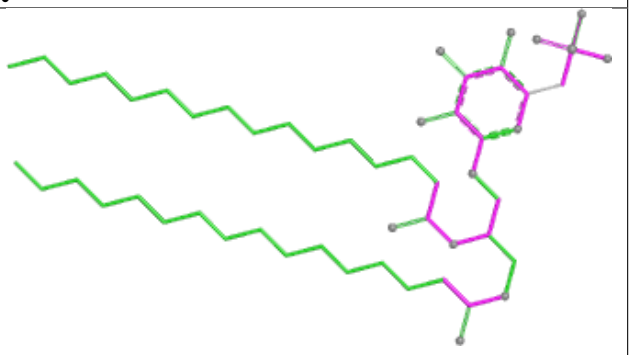


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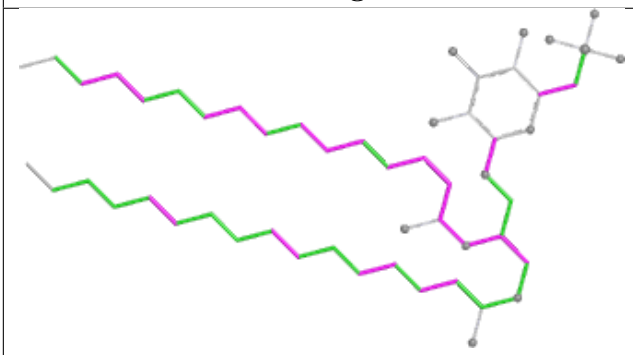
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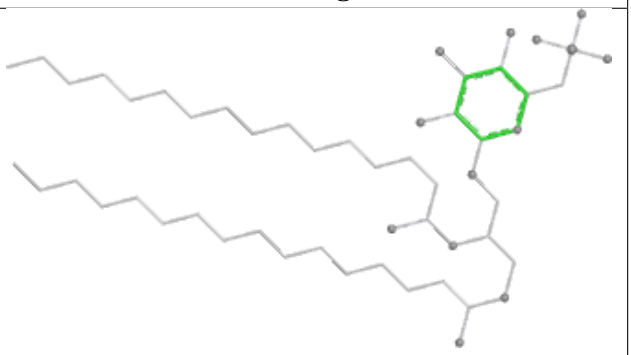
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Bond angles

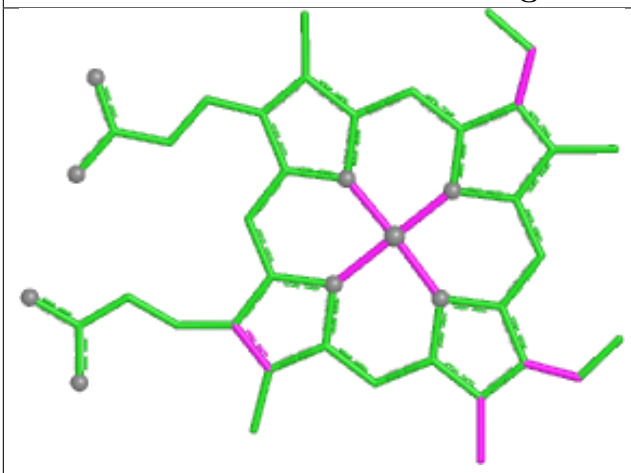


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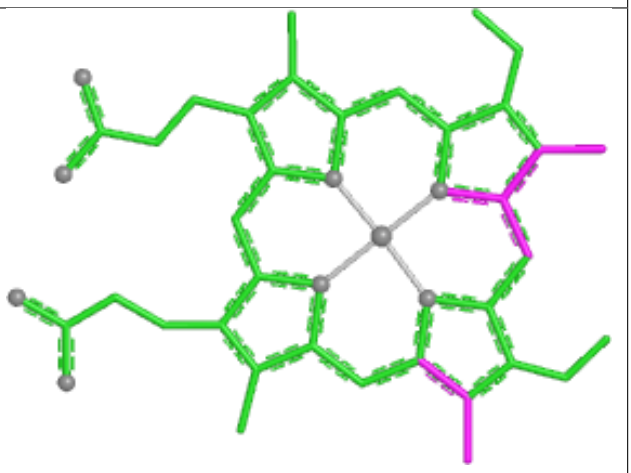


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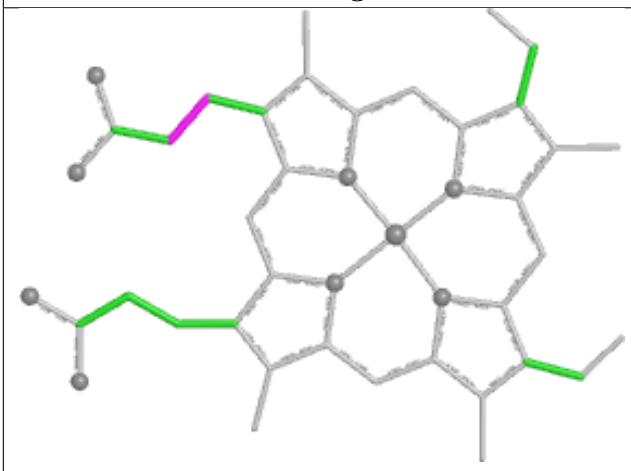
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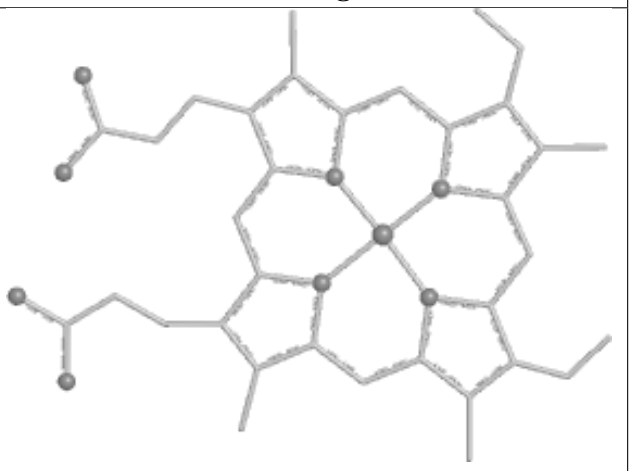
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Bond angles

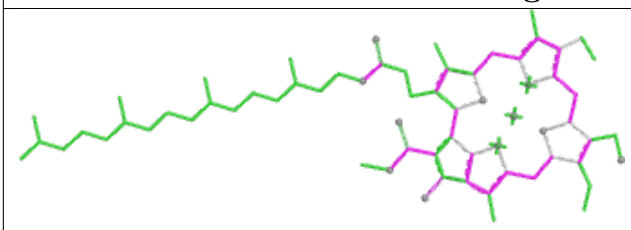


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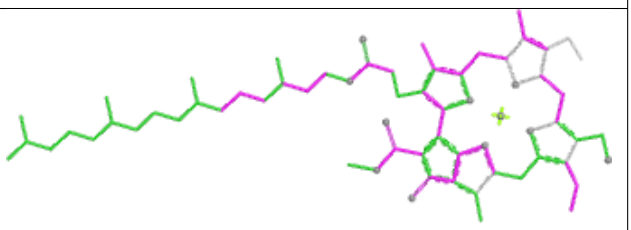


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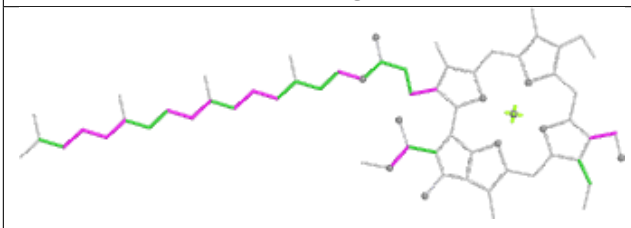
Ligand CHL Y 608



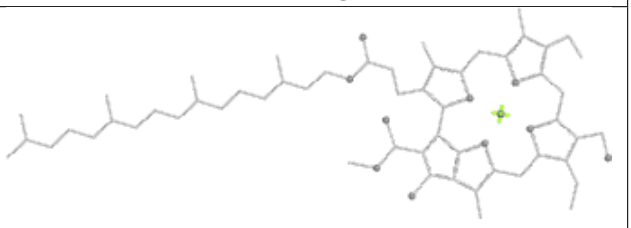
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Bond angles

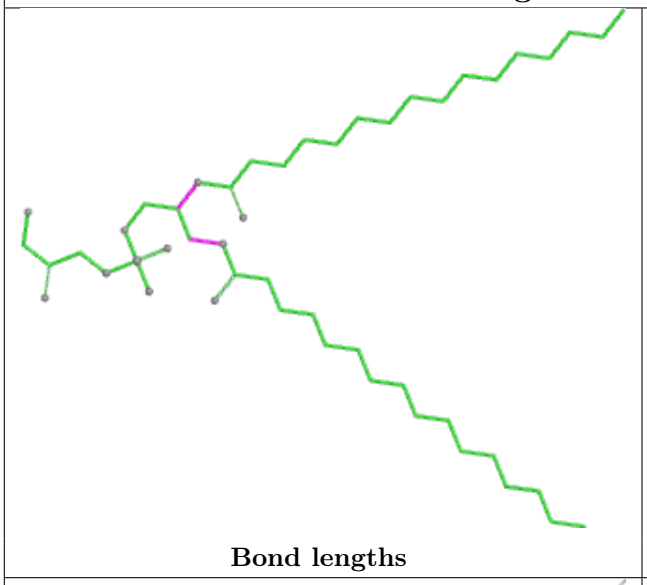


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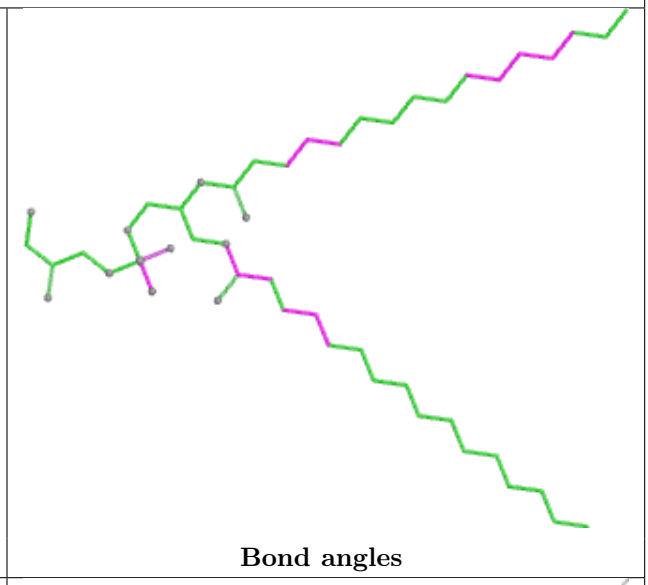


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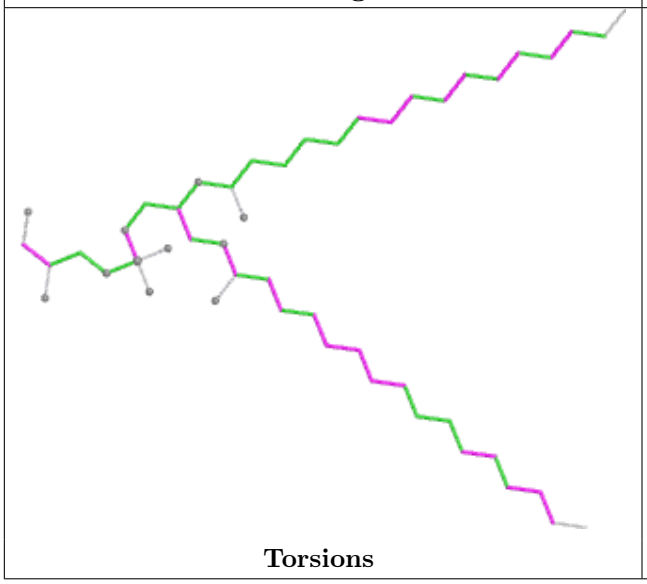
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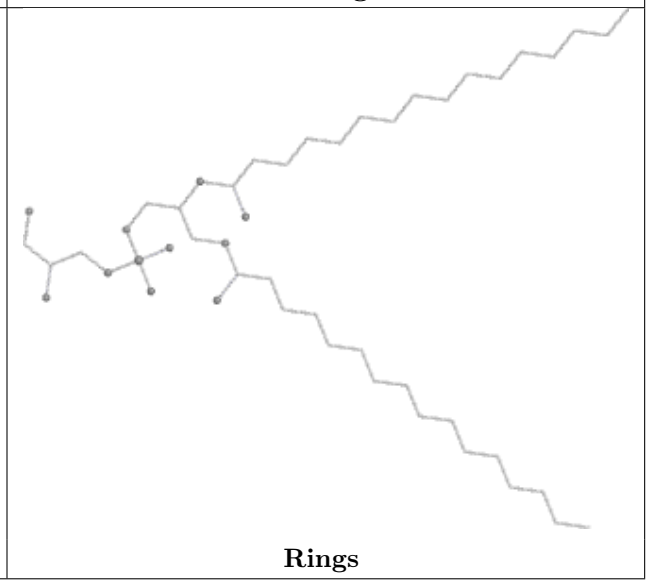
Bond lengths



Bond angles



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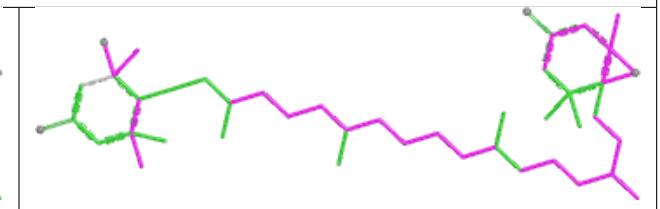


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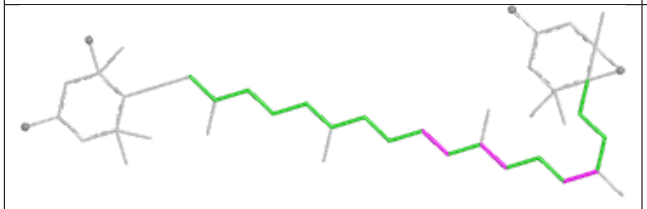
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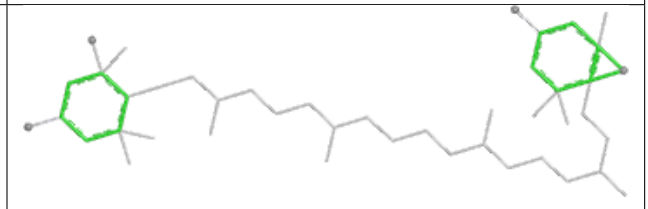
Bond lengths



Bond angles

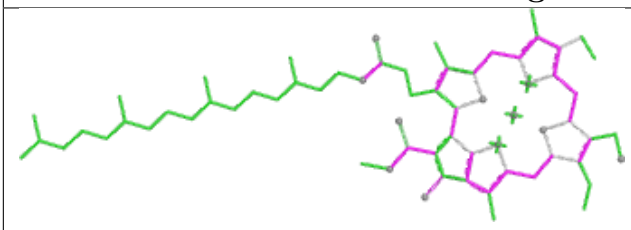


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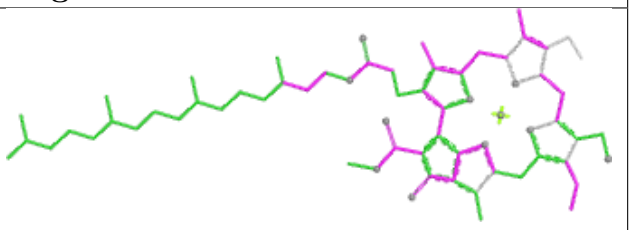


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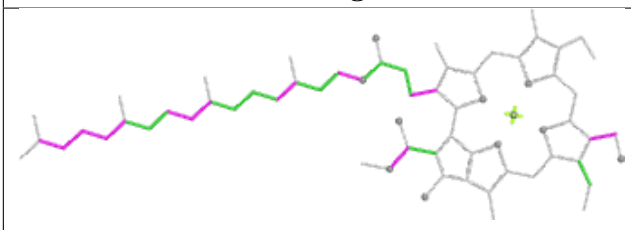
Ligand CHL g 608



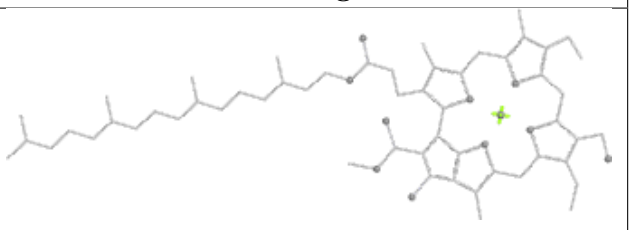
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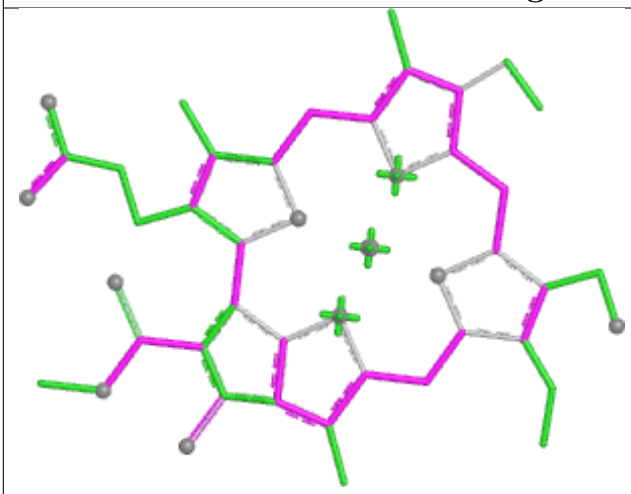


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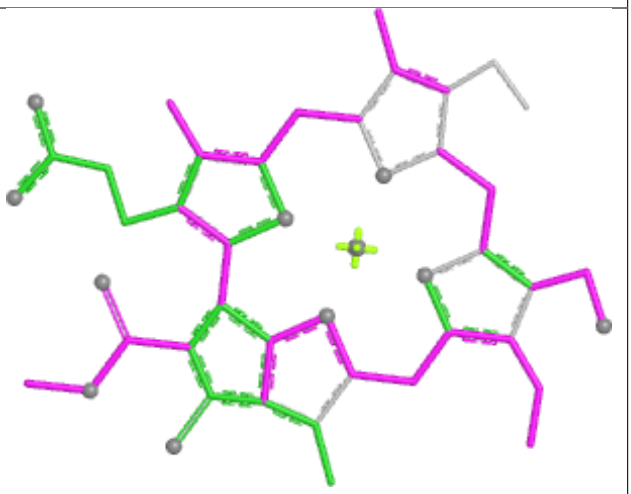


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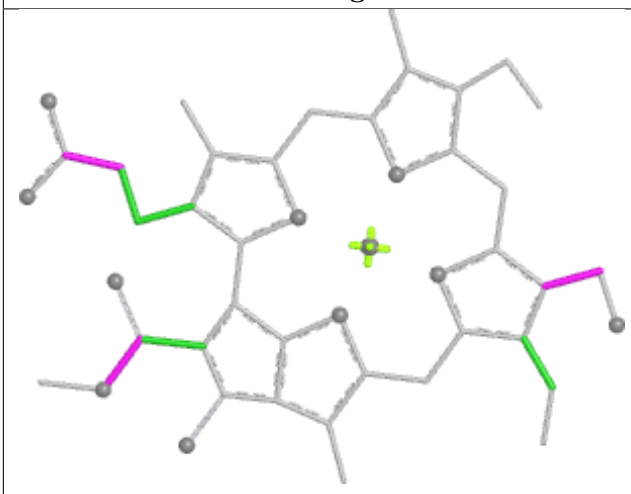
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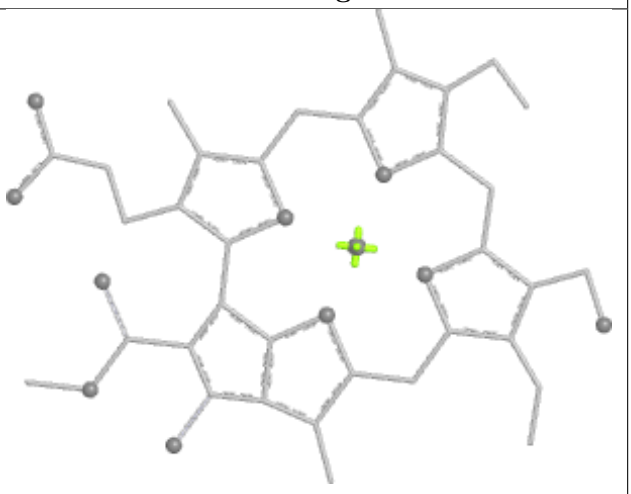
Bond lengths



Bond angles

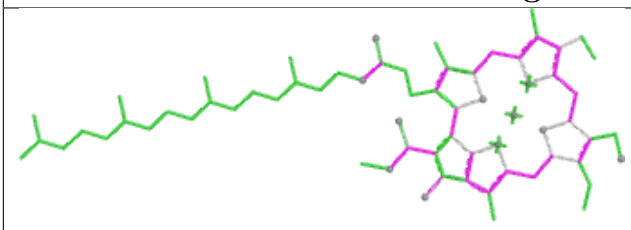


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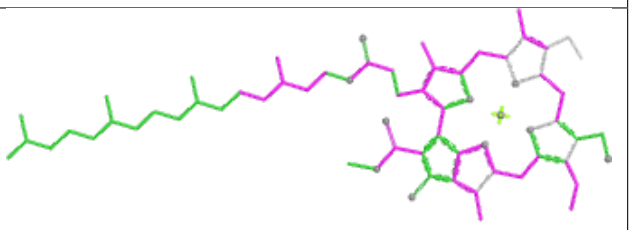


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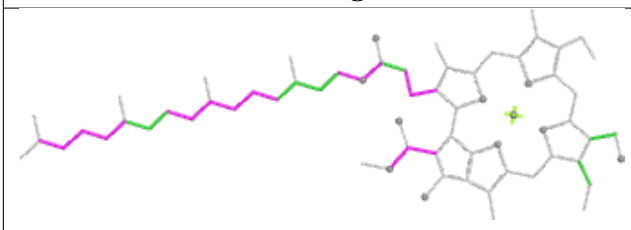
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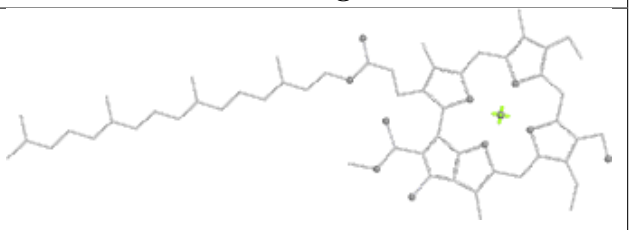
Bond lengths



Bond angles

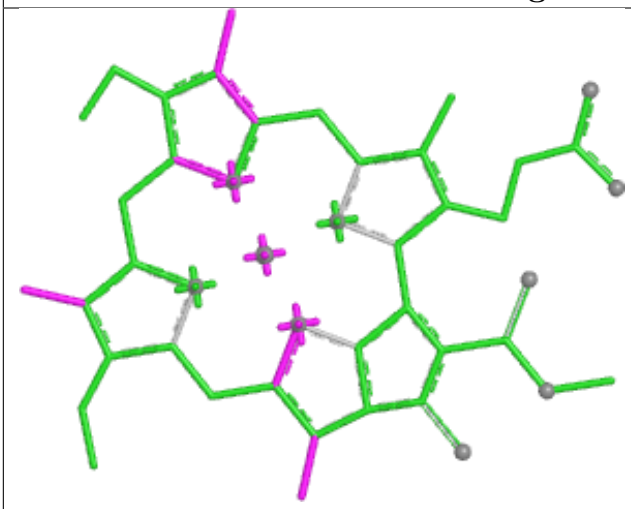


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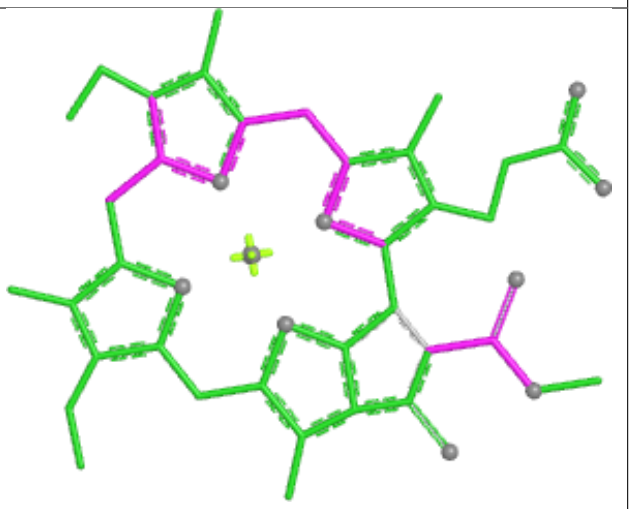


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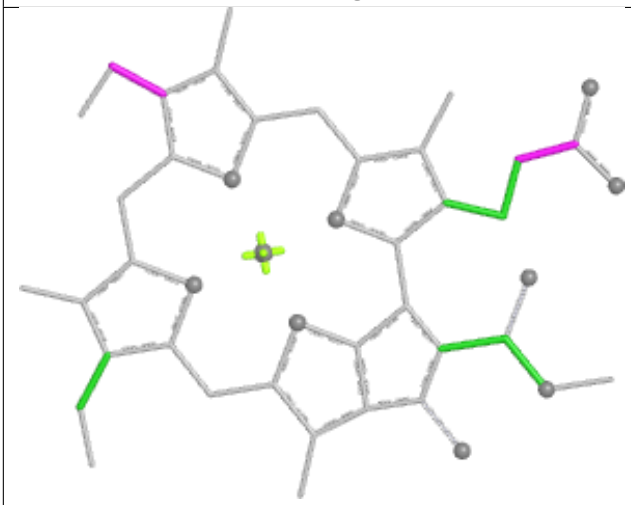
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Bond lengths



Bond angles

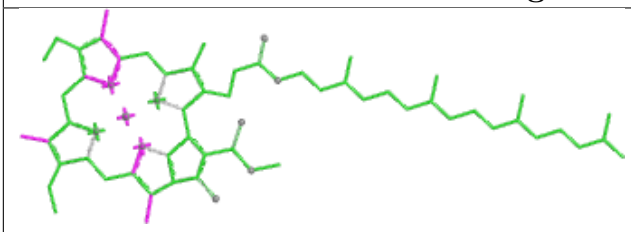


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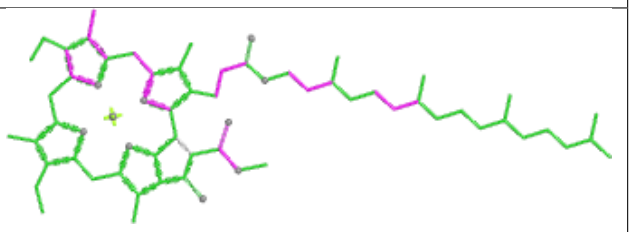


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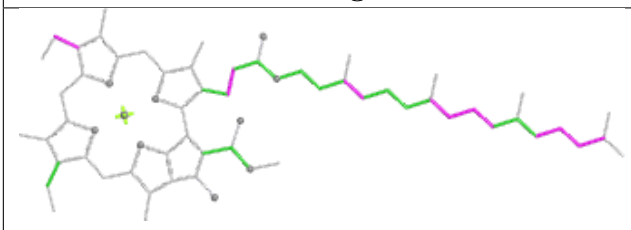
Ligand CLA b 607



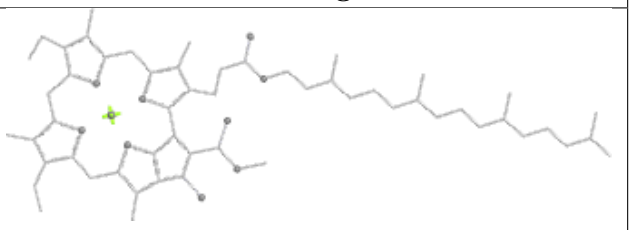
Bond lengths



Bond angles

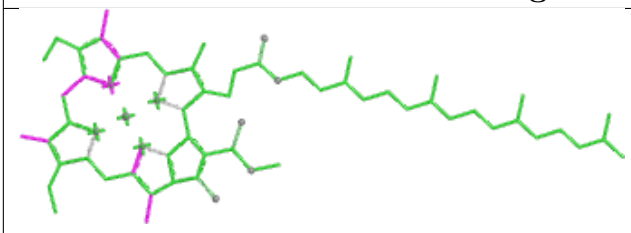


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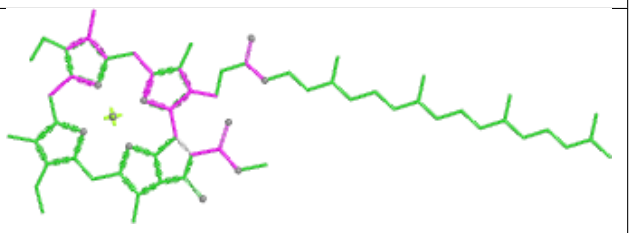


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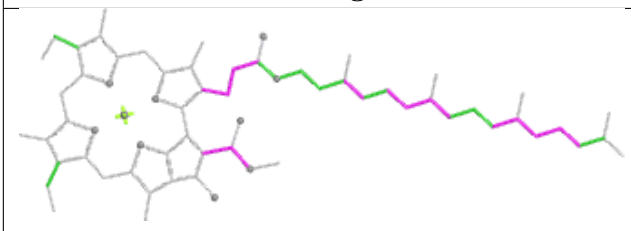
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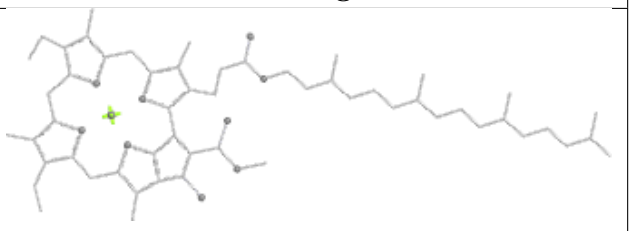
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Bond angles

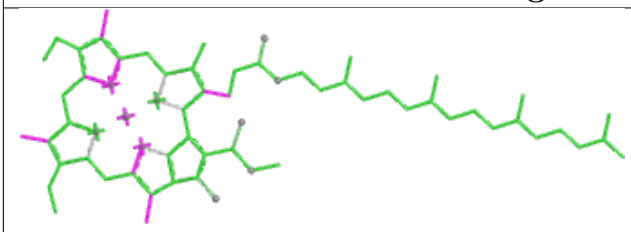


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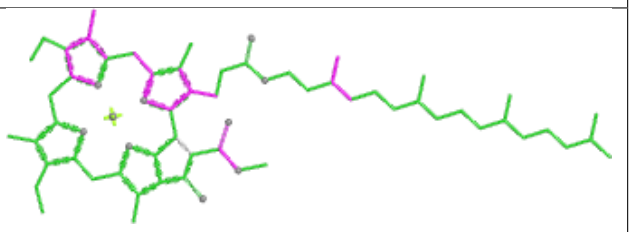


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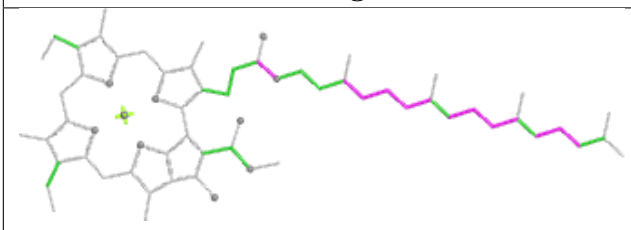
Ligand CLA b 614



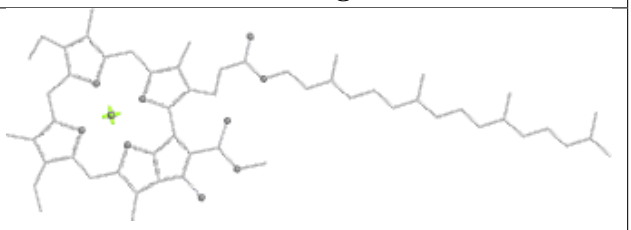
Bond lengths



Bond angles

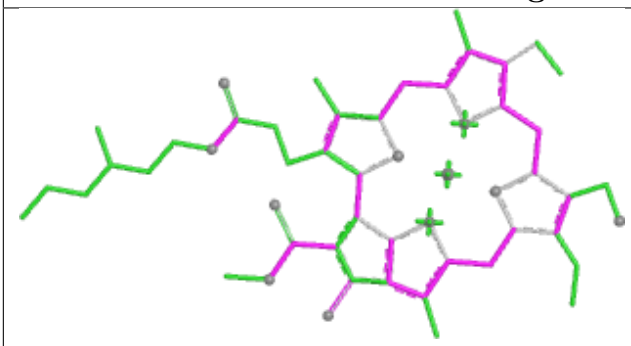


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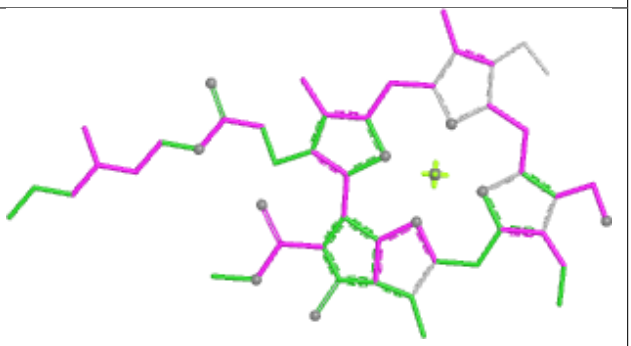


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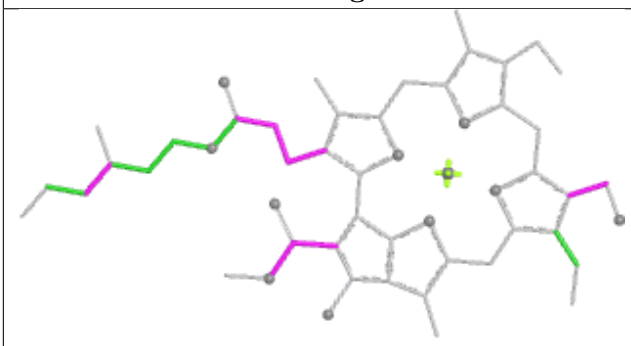
Ligand CHL 3 607



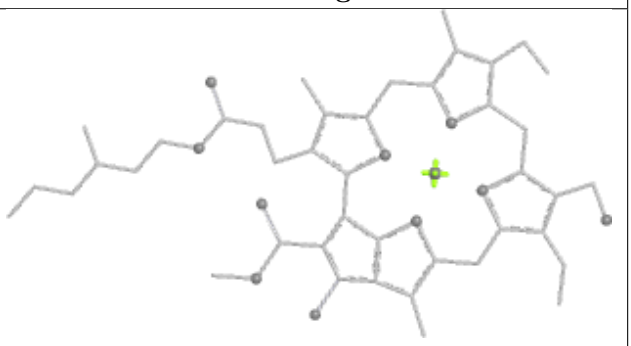
Bond lengths



Bond angles

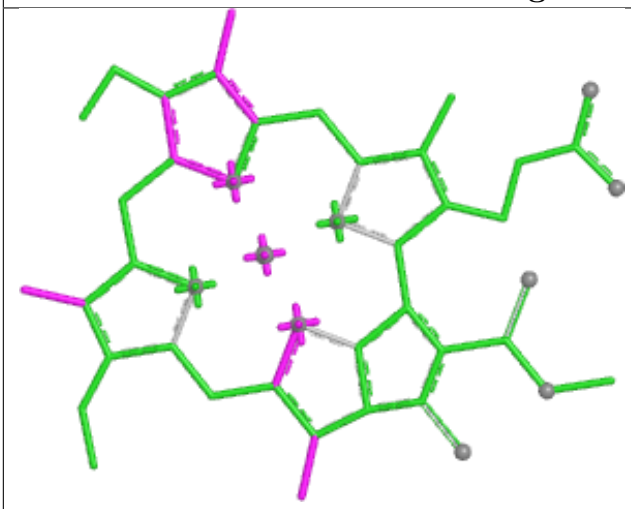


Torsions

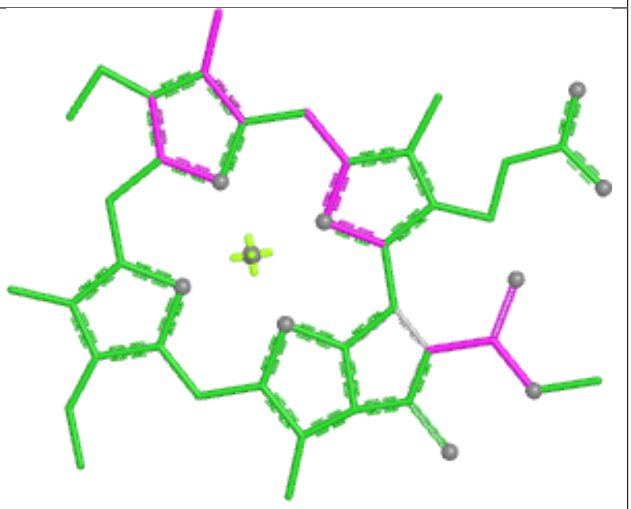


Rings

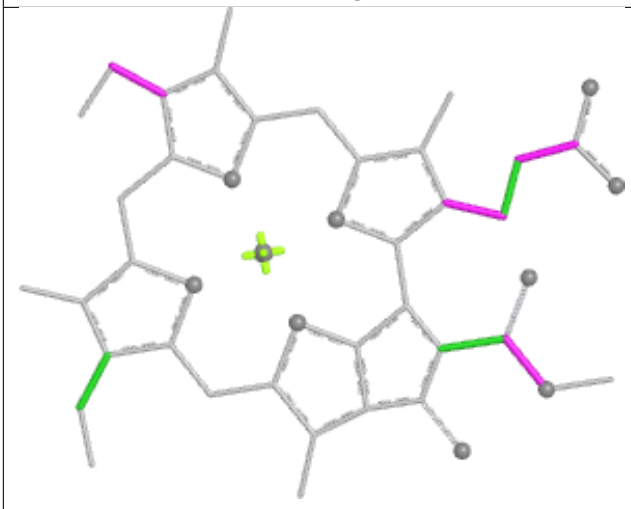
Ligand CLA 2 614



Bond lengths



Bond angles

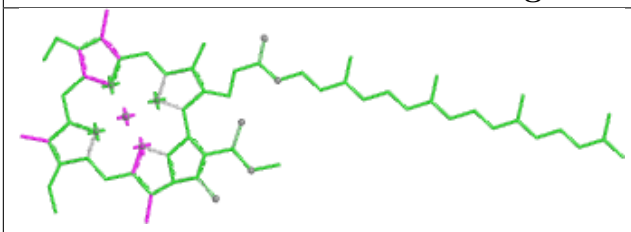


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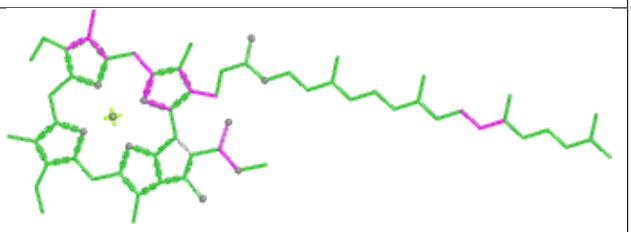


Rings

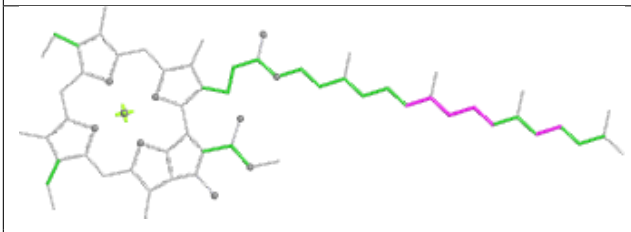
Ligand CLA C 509



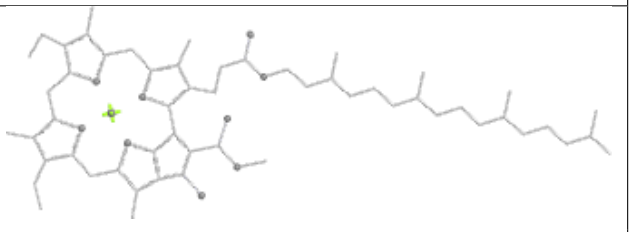
Bond lengths



Bond angles

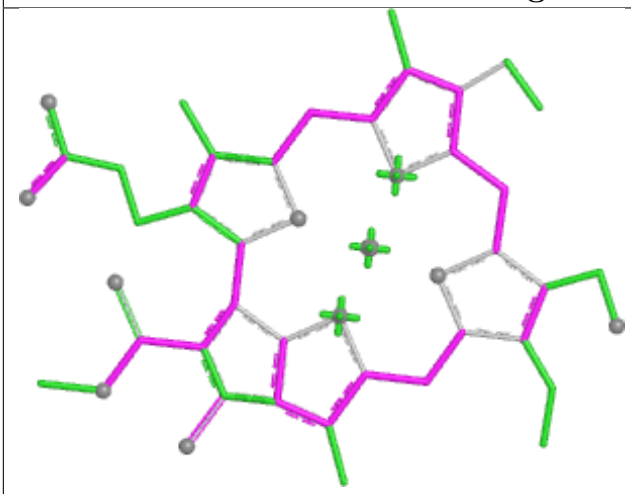


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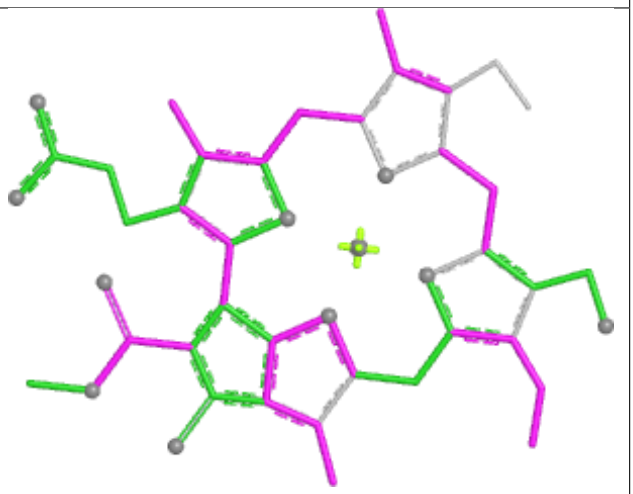


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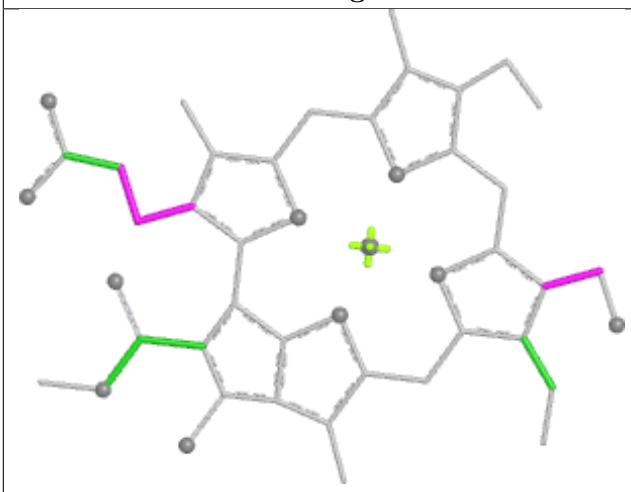
Ligand CHL 3 606



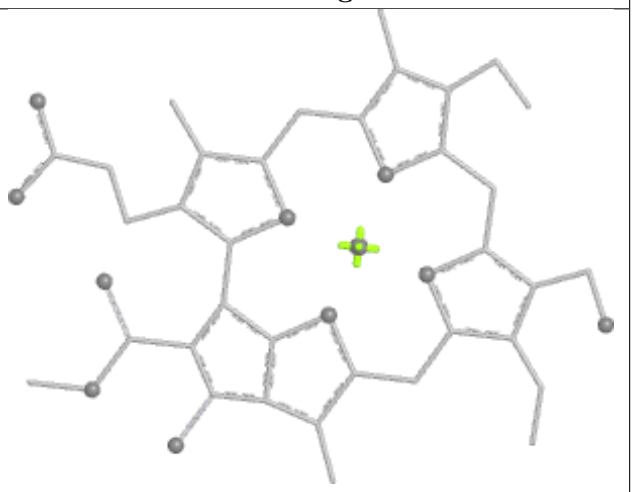
Bond lengths



Bond angles

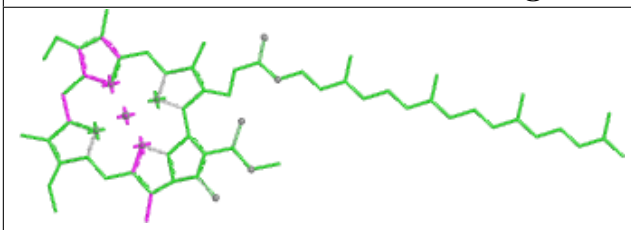


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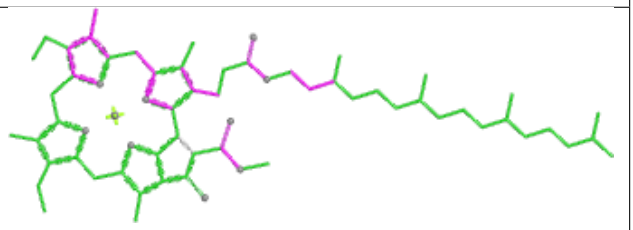


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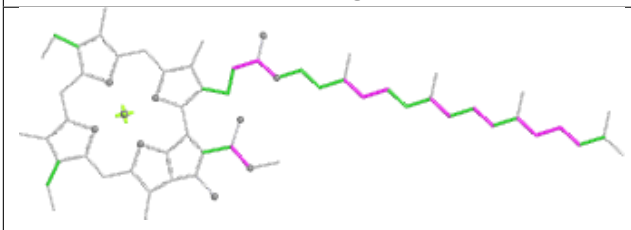
Ligand CLA C 510



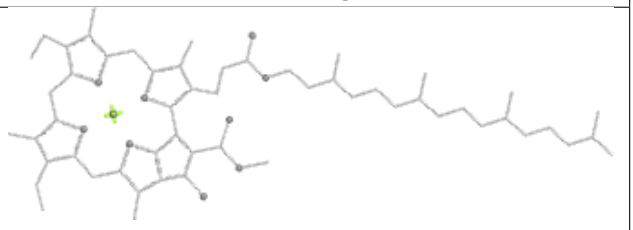
Bond lengths



Bond angles

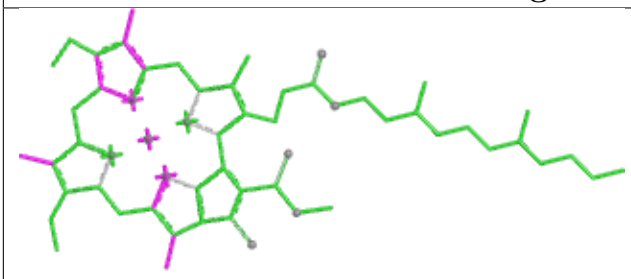


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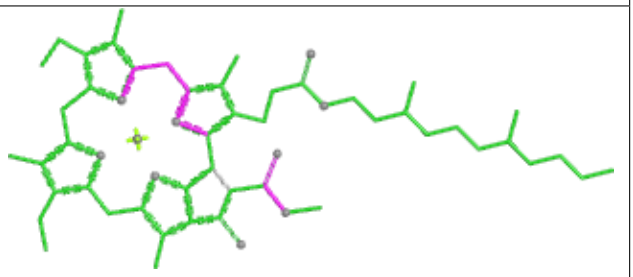


Rings

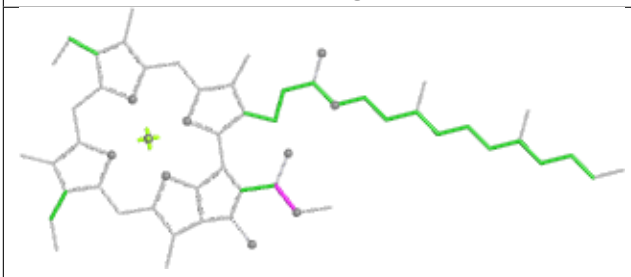
Ligand CLA r 609



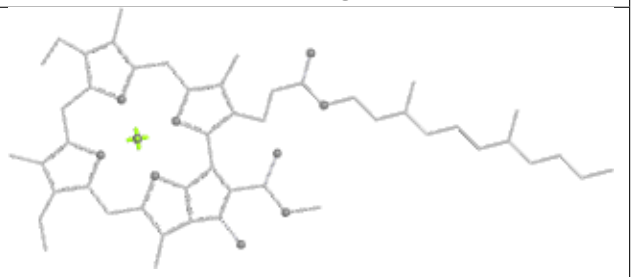
Bond lengths



Bond angles



Torsions

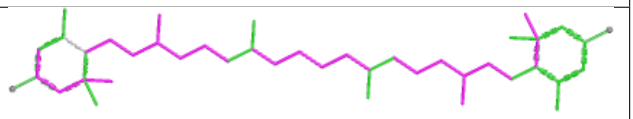


Rings

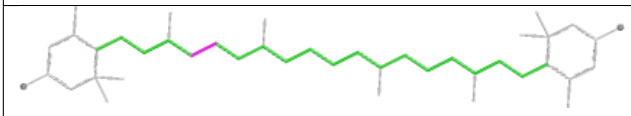
Ligand LUT n 1621



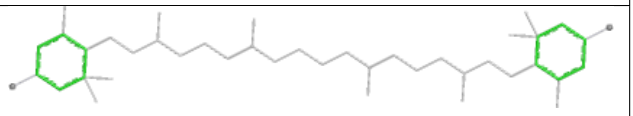
Bond lengths



Bond angles

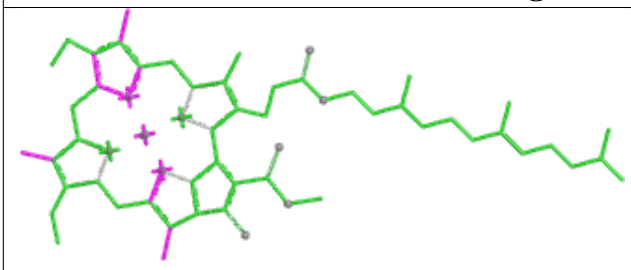


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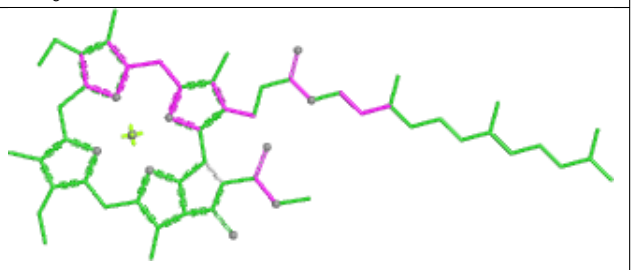


Rings

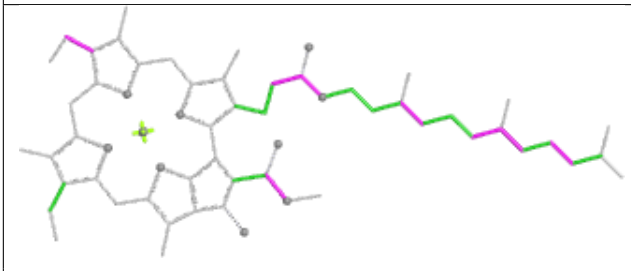
Ligand CLA y 612



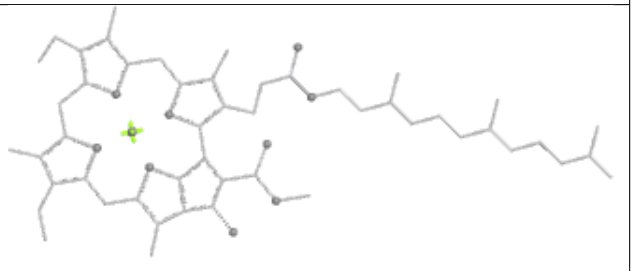
Bond lengths



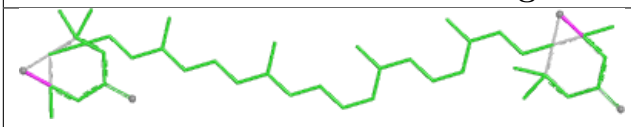
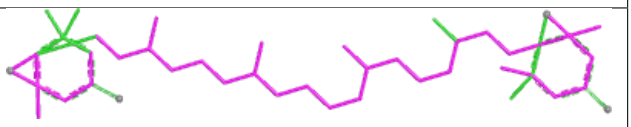
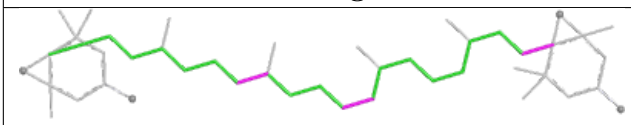
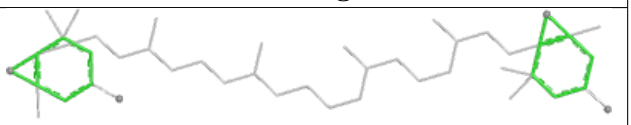
Bond angles

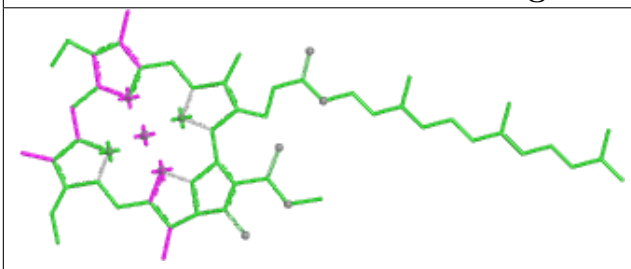
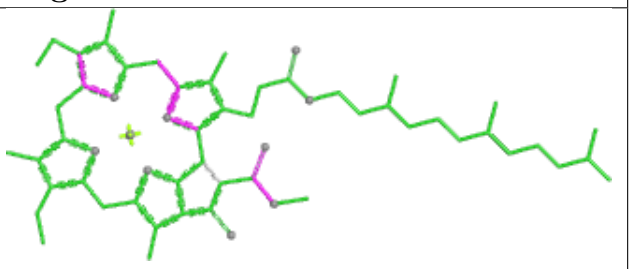
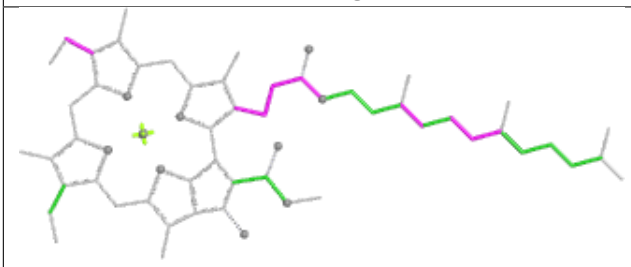
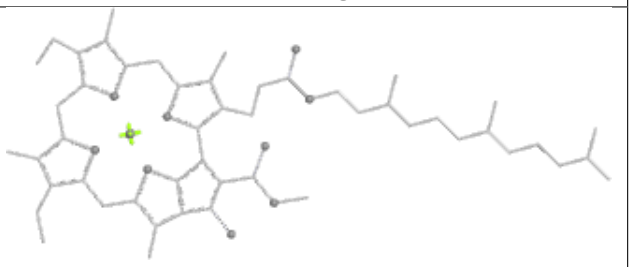


Torsions

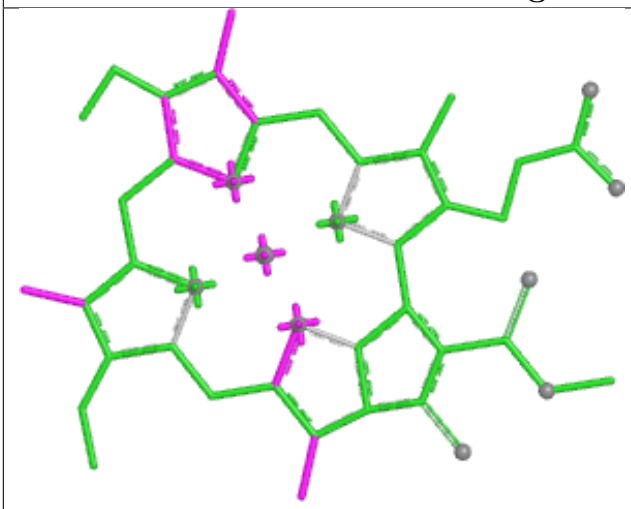


Rings

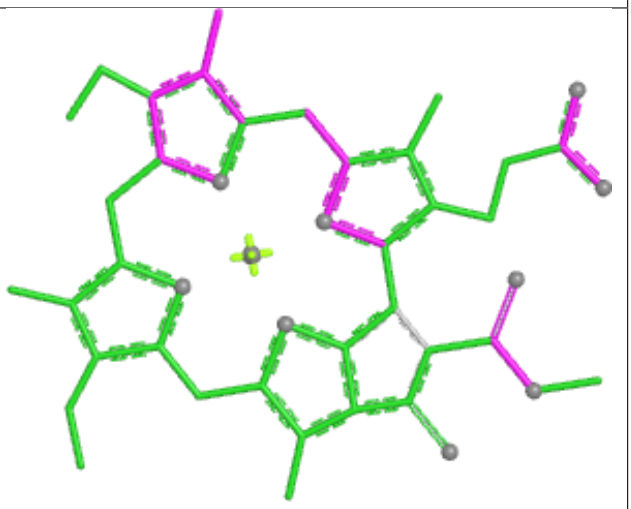
Ligand XAT 2 1622	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

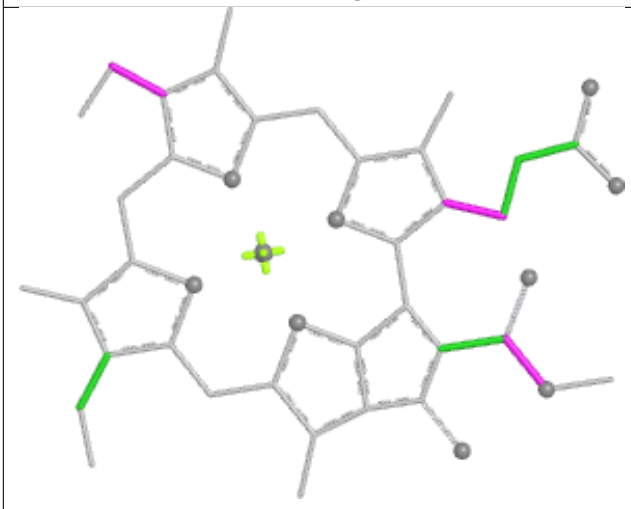
Ligand CLA 1 614



Bond lengths



Bond angles

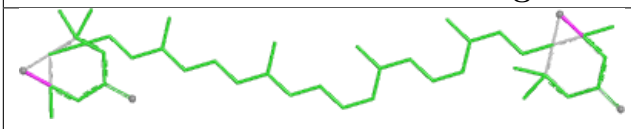


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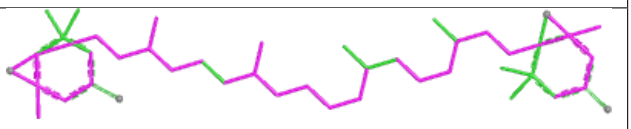


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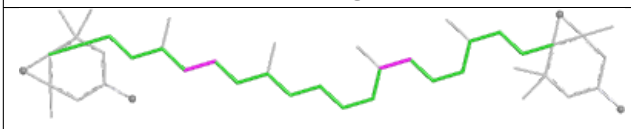
Ligand XAT N 1622



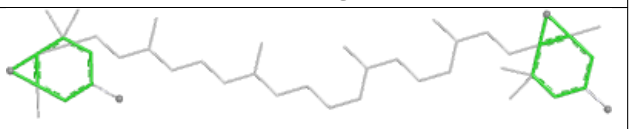
Bond lengths



Bond angles

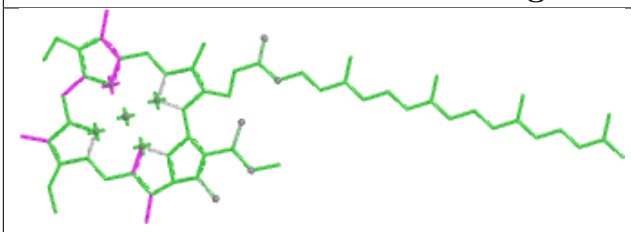


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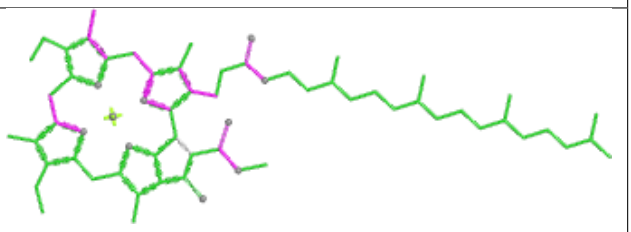


Rings

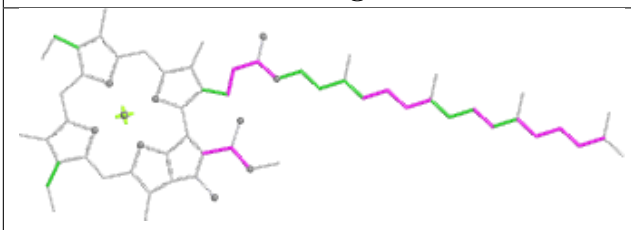
Ligand CLA b 617



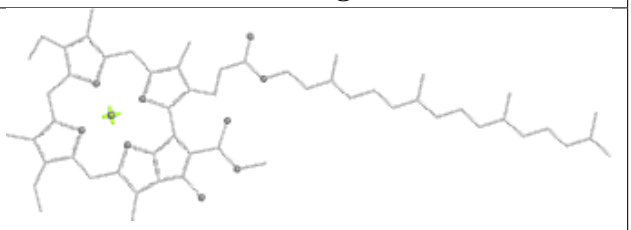
Bond lengths



Bond angles



Torsions



Rings

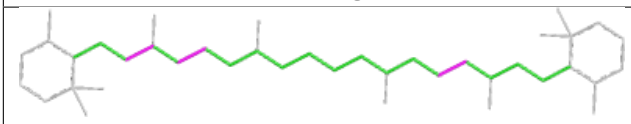
Ligand BCR C 517



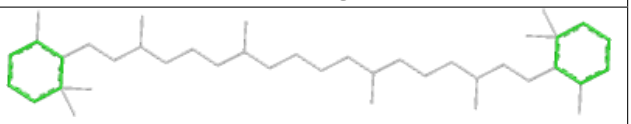
Bond lengths



Bond angles

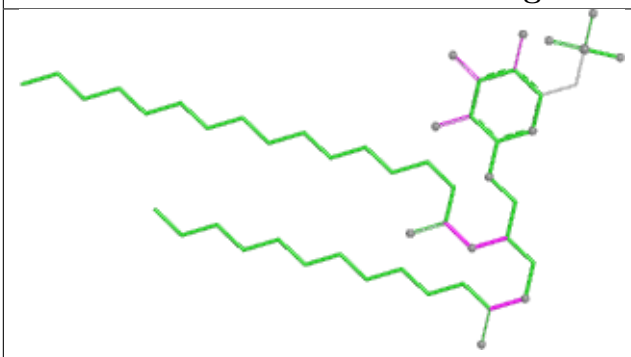


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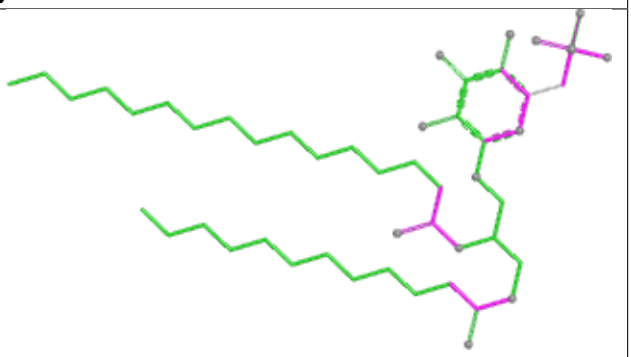


Rings

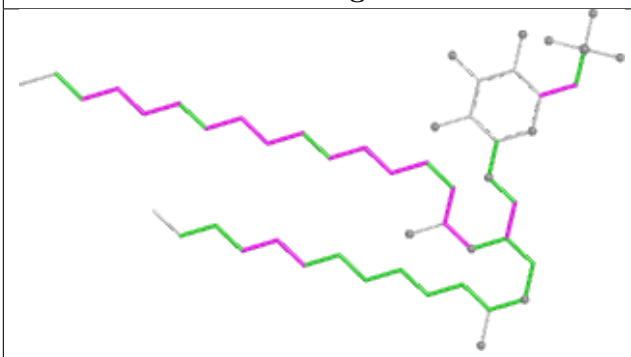
Ligand SQD A 412



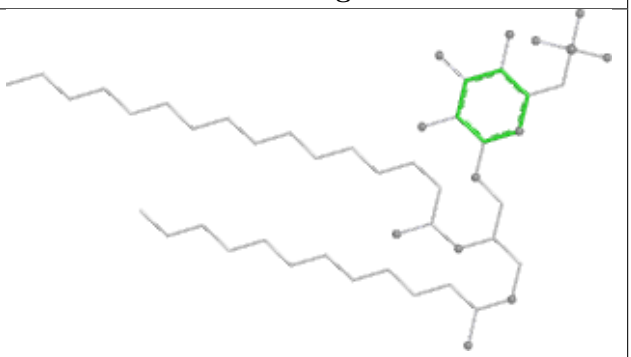
Bond lengths



Bond angles

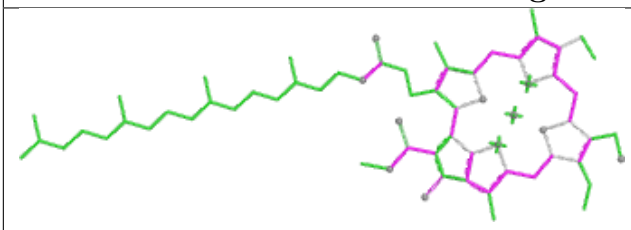


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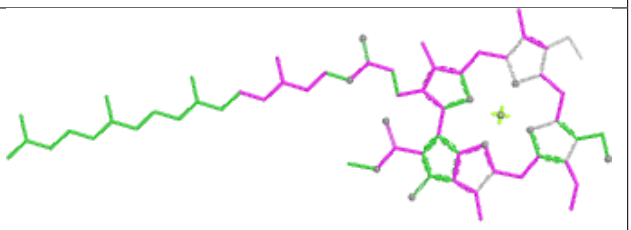


Rings

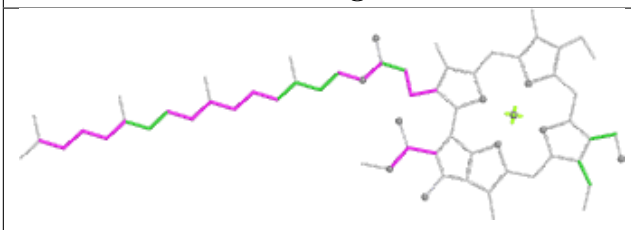
Ligand CHL r 606



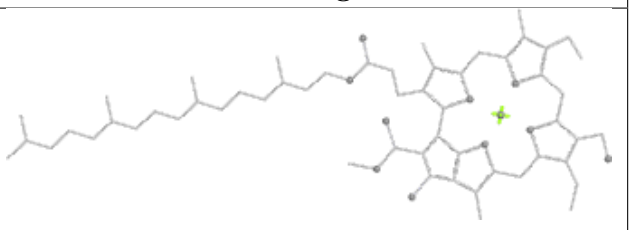
Bond lengths



Bond angles

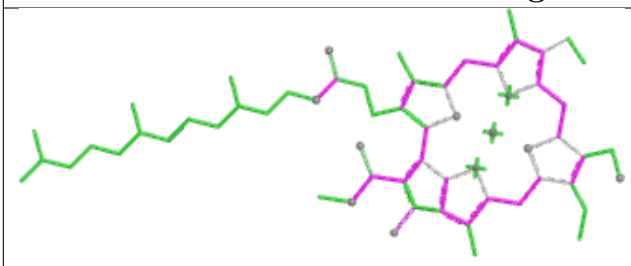


Torsions

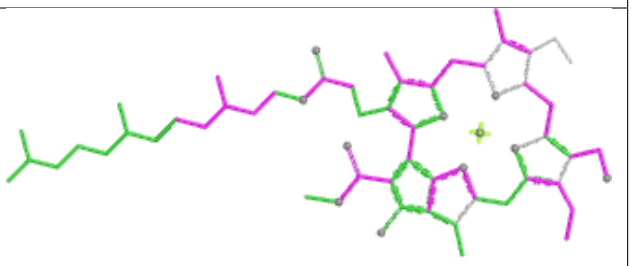


Rings

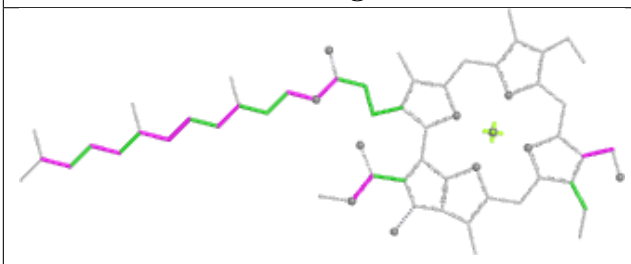
Ligand CHL 2 609



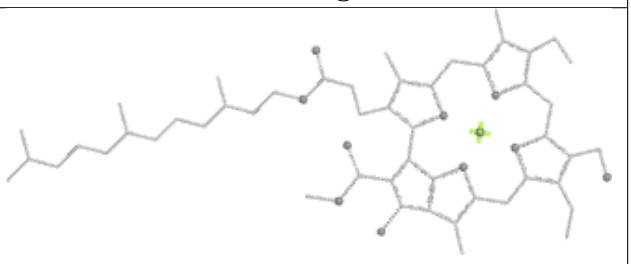
Bond lengths



Bond angles

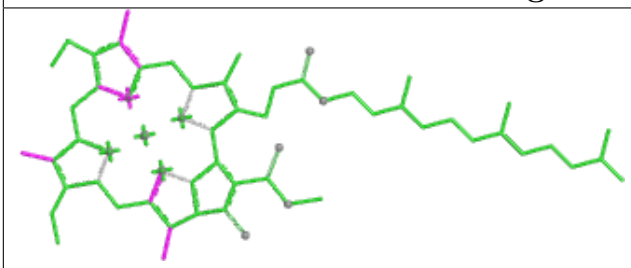


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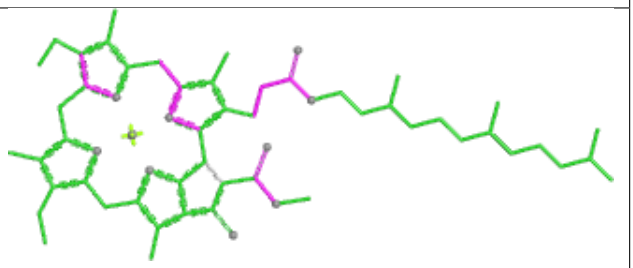


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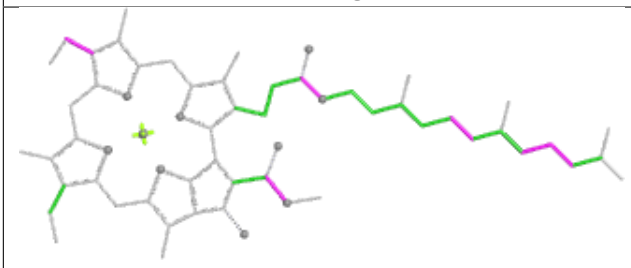
Ligand CLA n 611



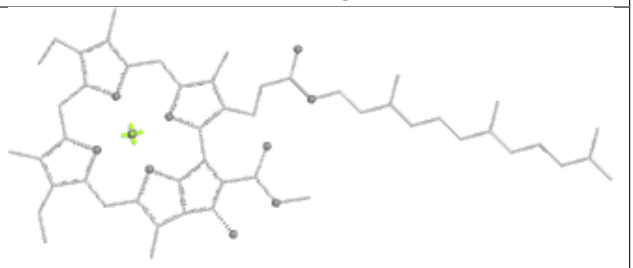
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Bond angles

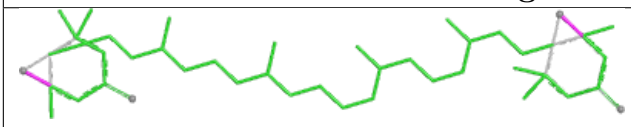


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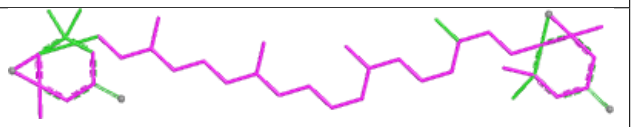


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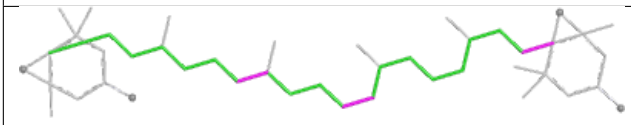
Ligand XAT 6 1622



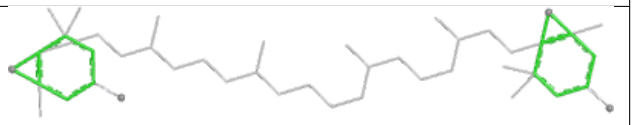
Bond lengths



Bond angles

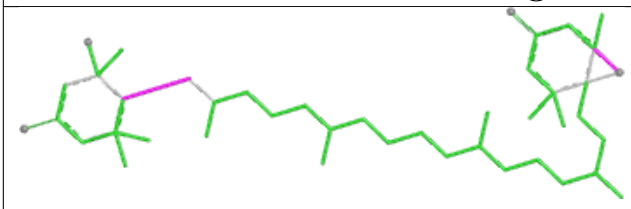


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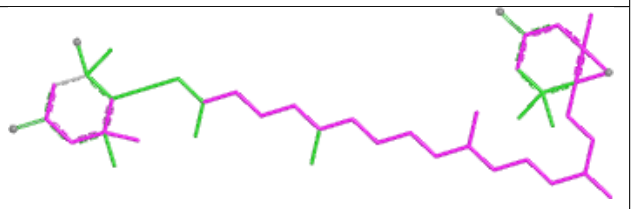


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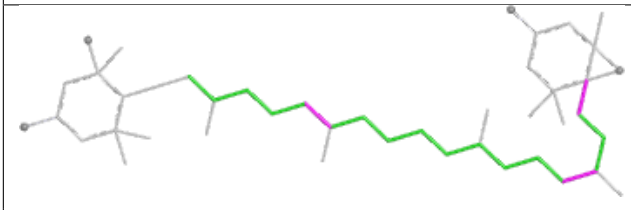
Ligand NEX r 623



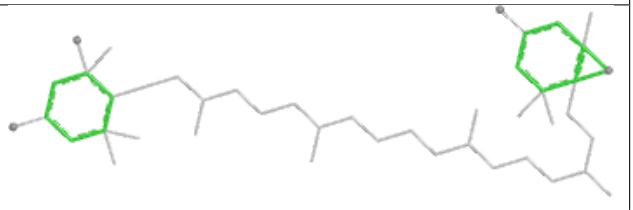
Bond lengths



Bond angles

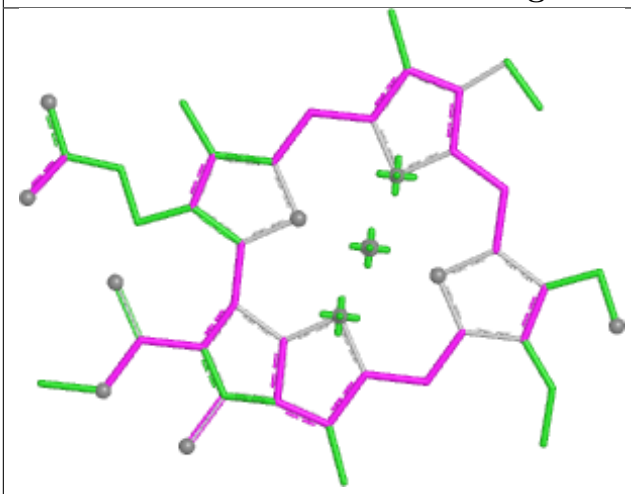


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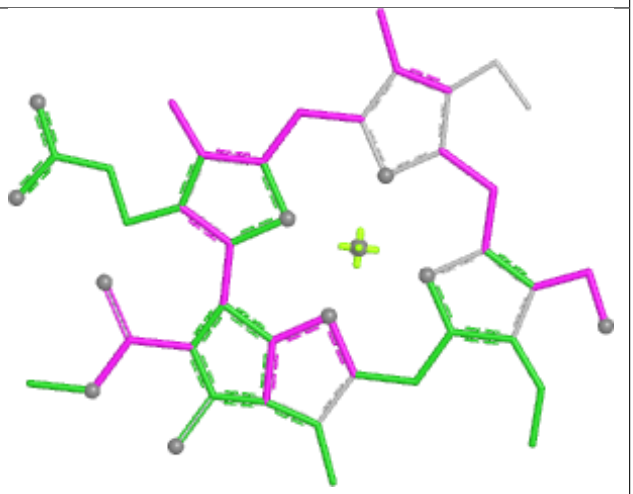


Rings

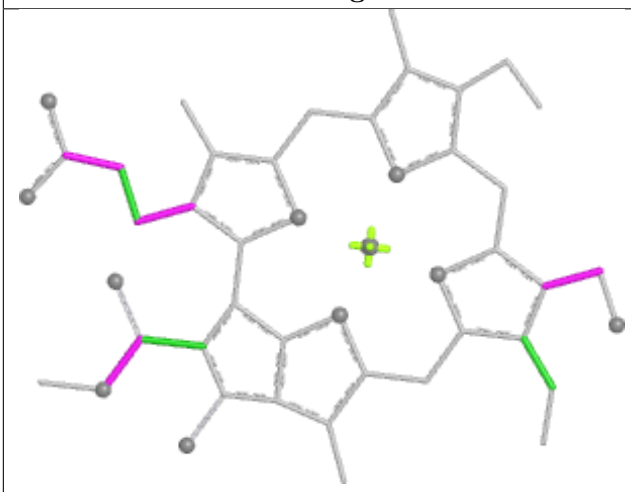
Ligand CHL 5 605



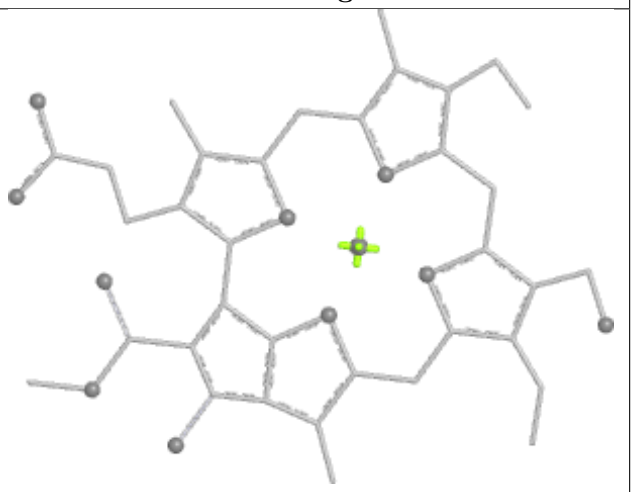
Bond lengths



Bond angles

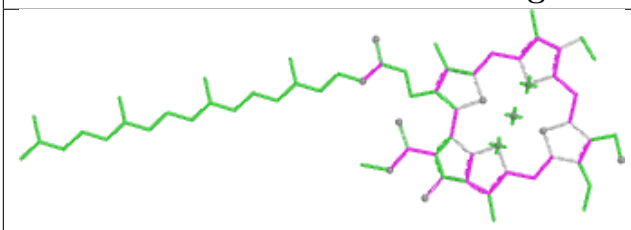


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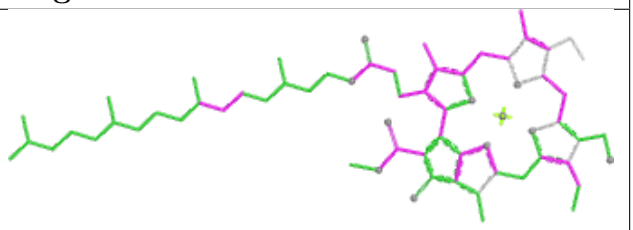


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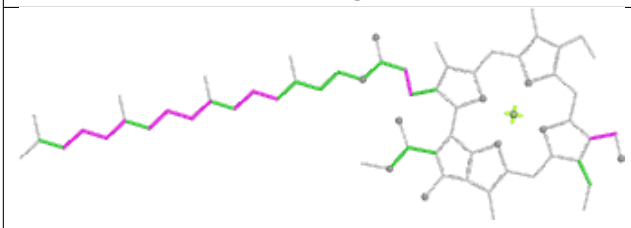
Ligand CHL g 607



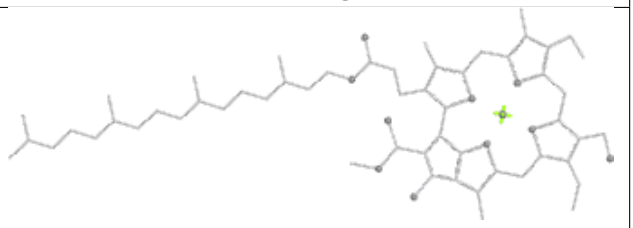
Bond lengths



Bond angles

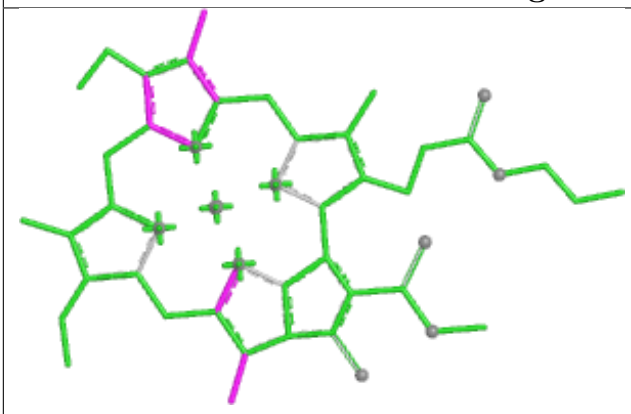


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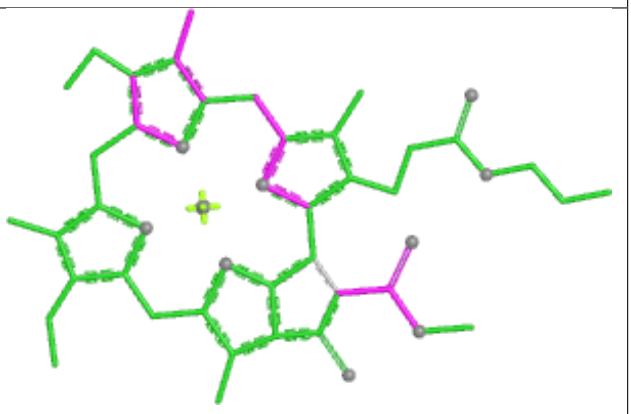


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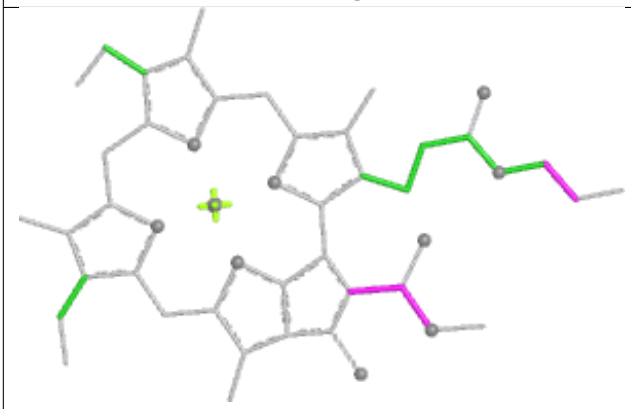
Ligand CLA 7 614



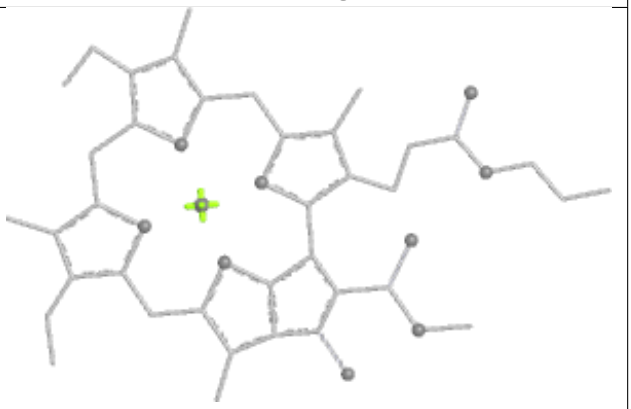
Bond lengths



Bond angles

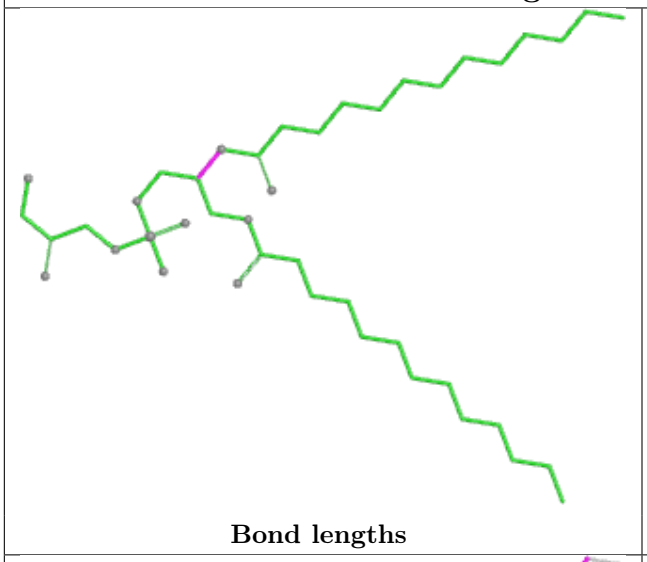


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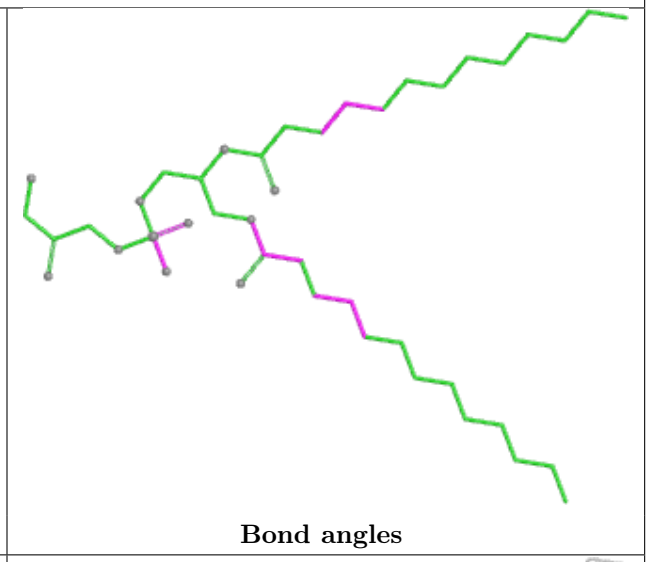


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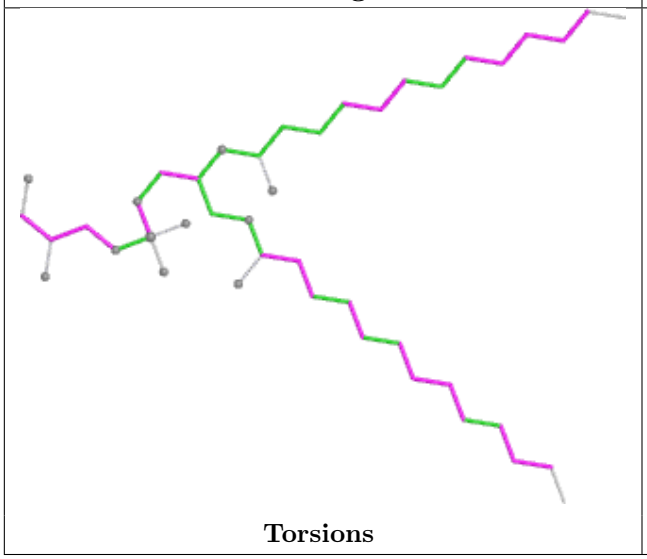
Ligand LHG D 410



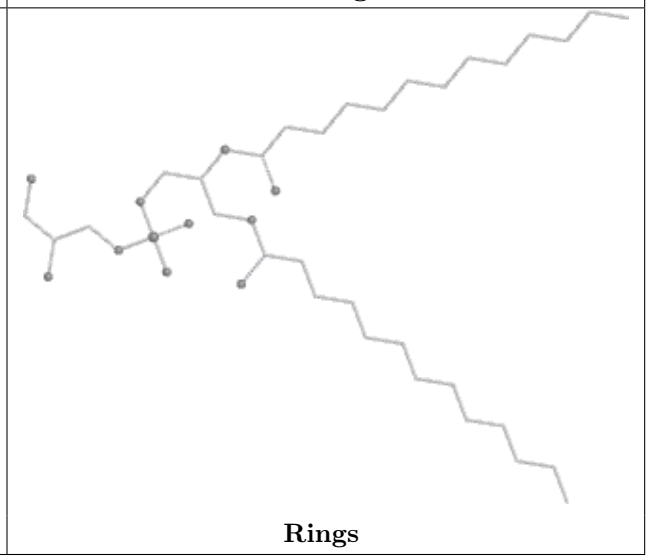
Bond lengths



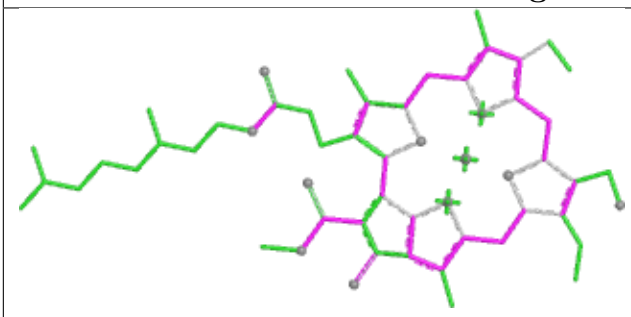
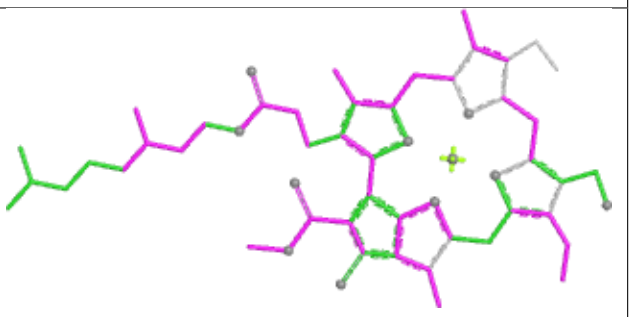
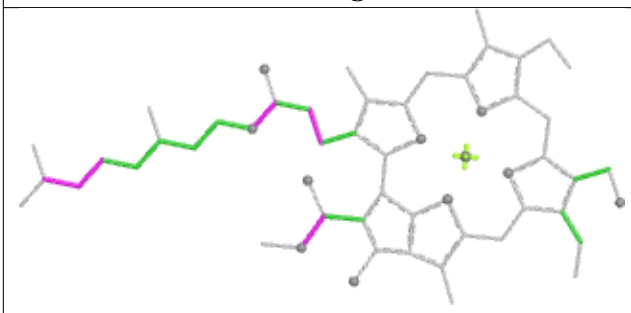
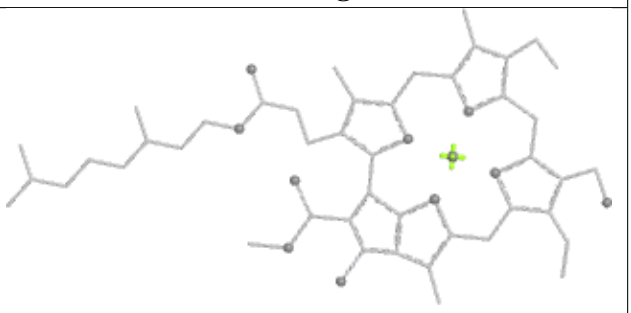
Bond angles

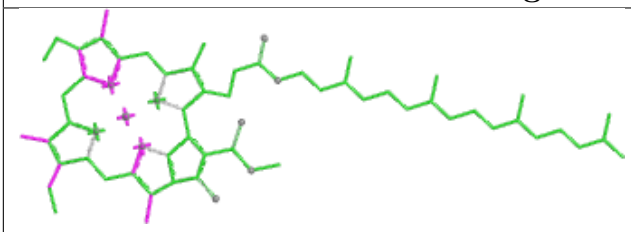
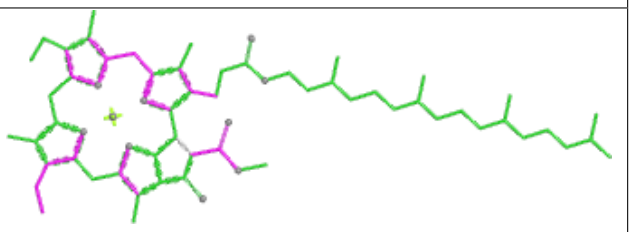
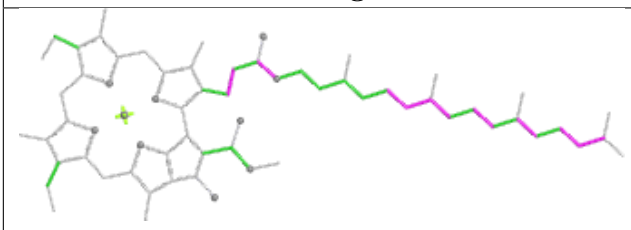
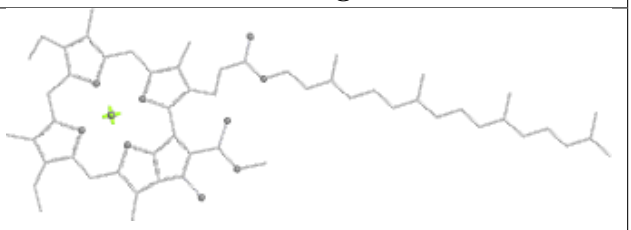


Torsions

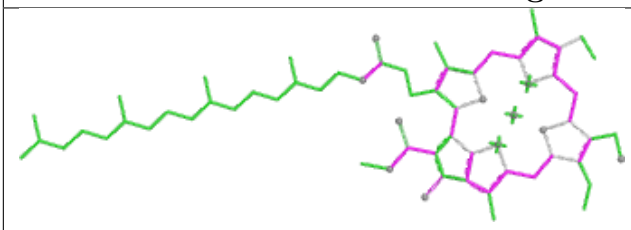


Rings

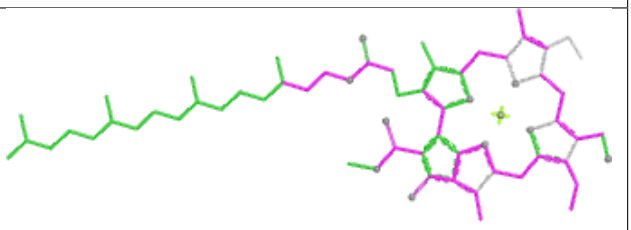
Ligand CHL r 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA N 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

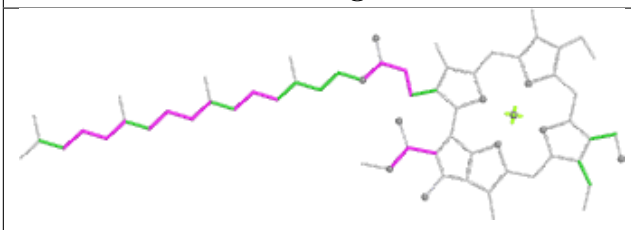
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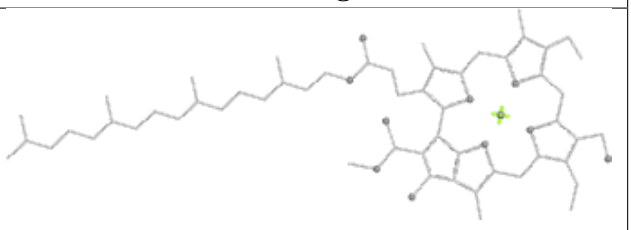
Bond lengths



Bond angles

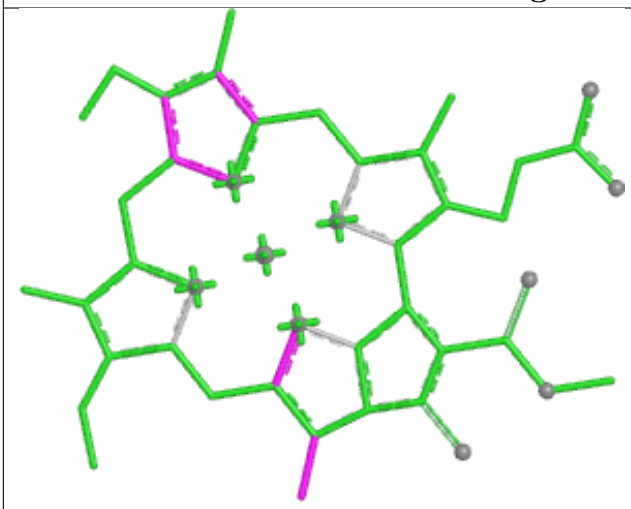


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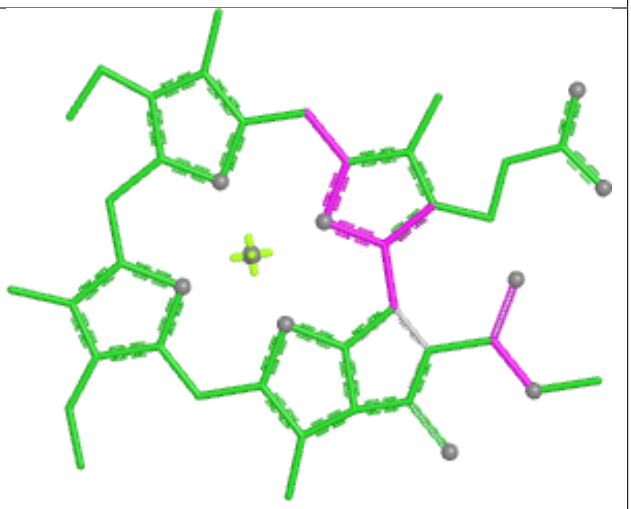


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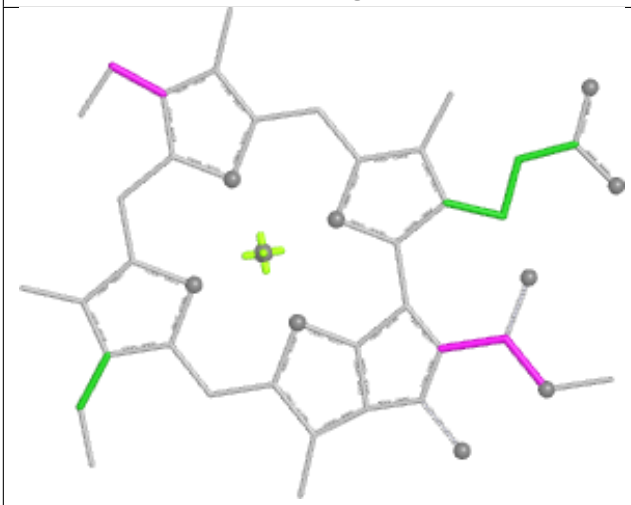
Ligand CLA s 603



Bond lengths



Bond angles

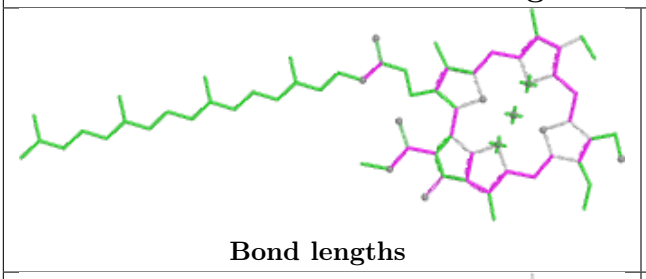


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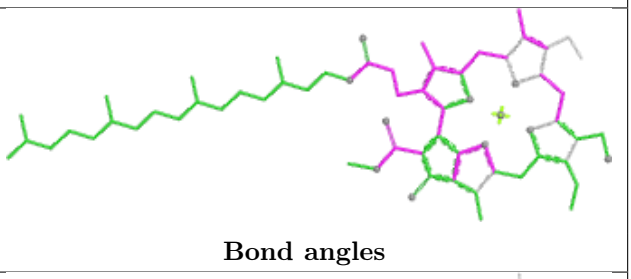


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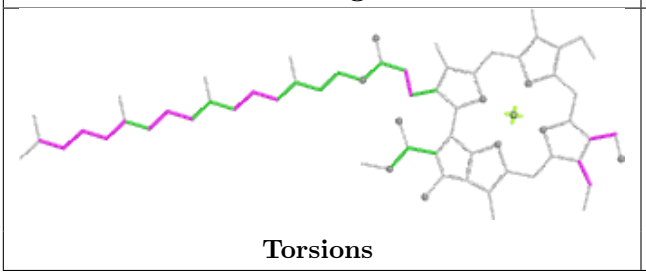
Ligand CHL n 607



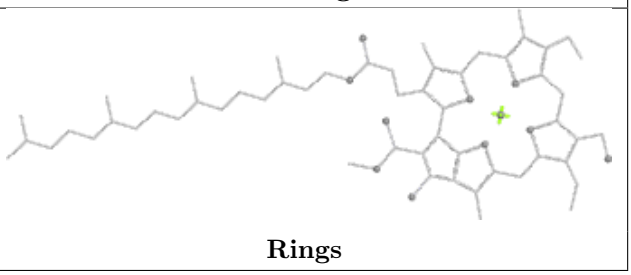
Bond lengths



Bond angles

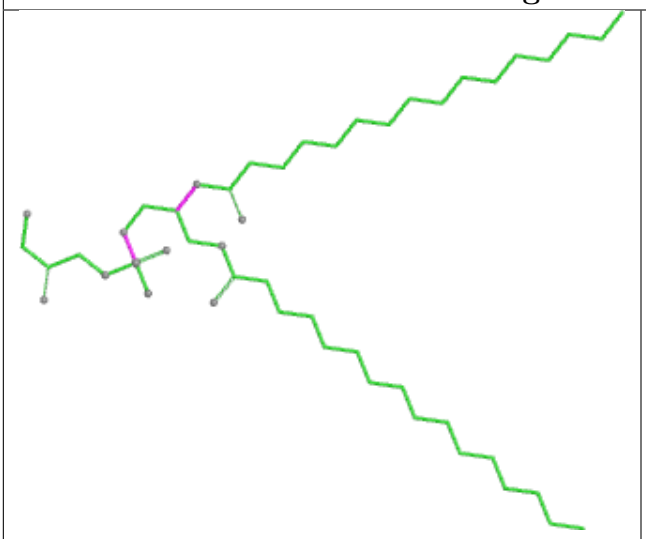


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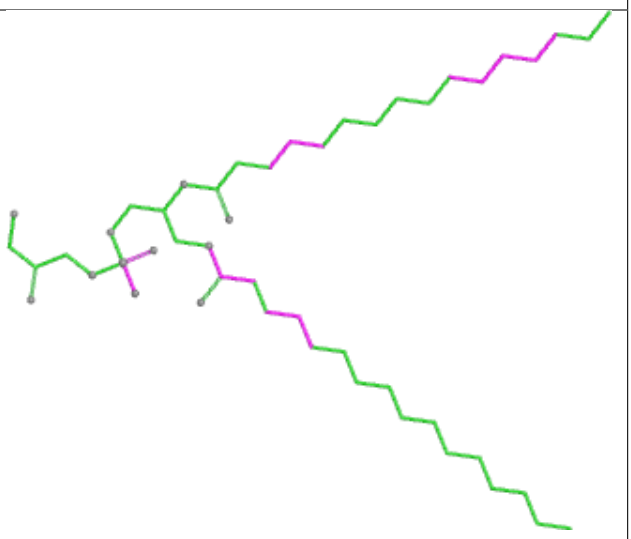


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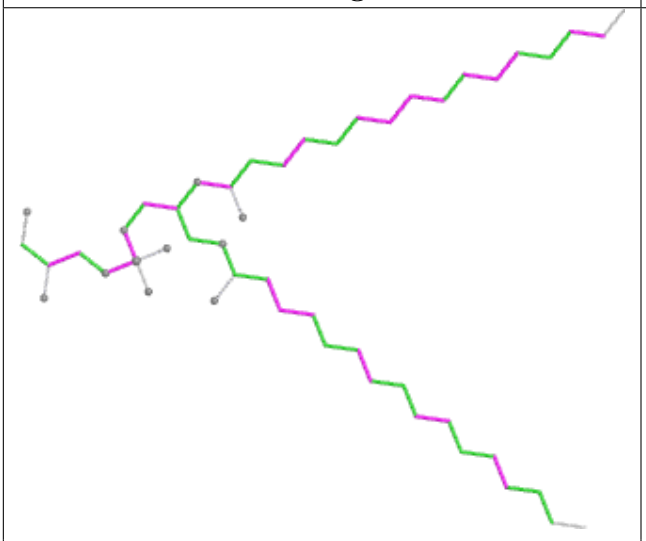
Ligand LHG C 523



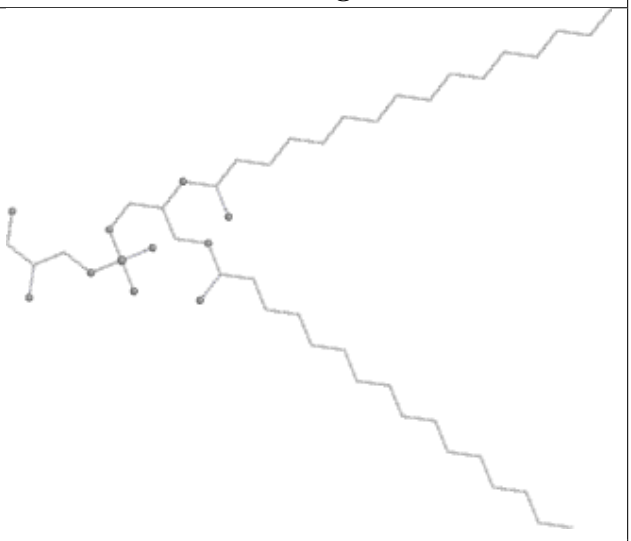
Bond lengths



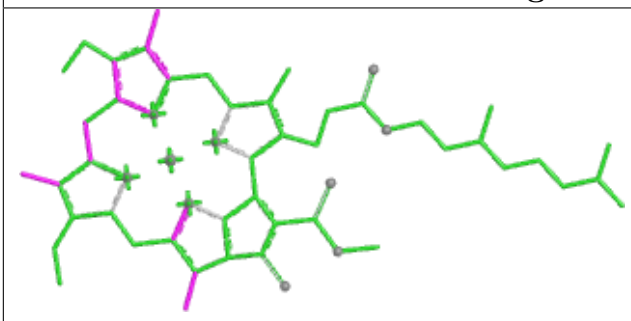
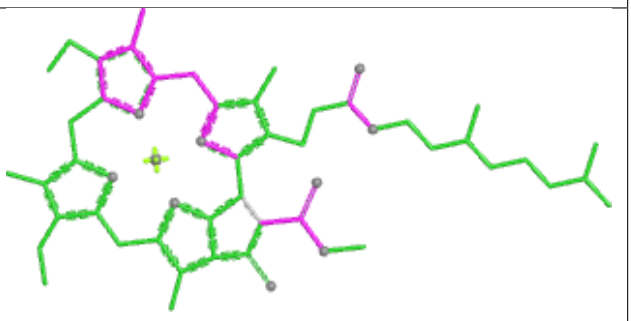
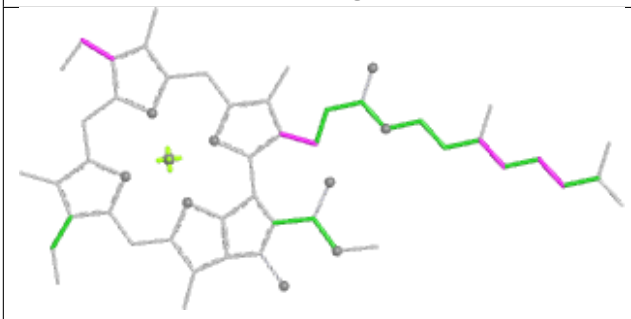
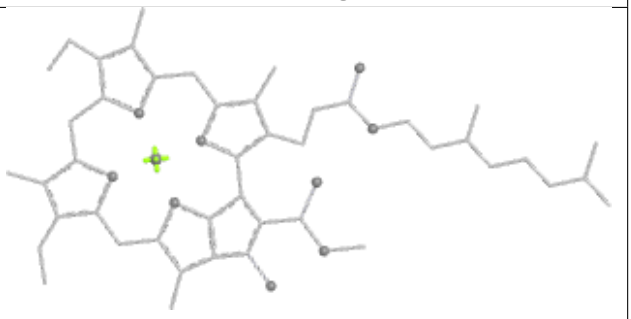
Bond angles

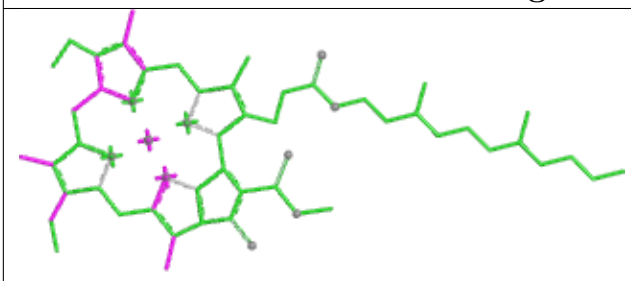
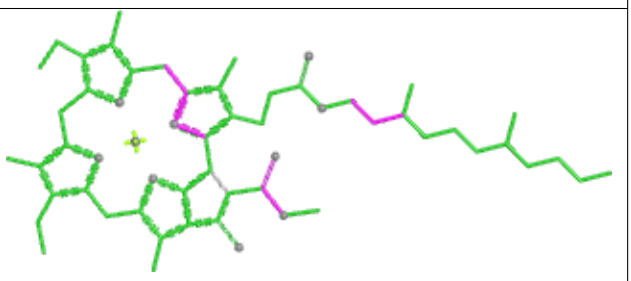
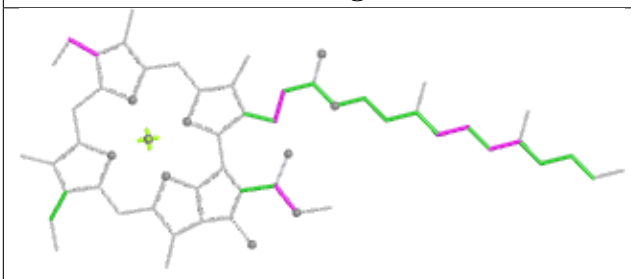
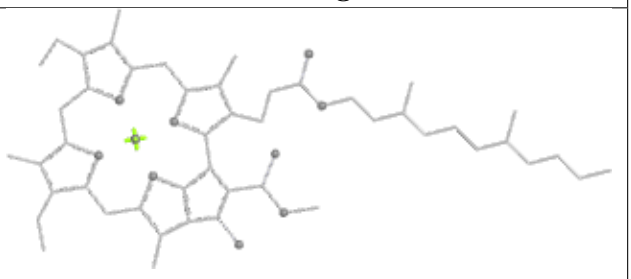


Torsions

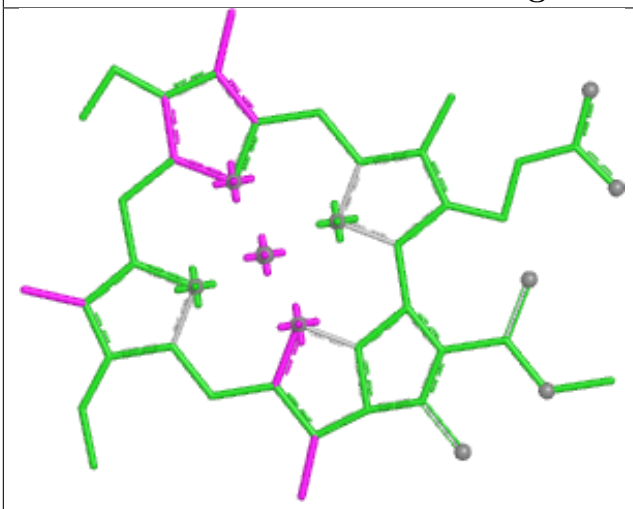


Rings

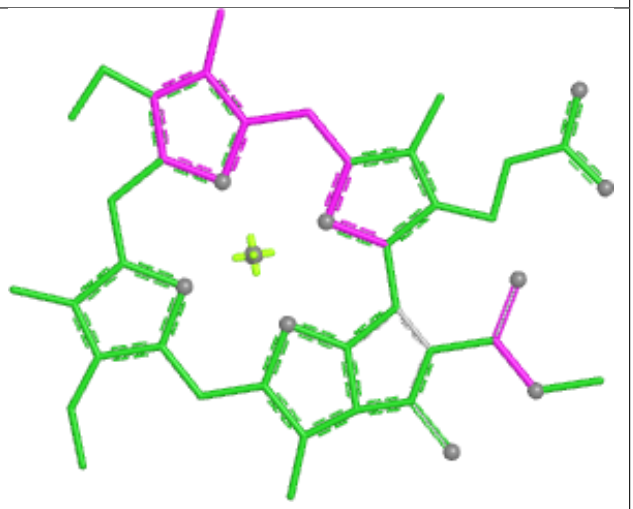
Ligand CLA S 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 7 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

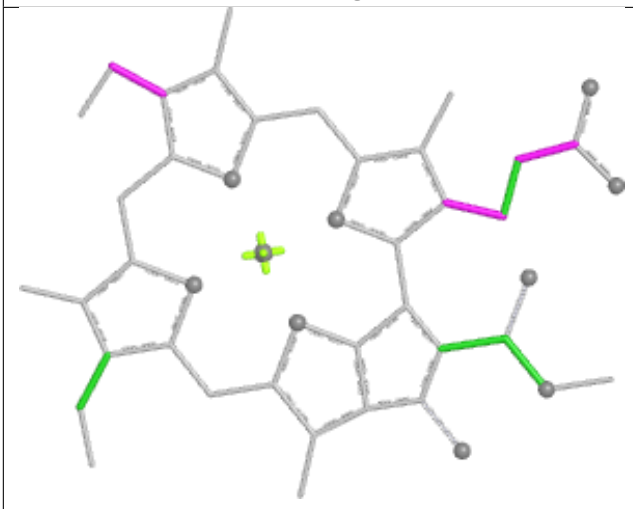
Ligand CLA 4 610



Bond lengths



Bond angles

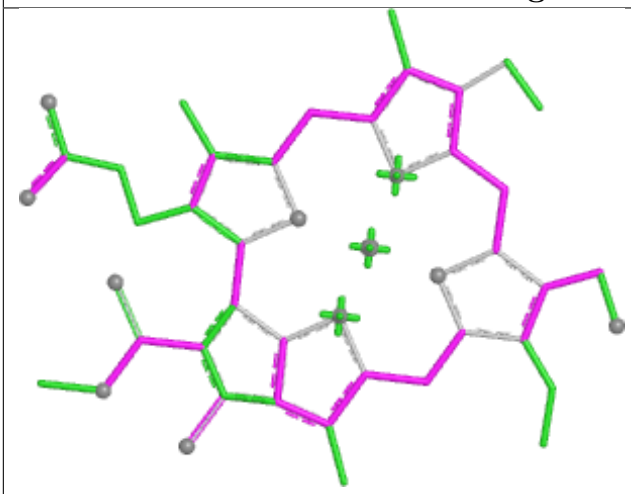


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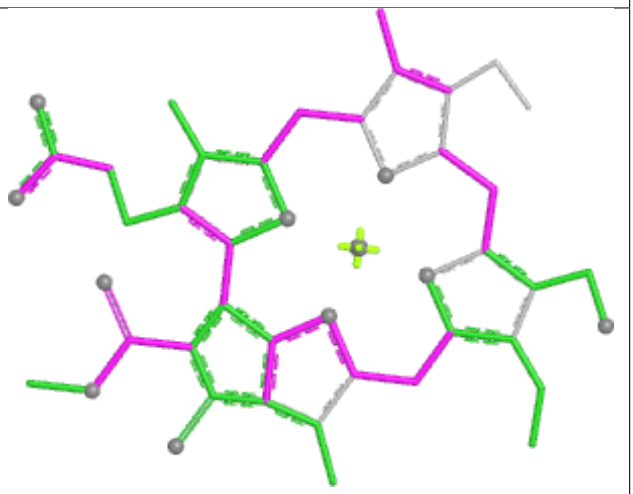


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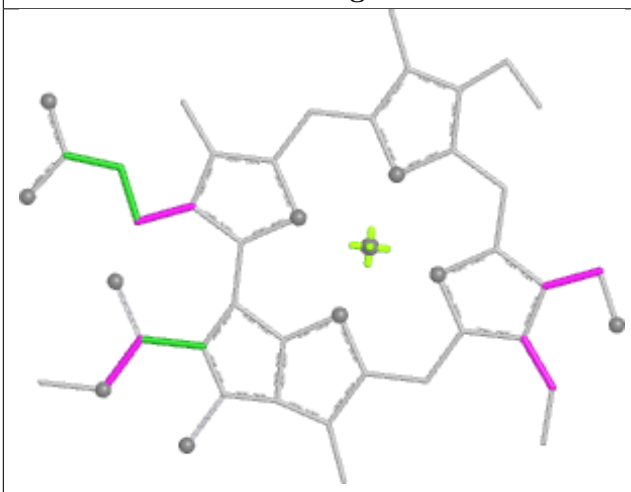
Ligand CHL 2 608



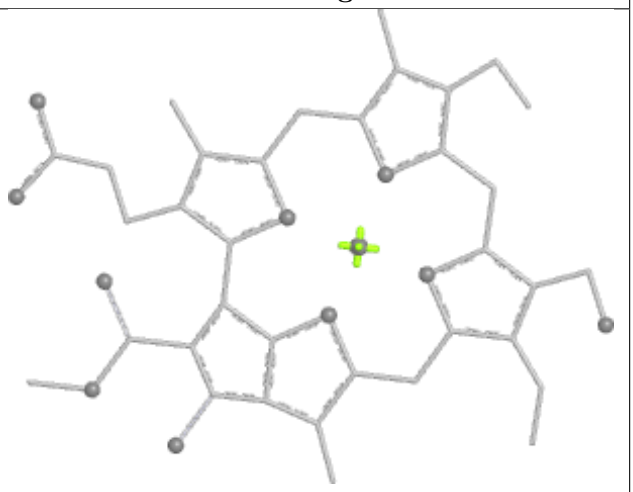
Bond lengths



Bond angles

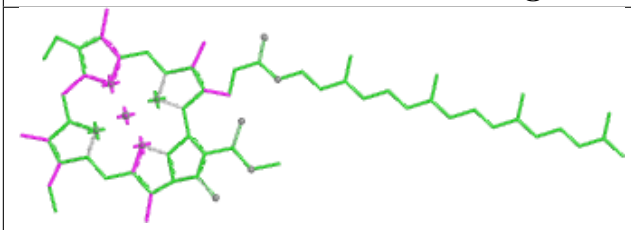


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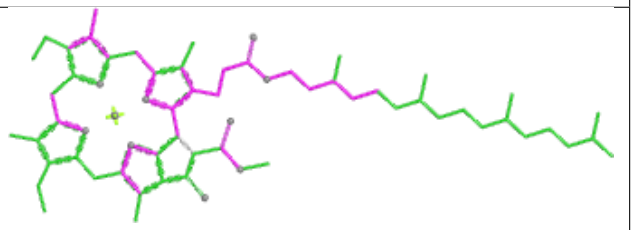


Rings

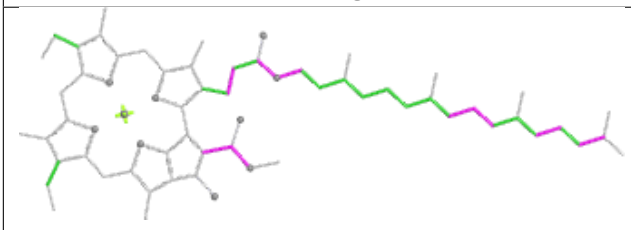
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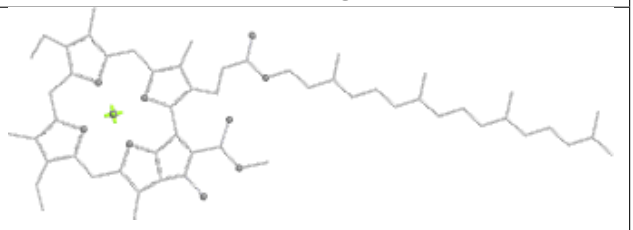
Bond lengths



Bond angles

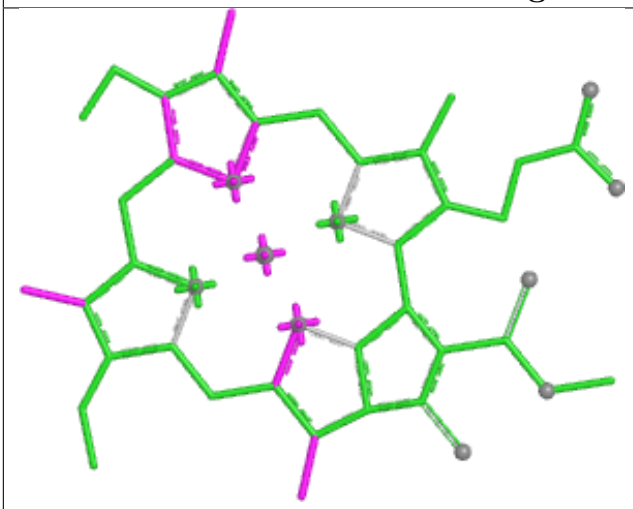


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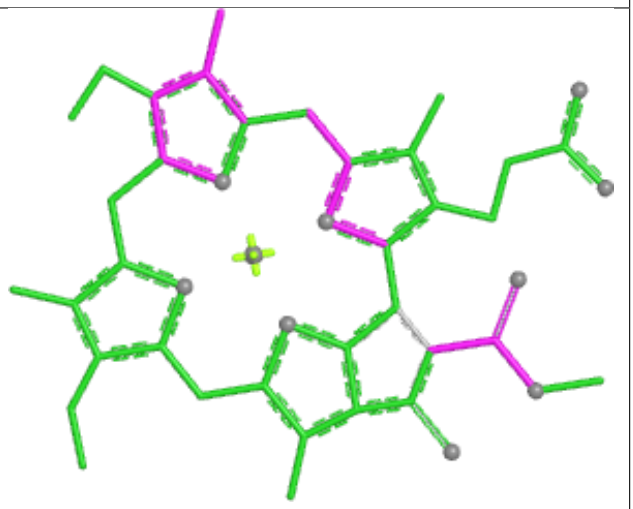


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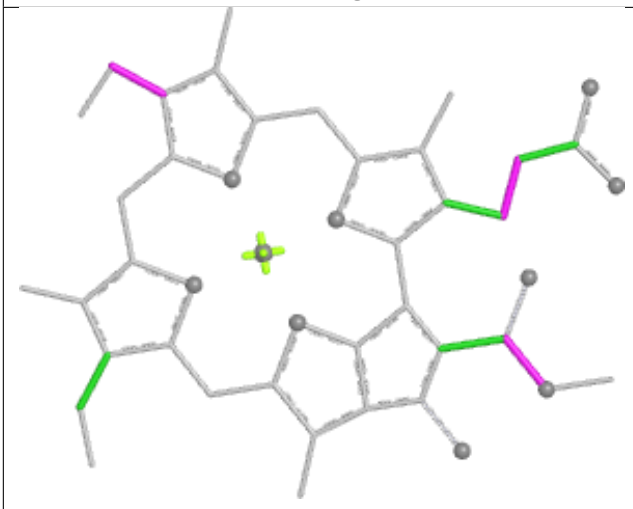
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Bond lengths



Bond angles

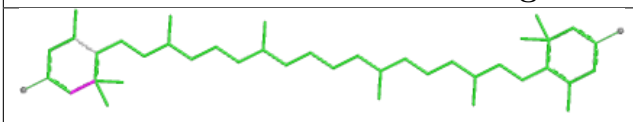


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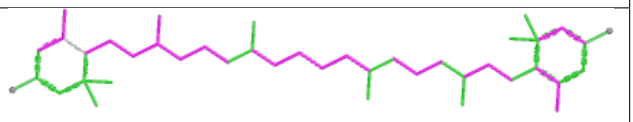


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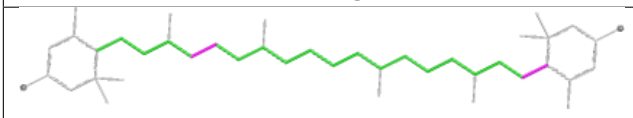
Ligand LUT 3 1621



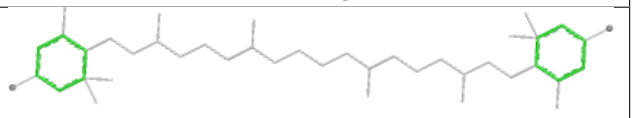
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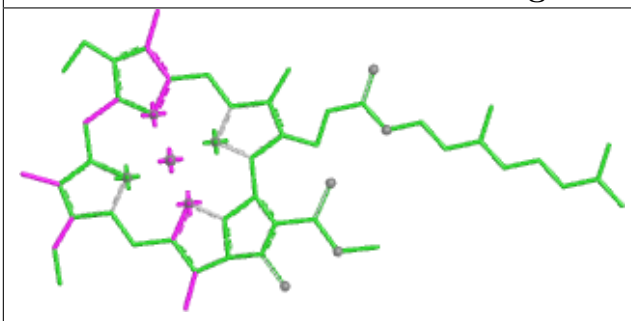
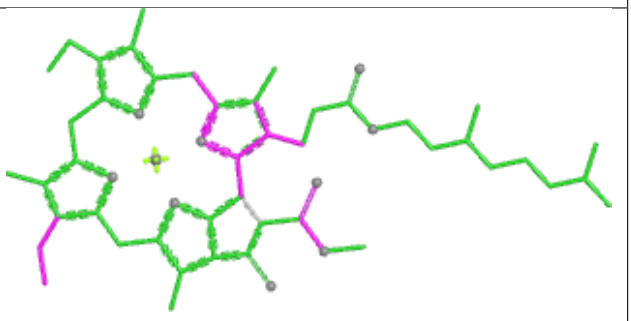
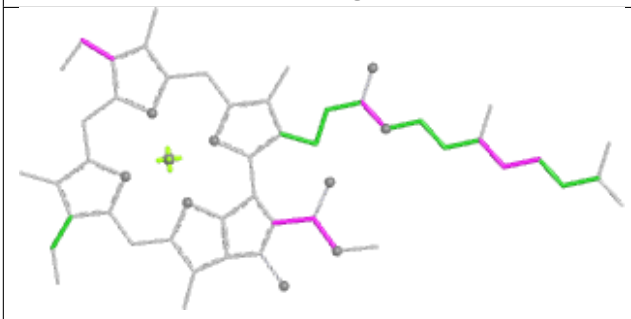
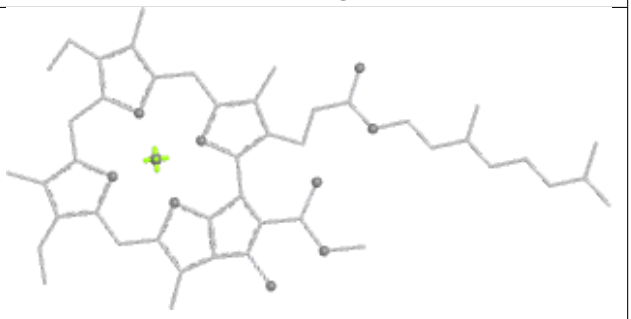
Bond angles

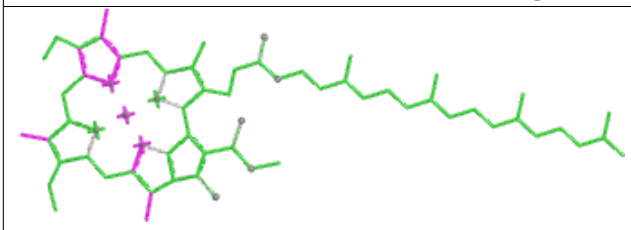
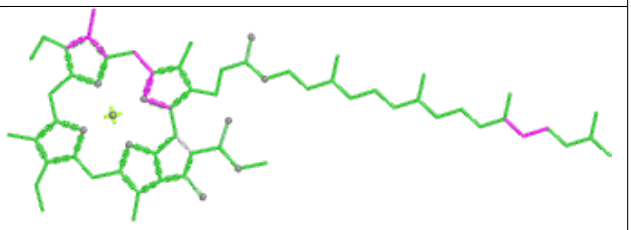
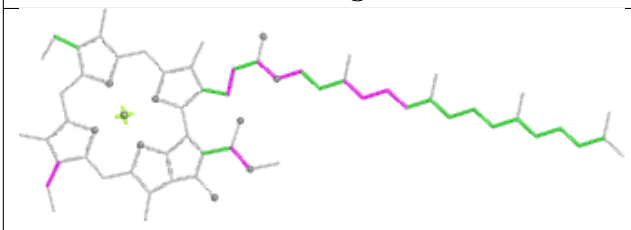
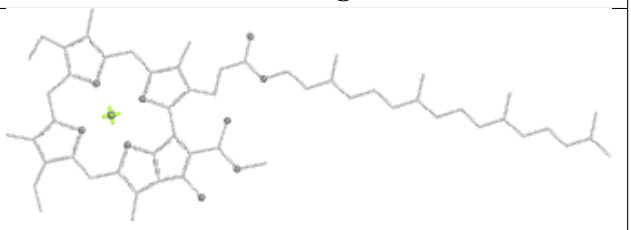


Torsions

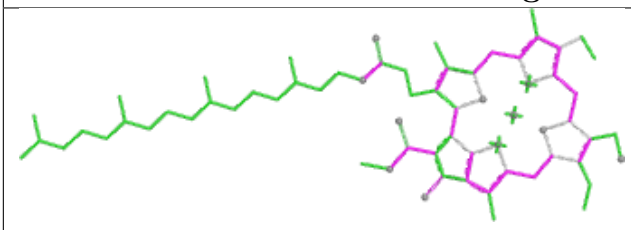


Rings

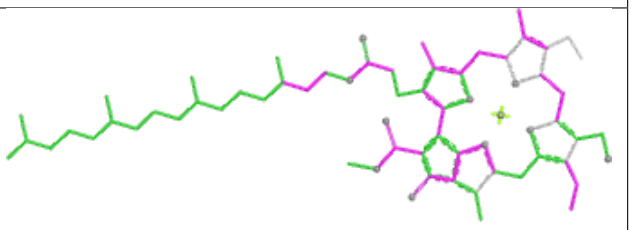
Ligand CLA 5 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

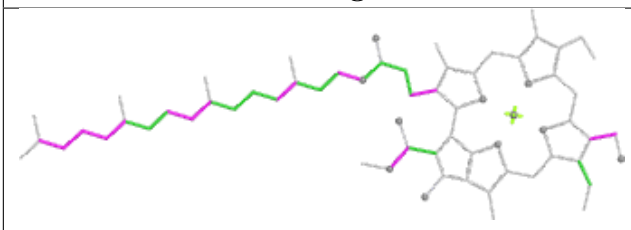
Ligand CHL G 608



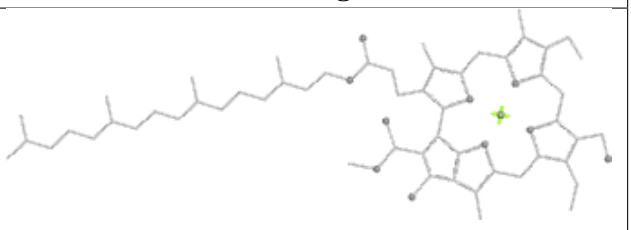
Bond lengths



Bond angles

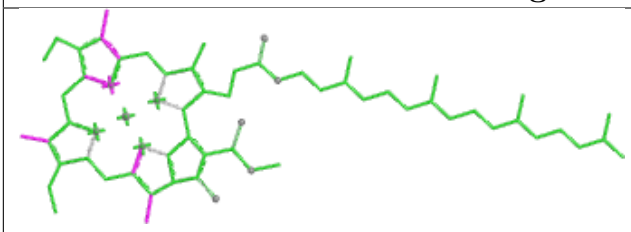


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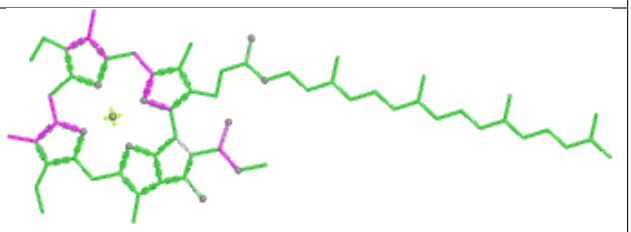


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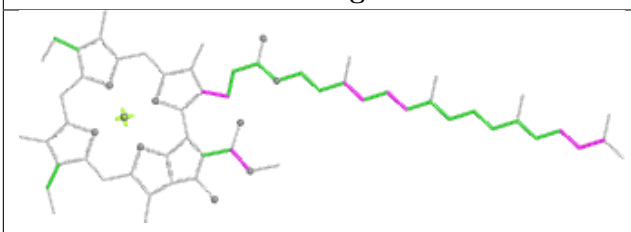
Ligand CLA c 508



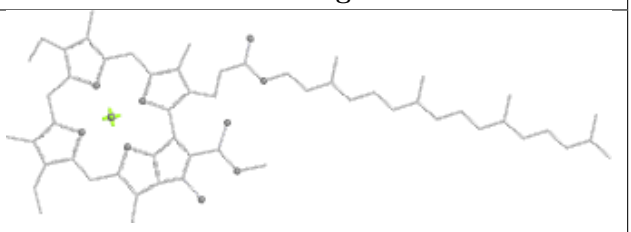
Bond lengths



Bond angles

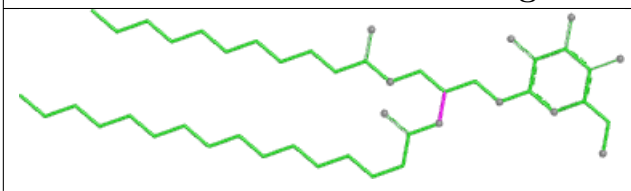


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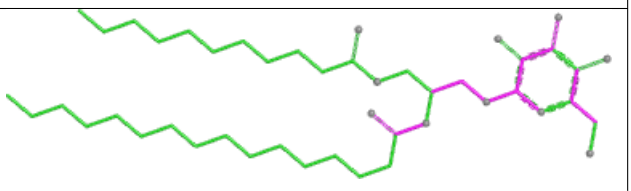


Rings

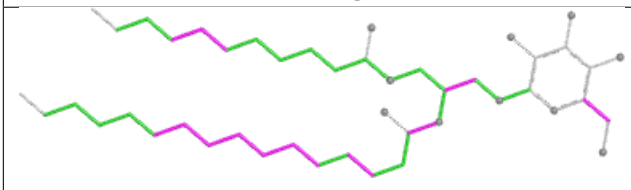
Ligand LMG D 411



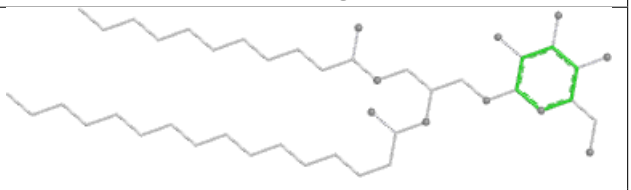
Bond lengths



Bond angles

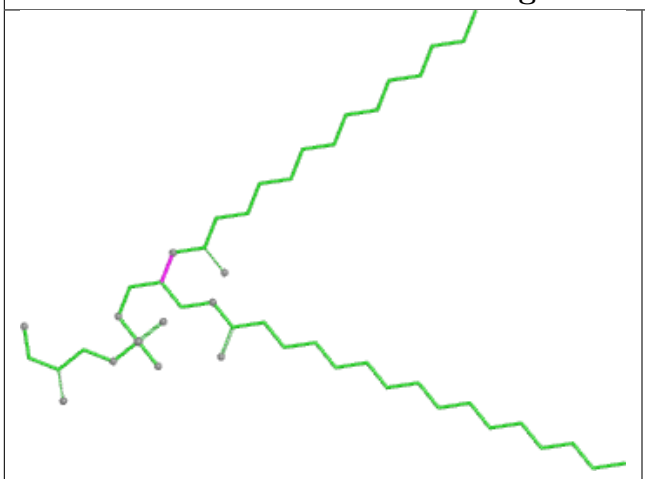


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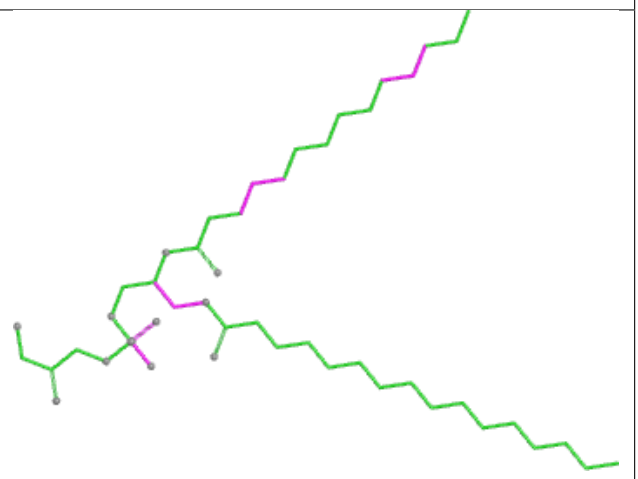


Rings

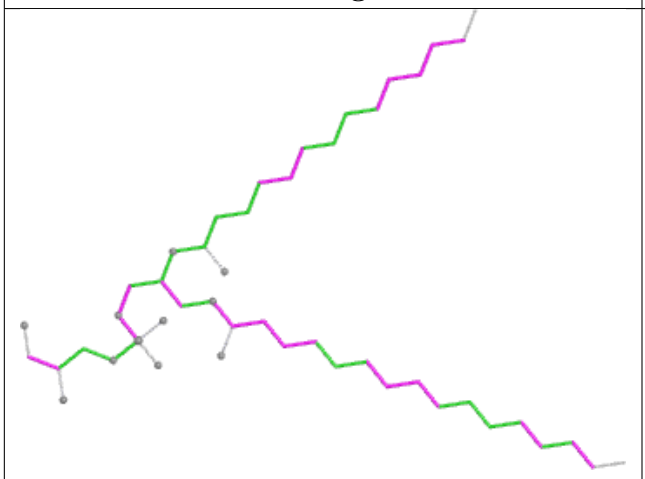
Ligand LHG 7 2630



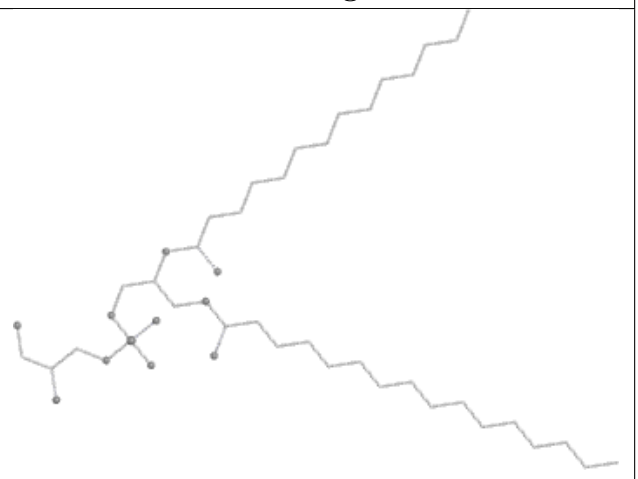
Bond lengths



Bond angles

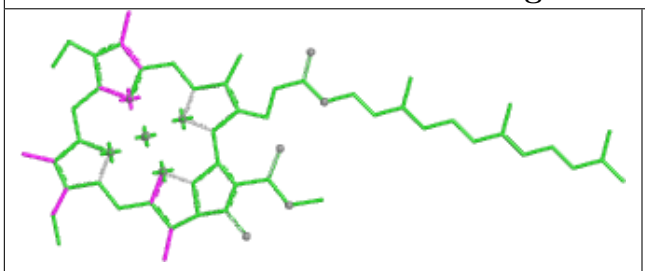


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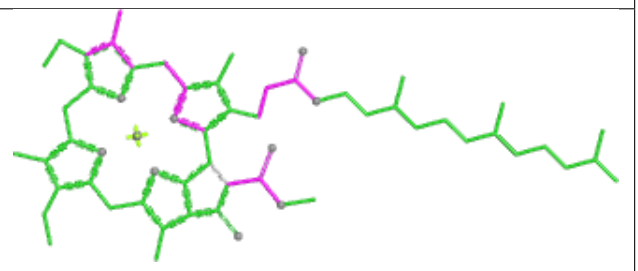


Rings

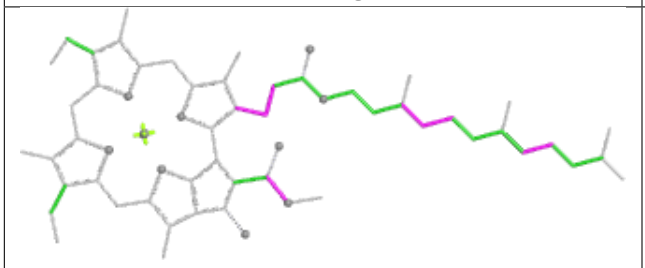
Ligand CLA R 602



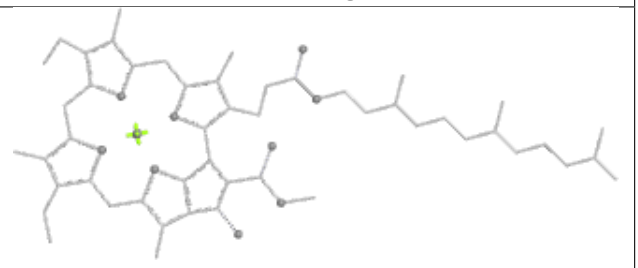
Bond lengths



Bond angles

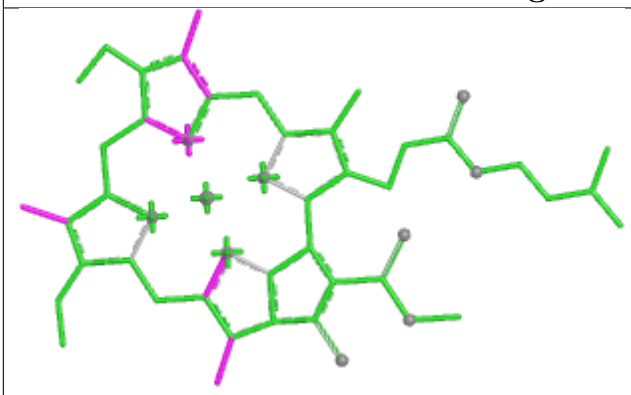


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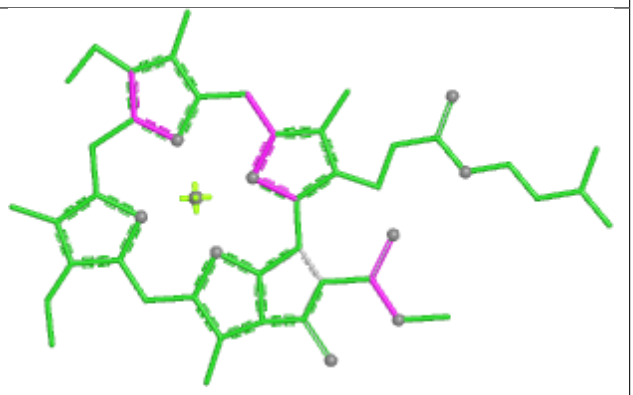


Rings

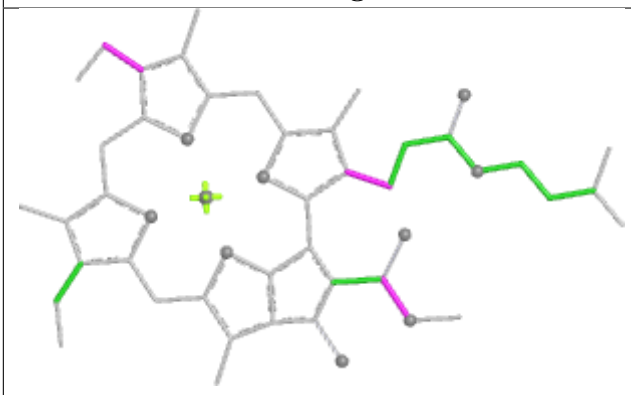
Ligand CLA 2 610



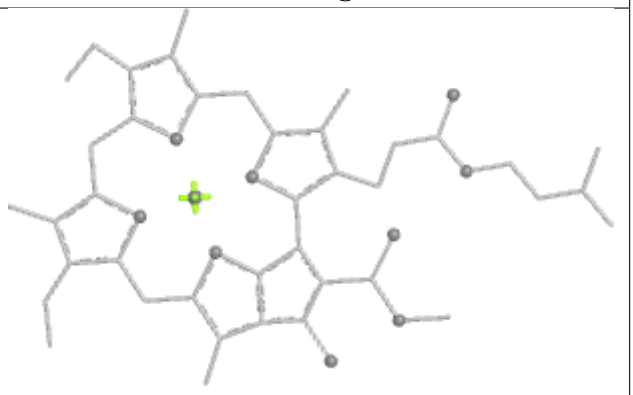
Bond lengths



Bond angles



Torsions

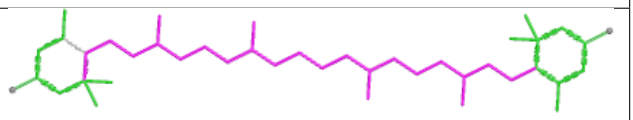


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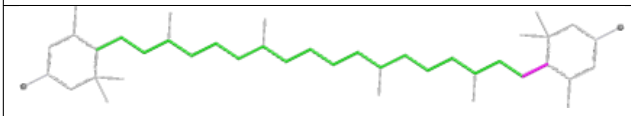
Ligand LUT 1 1620



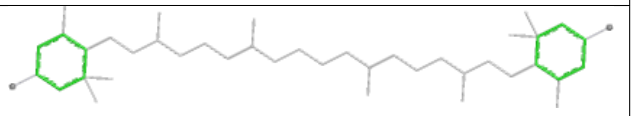
Bond lengths



Bond angles

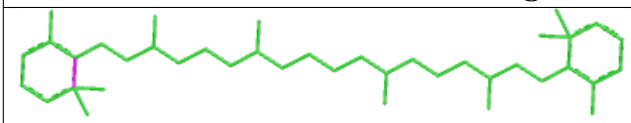


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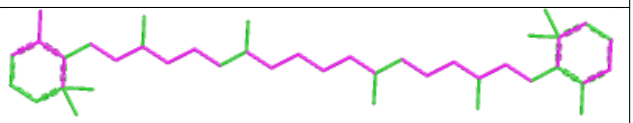


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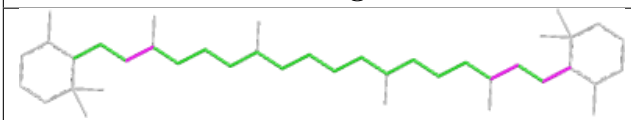
Ligand BCR B 620



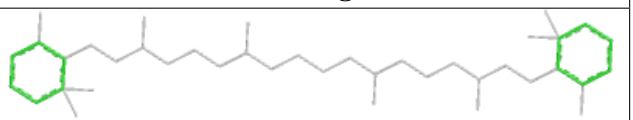
Bond lengths



Bond angles

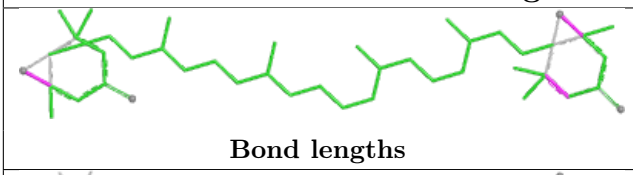


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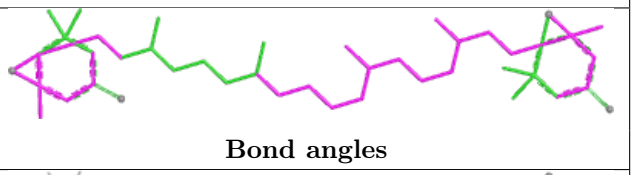


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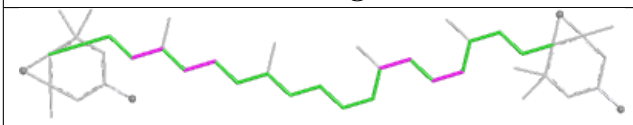
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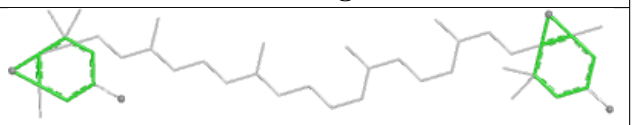
Bond lengths



Bond angles

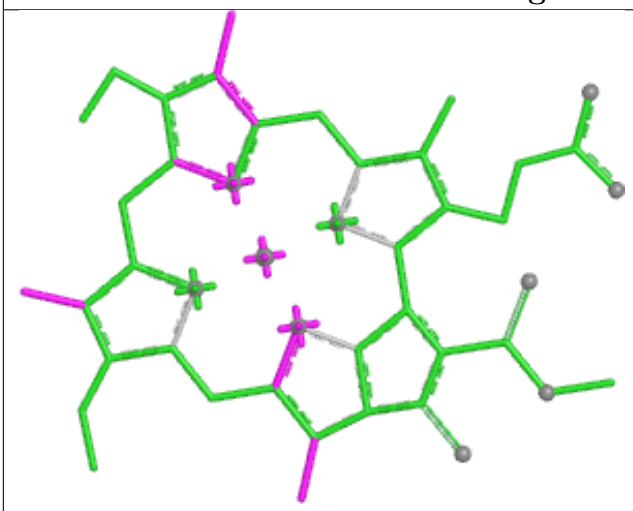


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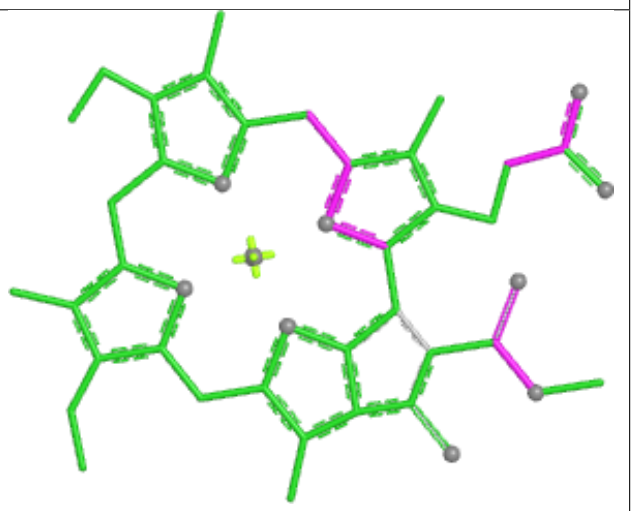


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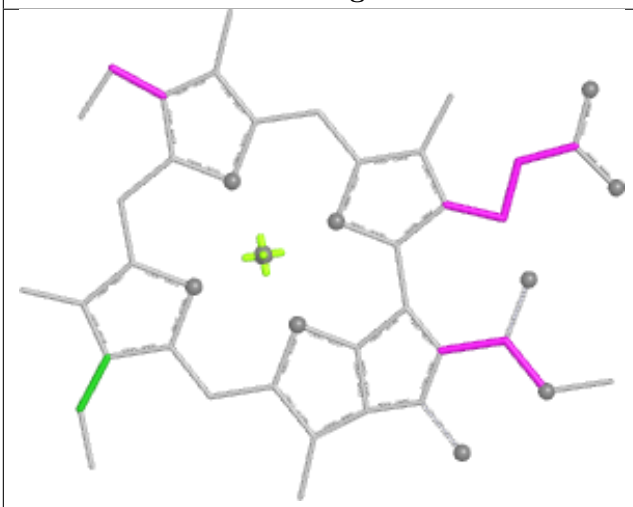
Ligand CLA 7 604



Bond lengths



Bond angles

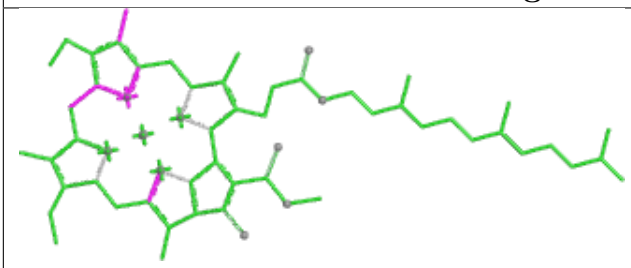


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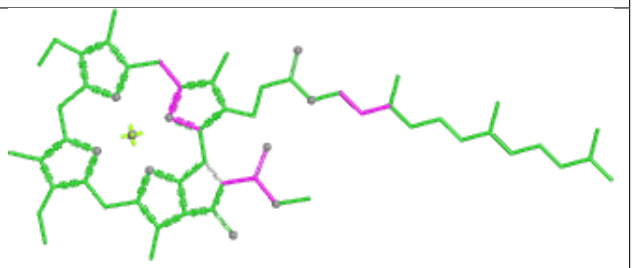


Rings

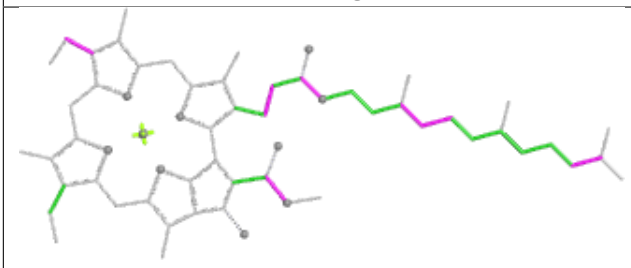
Ligand CLA R 613



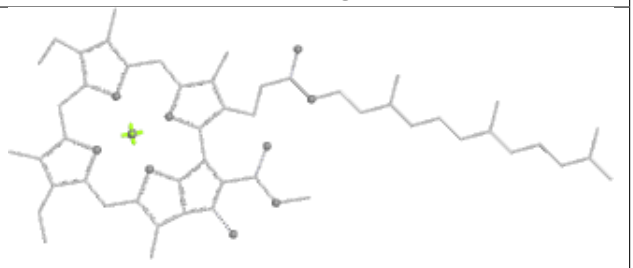
Bond lengths



Bond angles

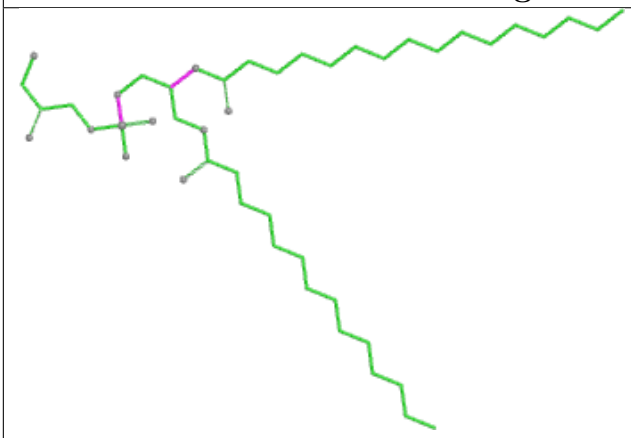


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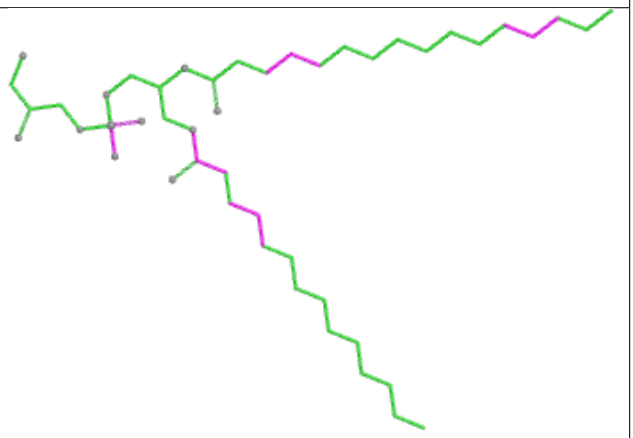


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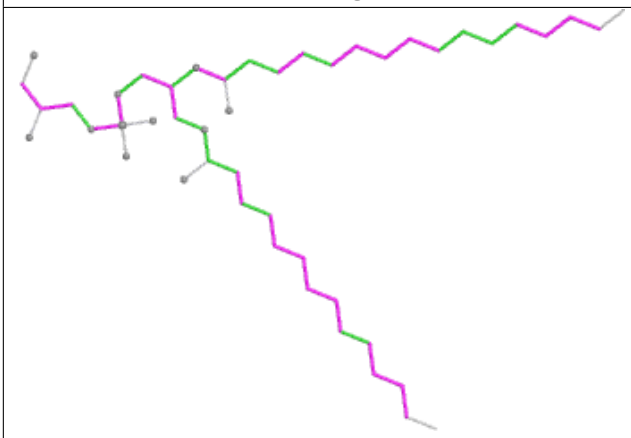
Ligand LHG B 2630



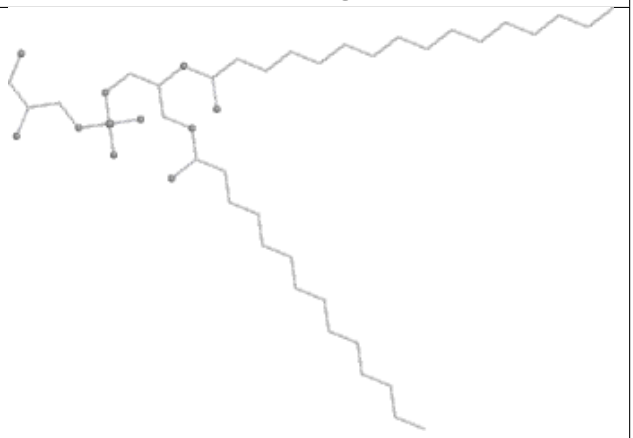
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Bond angles

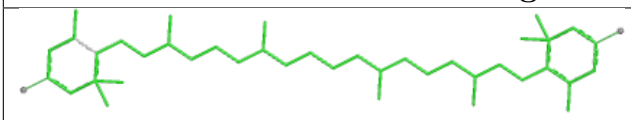


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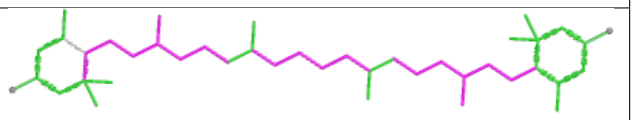


Rings

Ligand LUT 6 1620



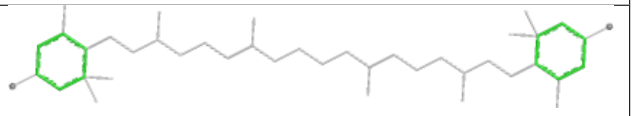
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Bond angles

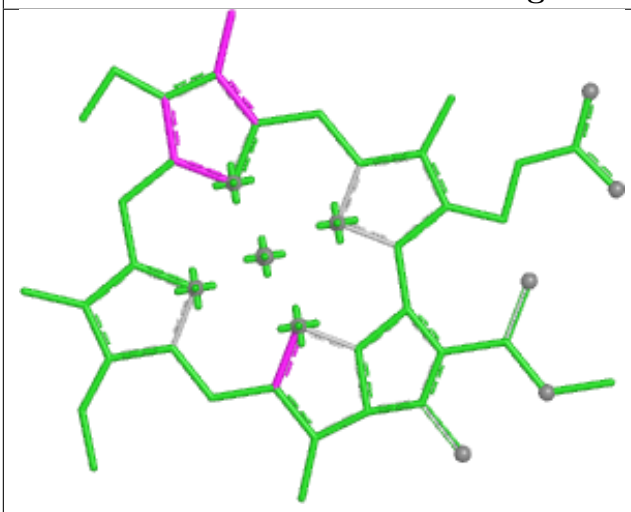


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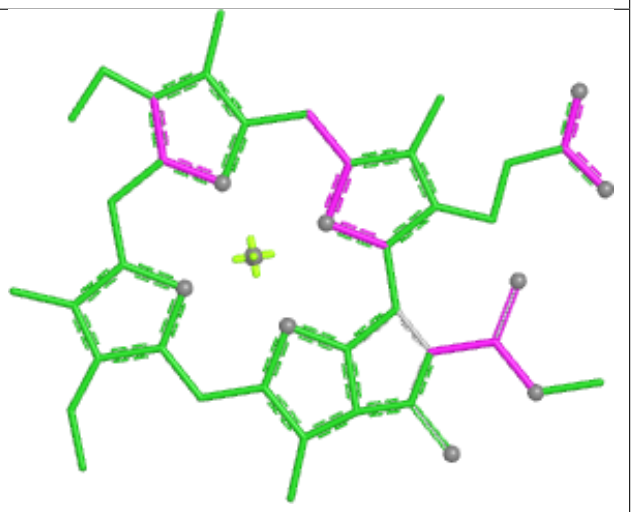


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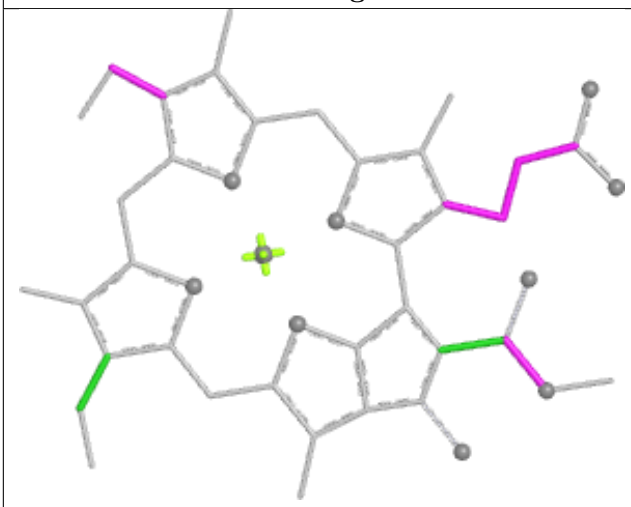
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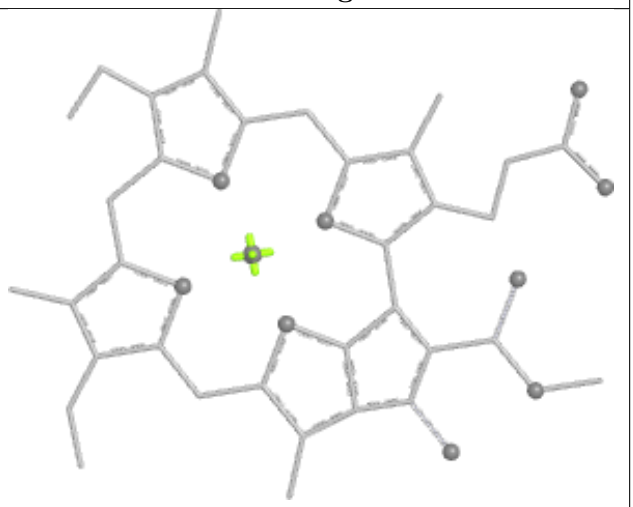
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Bond angles

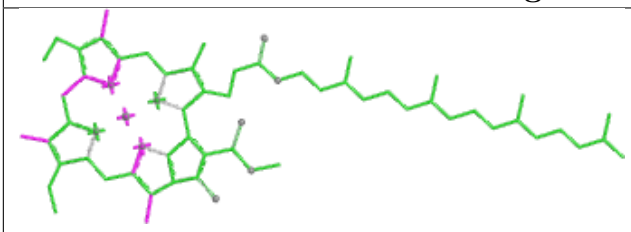


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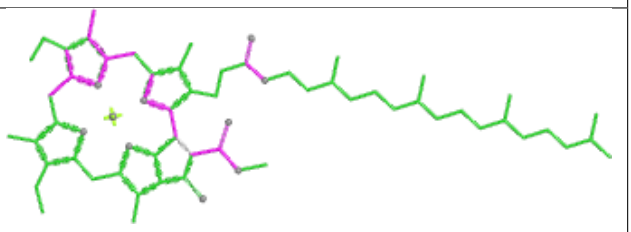


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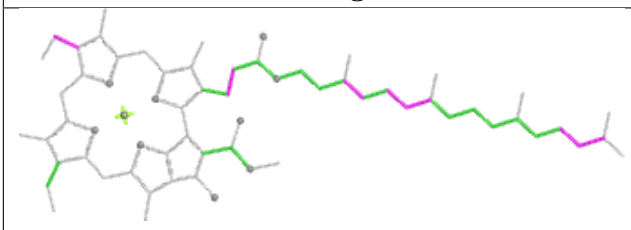
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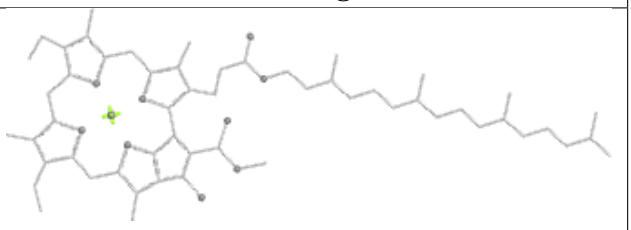
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Bond angles

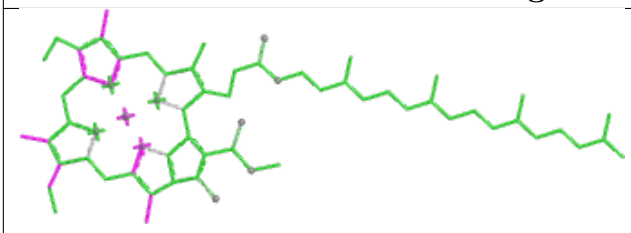


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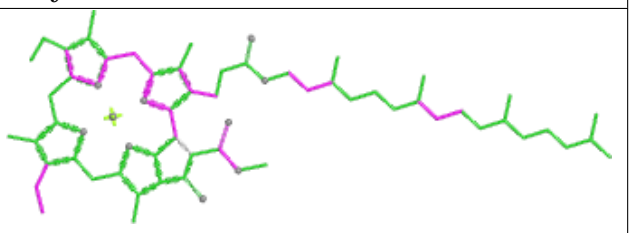


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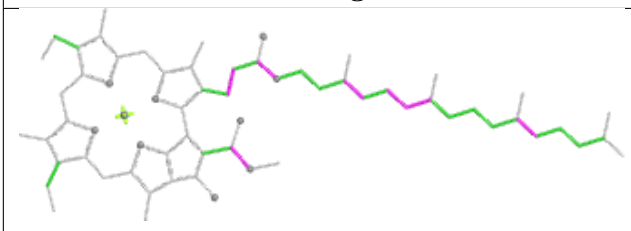
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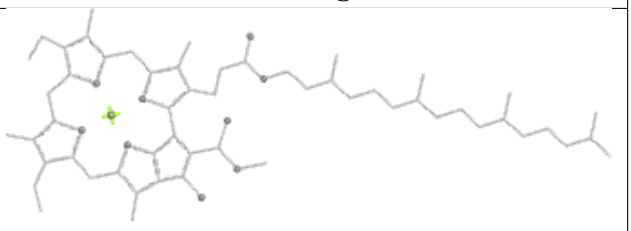
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Bond angles

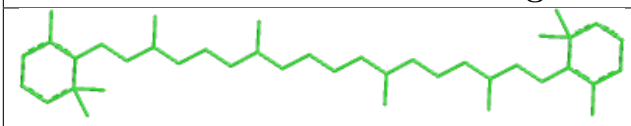


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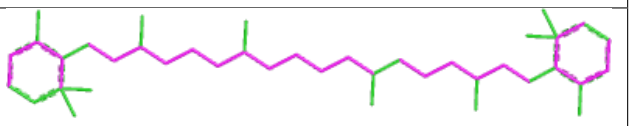


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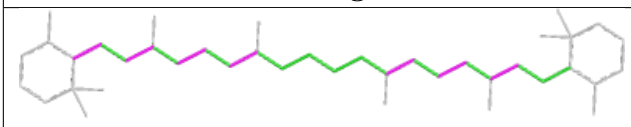
Ligand BCR 8 623



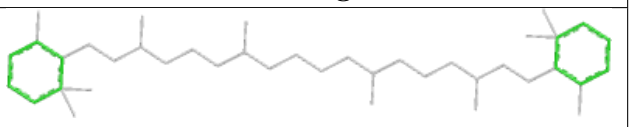
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Bond angles

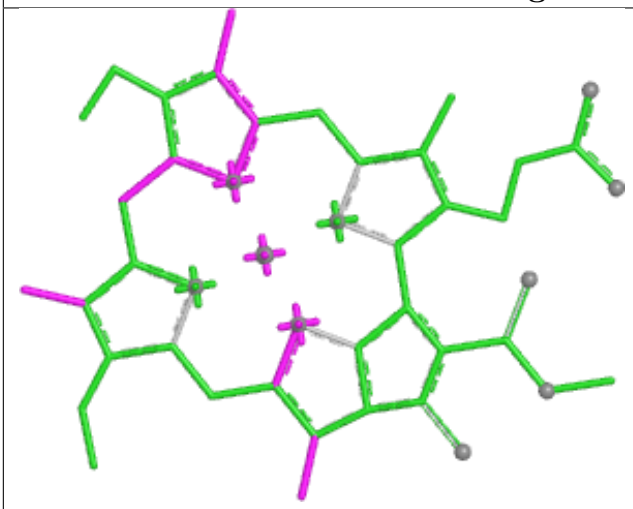


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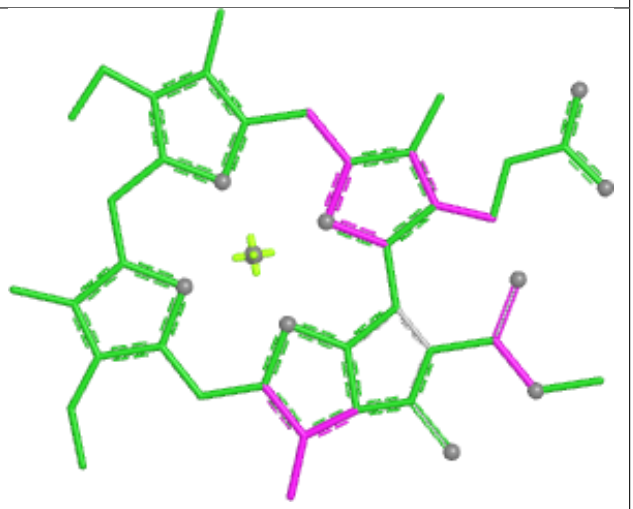


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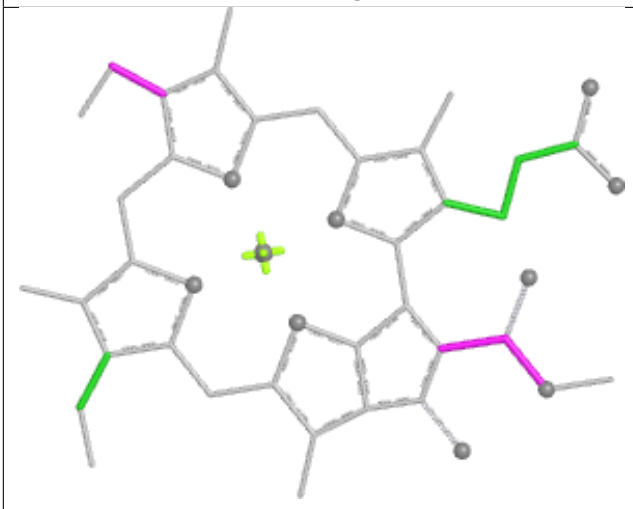
Ligand CLA 7 612



Bond lengths



Bond angles

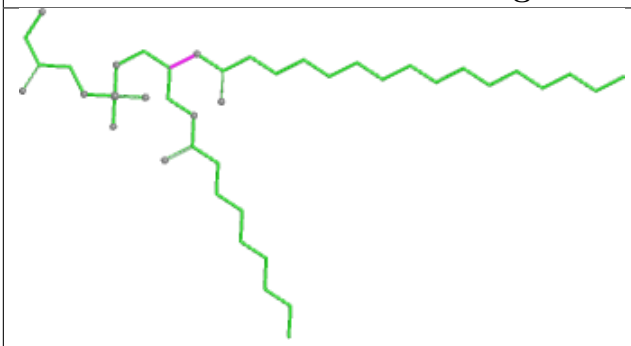


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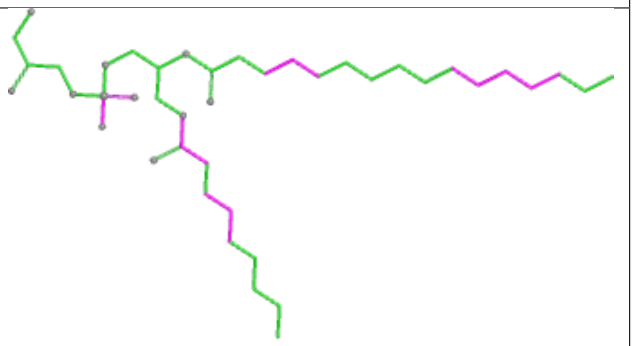


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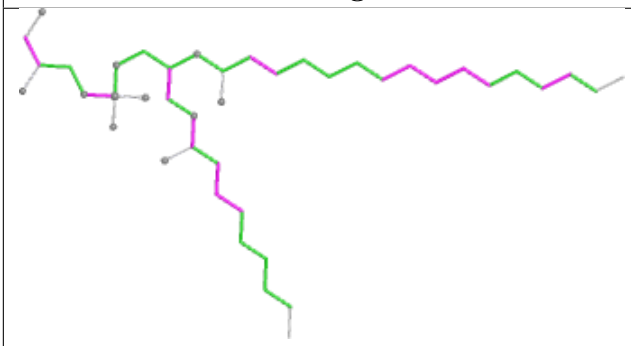
Ligand LHG R 2630



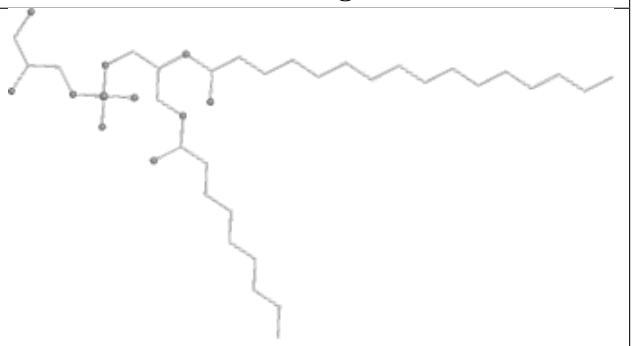
Bond lengths



Bond angles

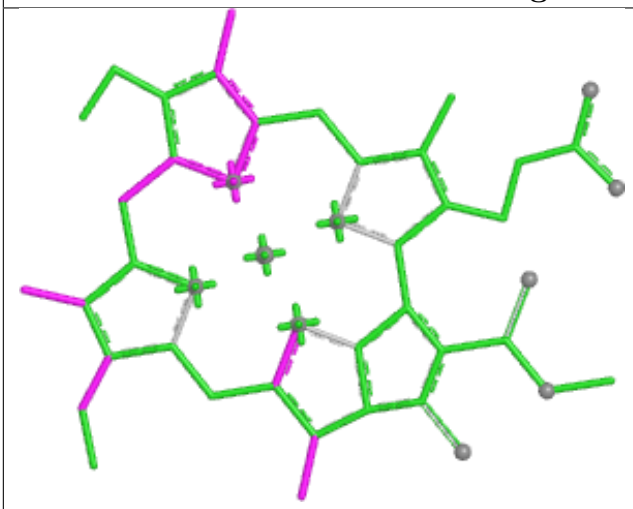


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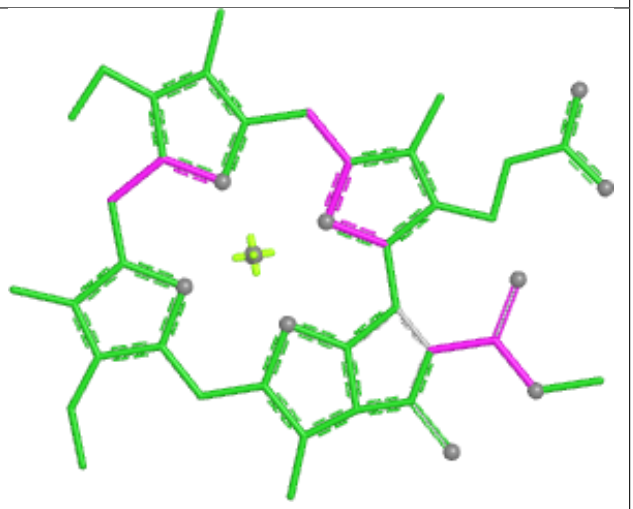


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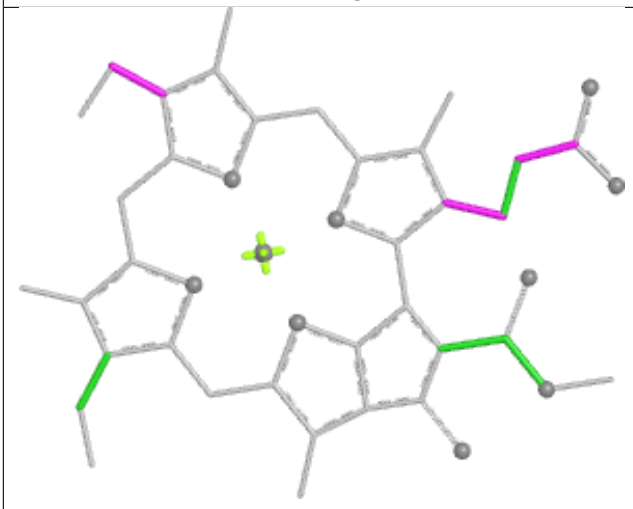
Ligand CLA r 616



Bond lengths



Bond angles

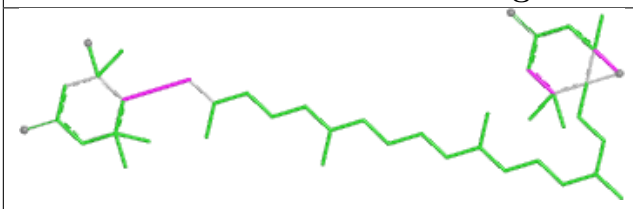


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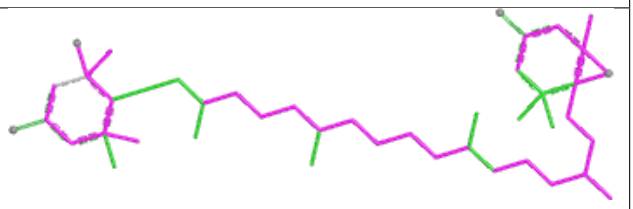


Rings

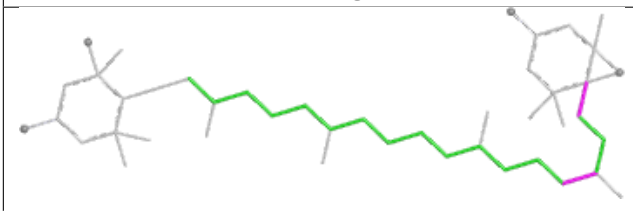
Ligand NEX Y 1623



Bond lengths



Bond angles

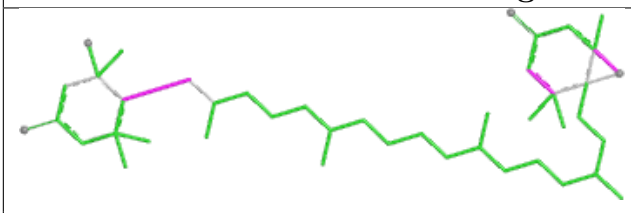


Torsions

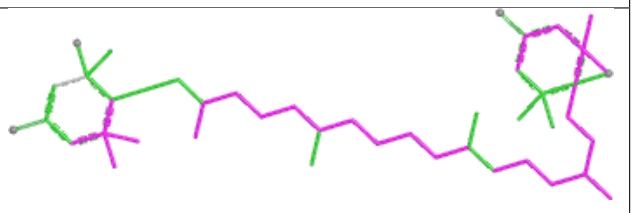


Rings

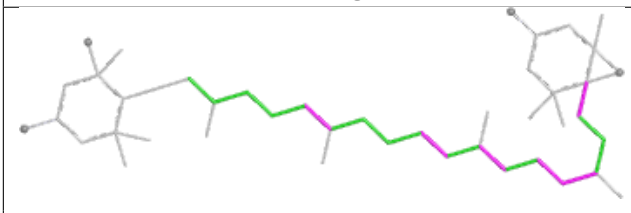
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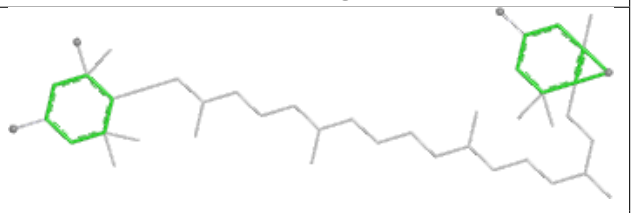
Bond lengths



Bond angles

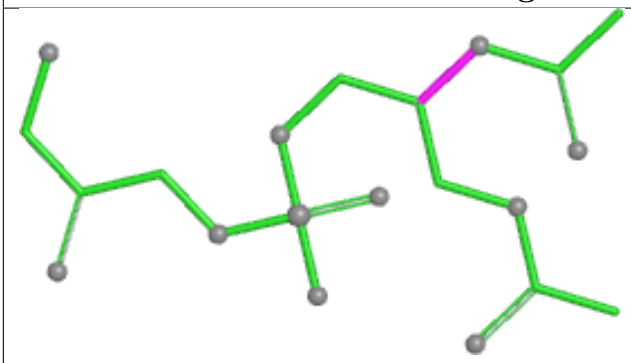


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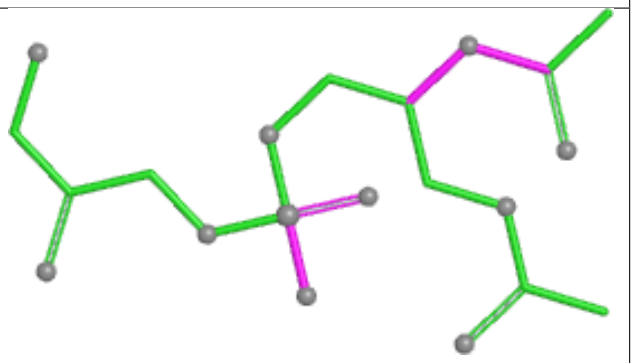


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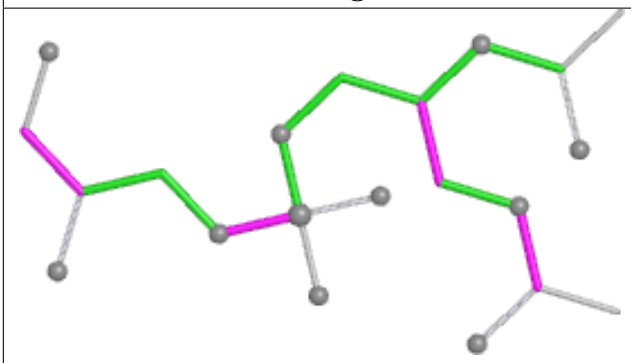
Ligand LHG 4 2630



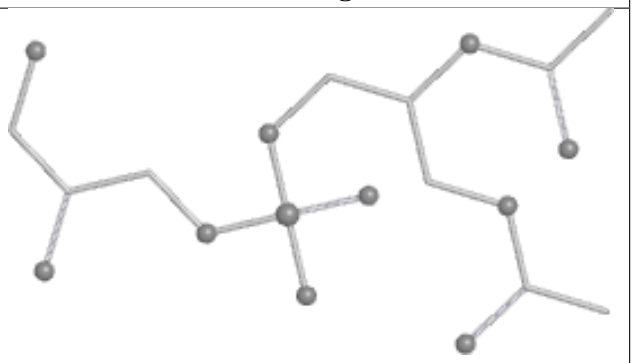
Bond lengths



Bond angles

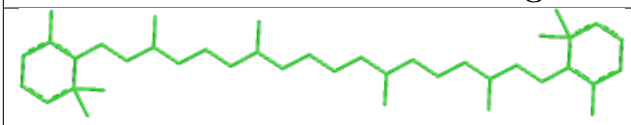


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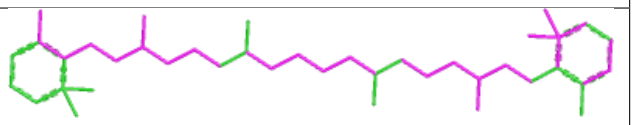


Rings

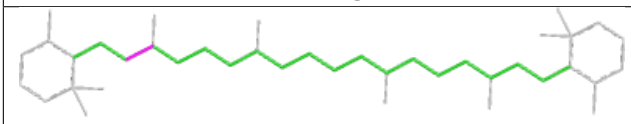
Ligand BCR b 619



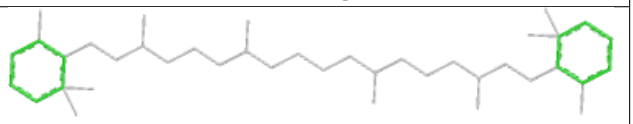
Bond lengths



Bond angles

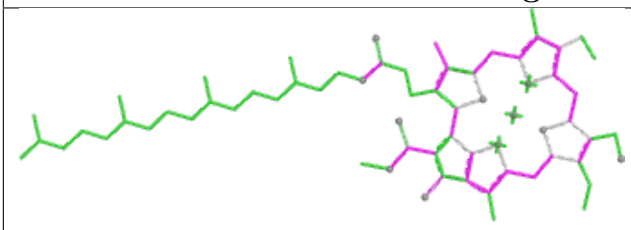


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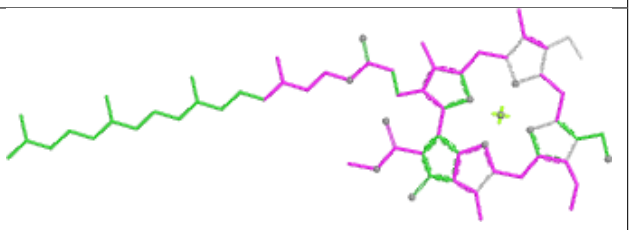


Rings

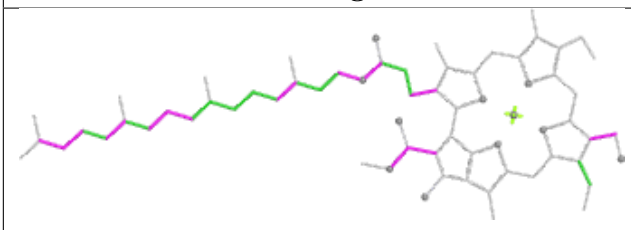
Ligand CHL N 609



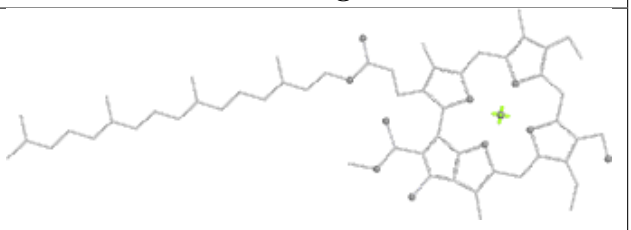
Bond lengths



Bond angles

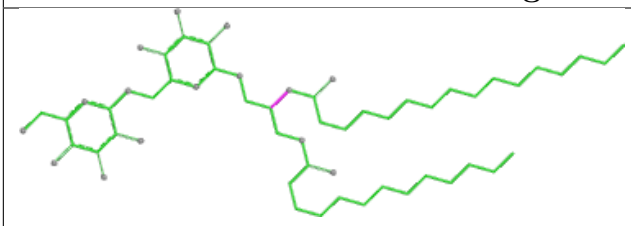


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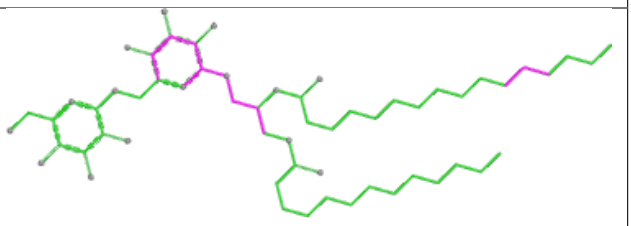


Rings

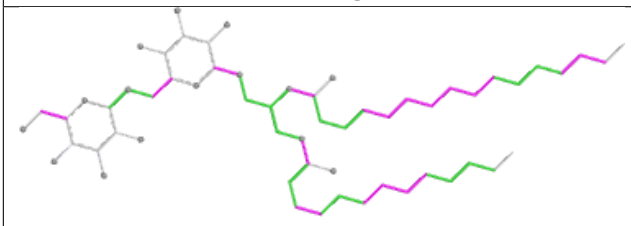
Ligand DGD b 626



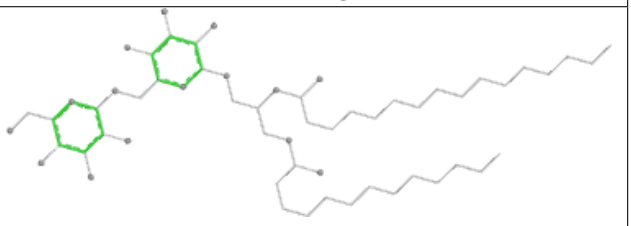
Bond lengths



Bond angles

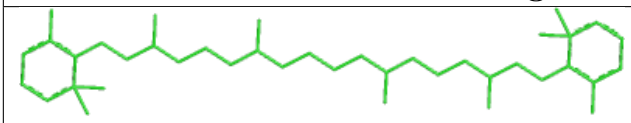


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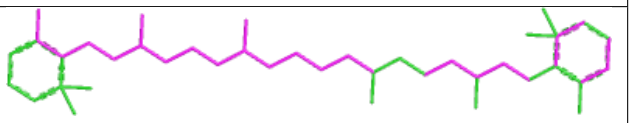


Rings

Ligand BCR c 516



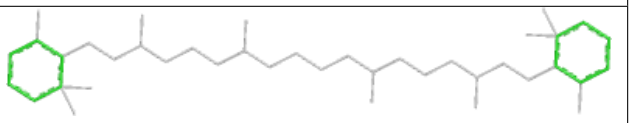
Bond lengths



Bond angles

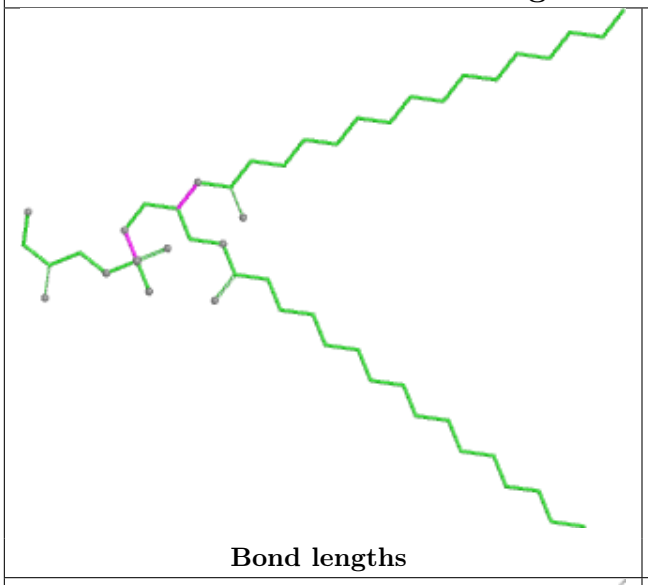


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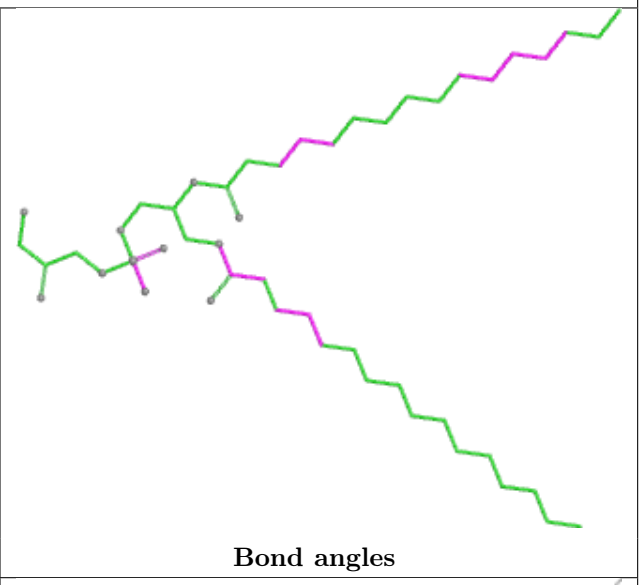


Rings

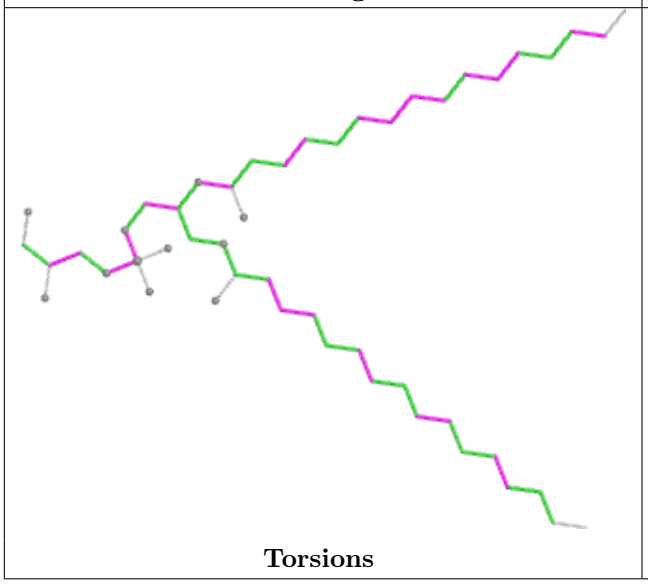
Ligand LHG c 523



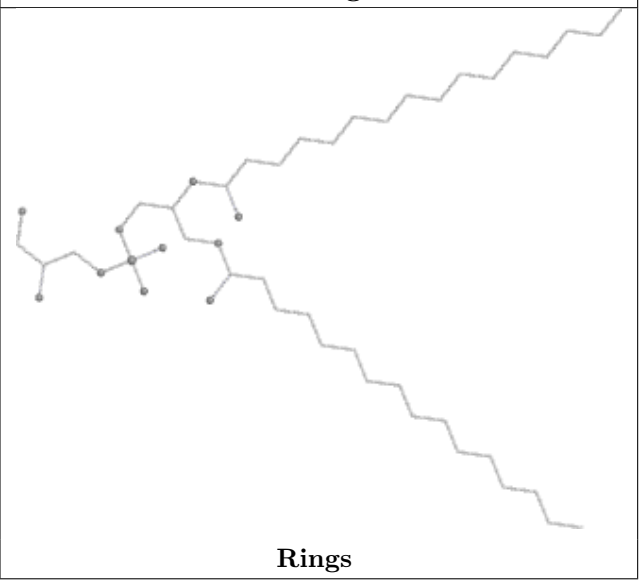
Bond lengths



Bond angles

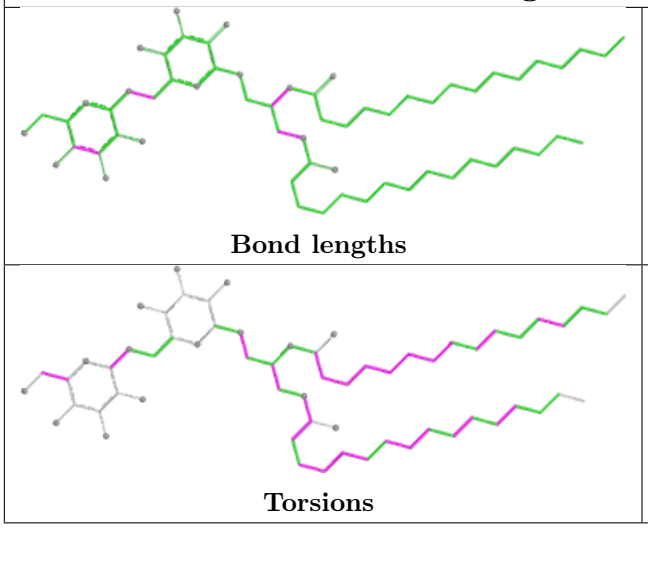


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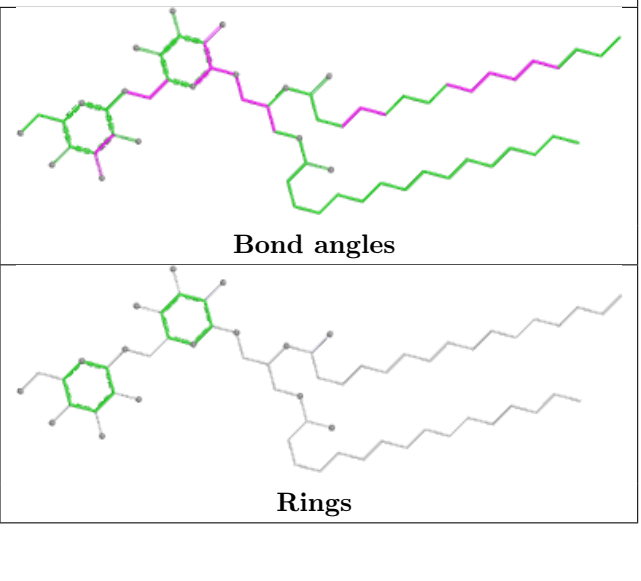


Rings

Ligand DGD C 519



Bond lengths

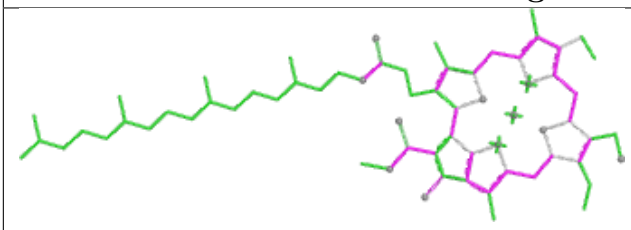


Bond angles

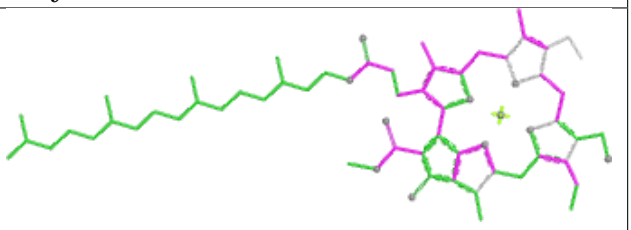
Torsions

Rings

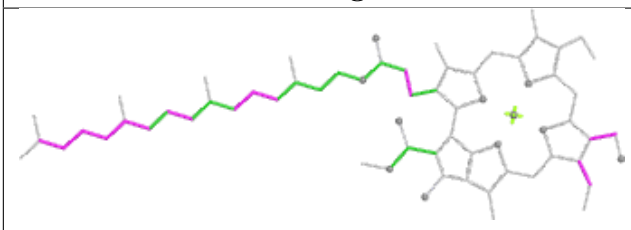
Ligand CHL y 607



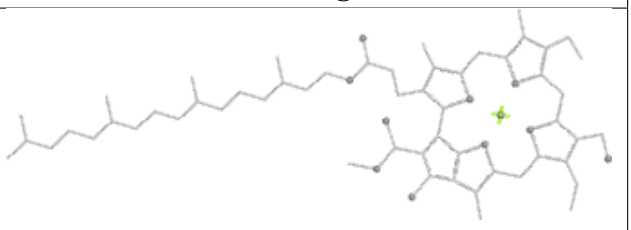
Bond lengths



Bond angles

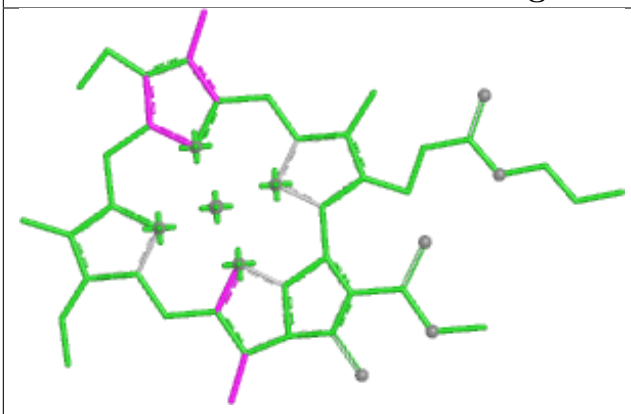


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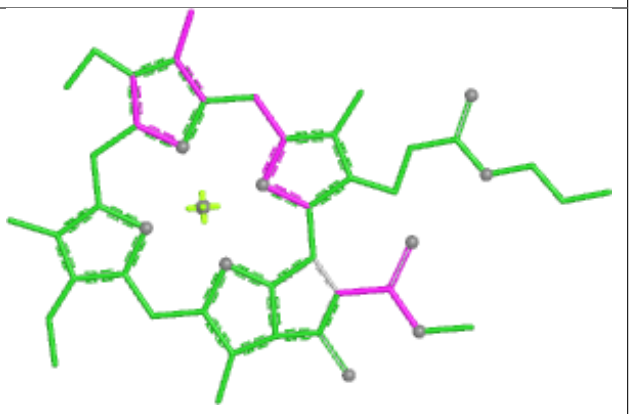


Rings

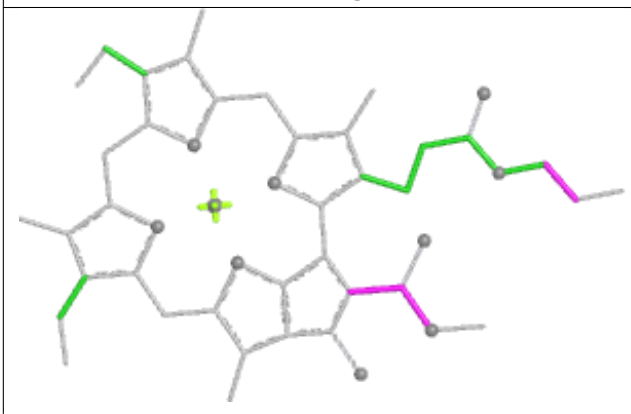
Ligand CLA 3 614



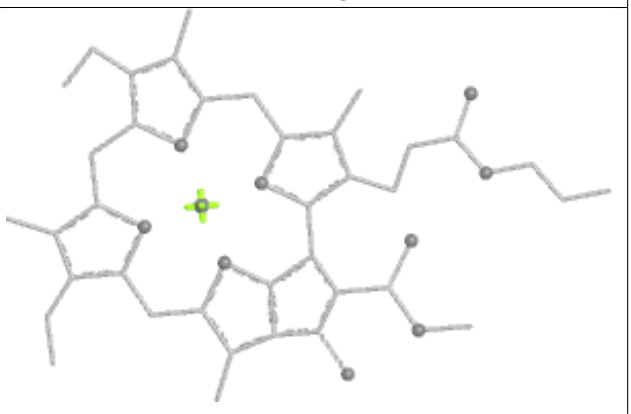
Bond lengths



Bond angles

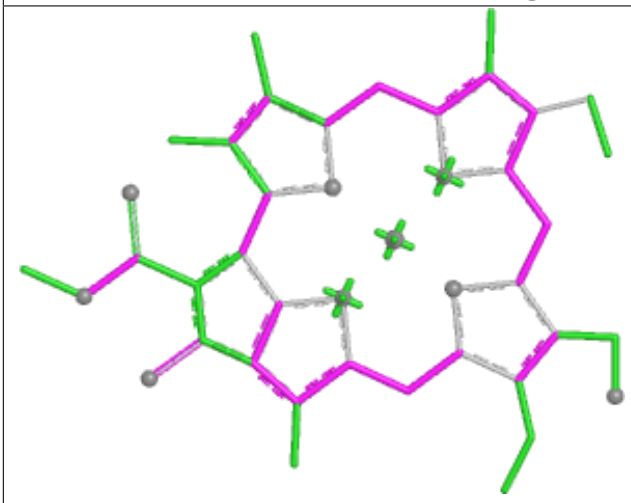


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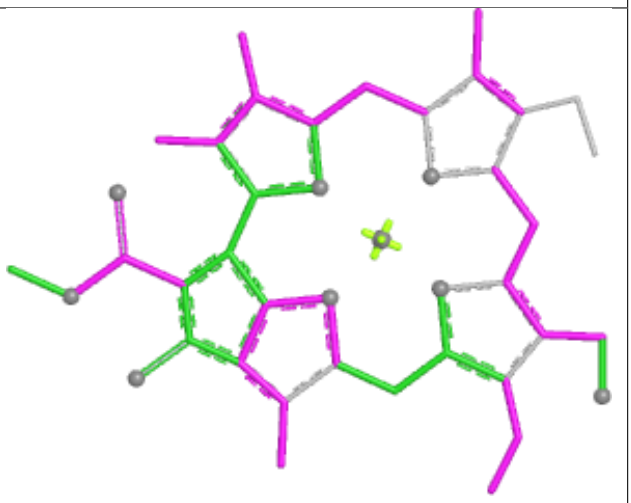


Rings

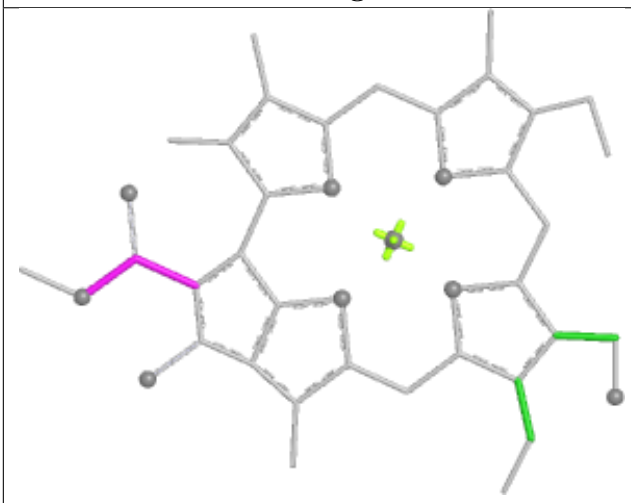
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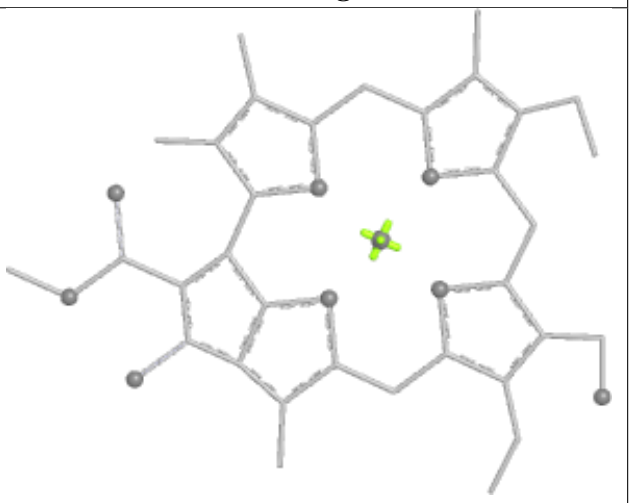
Bond lengths



Bond angles

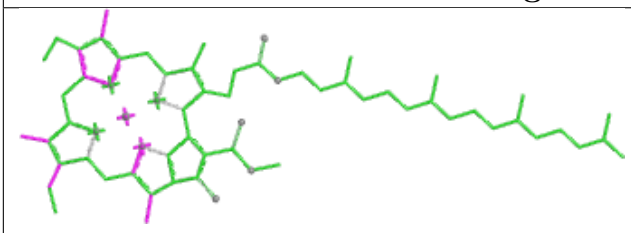


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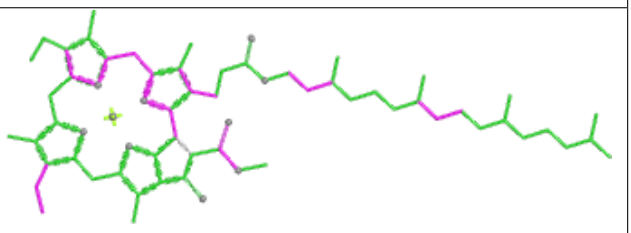


Rings

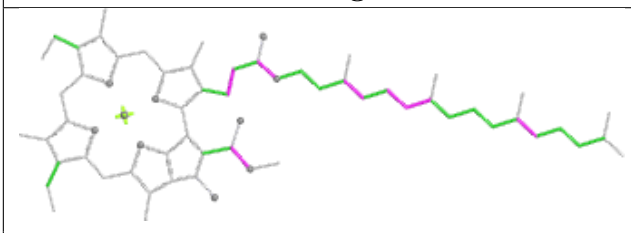
Ligand CLA Y 603



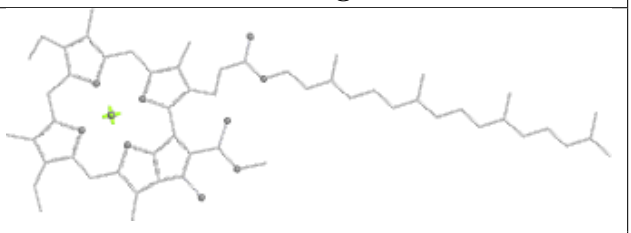
Bond lengths



Bond angles

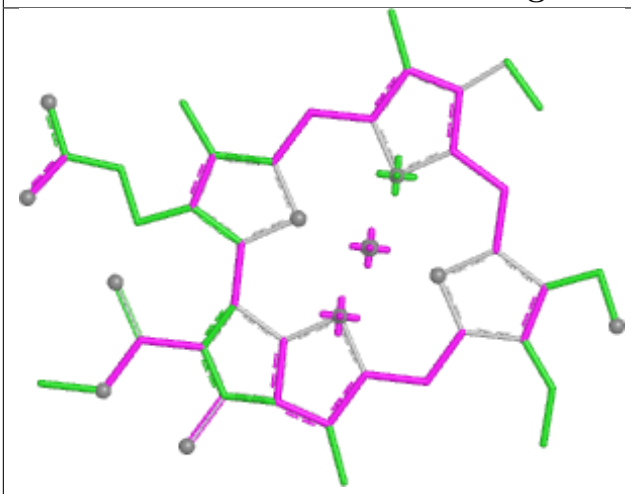


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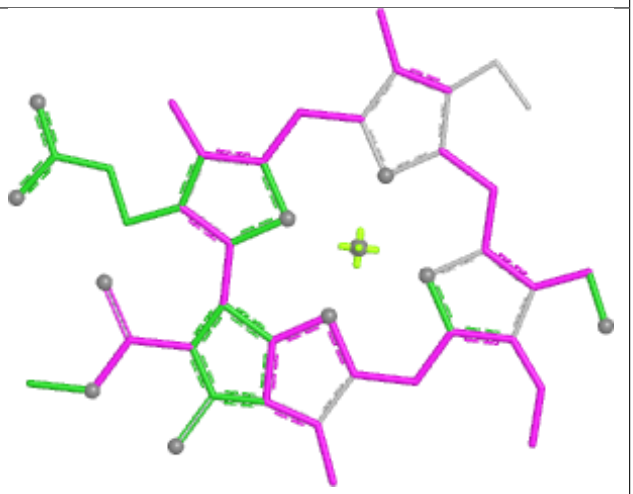


Rings

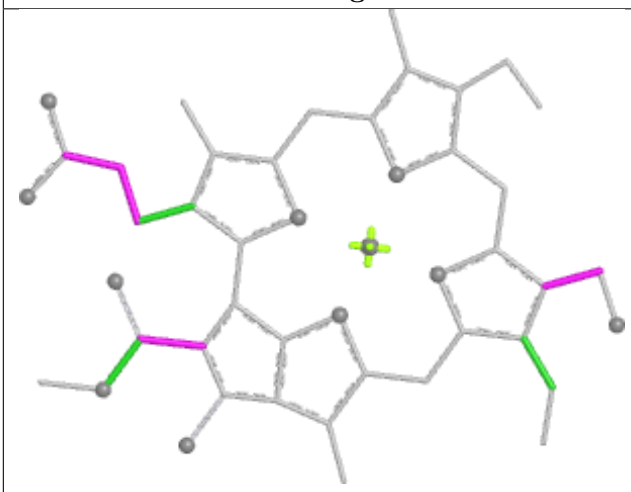
Ligand CHL 1 601



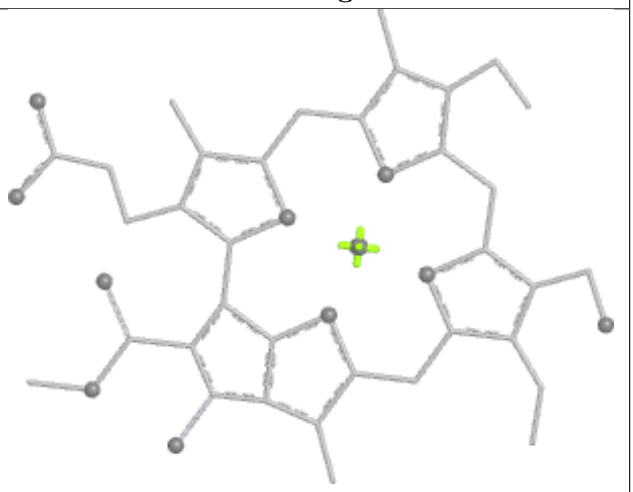
Bond lengths



Bond angles

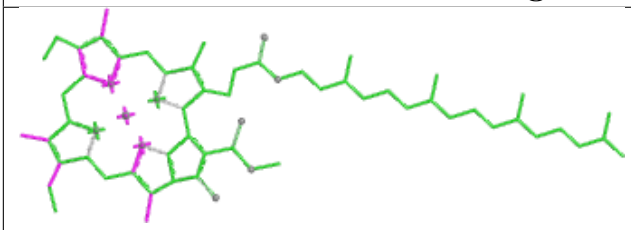


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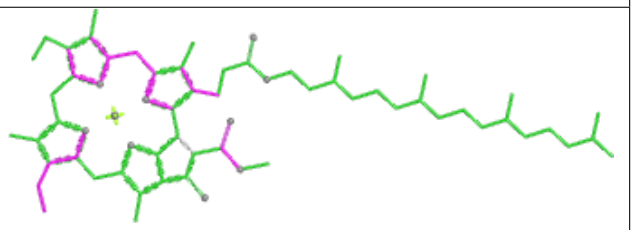


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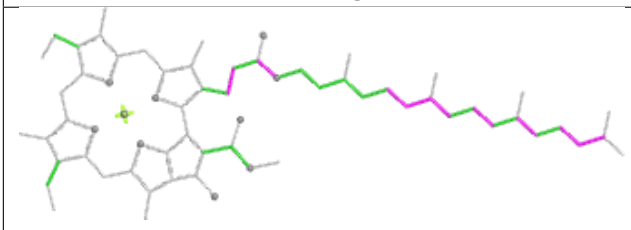
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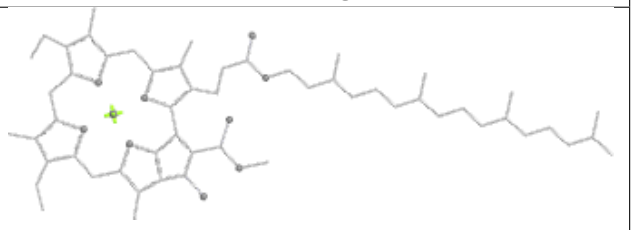
Bond lengths



Bond angles

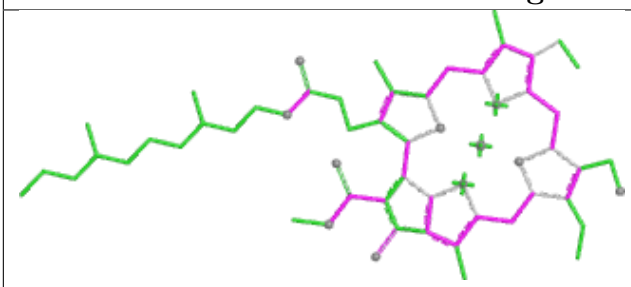


Torsions

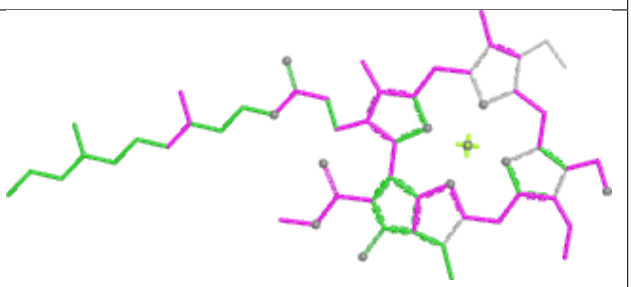


Rings

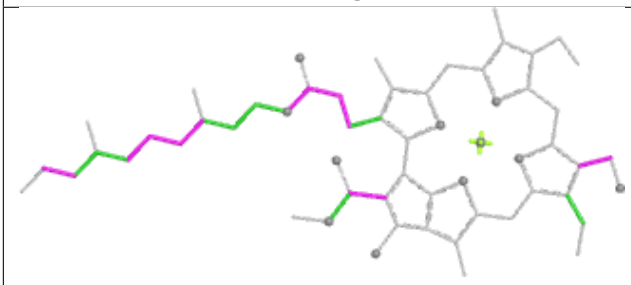
Ligand CHL S 607



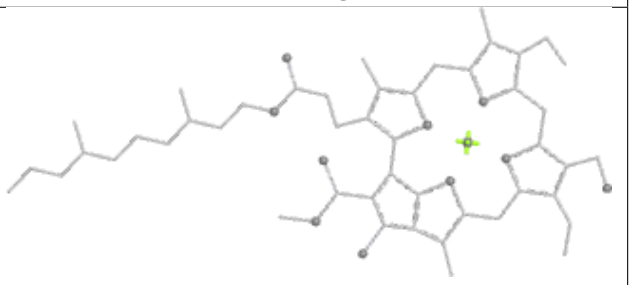
Bond lengths



Bond angles

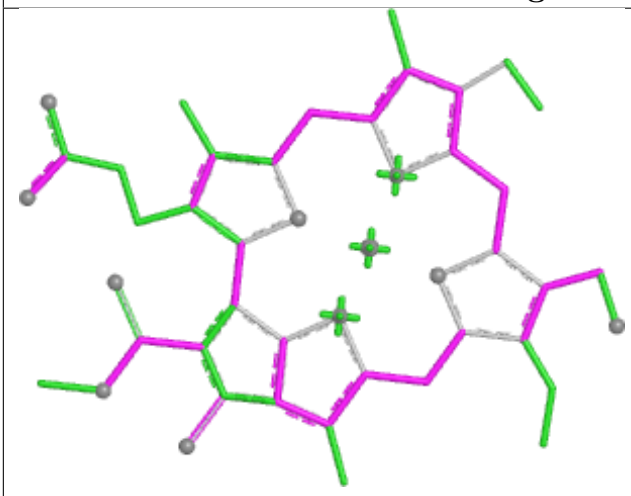


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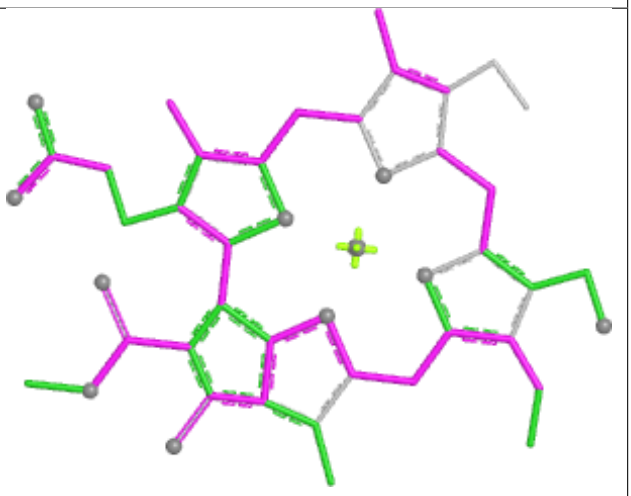


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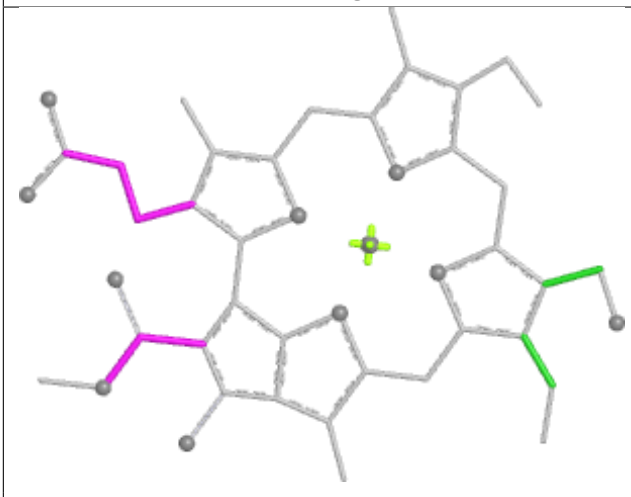
Ligand CHL 3 608



Bond lengths



Bond angles

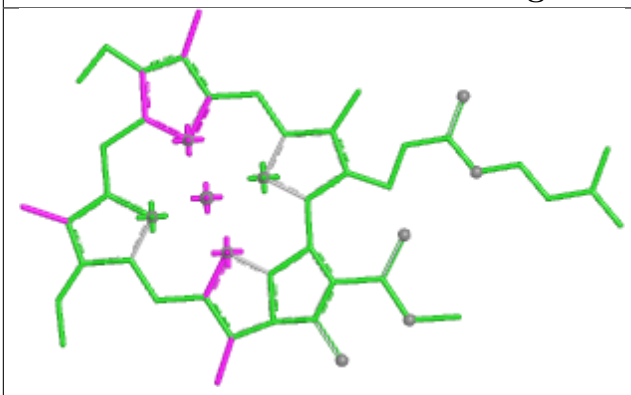


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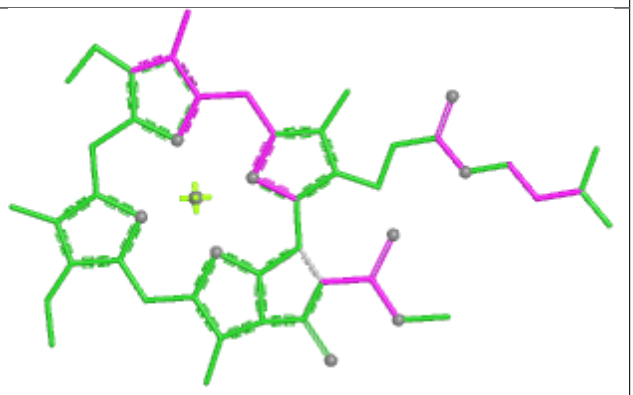


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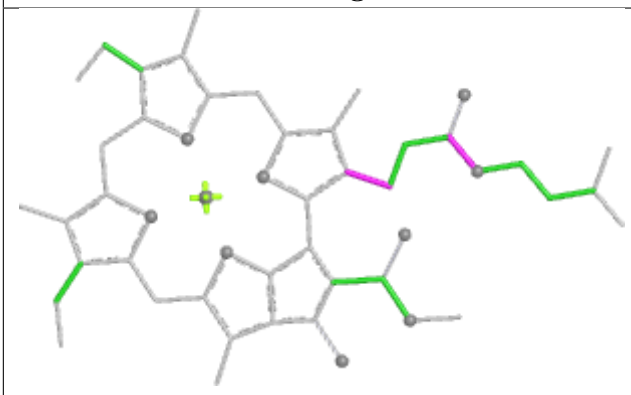
Ligand CLA n 604



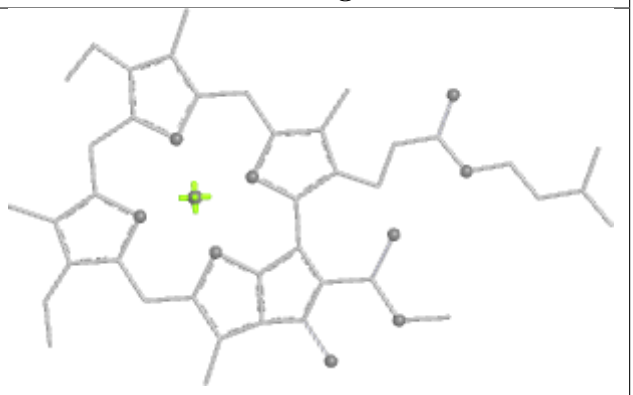
Bond lengths



Bond angles

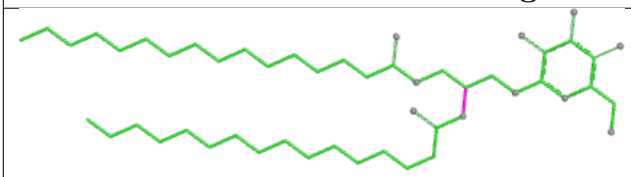


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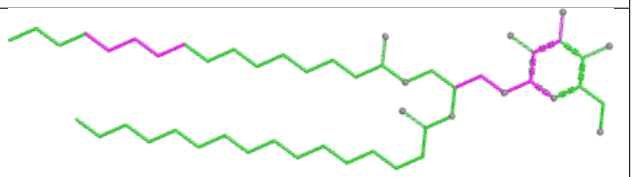


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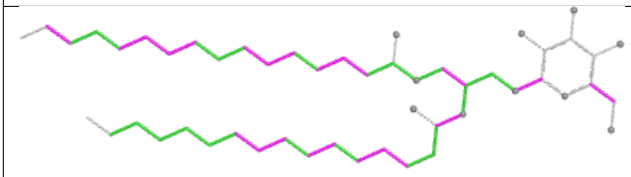
Ligand LMG C 521



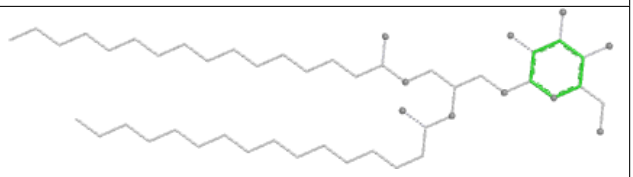
Bond lengths



Bond angles

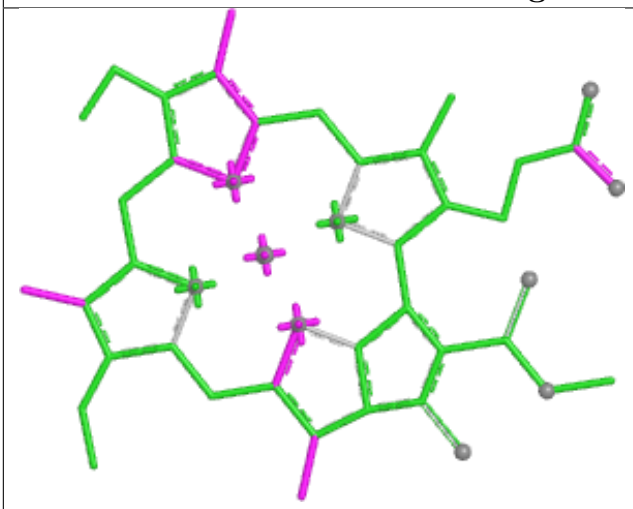


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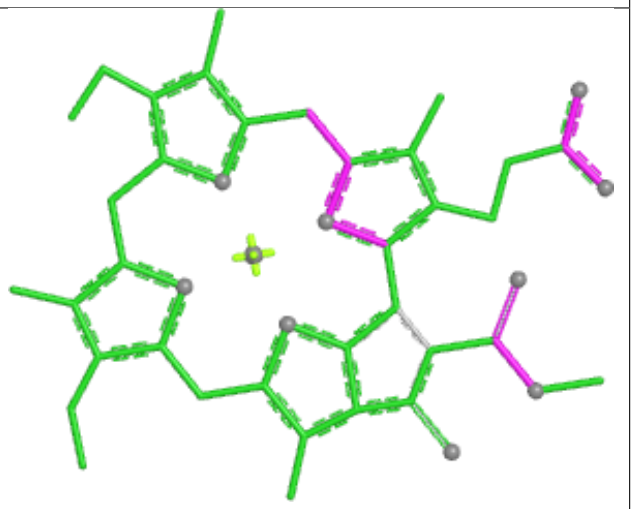


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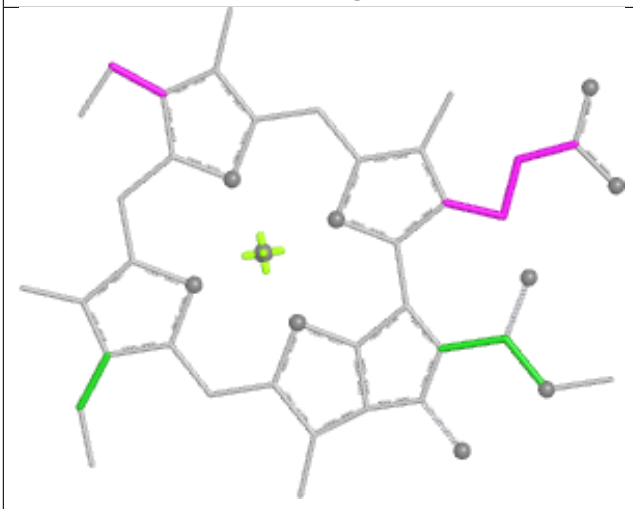
Ligand CLA 5 611



Bond lengths



Bond angles

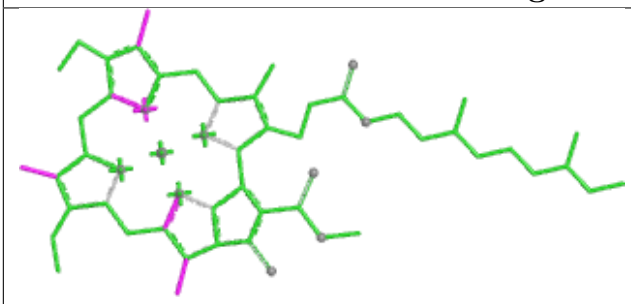


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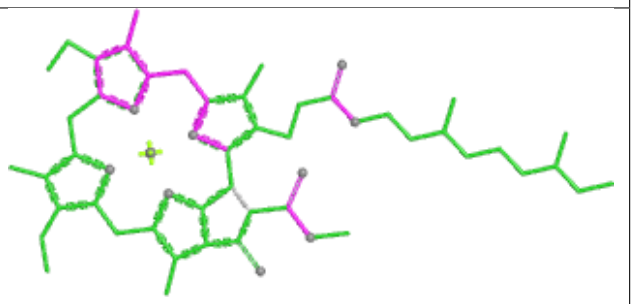


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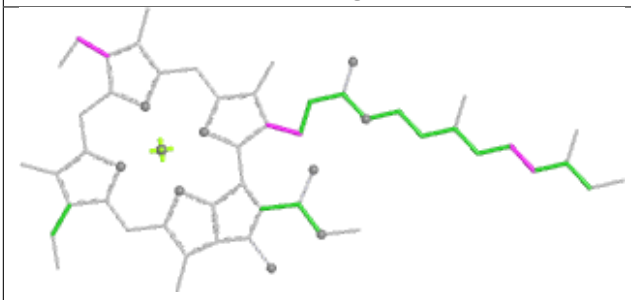
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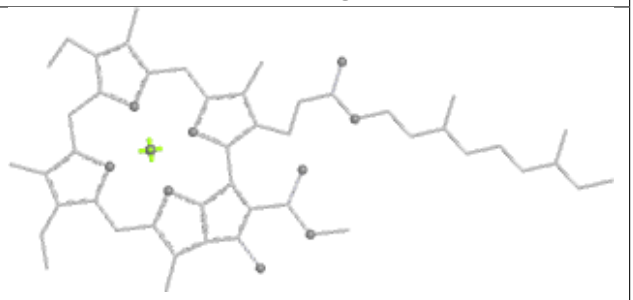
Bond lengths



Bond angles

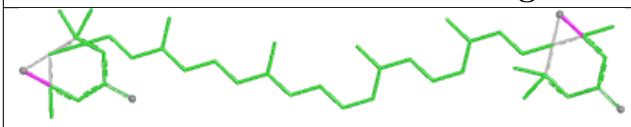


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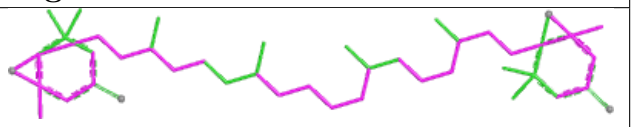


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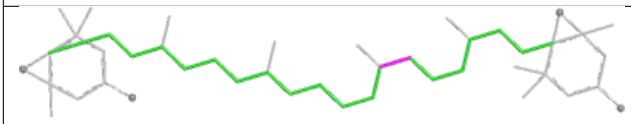
Ligand XAT g 1622



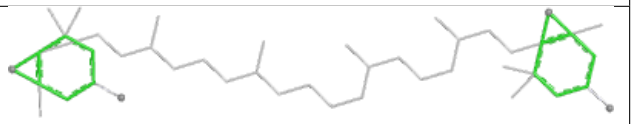
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Bond angles

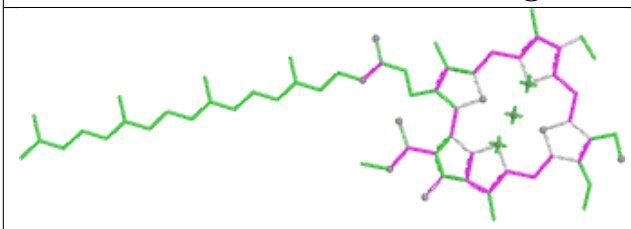


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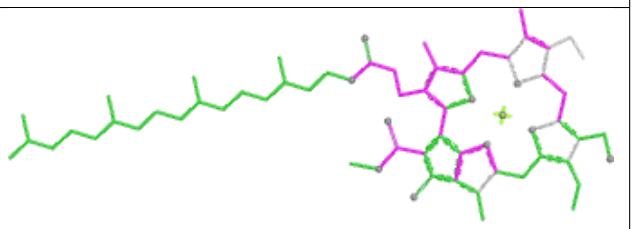


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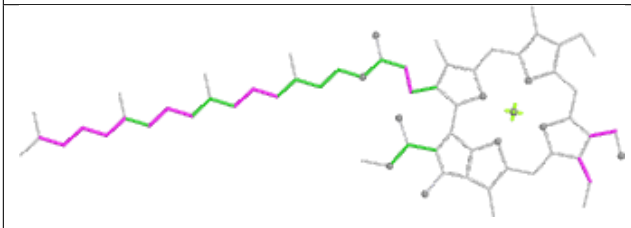
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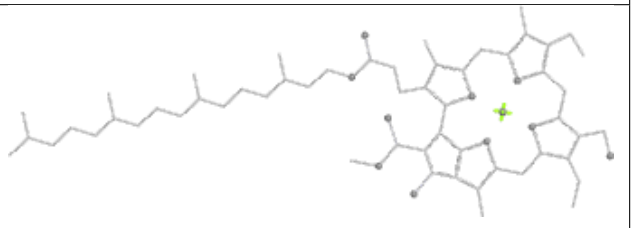
Bond lengths



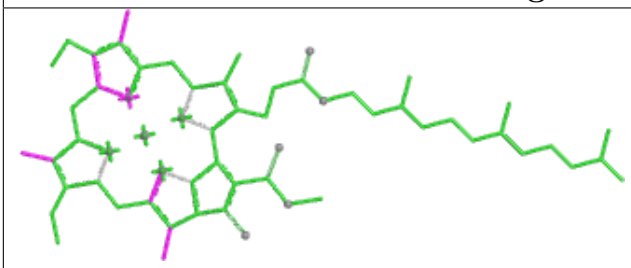
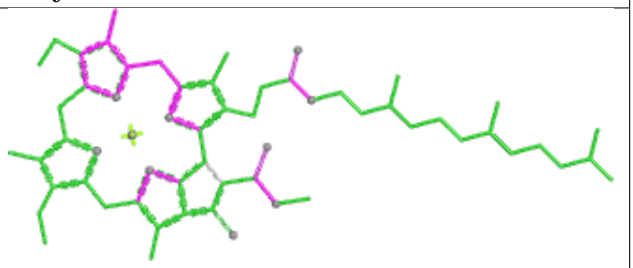
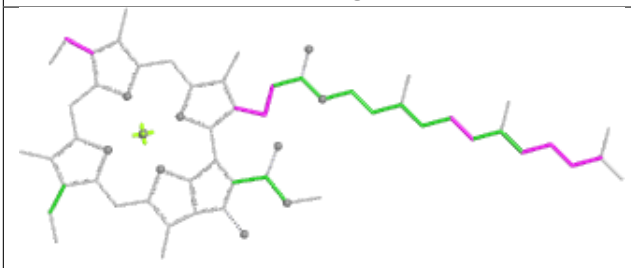
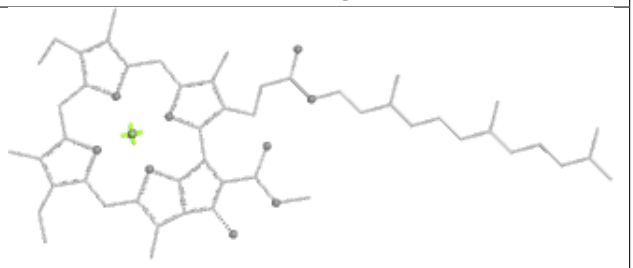
Bond angles

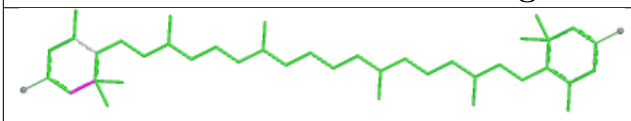
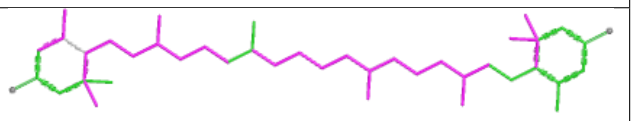
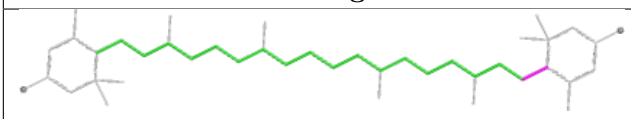
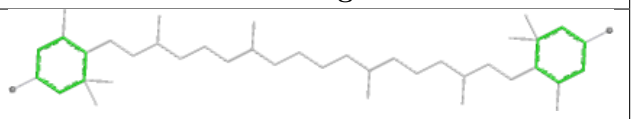


Torsions

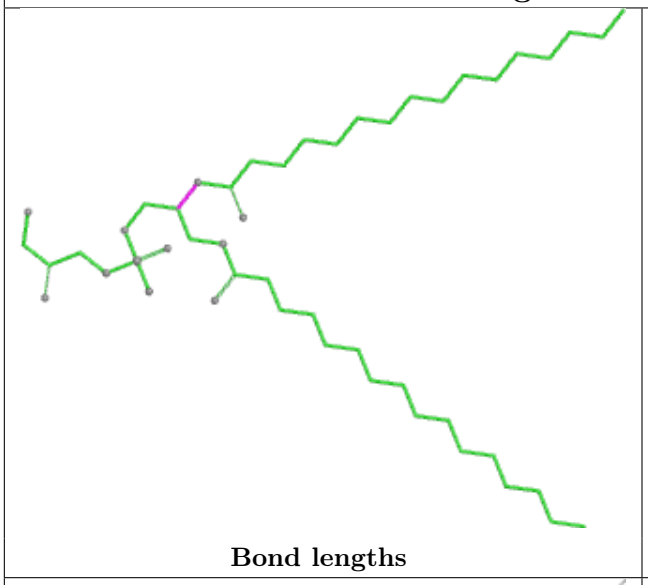


Rings

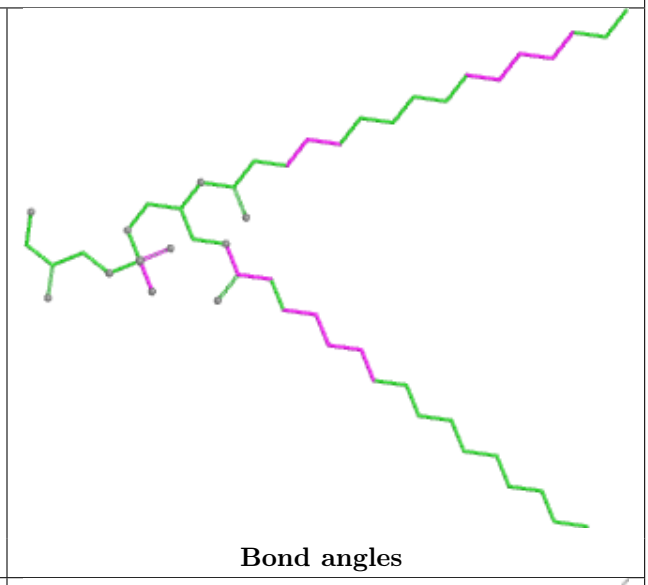
Ligand CLA y 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT n 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

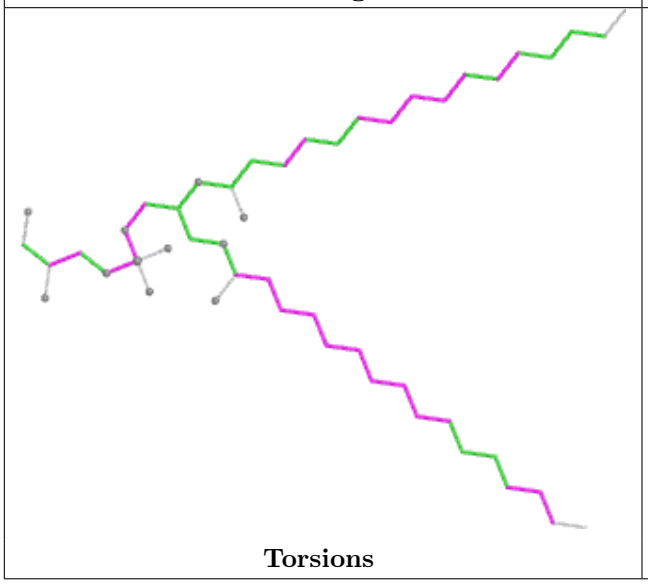
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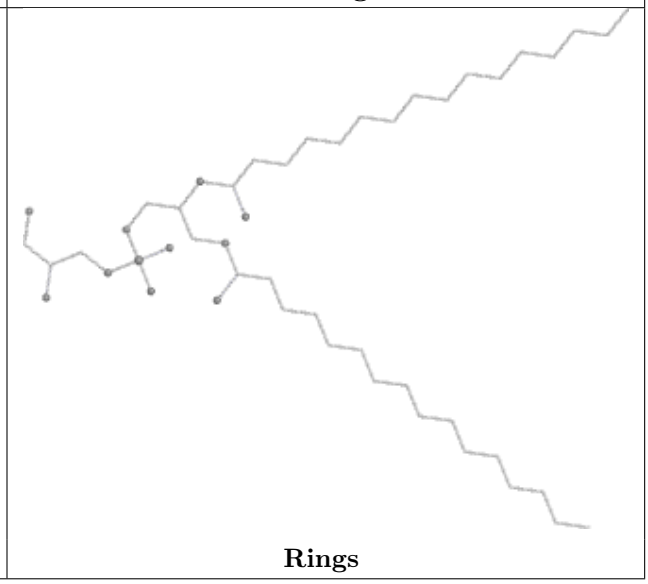
Bond lengths



Bond angles

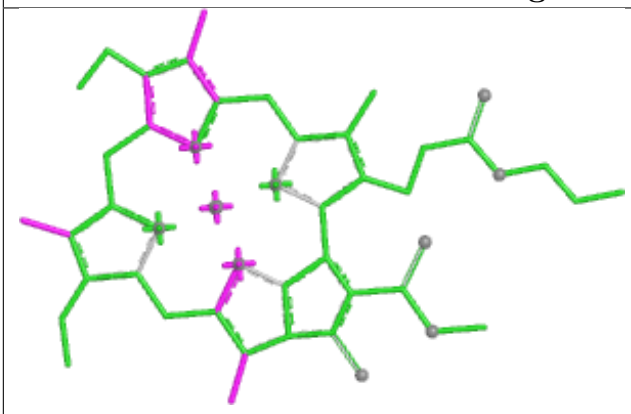


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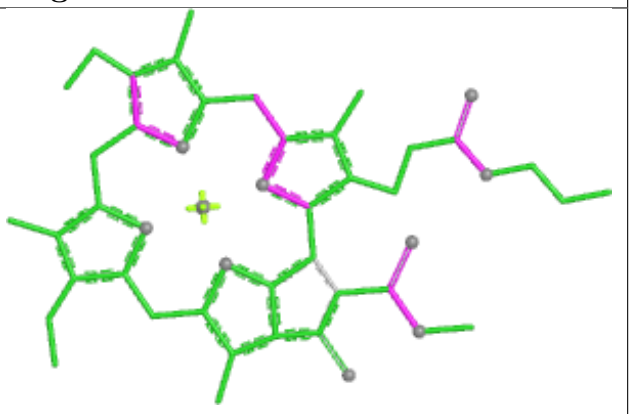


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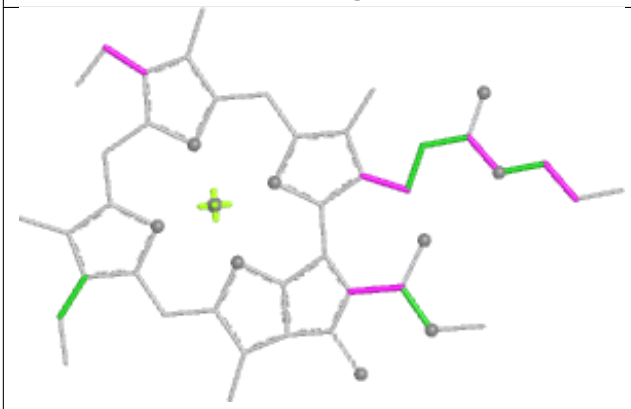
Ligand CLA g 614



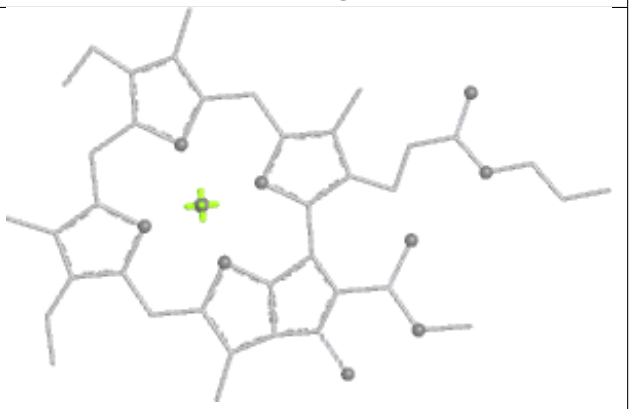
Bond lengths



Bond angles

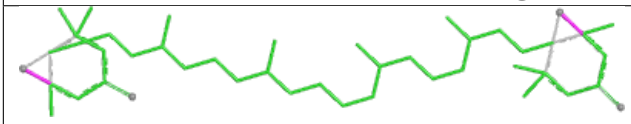


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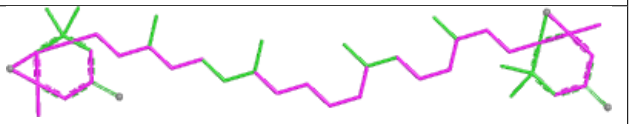


Rings

Ligand XAT G 1622



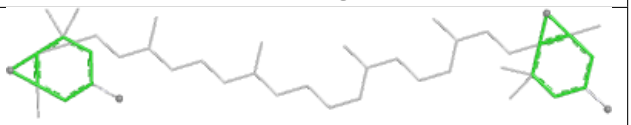
Bond lengths



Bond angles

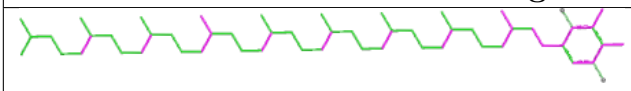


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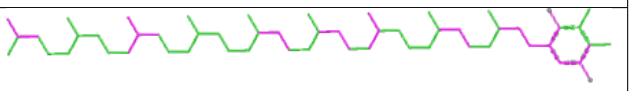


Rings

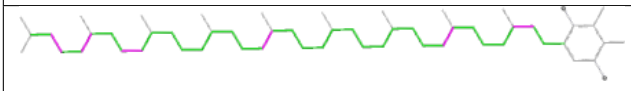
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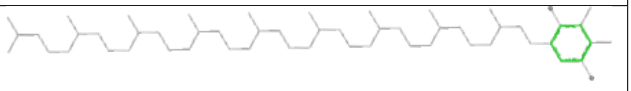
Bond lengths



Bond angles

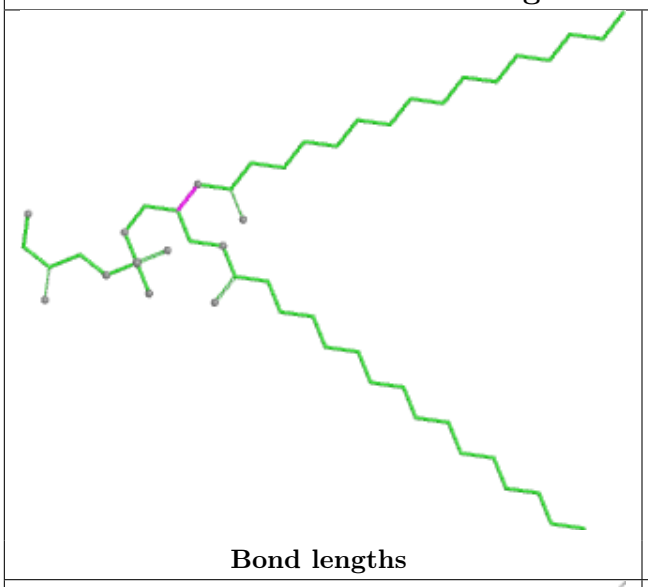


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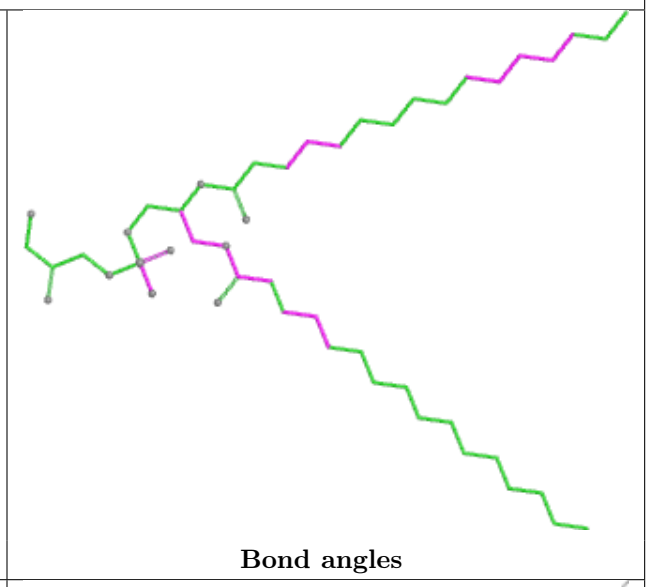


Rings

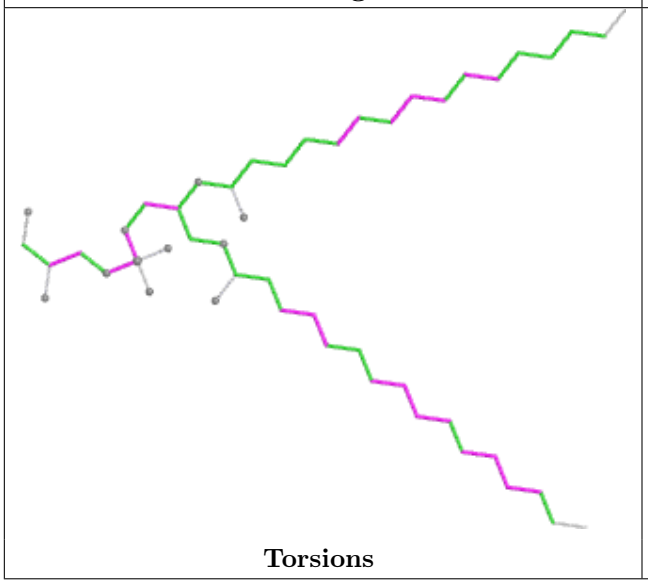
Ligand LHG D 409



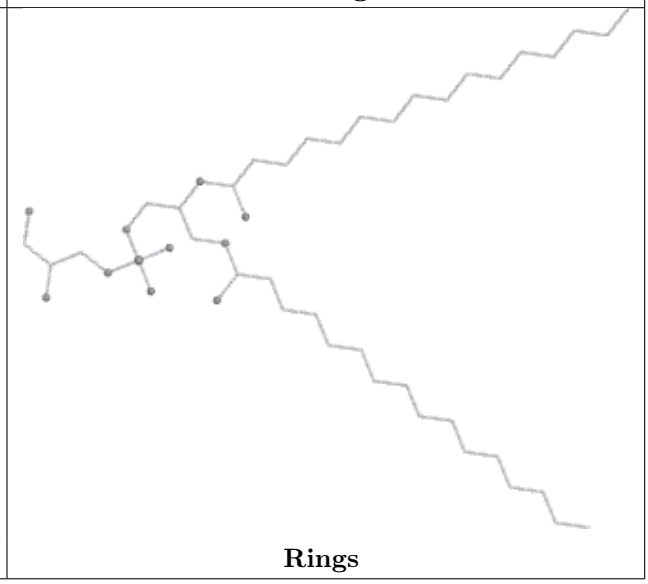
Bond lengths



Bond angles

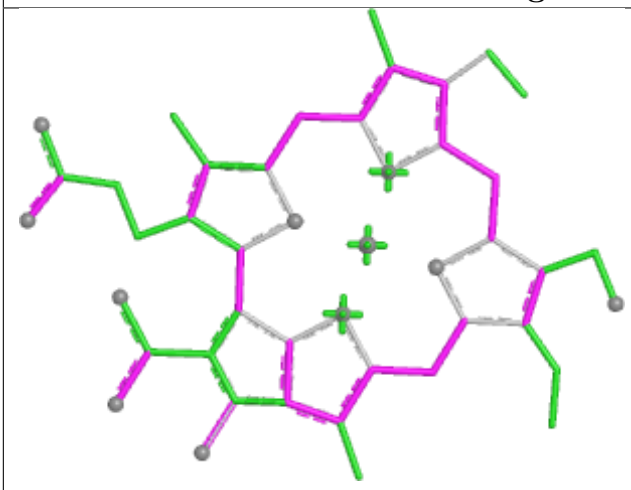


Torsions

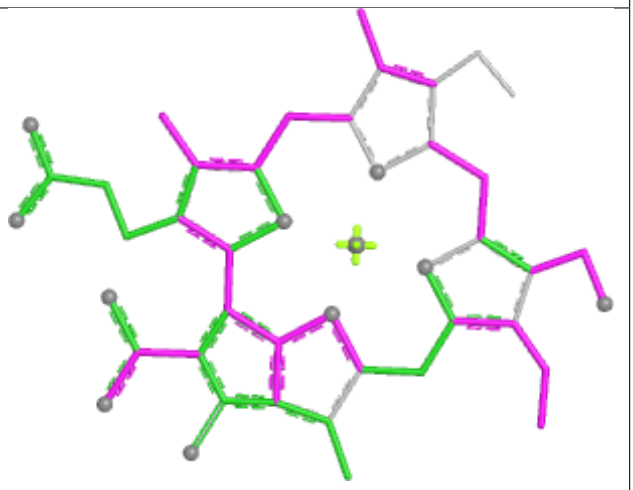


Rings

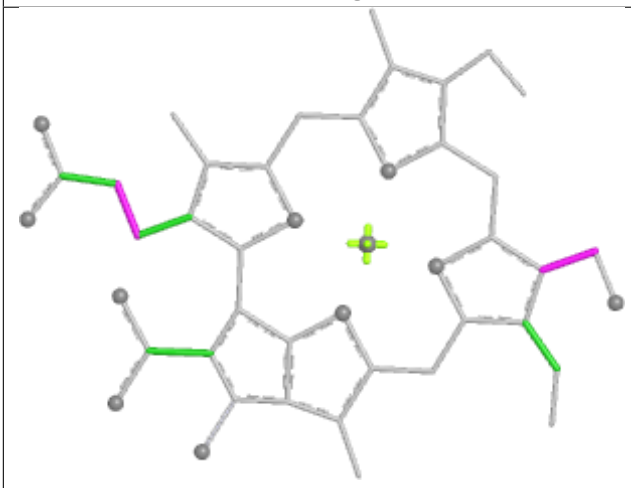
Ligand CHL 4 601



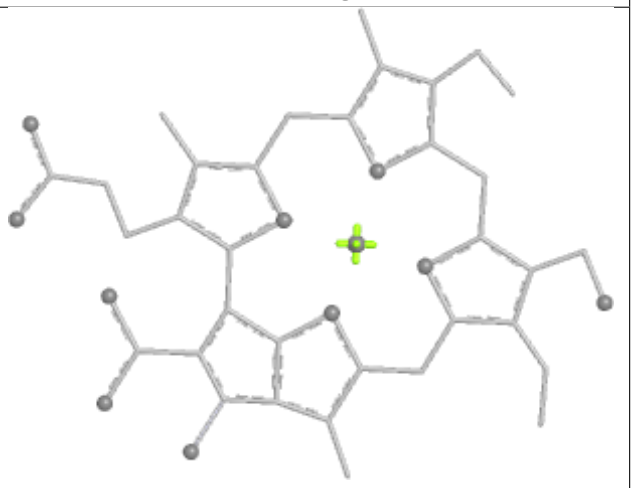
Bond lengths



Bond angles

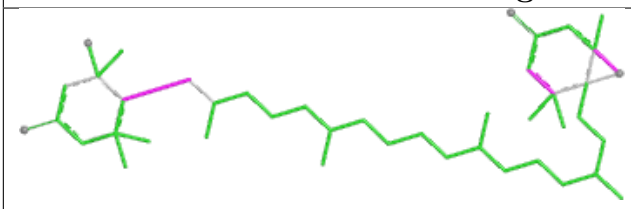


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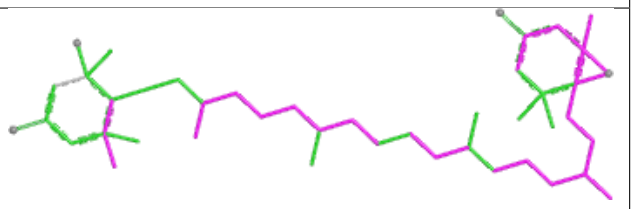


Rings

Ligand NEX n 1623



Bond lengths



Bond angles

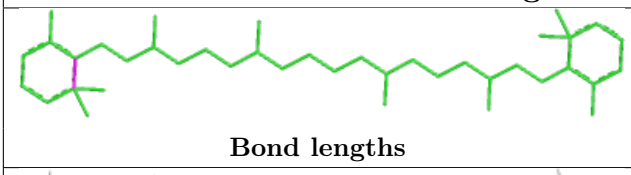


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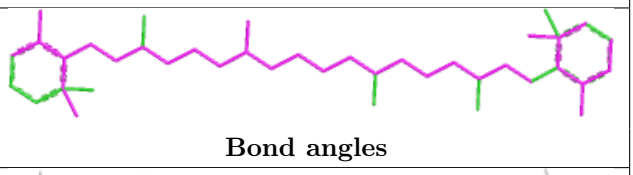


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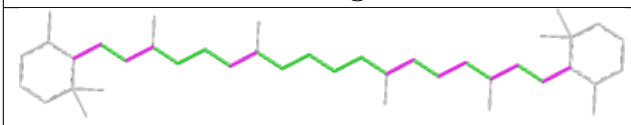
Ligand BCR T 101



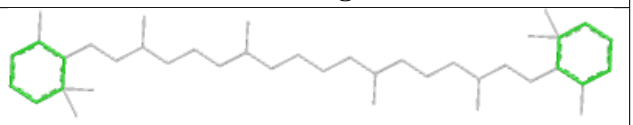
Bond lengths



Bond angles

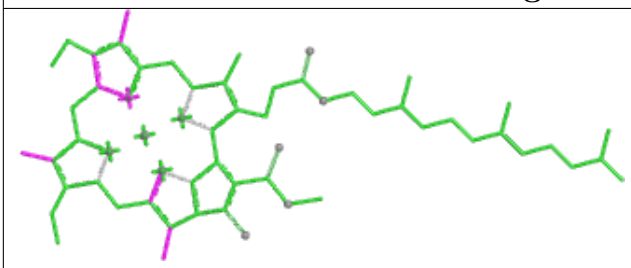


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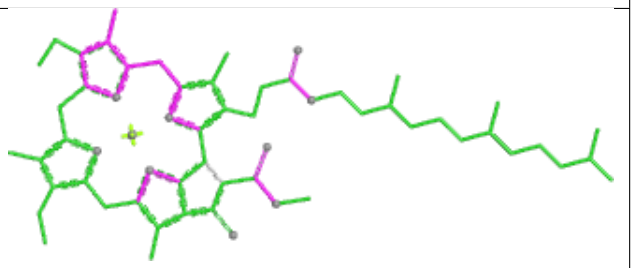


Rings

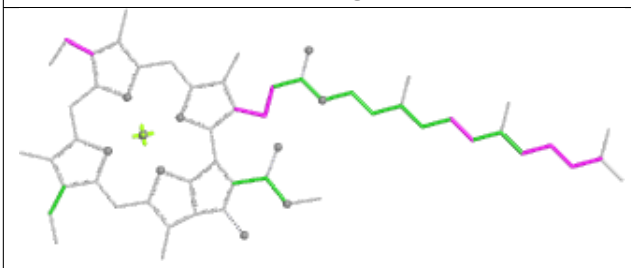
Ligand CLA Y 610



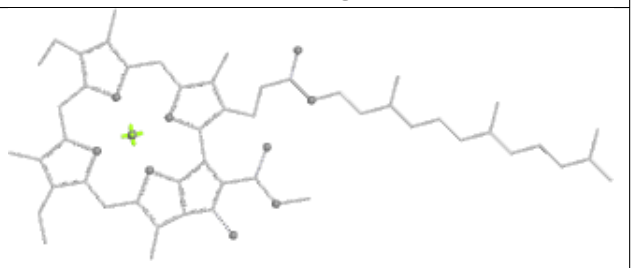
Bond lengths



Bond angles

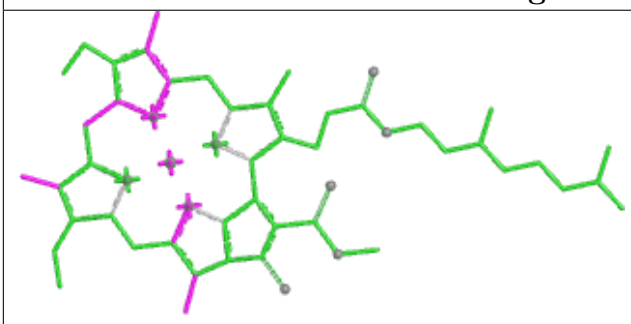


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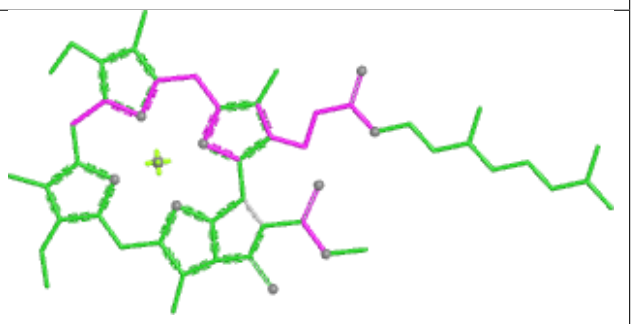


Rings

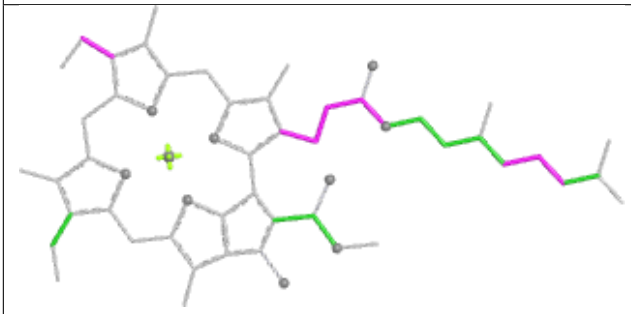
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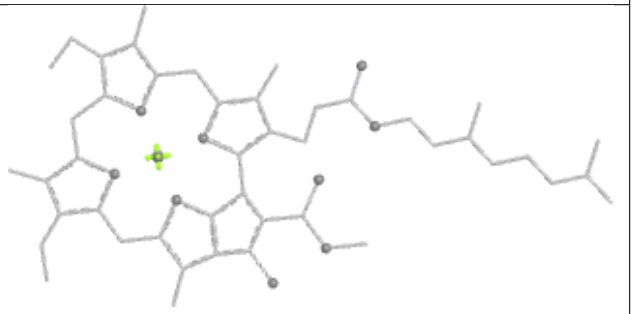
Bond lengths



Bond angles

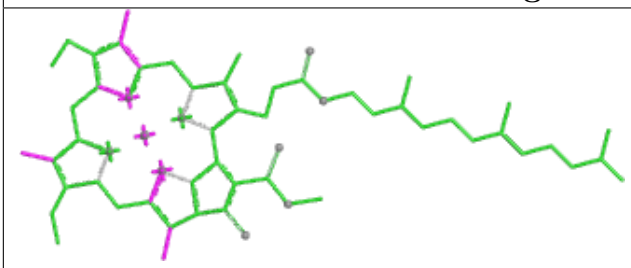


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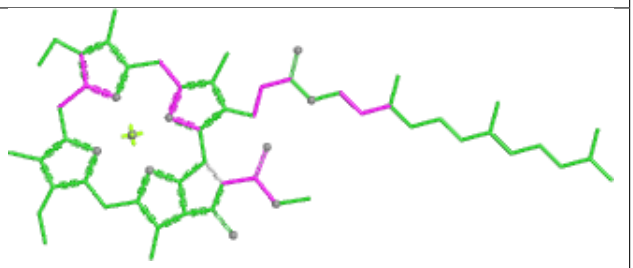


Rings

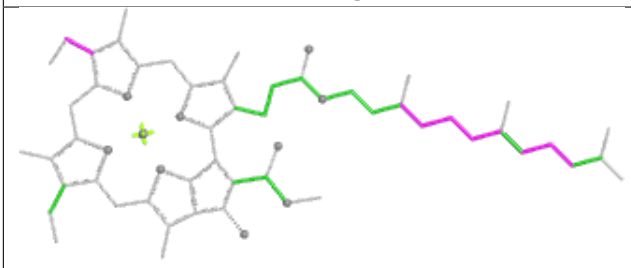
Ligand CLA A 410



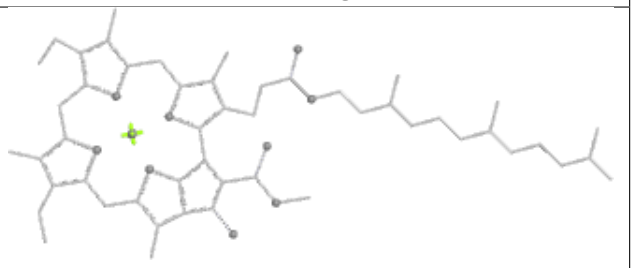
Bond lengths



Bond angles

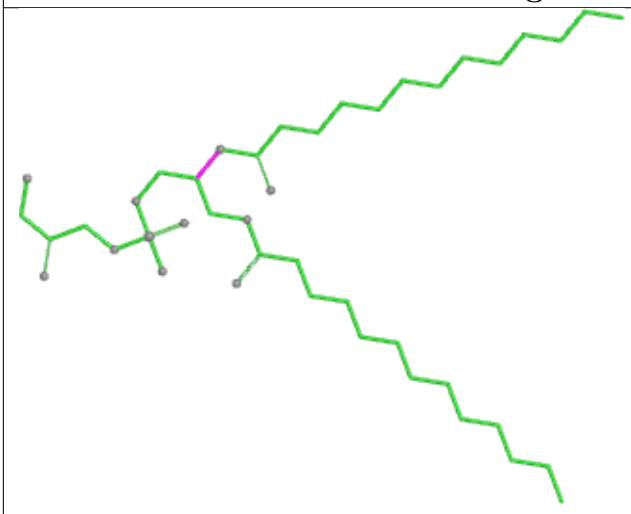


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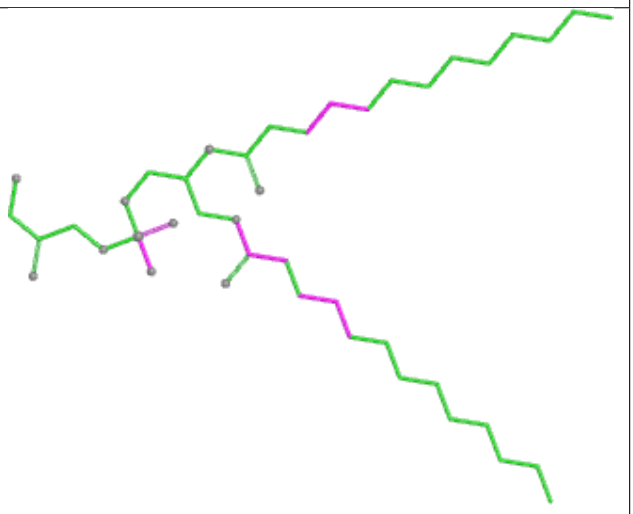


Rings

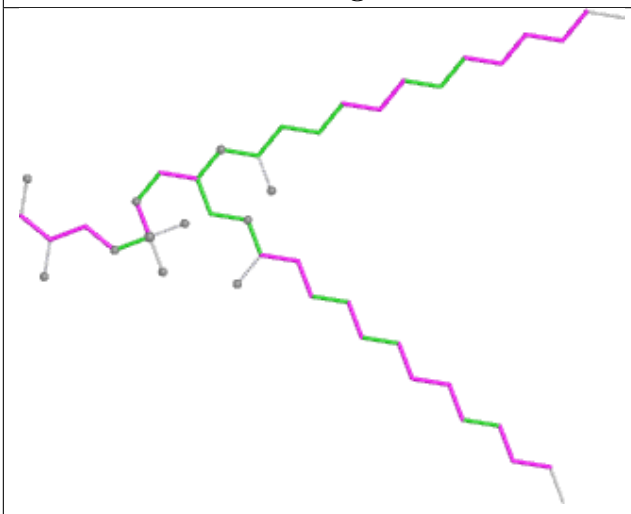
Ligand LHG d 410



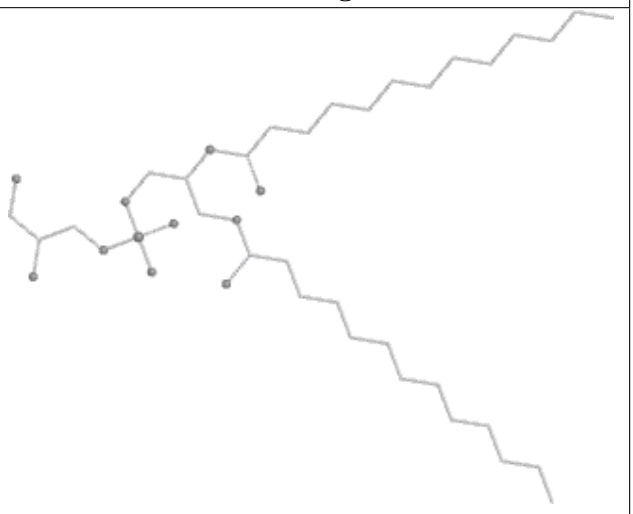
Bond lengths



Bond angles

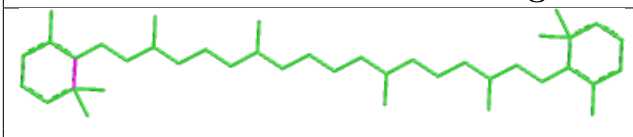


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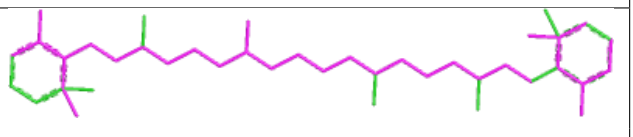


Rings

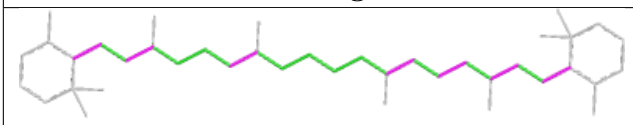
Ligand BCR t 101



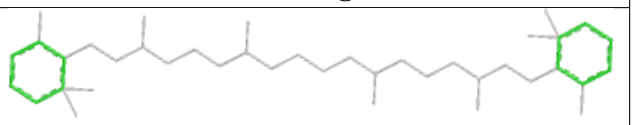
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Bond angles

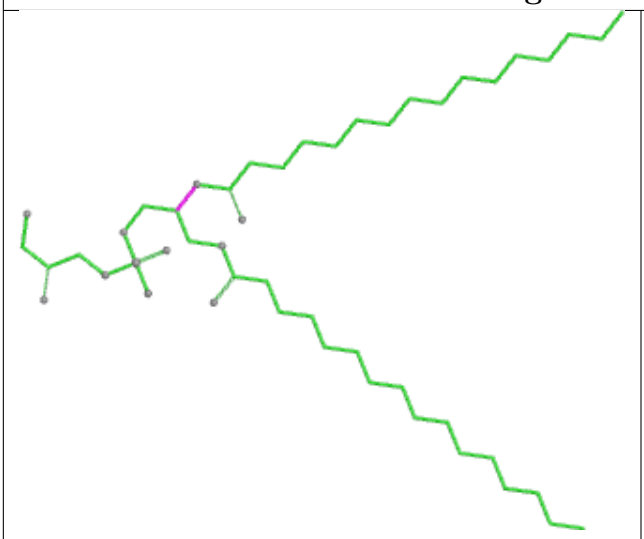


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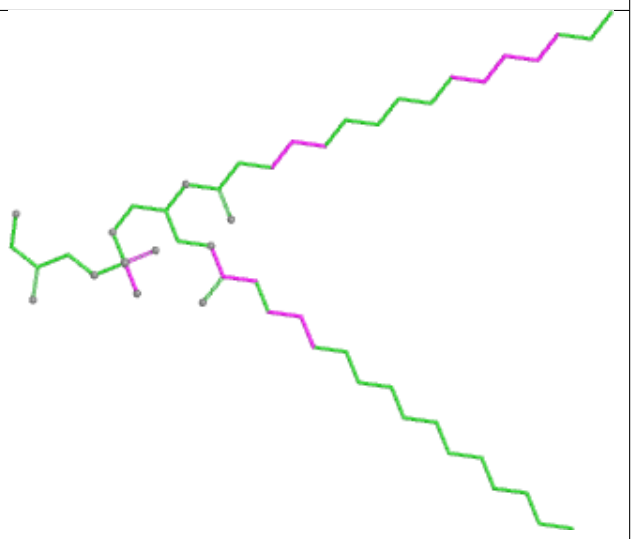


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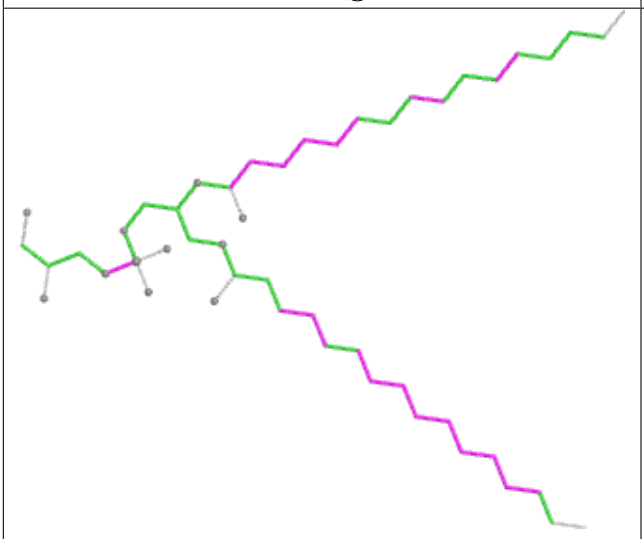
Ligand LHG L 101



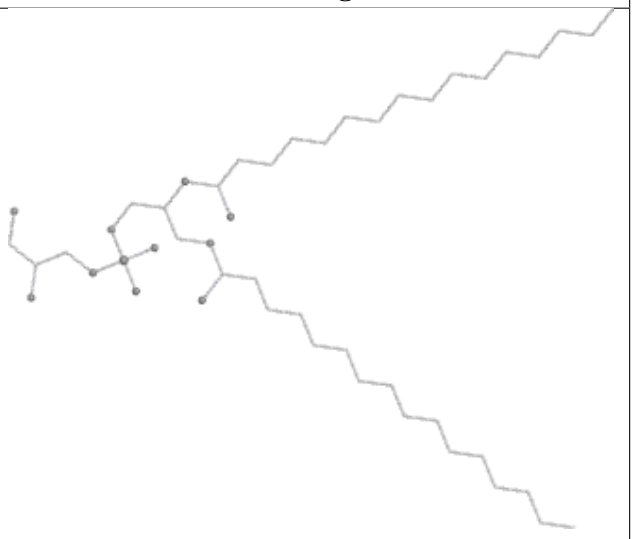
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Bond angles

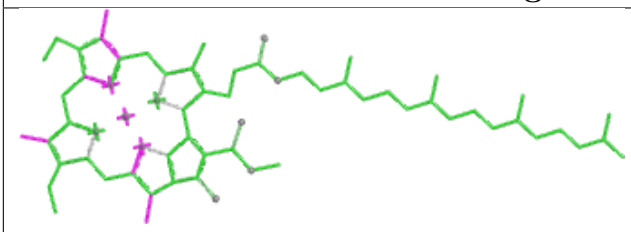


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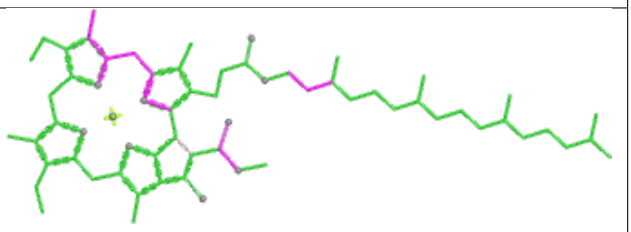


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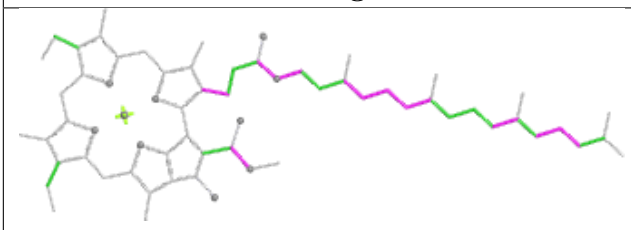
Ligand CLA C 506



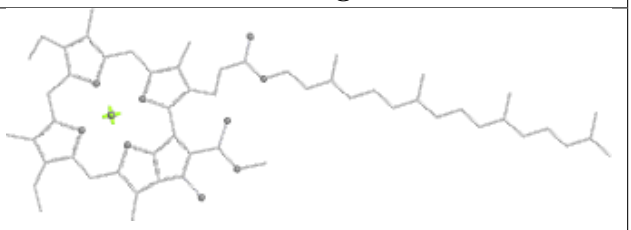
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Bond angles

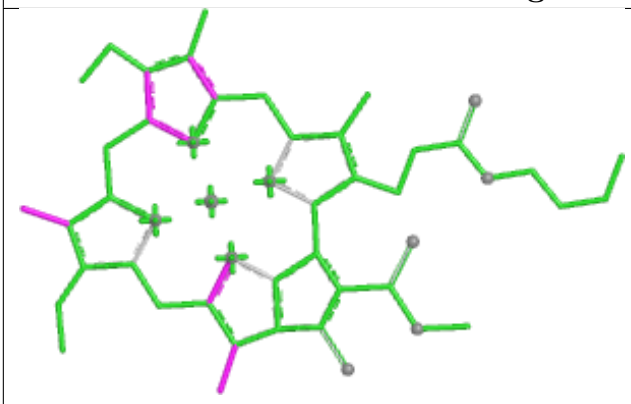


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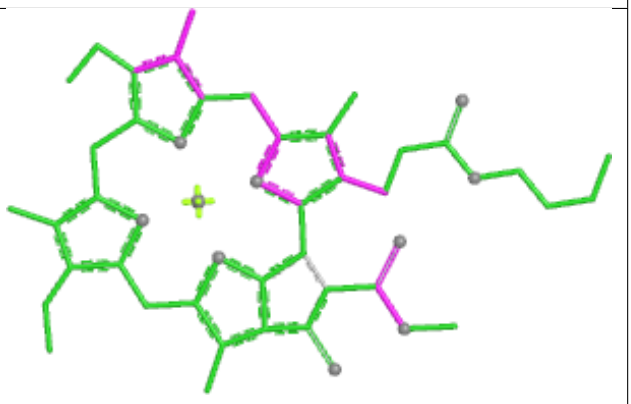


Rings

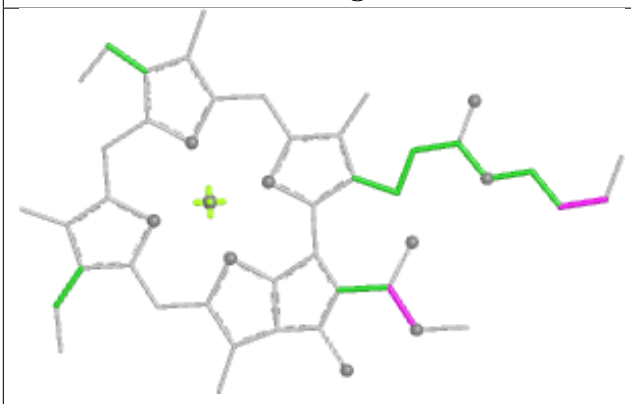
Ligand CLA S 612



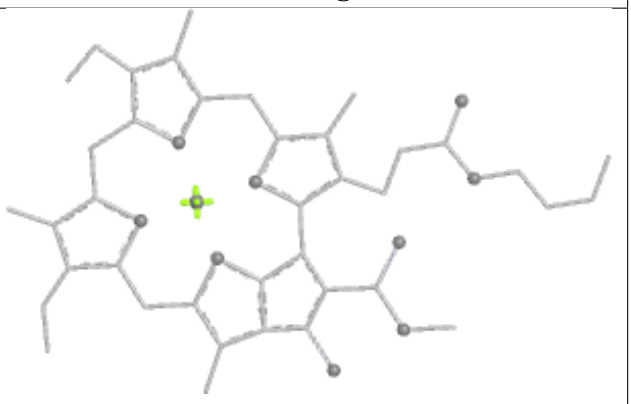
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Bond angles

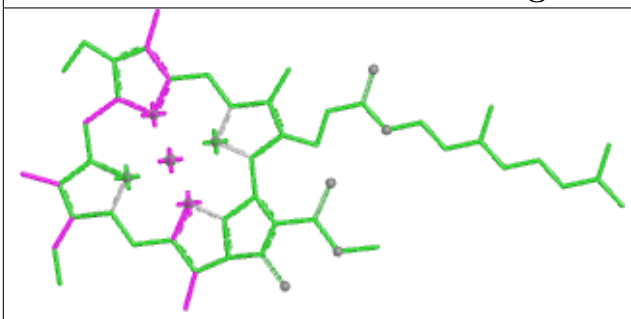


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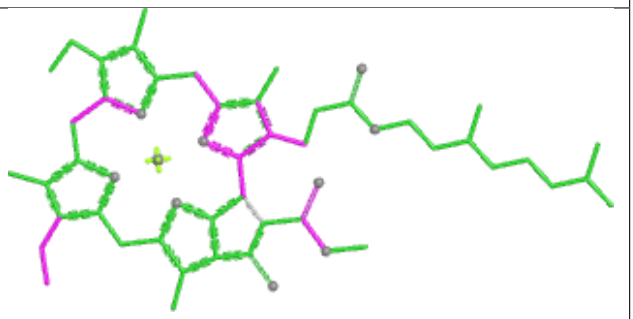


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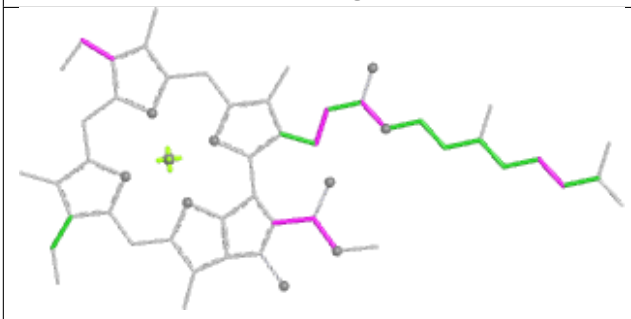
Ligand CLA 3 603



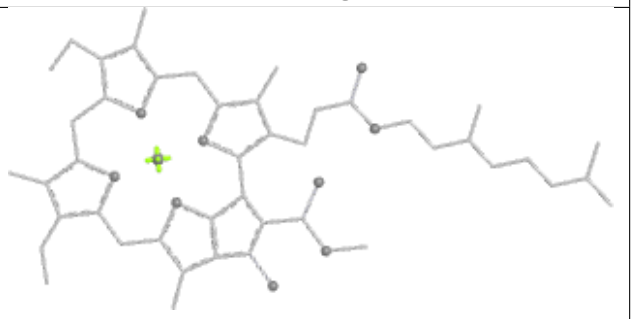
Bond lengths



Bond angles

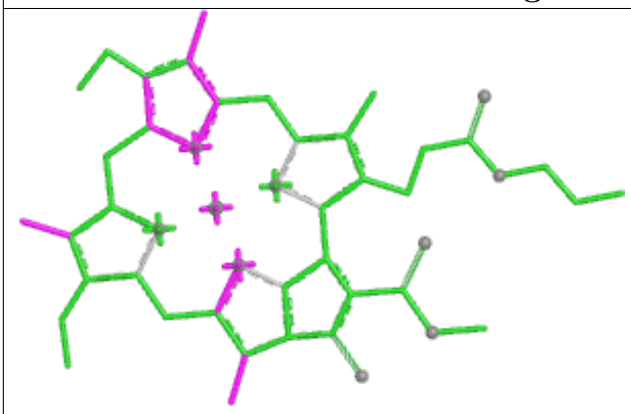


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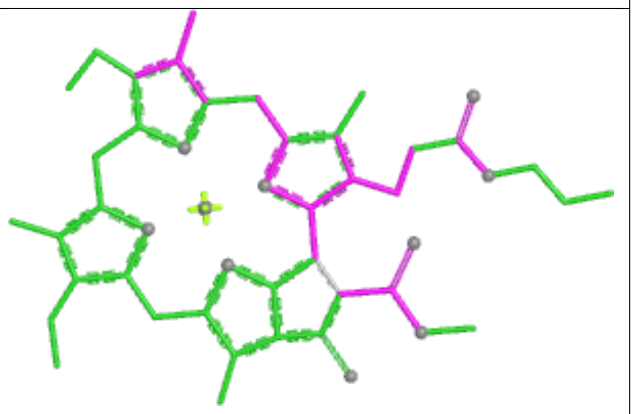


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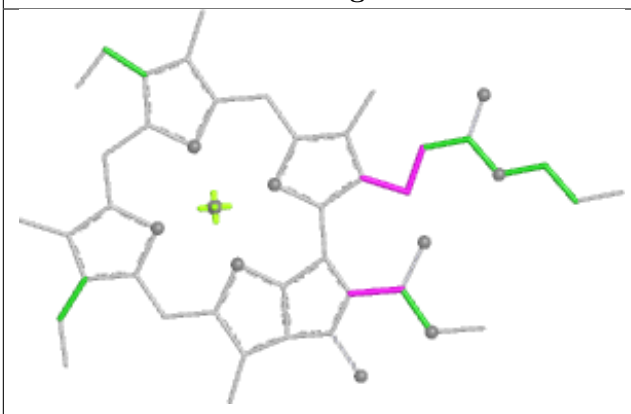
Ligand CLA R 604



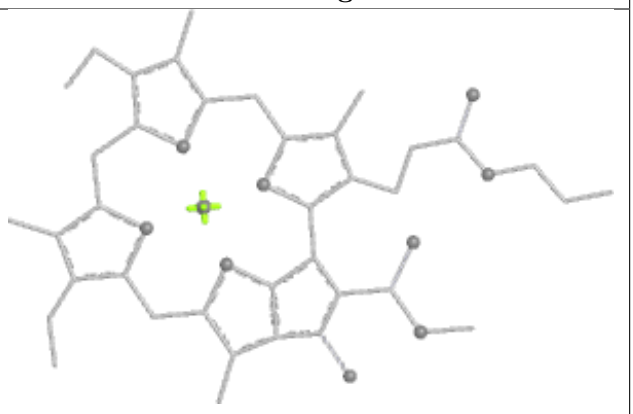
Bond lengths



Bond angles

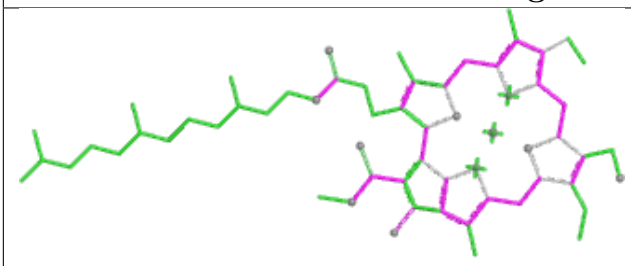


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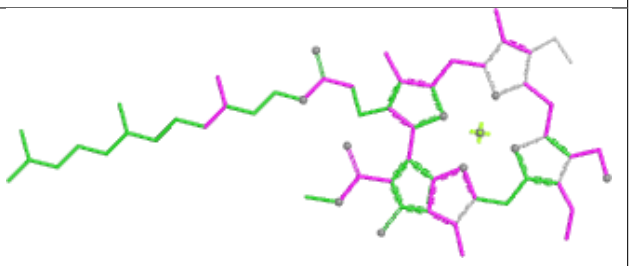


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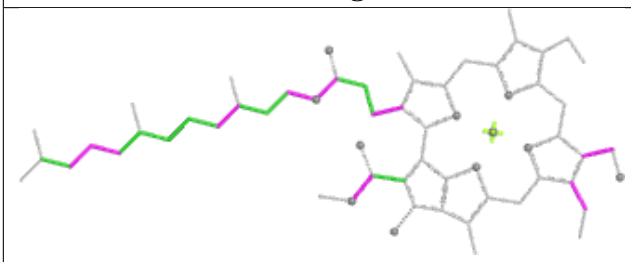
Ligand CHL 7 609



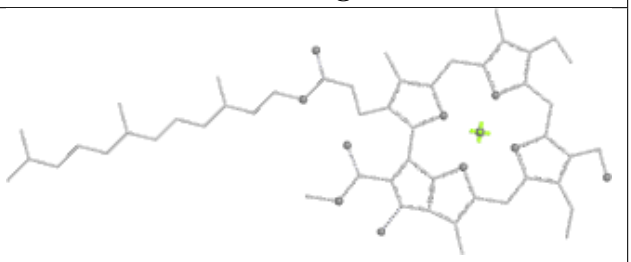
Bond lengths



Bond angles

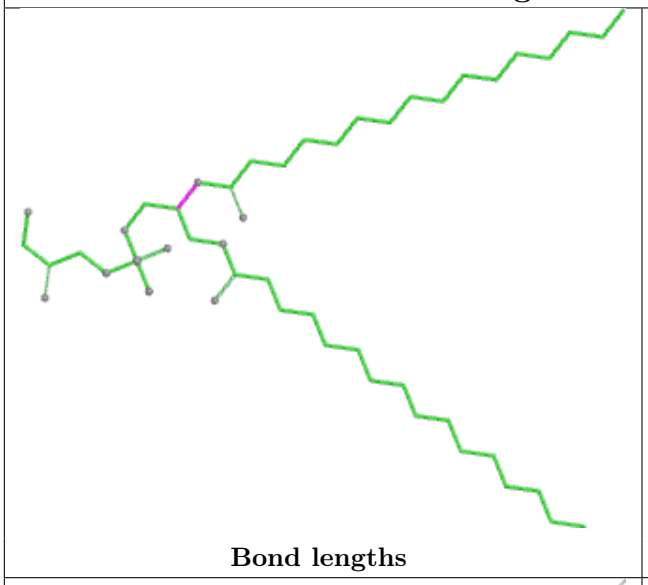


Torsions

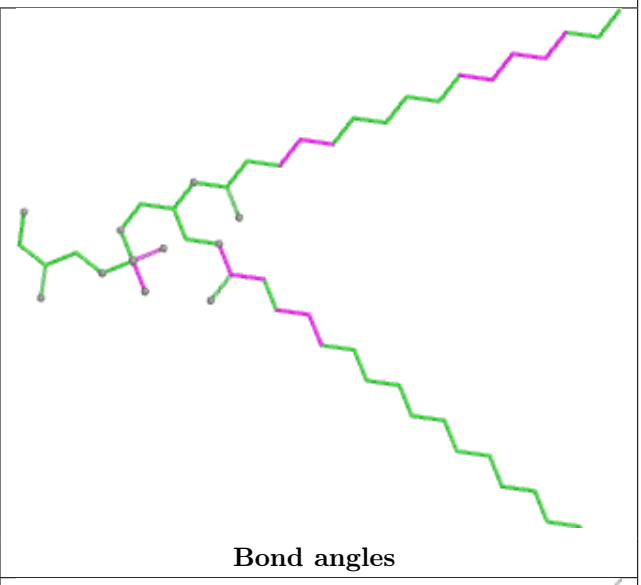


Rings

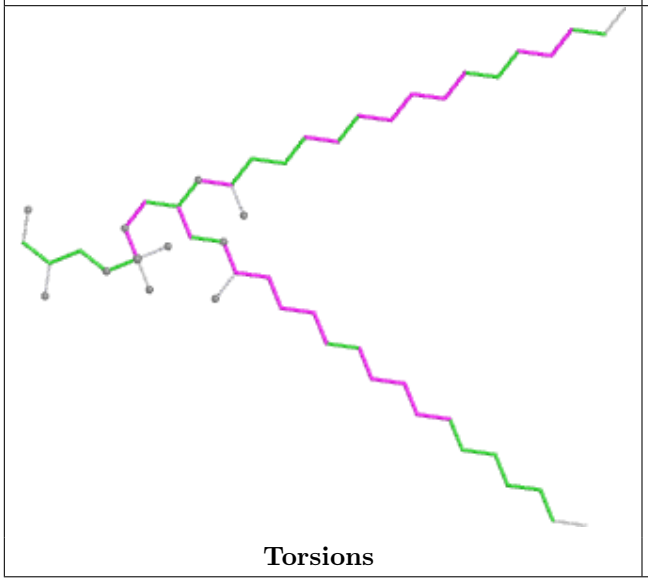
Ligand LHG G 2630



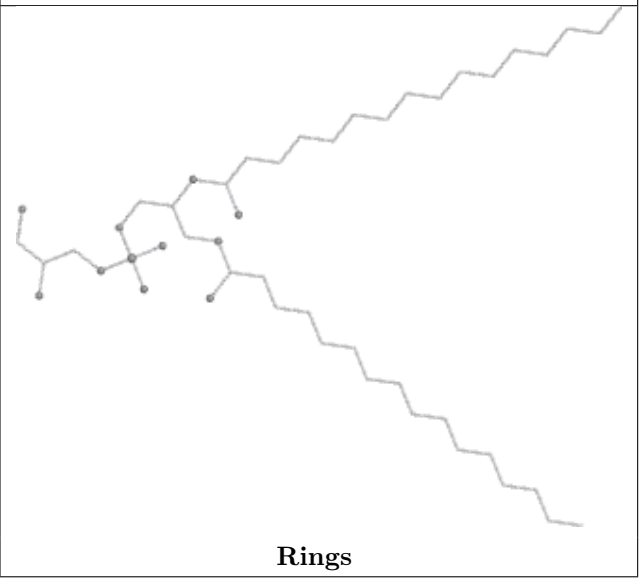
Bond lengths



Bond angles



Torsions

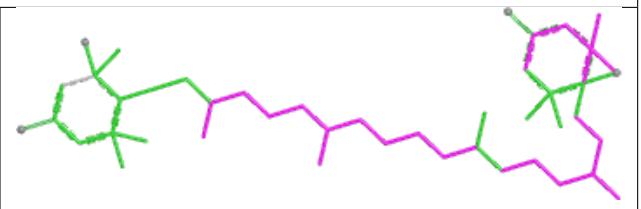


Rings

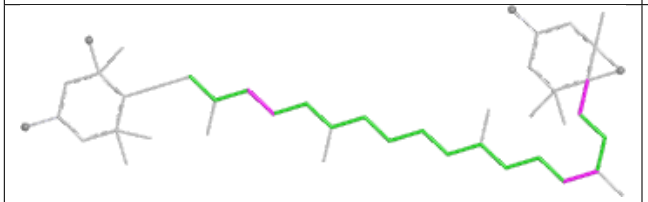
Ligand NEX 3 1623



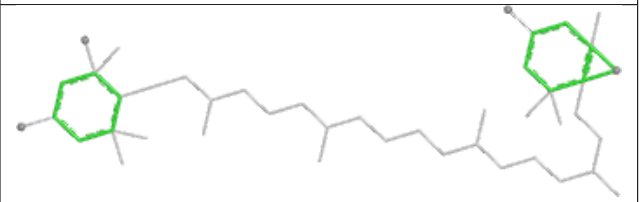
Bond lengths



Bond angles

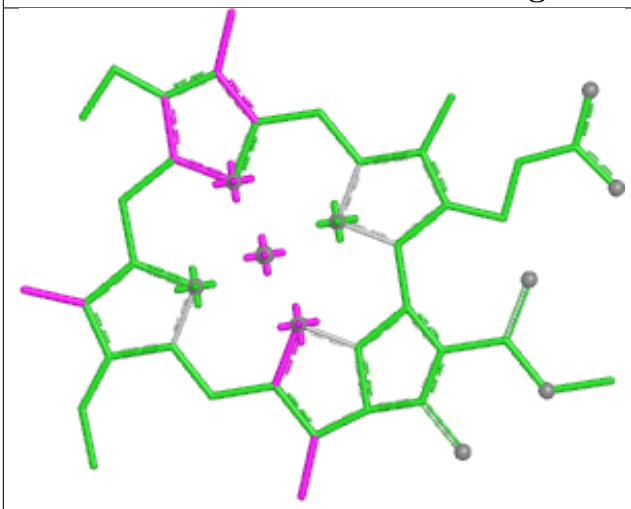


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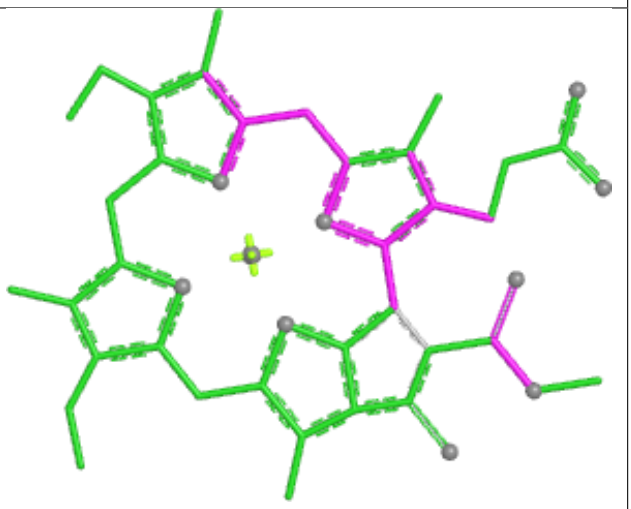


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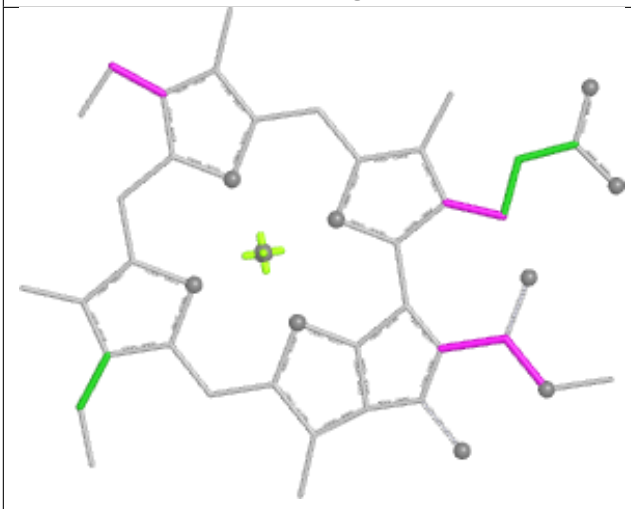
Ligand CLA 2 612



Bond lengths



Bond angles

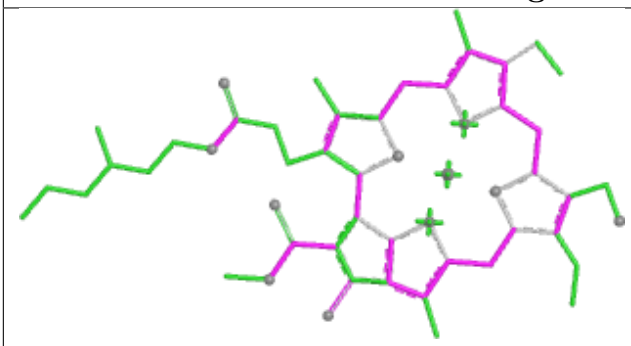


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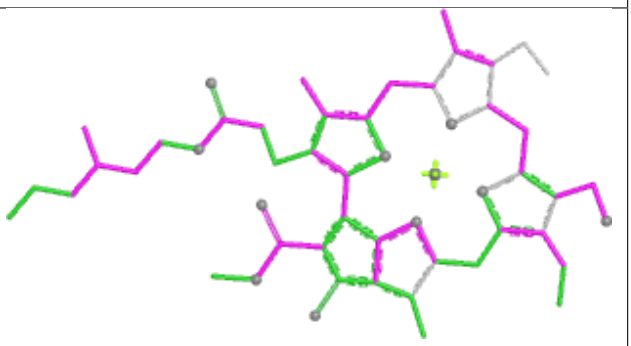


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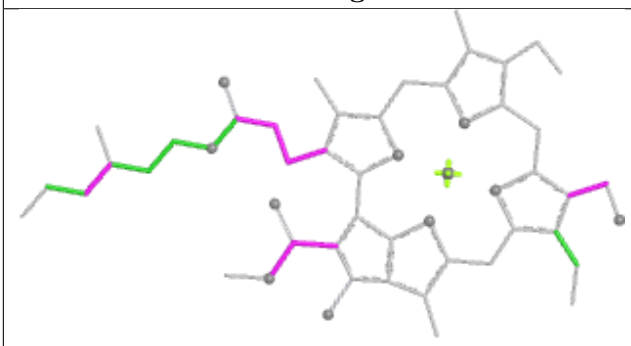
Ligand CHL 7 607



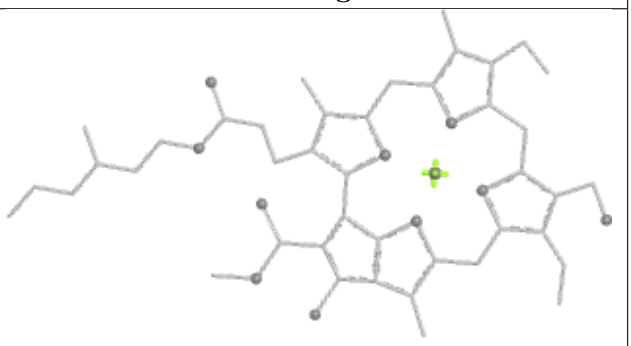
Bond lengths



Bond angles

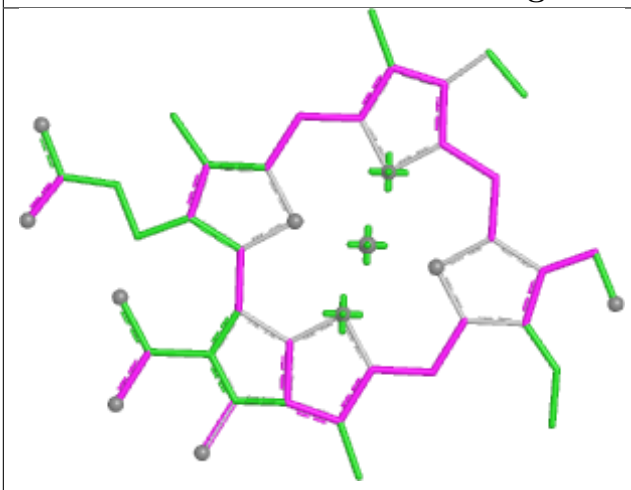


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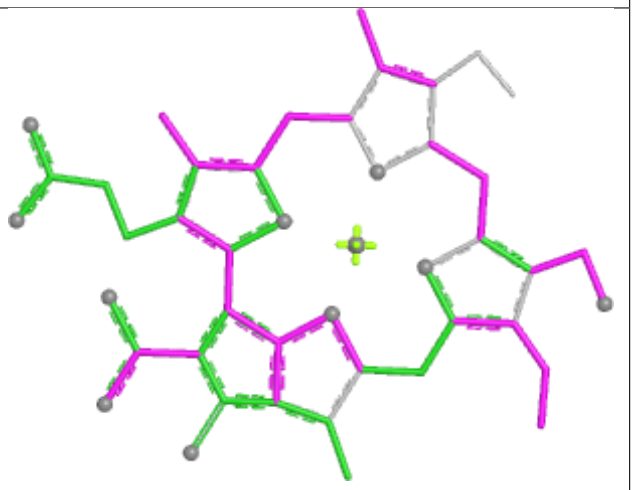


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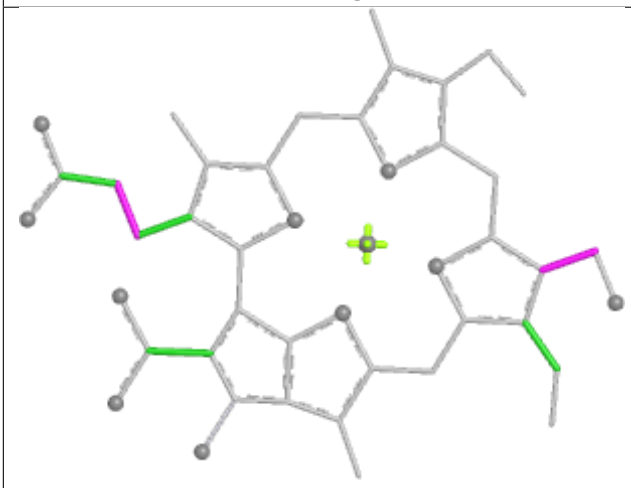
Ligand CHL 8 601



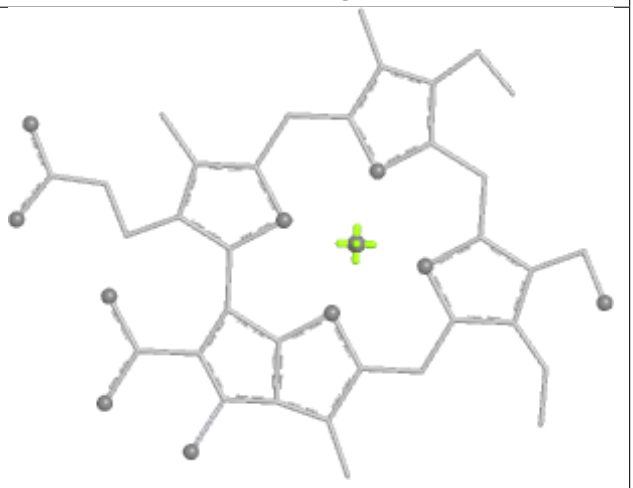
Bond lengths



Bond angles

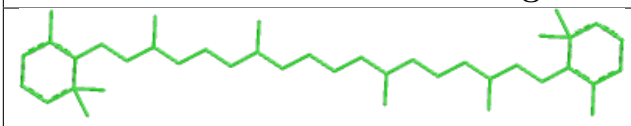


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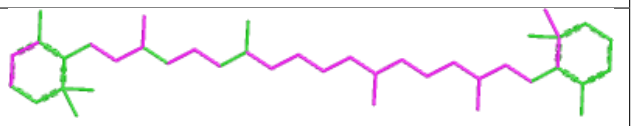


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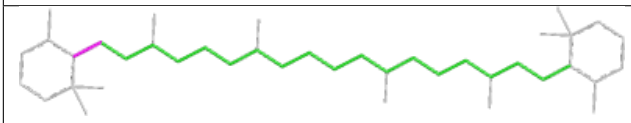
Ligand BCR C 514



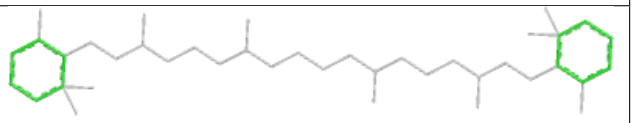
Bond lengths



Bond angles

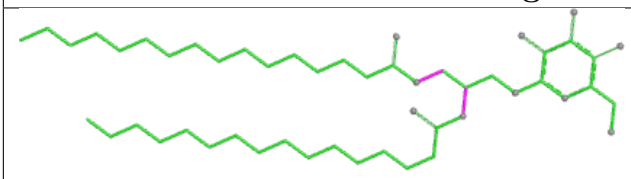


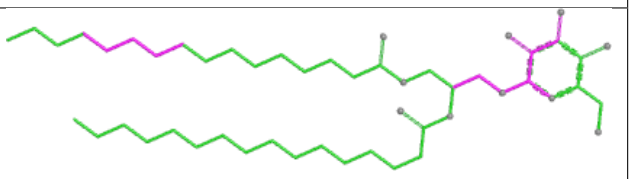
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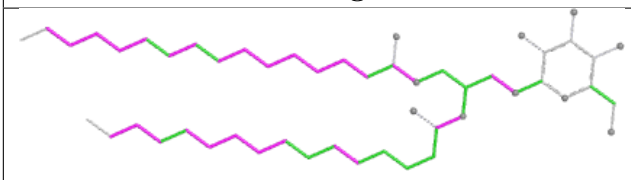


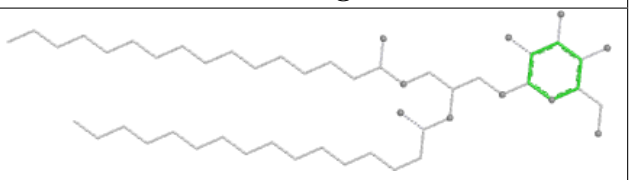
Rings

Ligand LMG b 622

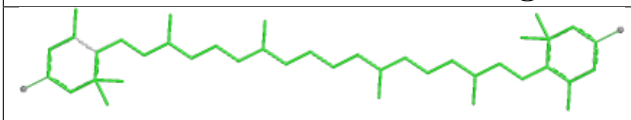

Bond lengths

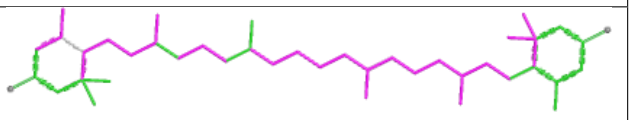

Bond angles

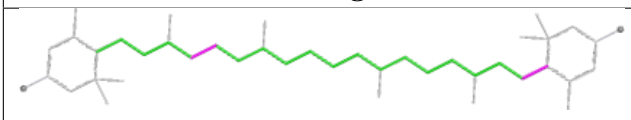

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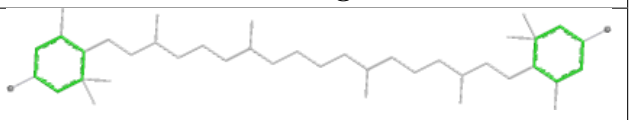

Rings

Ligand LUT S 1621


Bond lengths

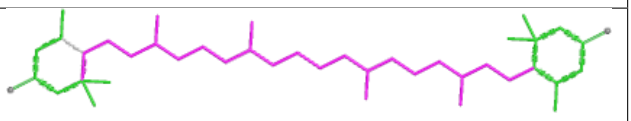

Bond angles


Torsions

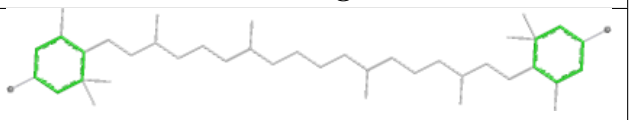

Rings

Ligand LUT 5 1620


Bond lengths

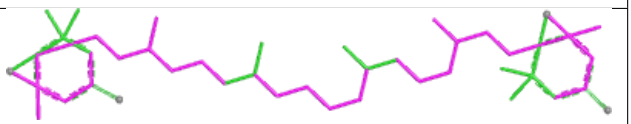

Bond angles

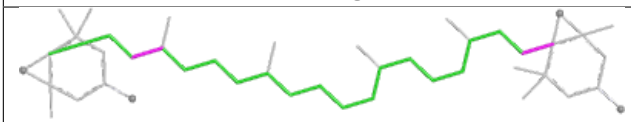

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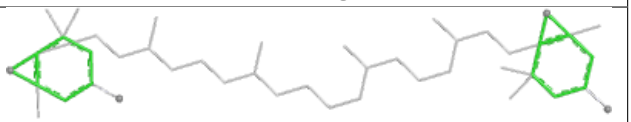

Rings

Ligand XAT 8 622

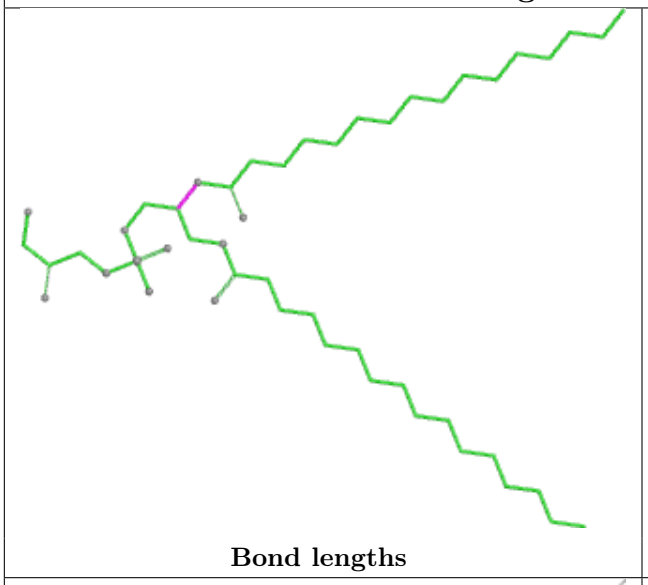

Bond lengths


Bond angles

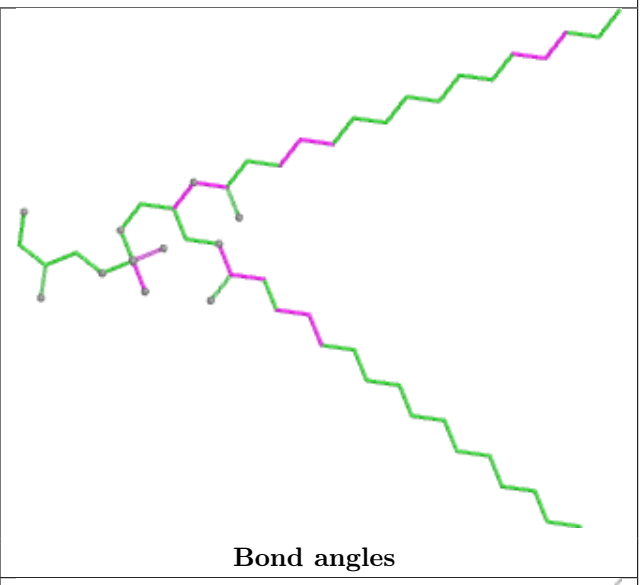

Torsions


Rings

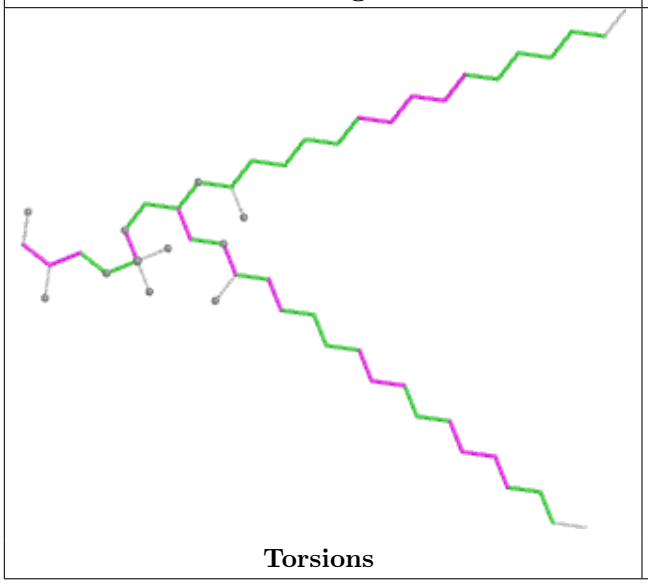
Ligand LHG b 2631



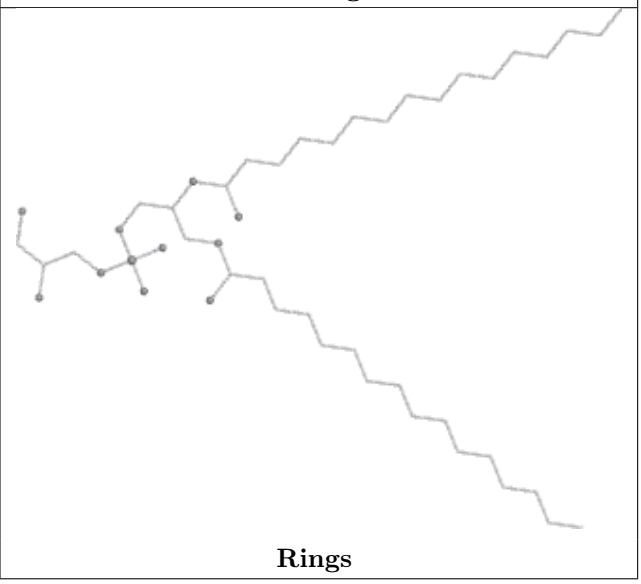
Bond lengths



Bond angles



Torsions



Rings

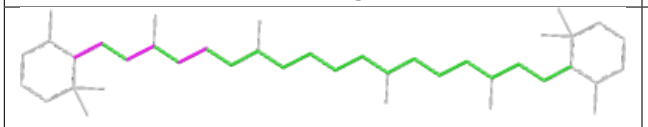
Ligand BCR d 404



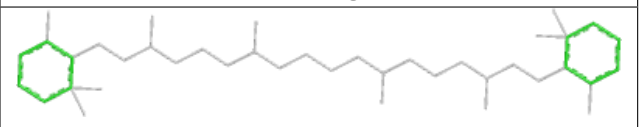
Bond lengths



Bond angles

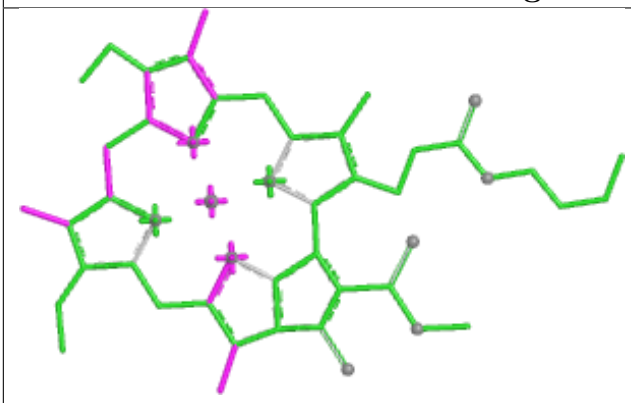


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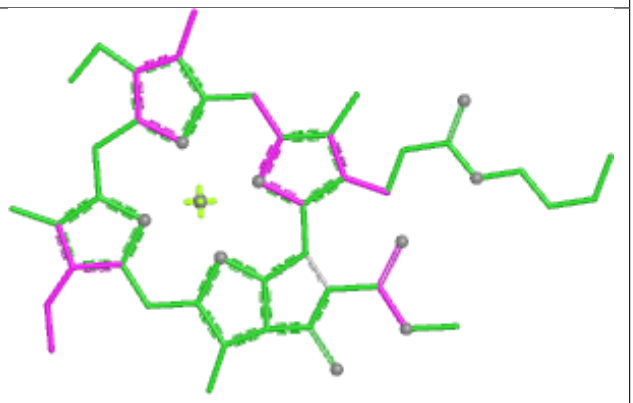


Rings

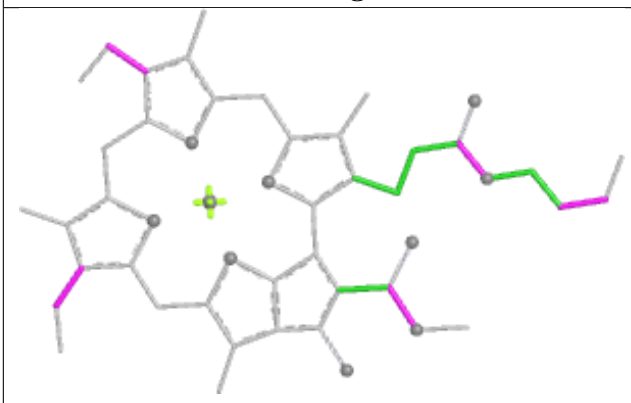
Ligand CLA R 601



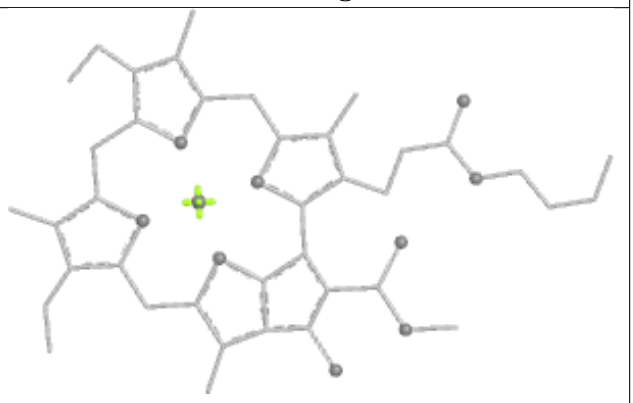
Bond lengths



Bond angles

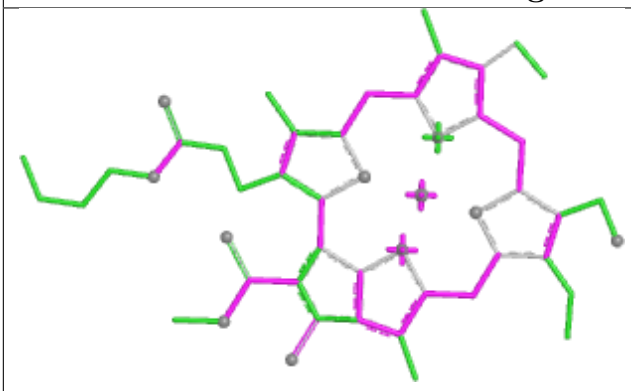


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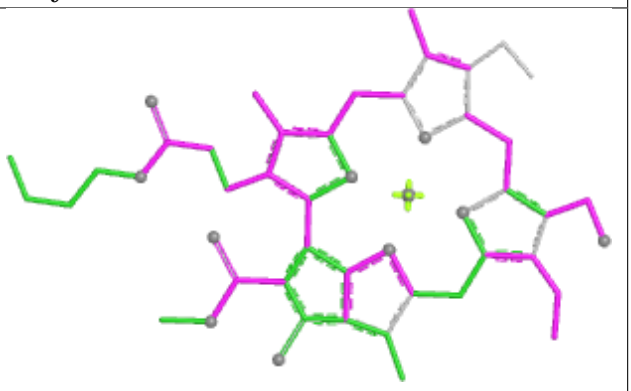


Rings

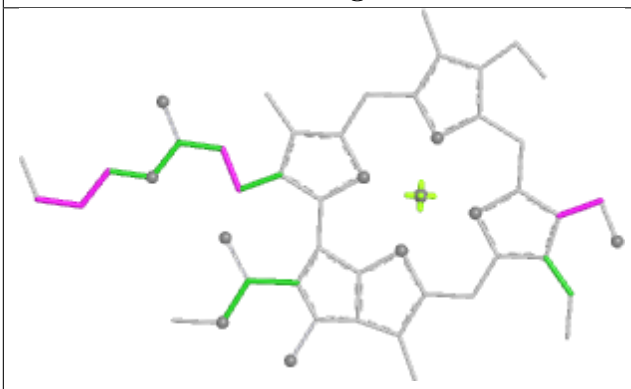
Ligand CHL y 606



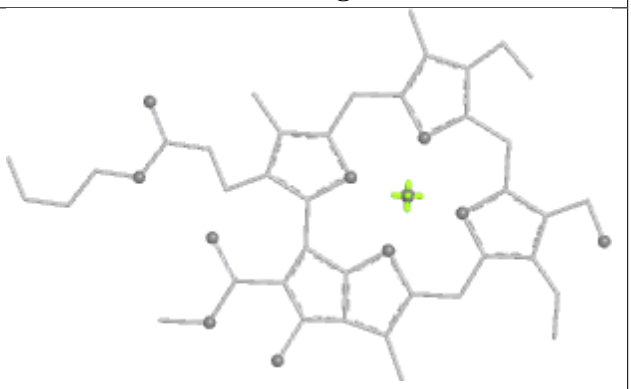
Bond lengths



Bond angles

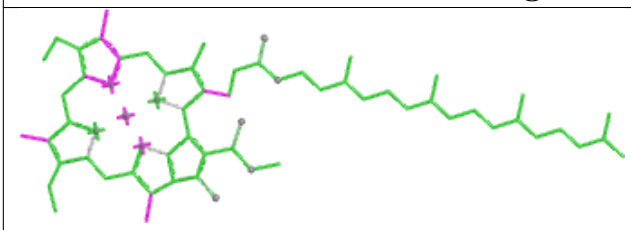


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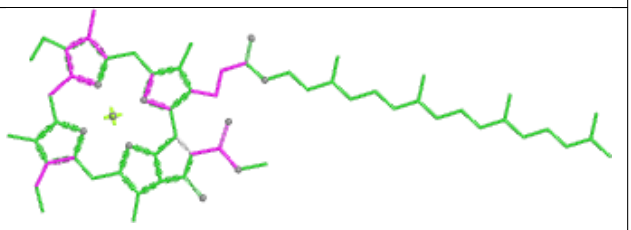


Rings

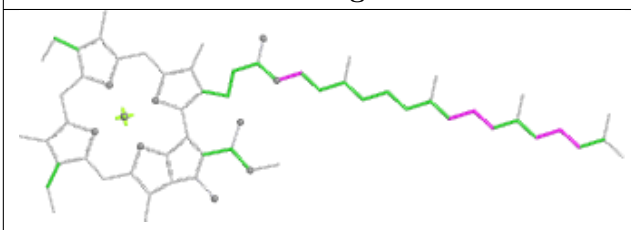
Ligand CLA D 402



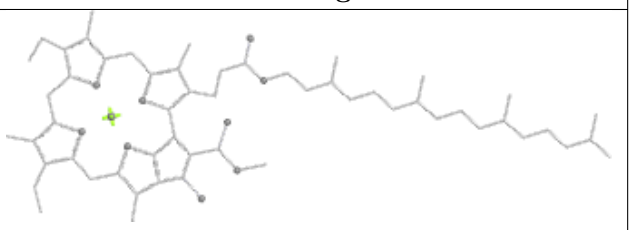
Bond lengths



Bond angles

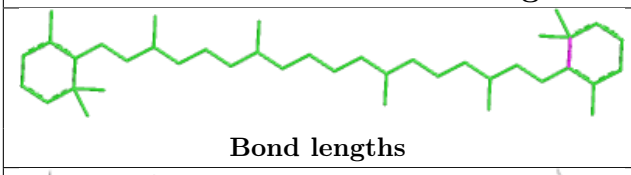


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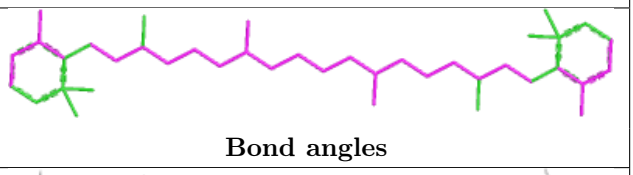


Rings

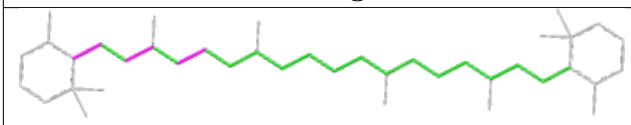
Ligand BCR D 404



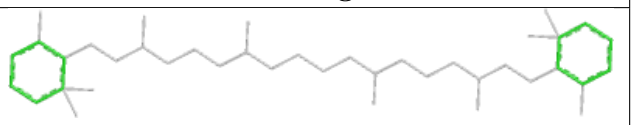
Bond lengths



Bond angles

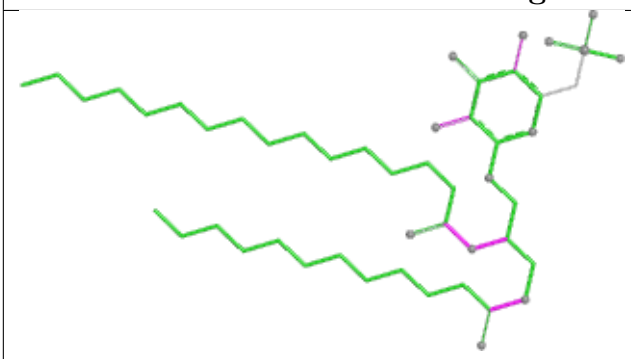


Torsions

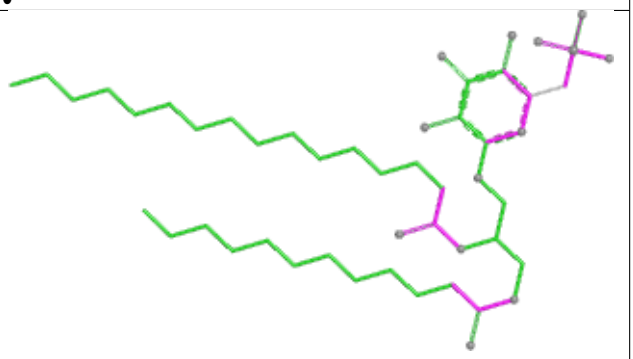


Rings

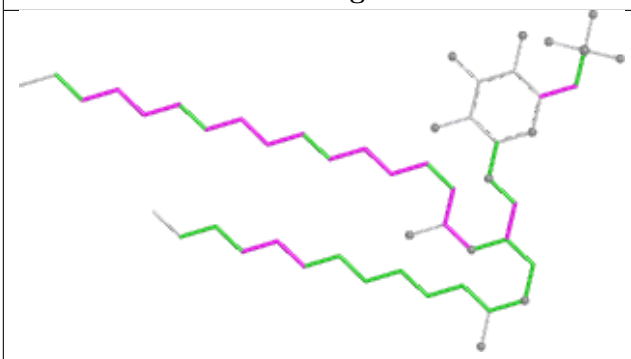
Ligand SQD a 412



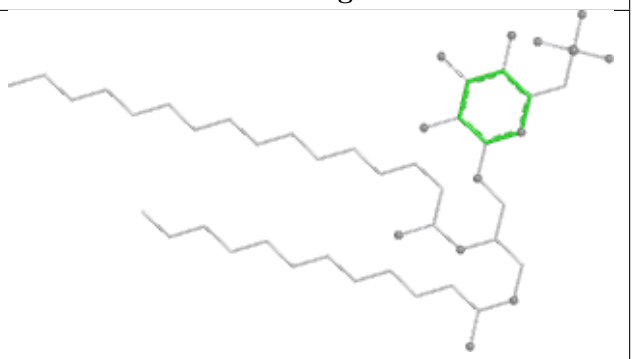
Bond lengths



Bond angles

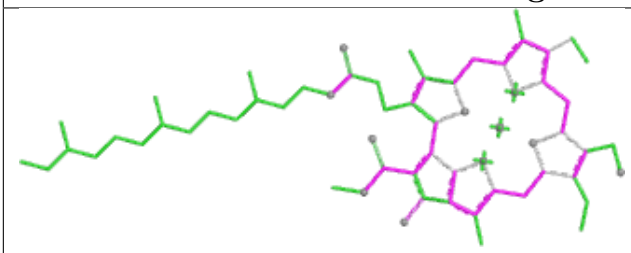


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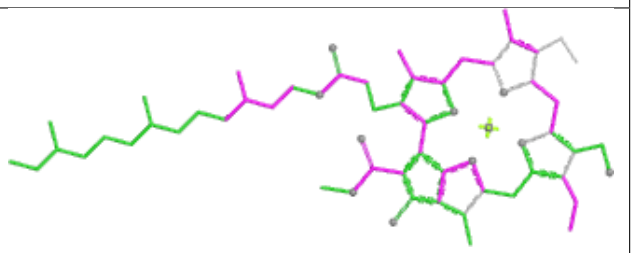


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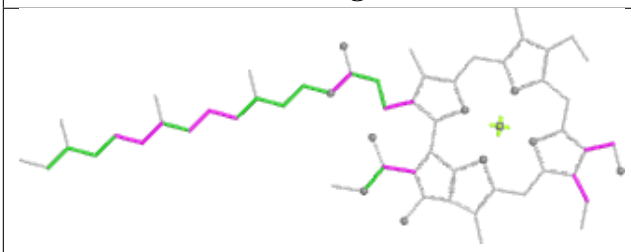
Ligand CHL 1 609



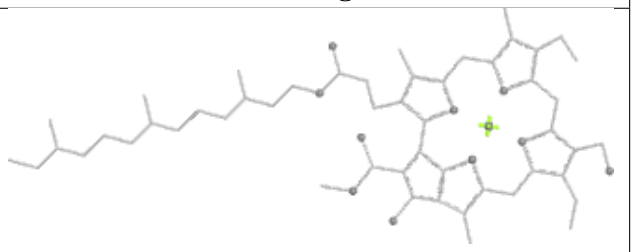
Bond lengths



Bond angles

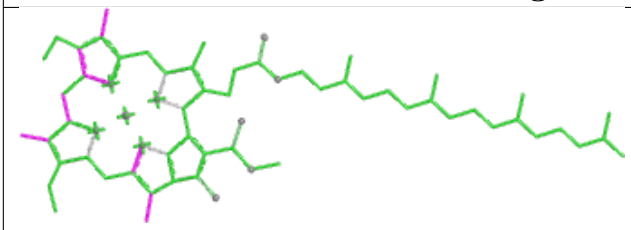


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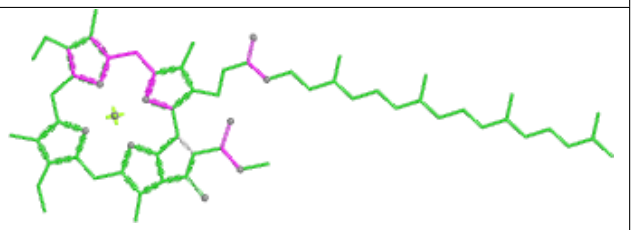


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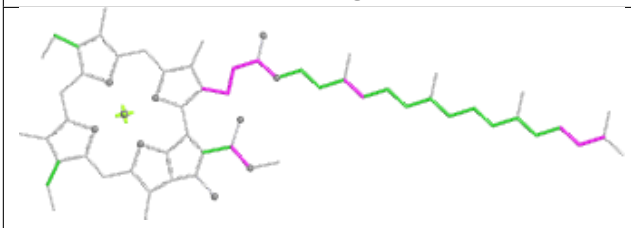
Ligand CLA c 501



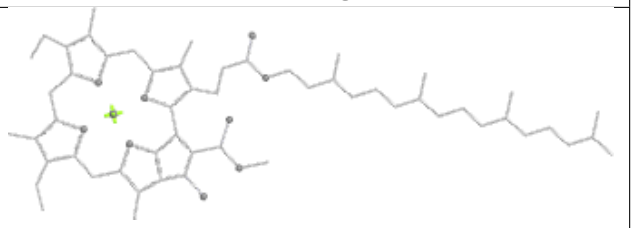
Bond lengths



Bond angles

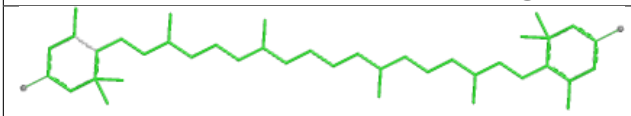


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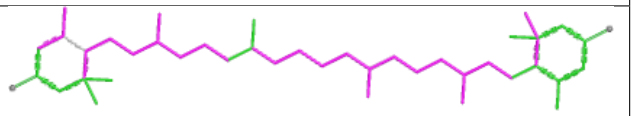


Rings

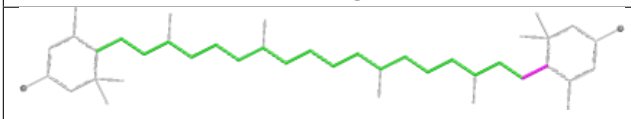
Ligand LUT S 1620



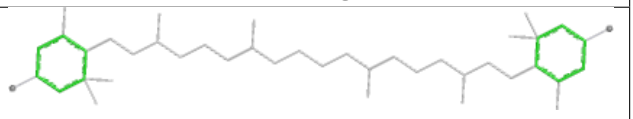
Bond lengths



Bond angles

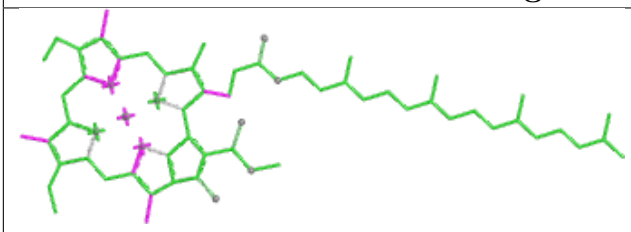


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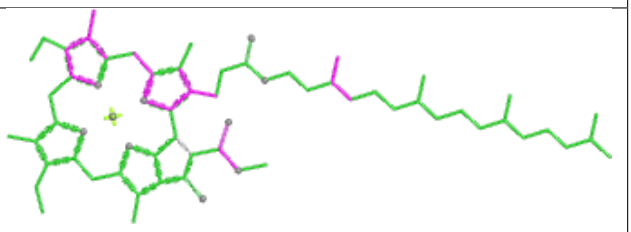


Rings

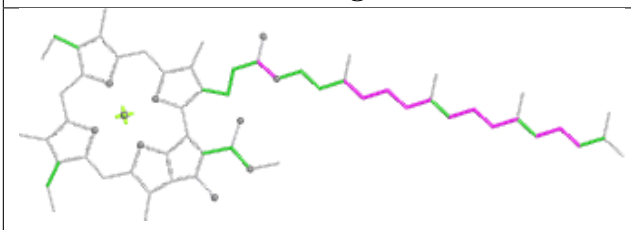
Ligand CLA B 614



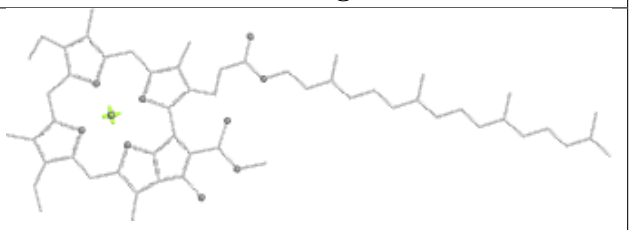
Bond lengths



Bond angles

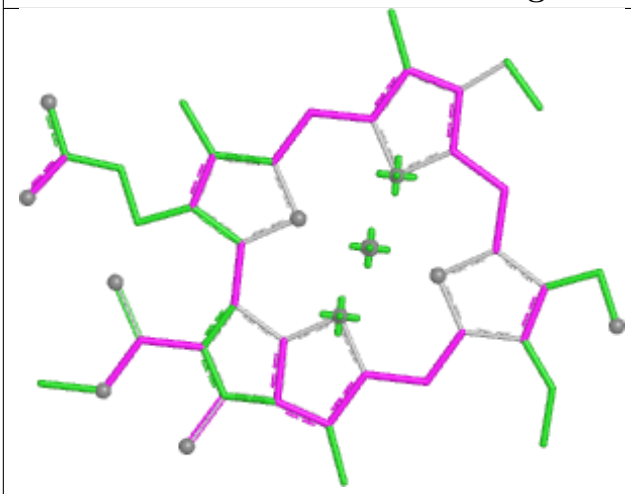


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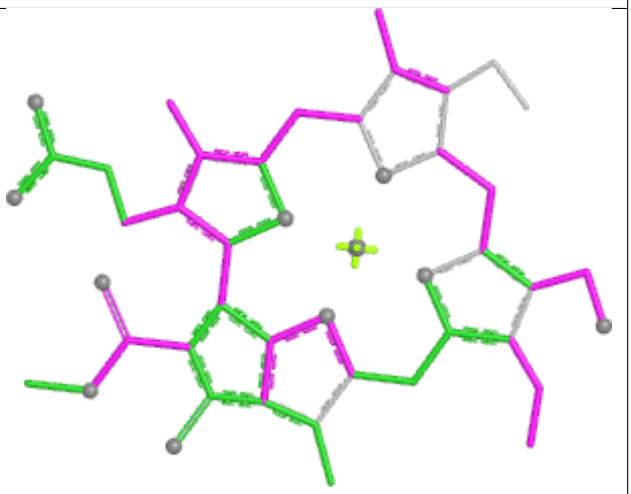


Rings

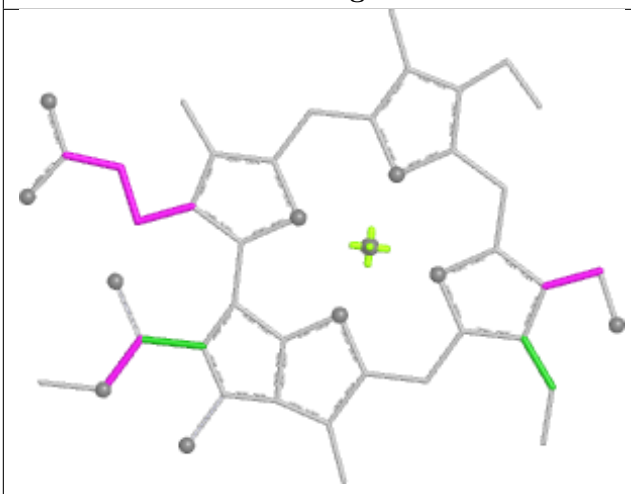
Ligand CHL 6 605



Bond lengths



Bond angles

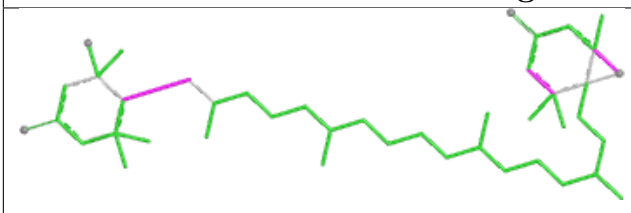


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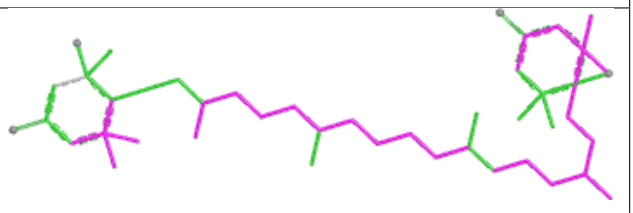


Rings

Ligand NEX 5 1623



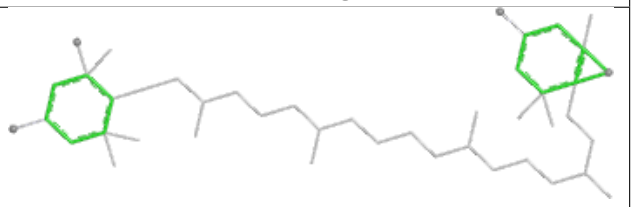
Bond lengths



Bond angles

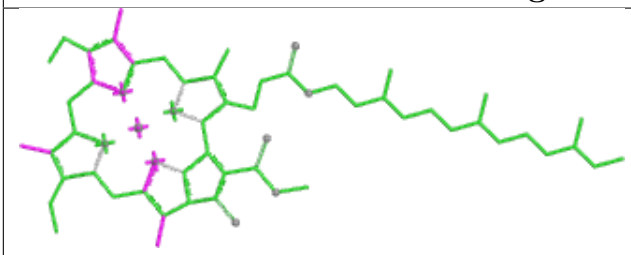


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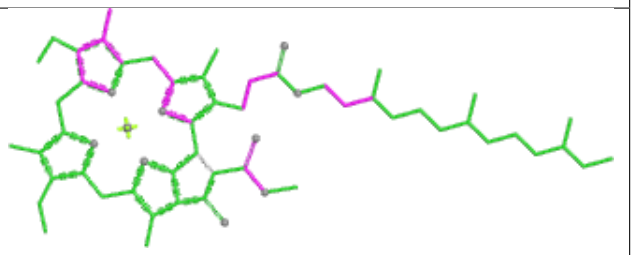


Rings

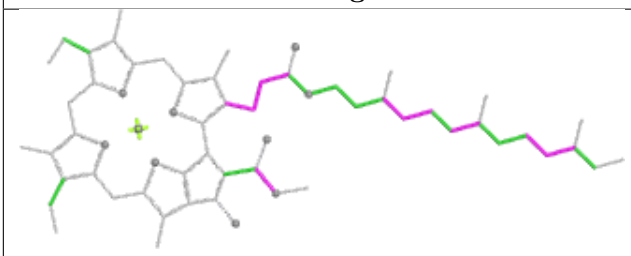
Ligand CLA 2 602



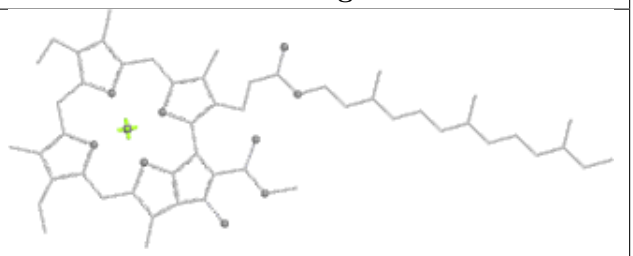
Bond lengths



Bond angles

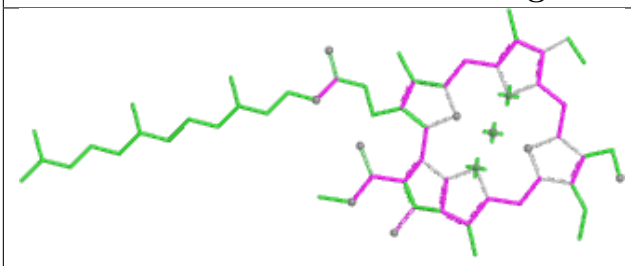


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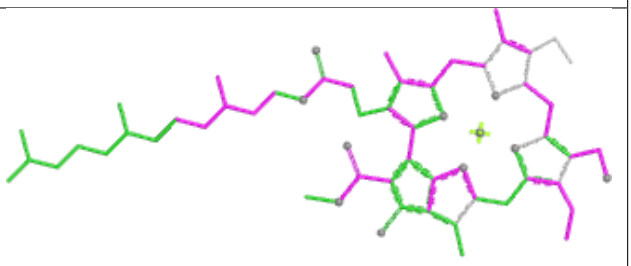


Rings

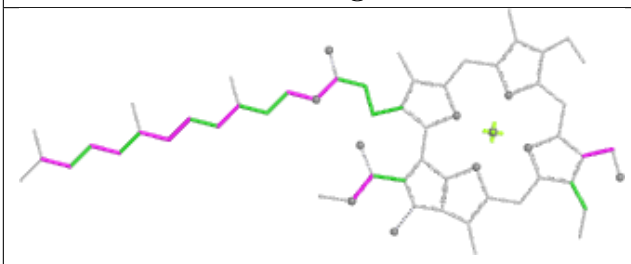
Ligand CHL 6 609



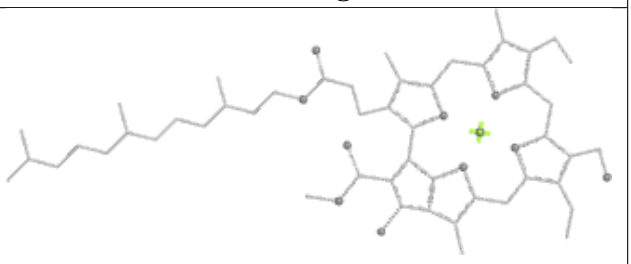
Bond lengths



Bond angles

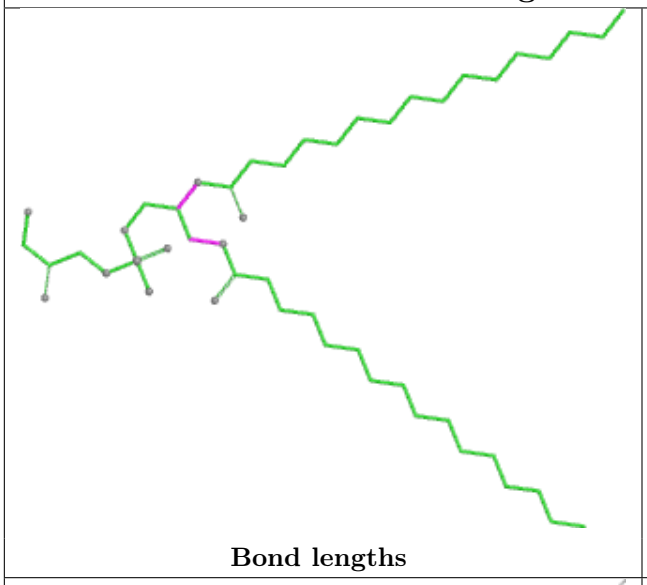


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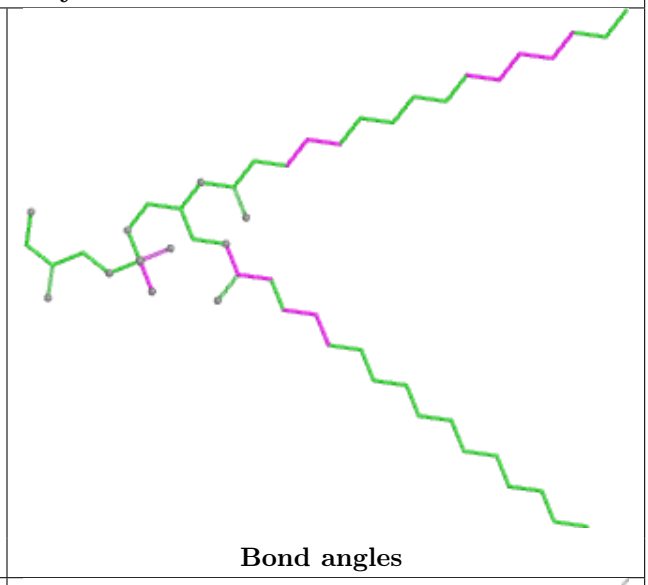


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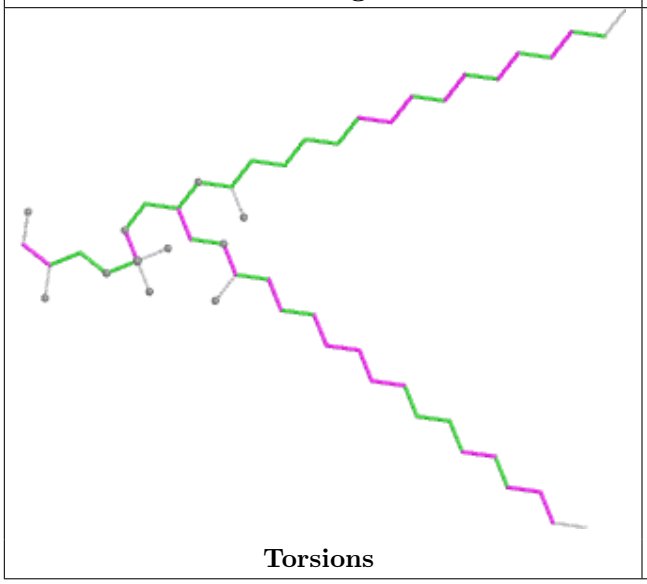
Ligand LHG y 2630



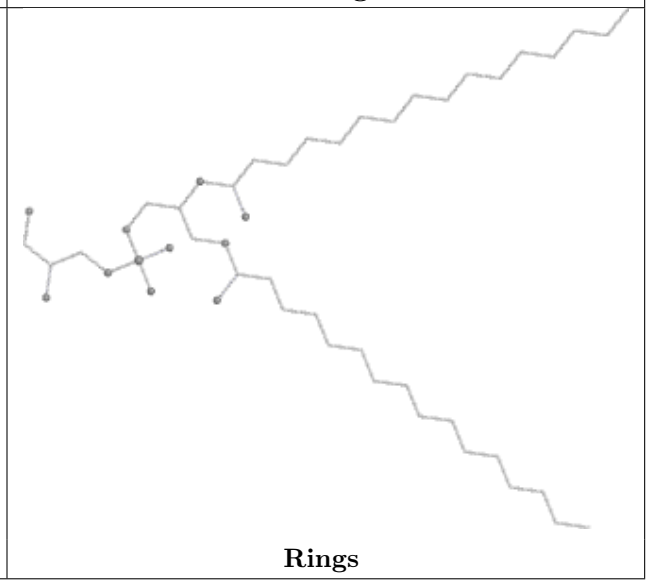
Bond lengths



Bond angles

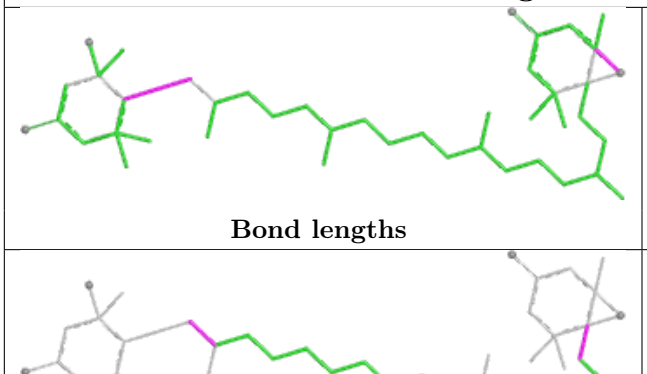


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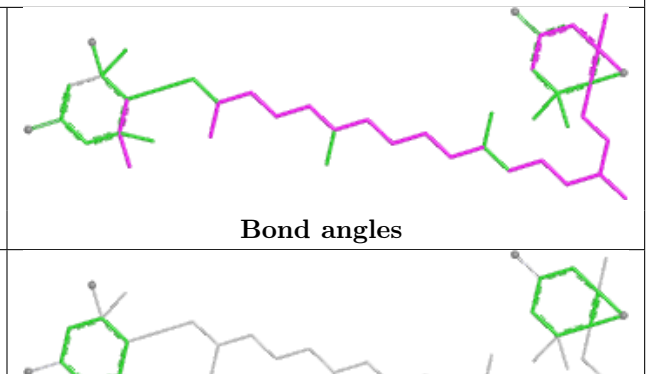


Rings

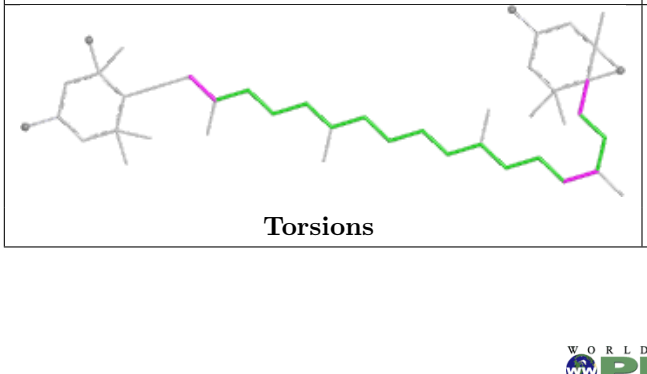
Ligand NEX S 1623



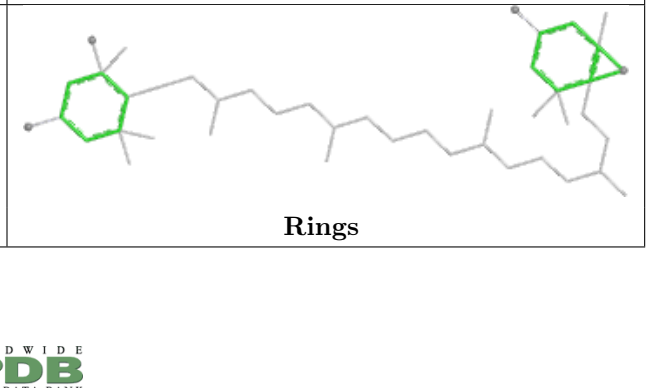
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Bond angles

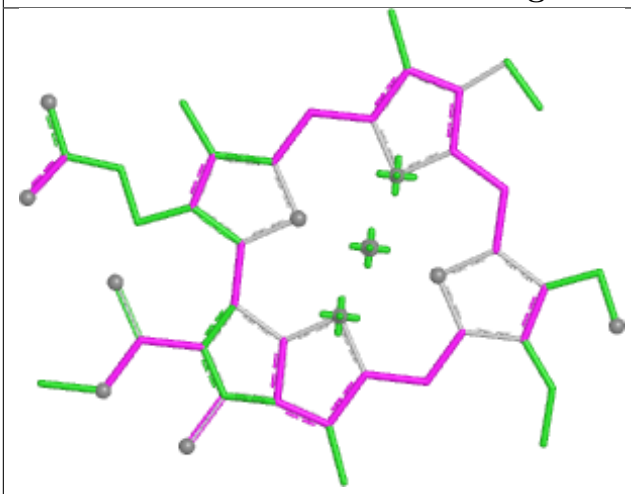


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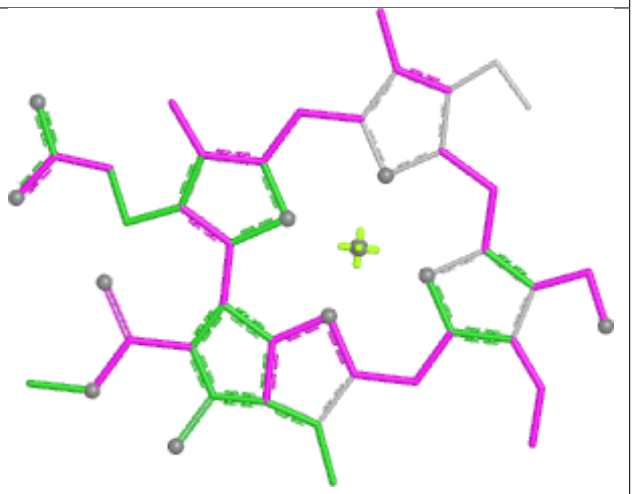


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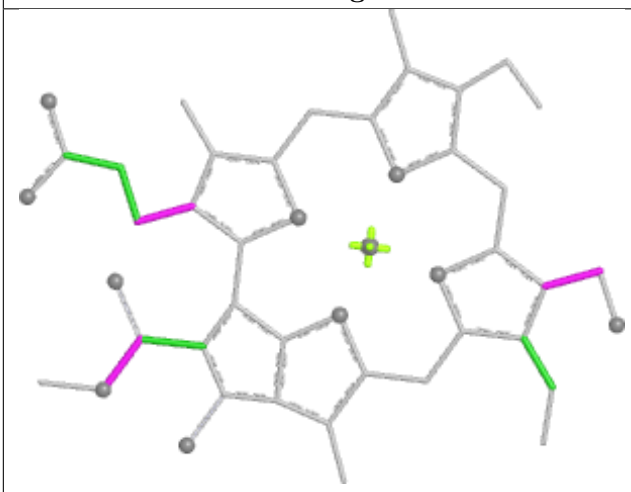
Ligand CHL 4 606



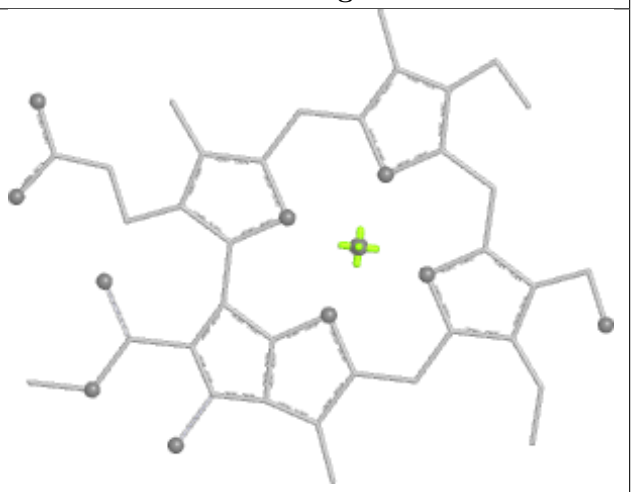
Bond lengths



Bond angles



Torsions

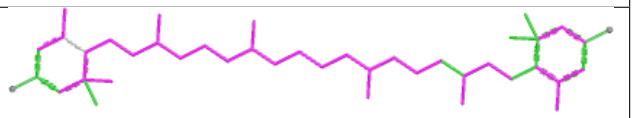


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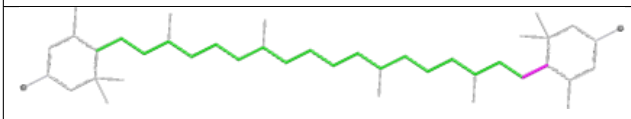
Ligand LUT R 620



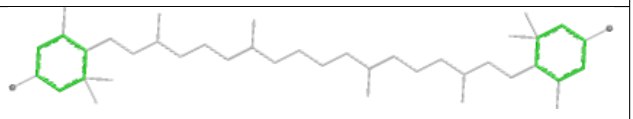
Bond lengths



Bond angles

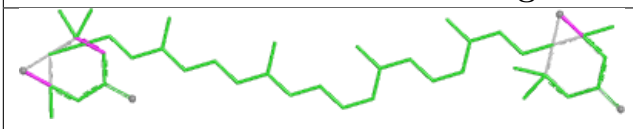


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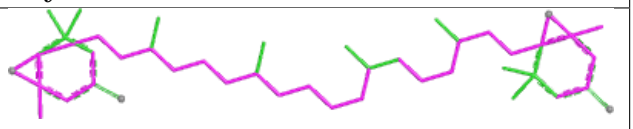


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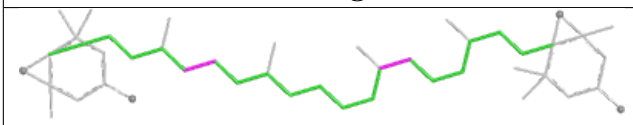
Ligand XAT y 1622



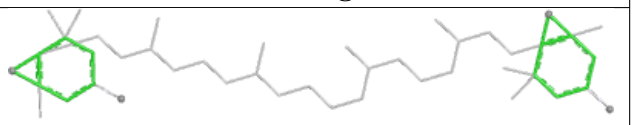
Bond lengths



Bond angles

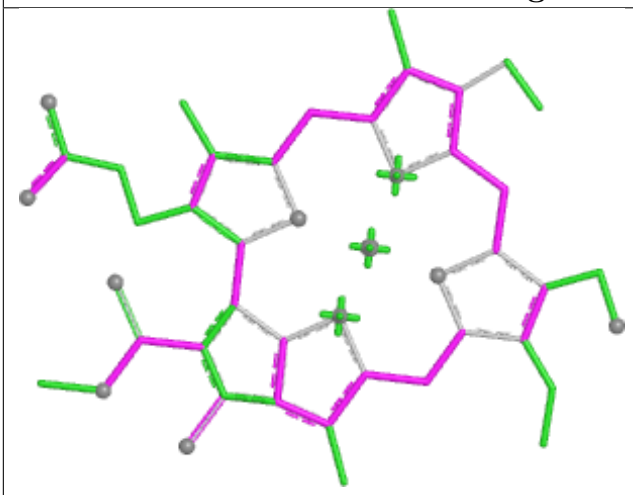


Torsions

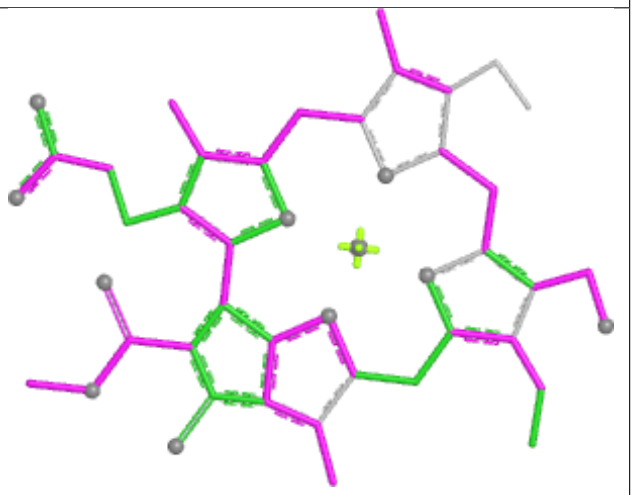


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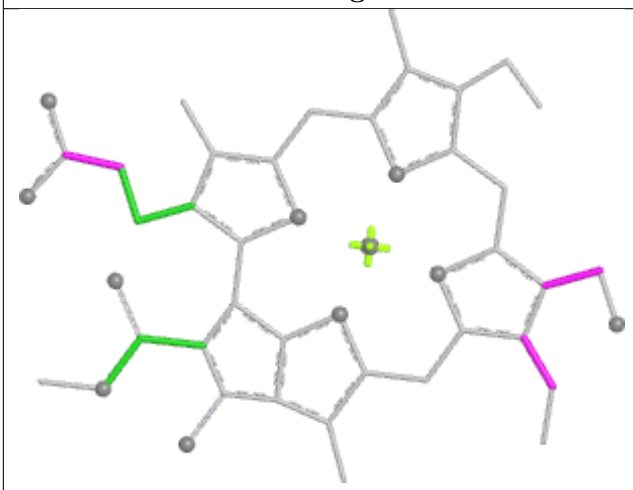
Ligand CHL 4 609



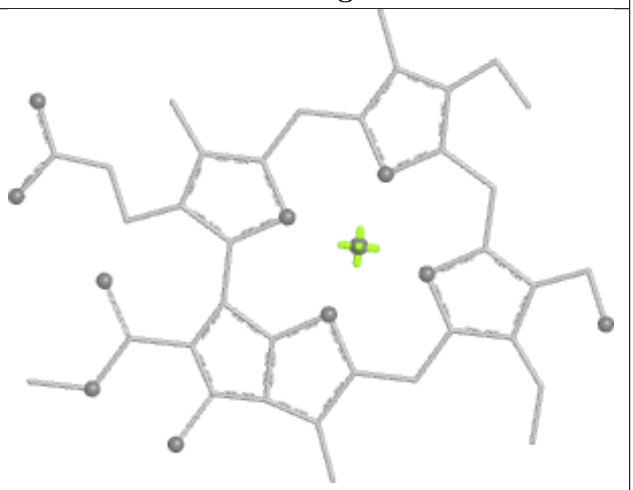
Bond lengths



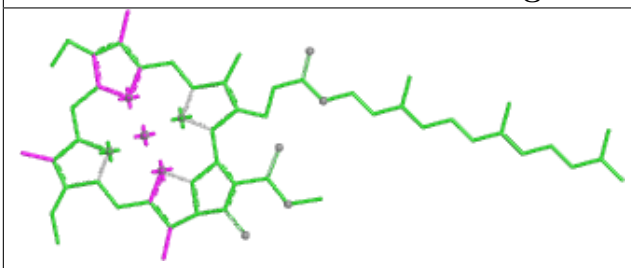
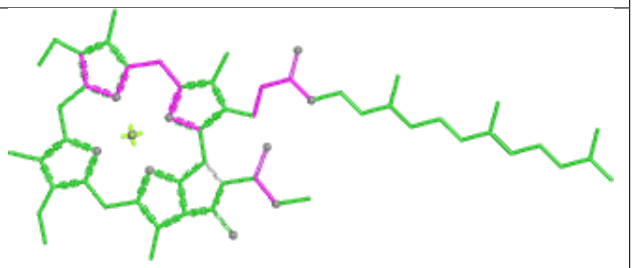
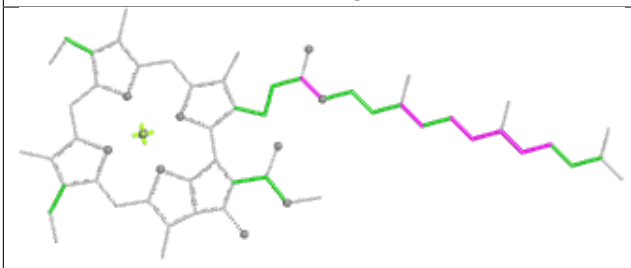
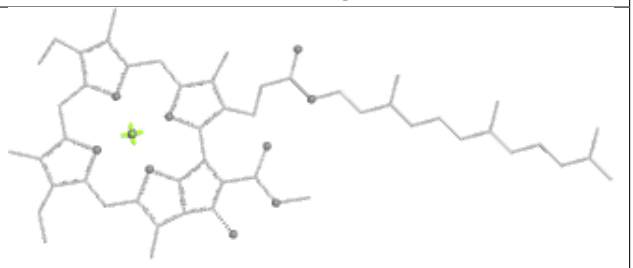
Bond angles

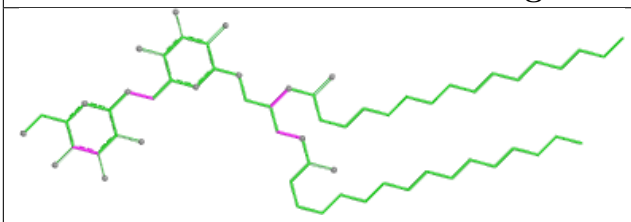
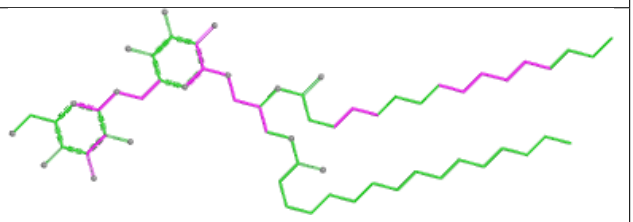
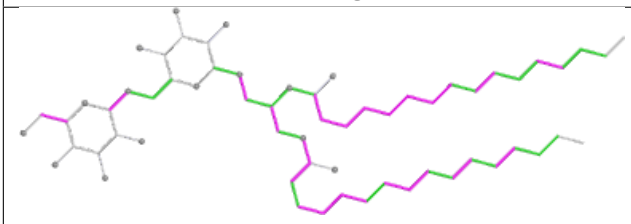
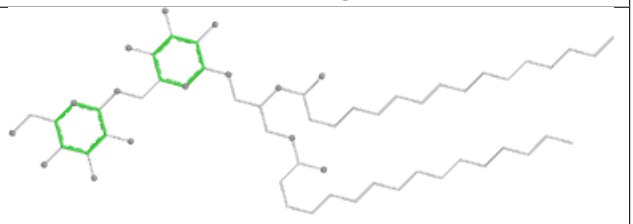


Torsions

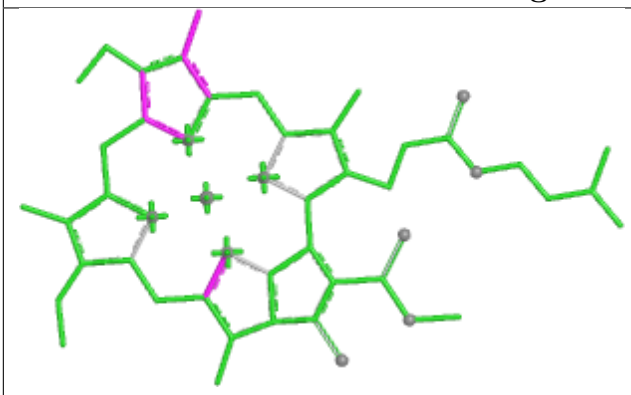


Rings

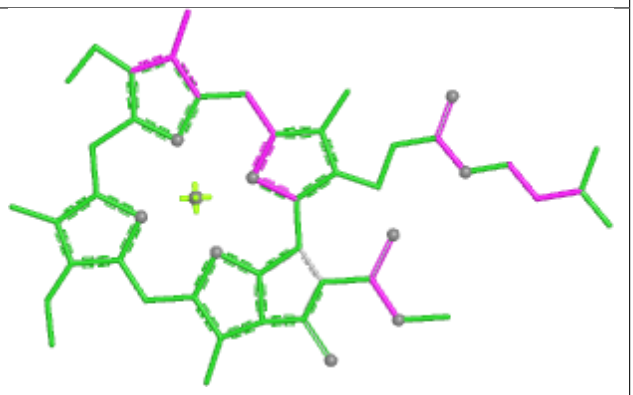
Ligand CLA Y 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD c 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

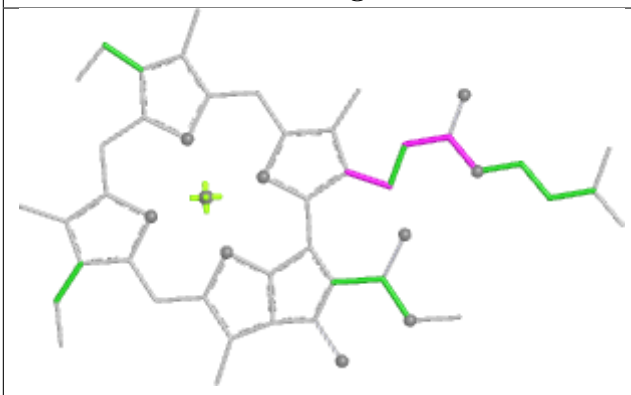
Ligand CLA s 604



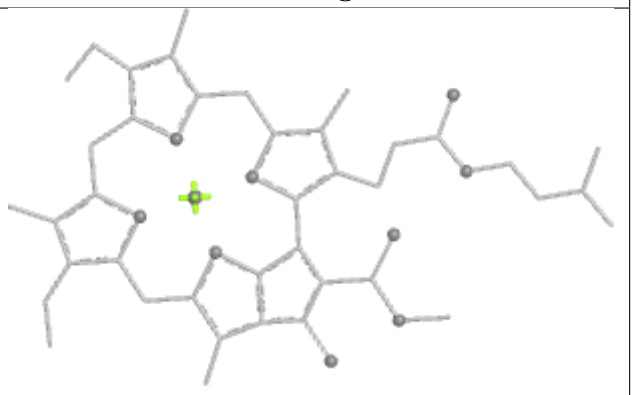
Bond lengths



Bond angles

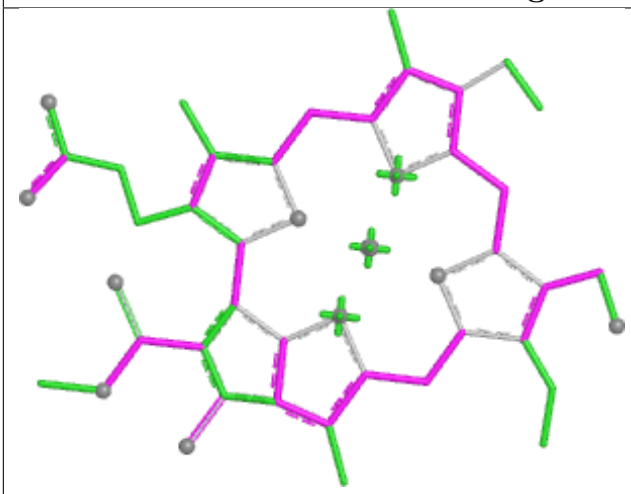


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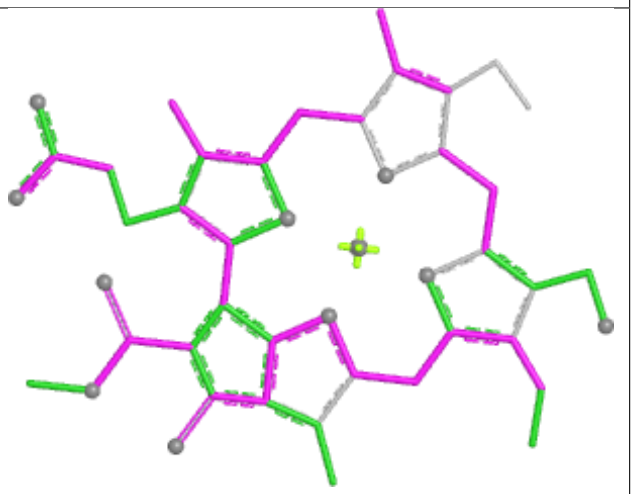


Rings

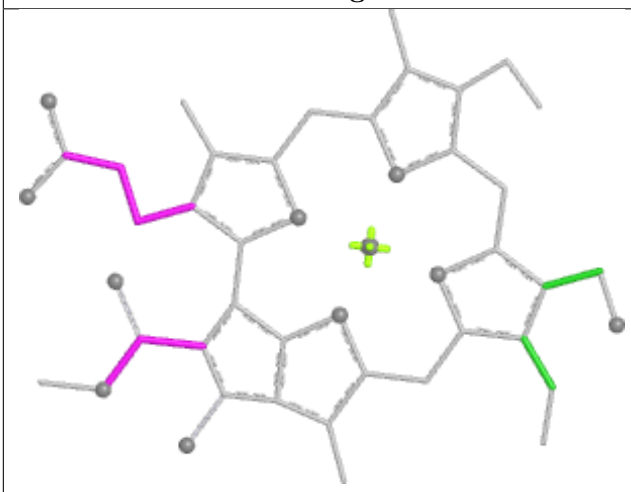
Ligand CHL 7 608



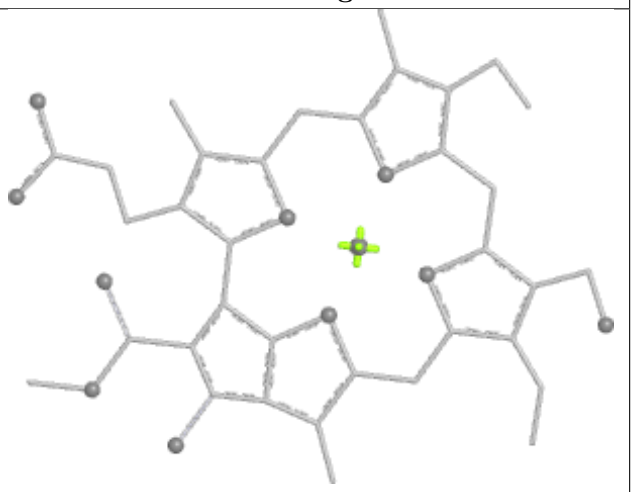
Bond lengths



Bond angles

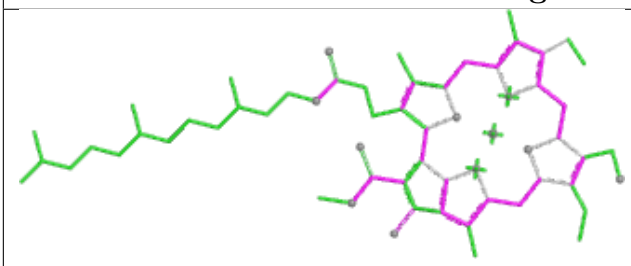


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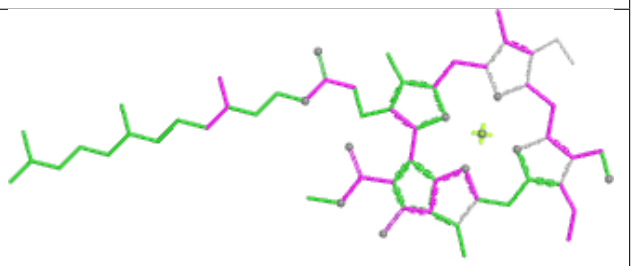


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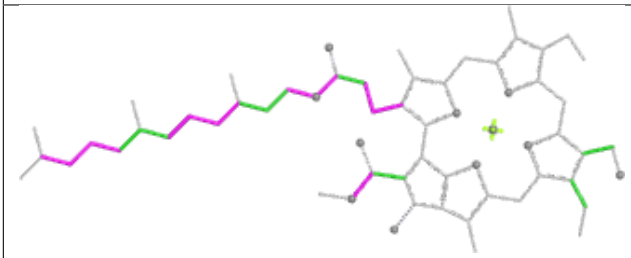
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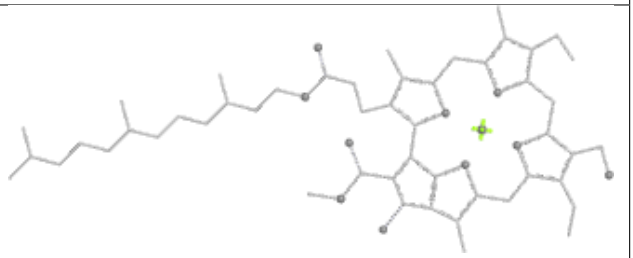
Bond lengths



Bond angles

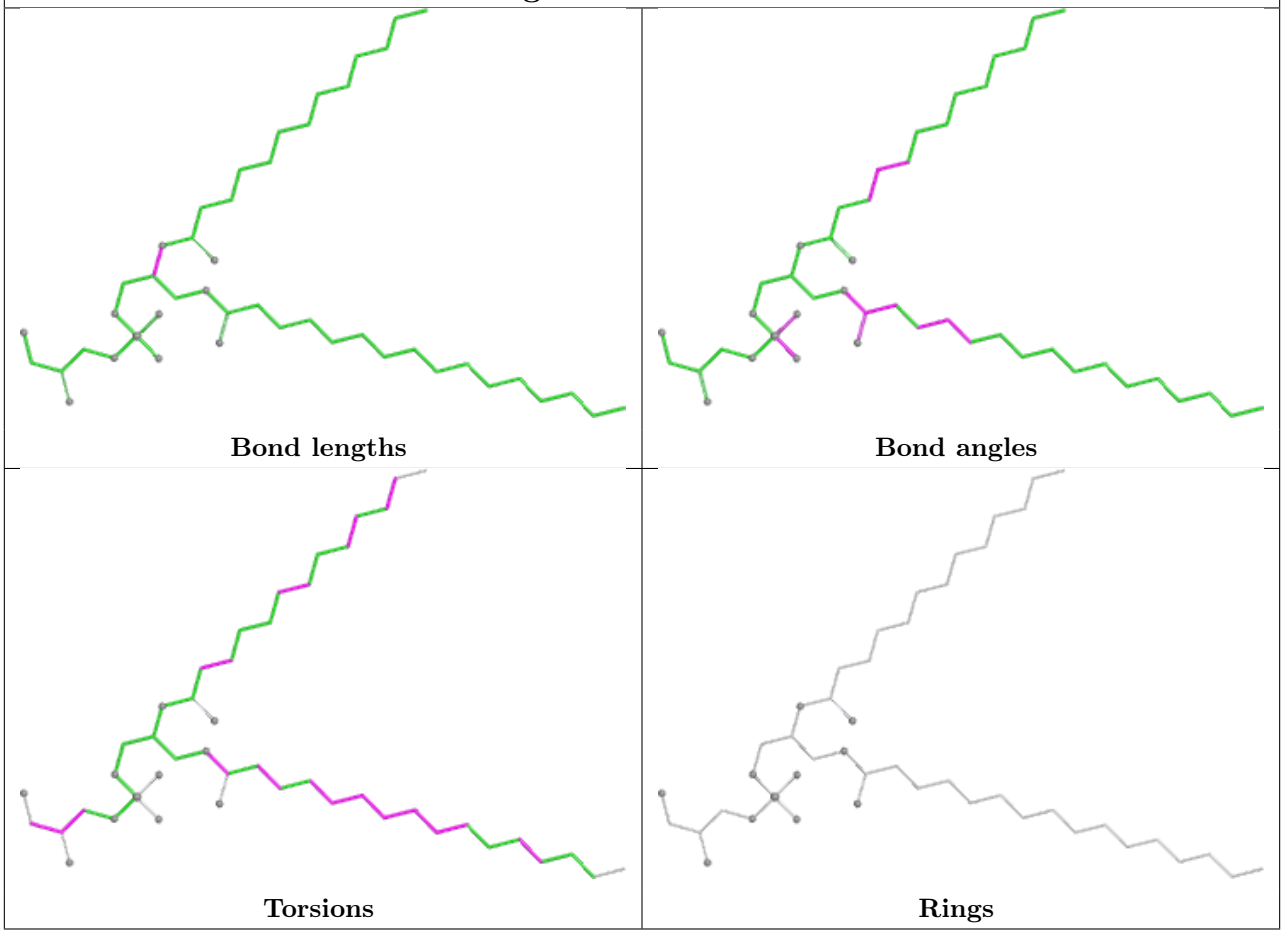


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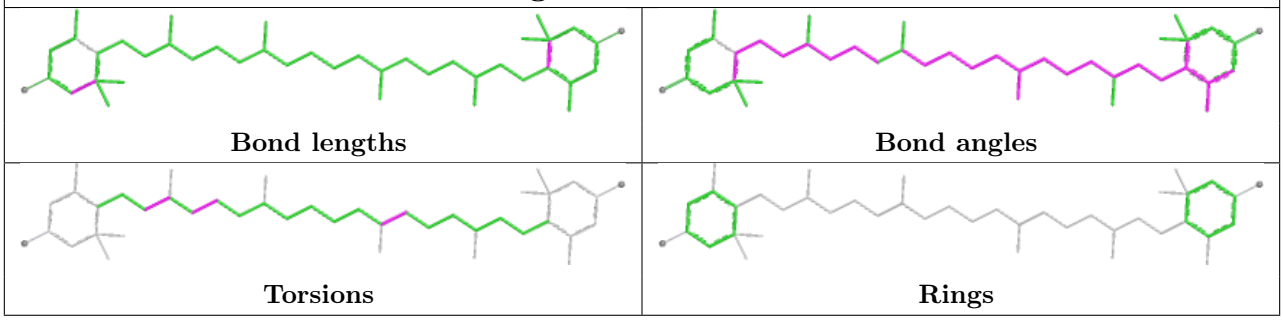


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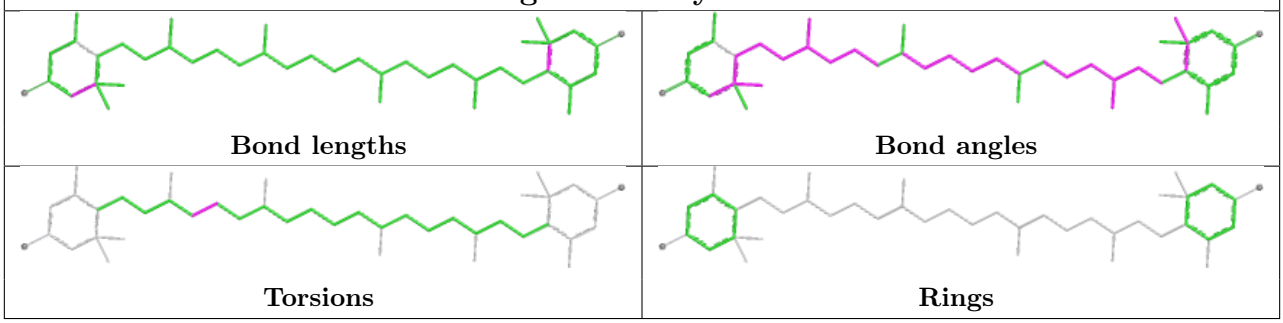
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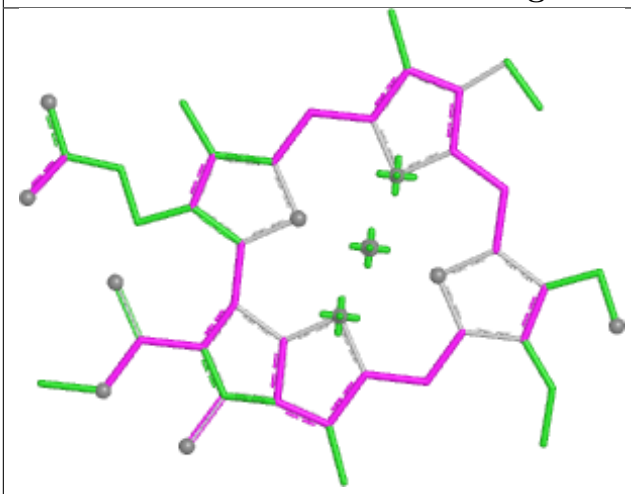
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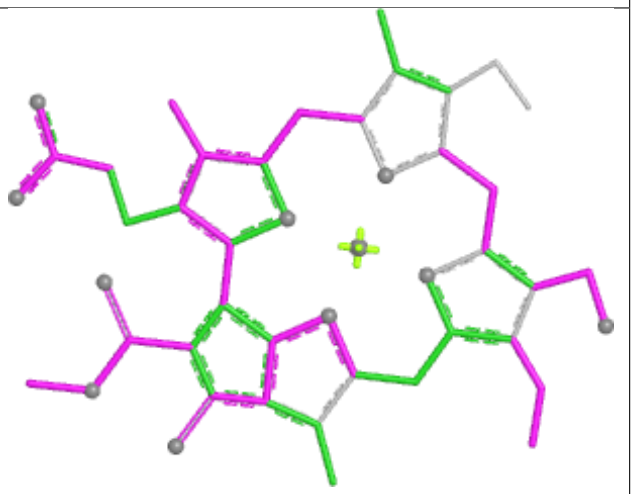
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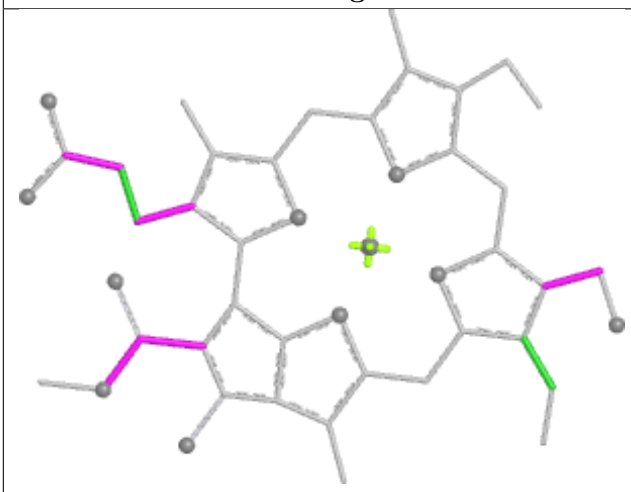
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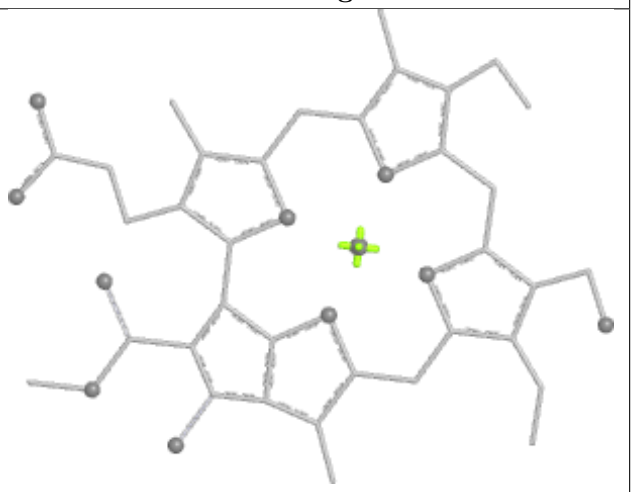
Bond lengths



Bond angles

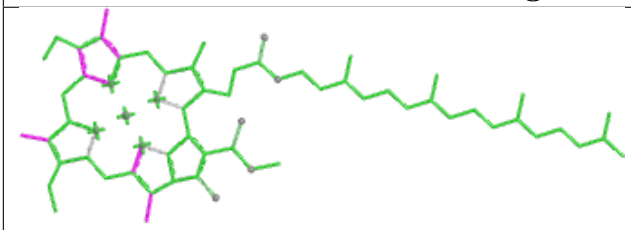


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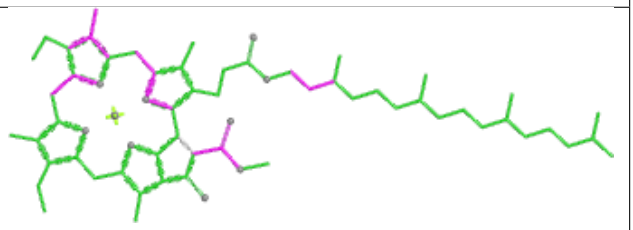


Rings

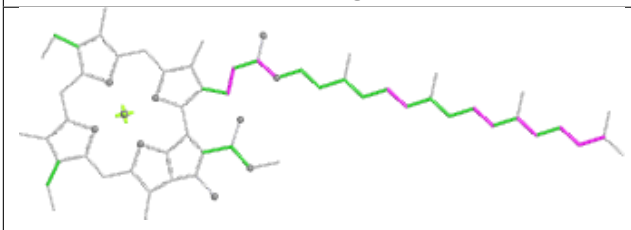
Ligand CLA C 505



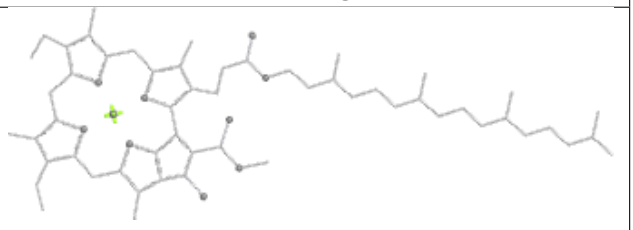
Bond lengths



Bond angles

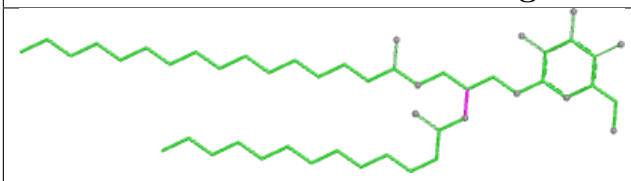


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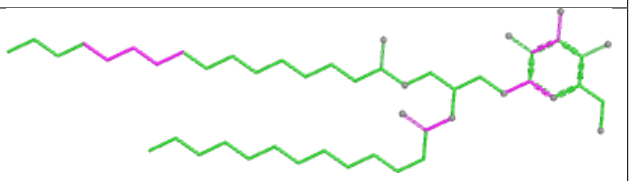


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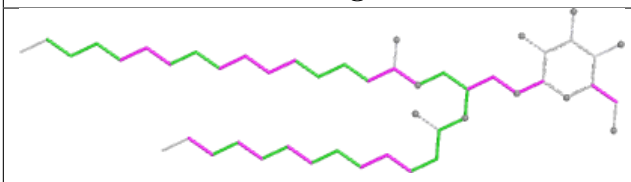
Ligand LMG A 413



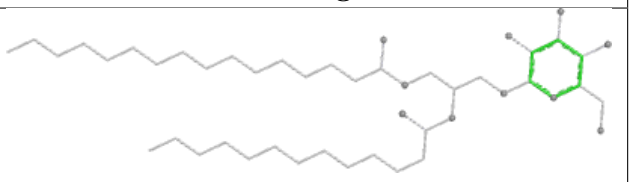
Bond lengths



Bond angles

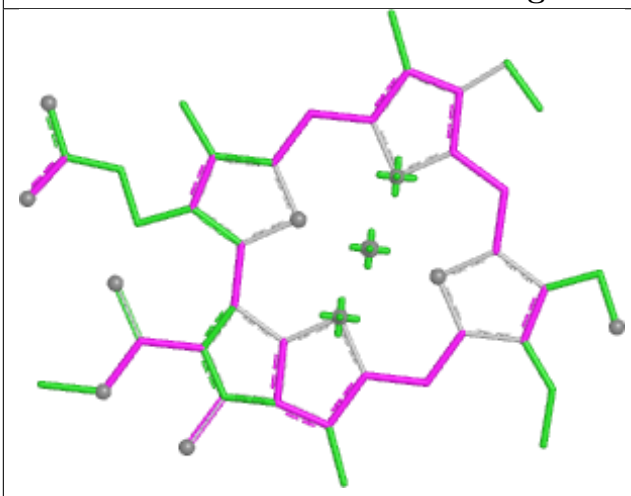


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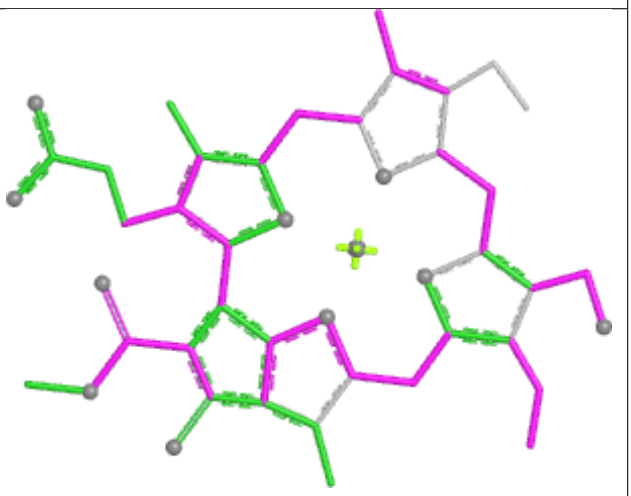


Rings

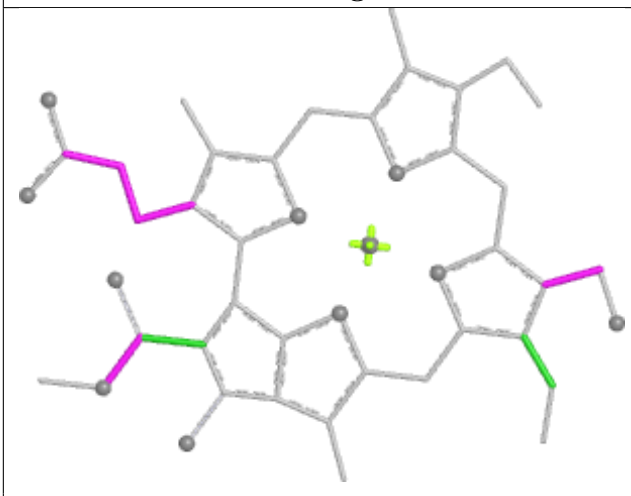
Ligand CHL 3 605



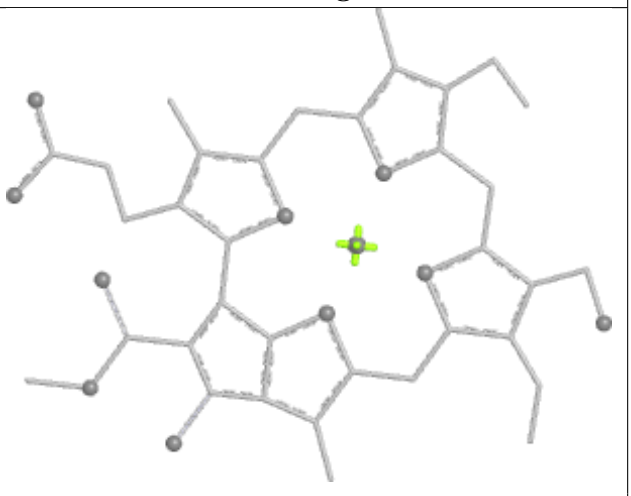
Bond lengths



Bond angles

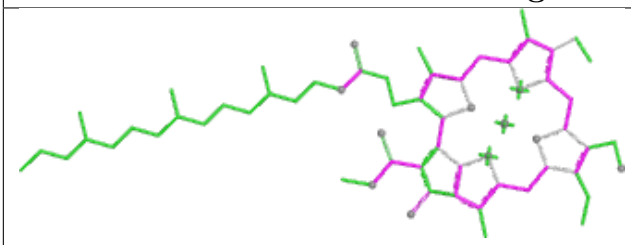


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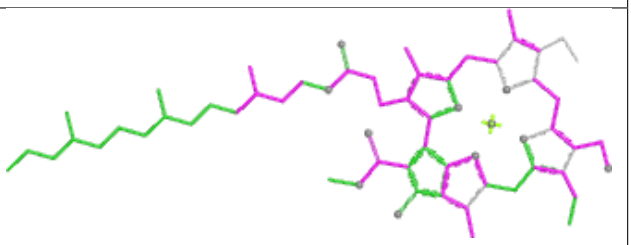


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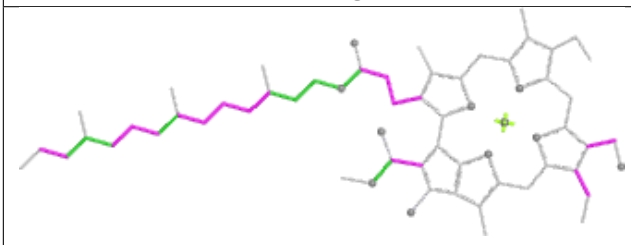
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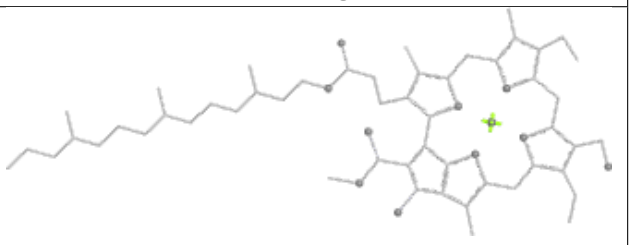
Bond lengths



Bond angles

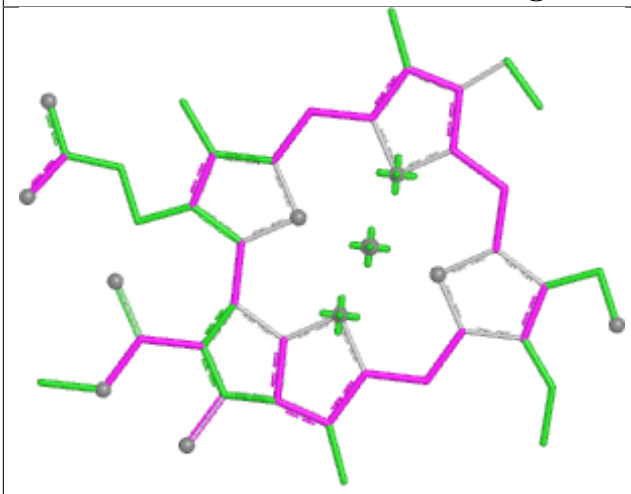


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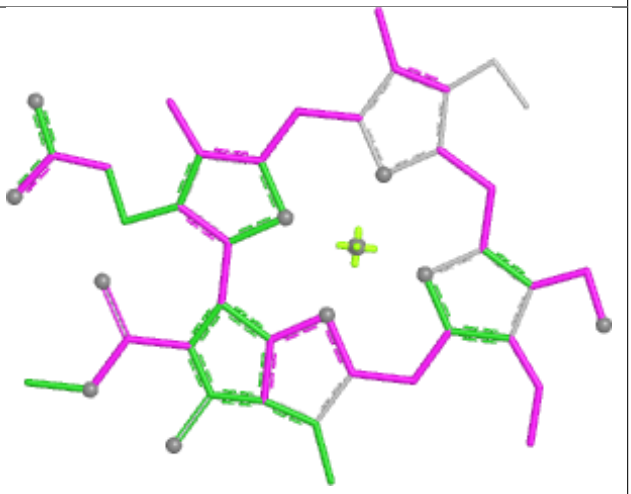


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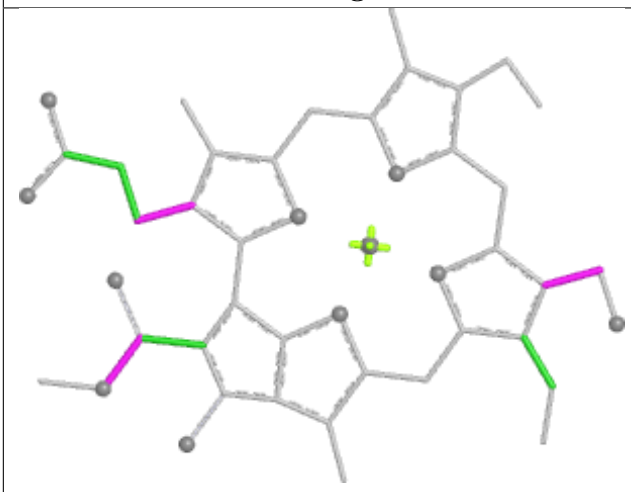
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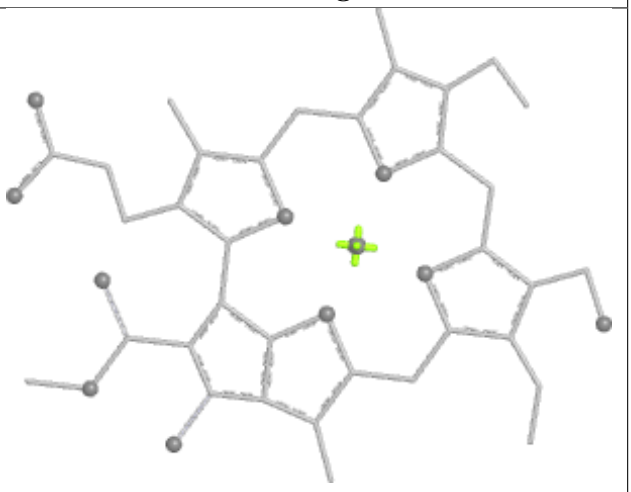
Bond lengths



Bond angles

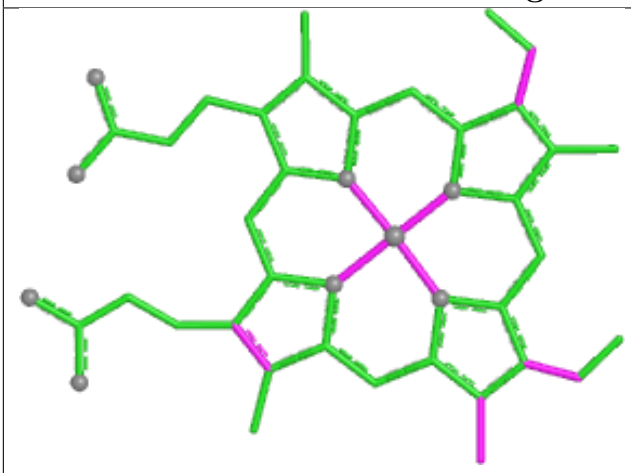


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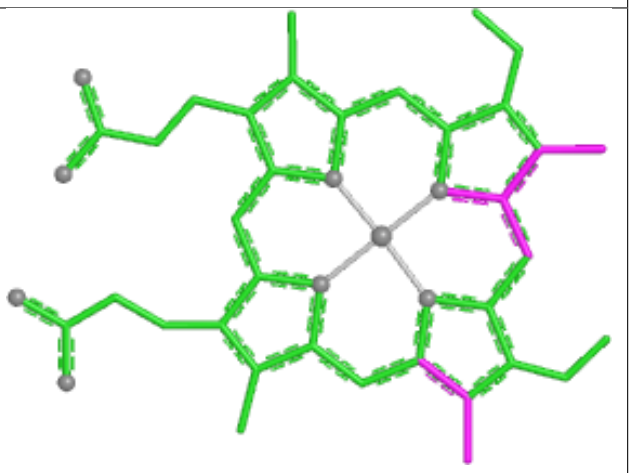


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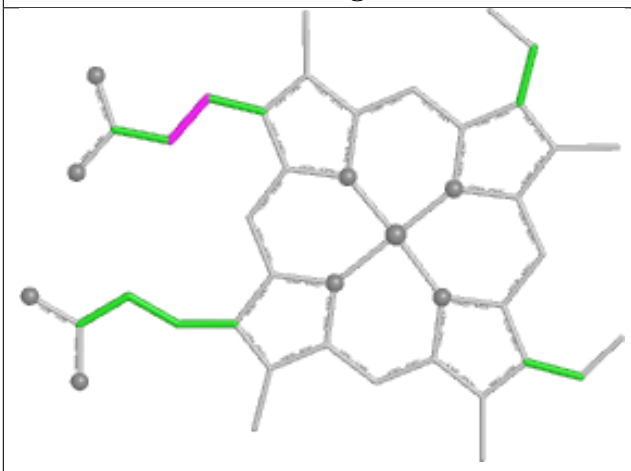
Ligand HEM f 101



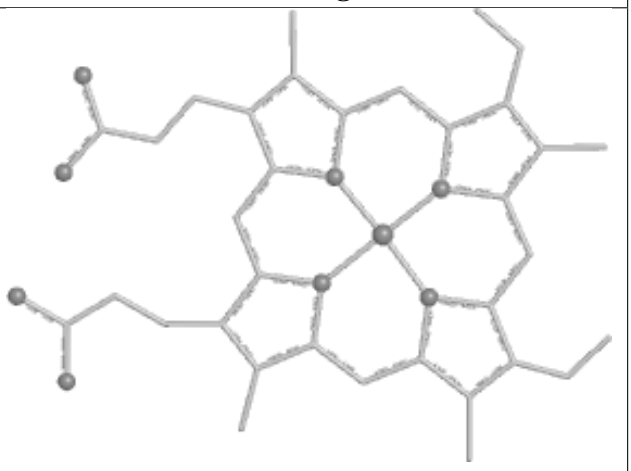
Bond lengths



Bond angles

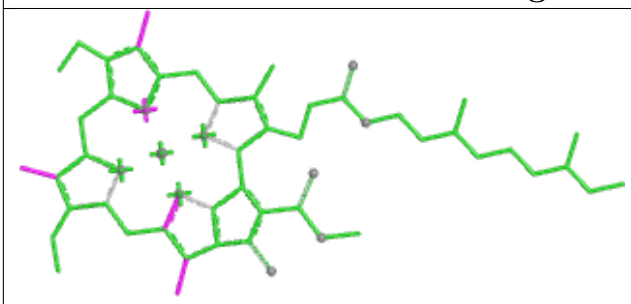


Torsions

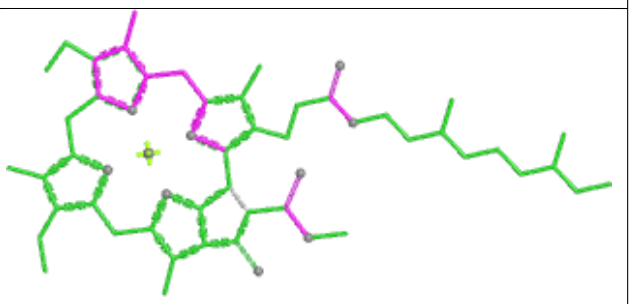


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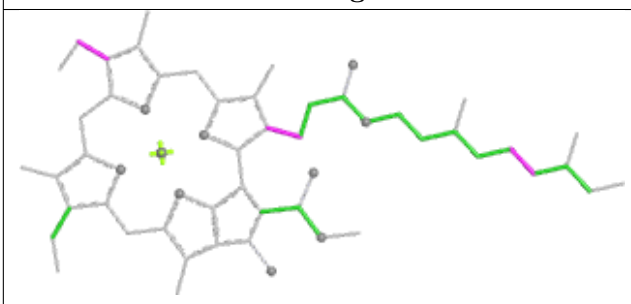
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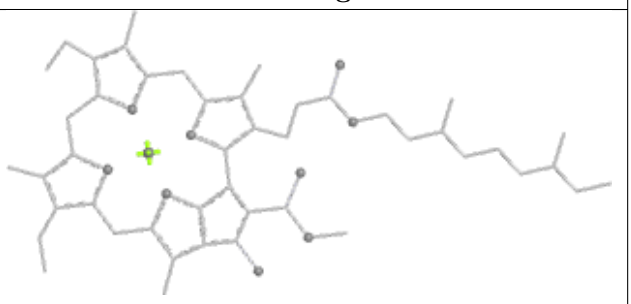
Bond lengths



Bond angles

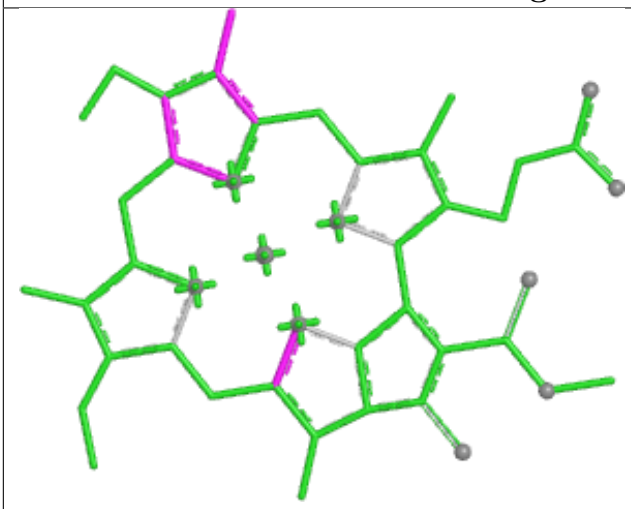


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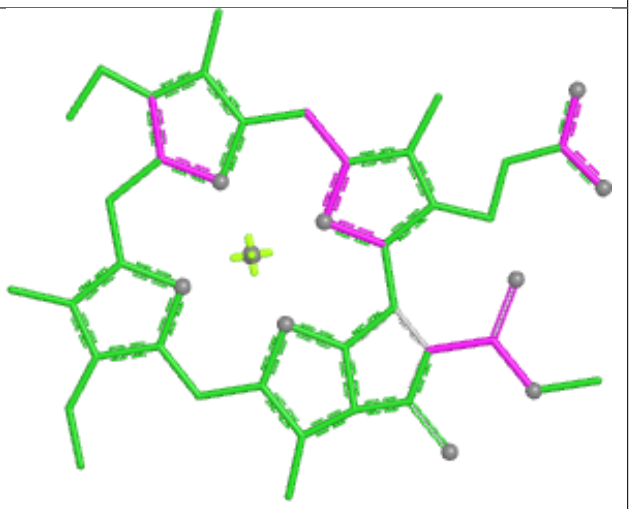


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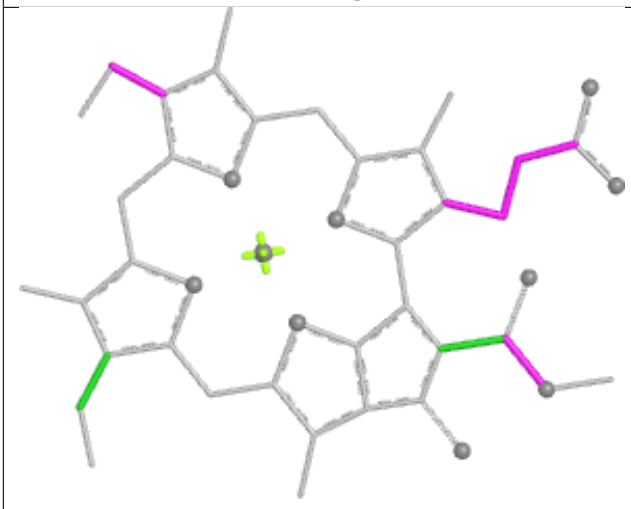
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Bond lengths



Bond angles

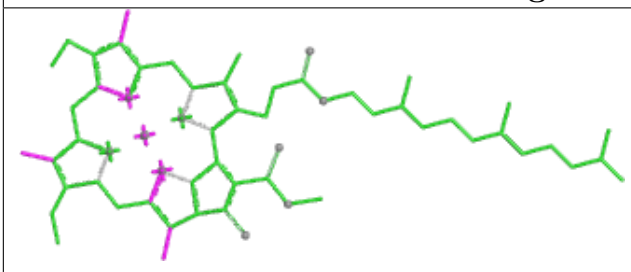


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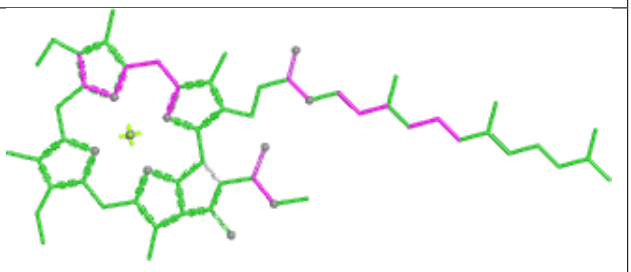


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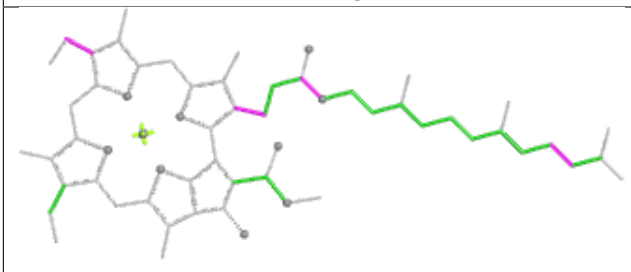
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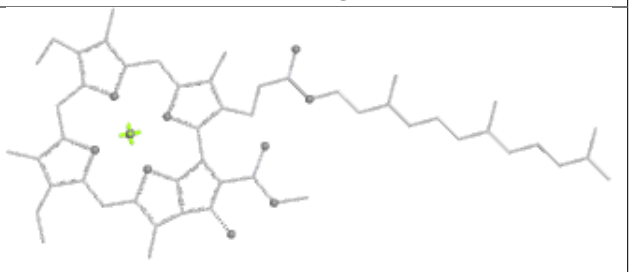
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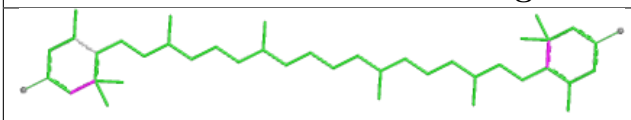


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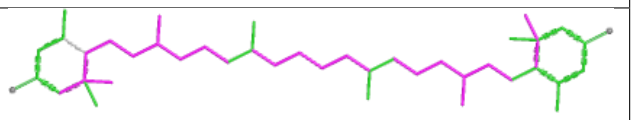


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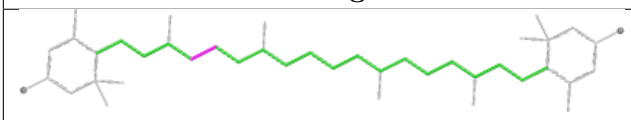
Ligand LUT Y 1621



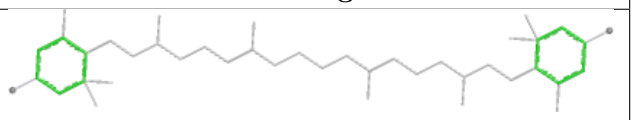
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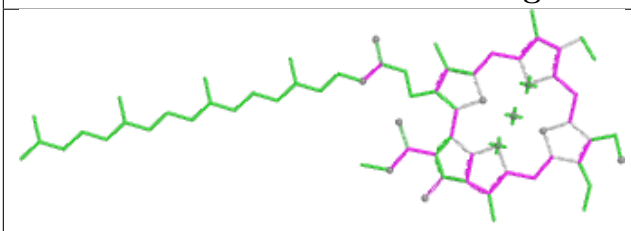


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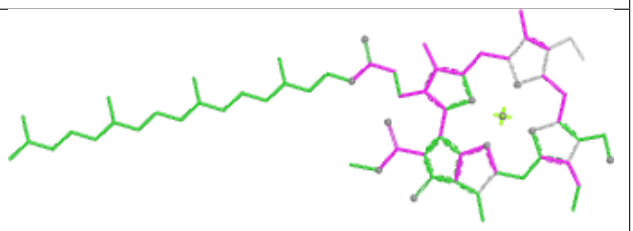


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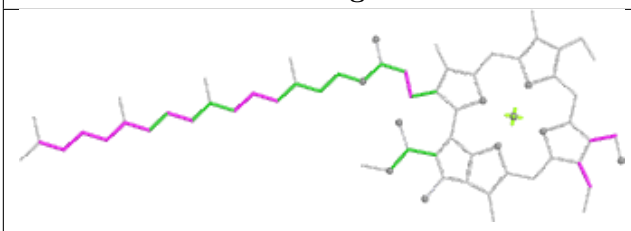
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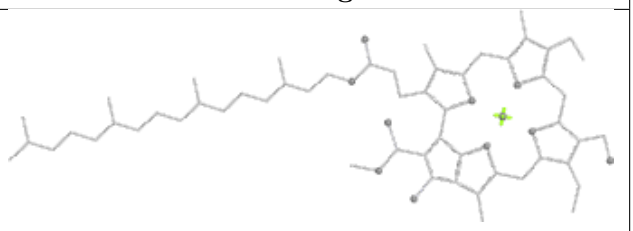
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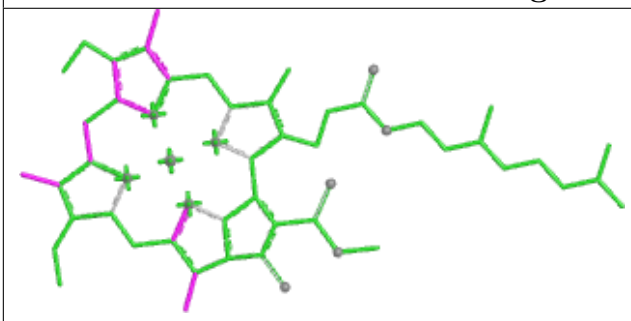


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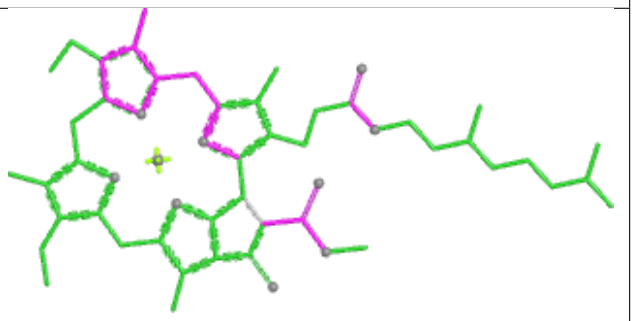


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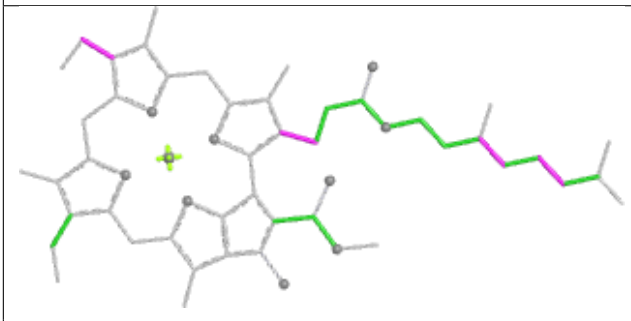
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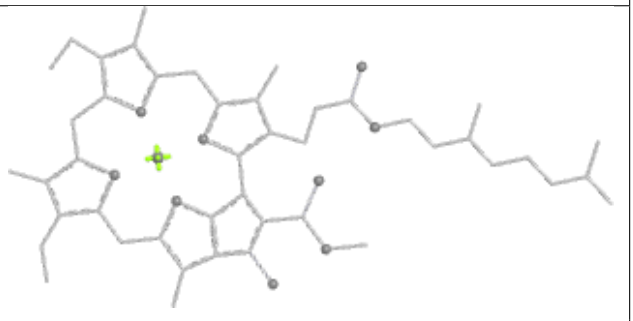
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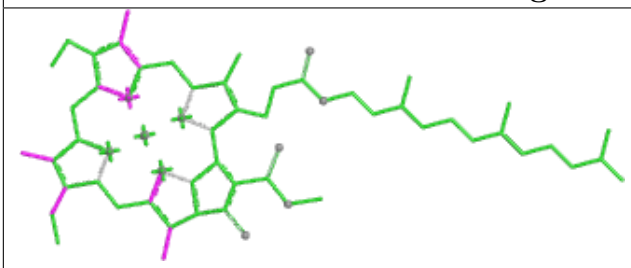


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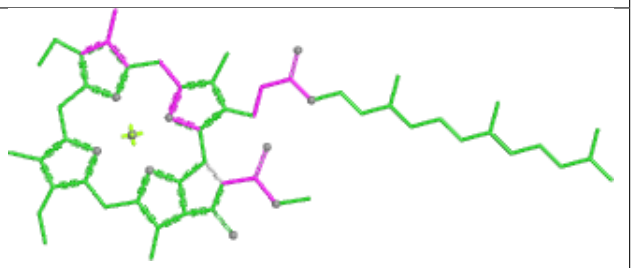


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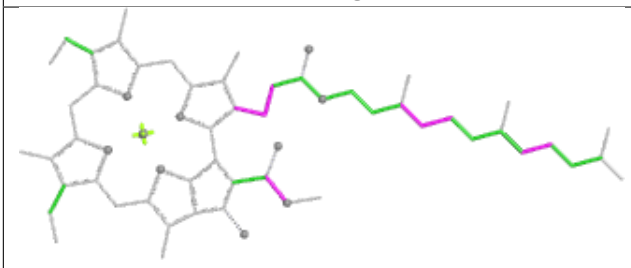
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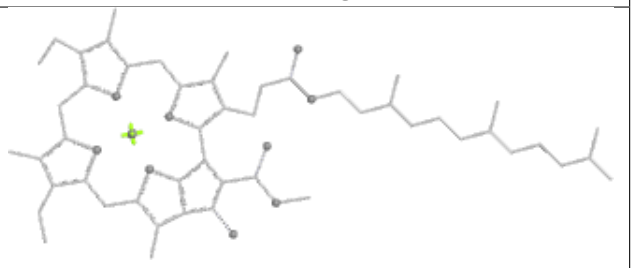
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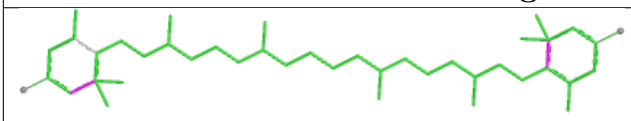


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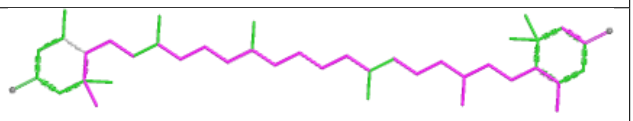


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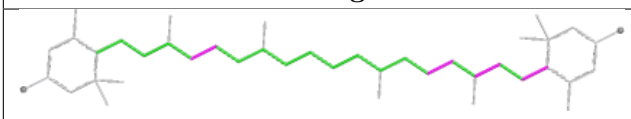
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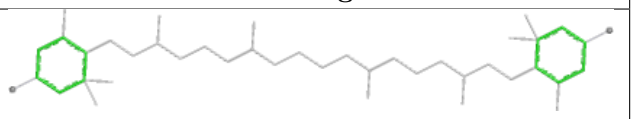
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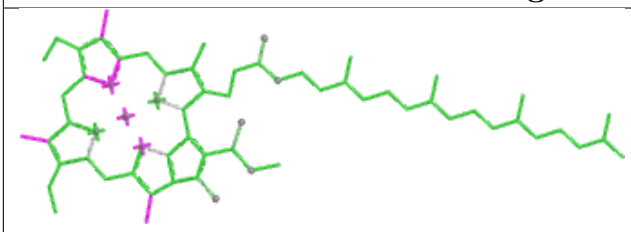


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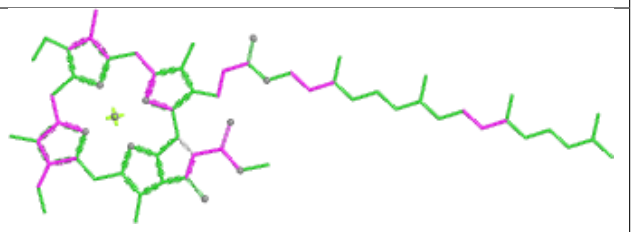


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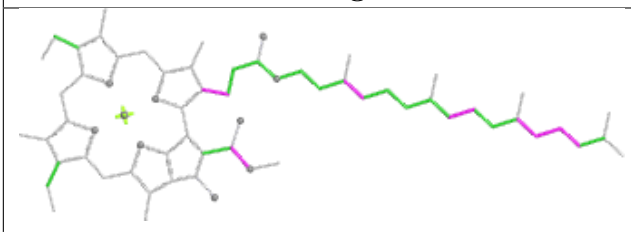
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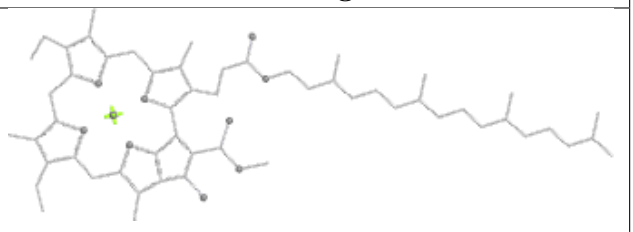
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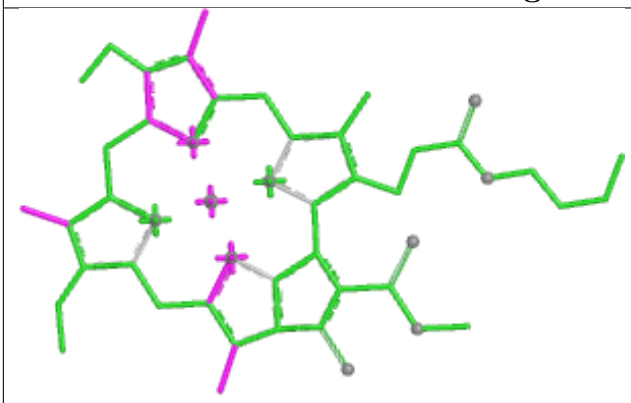


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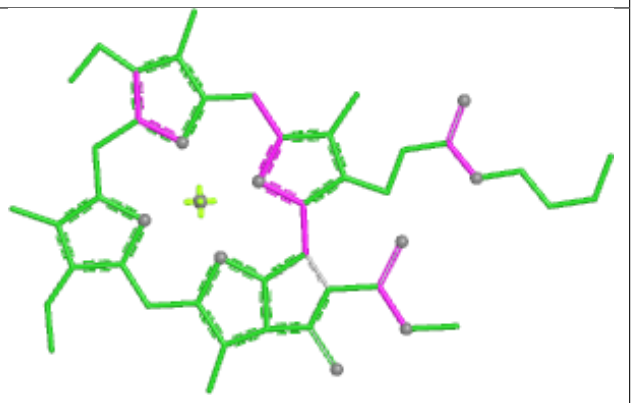


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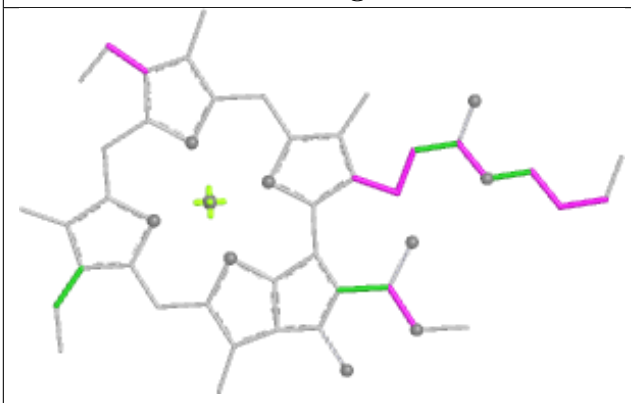
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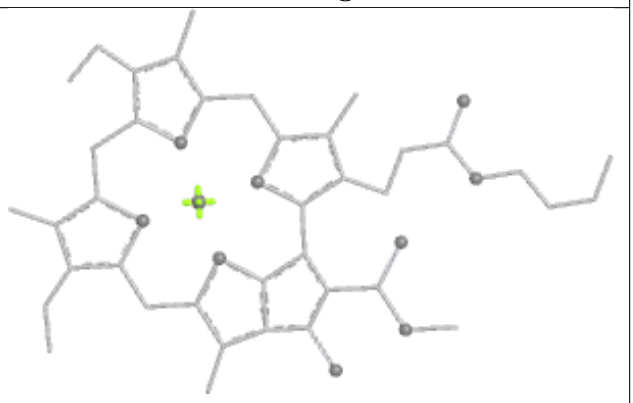
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Bond angles



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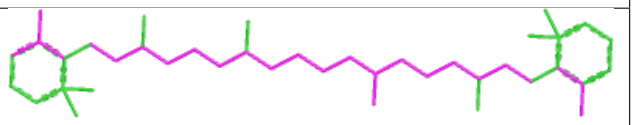


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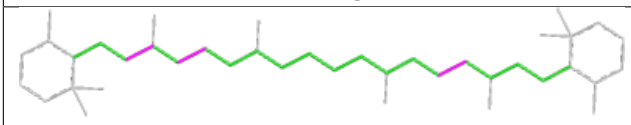
Ligand BCR c 517



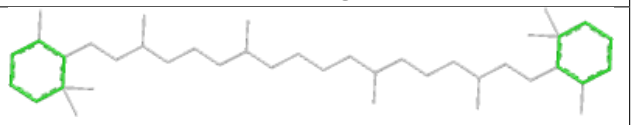
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Bond angles

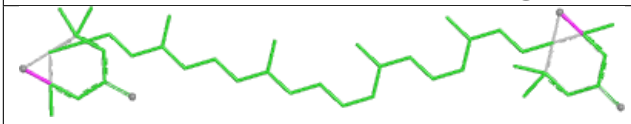


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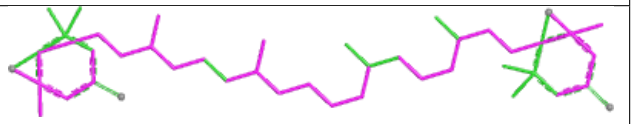


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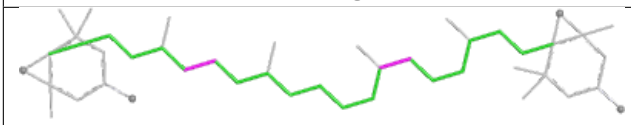
Ligand XAT n 1622



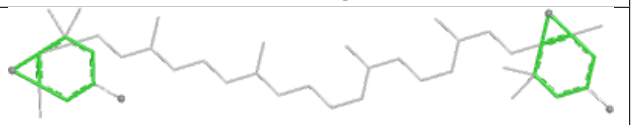
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Bond angles

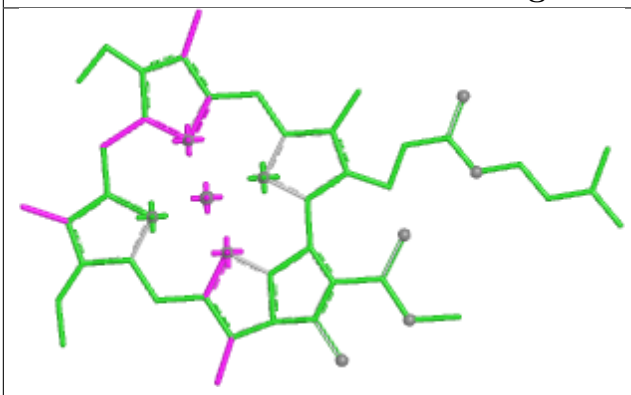


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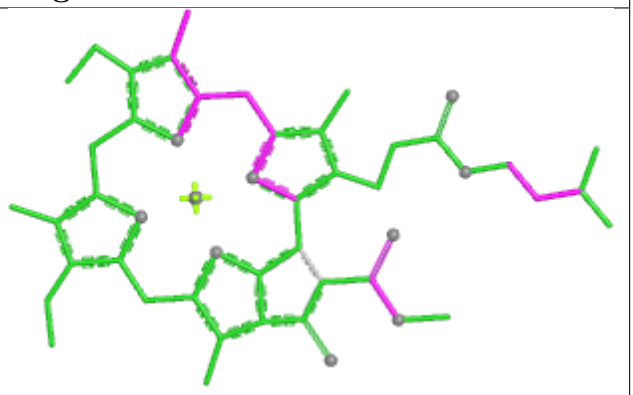


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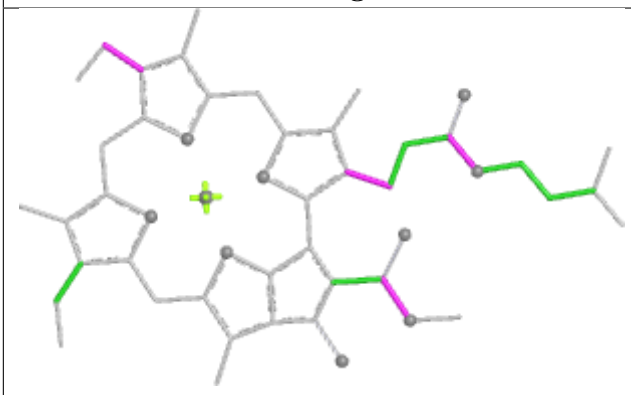
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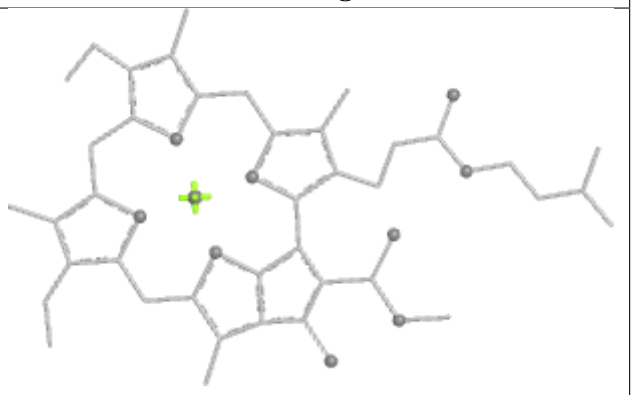
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Bond angles

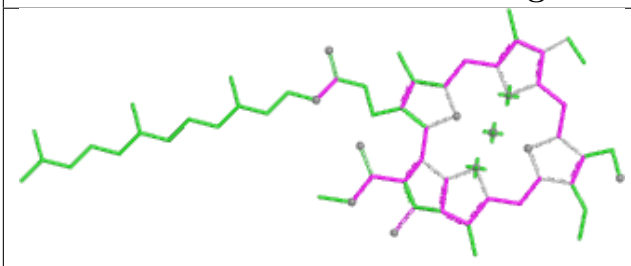


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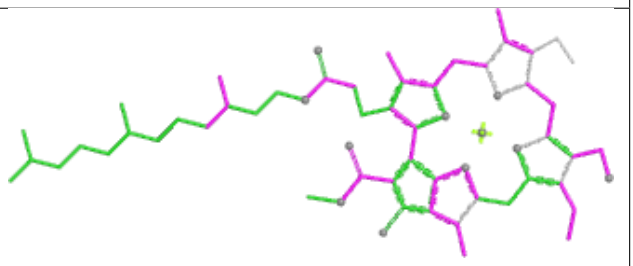


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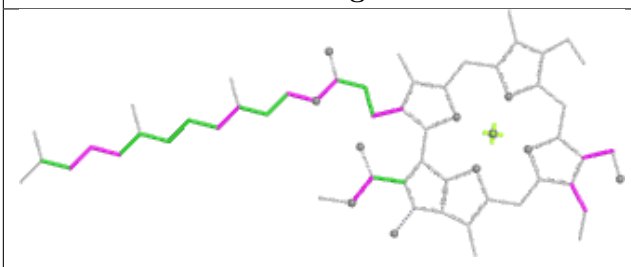
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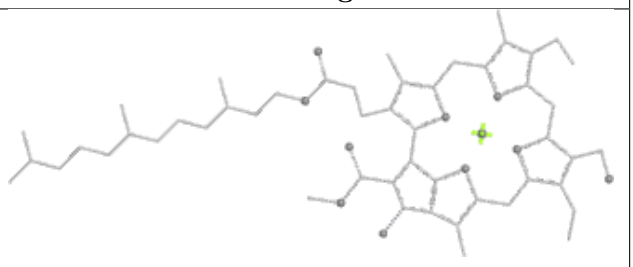
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Bond angles

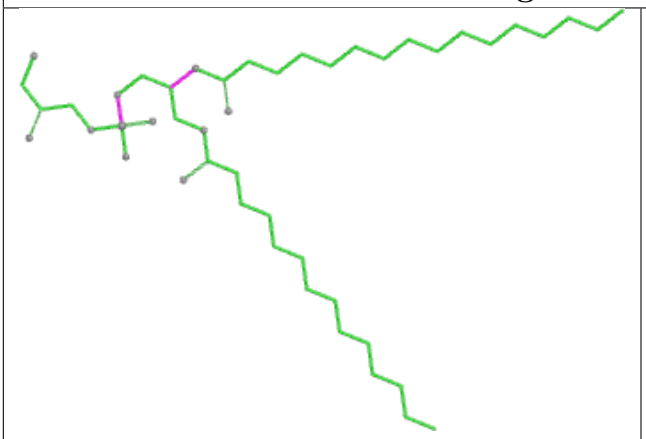


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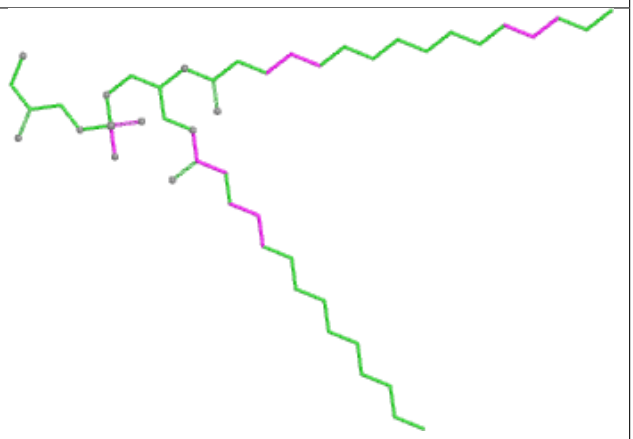


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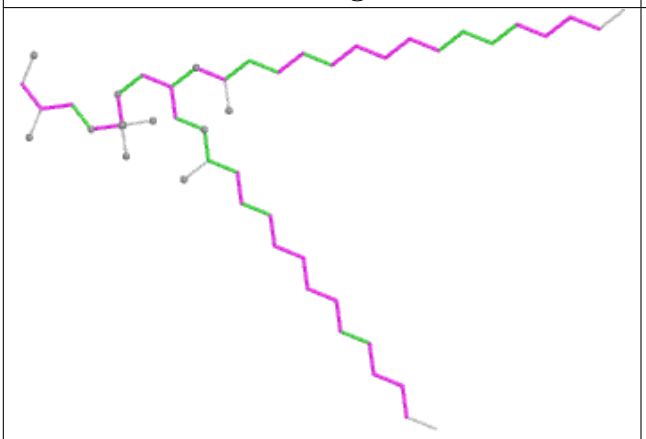
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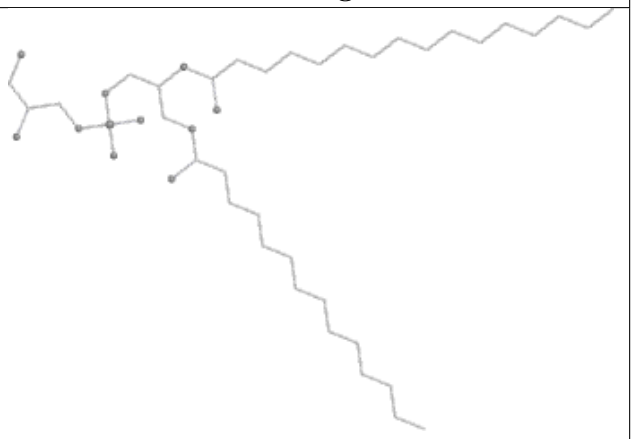
Bond lengths



Bond angles

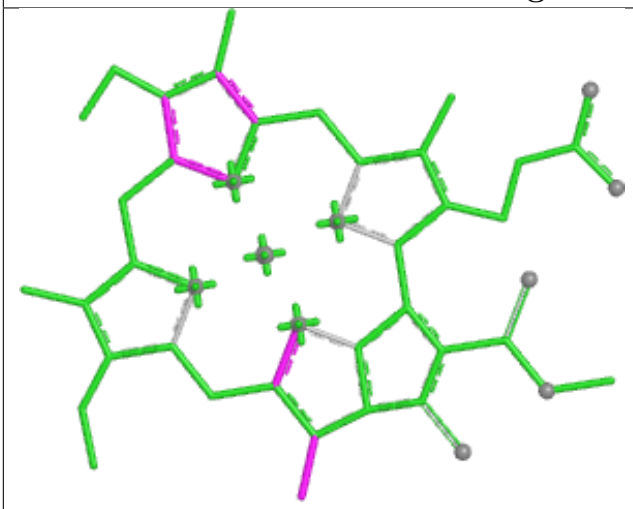


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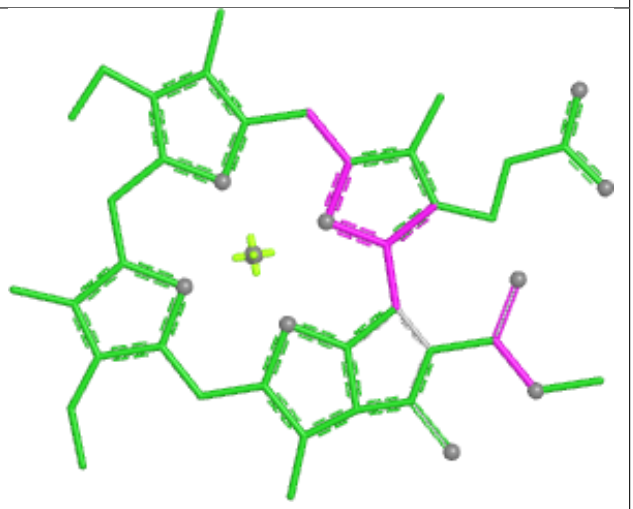


Rings

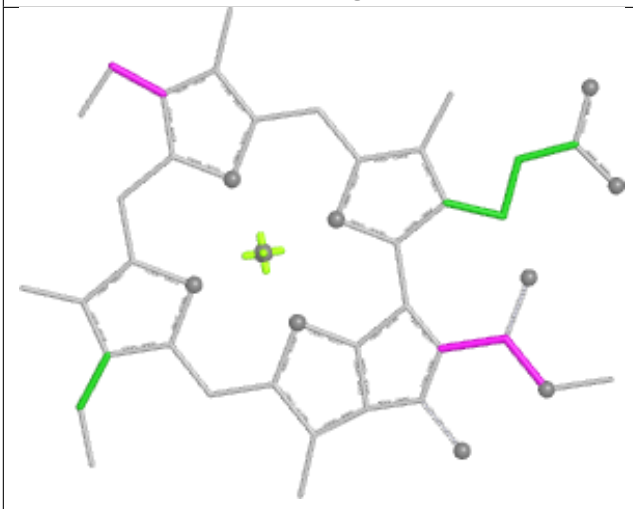
Ligand CLA S 603



Bond lengths



Bond angles

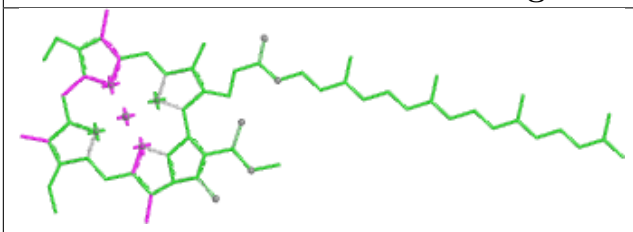


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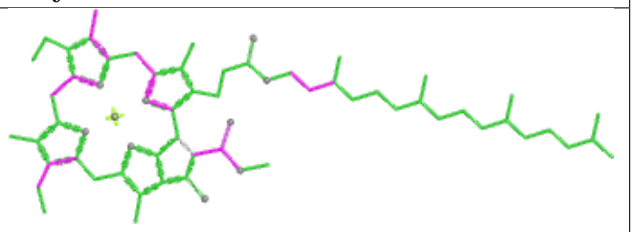


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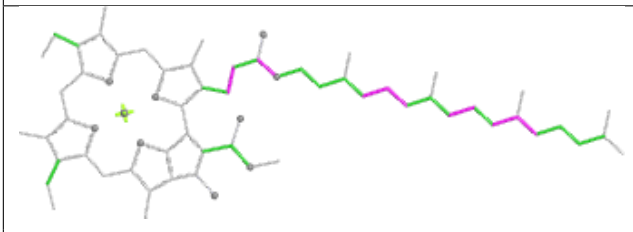
Ligand CLA y 613



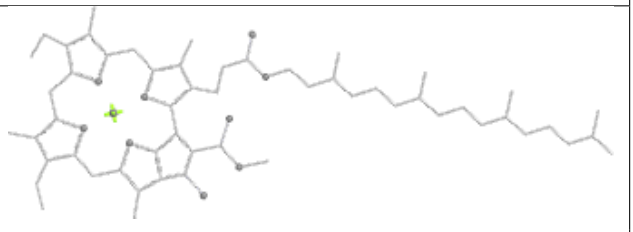
Bond lengths



Bond angles

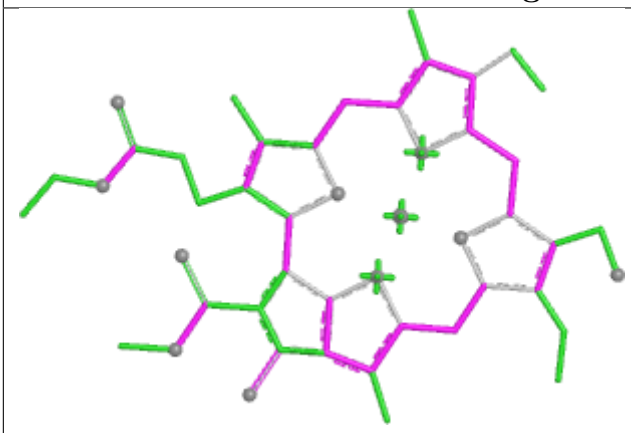


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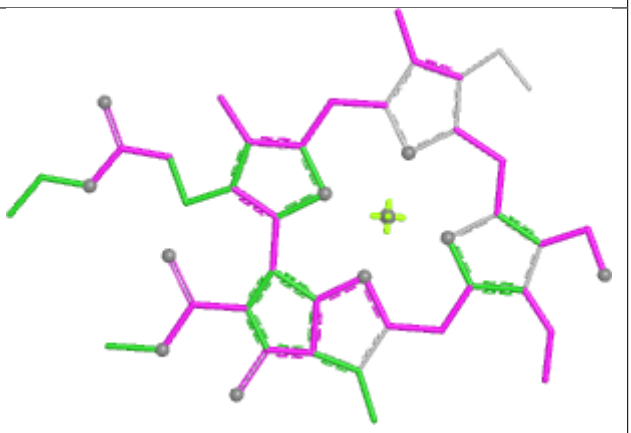


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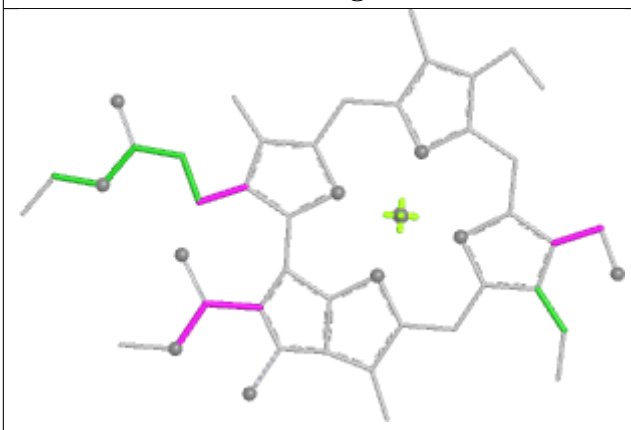
Ligand CHL N 605



Bond lengths



Bond angles

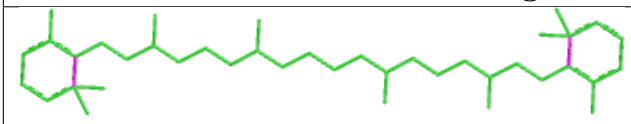


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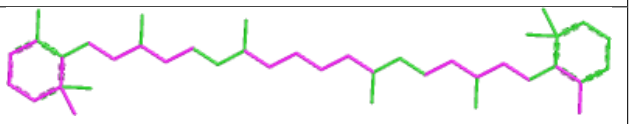


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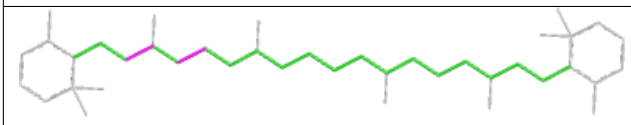
Ligand BCR H 101



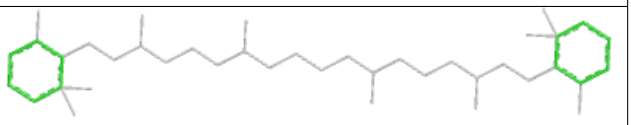
Bond lengths



Bond angles

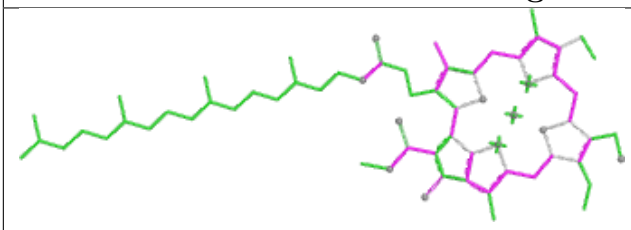


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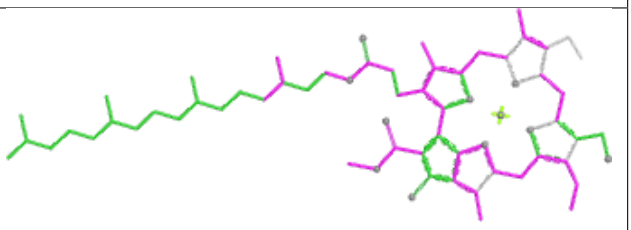


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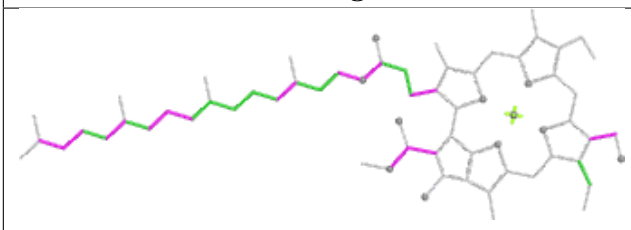
Ligand CHL n 609



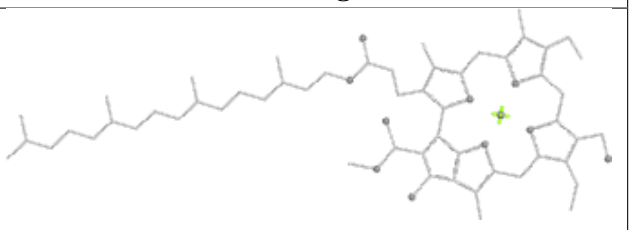
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Bond angles

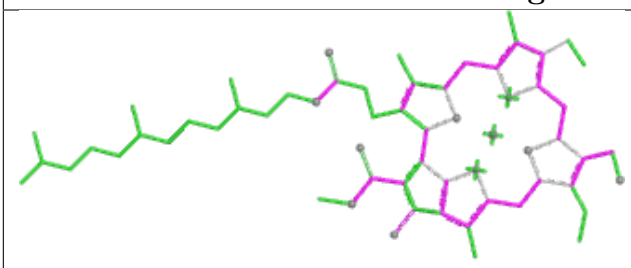


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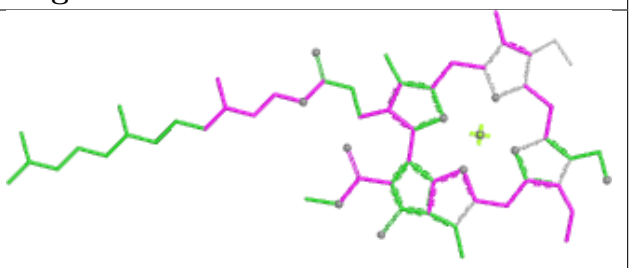


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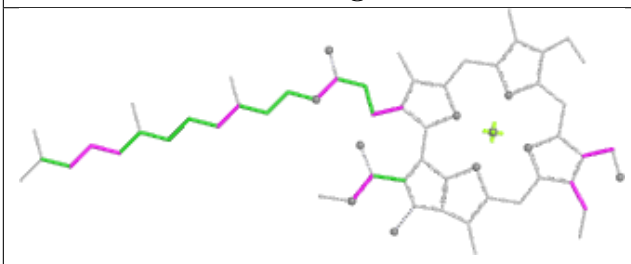
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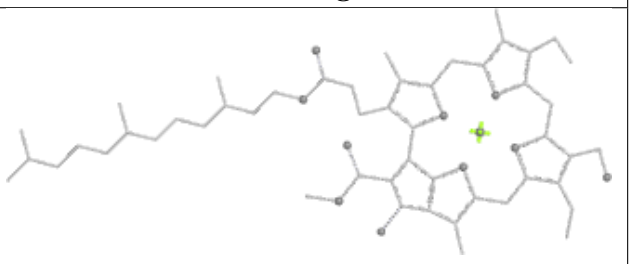
Bond lengths



Bond angles

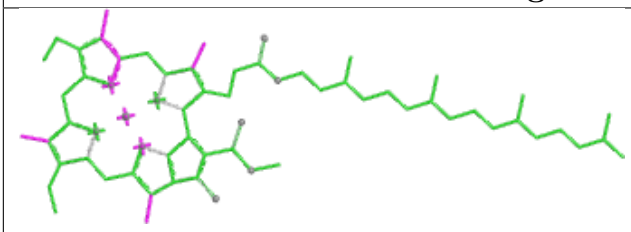


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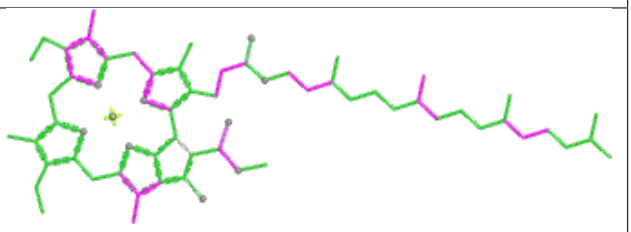


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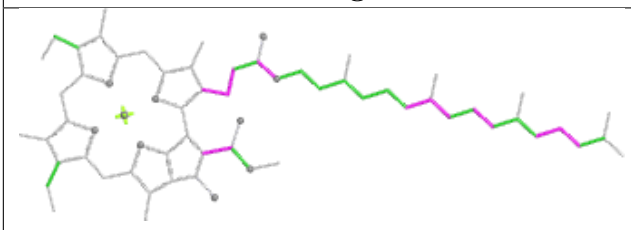
Ligand CLA b 613



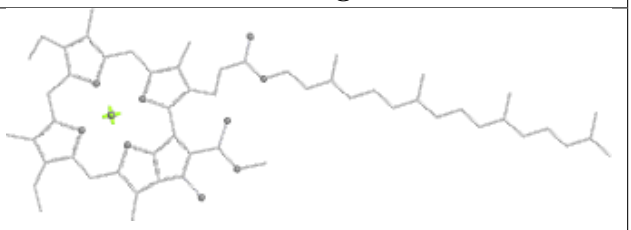
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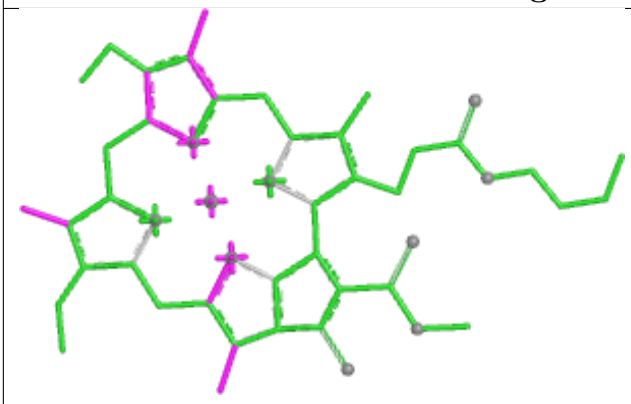


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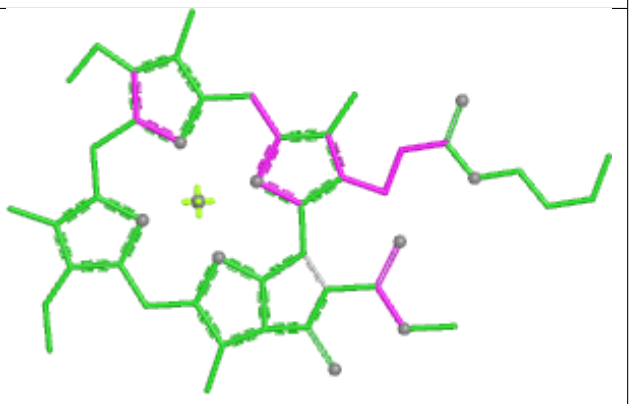


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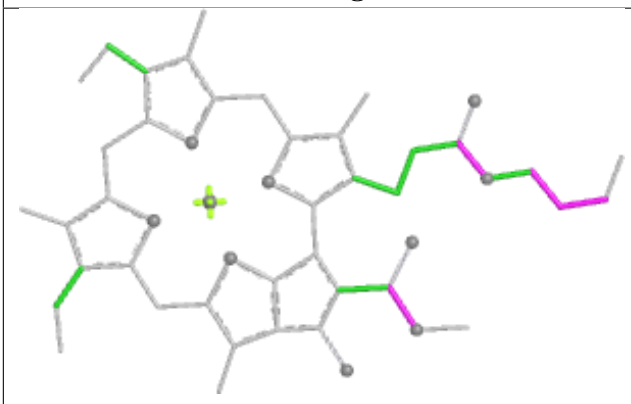
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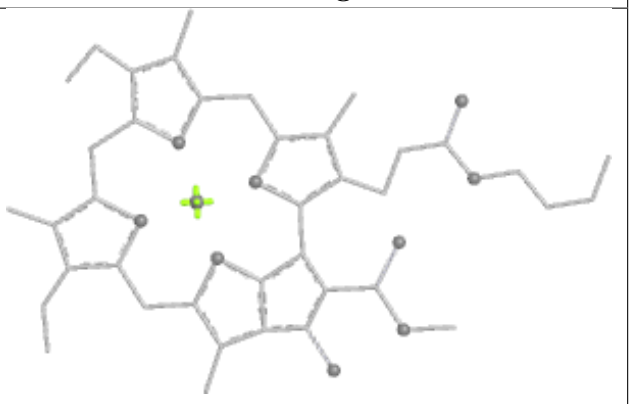
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Bond angles

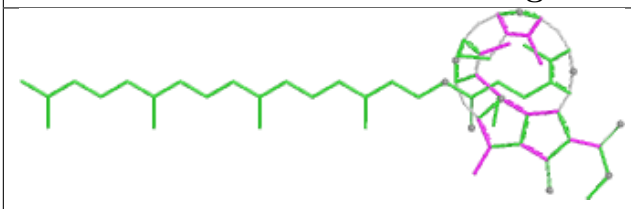


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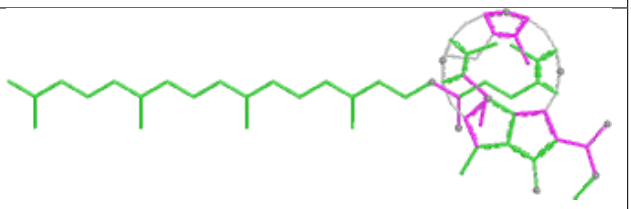


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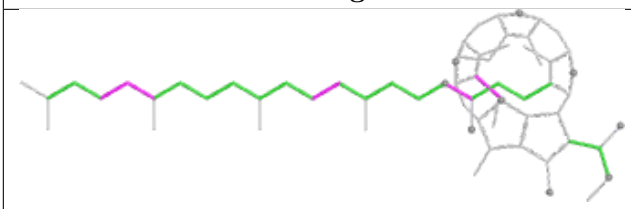
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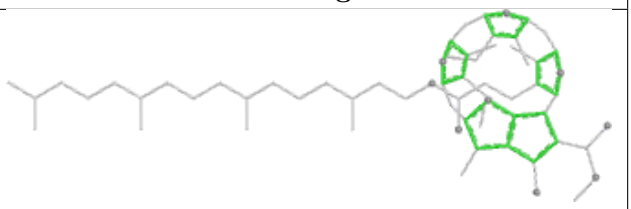
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Bond angles

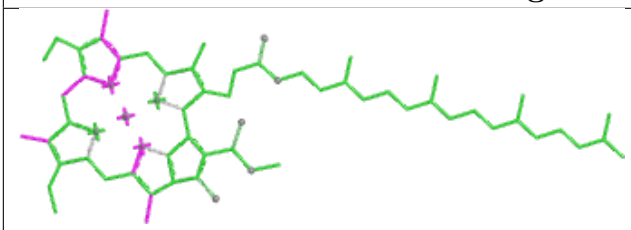


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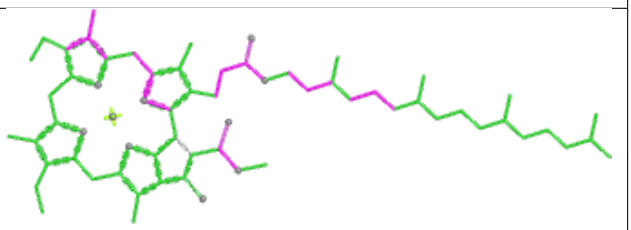


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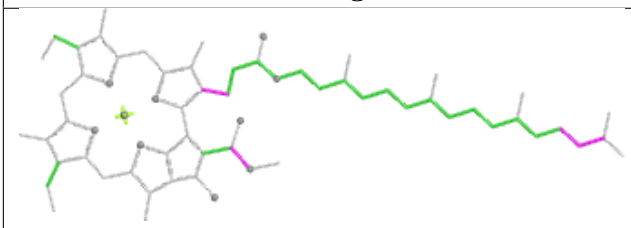
Ligand CLA b 610



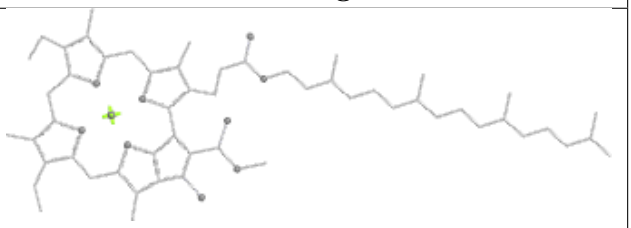
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Bond angles

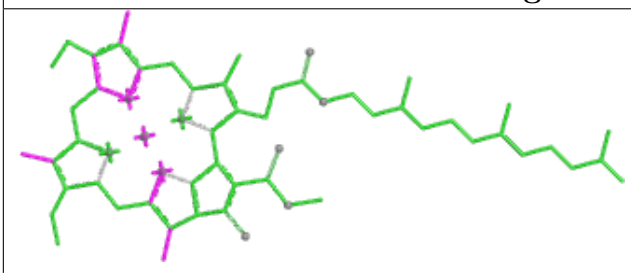


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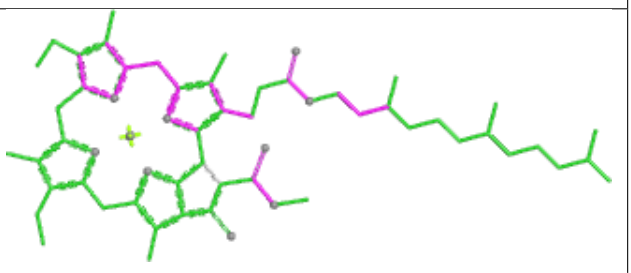


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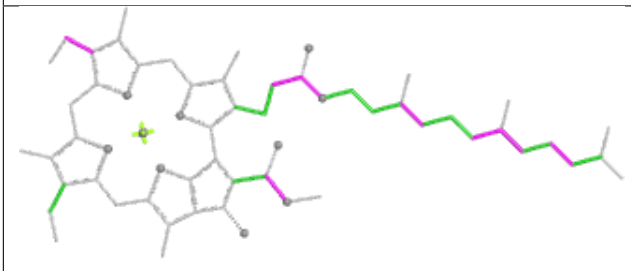
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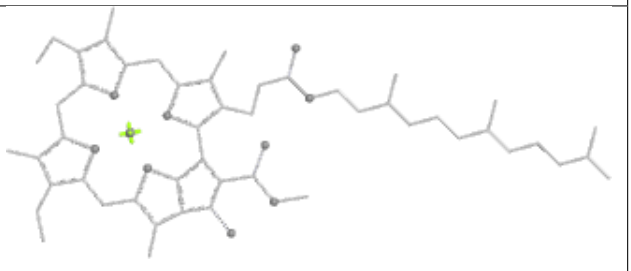
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Bond angles

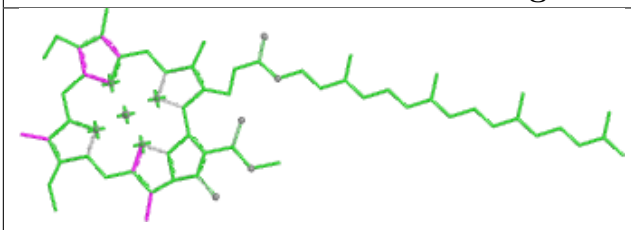


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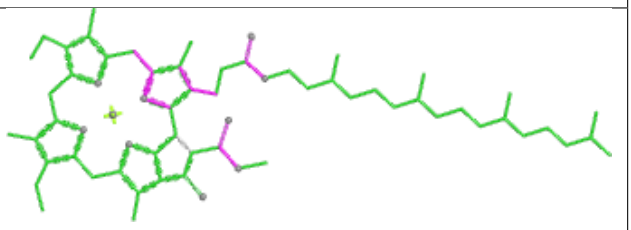


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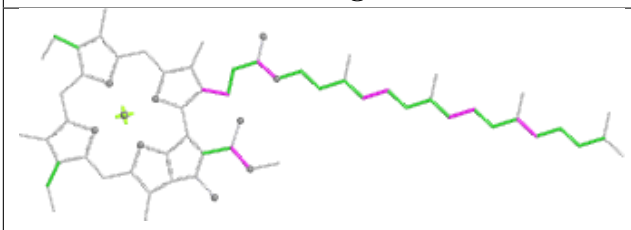
Ligand CLA c 512



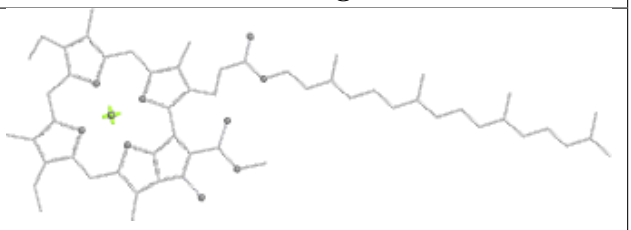
Bond lengths



Bond angles

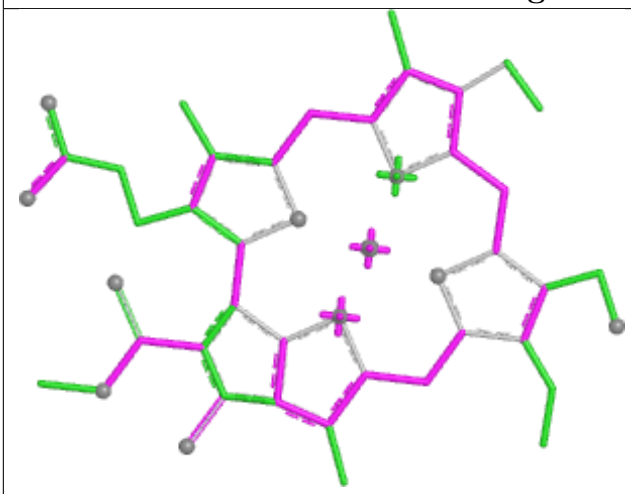


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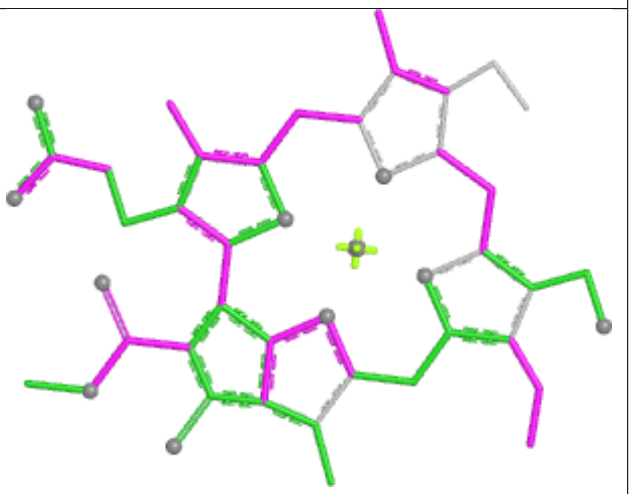


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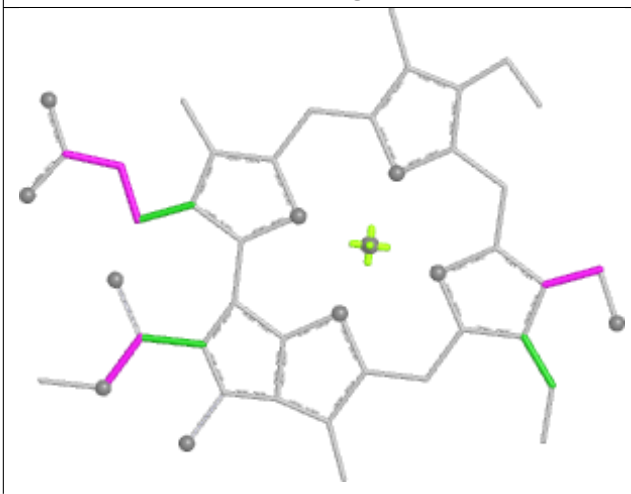
Ligand CHL 5 606



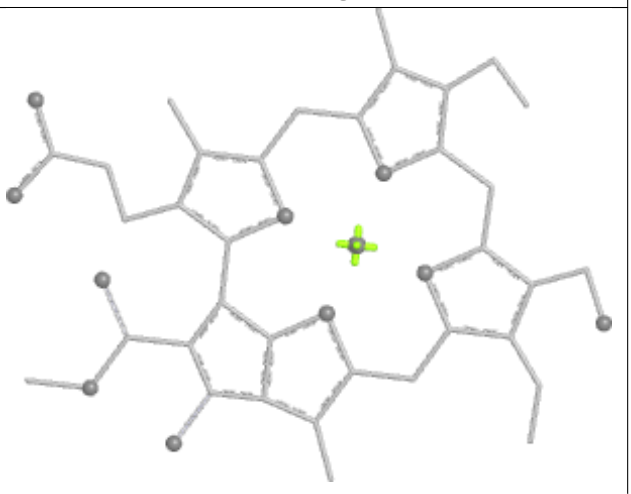
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Bond angles

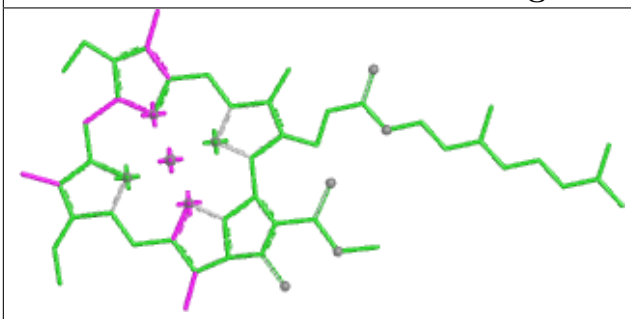


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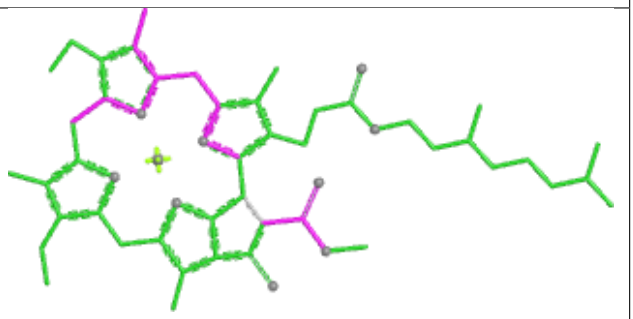


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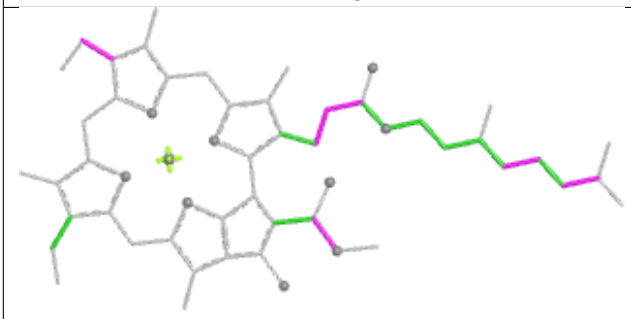
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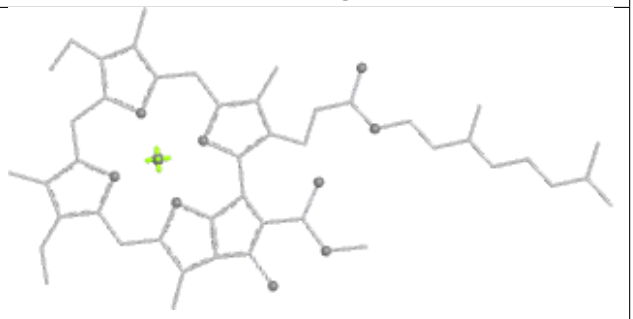
Bond lengths



Bond angles

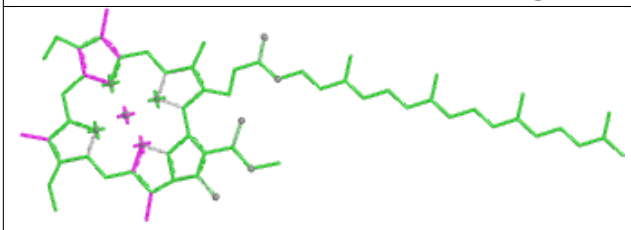


Torsions

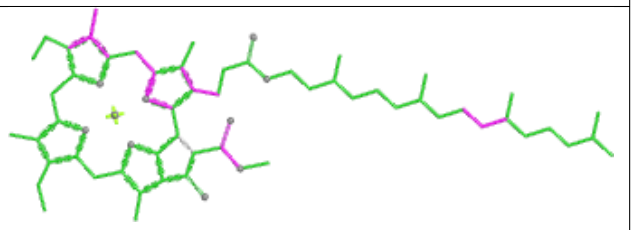


Rings

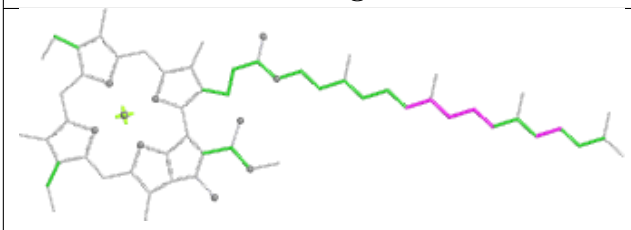
Ligand CLA c 509



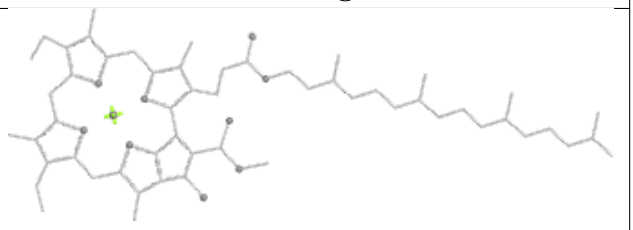
Bond lengths



Bond angles

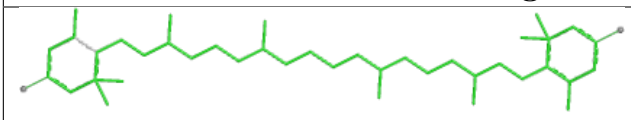


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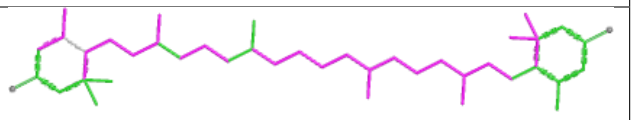


Rings

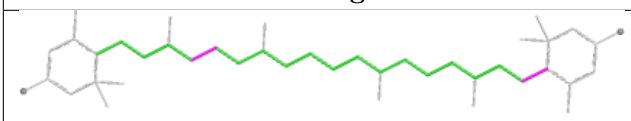
Ligand LUT s 1621



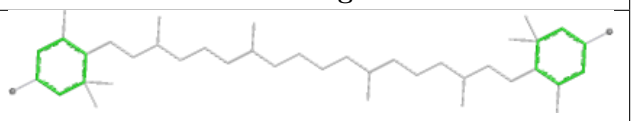
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Bond angles

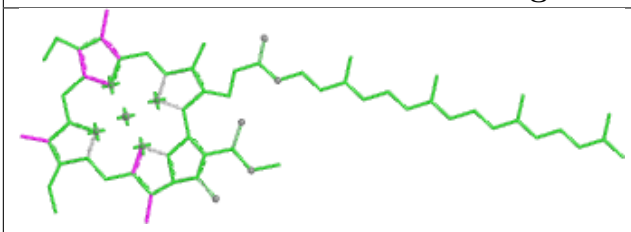


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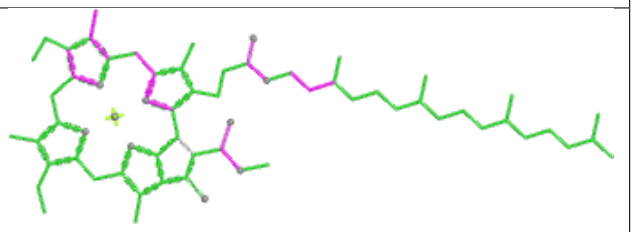


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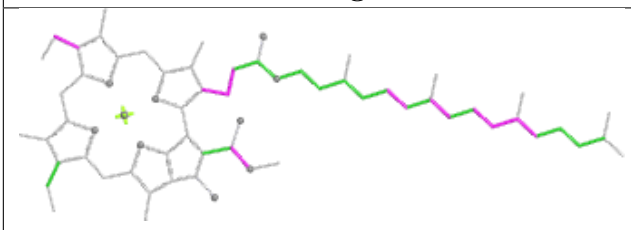
Ligand CLA r 610



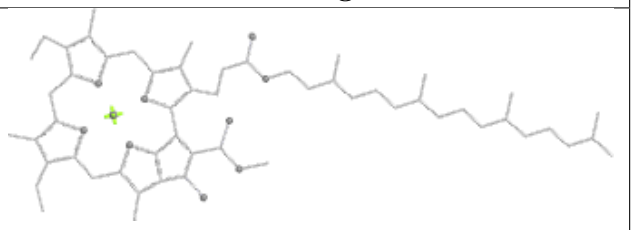
Bond lengths



Bond angles

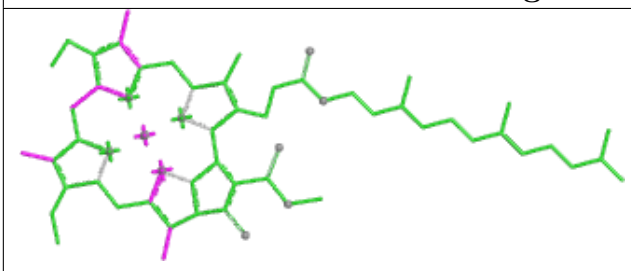


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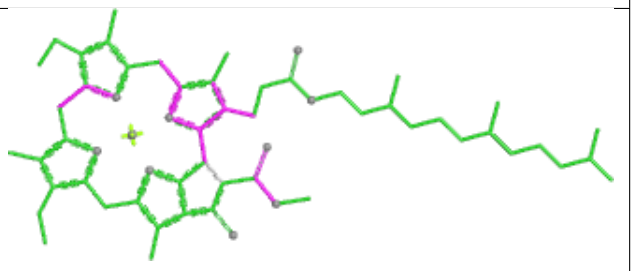


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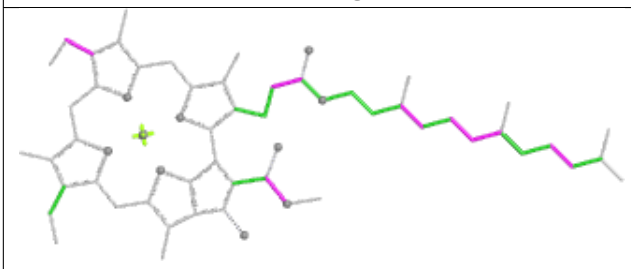
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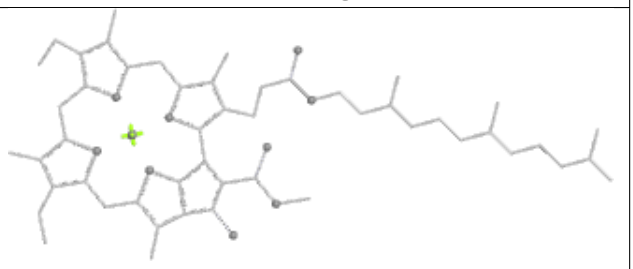
Bond lengths



Bond angles

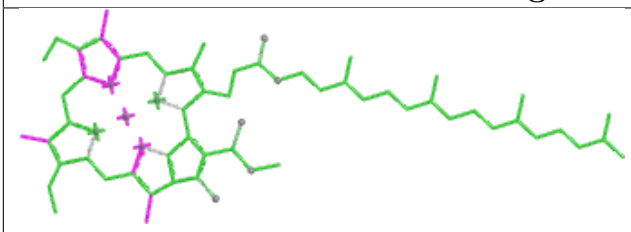


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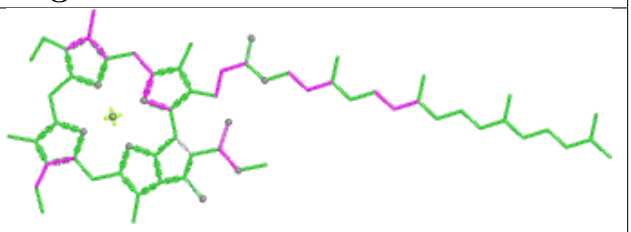


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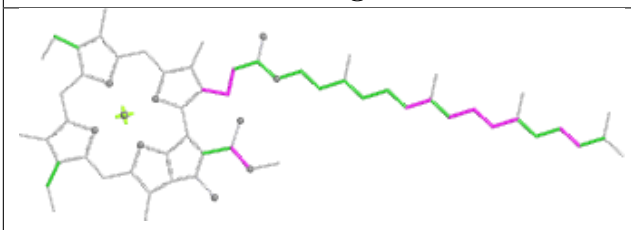
Ligand CLA g 602



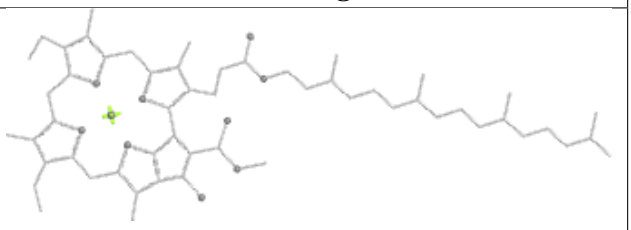
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Bond angles

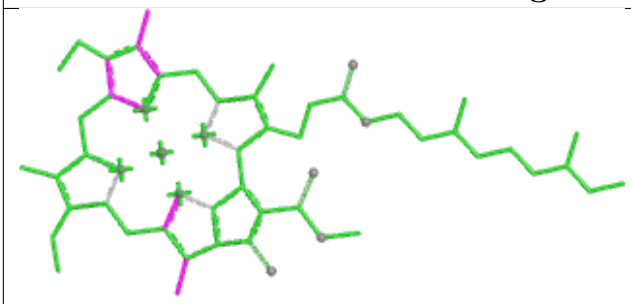


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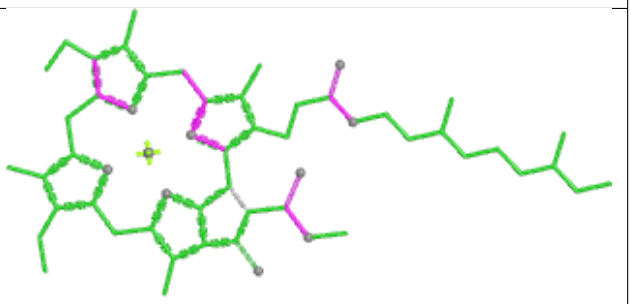


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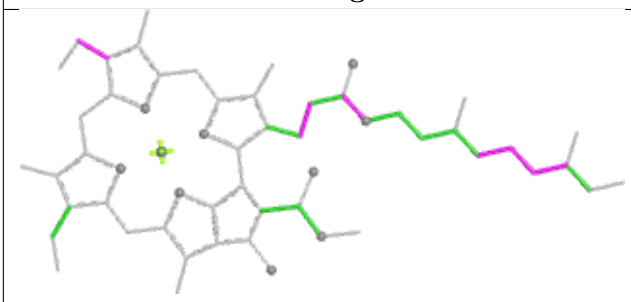
Ligand CLA s 611



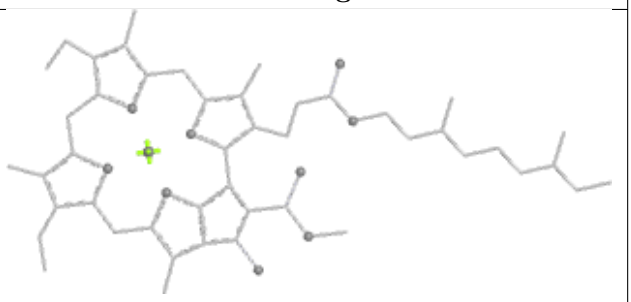
Bond lengths



Bond angles

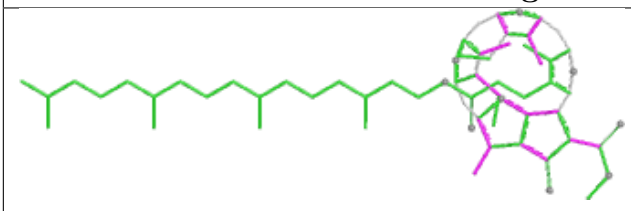


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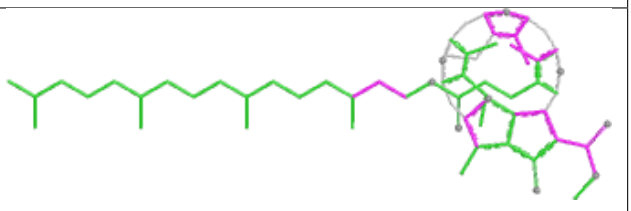


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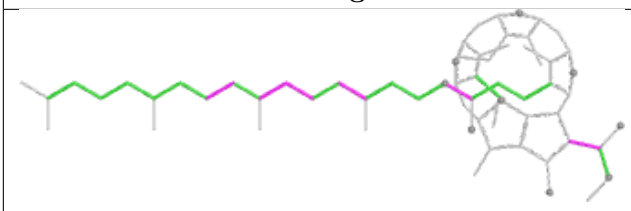
Ligand PHO A 409



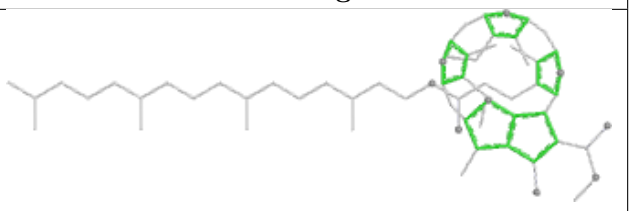
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Bond angles

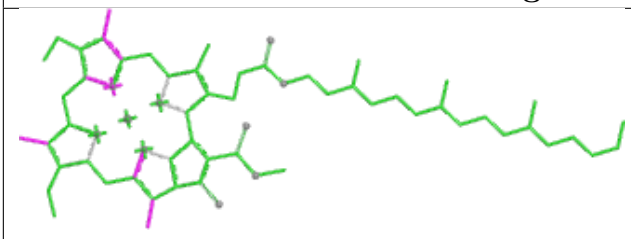


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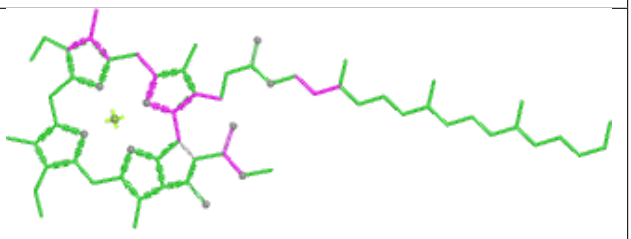


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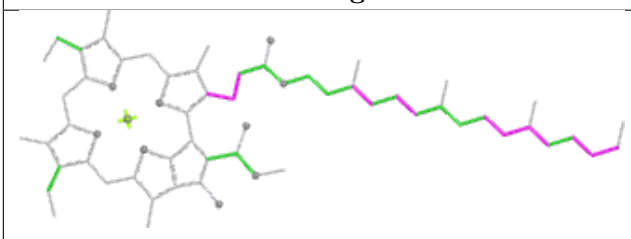
Ligand CLA G 610



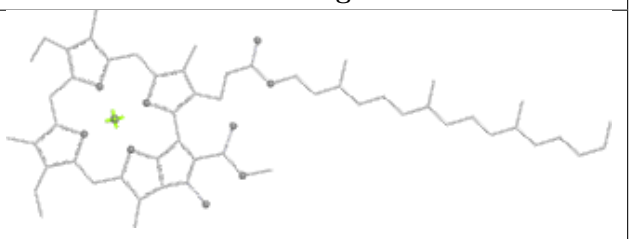
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Bond angles

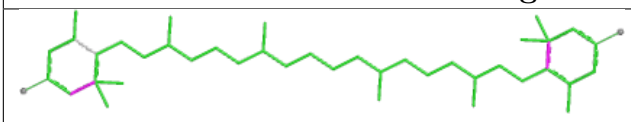


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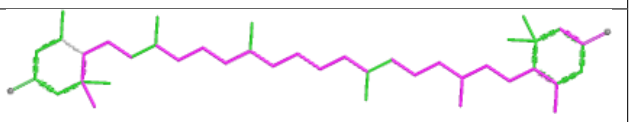


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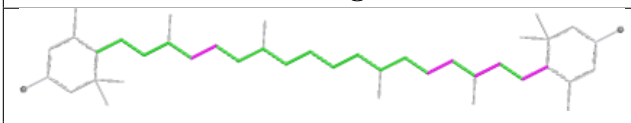
Ligand LUT 5 1621



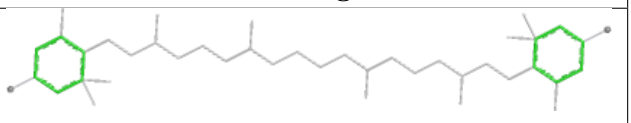
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Bond angles

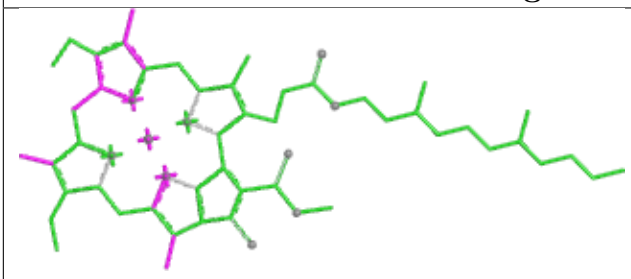


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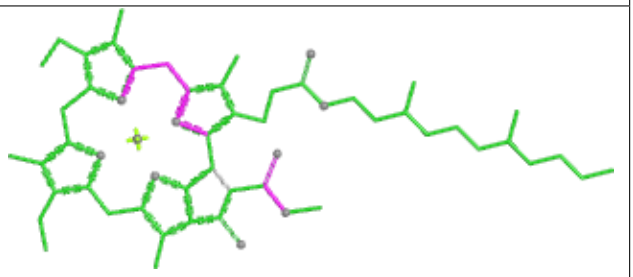


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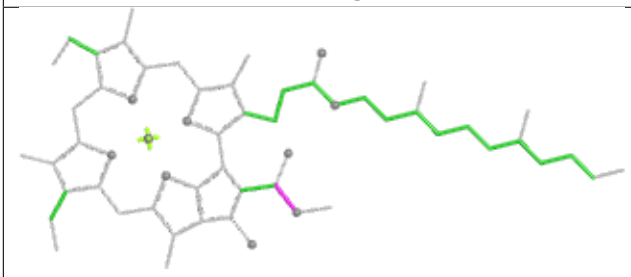
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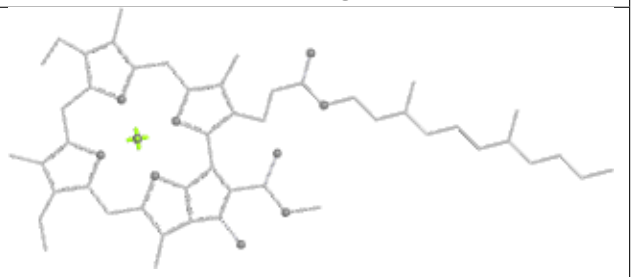
Bond lengths



Bond angles

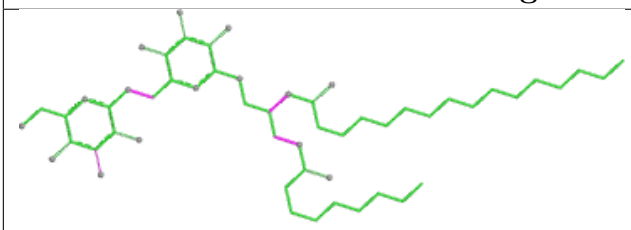


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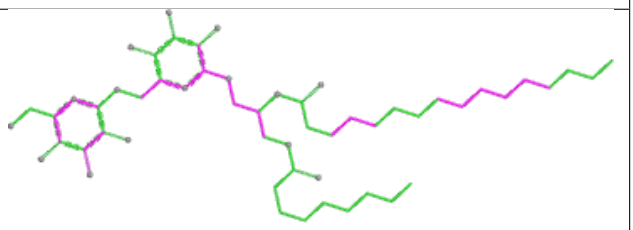


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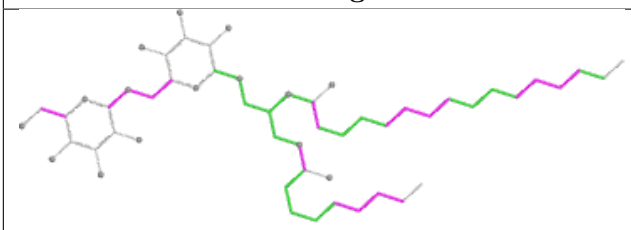
Ligand DGD C 518



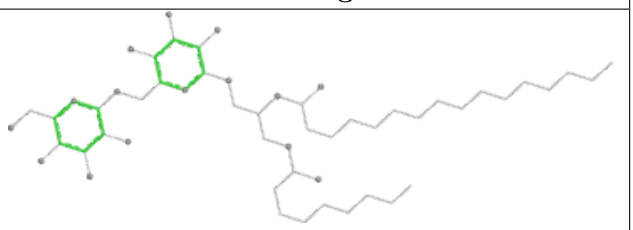
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Bond angles

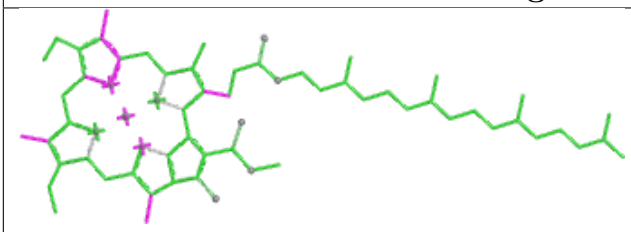


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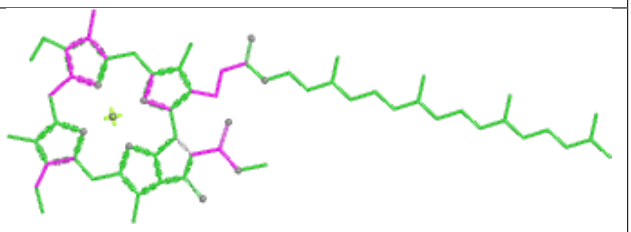


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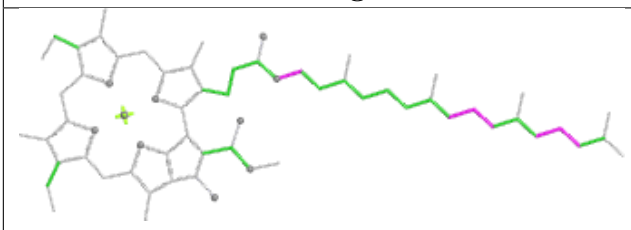
Ligand CLA d 402



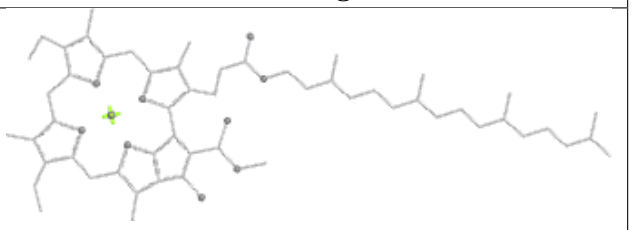
Bond lengths



Bond angles



Torsions

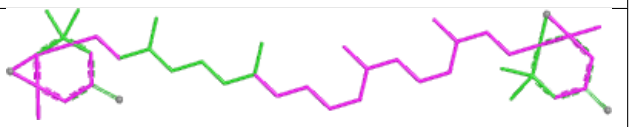


Rings

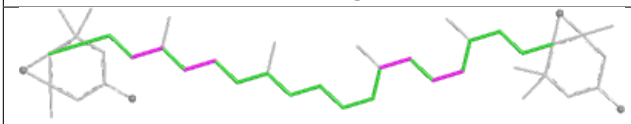
Ligand XAT r 622



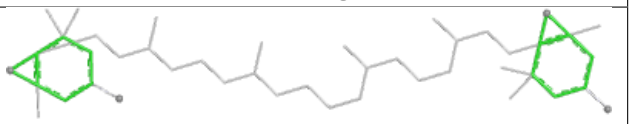
Bond lengths



Bond angles

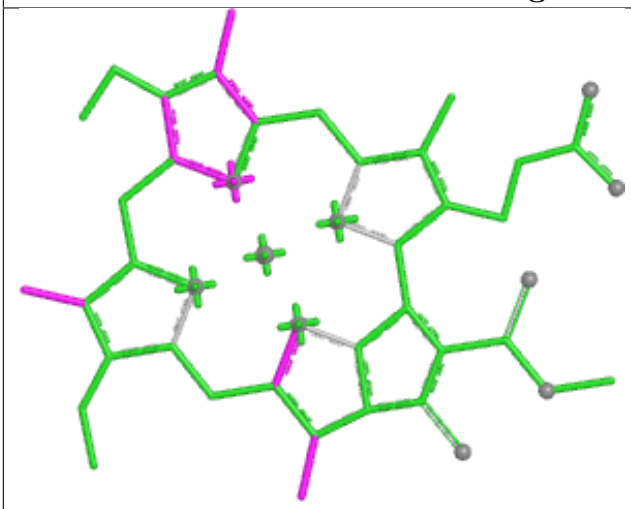


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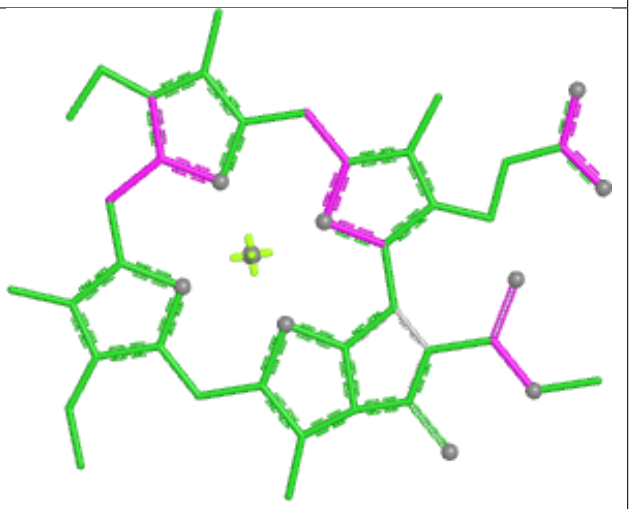


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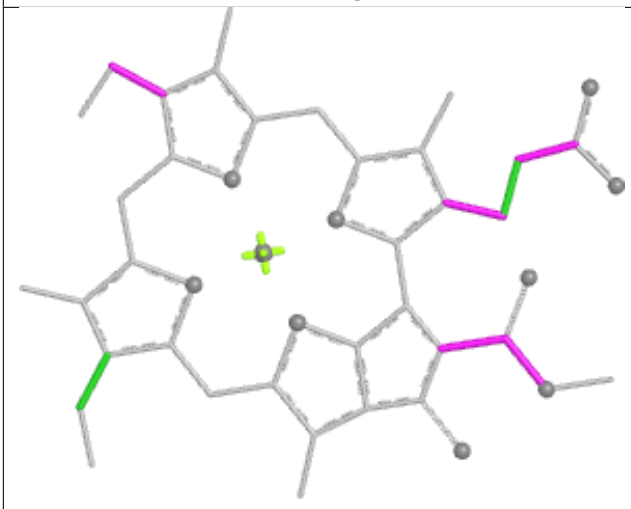
Ligand CLA 4 611



Bond lengths



Bond angles

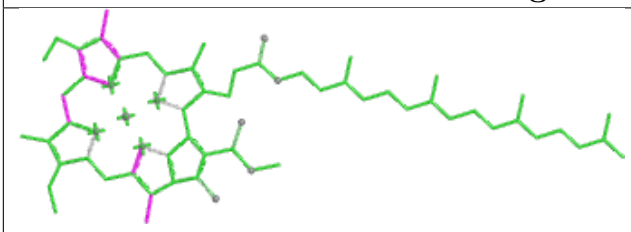


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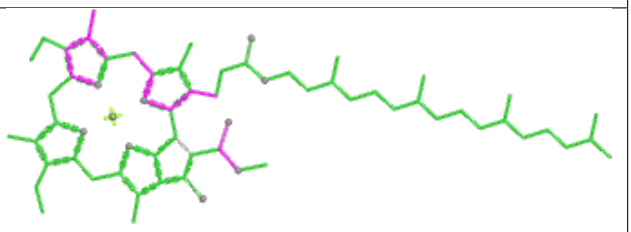


Rings

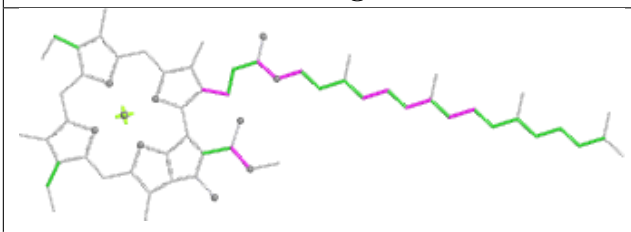
Ligand CLA c 511



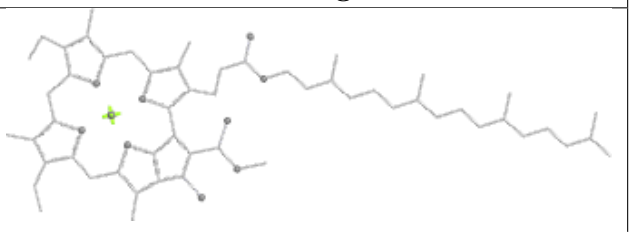
Bond lengths



Bond angles

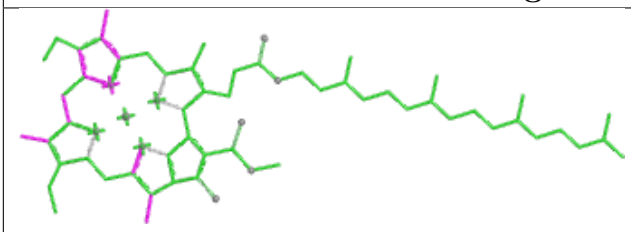


Torsions

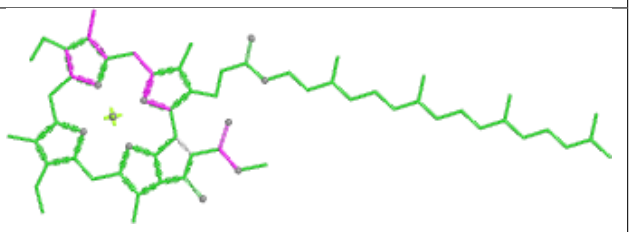


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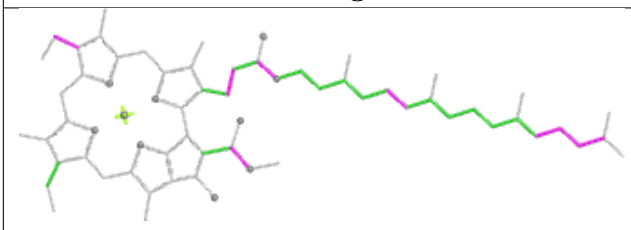
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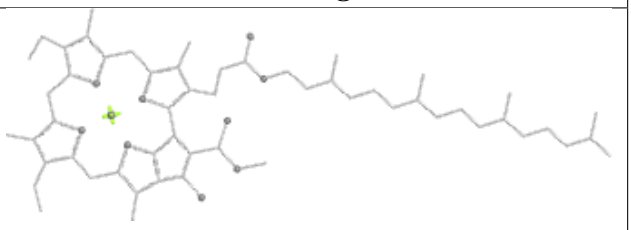
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Bond angles

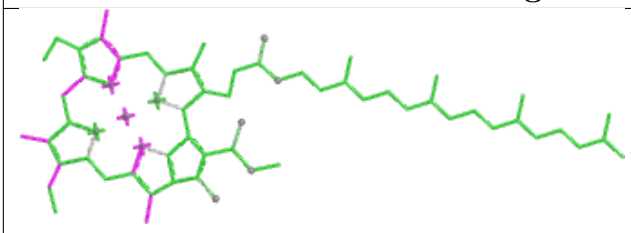


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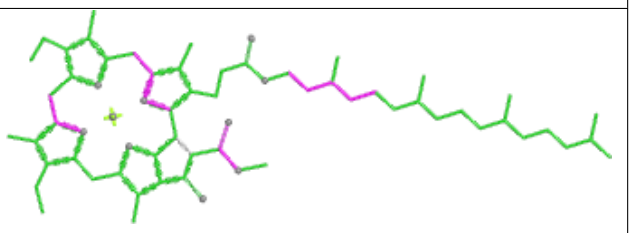


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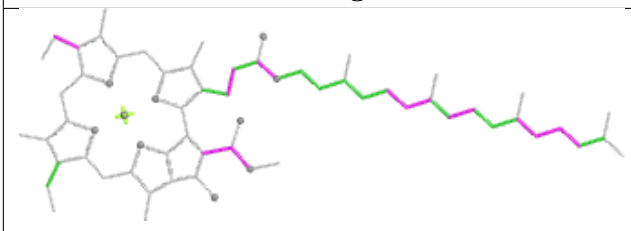
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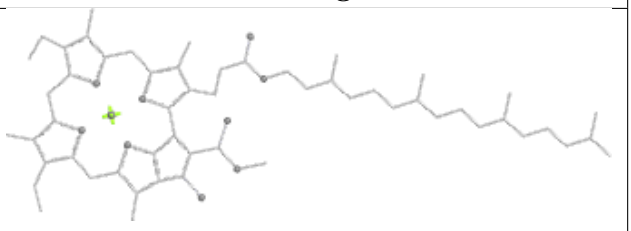
Bond lengths



Bond angles

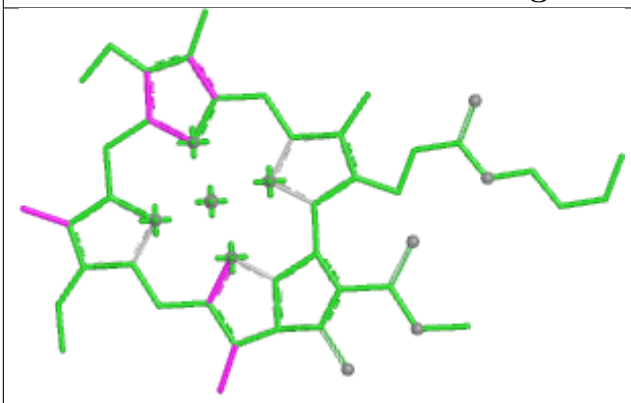


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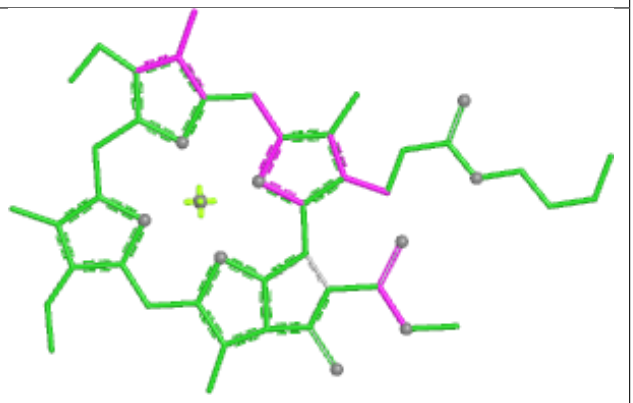


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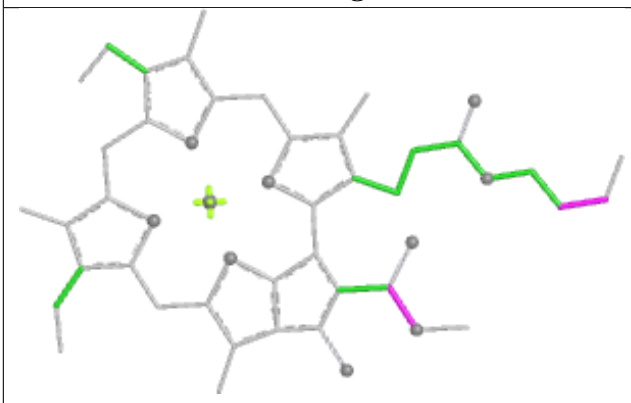
Ligand CLA s 612



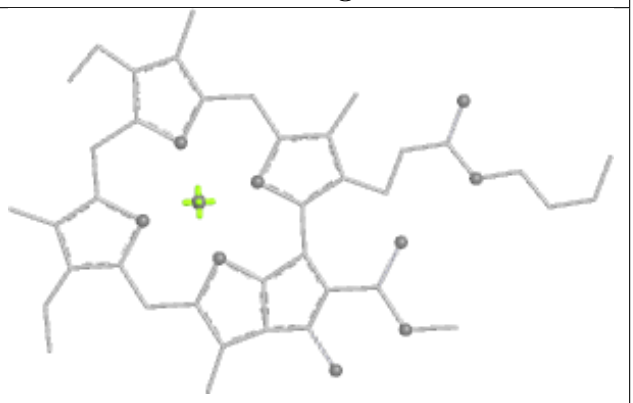
Bond lengths



Bond angles

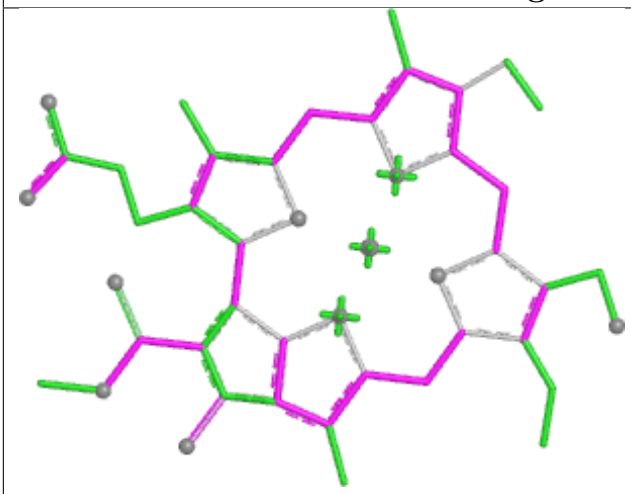


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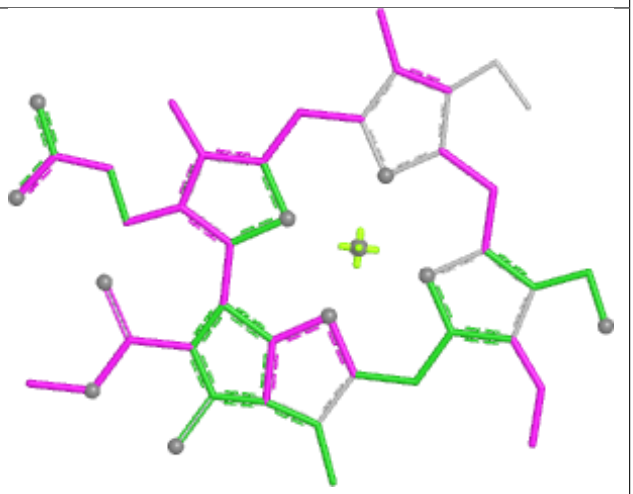


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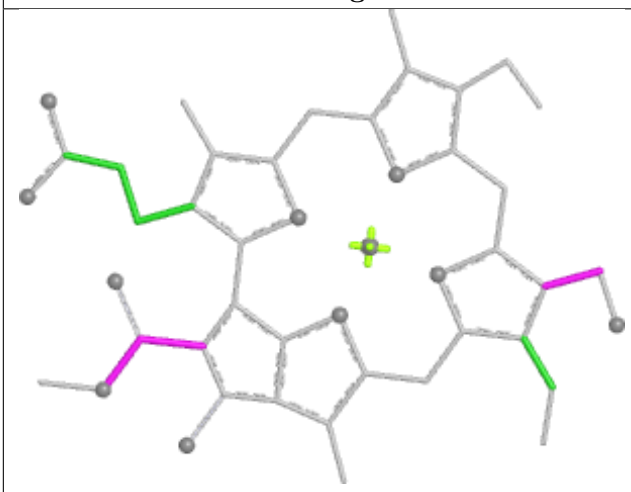
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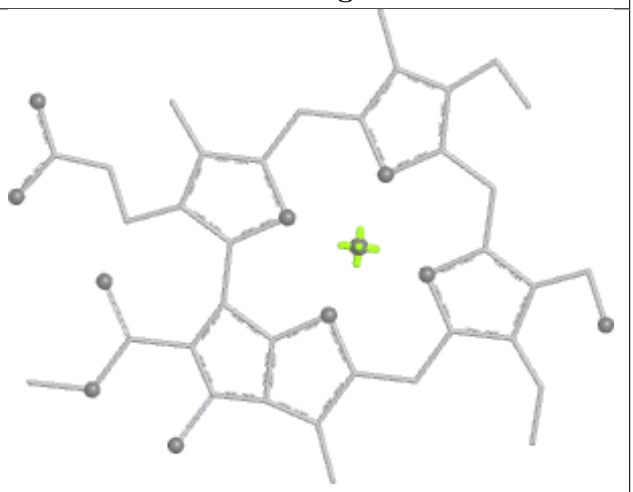
Bond lengths



Bond angles

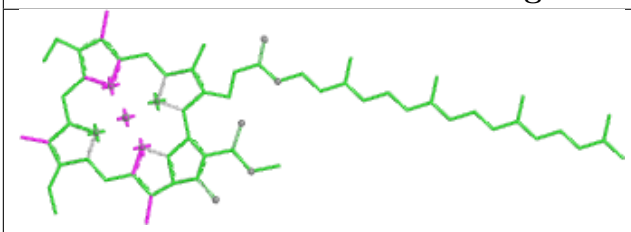


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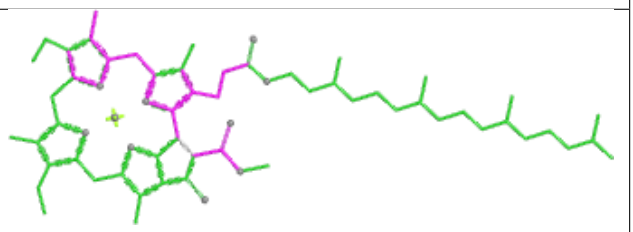


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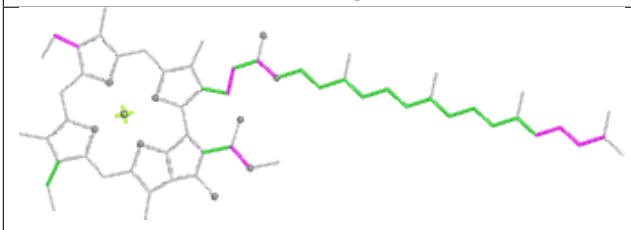
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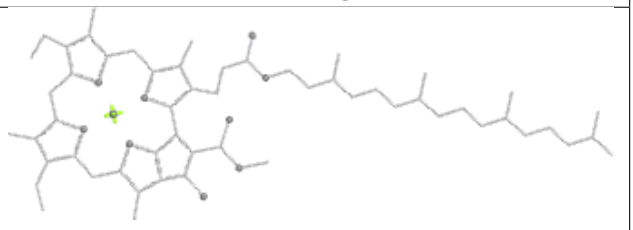
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Bond angles

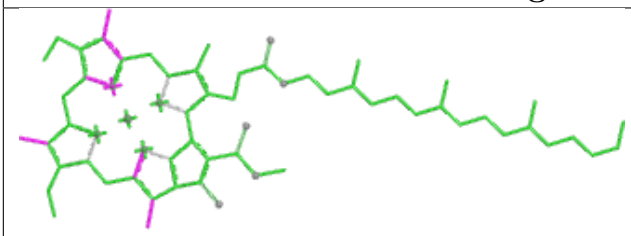


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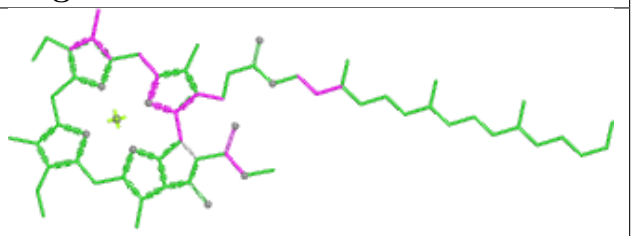


Rings

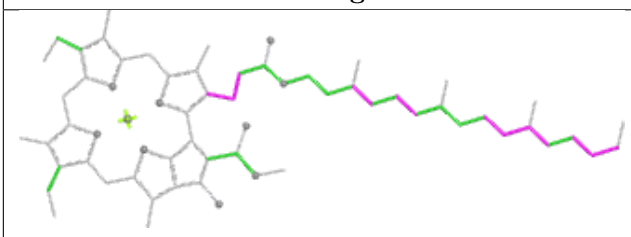
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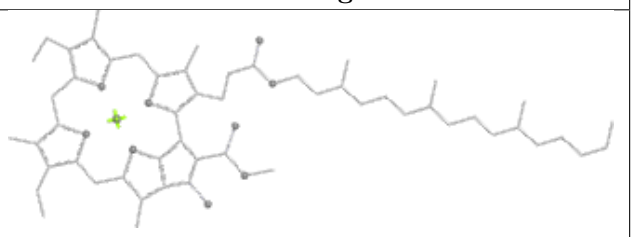
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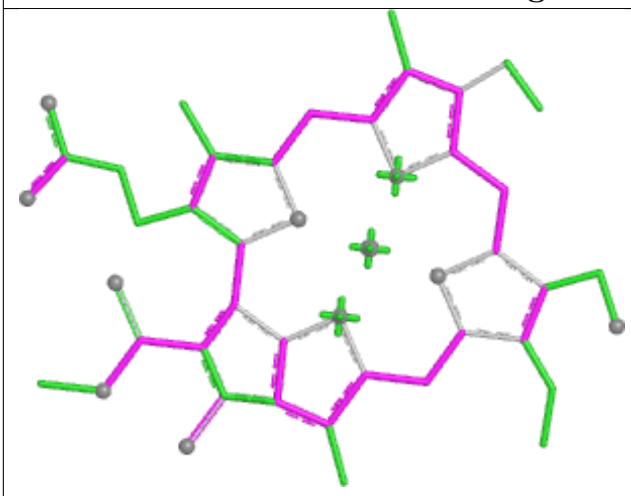


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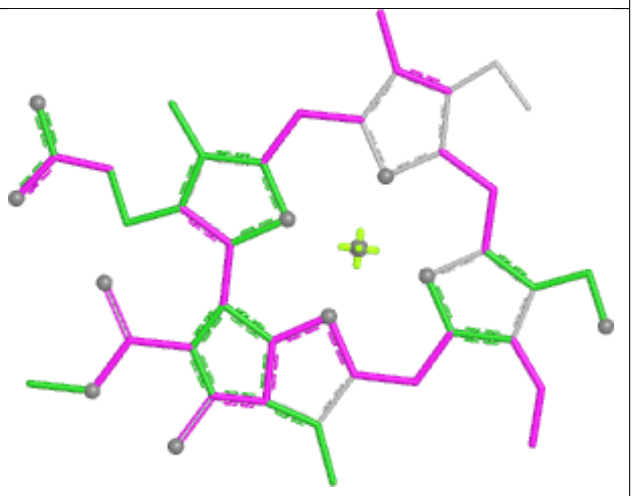


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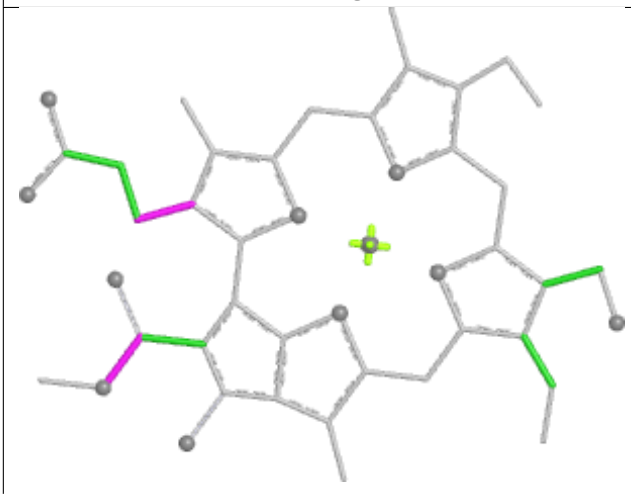
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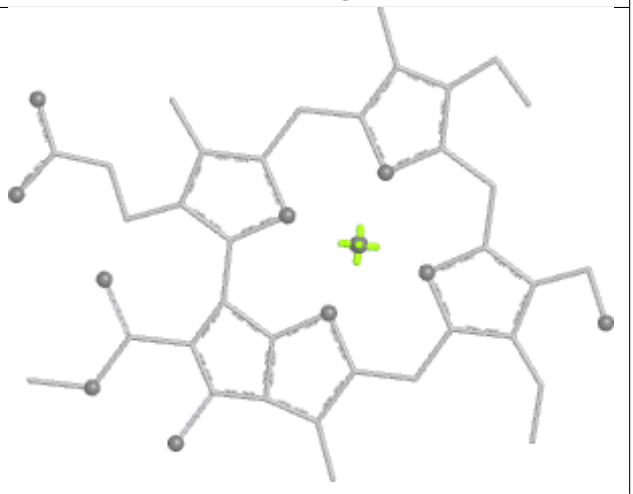
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Bond angles

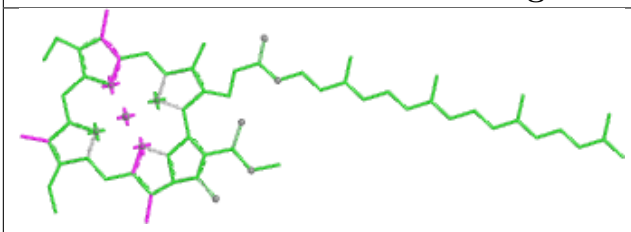


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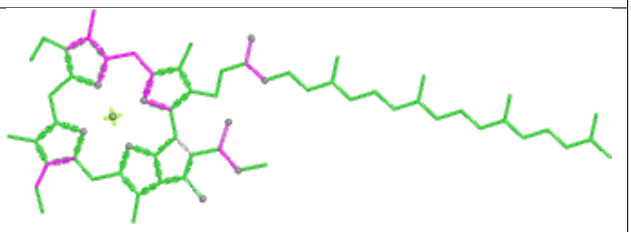


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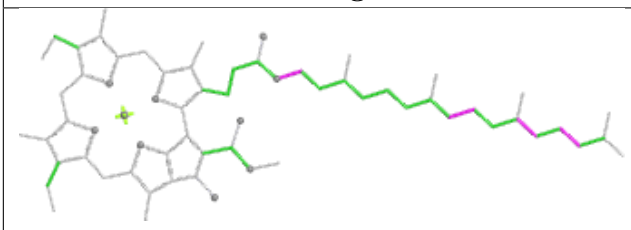
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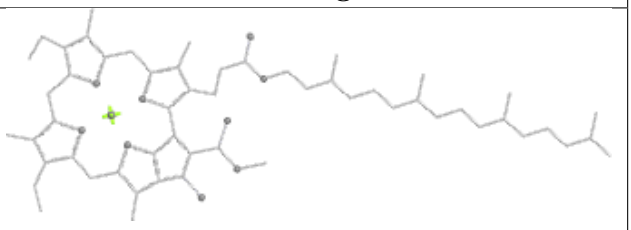
Bond lengths



Bond angles

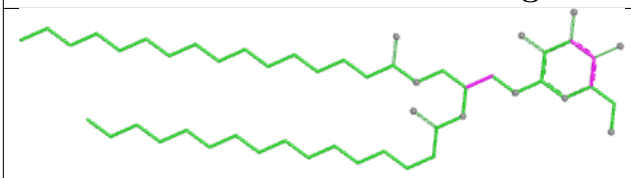


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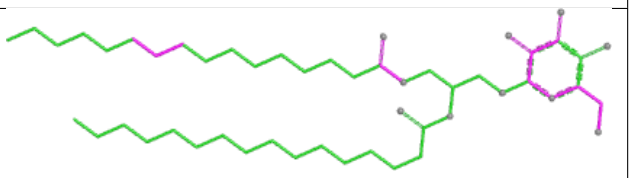


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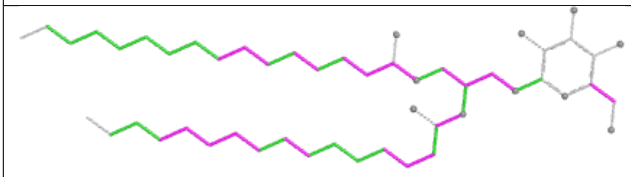
Ligand LMG Z 101



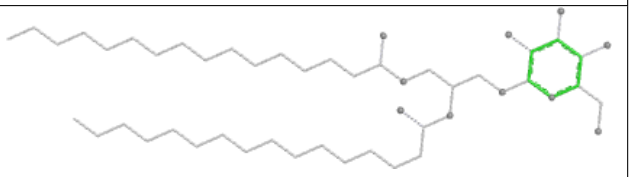
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Bond angles

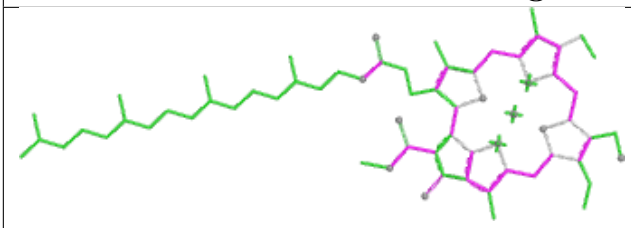


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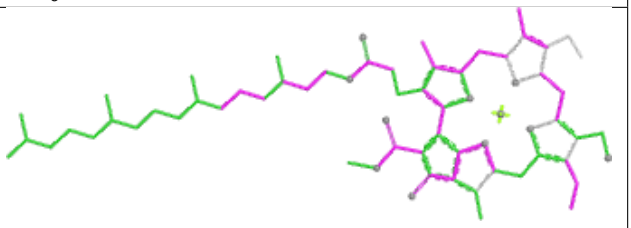


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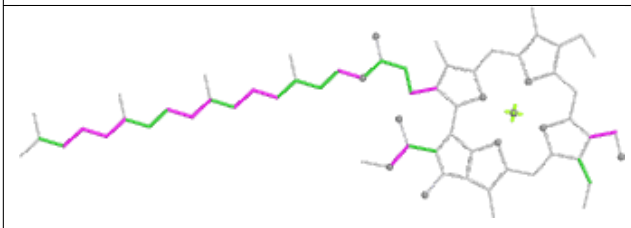
Ligand CHL y 608



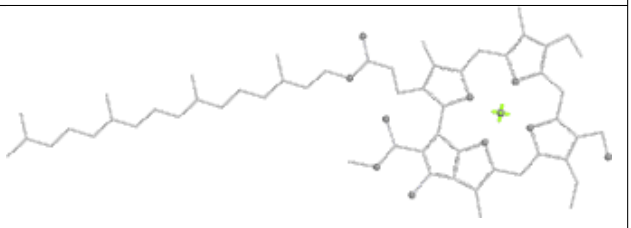
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Bond angles

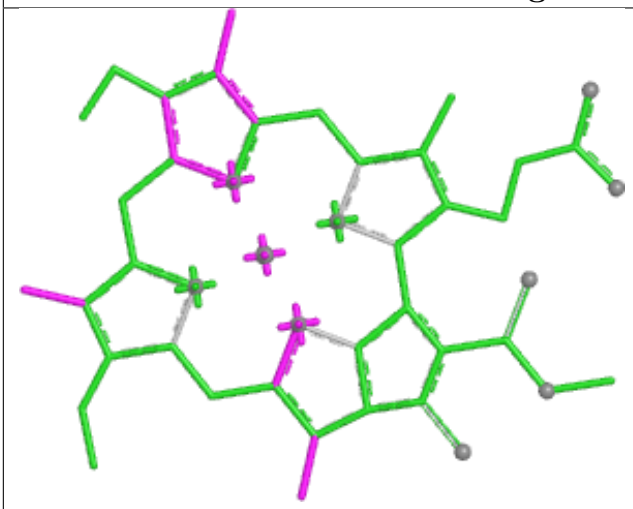


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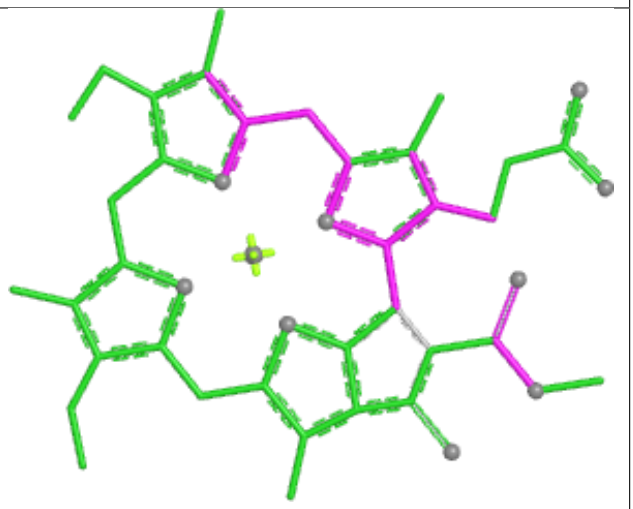


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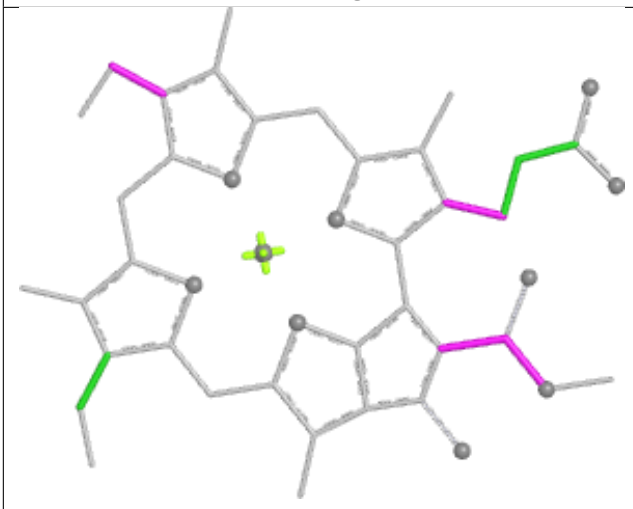
Ligand CLA 6 612



Bond lengths



Bond angles

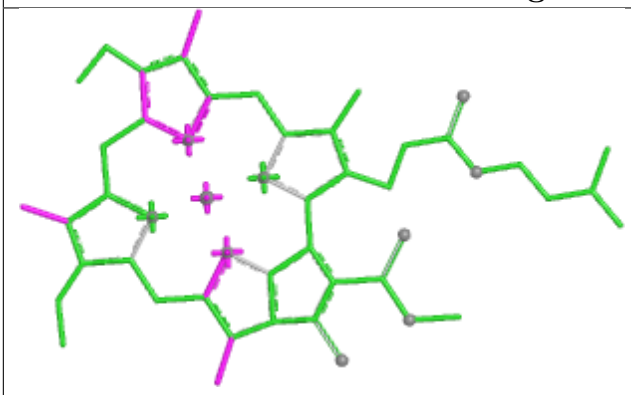


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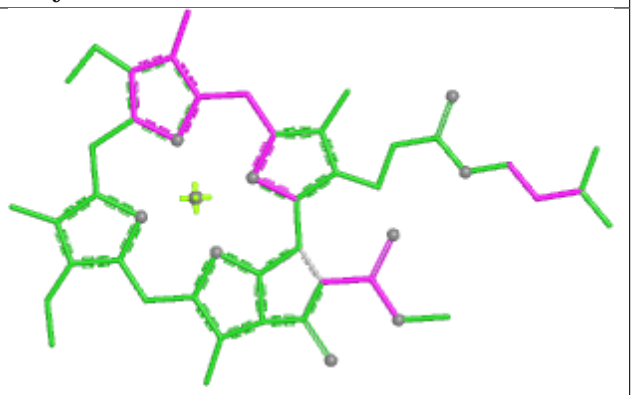


Rings

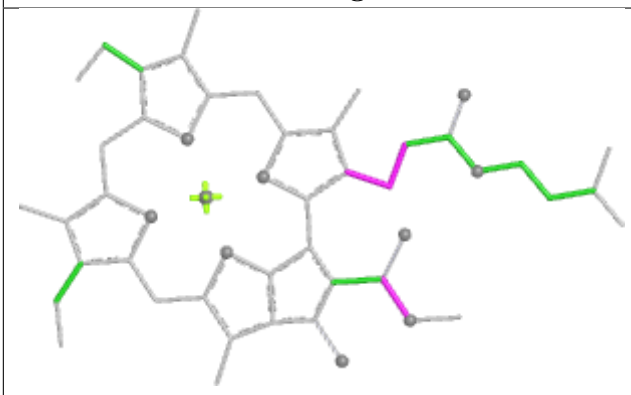
Ligand CLA y 604



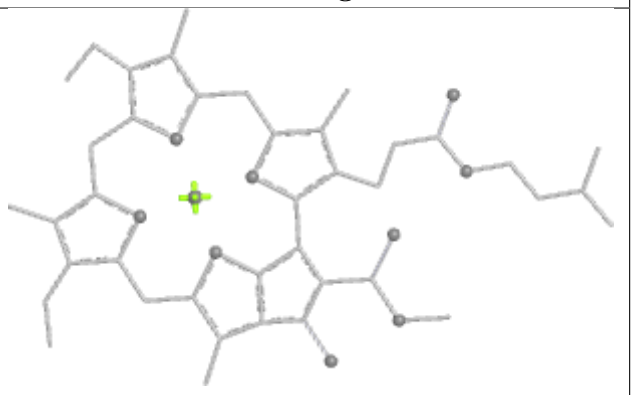
Bond lengths



Bond angles

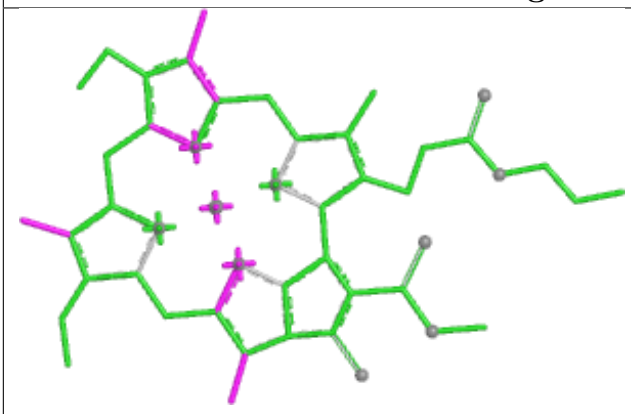


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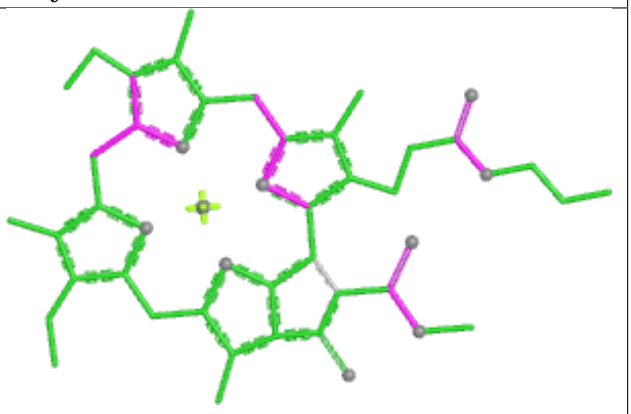


Rings

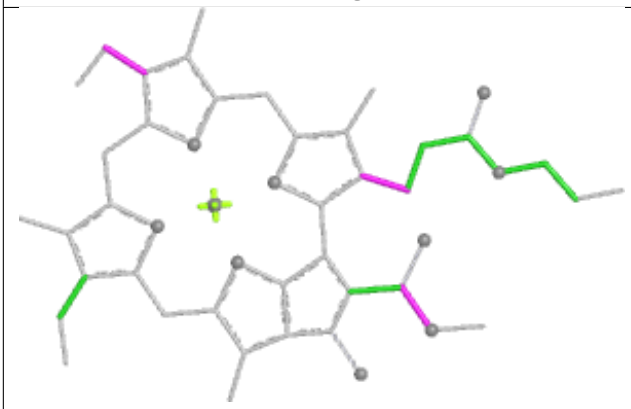
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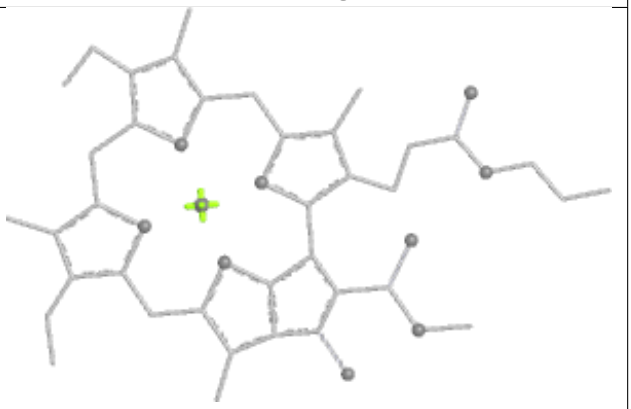
Bond lengths



Bond angles

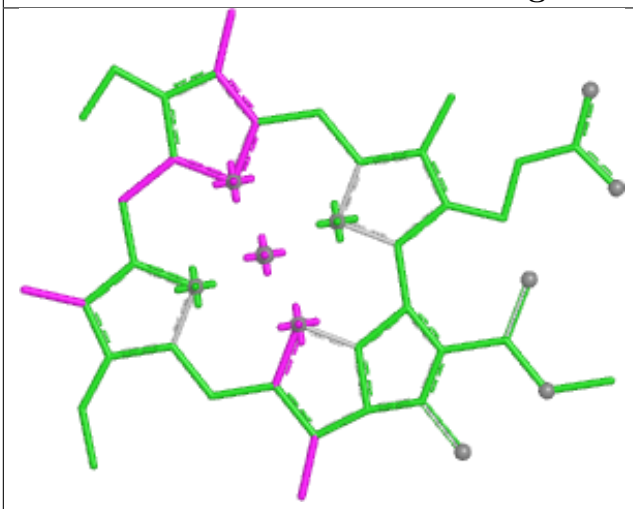


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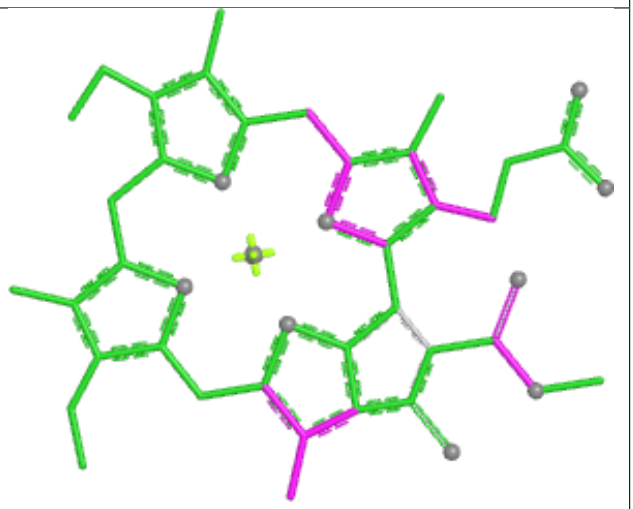


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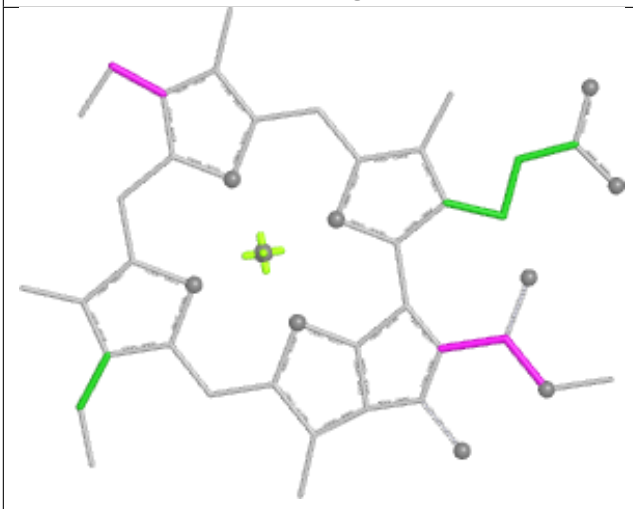
Ligand CLA 3 612



Bond lengths



Bond angles

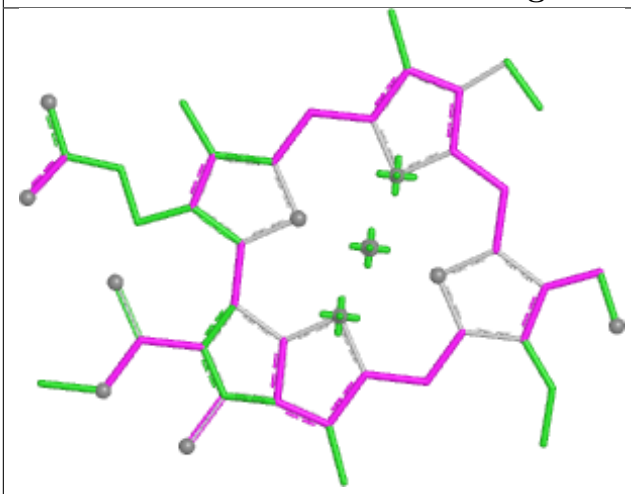


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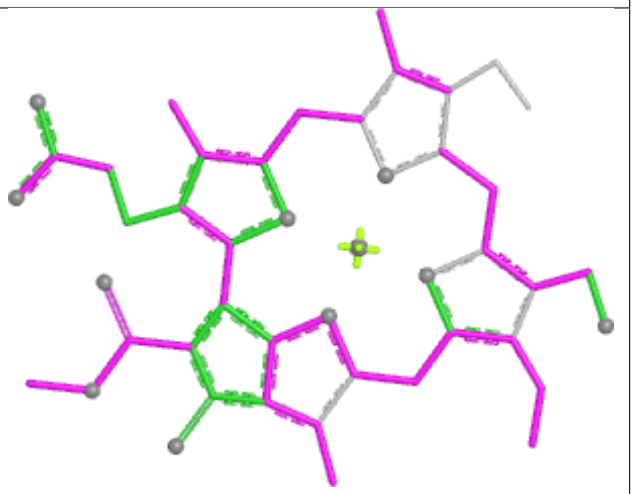


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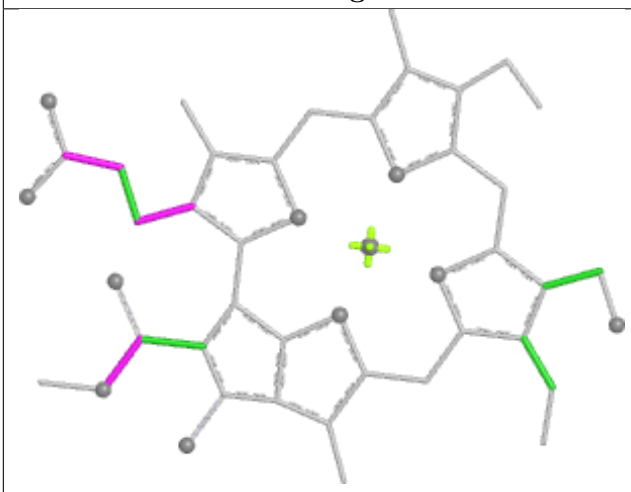
Ligand CHL 2 601



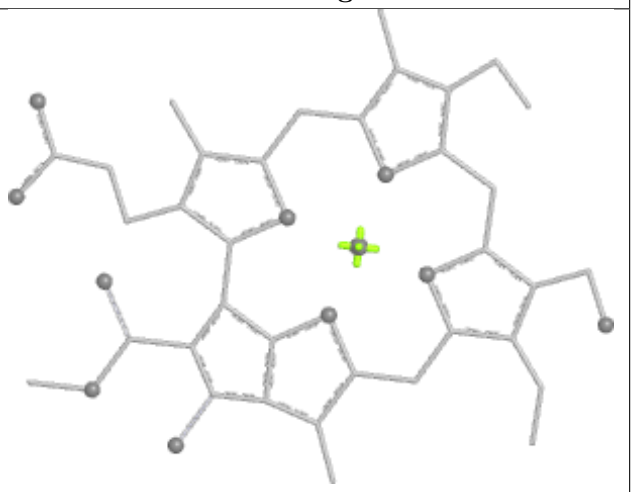
Bond lengths



Bond angles



Torsions

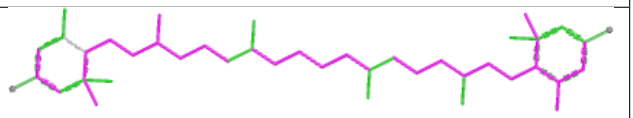


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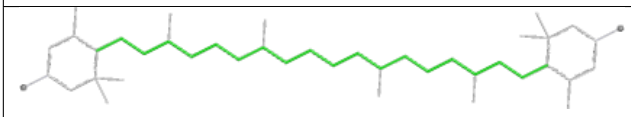
Ligand LUT 2 1621



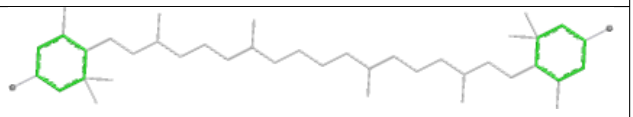
Bond lengths



Bond angles

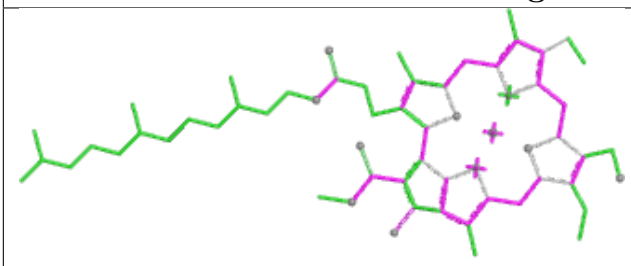


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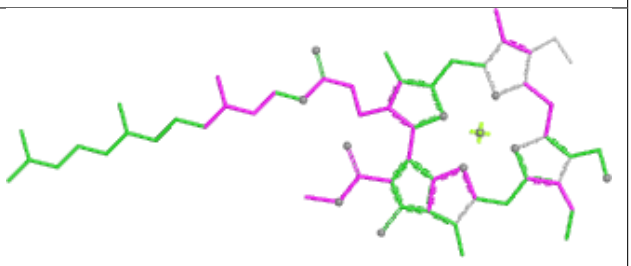


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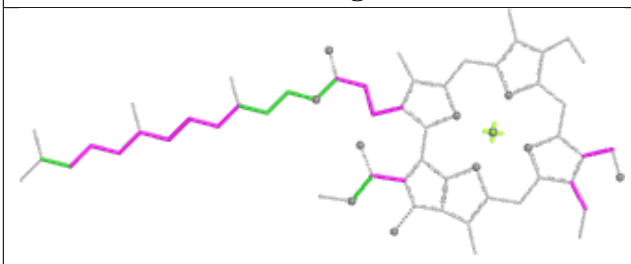
Ligand CHL 2 607



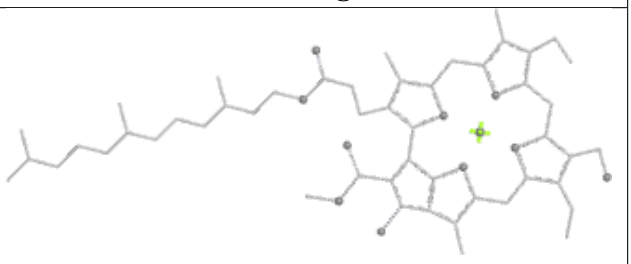
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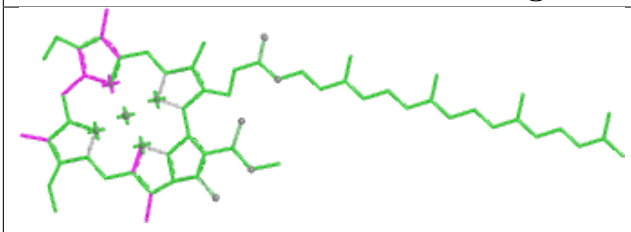


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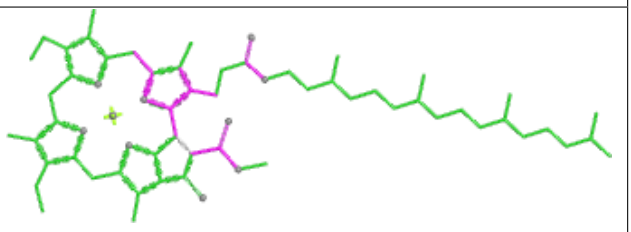


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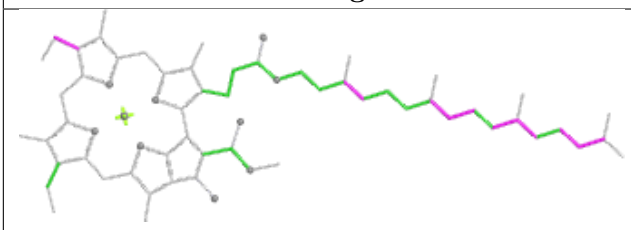
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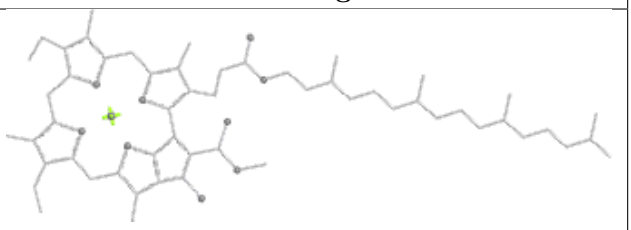
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Bond angles

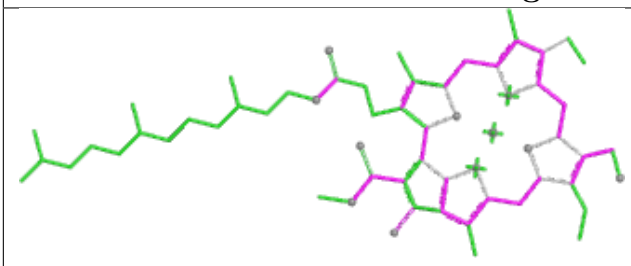


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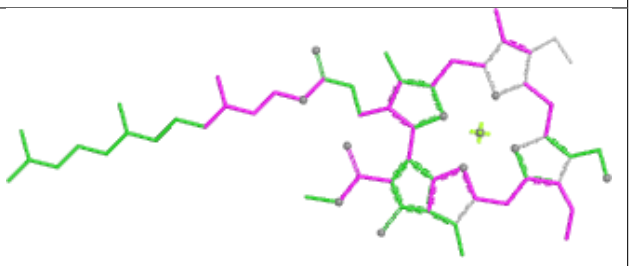


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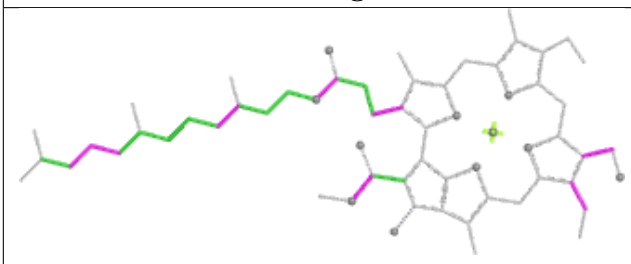
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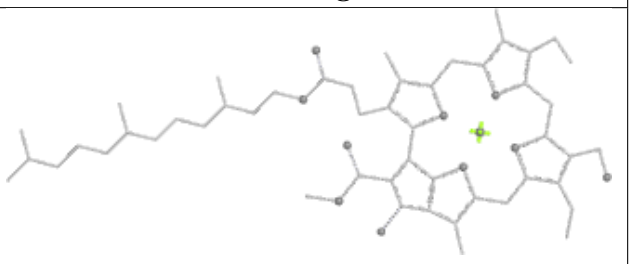
Bond lengths



Bond angles

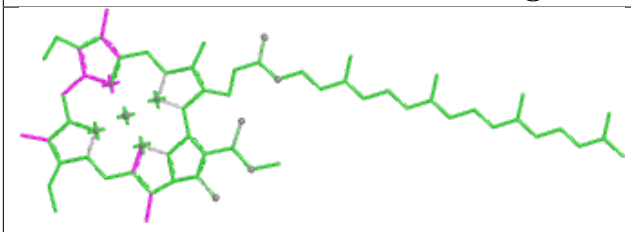


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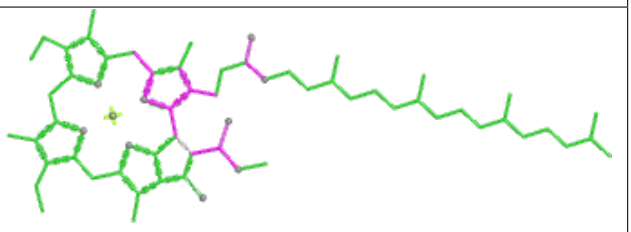


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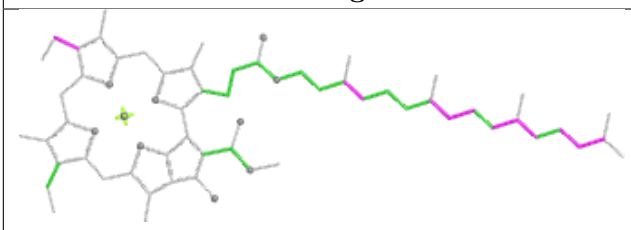
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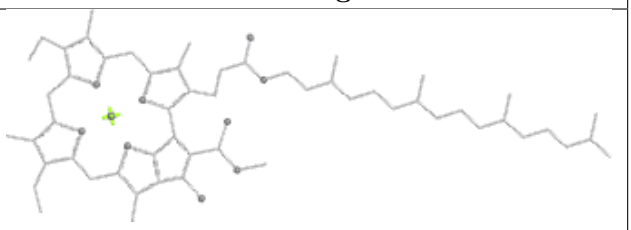
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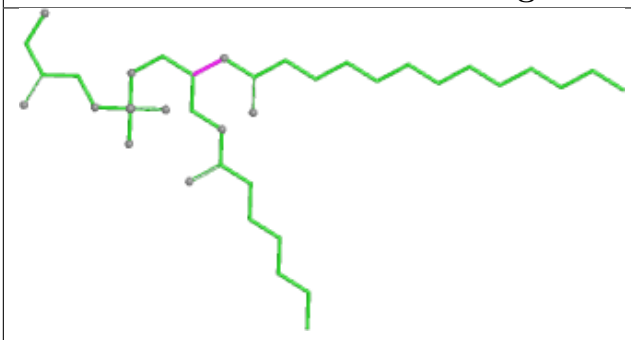


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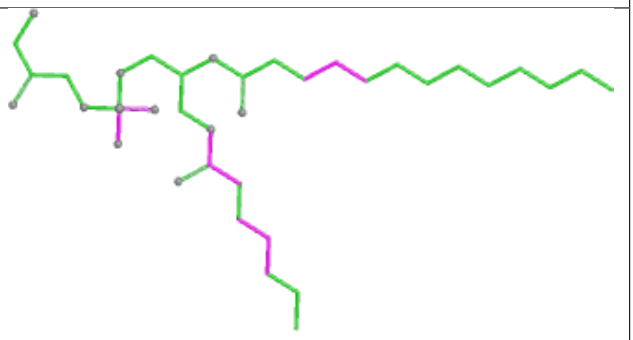


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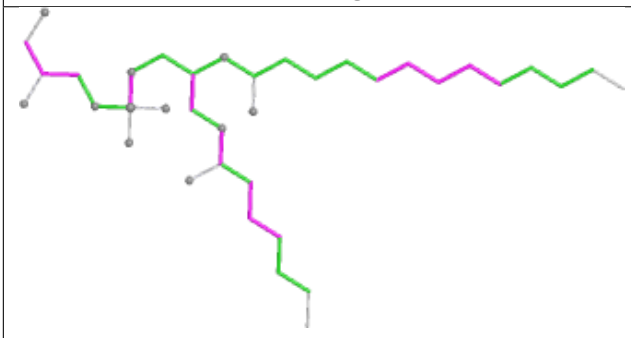
Ligand LHG 6 2630



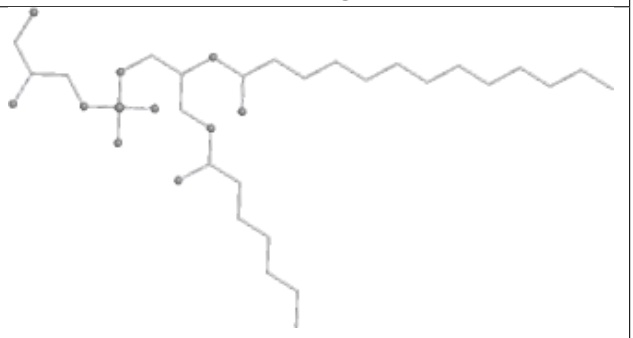
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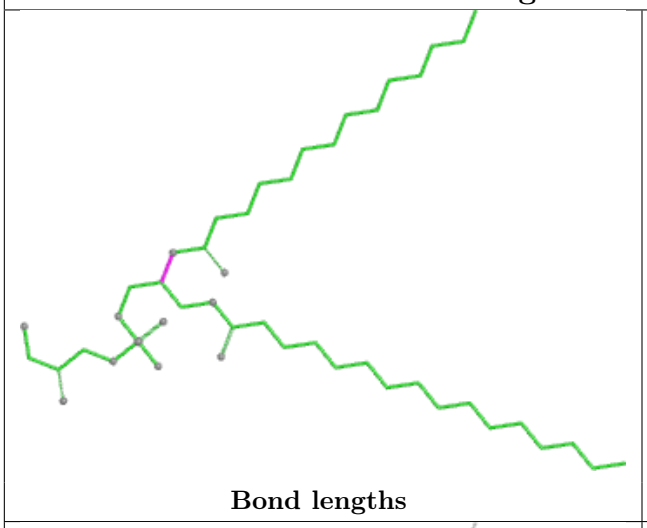


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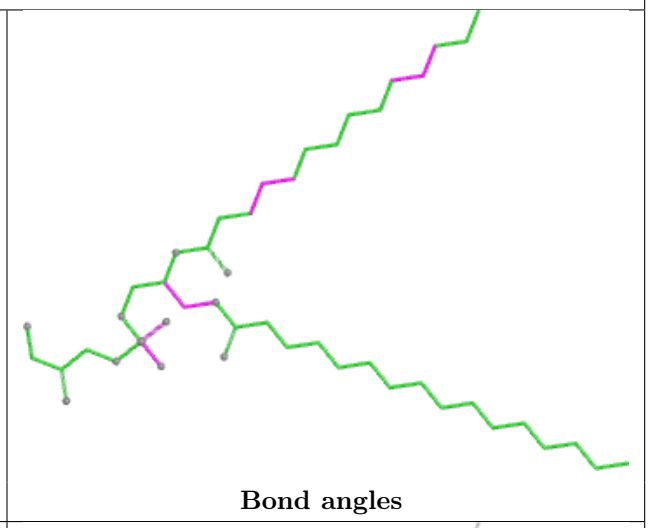


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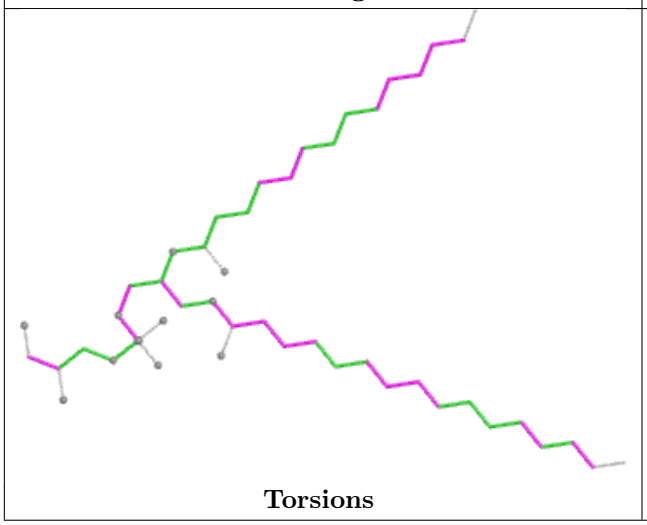
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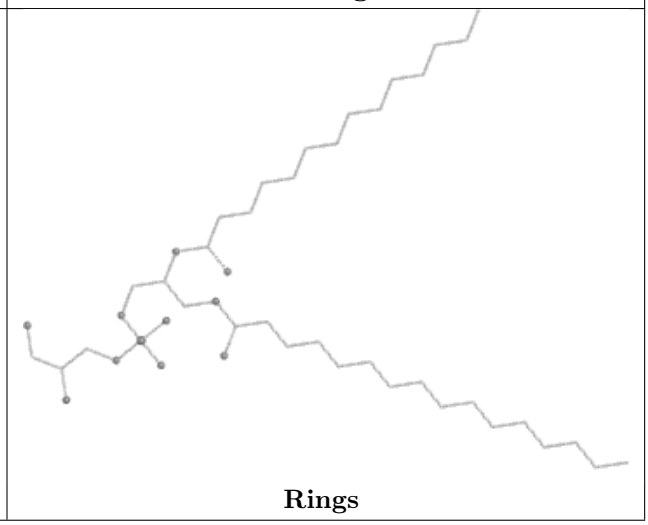
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Bond angles

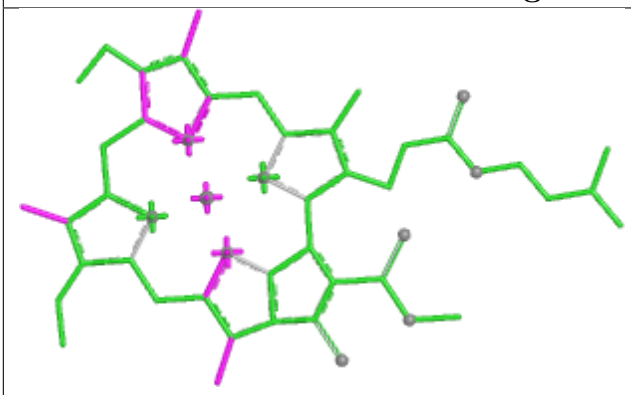


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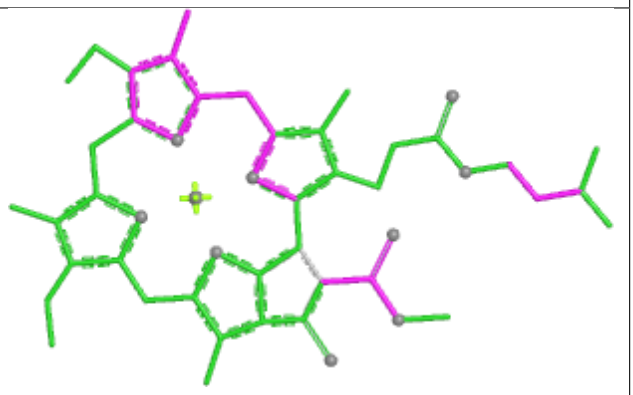


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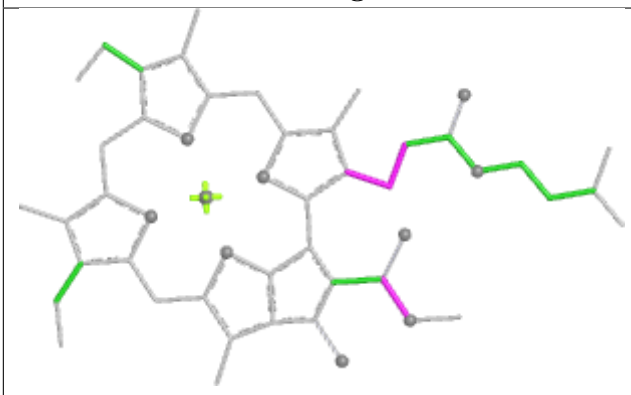
Ligand CLA Y 604



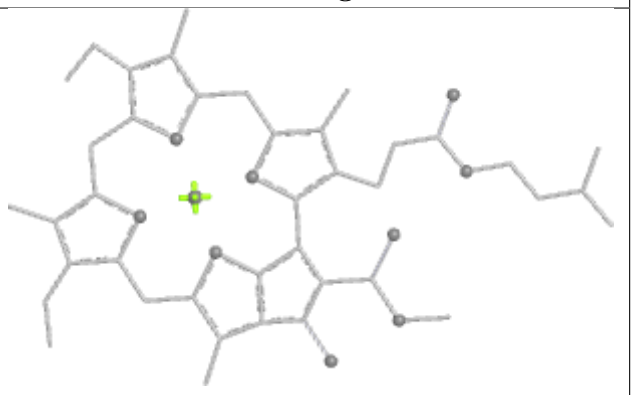
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Bond angles

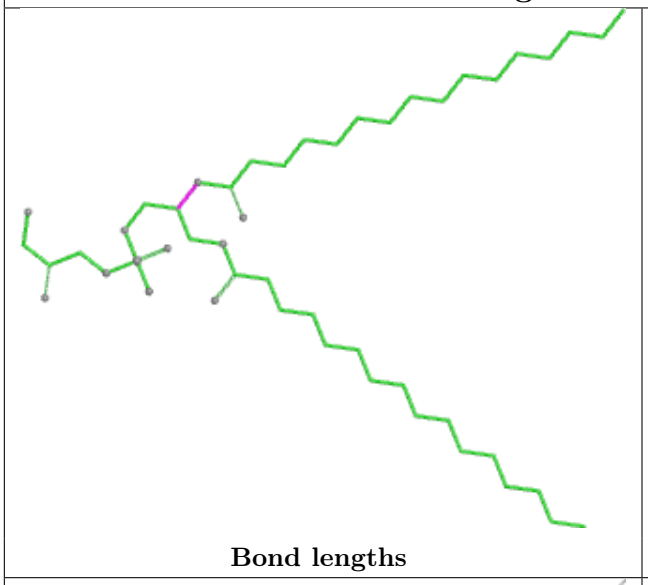


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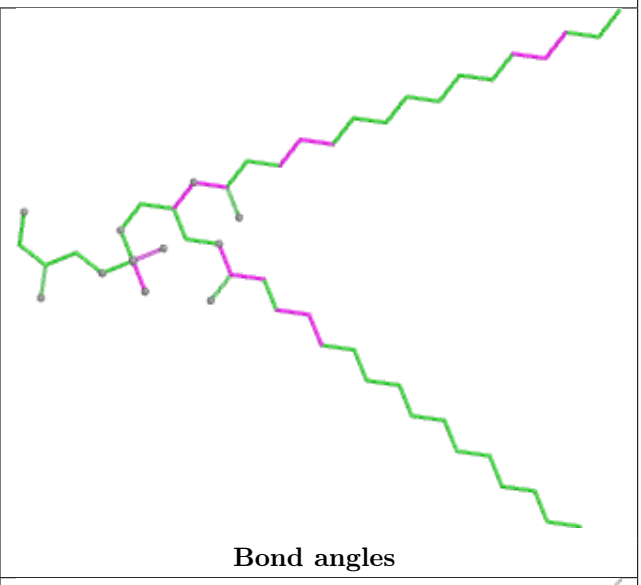


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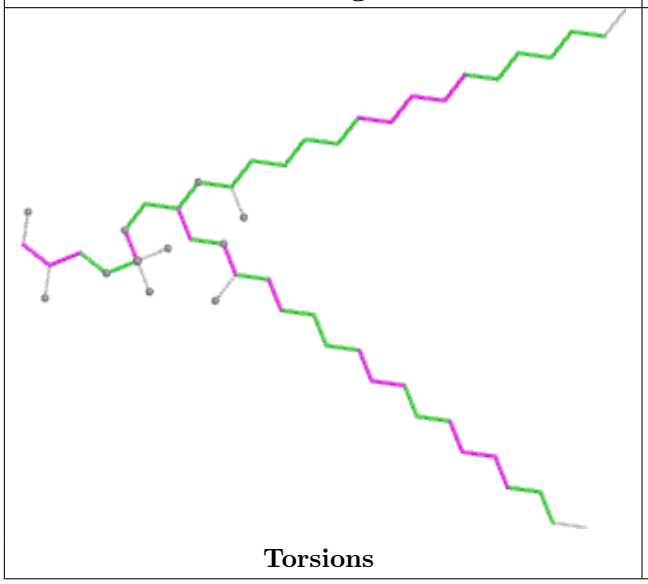
Ligand LHG B 2631



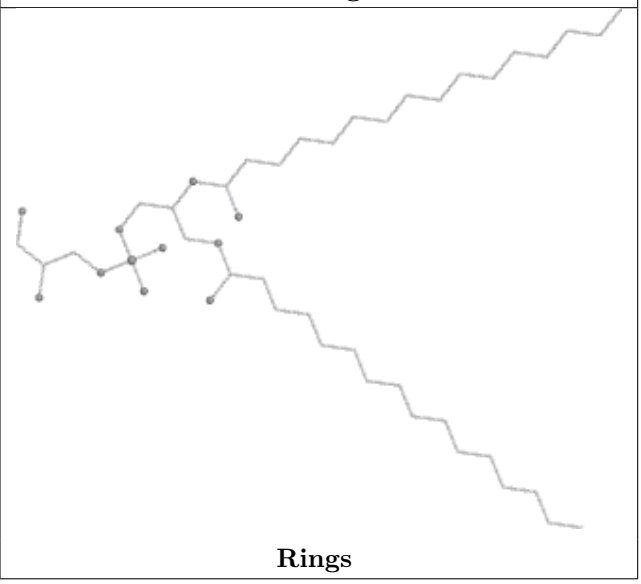
Bond lengths



Bond angles

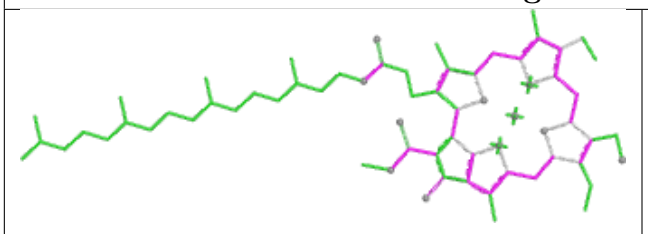


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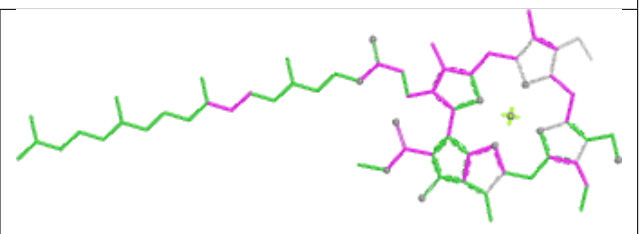


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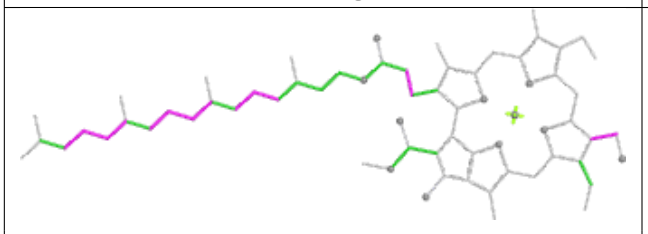
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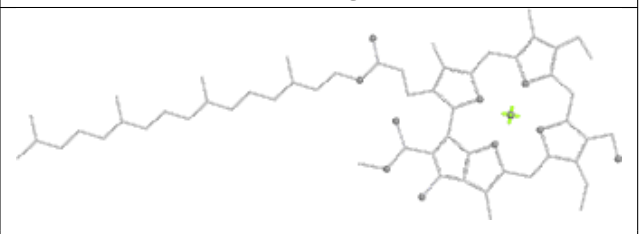
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Bond angles

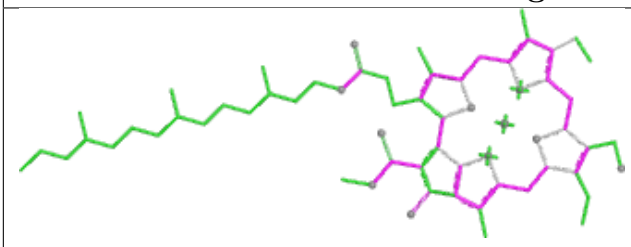


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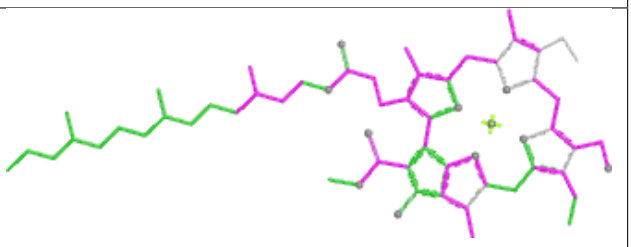


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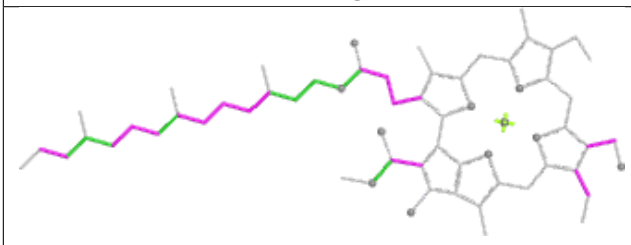
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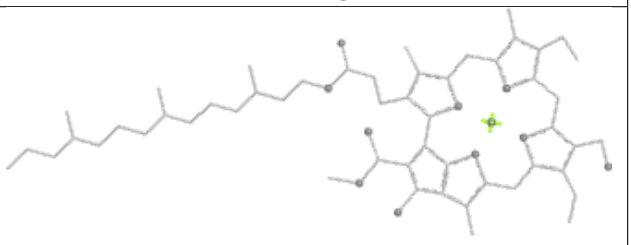
Bond lengths



Bond angles

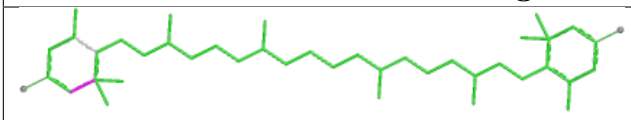


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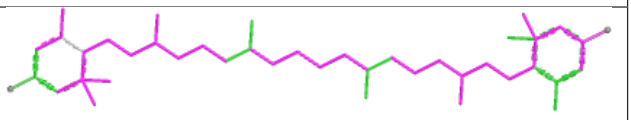


Rings

Ligand LUT Y 1620



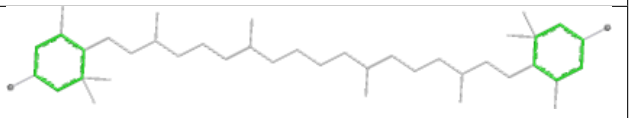
Bond lengths



Bond angles

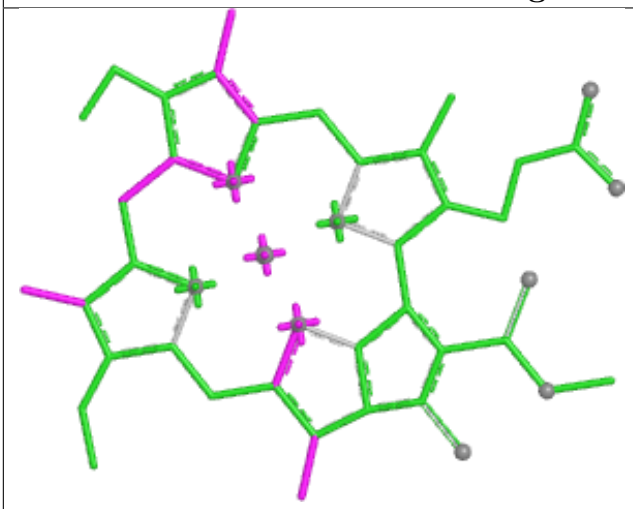


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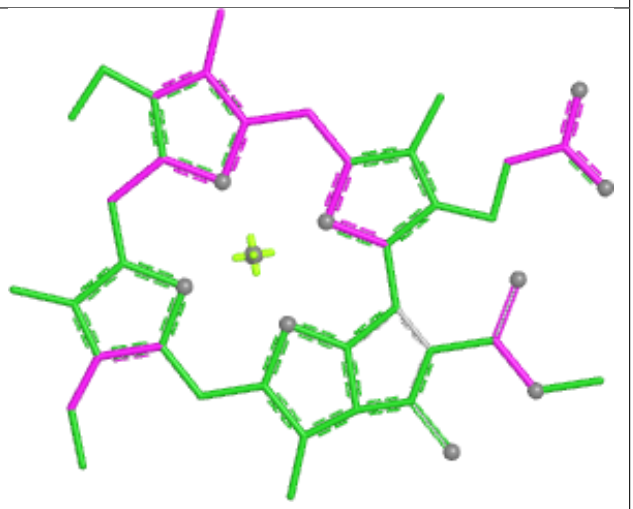


Rings

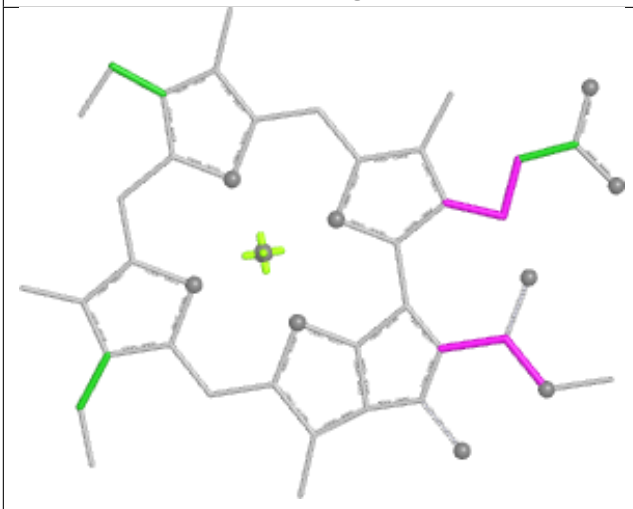
Ligand CLA 6 604



Bond lengths



Bond angles

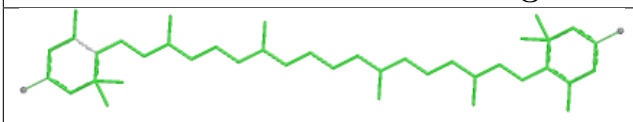


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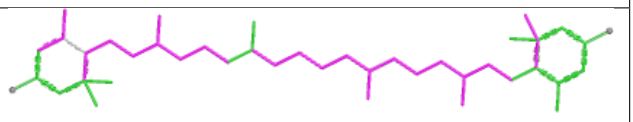


Rings

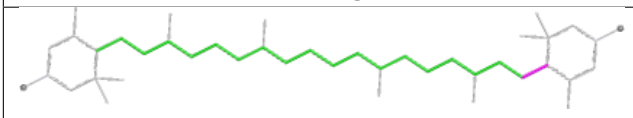
Ligand LUT s 1620



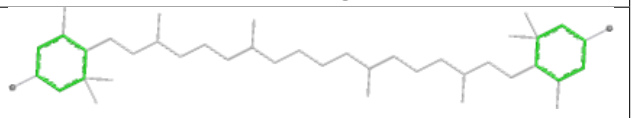
Bond lengths



Bond angles

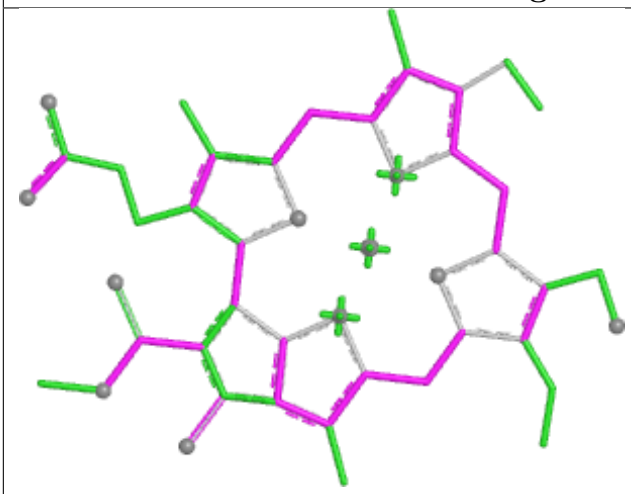


Torsions

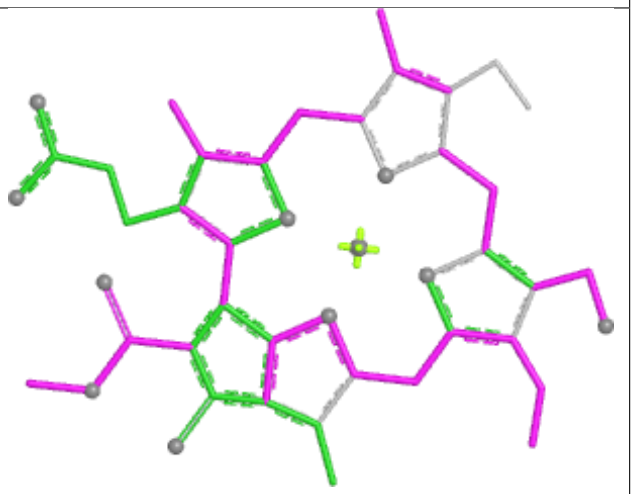


Rings

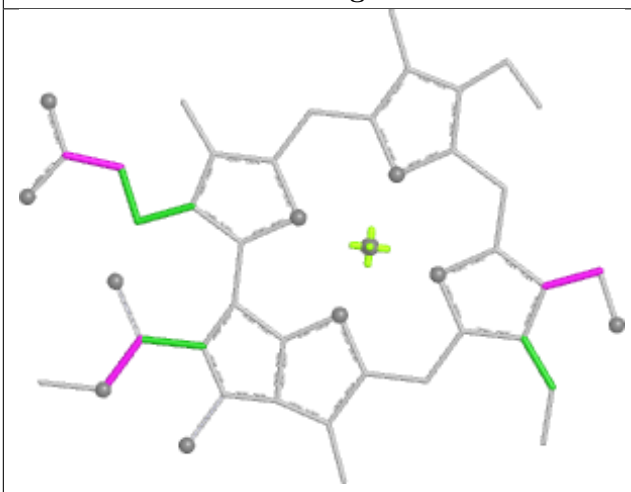
Ligand CHL s 601



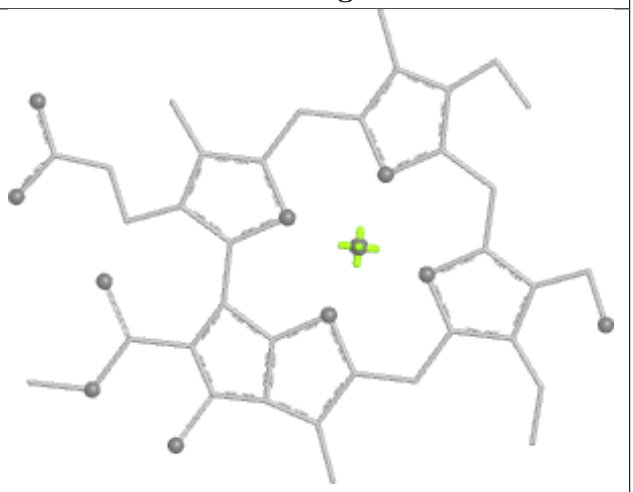
Bond lengths



Bond angles

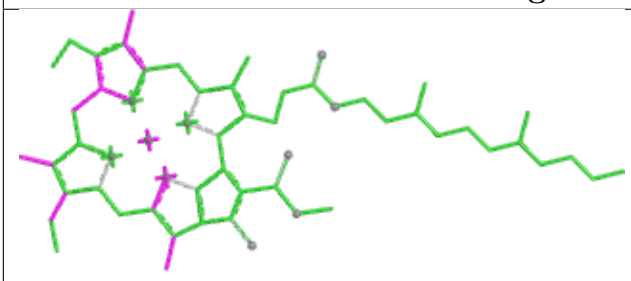


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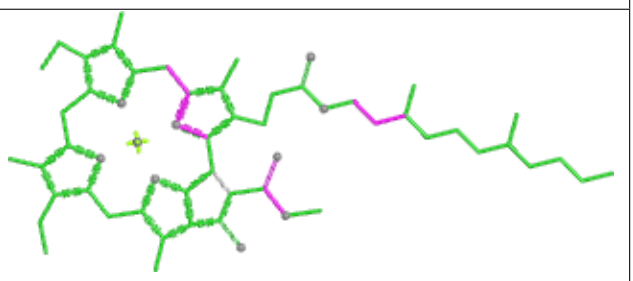


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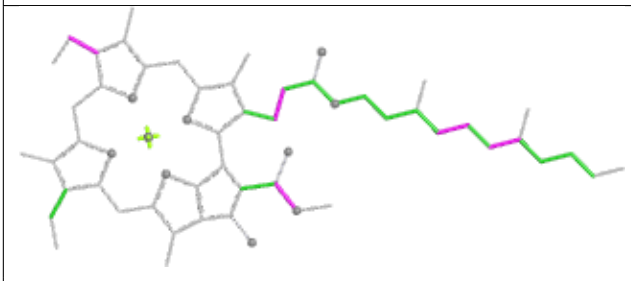
Ligand CLA 3 613



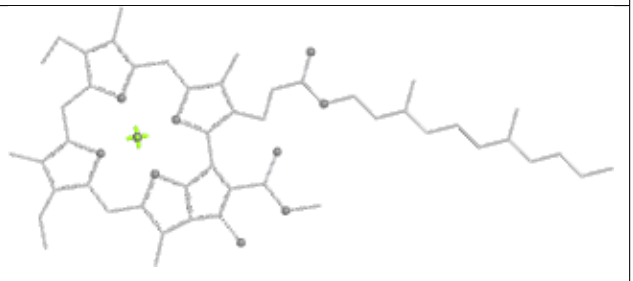
Bond lengths



Bond angles

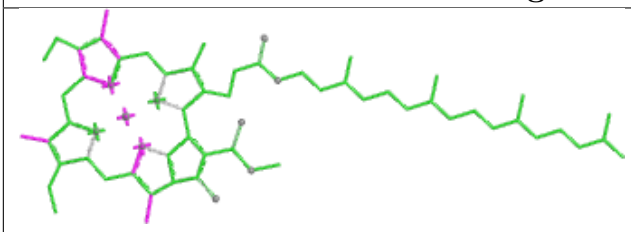


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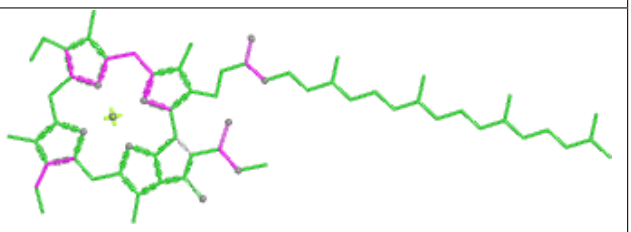


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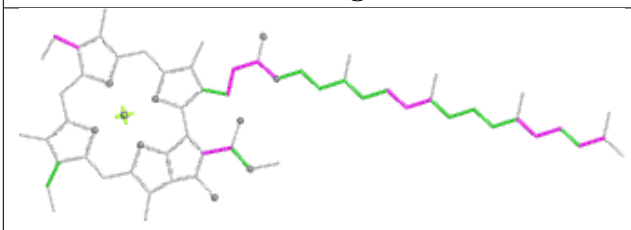
Ligand CLA b 602



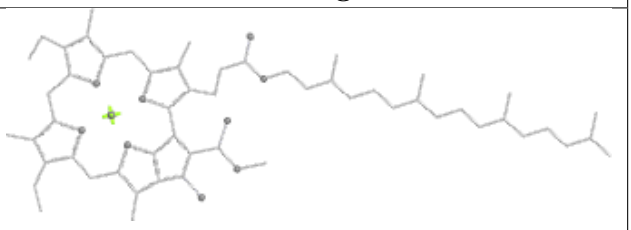
Bond lengths



Bond angles

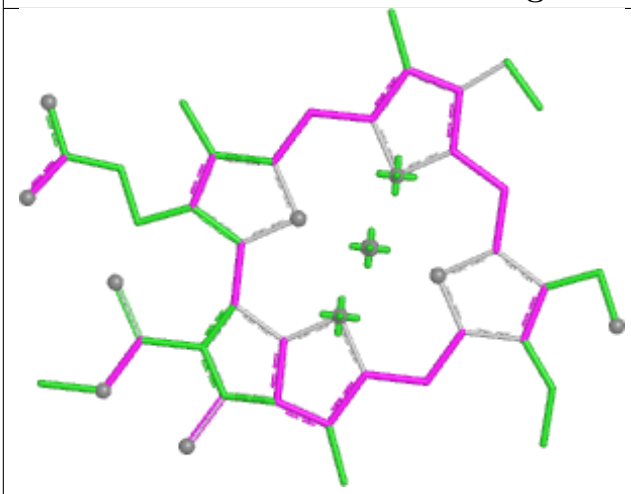


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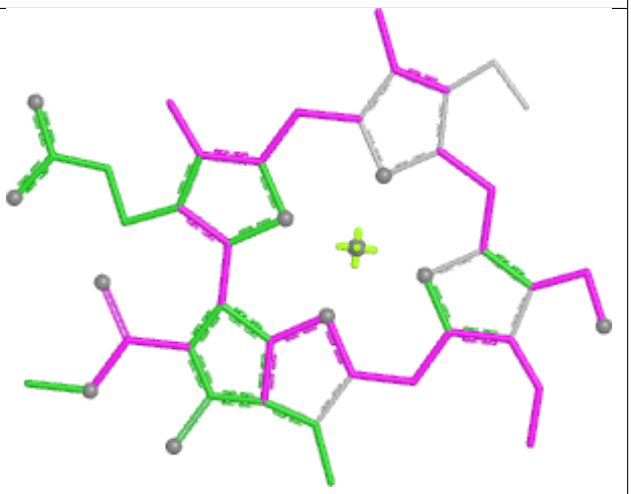


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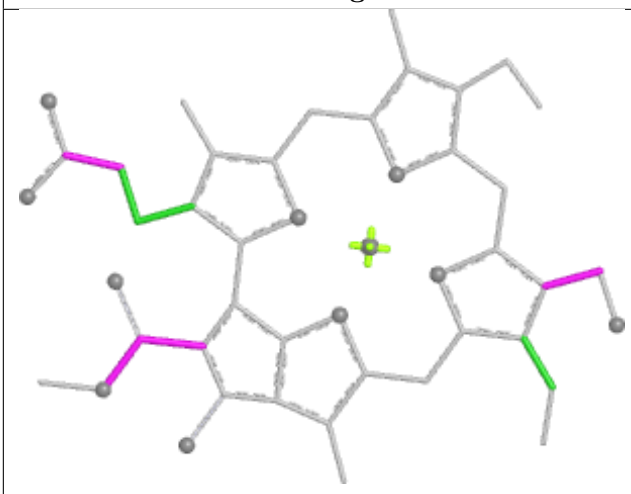
Ligand CHL S 606



Bond lengths



Bond angles

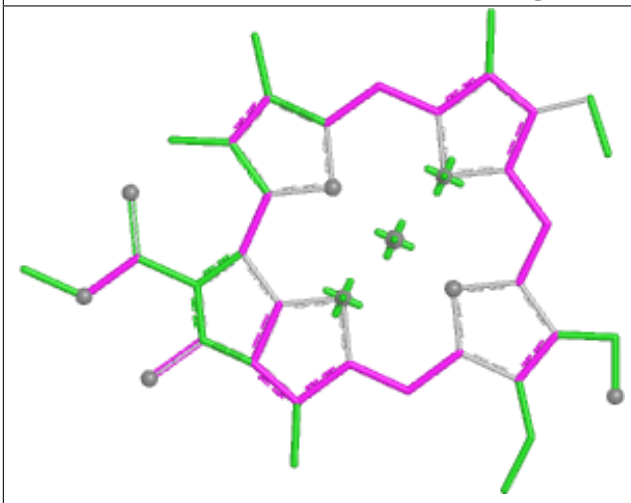


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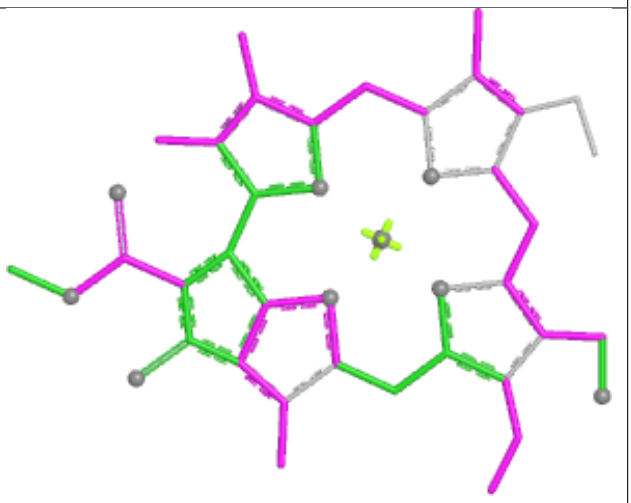


Rings

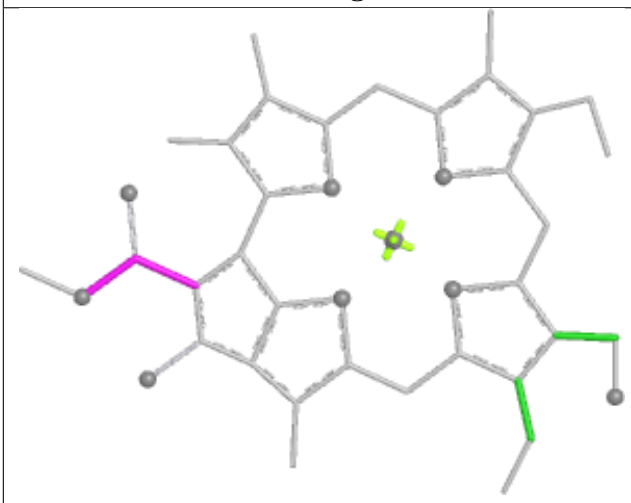
Ligand CHL r 614



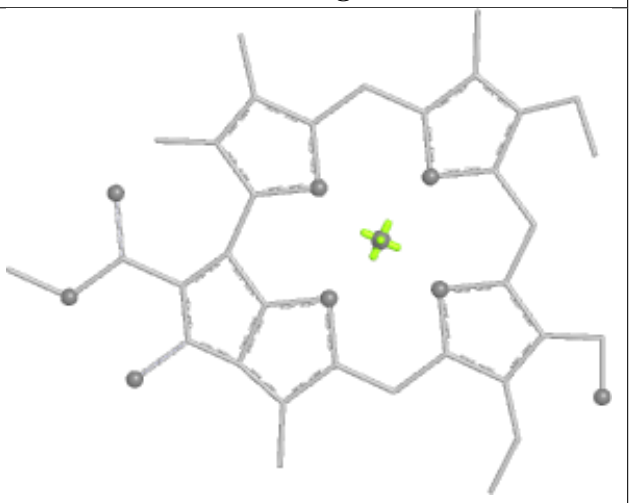
Bond lengths



Bond angles

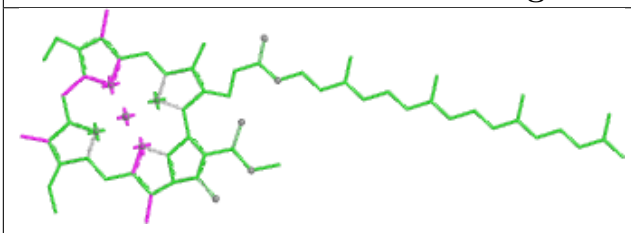


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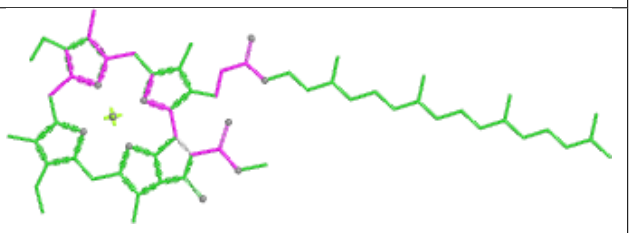


Rings

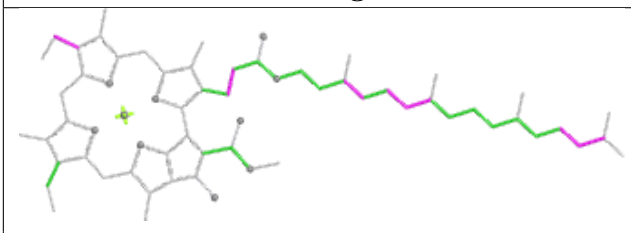
Ligand CLA b 604



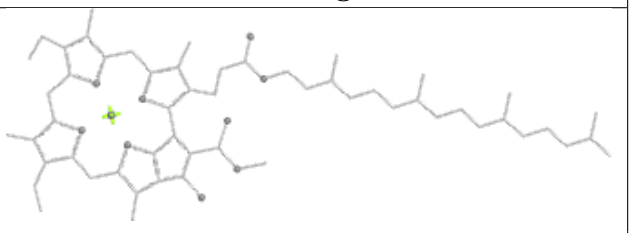
Bond lengths



Bond angles

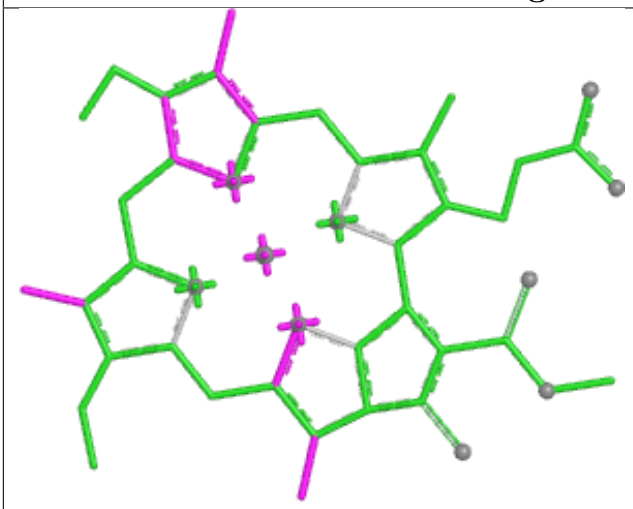


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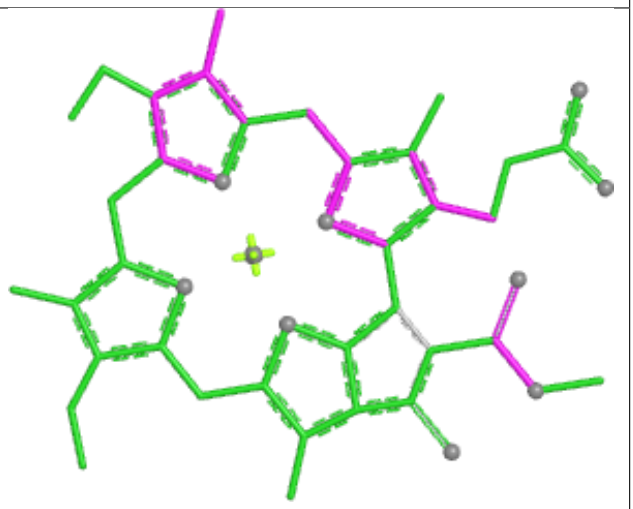


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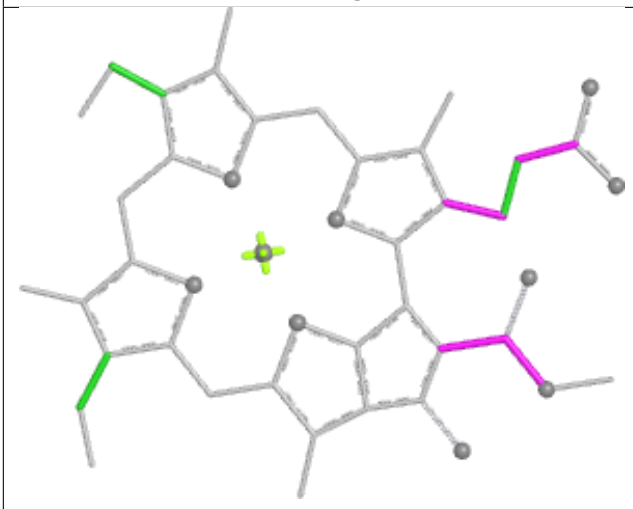
Ligand CLA 4 612



Bond lengths



Bond angles

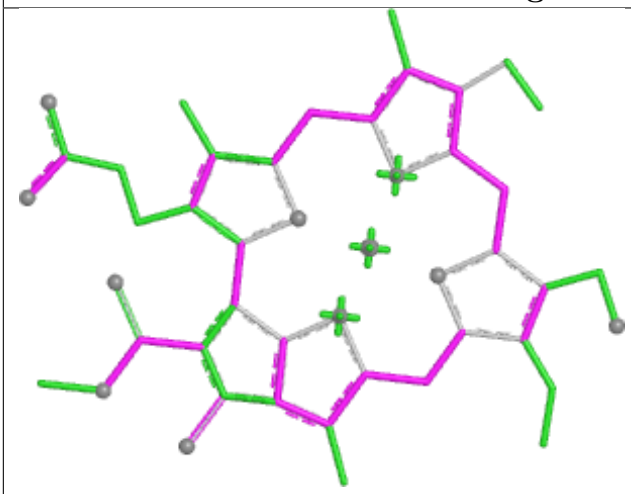


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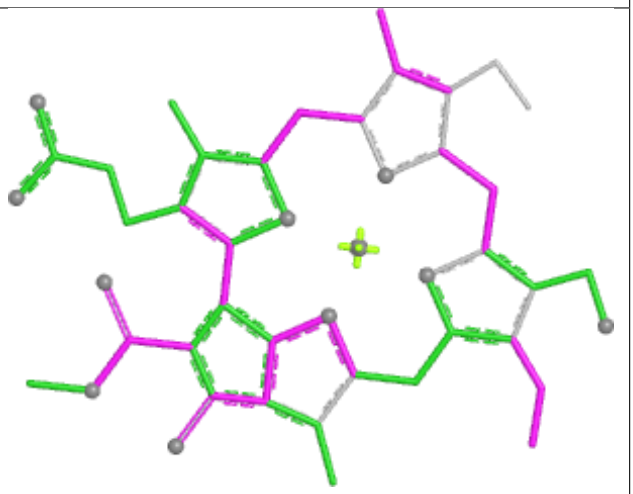


Rings

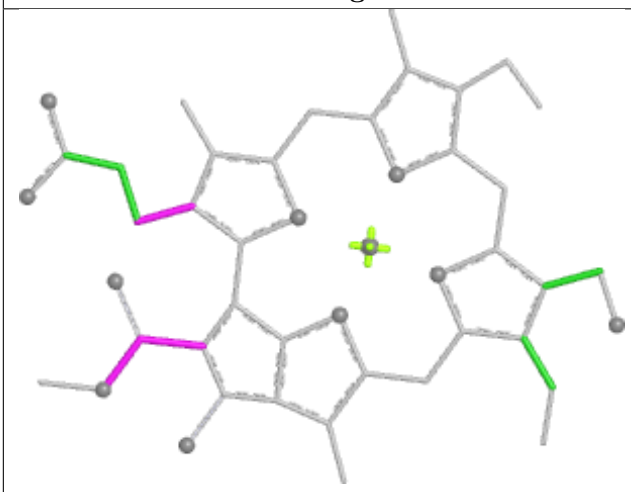
Ligand CHL S 608



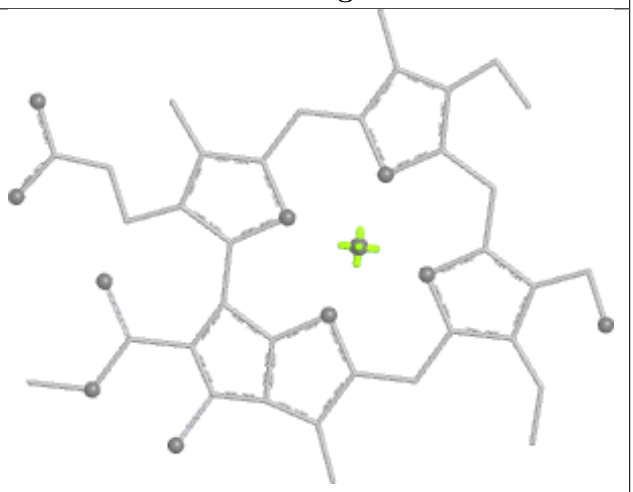
Bond lengths



Bond angles

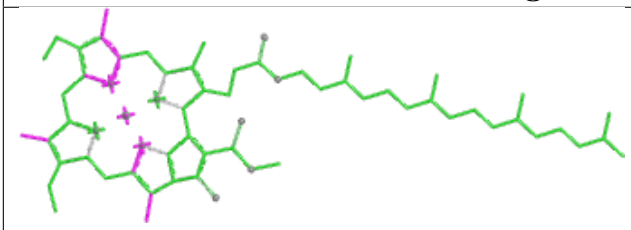


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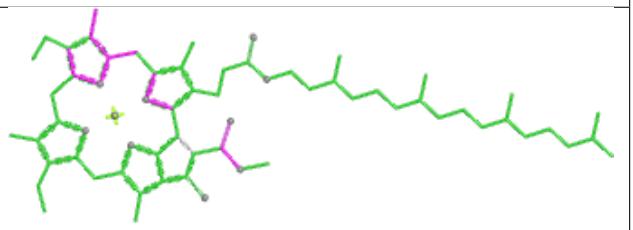


Rings

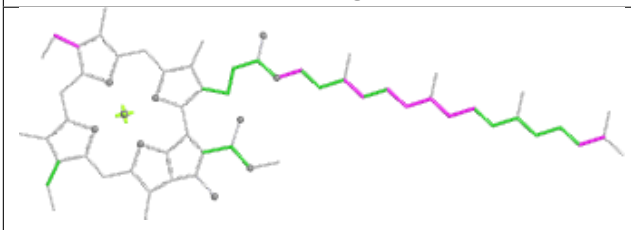
Ligand CLA B 603



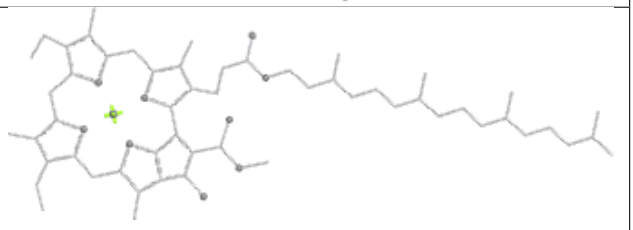
Bond lengths



Bond angles

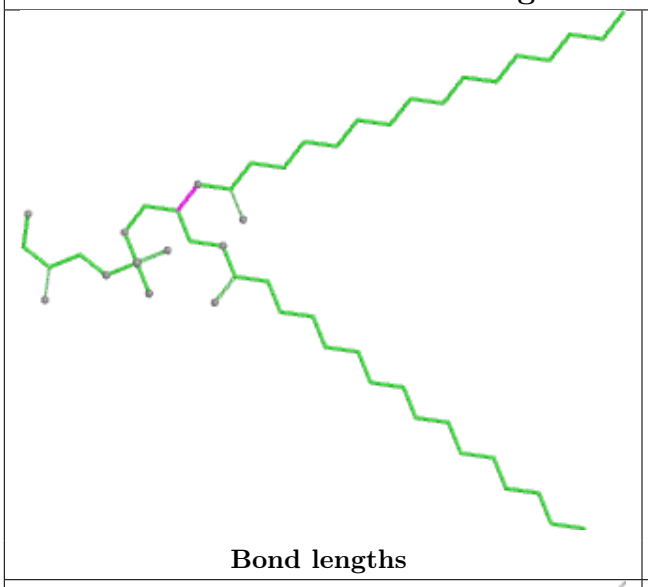


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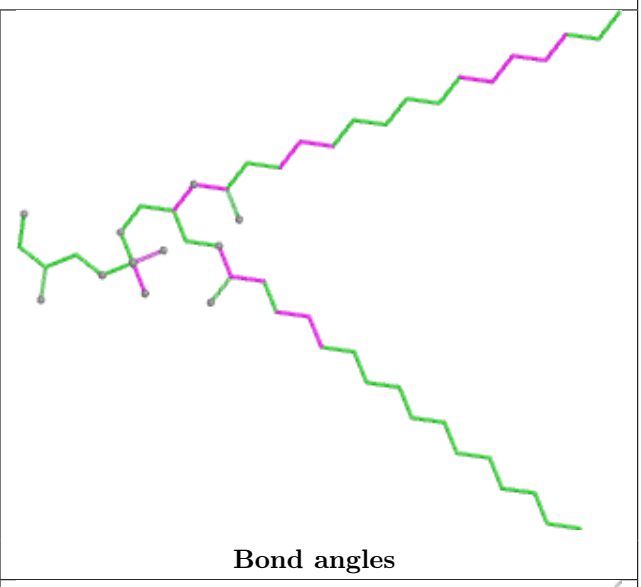


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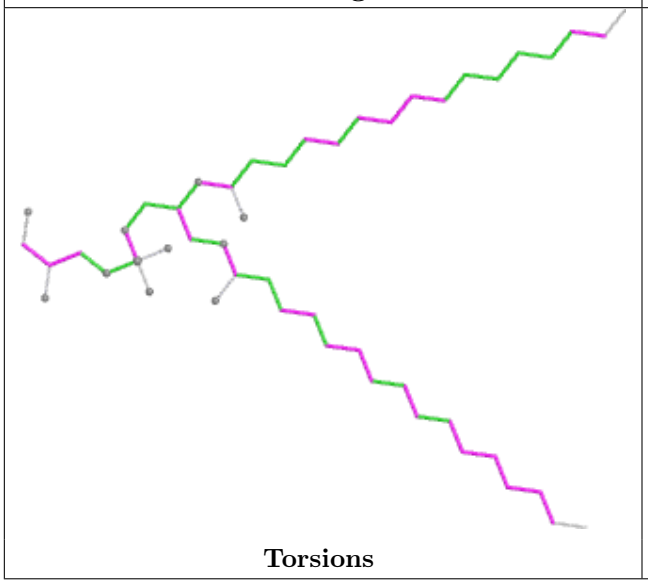
Ligand LHG S 2630



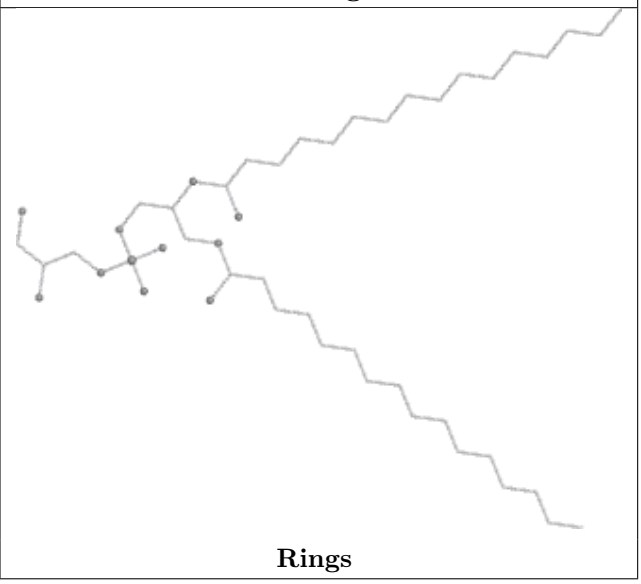
Bond lengths



Bond angles

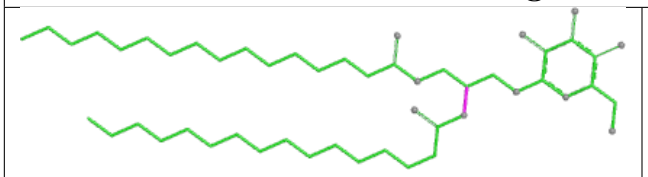


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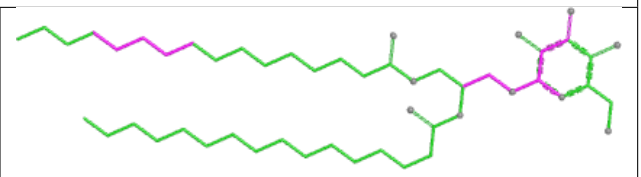


Rings

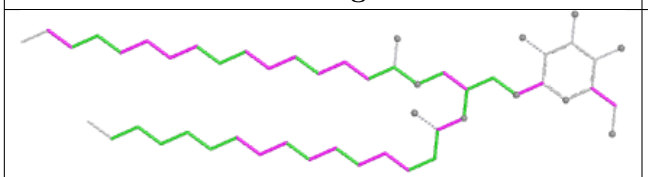
Ligand LMG c 521



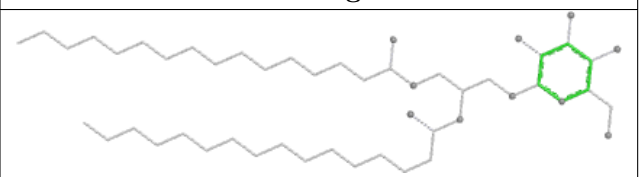
Bond lengths



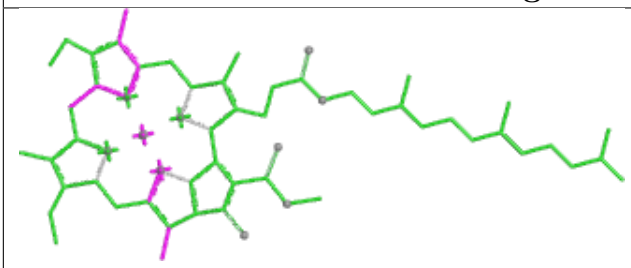
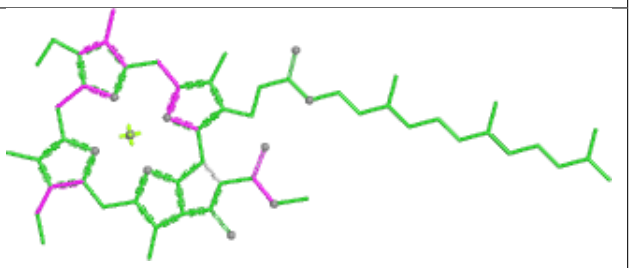
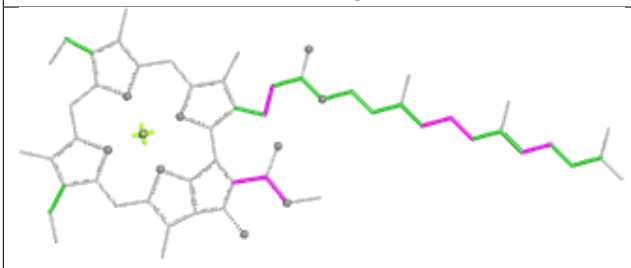
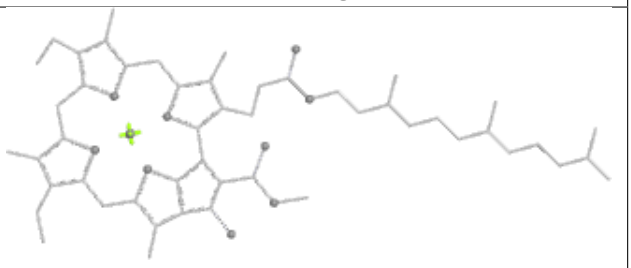
Bond angles

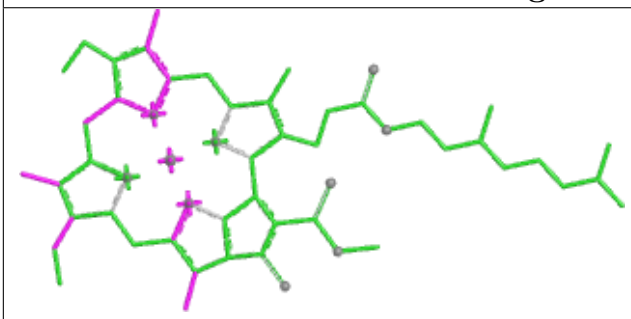
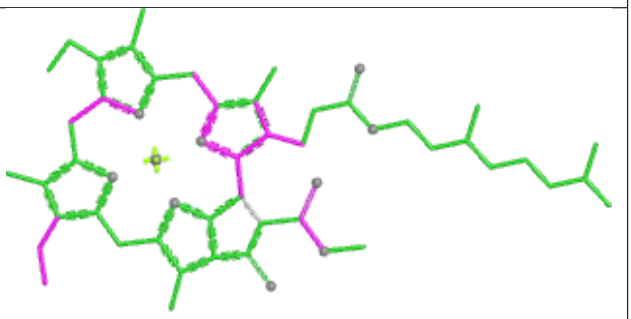
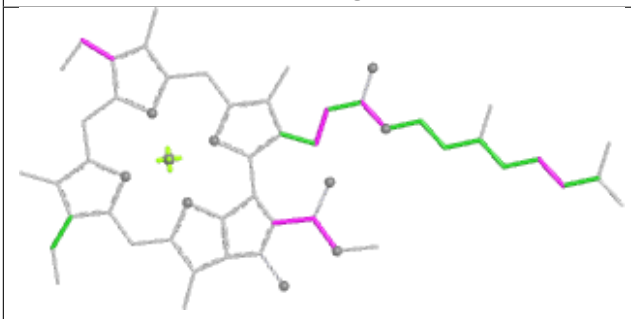
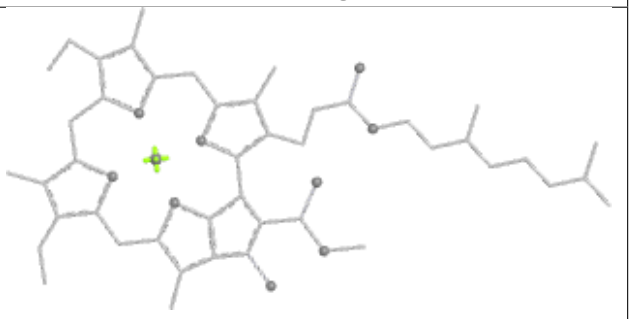


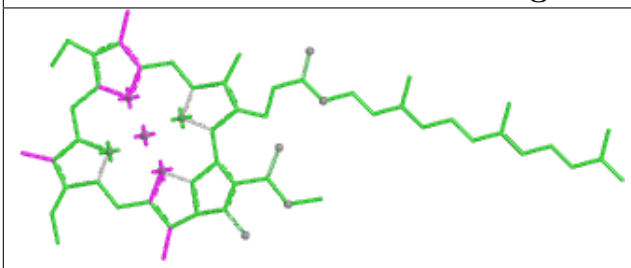
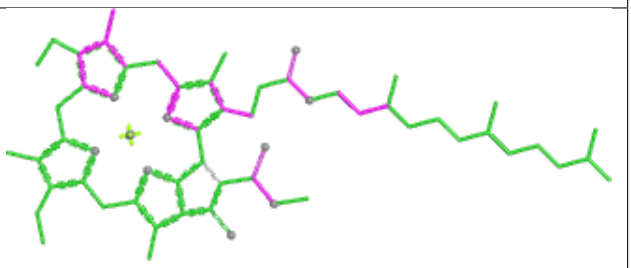
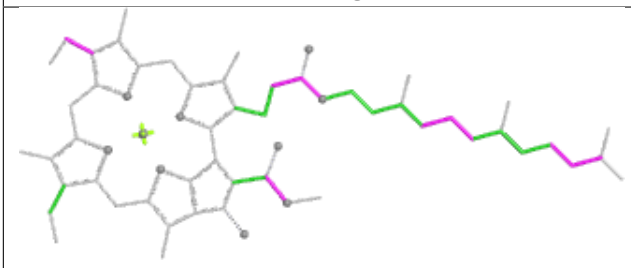
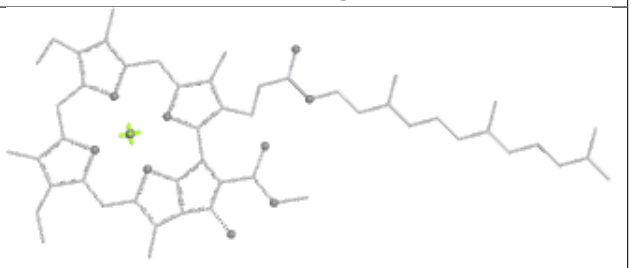
Torsions

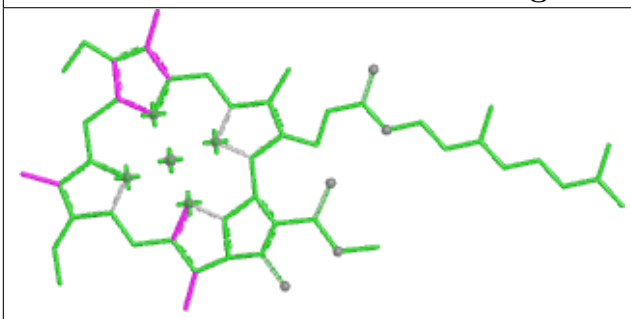
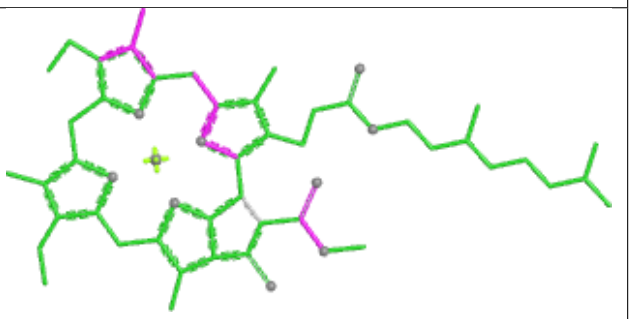
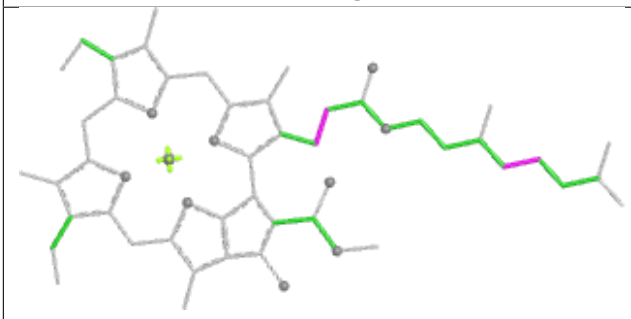
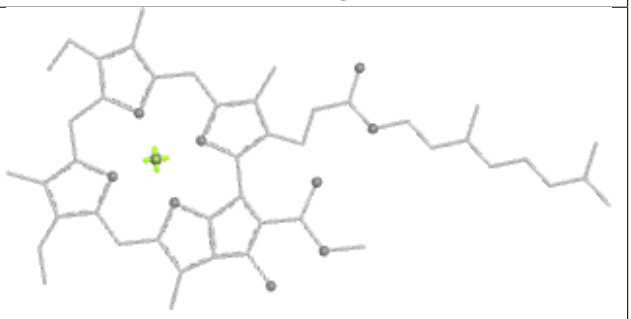


Rings

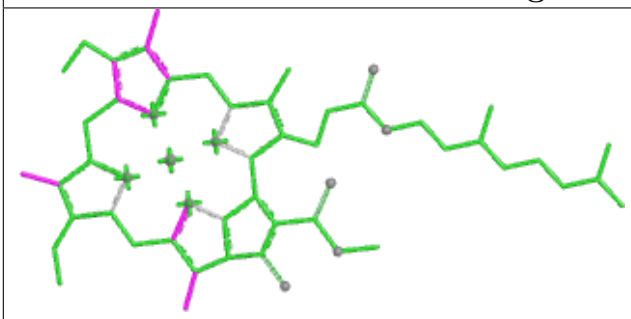
Ligand CLA N 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 7 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

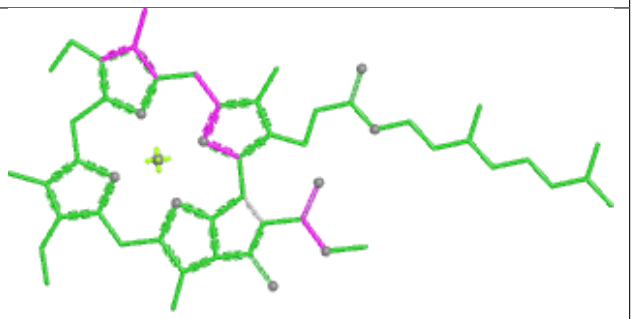
Ligand CLA r 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA s 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

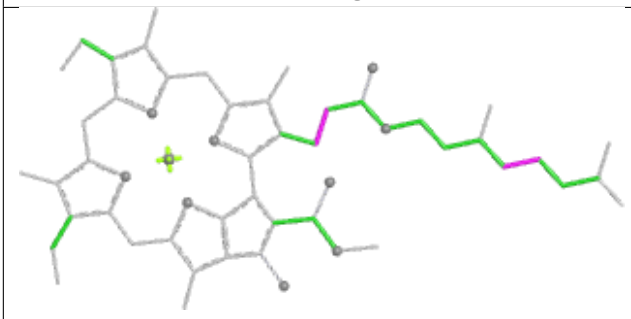
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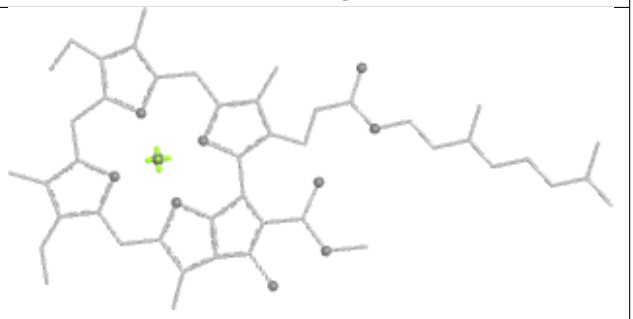
Bond lengths



Bond angles

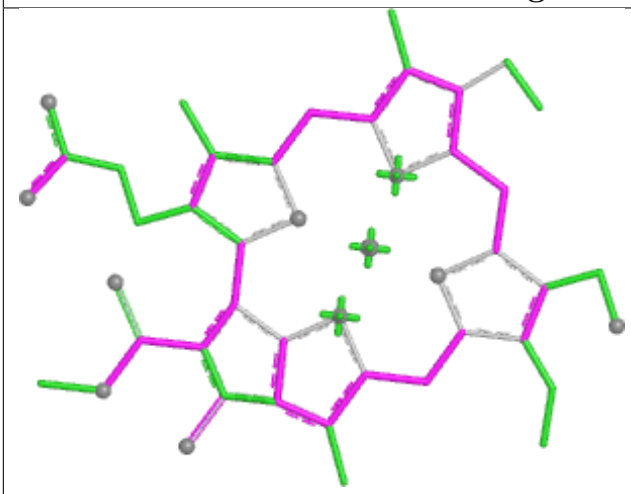


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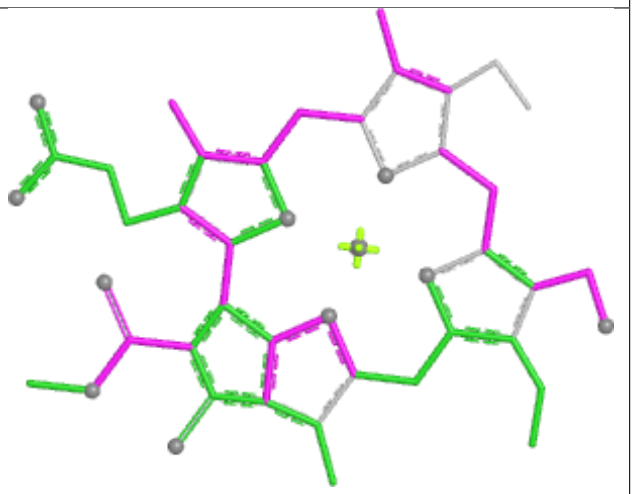


Rings

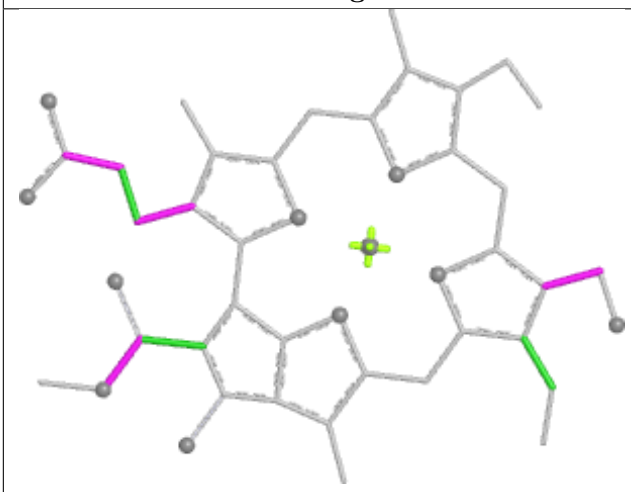
Ligand CHL 1 605



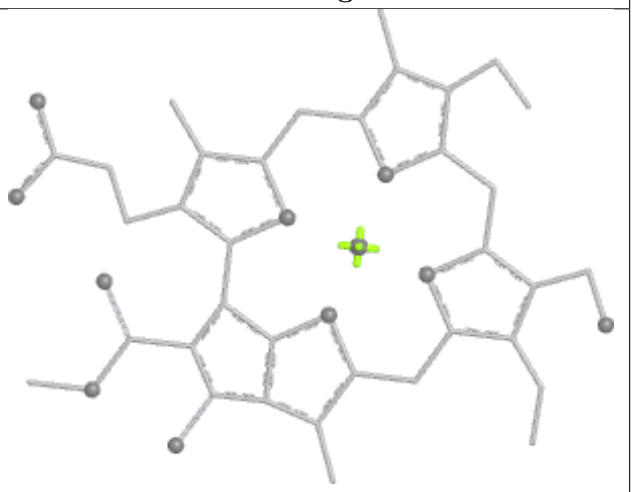
Bond lengths



Bond angles



Torsions

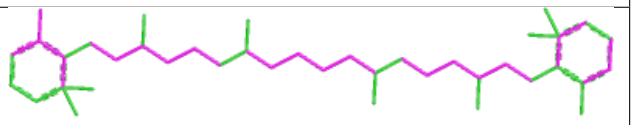


Rings

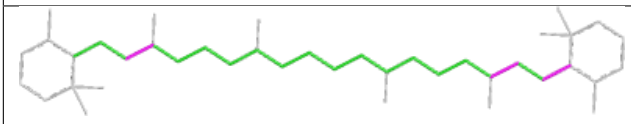
Ligand BCR b 620



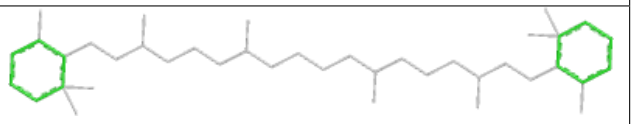
Bond lengths



Bond angles

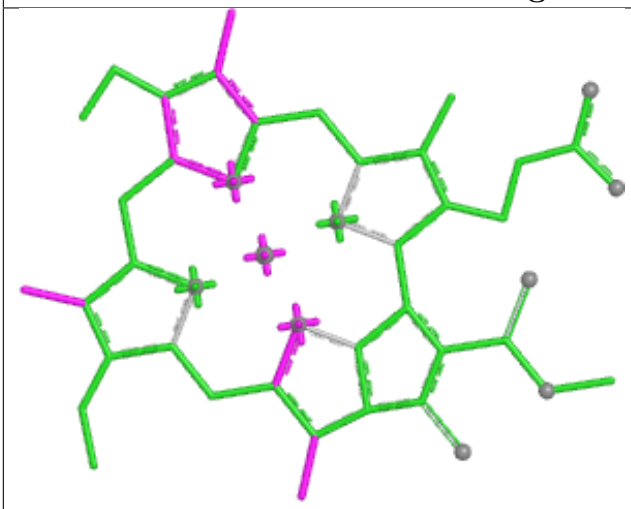


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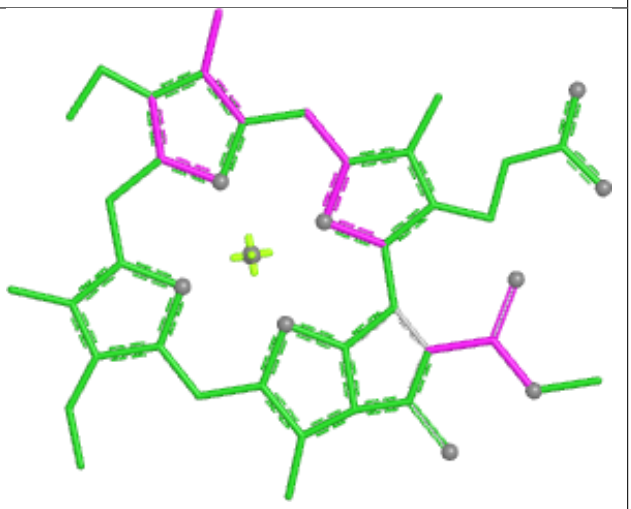


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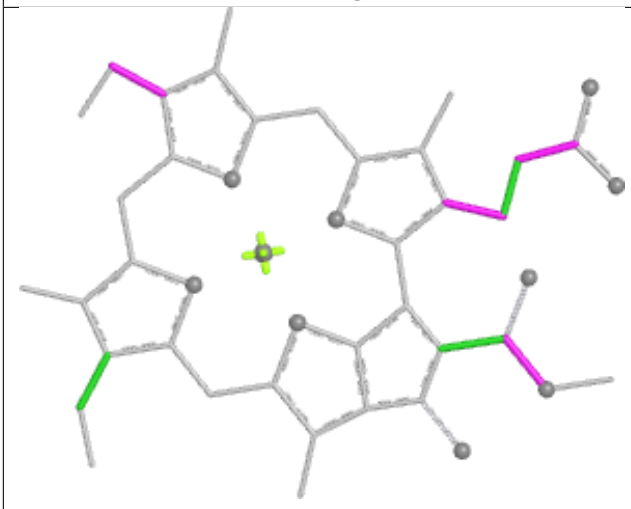
Ligand CLA 6 614



Bond lengths



Bond angles

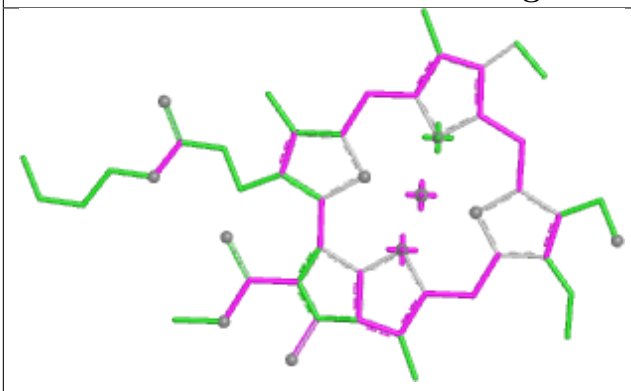


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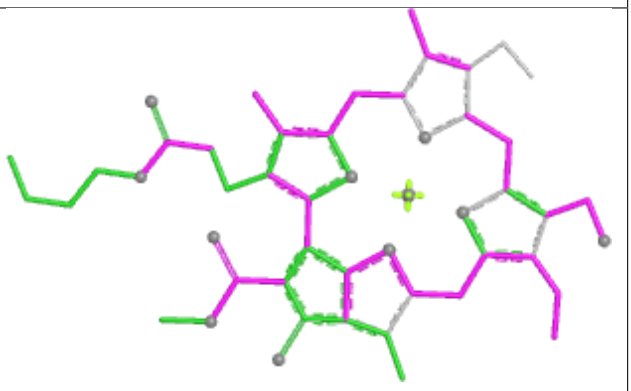


Rings

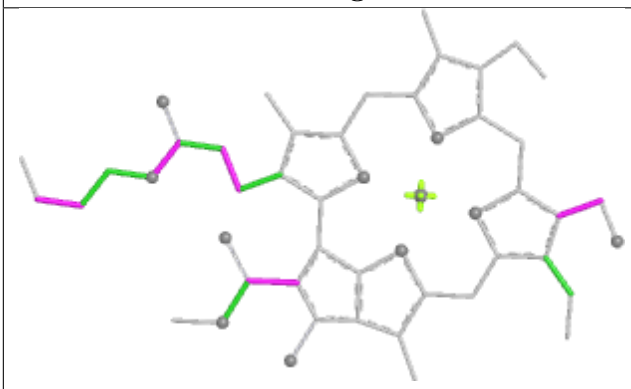
Ligand CHL N 606



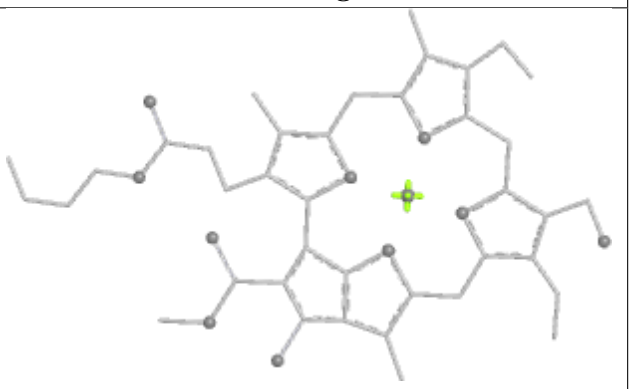
Bond lengths



Bond angles

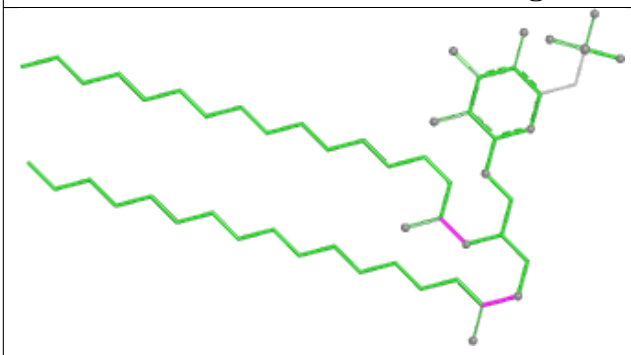


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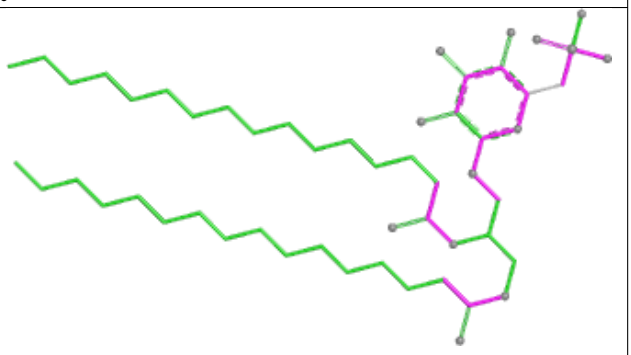


Rings

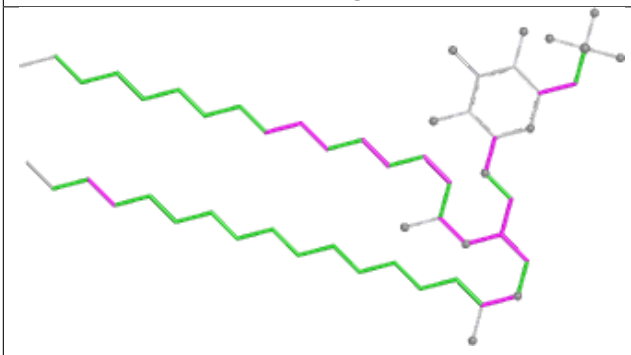
Ligand SQD b 621



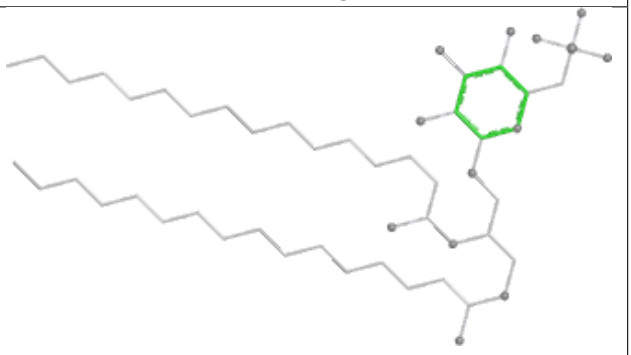
Bond lengths



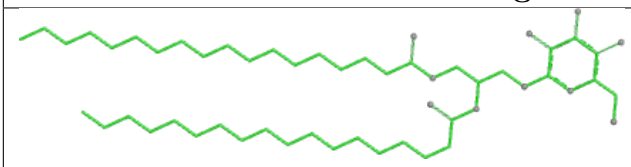
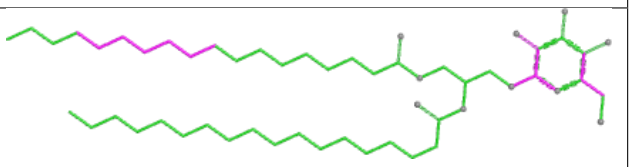
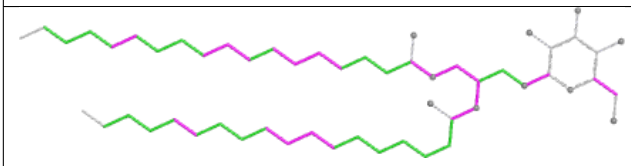
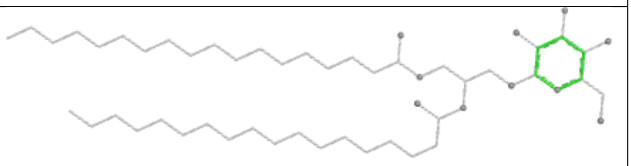
Bond angles

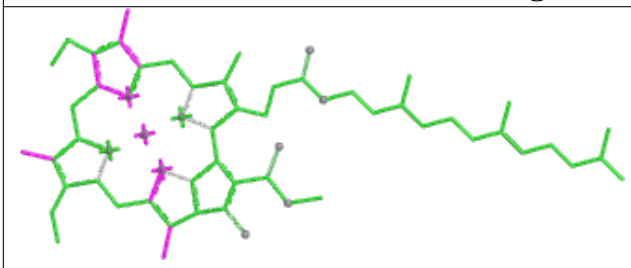
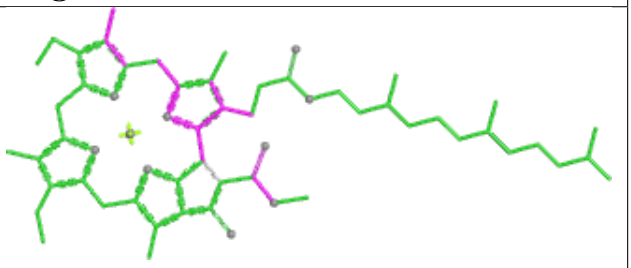
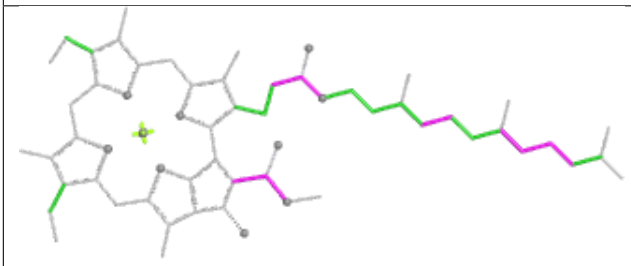
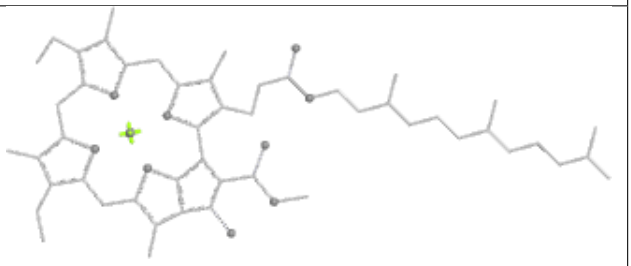


Torsions

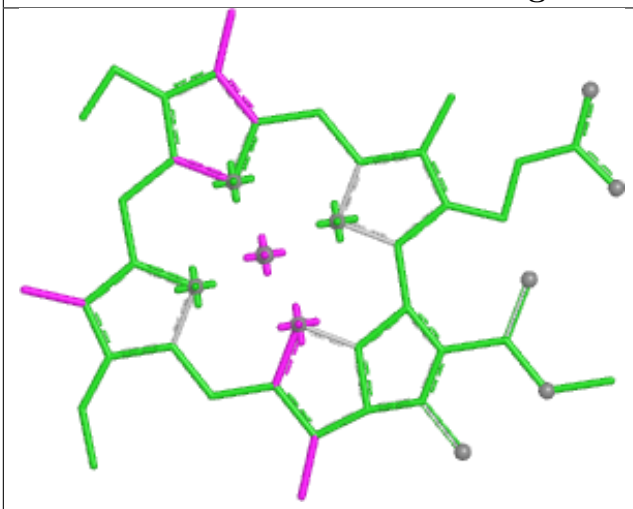


Rings

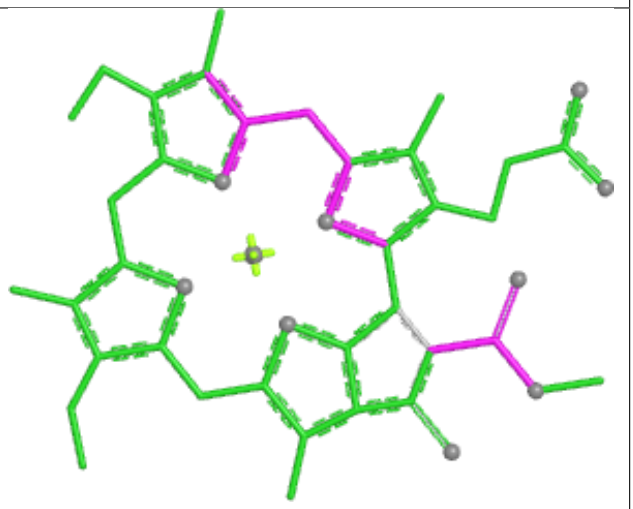
Ligand LMG b 2633	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

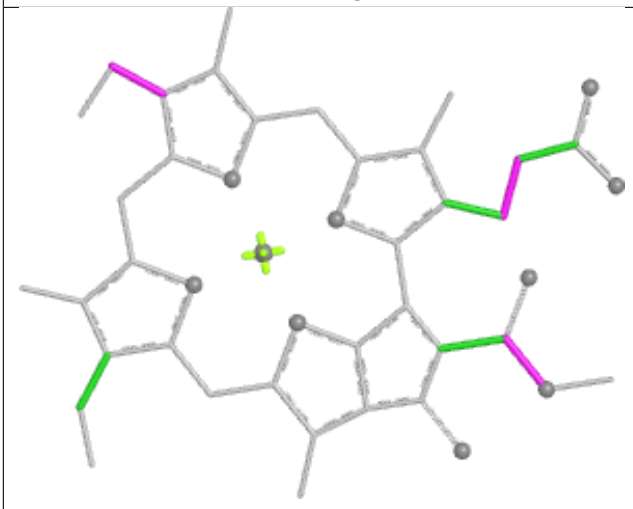
Ligand CLA 6 613



Bond lengths



Bond angles

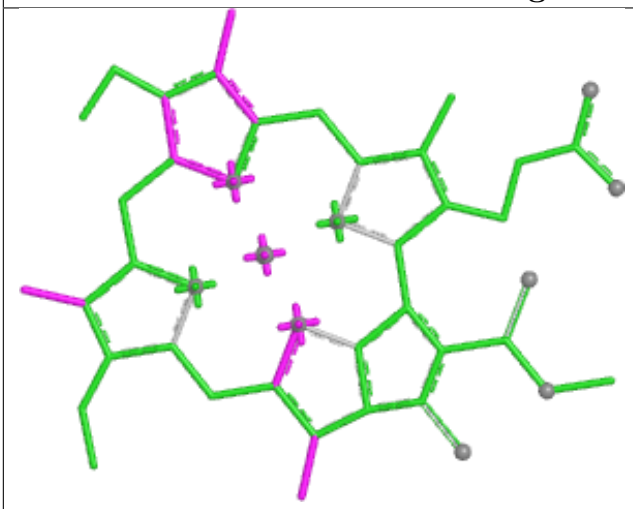


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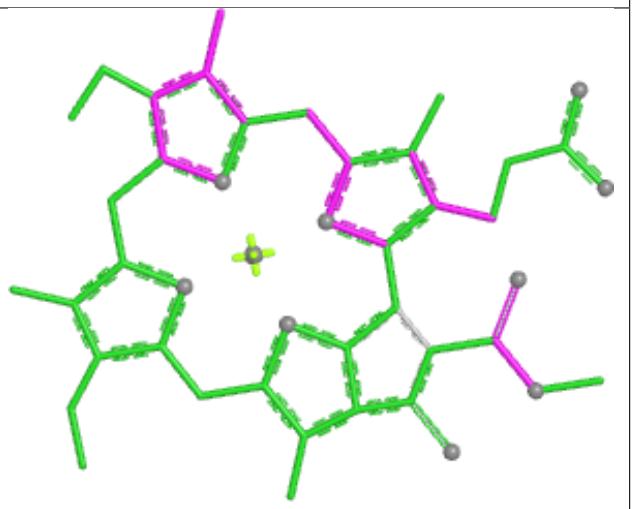


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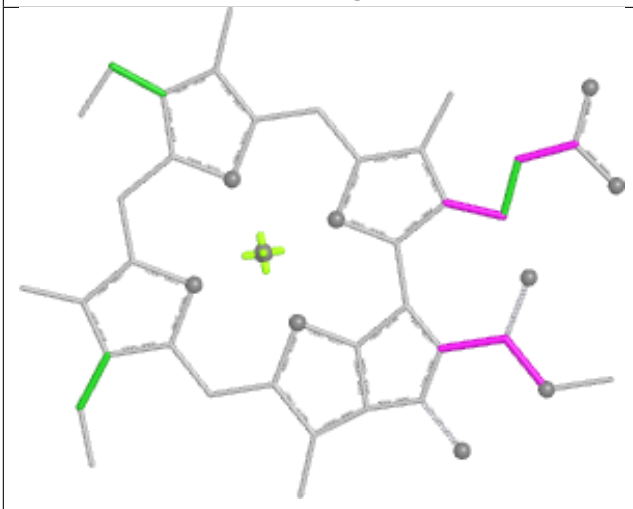
Ligand CLA 8 612



Bond lengths



Bond angles

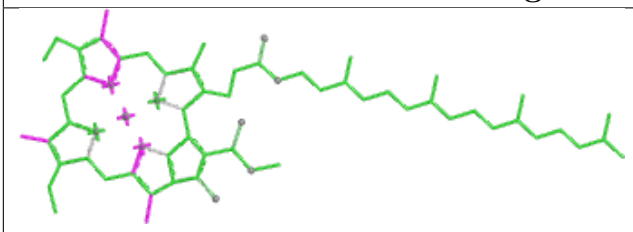


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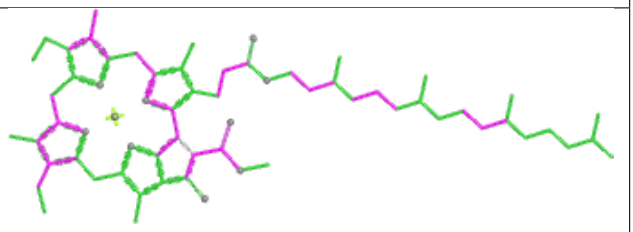


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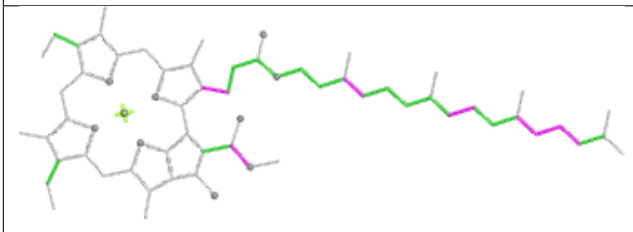
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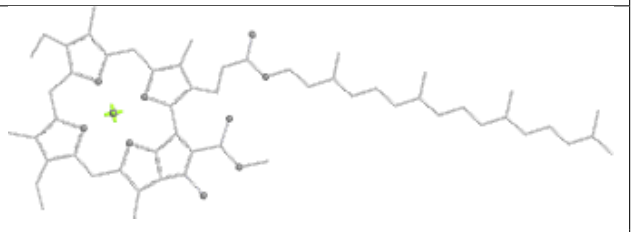
Bond lengths



Bond angles

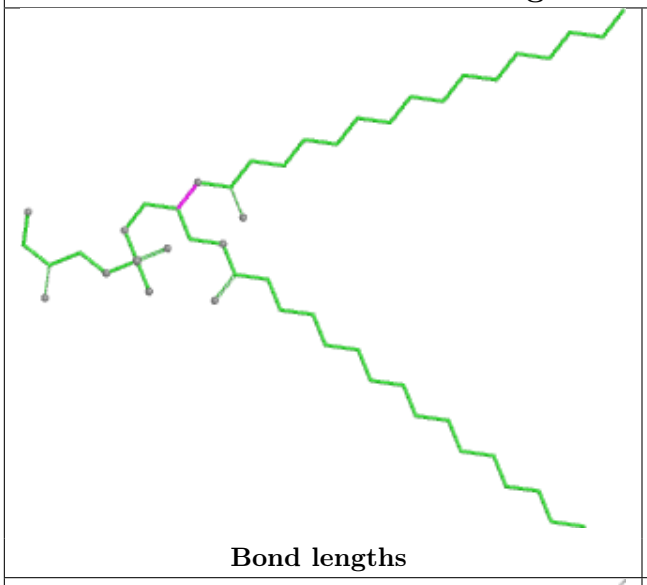


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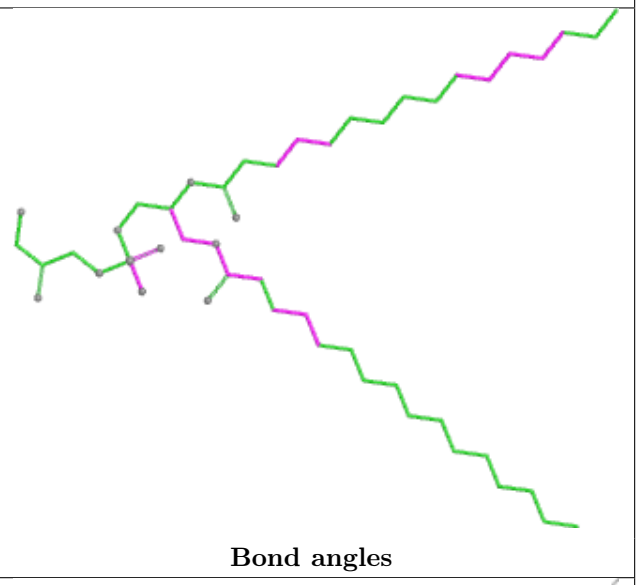


Rings

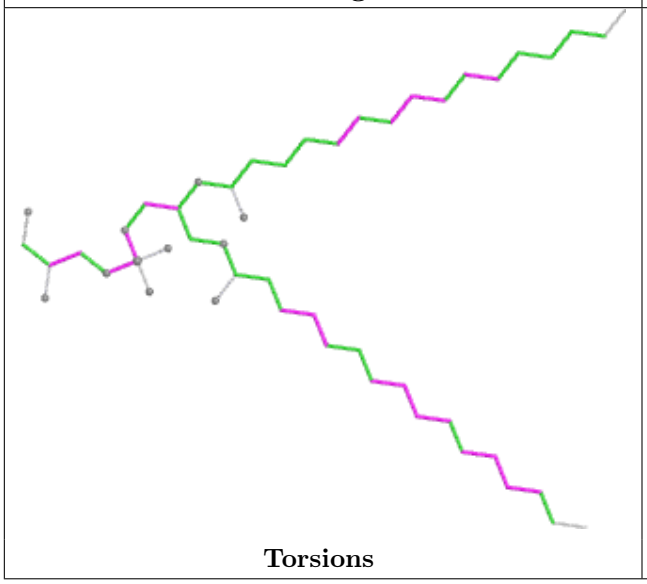
Ligand LHG d 409



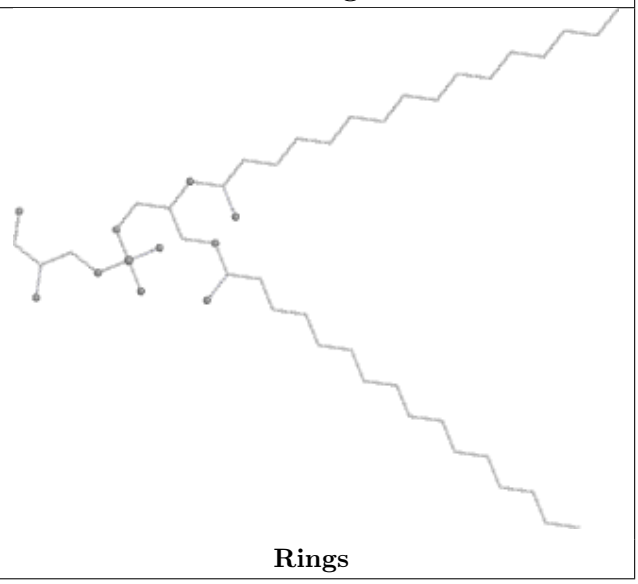
Bond lengths



Bond angles

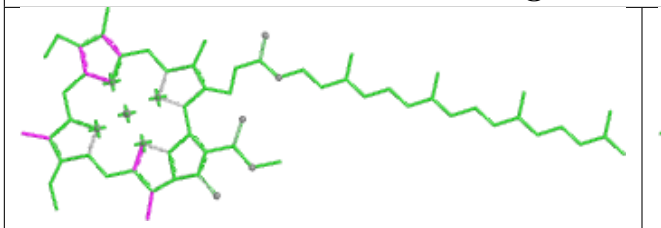


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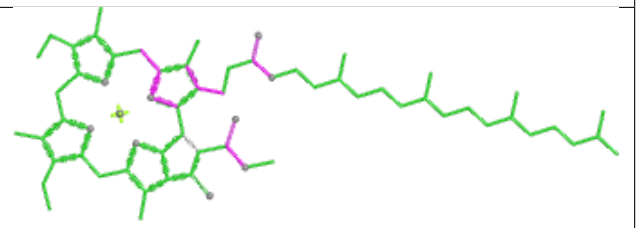


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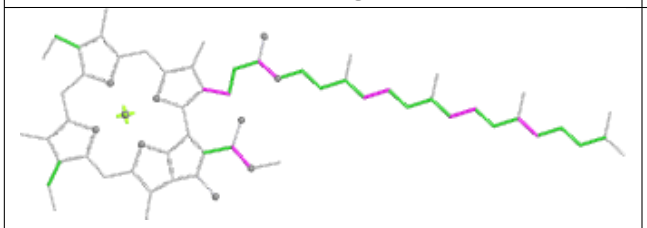
Ligand CLA C 512



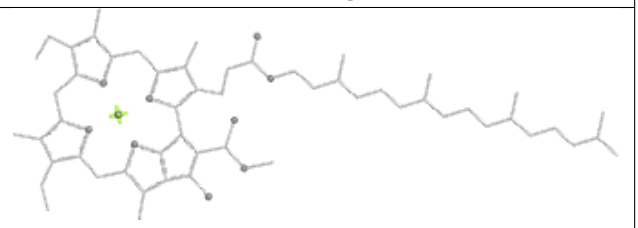
Bond lengths



Bond angles

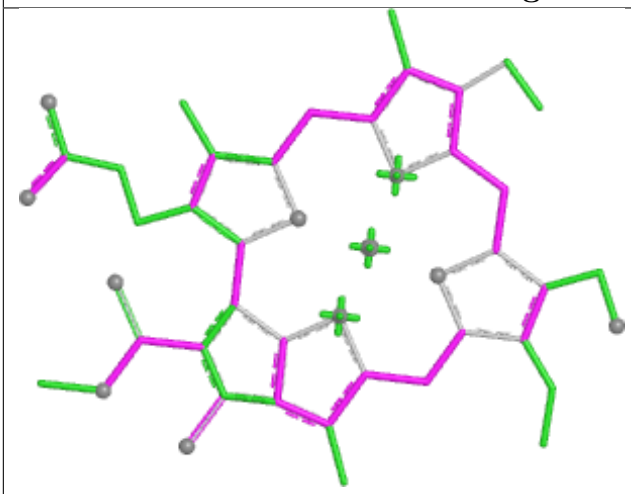


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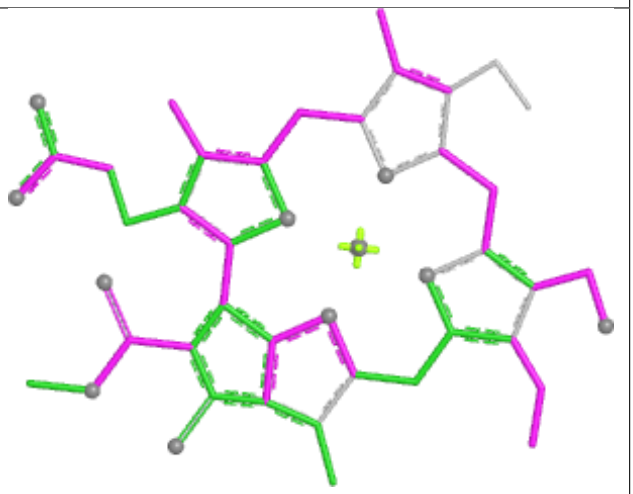


Rings

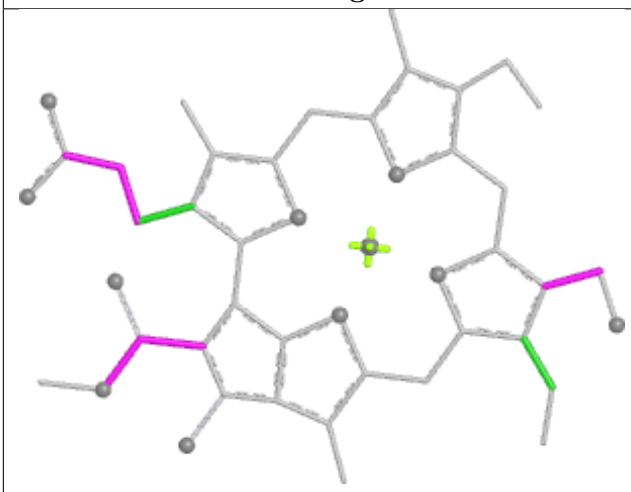
Ligand CHL G 605



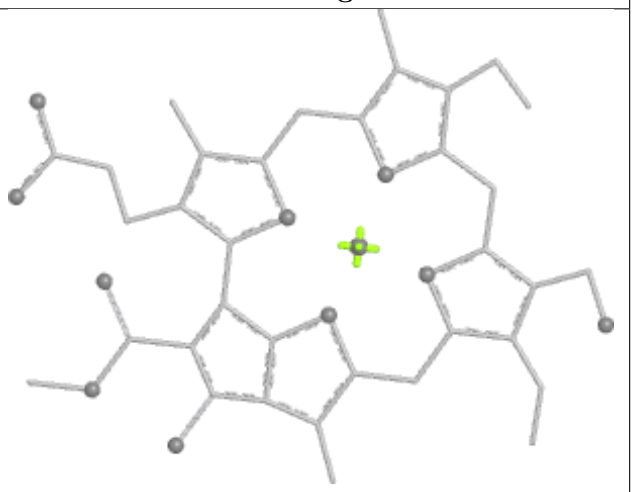
Bond lengths



Bond angles

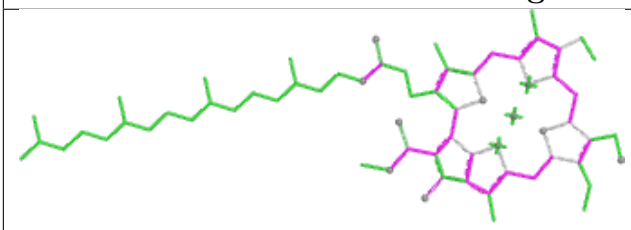


Torsions

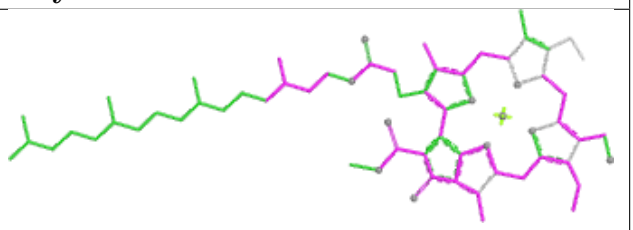


Rings

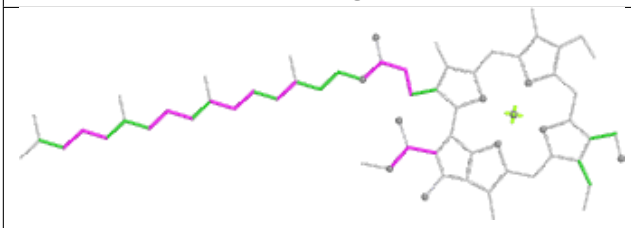
Ligand CHL y 601



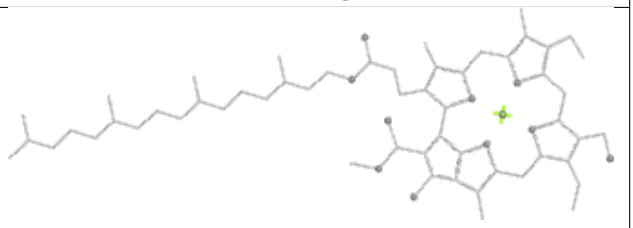
Bond lengths



Bond angles

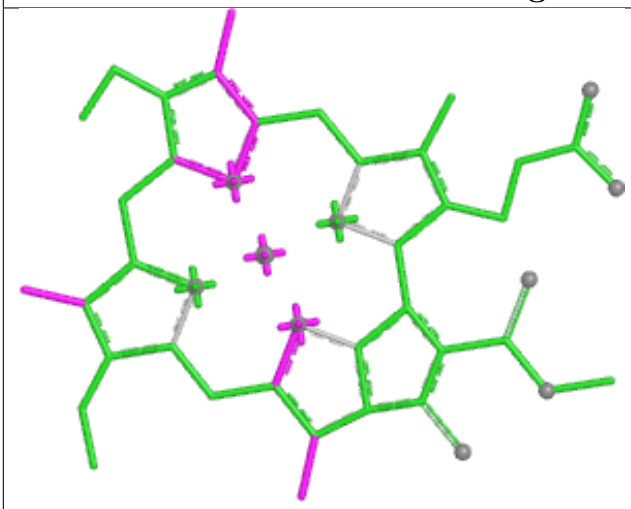


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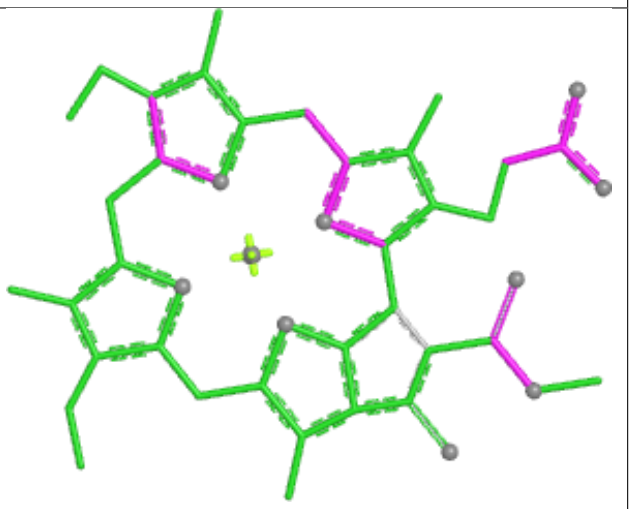


Rings

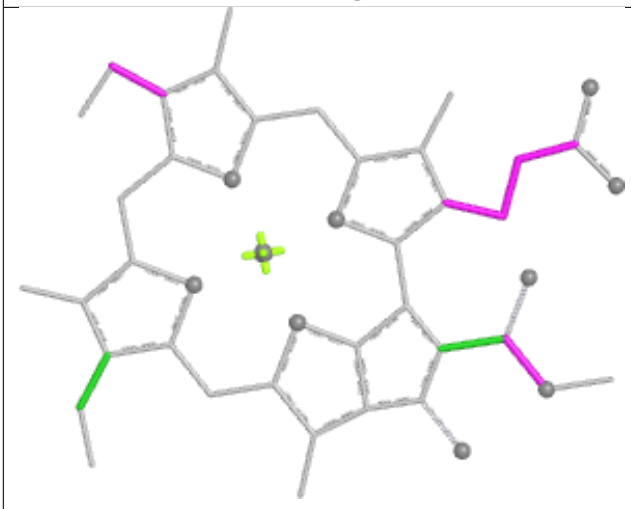
Ligand CLA 4 604



Bond lengths



Bond angles

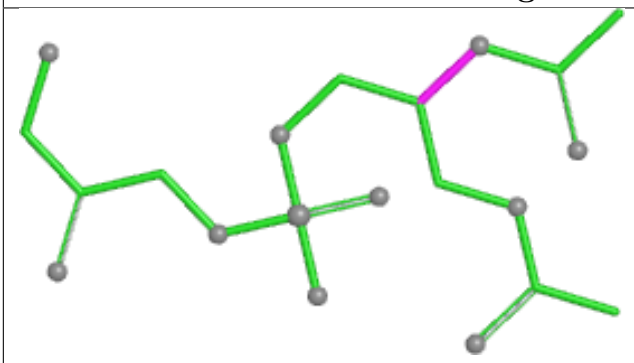


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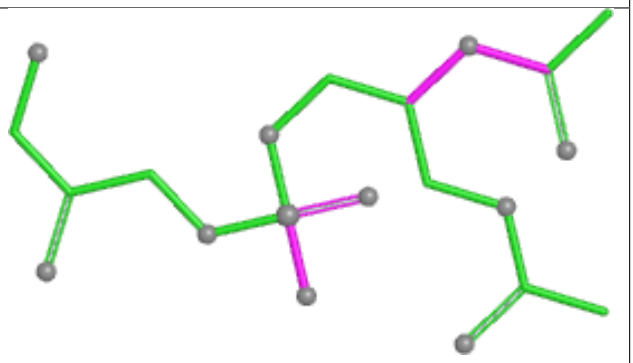


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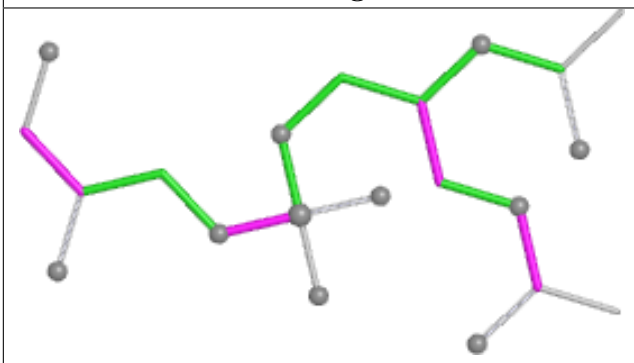
Ligand LHG 8 2630



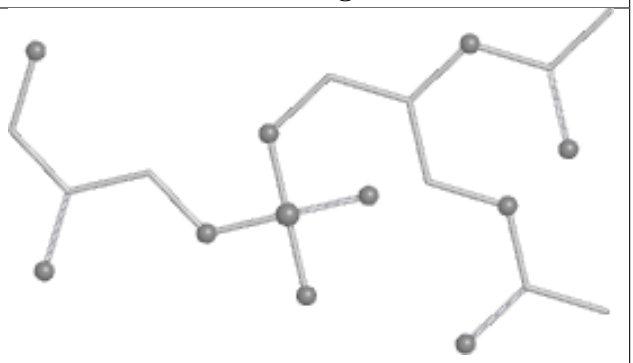
Bond lengths



Bond angles

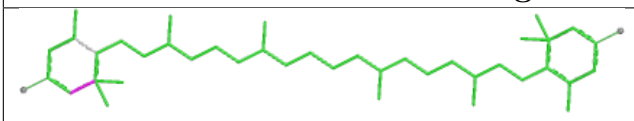


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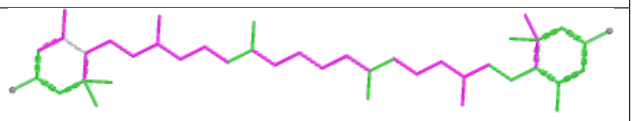


Rings

Ligand LUT G 1620



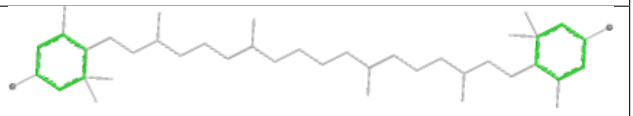
Bond lengths



Bond angles

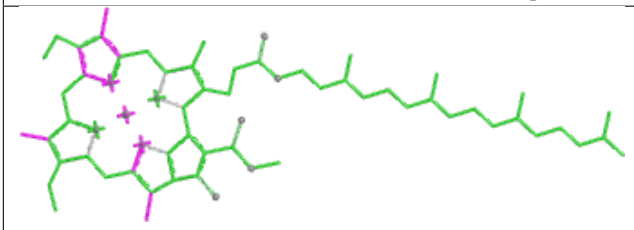


Torsions

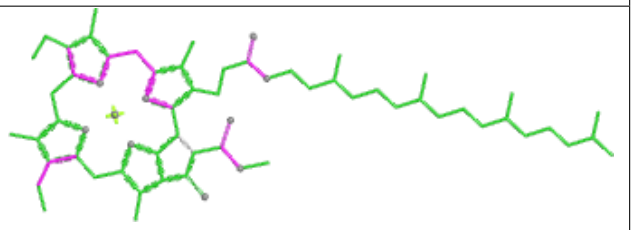


Rings

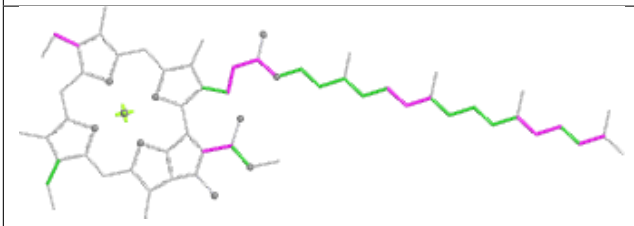
Ligand CLA B 602



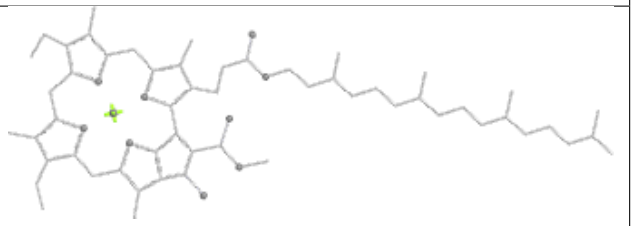
Bond lengths



Bond angles

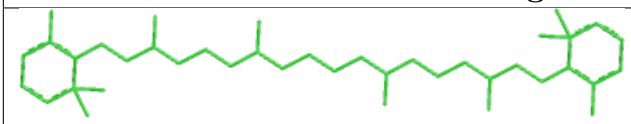


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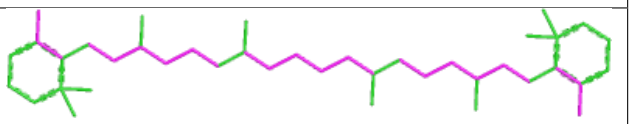


Rings

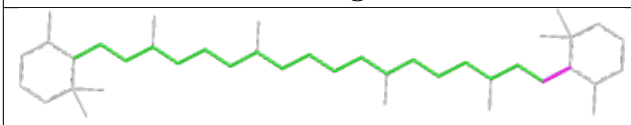
Ligand BCR a 411



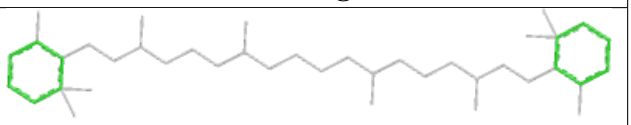
Bond lengths



Bond angles

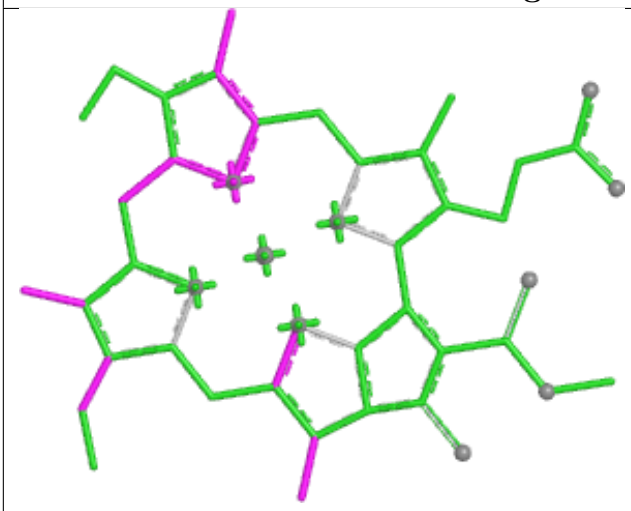


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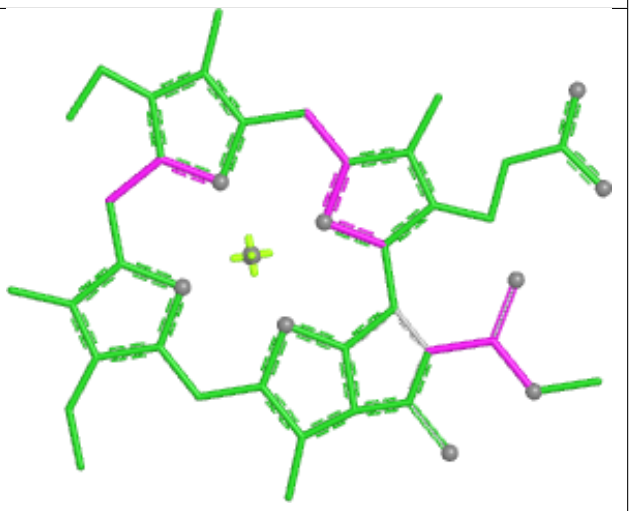


Rings

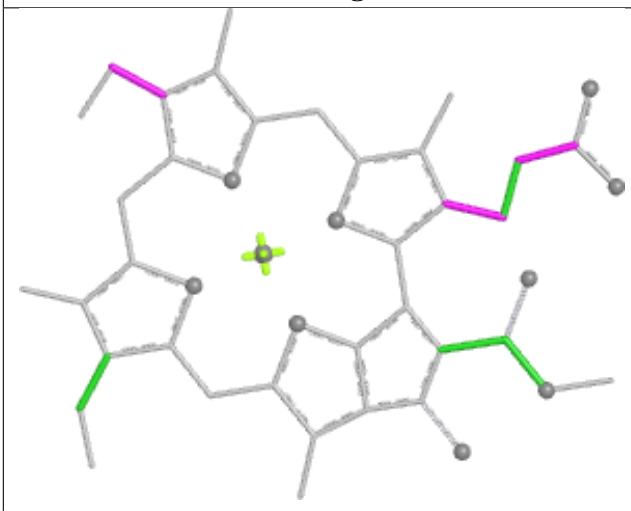
Ligand CLA R 616



Bond lengths



Bond angles

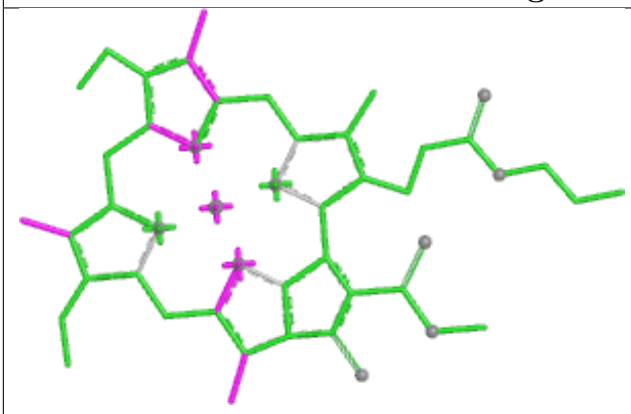


Torsions

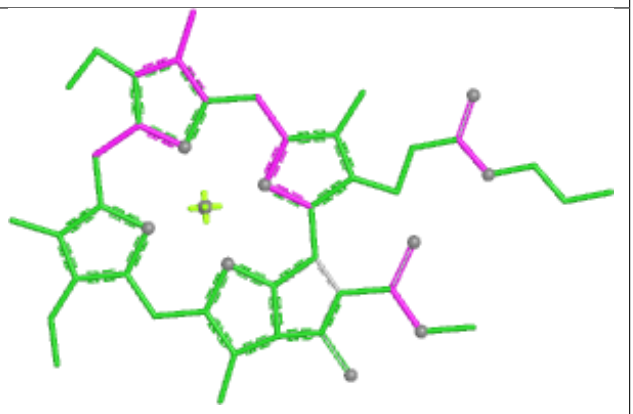


Rings

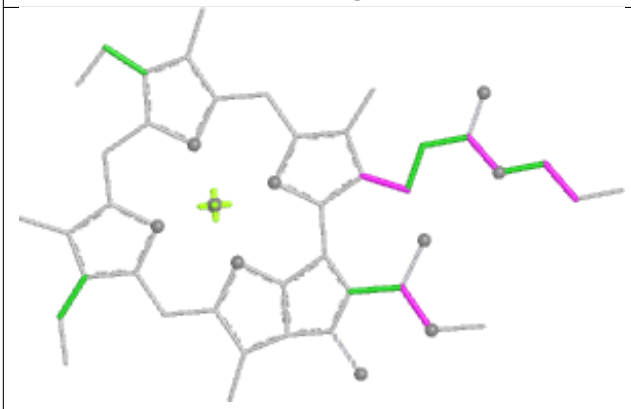
Ligand CLA n 614



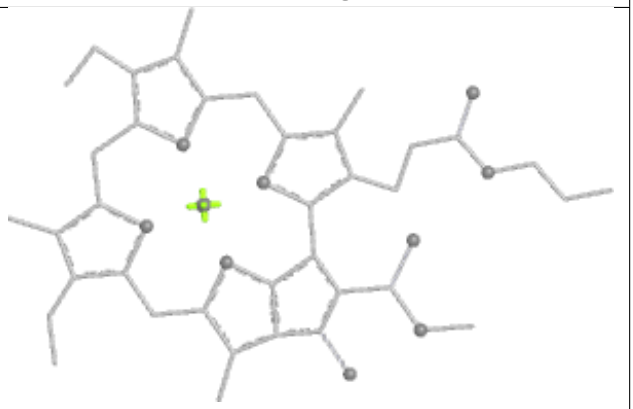
Bond lengths



Bond angles

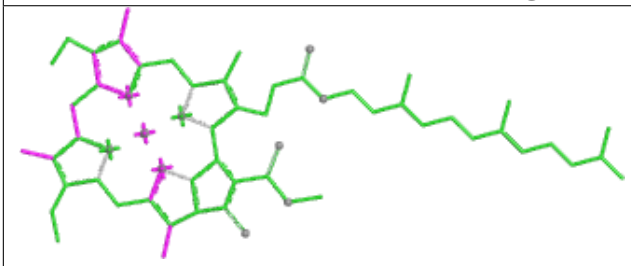


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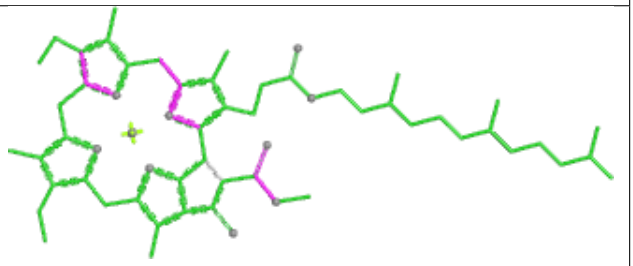


Rings

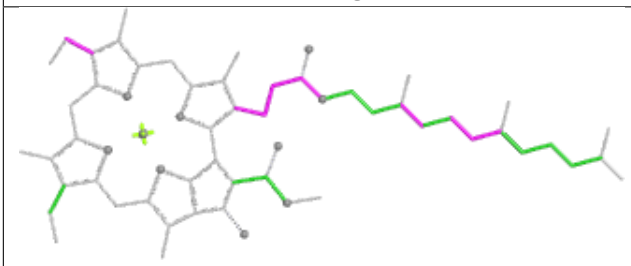
Ligand CLA G 611



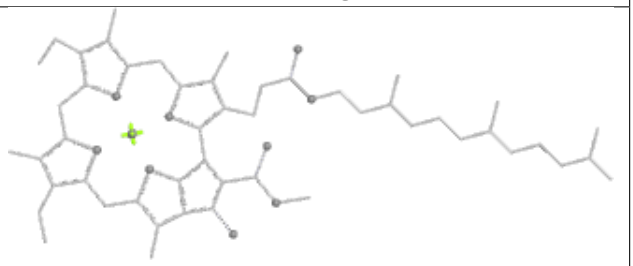
Bond lengths



Bond angles

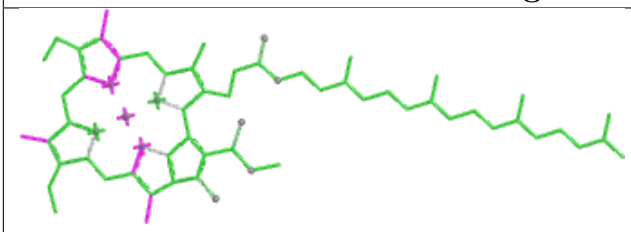


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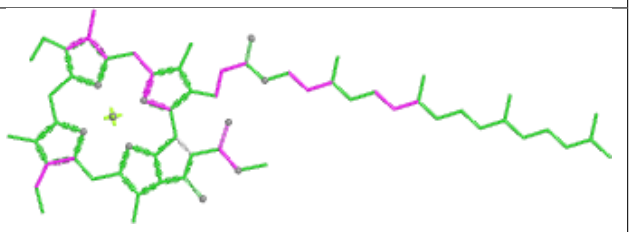


Rings

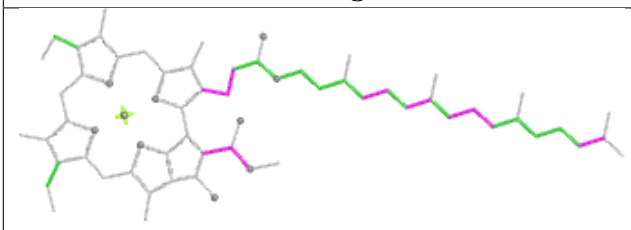
Ligand CLA N 602



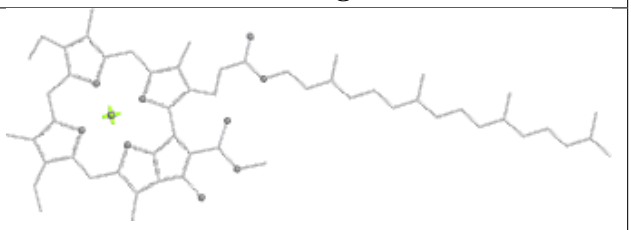
Bond lengths



Bond angles

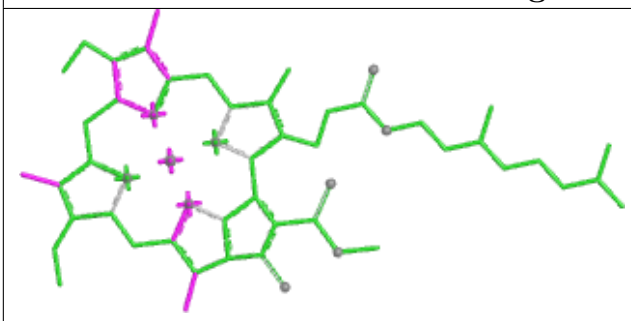


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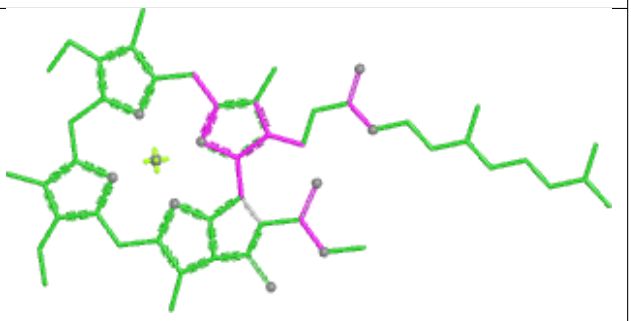


Rings

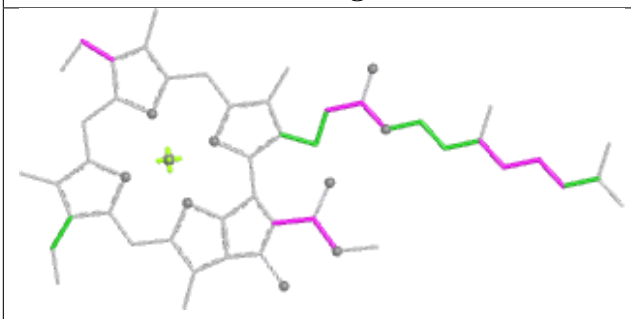
Ligand CLA 2 603



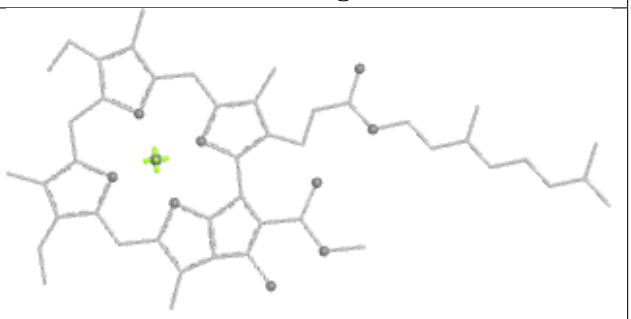
Bond lengths



Bond angles

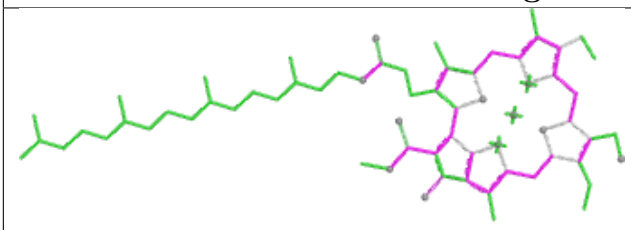


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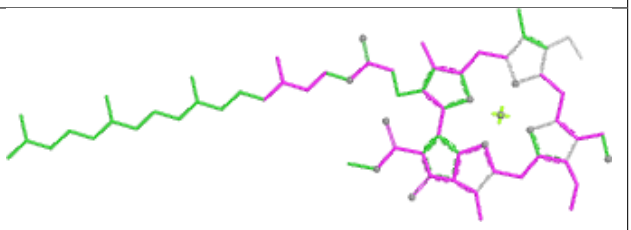


Rings

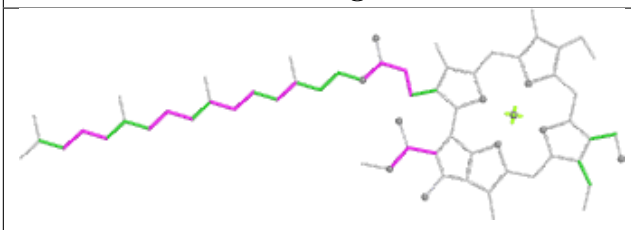
Ligand CHL Y 601



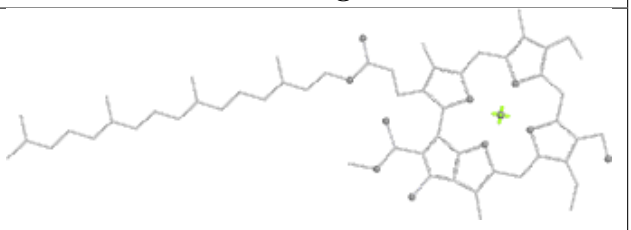
Bond lengths



Bond angles

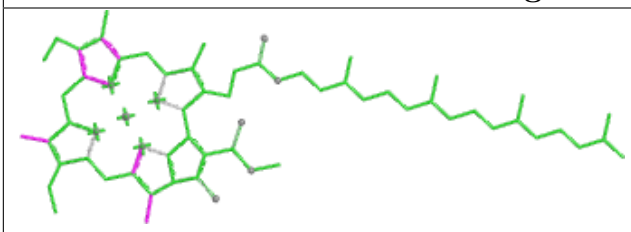


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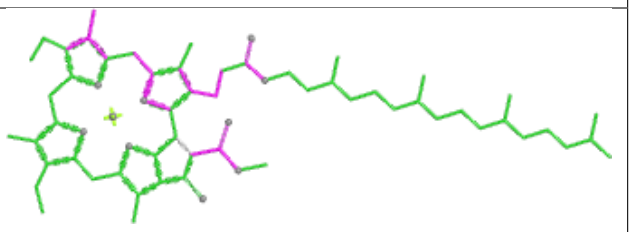


Rings

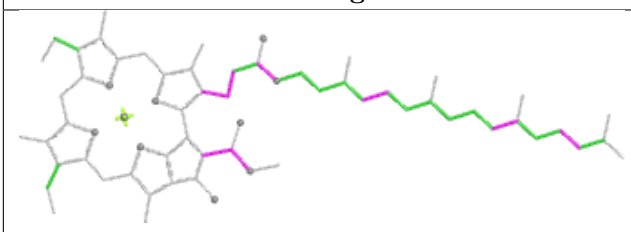
Ligand CLA C 513



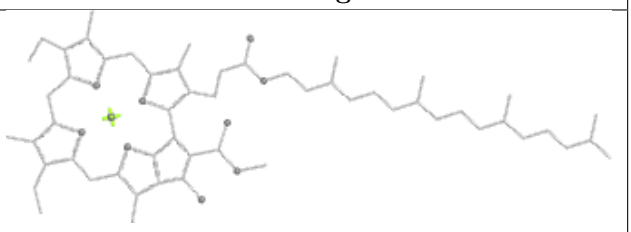
Bond lengths



Bond angles

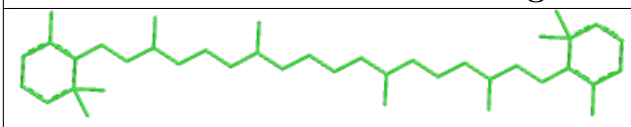


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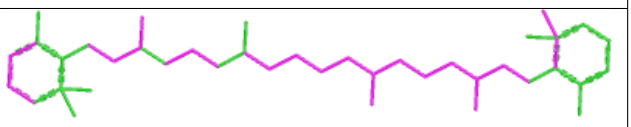


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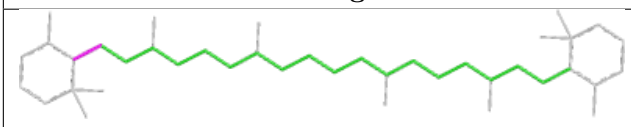
Ligand BCR c 514



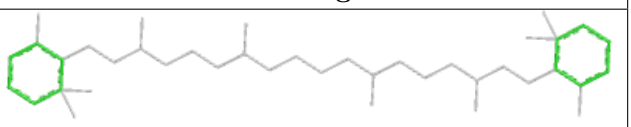
Bond lengths



Bond angles

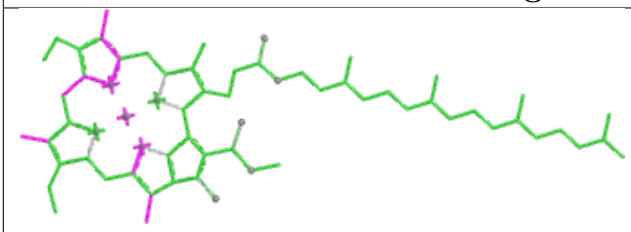


Torsions

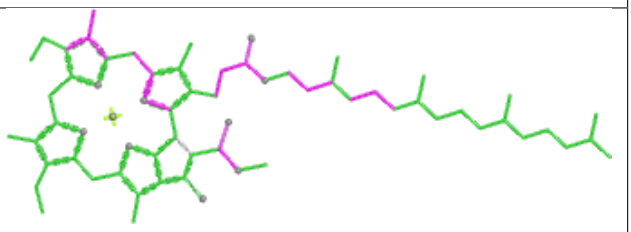


Rings

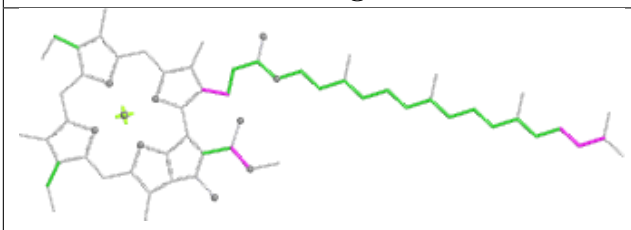
Ligand CLA B 610



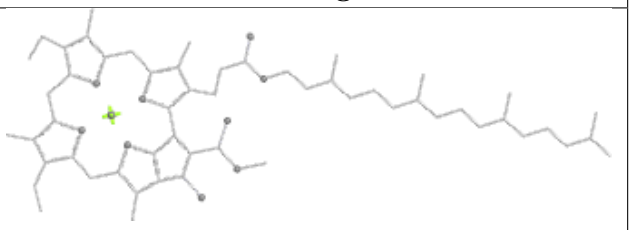
Bond lengths



Bond angles

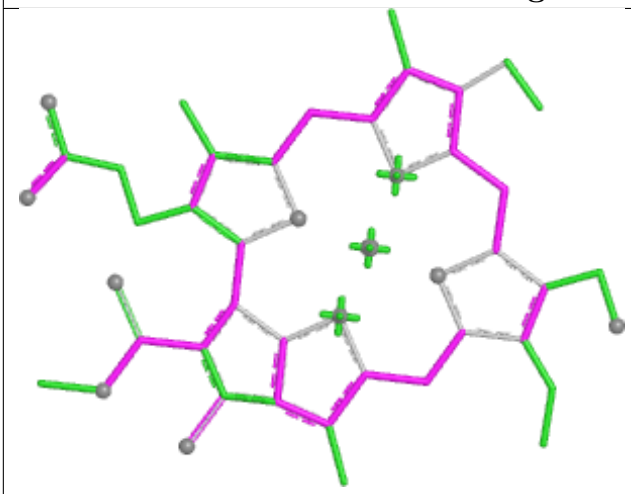


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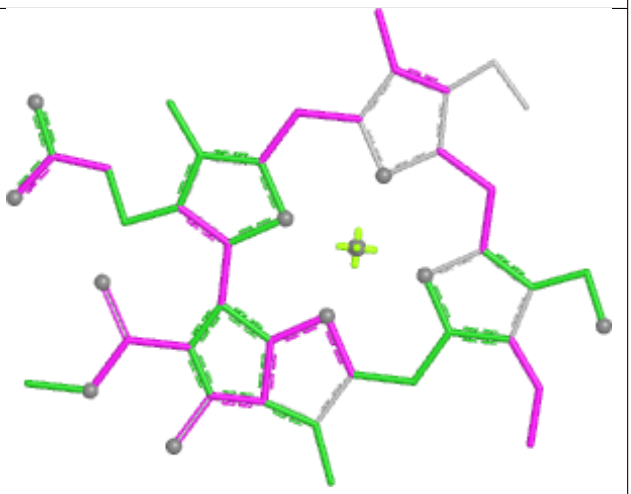


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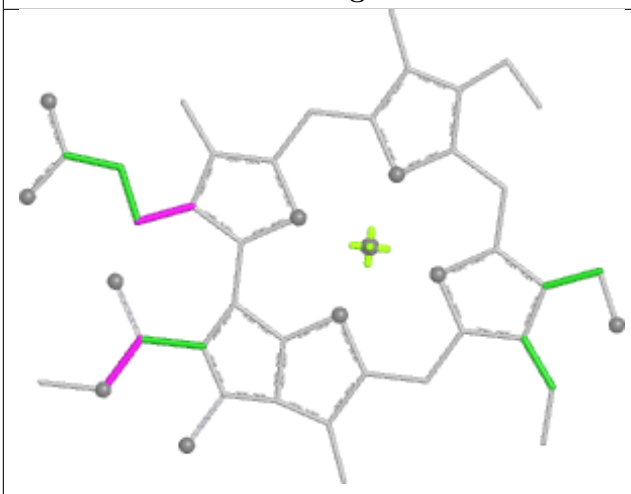
Ligand CHL 5 608



Bond lengths



Bond angles

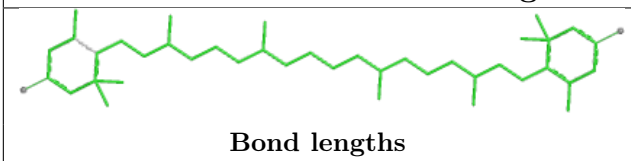


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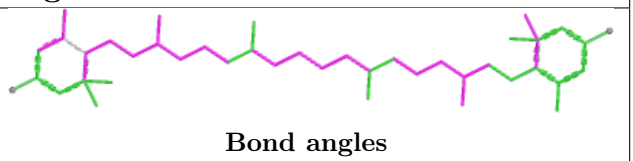


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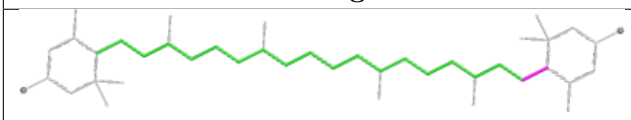
Ligand LUT g 1620



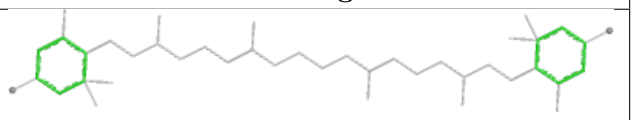
Bond lengths



Bond angles

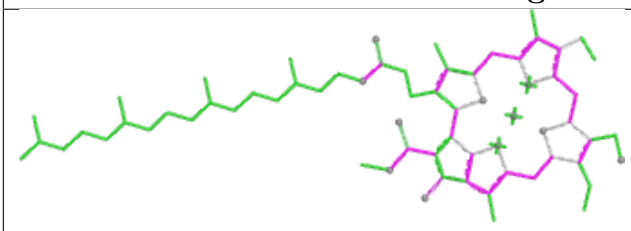


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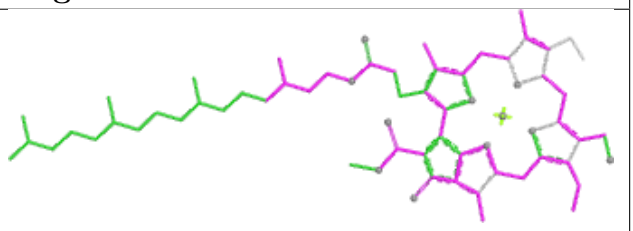


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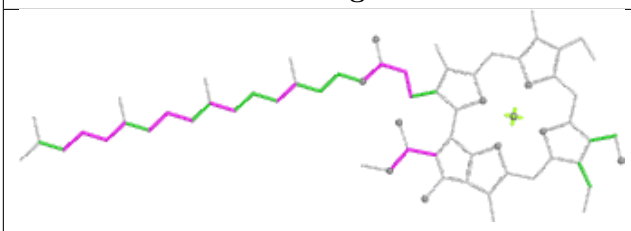
Ligand CHL g 601



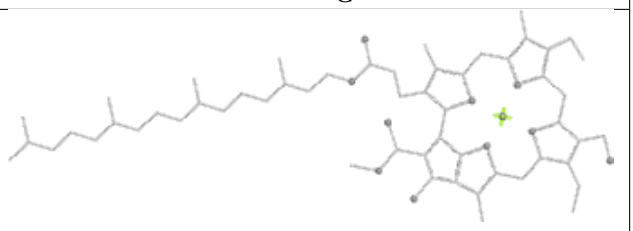
Bond lengths



Bond angles

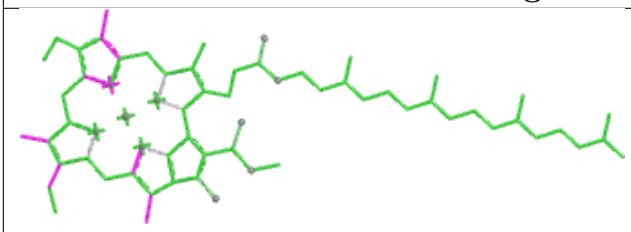


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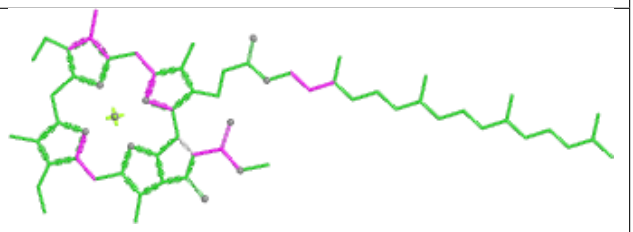


Rings

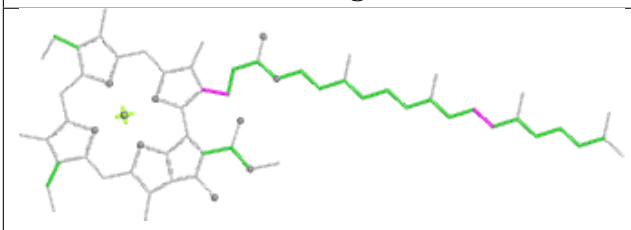
Ligand CLA A 406



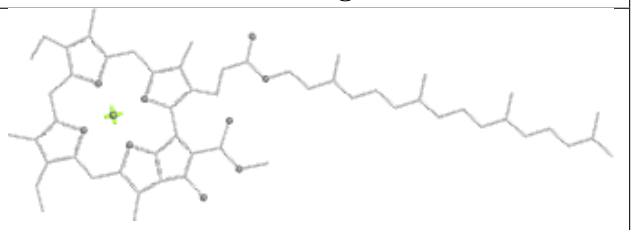
Bond lengths



Bond angles

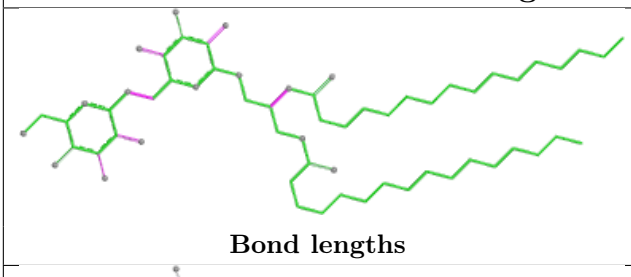


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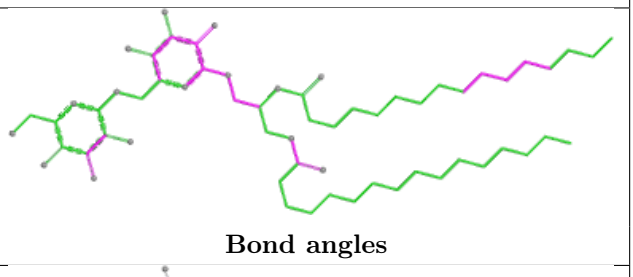


Rings

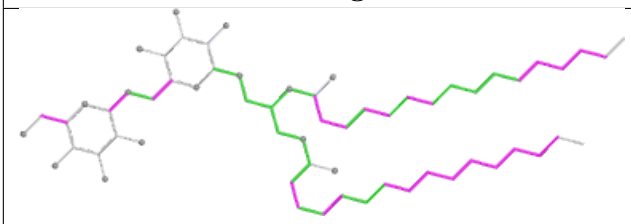
Ligand DGD H 102



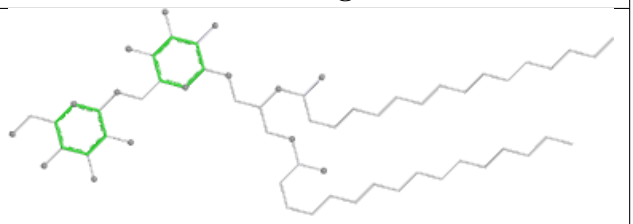
Bond lengths



Bond angles

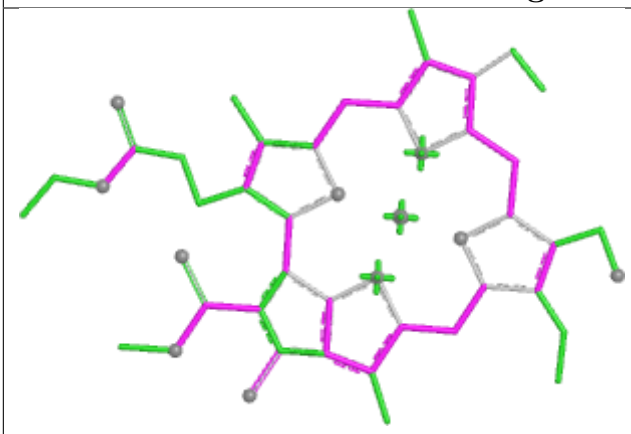


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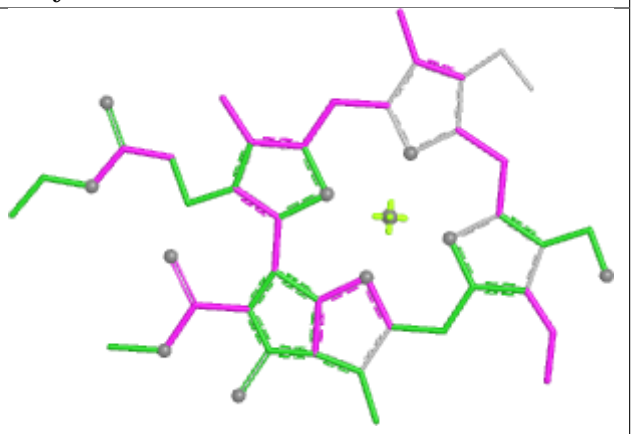


Rings

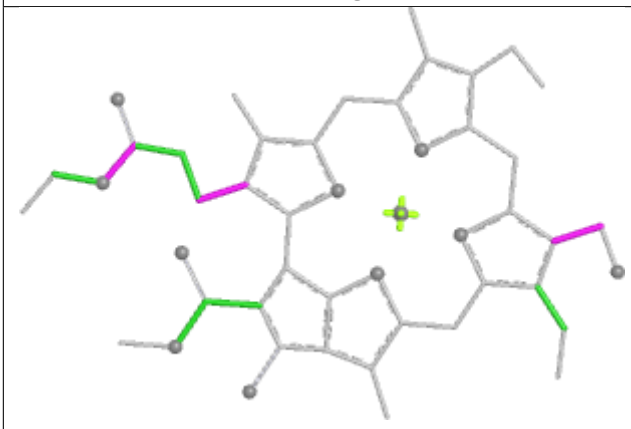
Ligand CHL y 605



Bond lengths



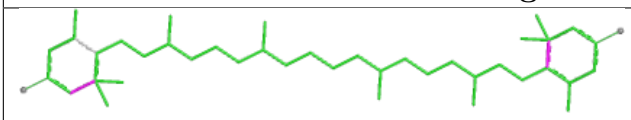
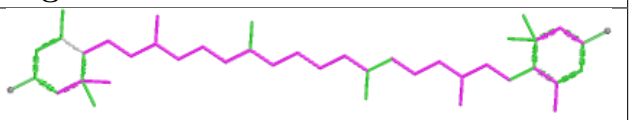
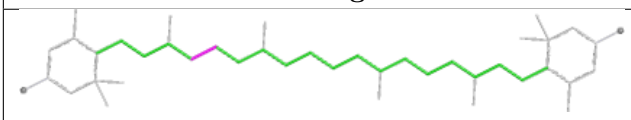
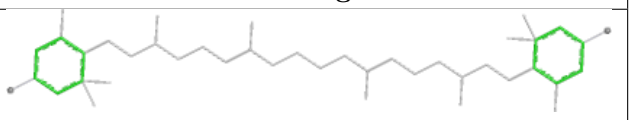
Bond angles

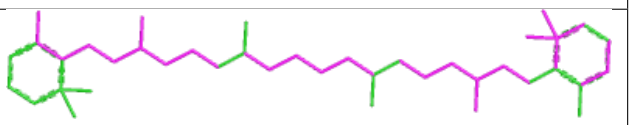
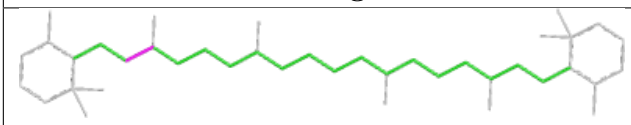
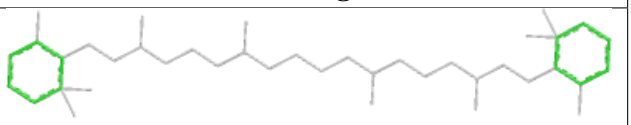


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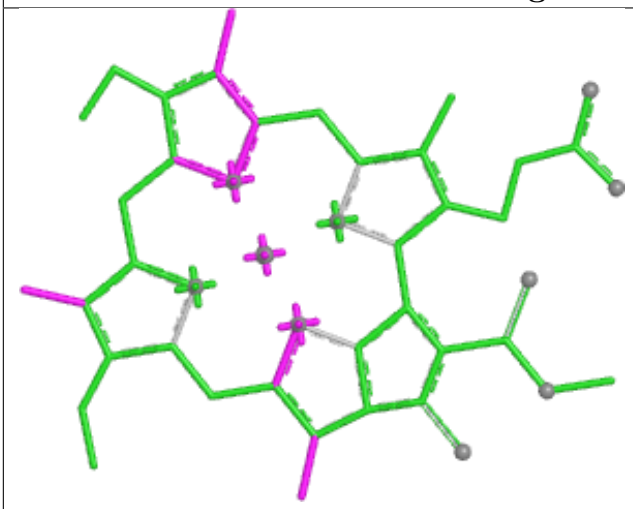


Rings

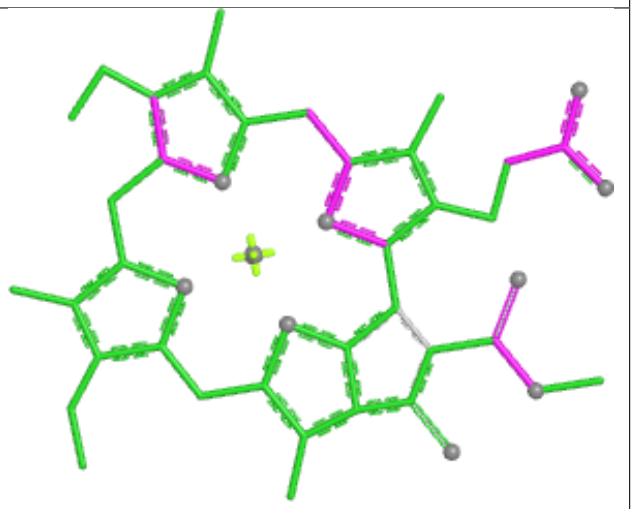
Ligand LUT g 1621	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

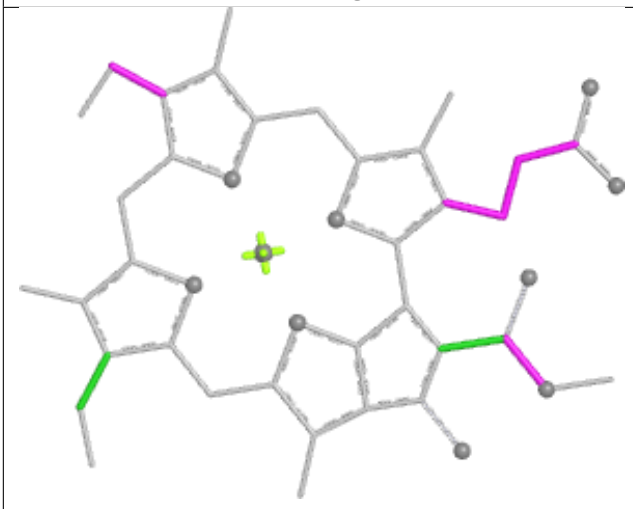
Ligand CLA 8 604



Bond lengths



Bond angles

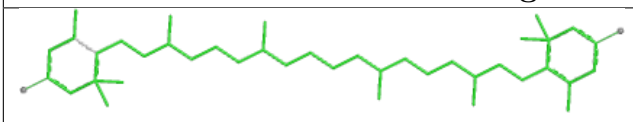


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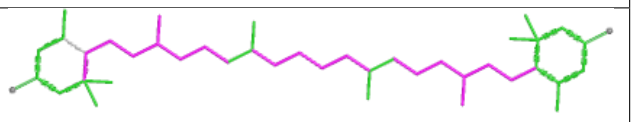


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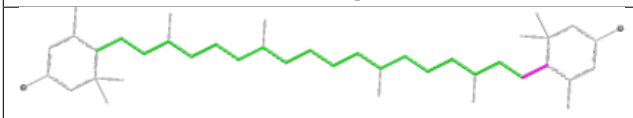
Ligand LUT 2 1620



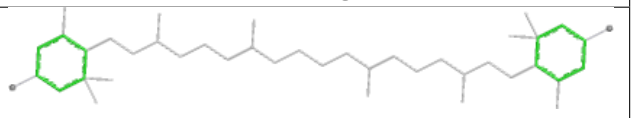
Bond lengths



Bond angles

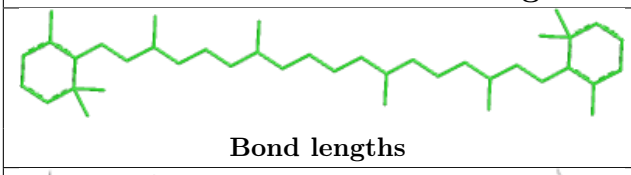


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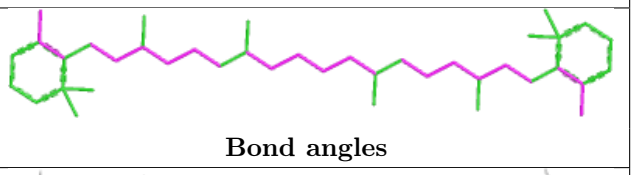


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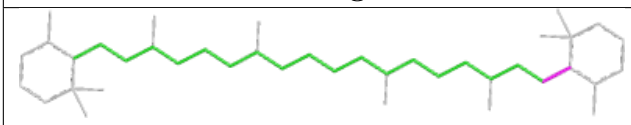
Ligand BCR A 411



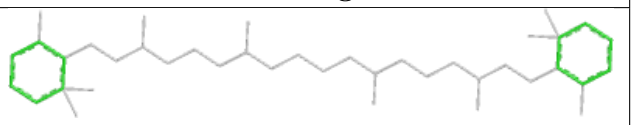
Bond lengths



Bond angles

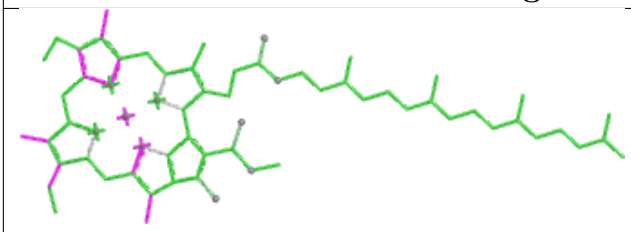


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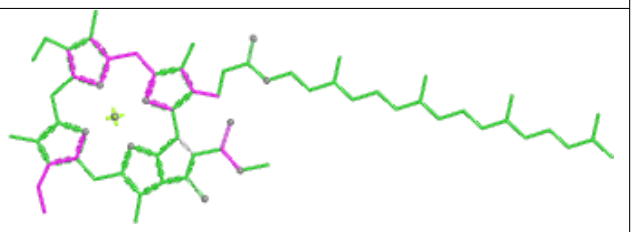


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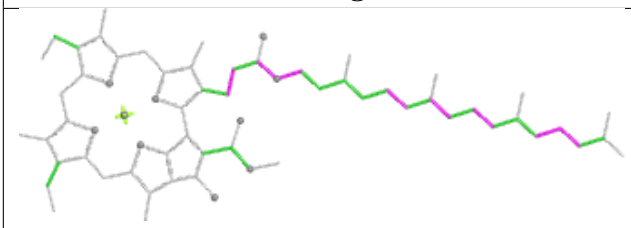
Ligand CLA G 603



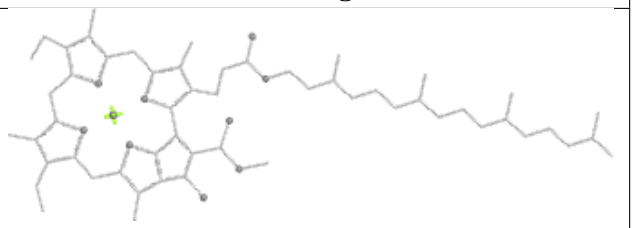
Bond lengths



Bond angles

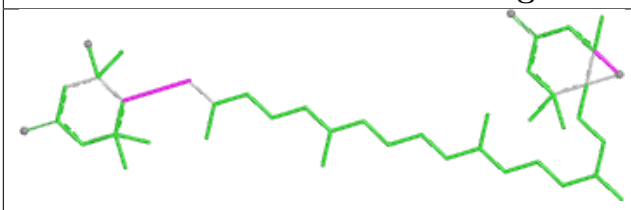


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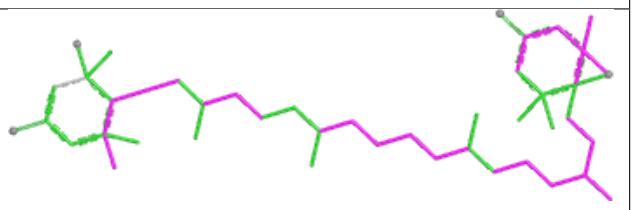


Rings

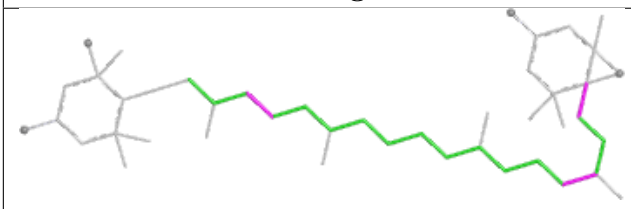
Ligand NEX 2 1623



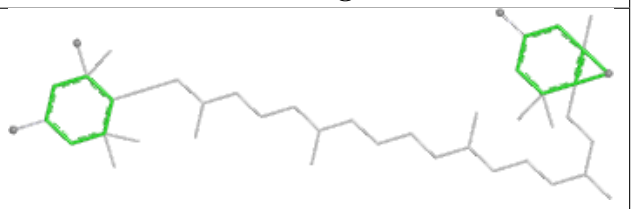
Bond lengths



Bond angles

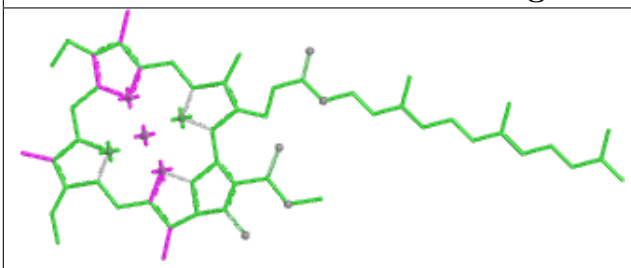


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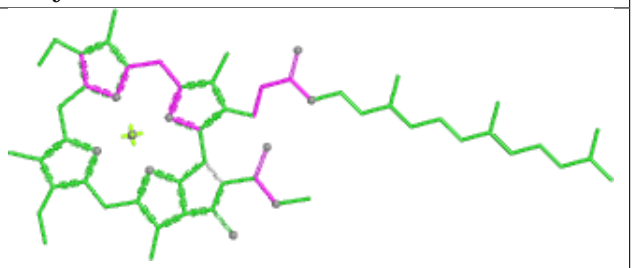


Rings

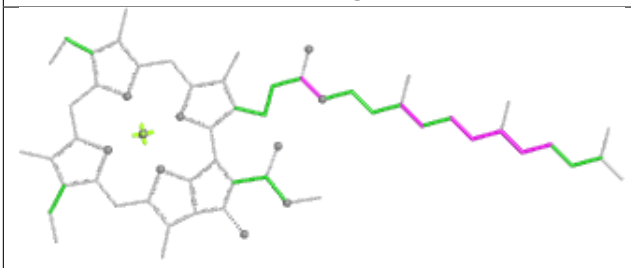
Ligand CLA y 611



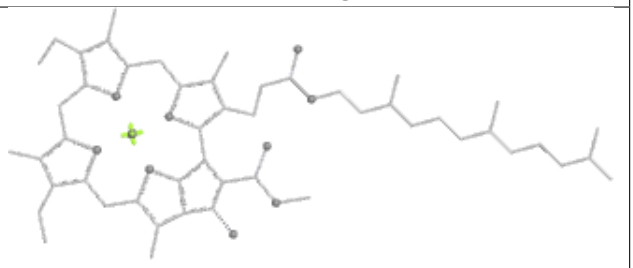
Bond lengths



Bond angles

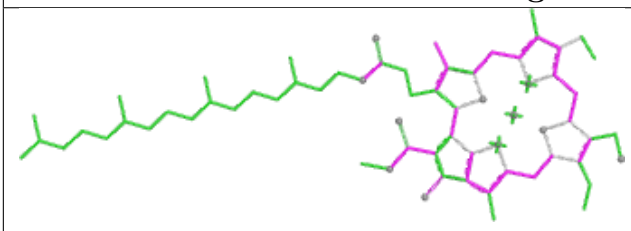


Torsions

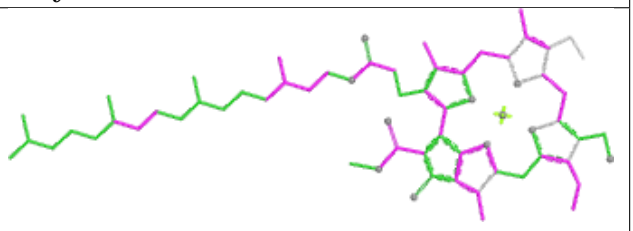


Rings

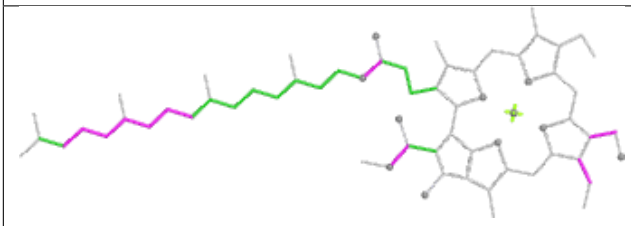
Ligand CHL y 609



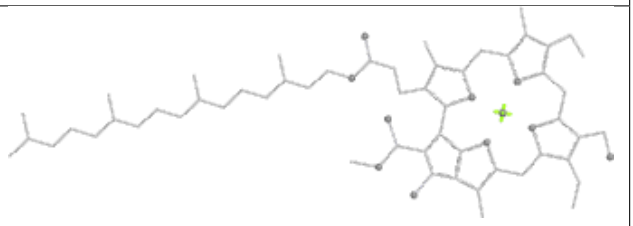
Bond lengths



Bond angles

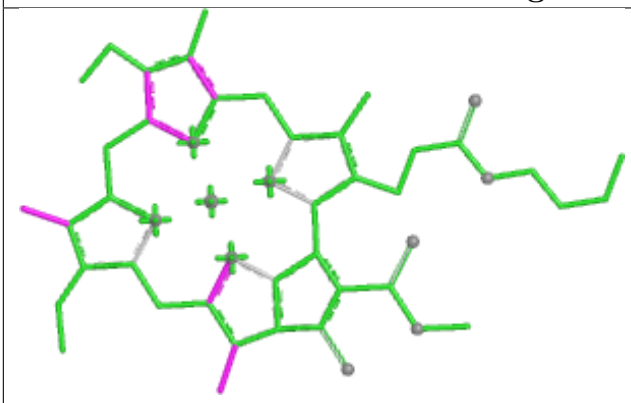


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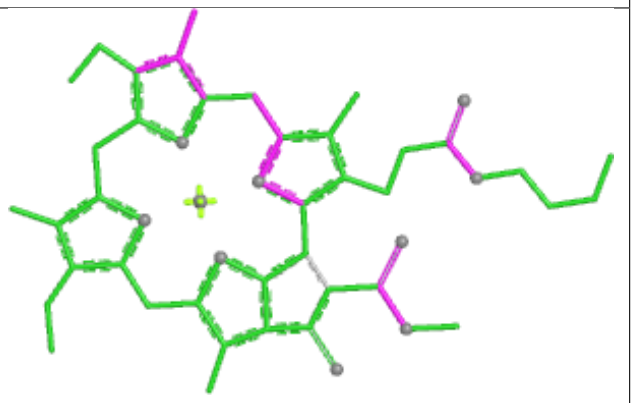


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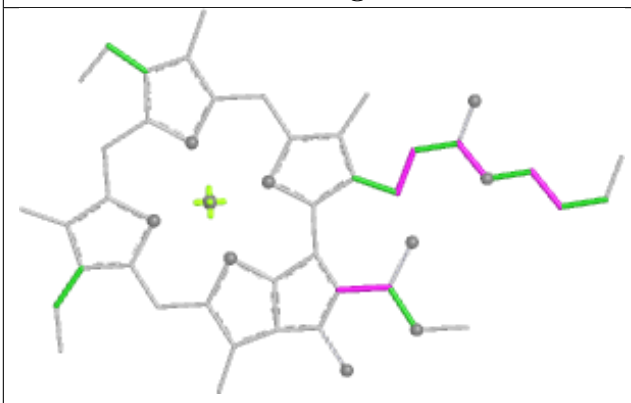
Ligand CLA S 614



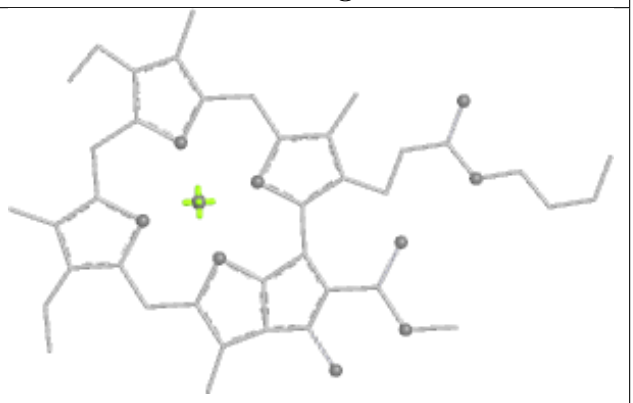
Bond lengths



Bond angles

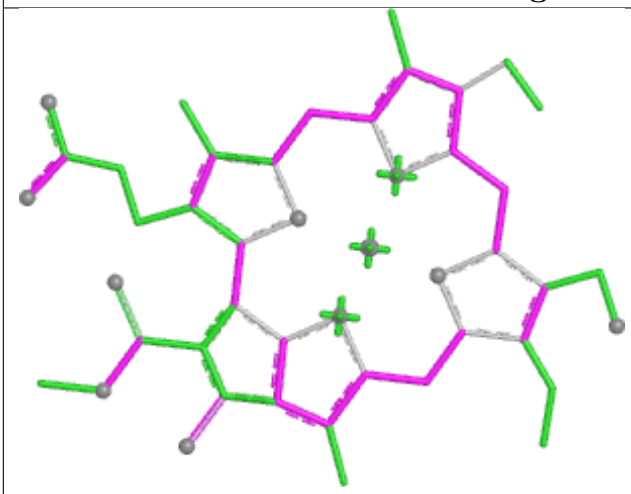


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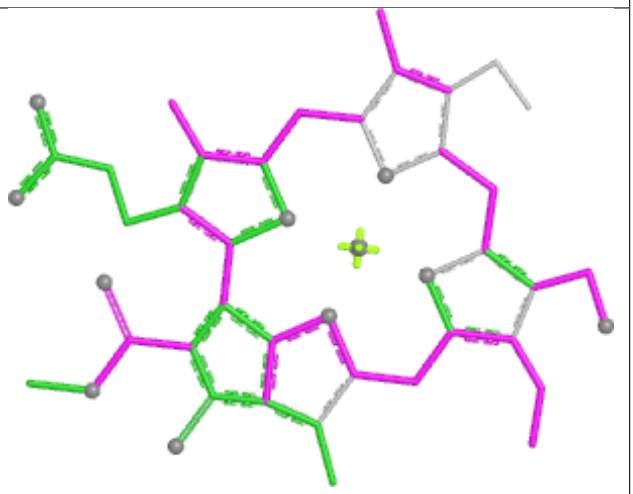


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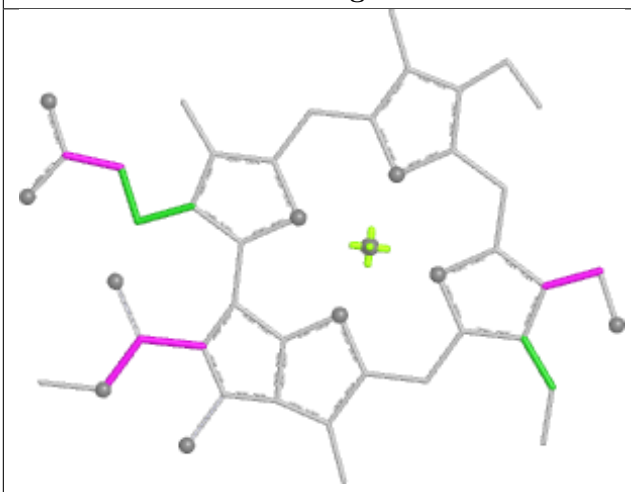
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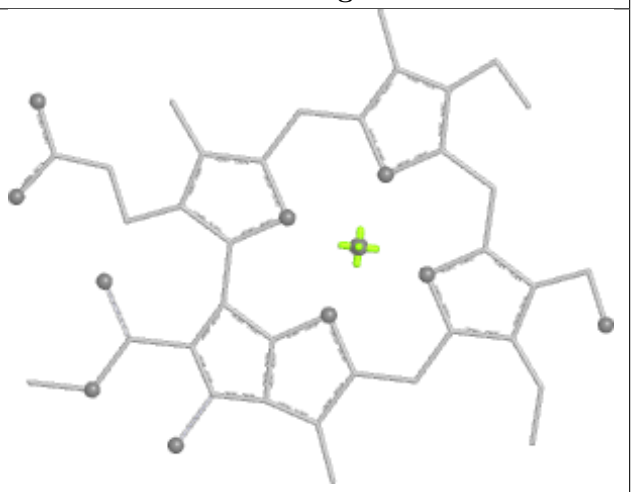
Bond lengths



Bond angles

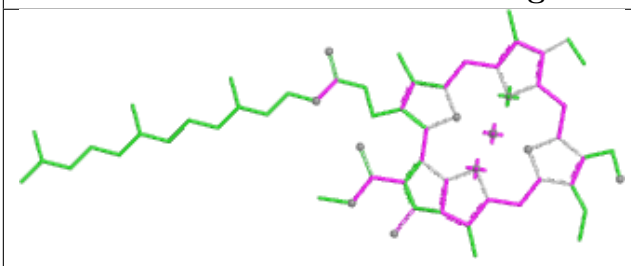


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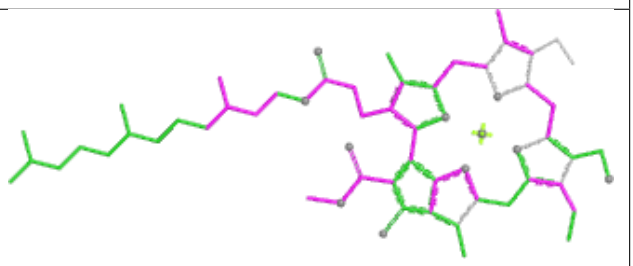


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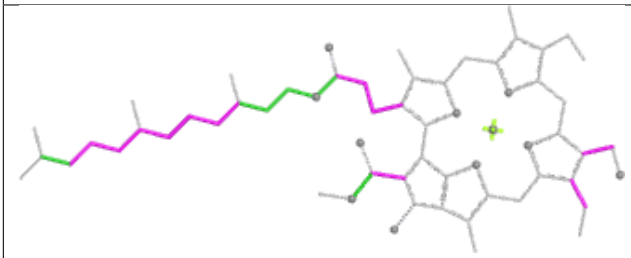
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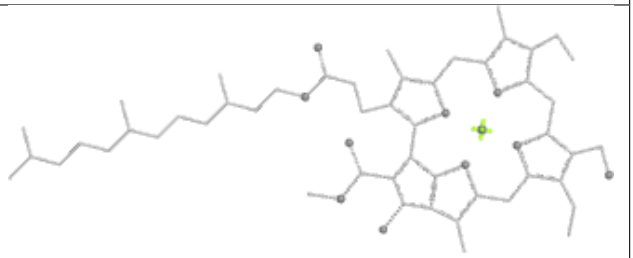
Bond lengths



Bond angles

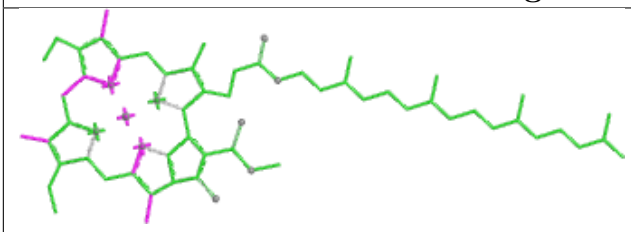


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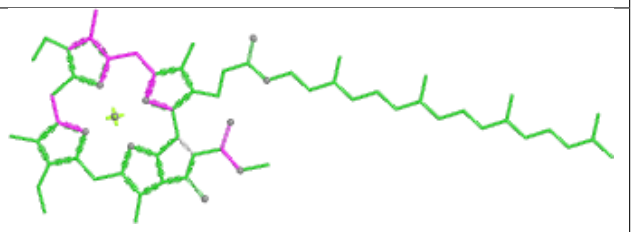


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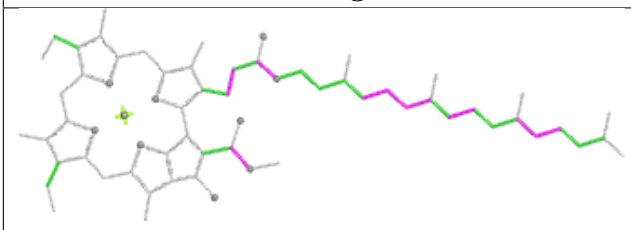
Ligand CLA B 608



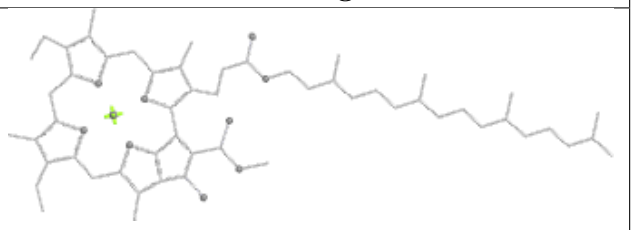
Bond lengths



Bond angles

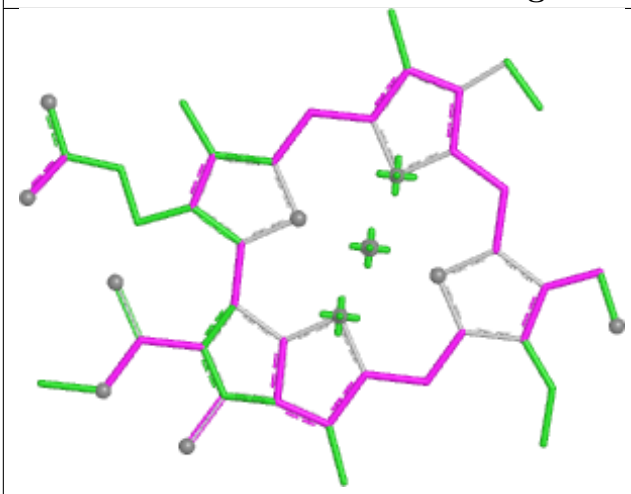


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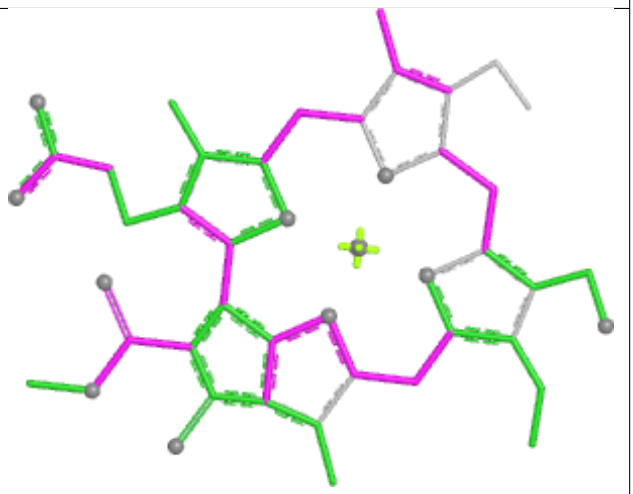


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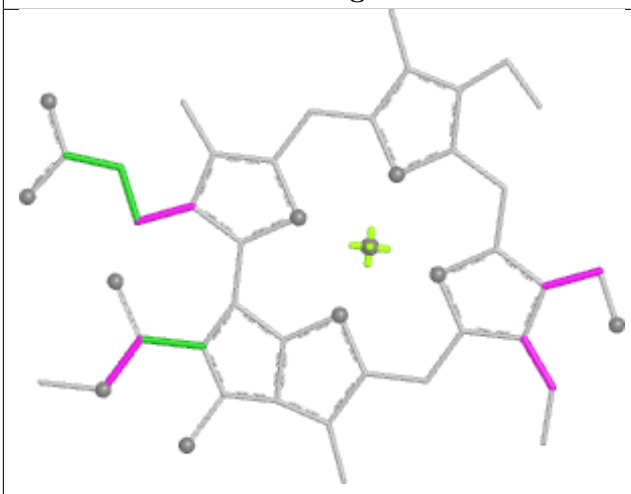
Ligand CHL 6 608



Bond lengths



Bond angles

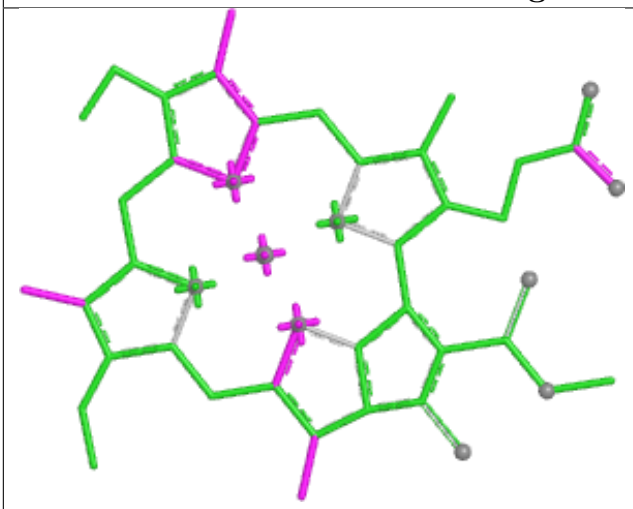


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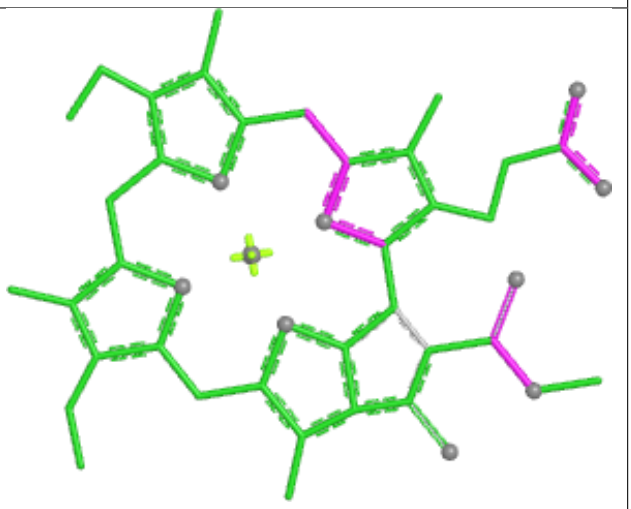


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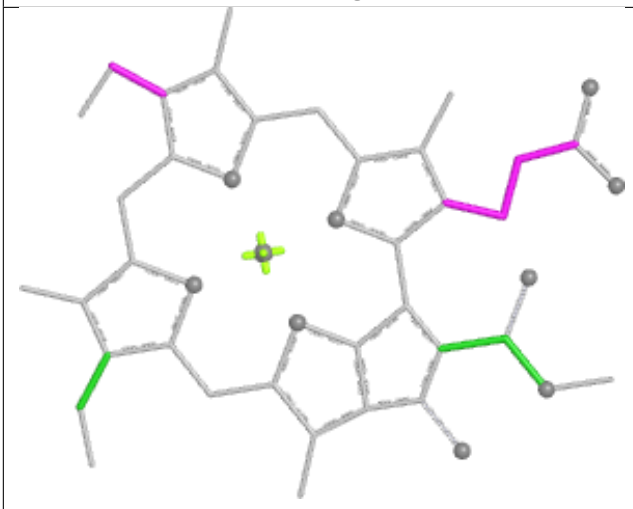
Ligand CLA 1 611



Bond lengths



Bond angles

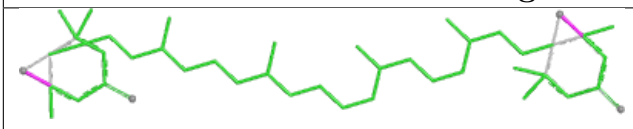


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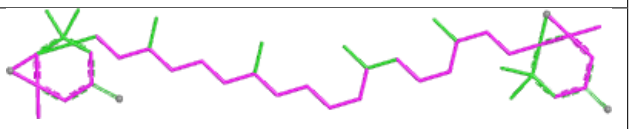


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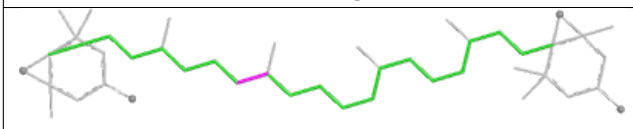
Ligand XAT 1 1622



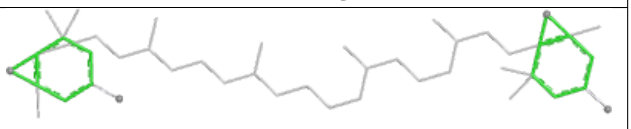
Bond lengths



Bond angles

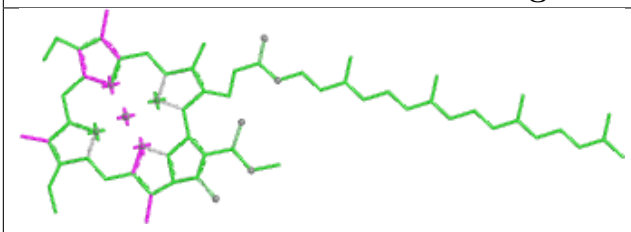


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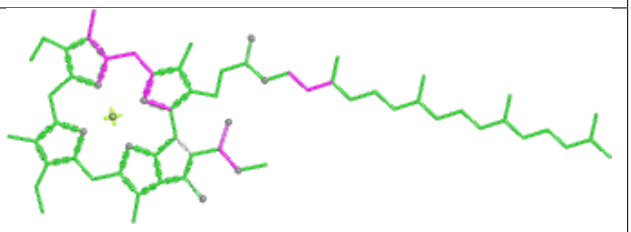


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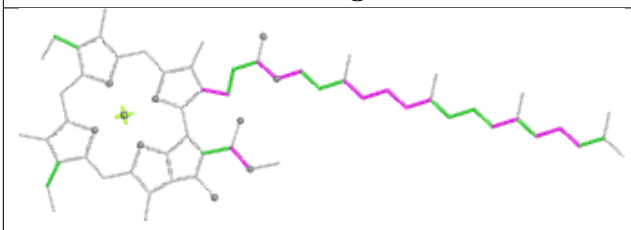
Ligand CLA c 506



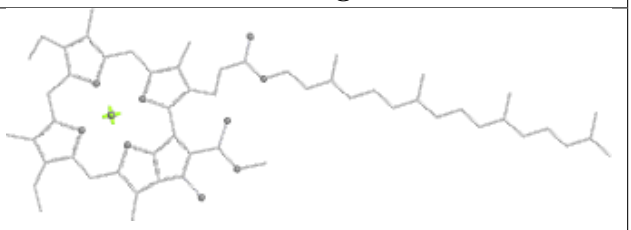
Bond lengths



Bond angles



Torsions

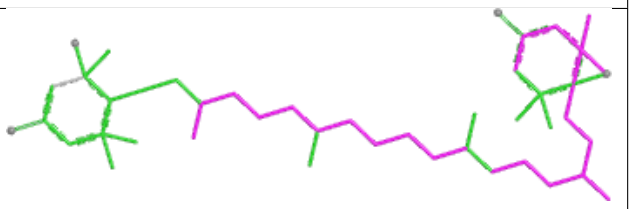


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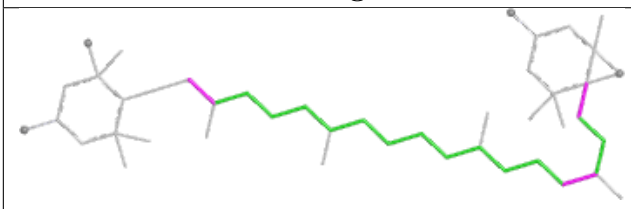
Ligand NEX s 1623



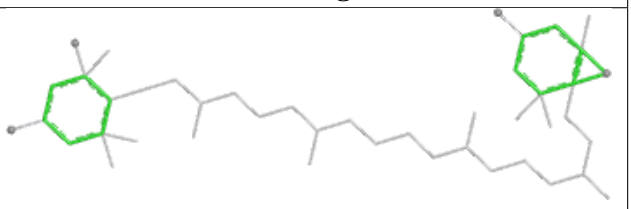
Bond lengths



Bond angles

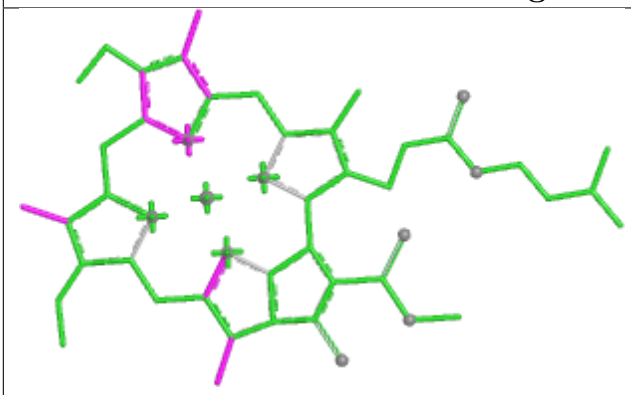


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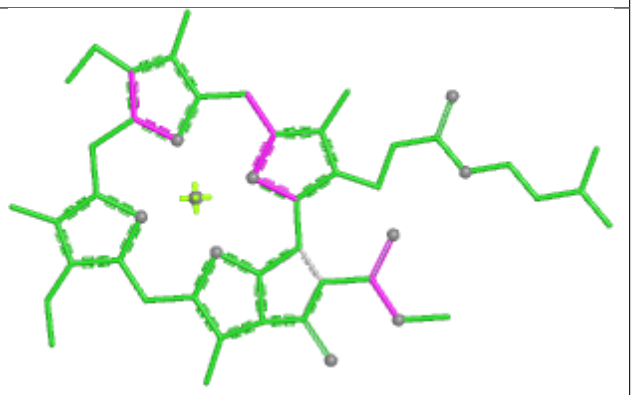


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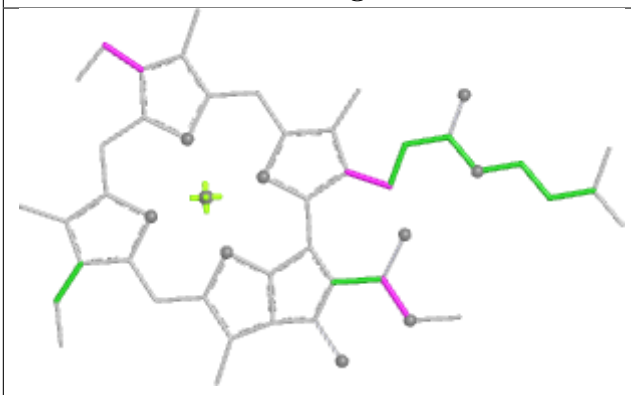
Ligand CLA 6 610



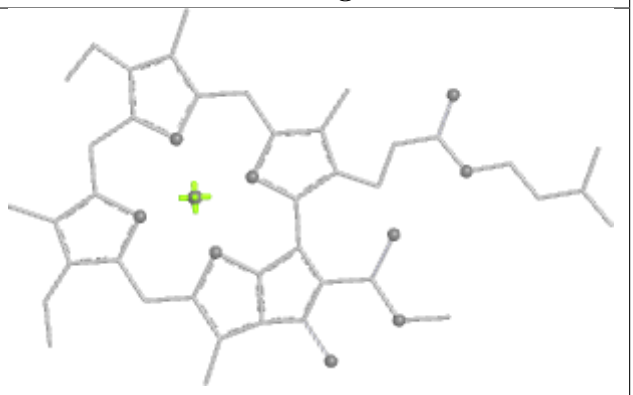
Bond lengths



Bond angles

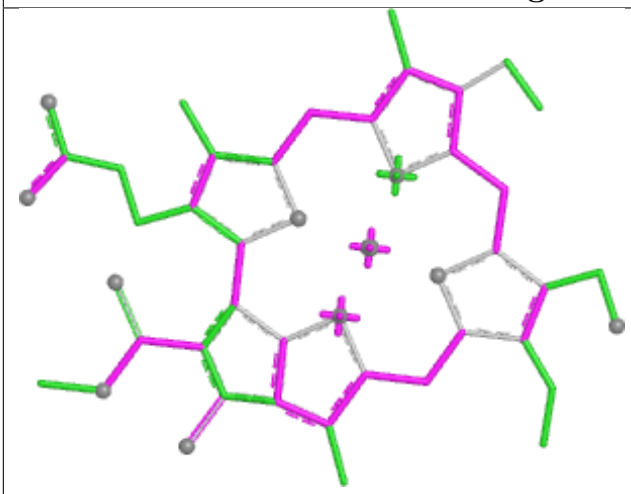


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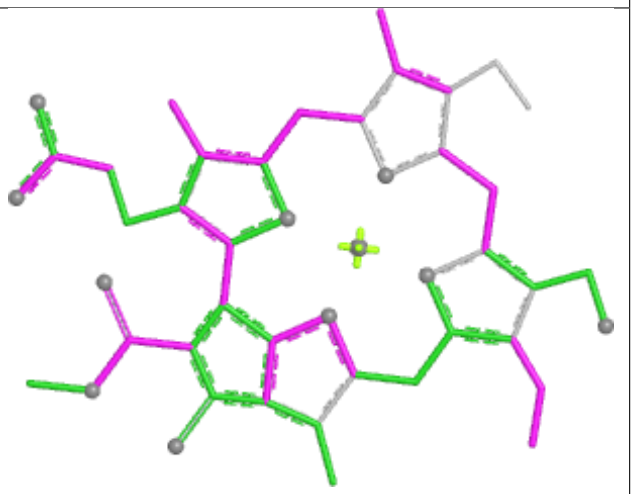


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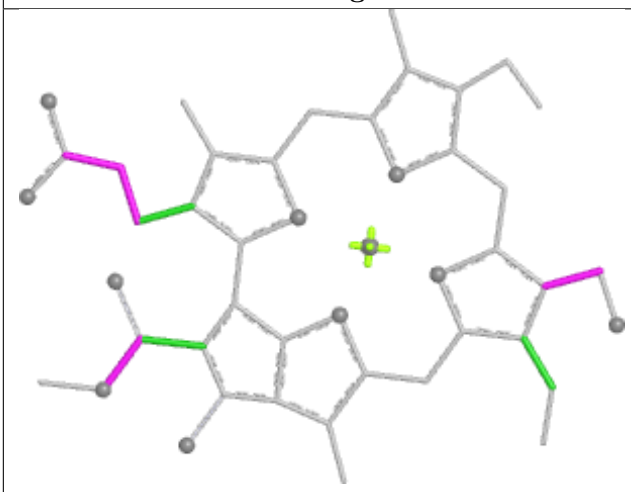
Ligand CHL 1 606



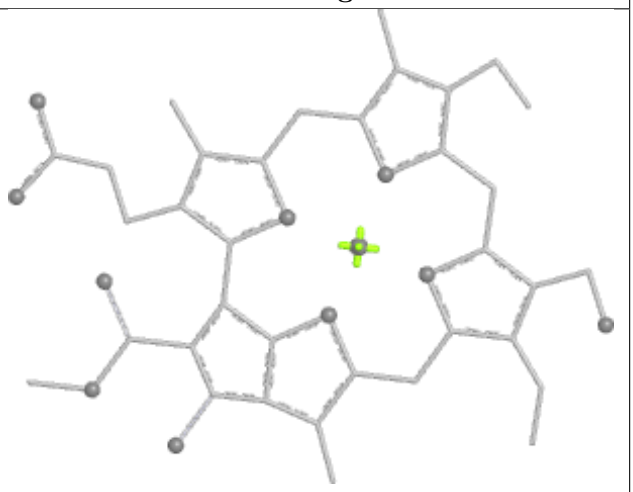
Bond lengths



Bond angles

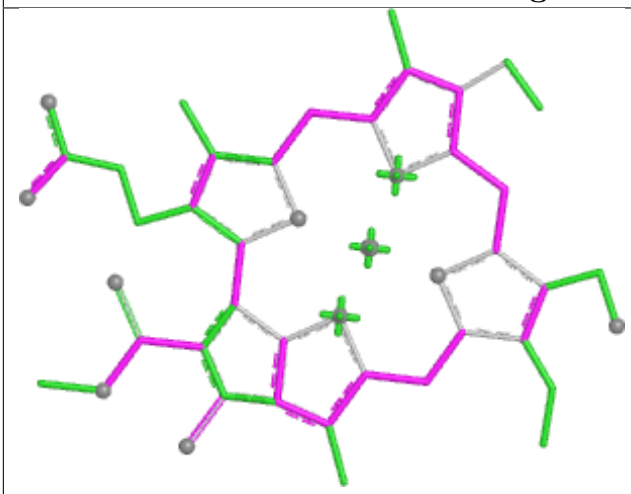


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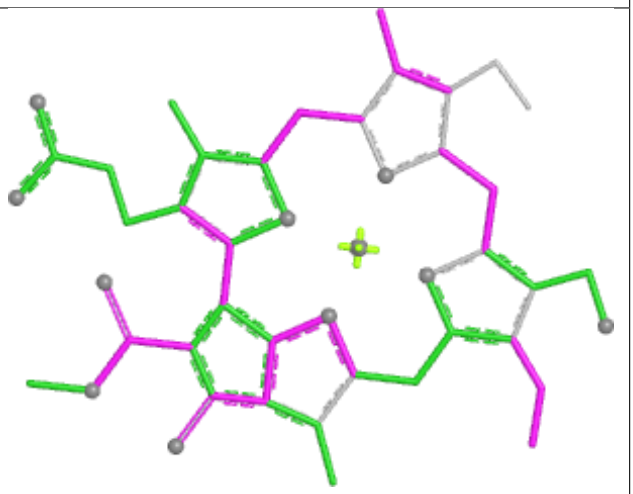


Rings

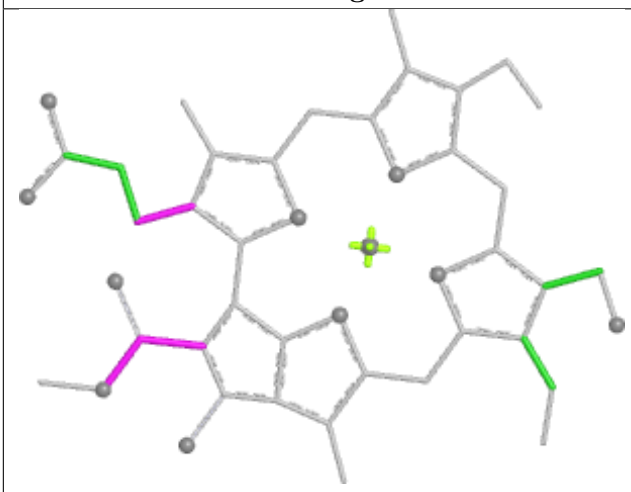
Ligand CHL s 608



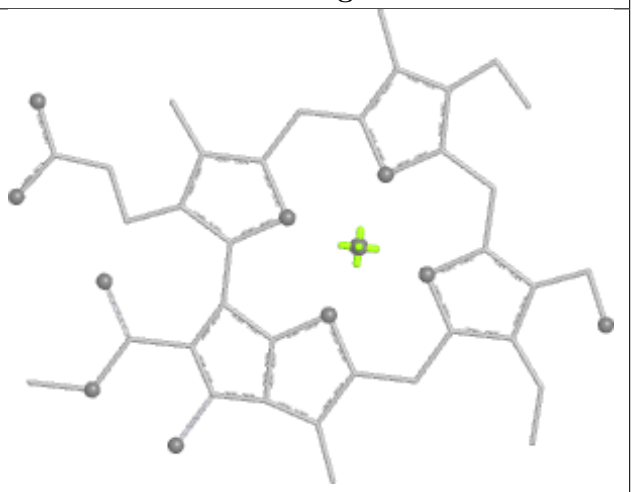
Bond lengths



Bond angles

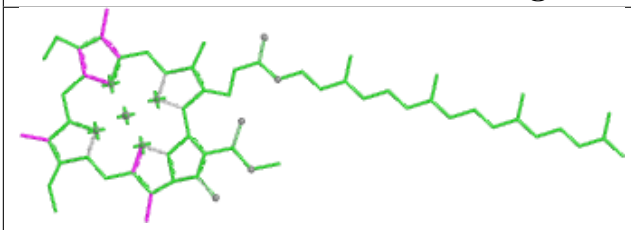


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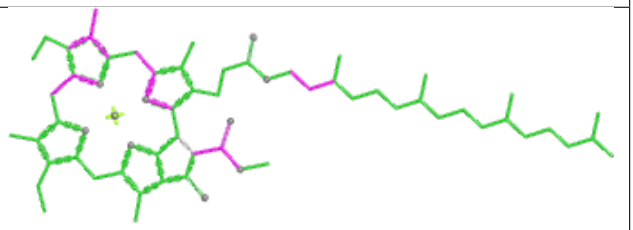


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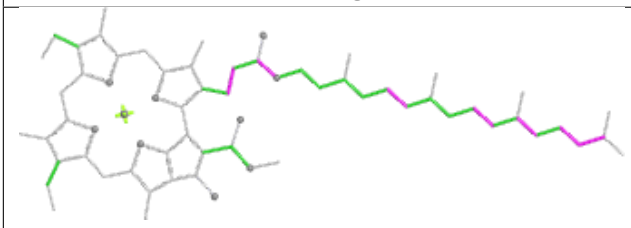
Ligand CLA c 505



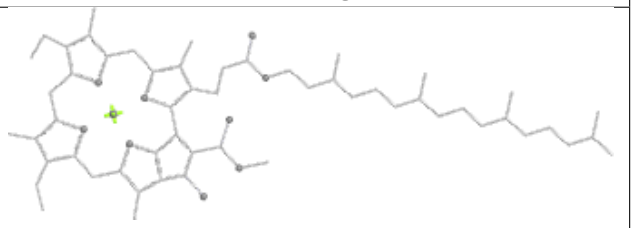
Bond lengths



Bond angles

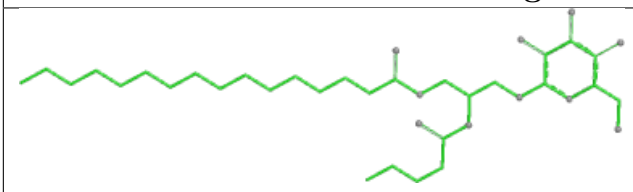


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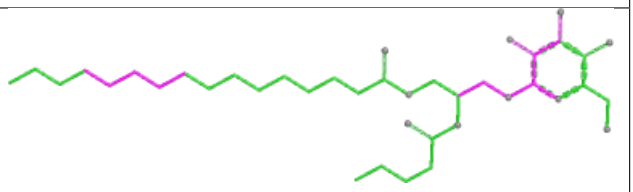


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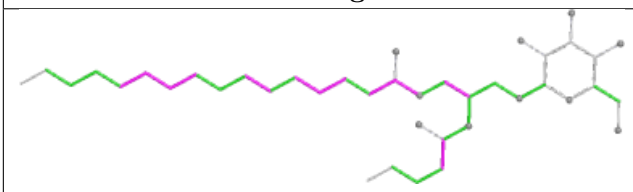
Ligand LMG a 415



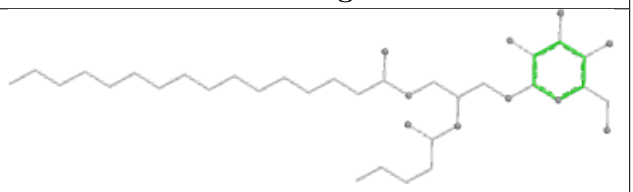
Bond lengths



Bond angles

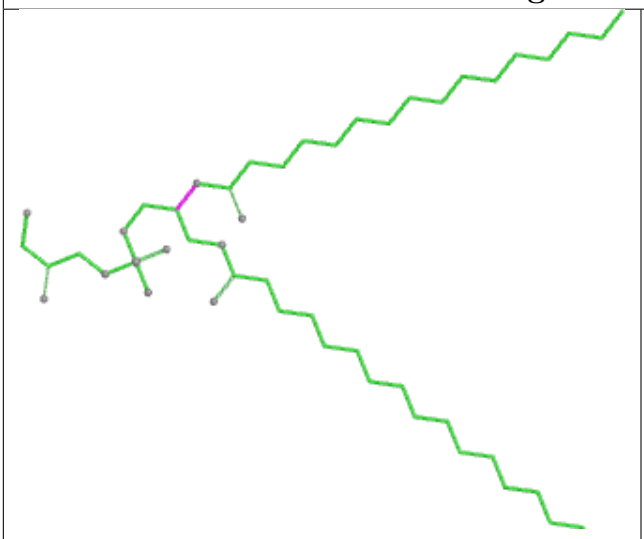


Torsions

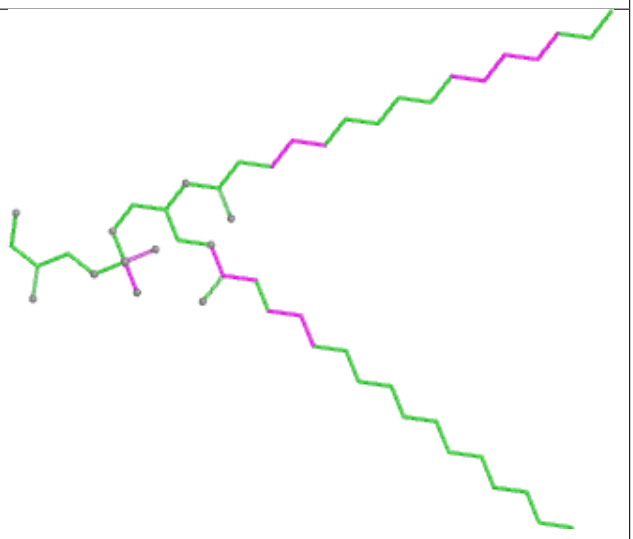


Rings

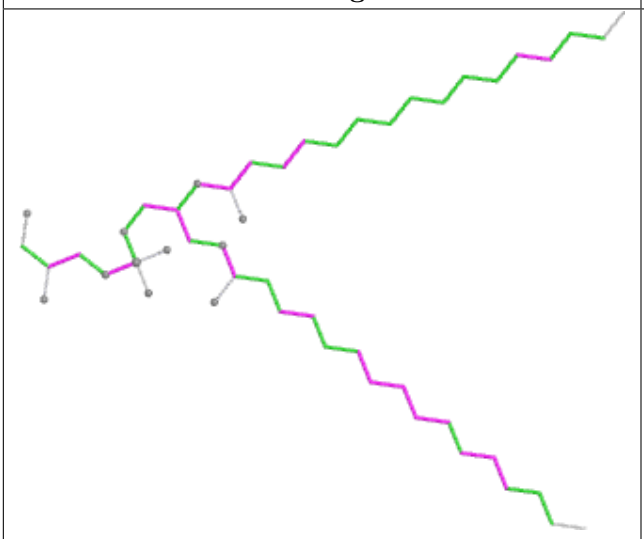
Ligand LHG c 522



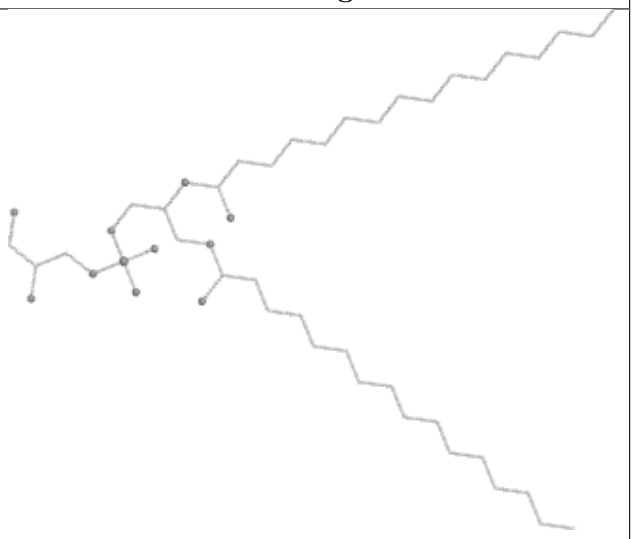
Bond lengths



Bond angles

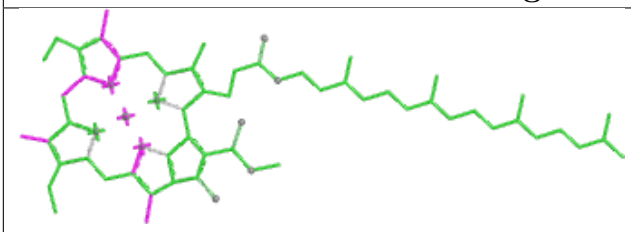


Torsions

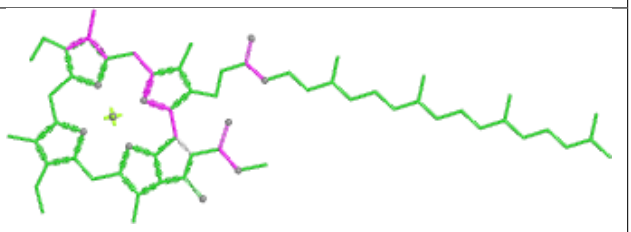


Rings

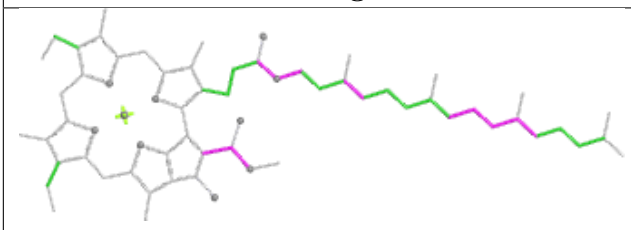
Ligand CLA D 403



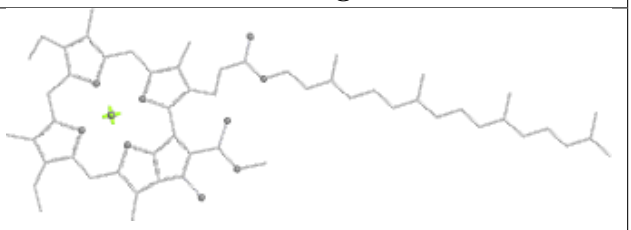
Bond lengths



Bond angles



Torsions



Rings

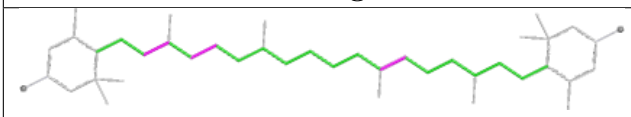
Ligand LUT 8 620



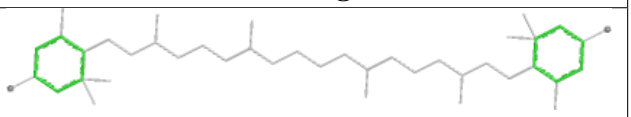
Bond lengths



Bond angles

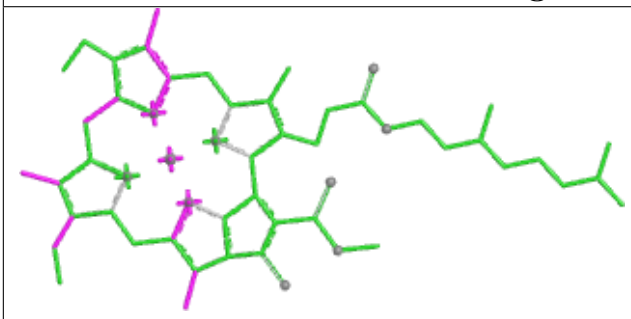


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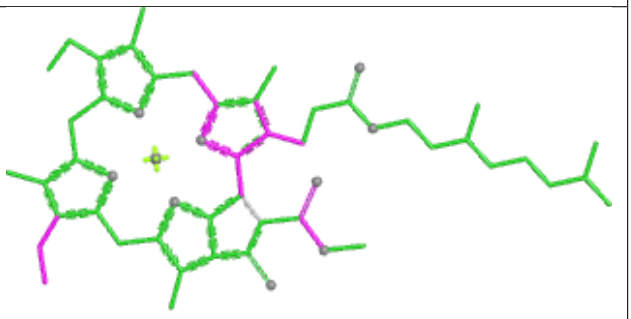


Rings

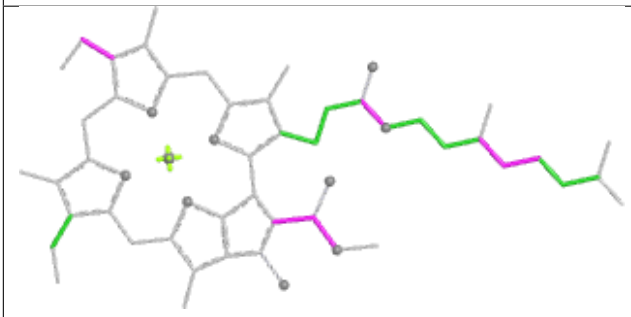
Ligand CLA 1 603



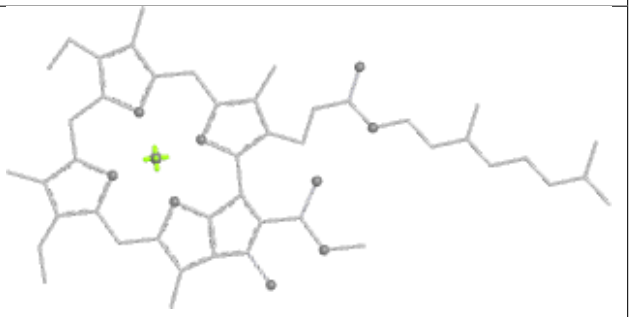
Bond lengths



Bond angles

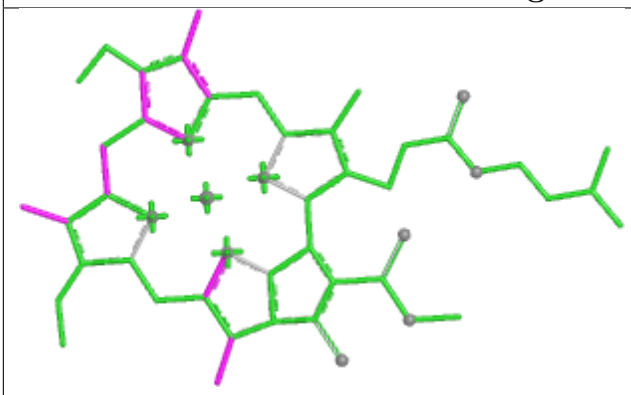


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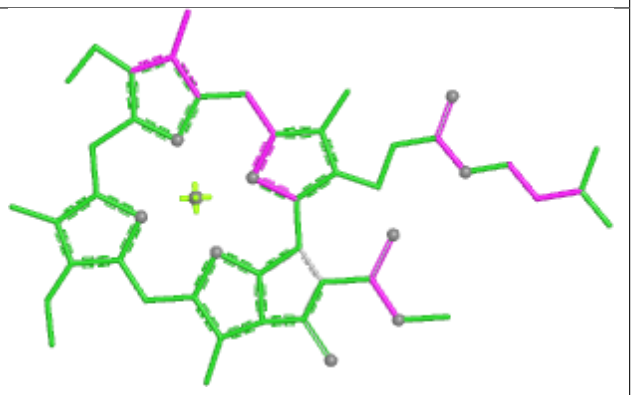


Rings

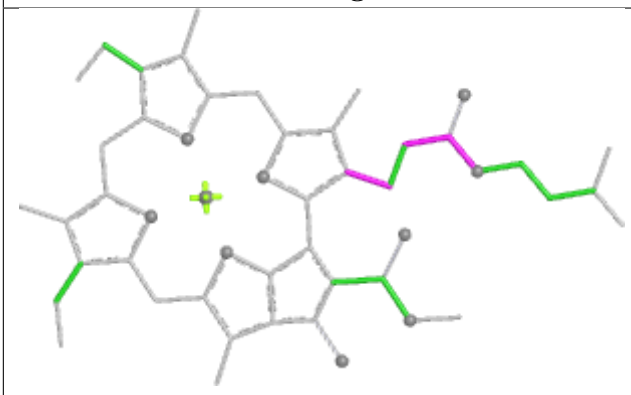
Ligand CLA S 604



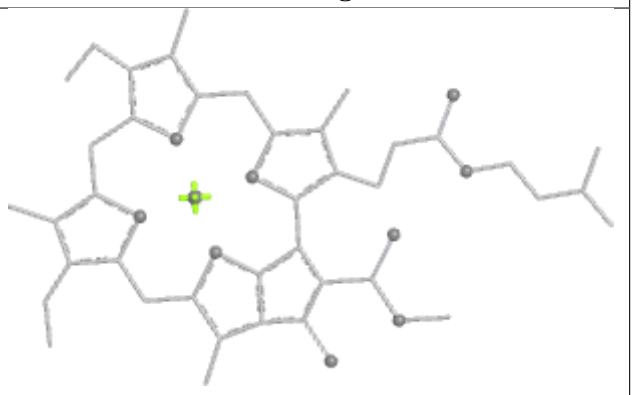
Bond lengths



Bond angles

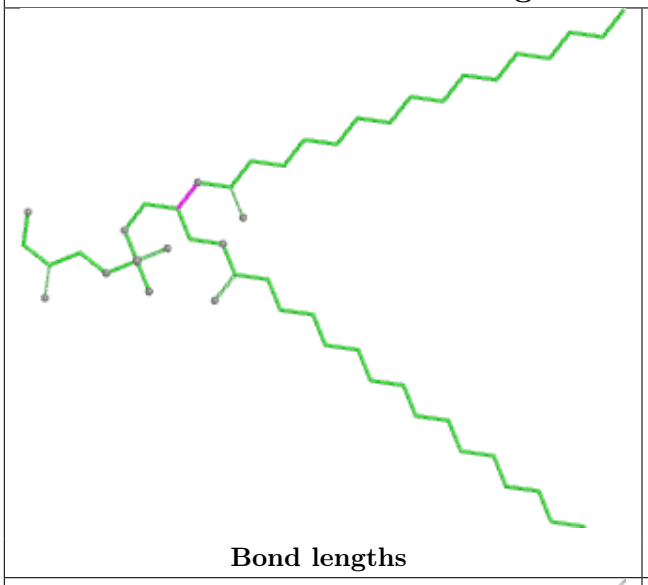


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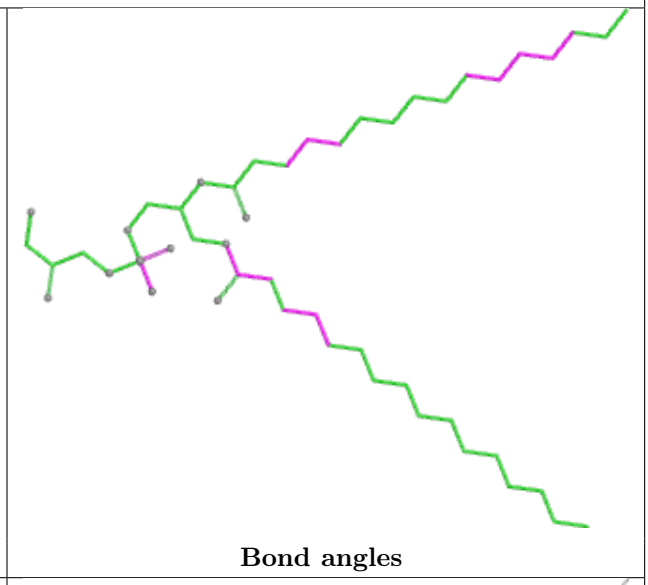


Rings

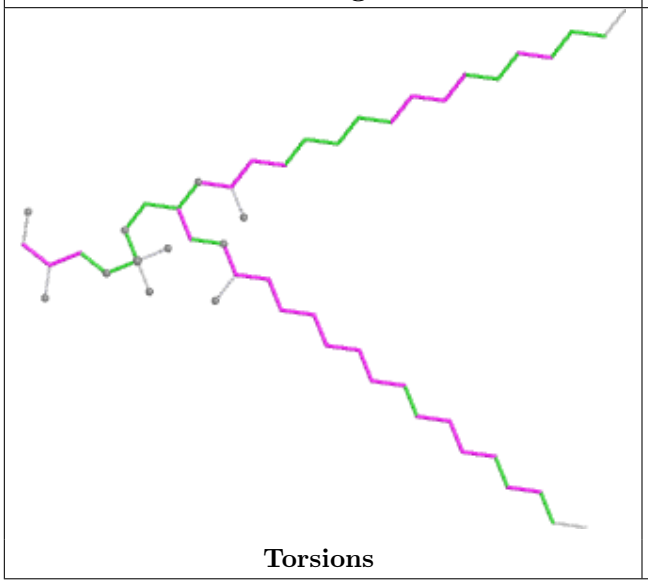
Ligand LHG C 2630



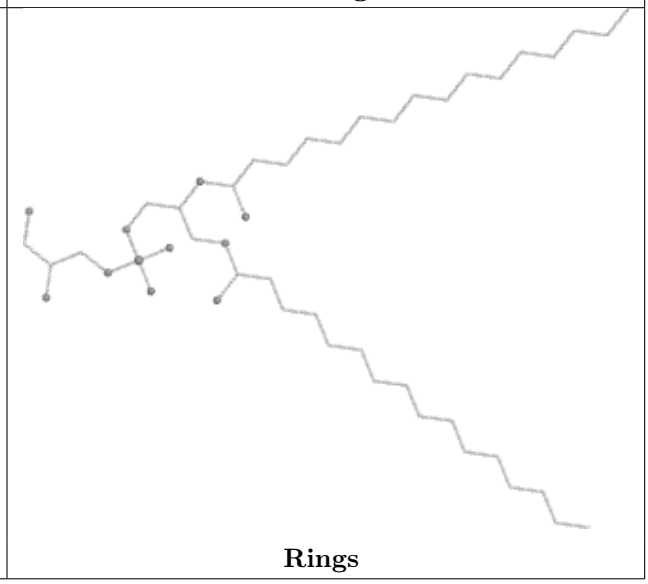
Bond lengths



Bond angles

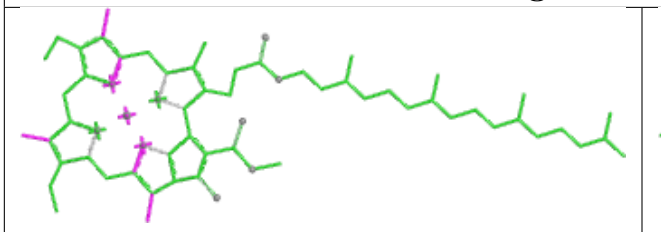


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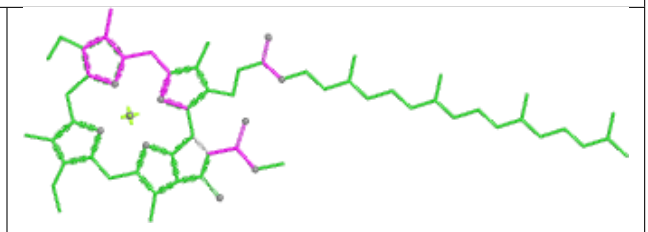


Rings

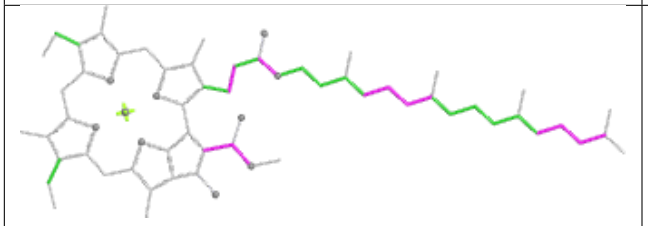
Ligand CLA b 615



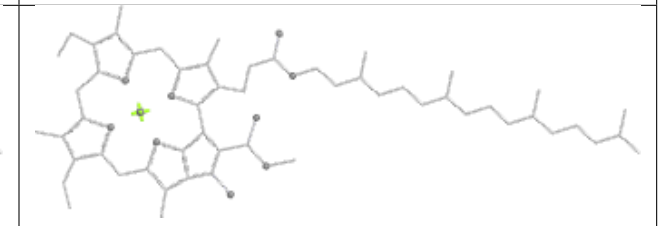
Bond lengths



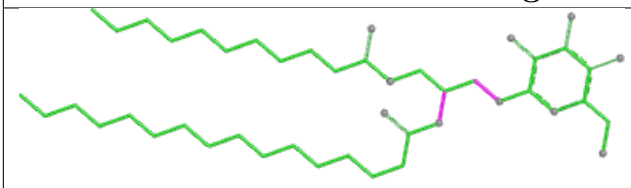
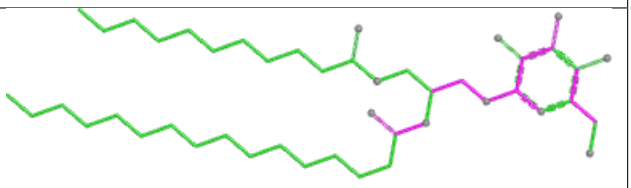
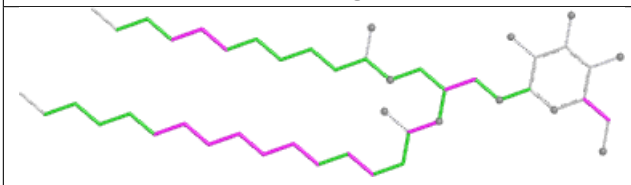
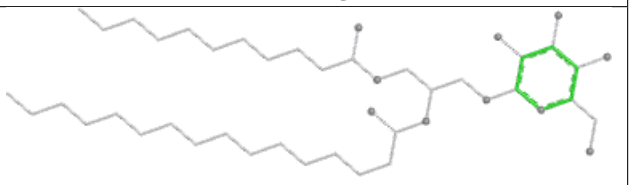
Bond angles

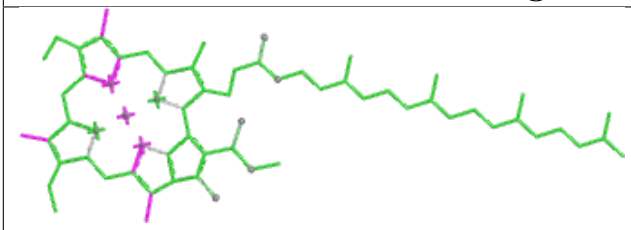
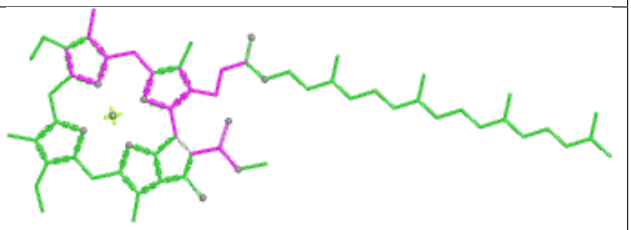
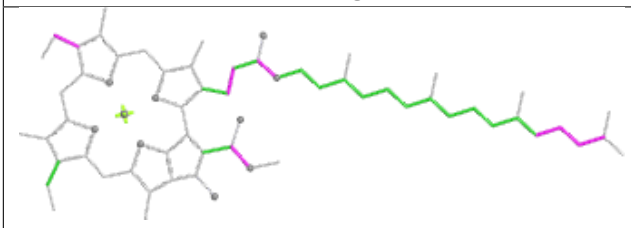
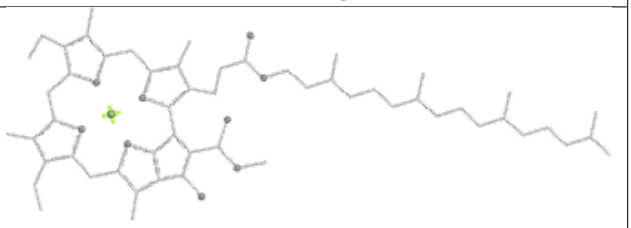


Torsions

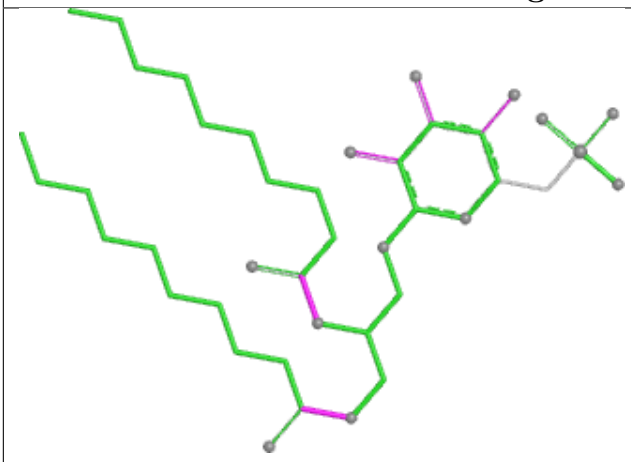


Rings

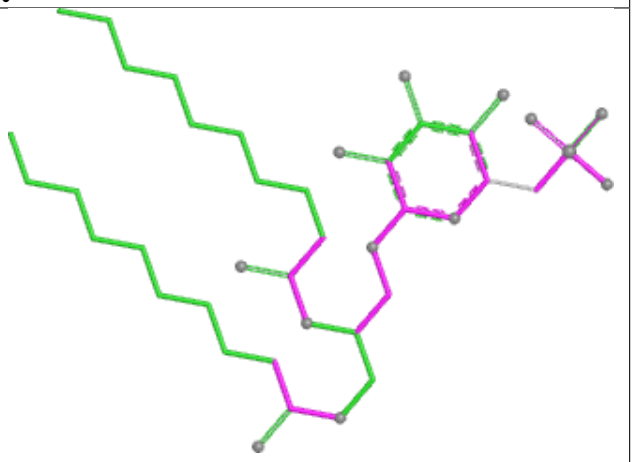
Ligand LMG d 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

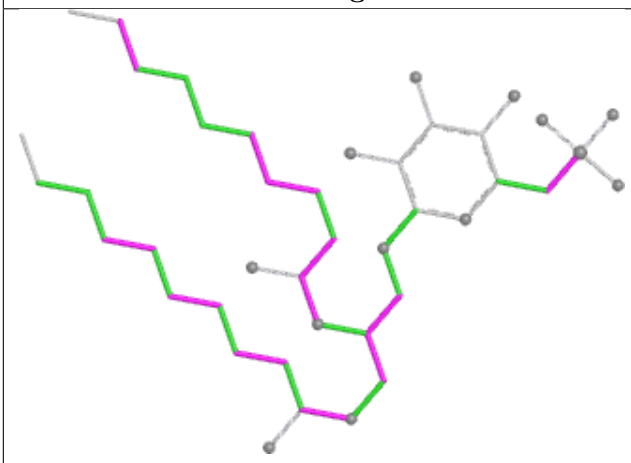
Ligand SQD b 623



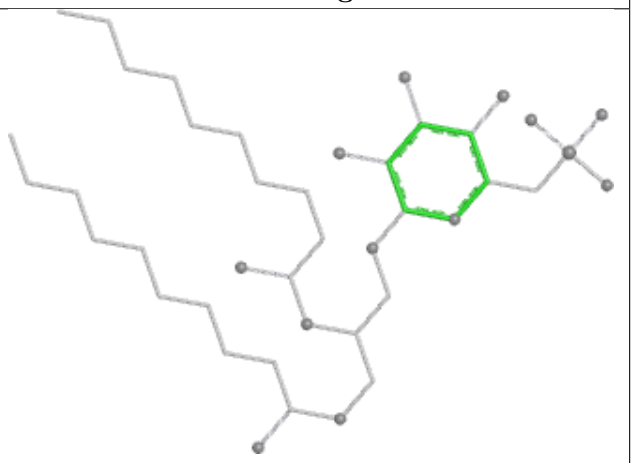
Bond lengths



Bond angles

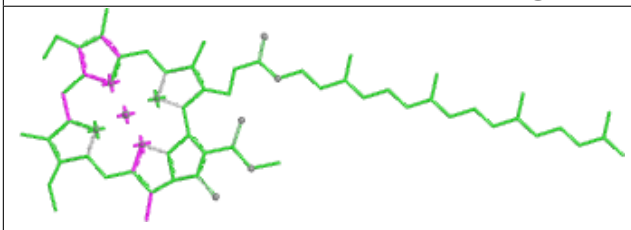


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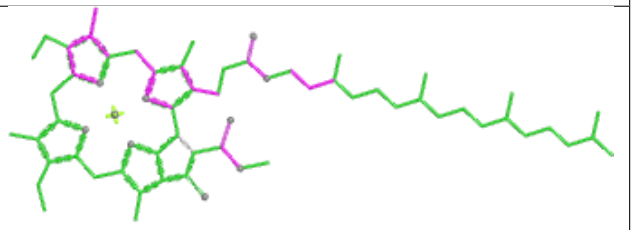


Rings

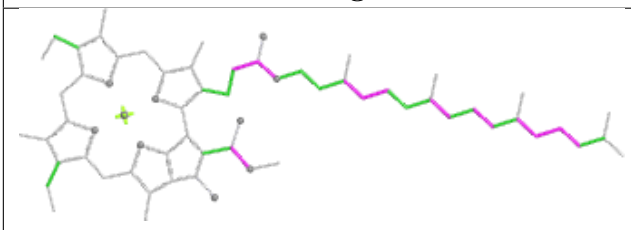
Ligand CLA c 510



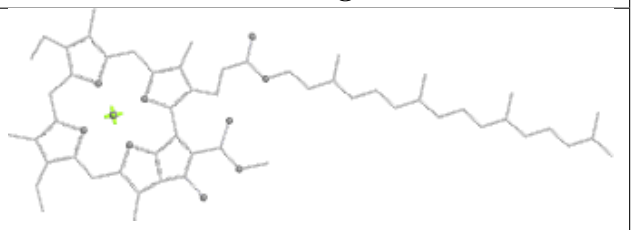
Bond lengths



Bond angles

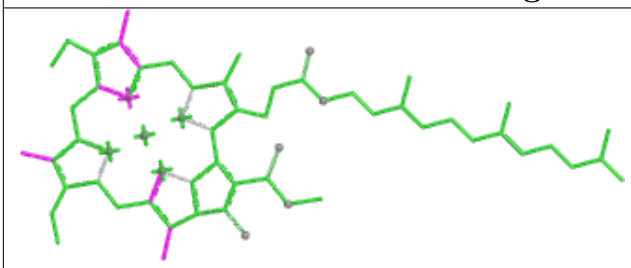


Torsions

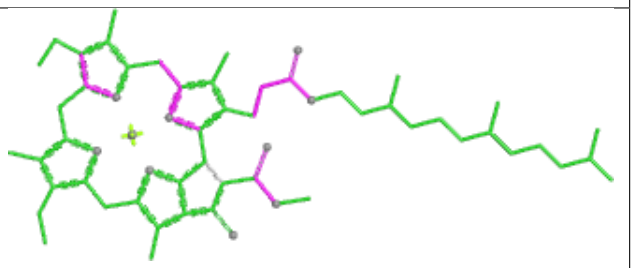


Rings

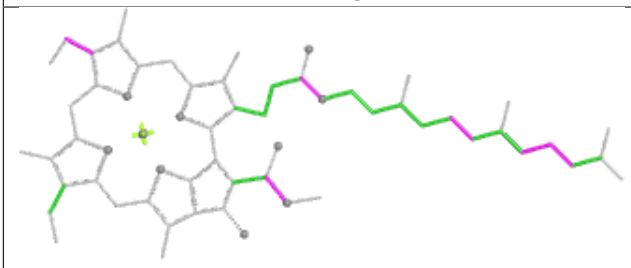
Ligand CLA N 611



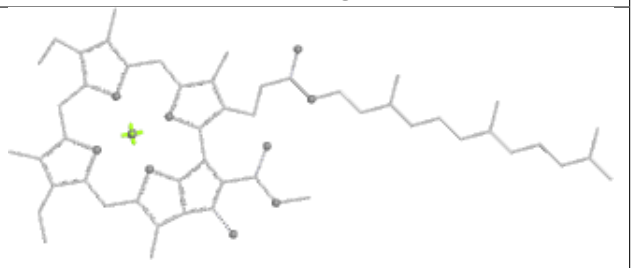
Bond lengths



Bond angles

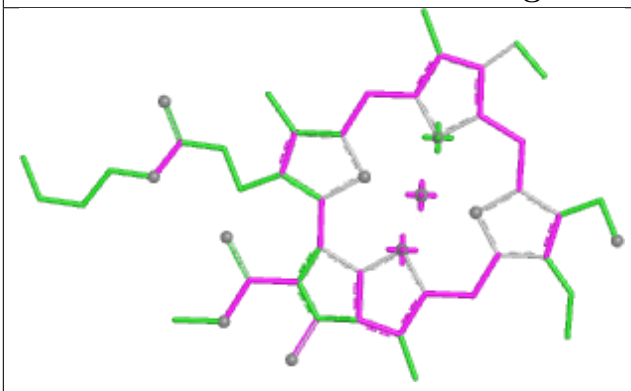


Torsions

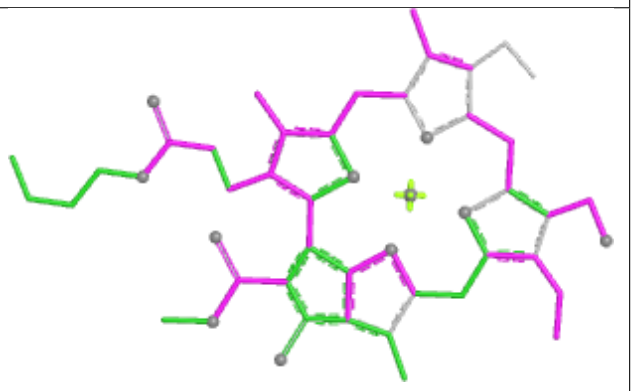


Rings

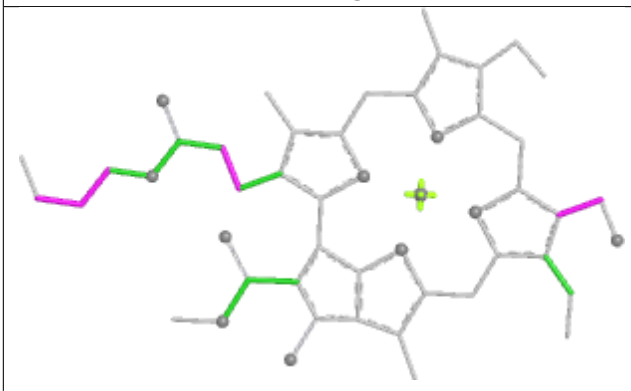
Ligand CHL Y 606



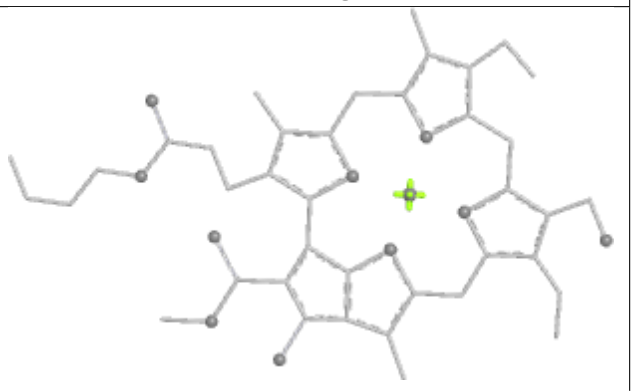
Bond lengths



Bond angles

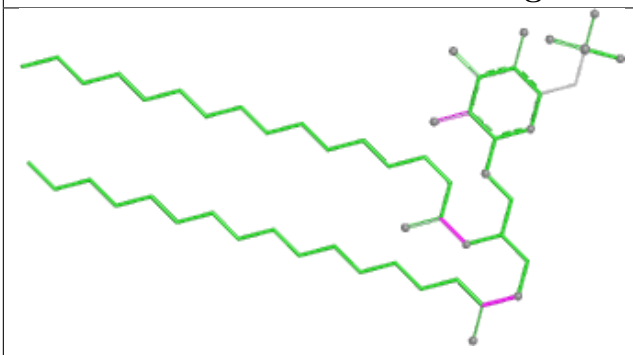


Torsions

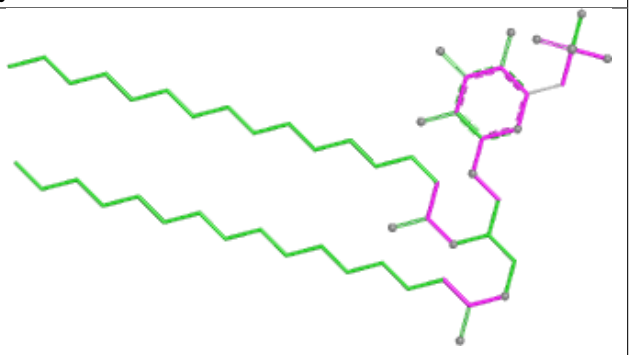


Rings

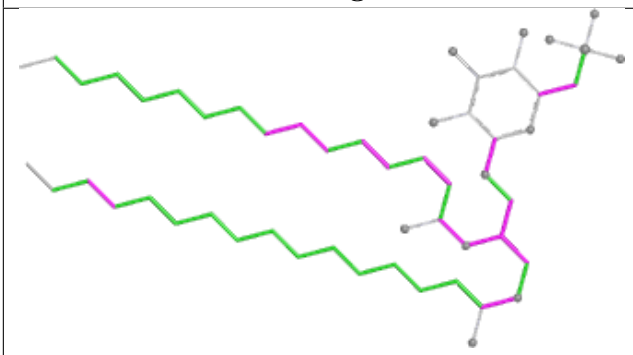
Ligand SQD B 621



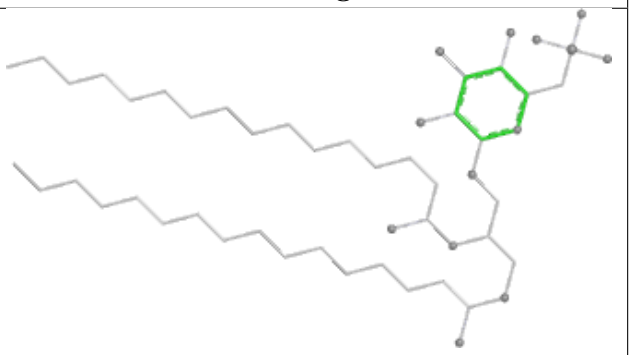
Bond lengths



Bond angles

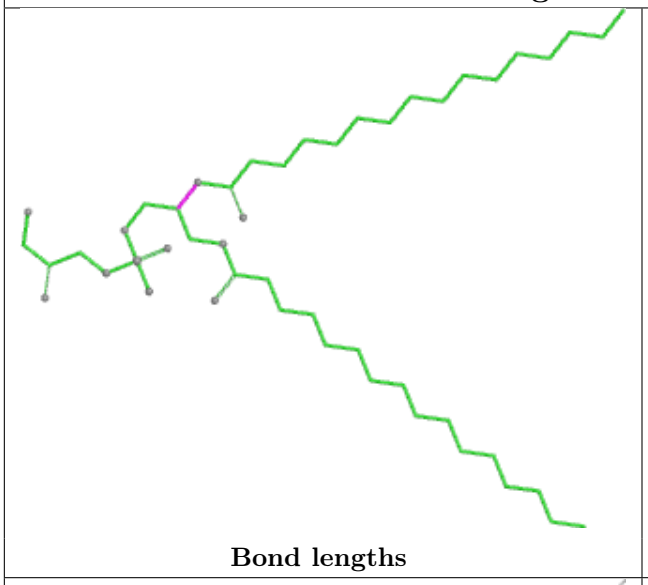


Torsions

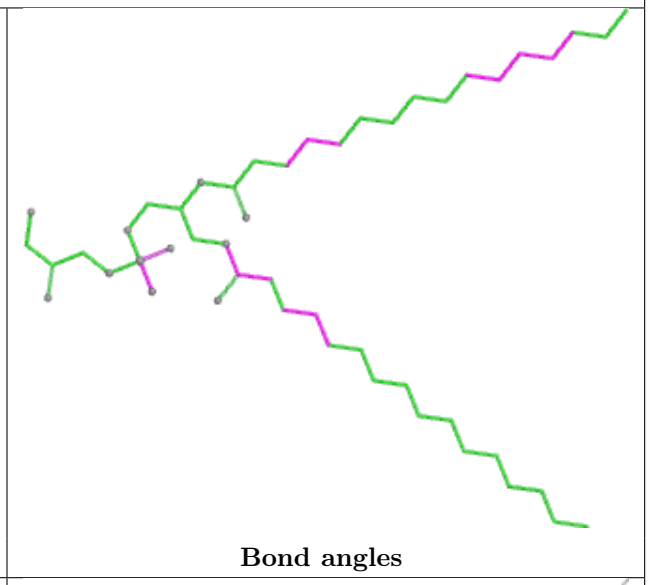


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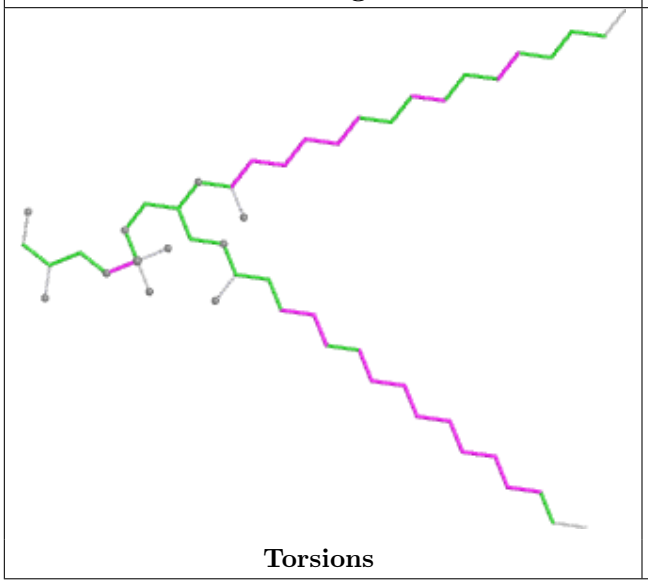
Ligand LHG l 101



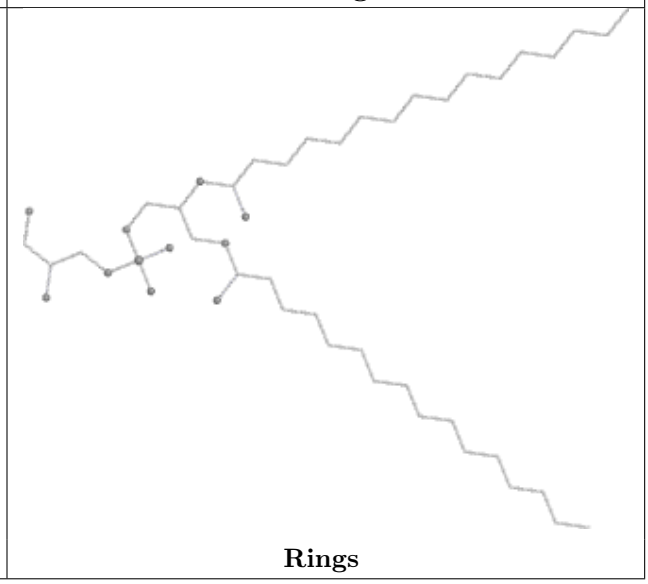
Bond lengths



Bond angles

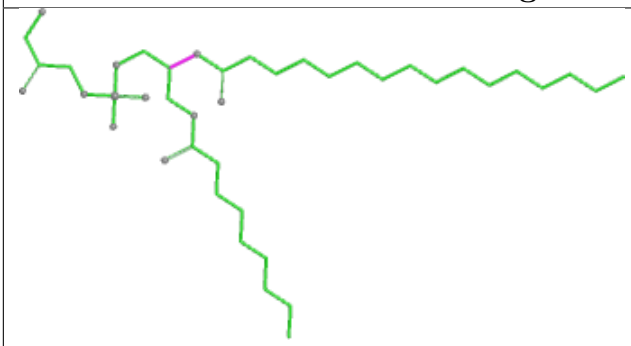


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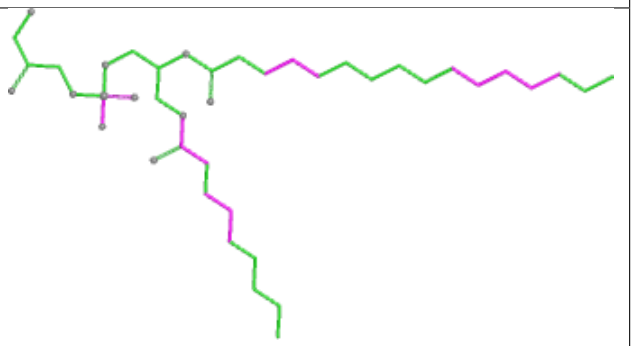


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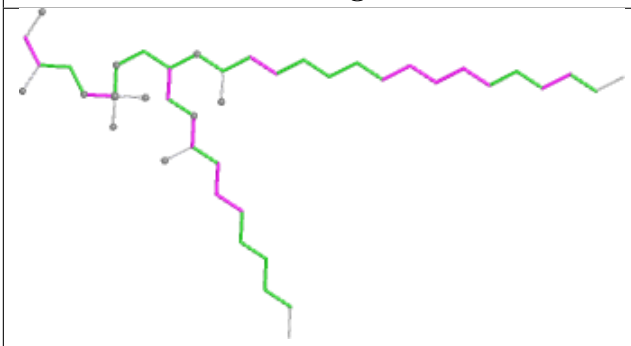
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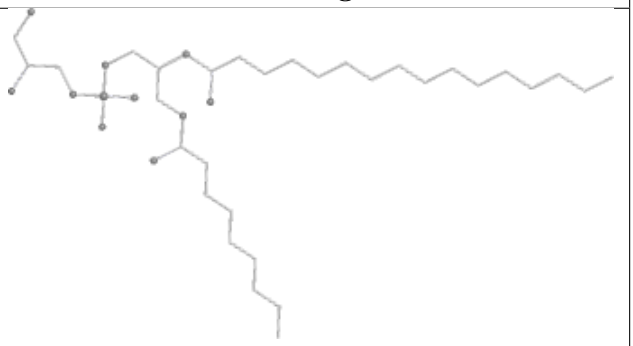
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Bond angles

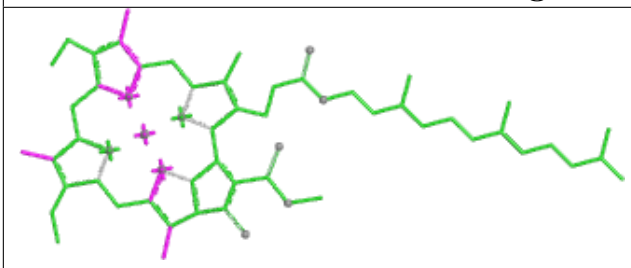


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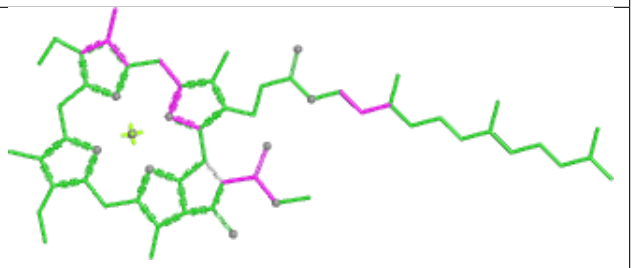


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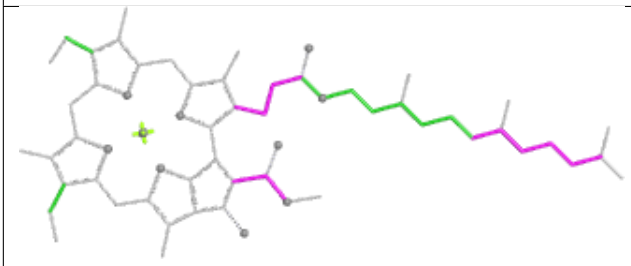
Ligand CLA 7 602



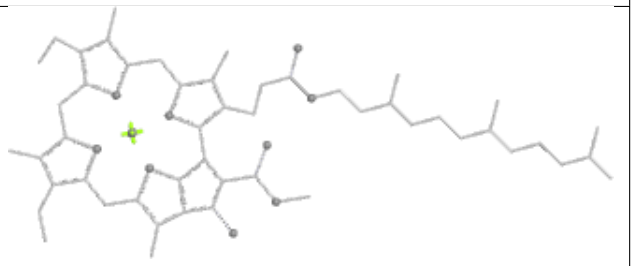
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Bond angles

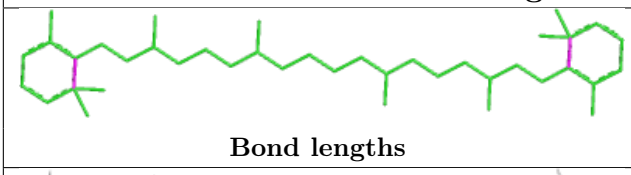


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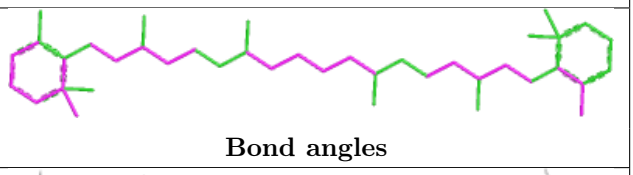


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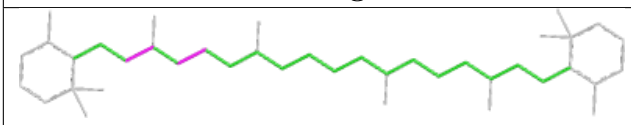
Ligand BCR h 101



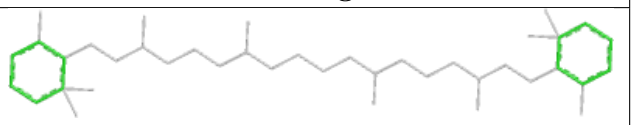
Bond lengths



Bond angles

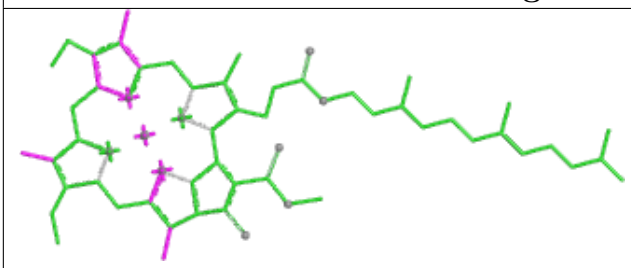


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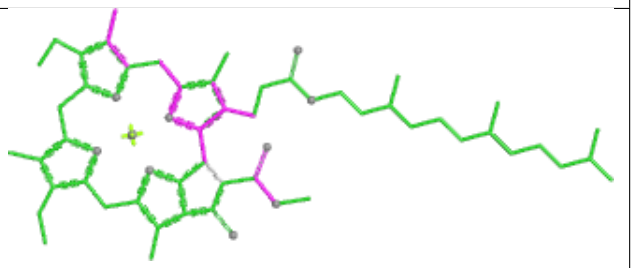


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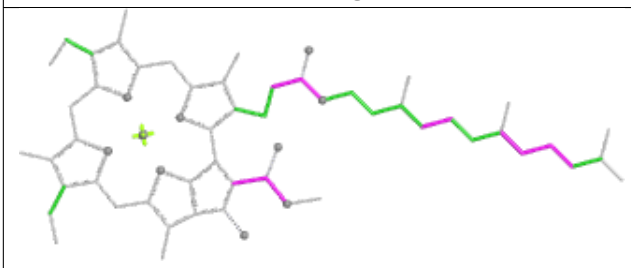
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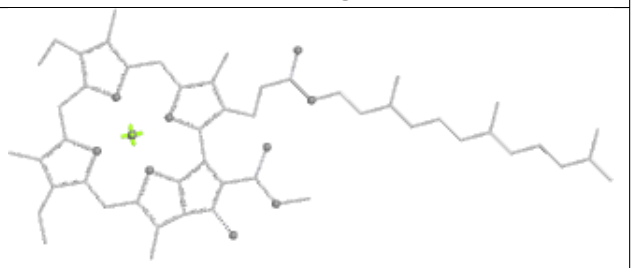
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Bond angles

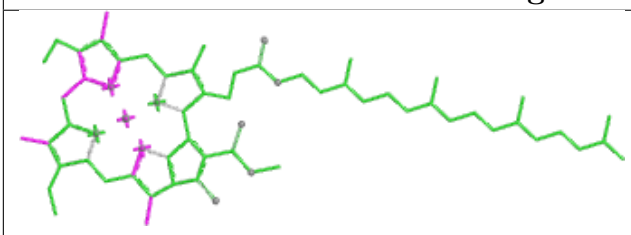


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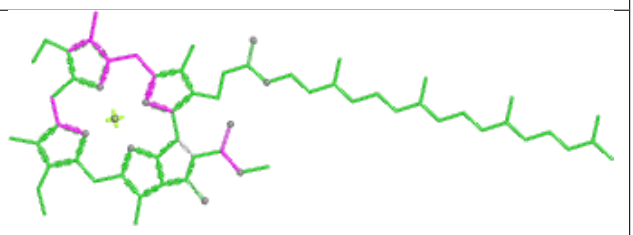


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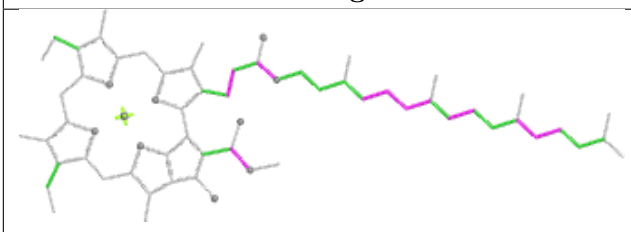
Ligand CLA b 608



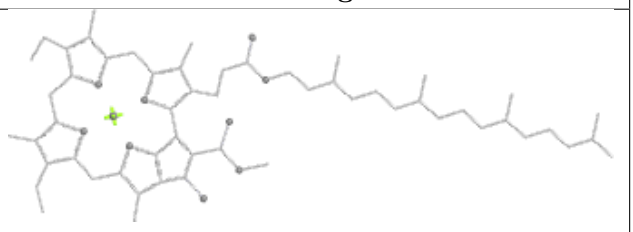
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Bond angles

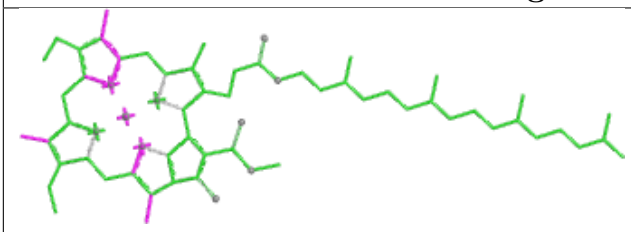


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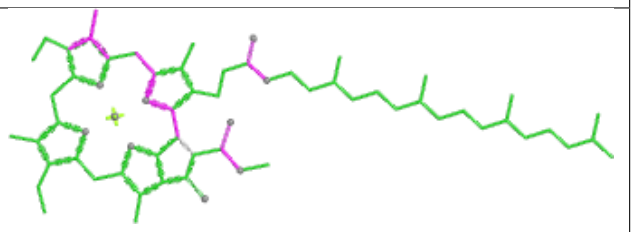


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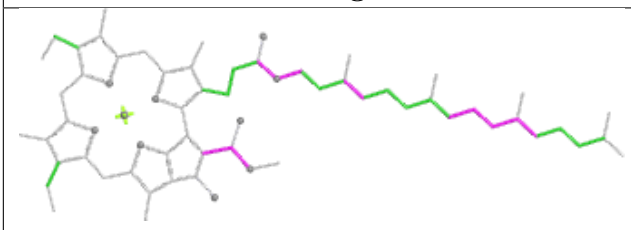
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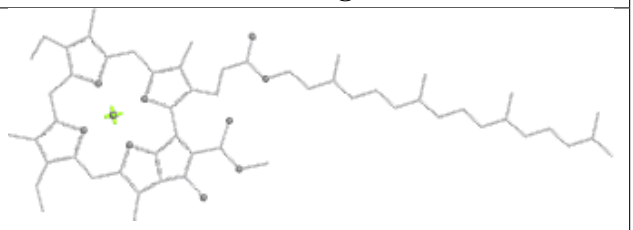
Bond lengths



Bond angles



Torsions

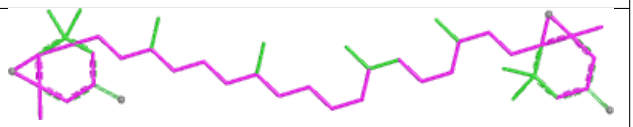


Rings

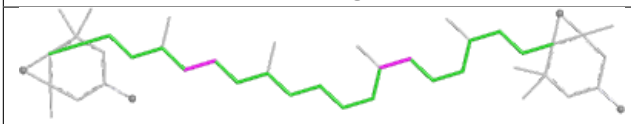
Ligand XAT Y 1622



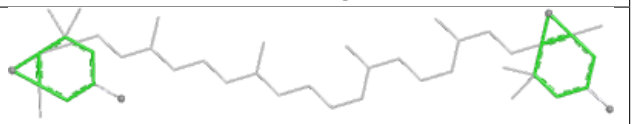
Bond lengths



Bond angles



Torsions



Rings

Ligand PL9 d 405



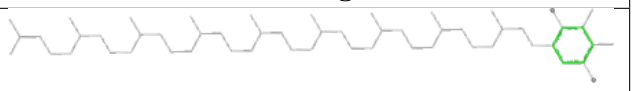
Bond lengths



Bond angles

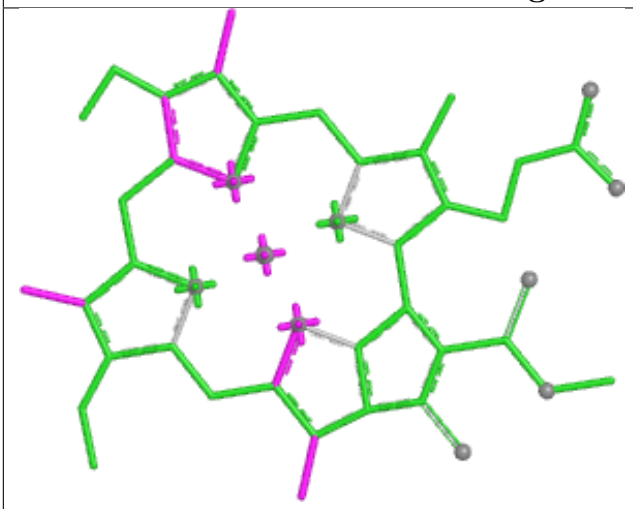


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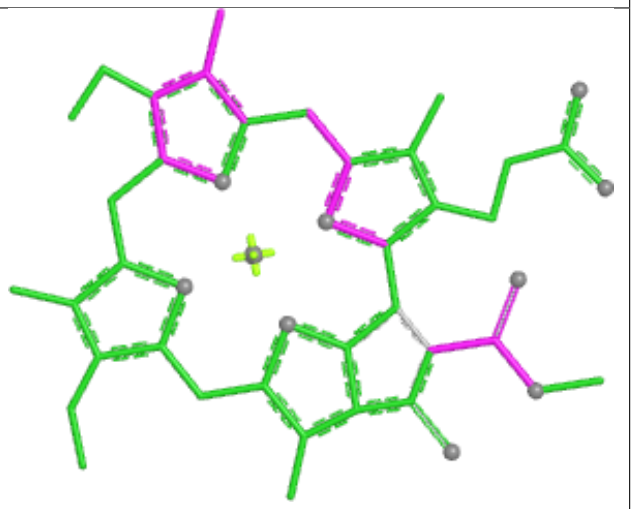


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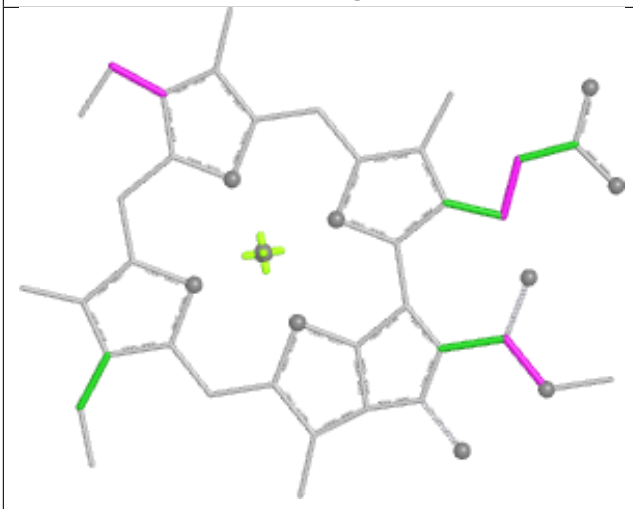
Ligand CLA 4 602



Bond lengths



Bond angles

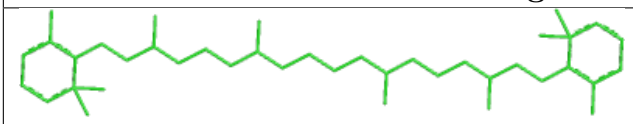


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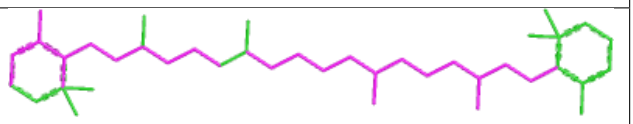


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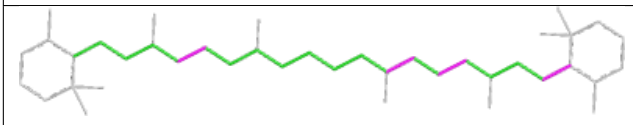
Ligand BCR c 515



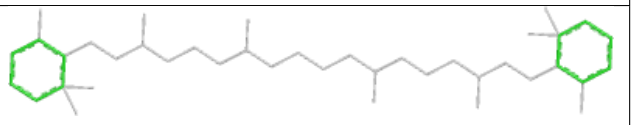
Bond lengths



Bond angles

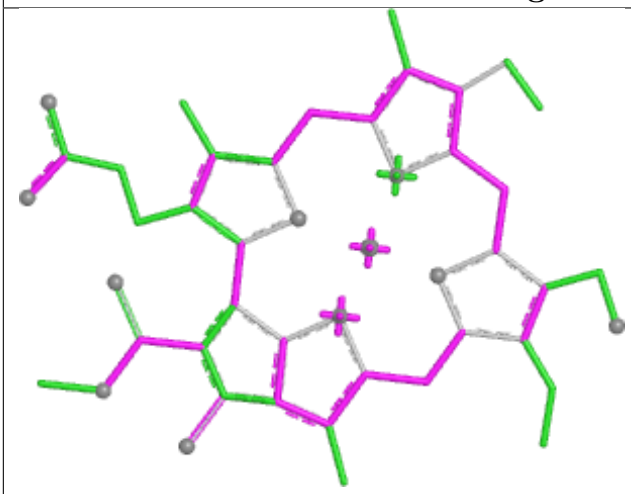


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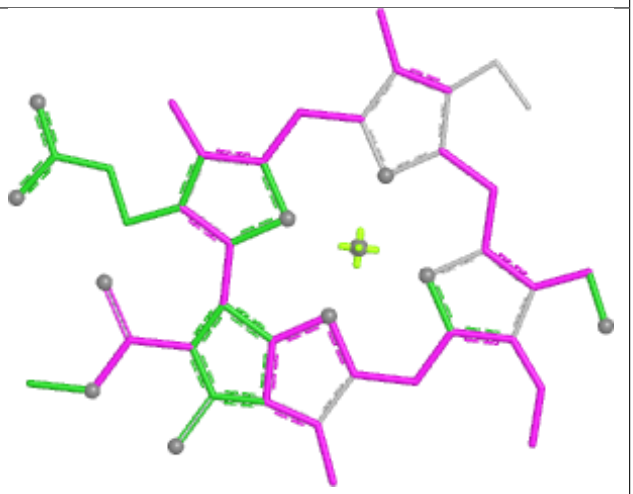


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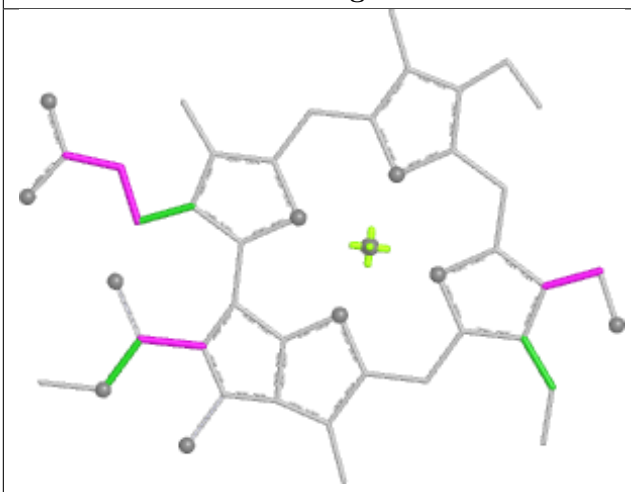
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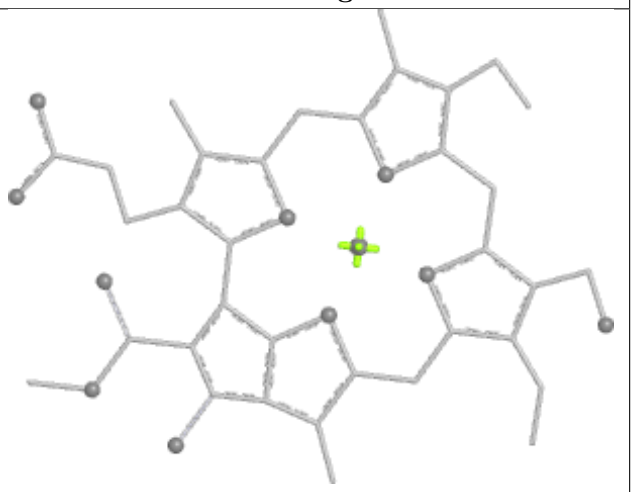
Bond lengths



Bond angles

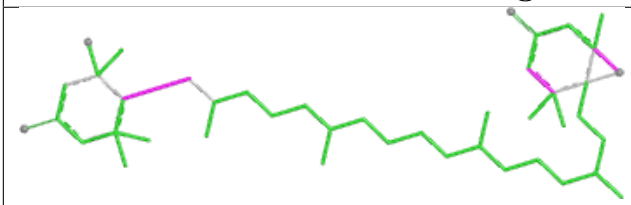


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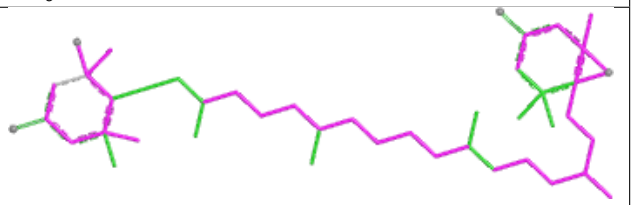


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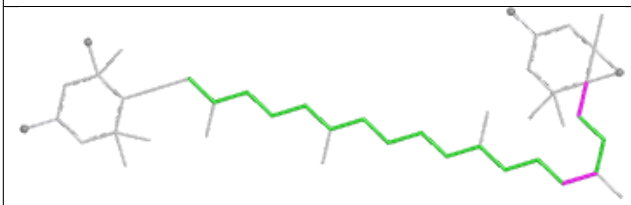
Ligand NEX y 1623



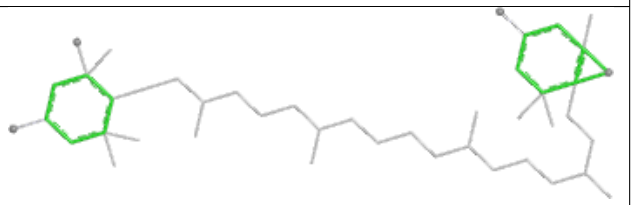
Bond lengths



Bond angles

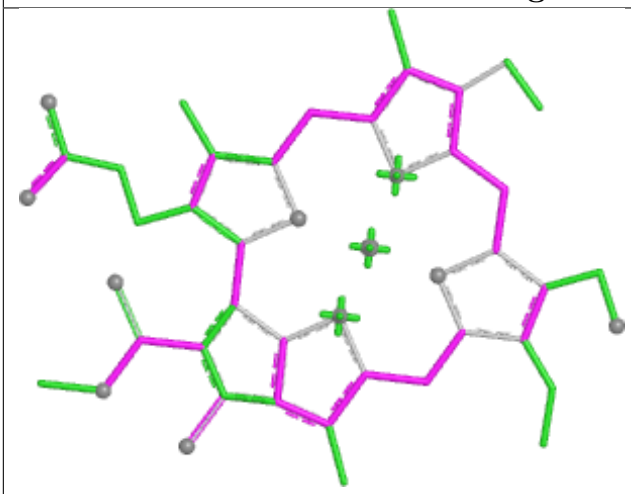


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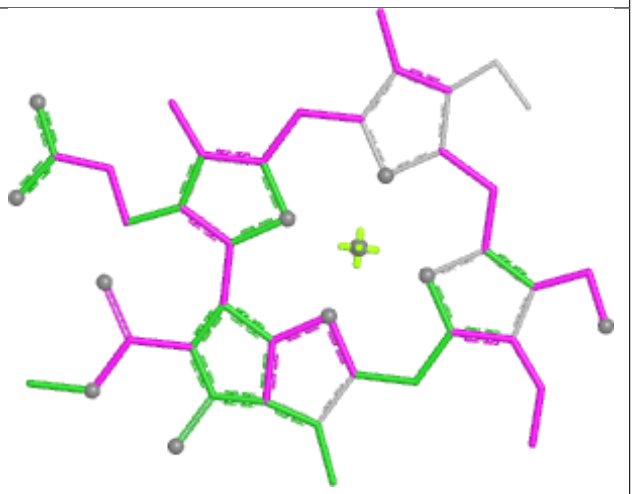


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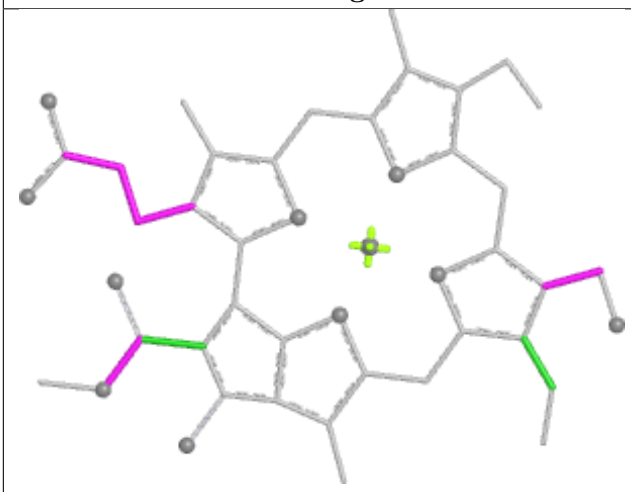
Ligand CHL 4 607



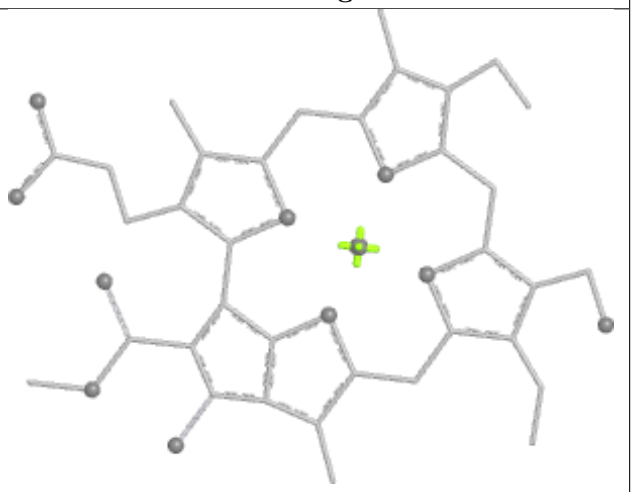
Bond lengths



Bond angles

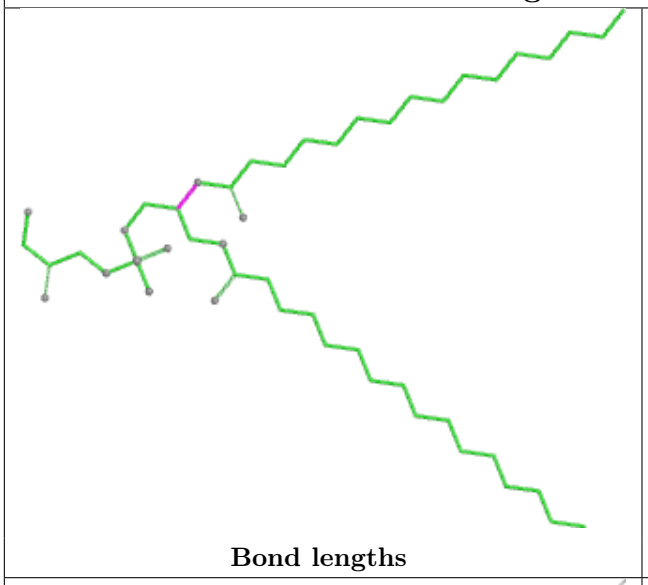


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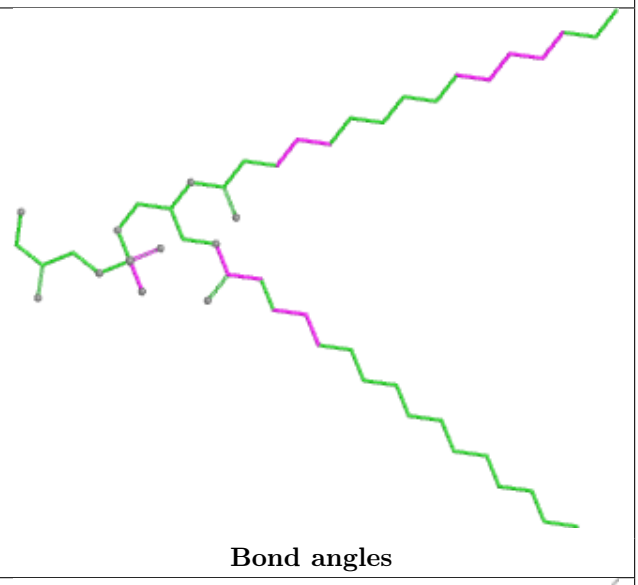


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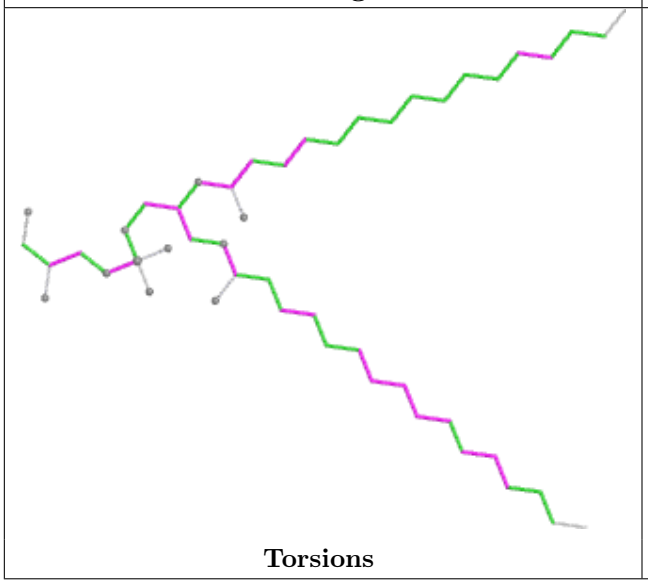
Ligand LHG C 522



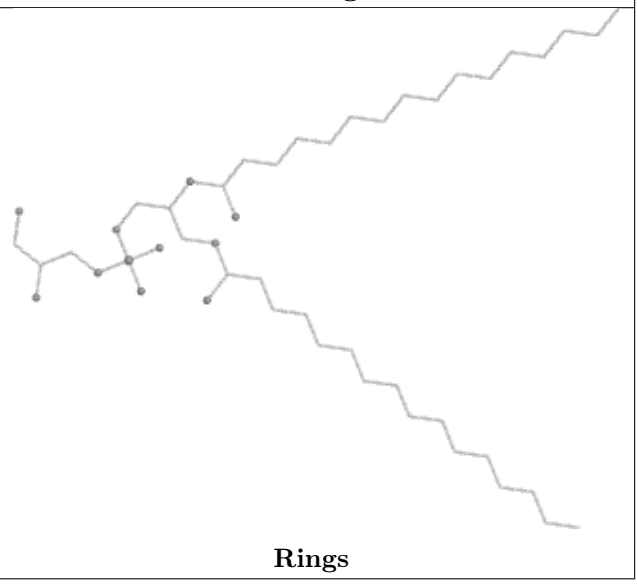
Bond lengths



Bond angles

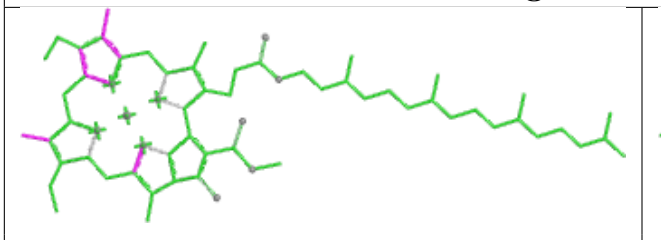


Torsions

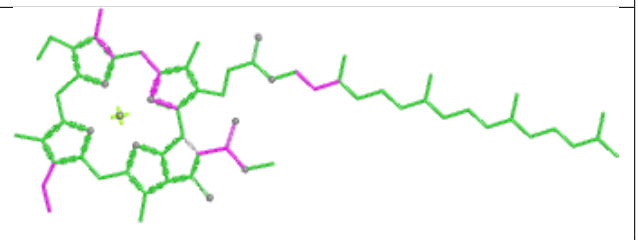


Rings

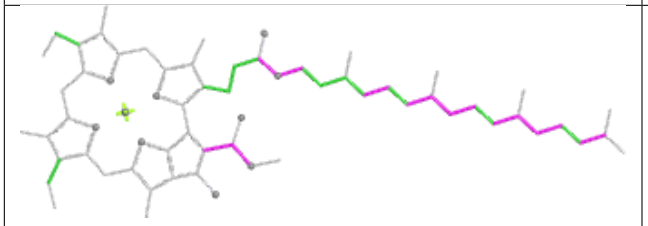
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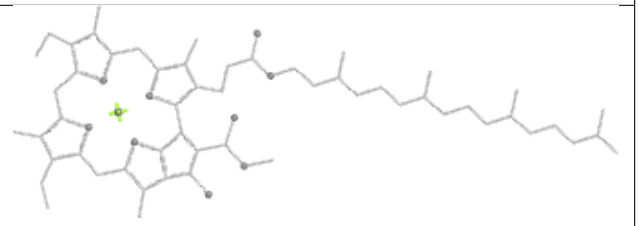
Bond lengths



Bond angles

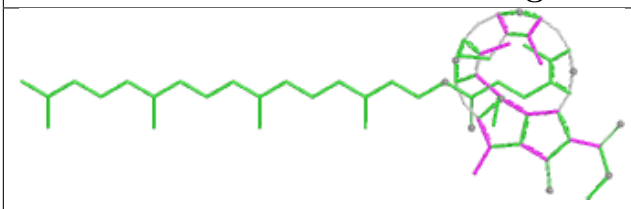


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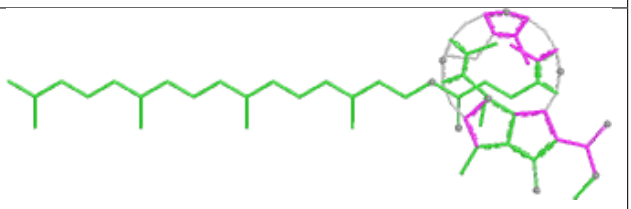


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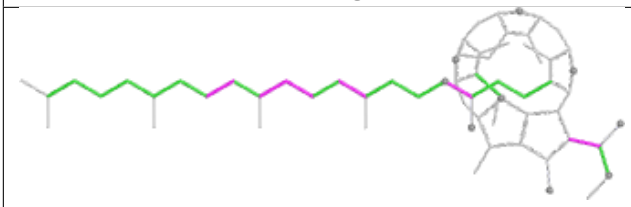
Ligand PHO a 409



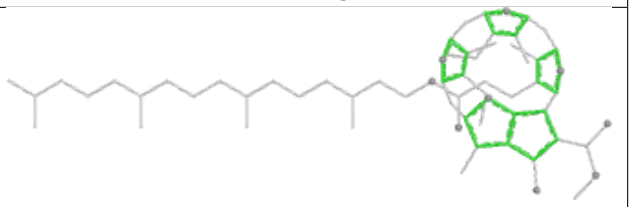
Bond lengths



Bond angles

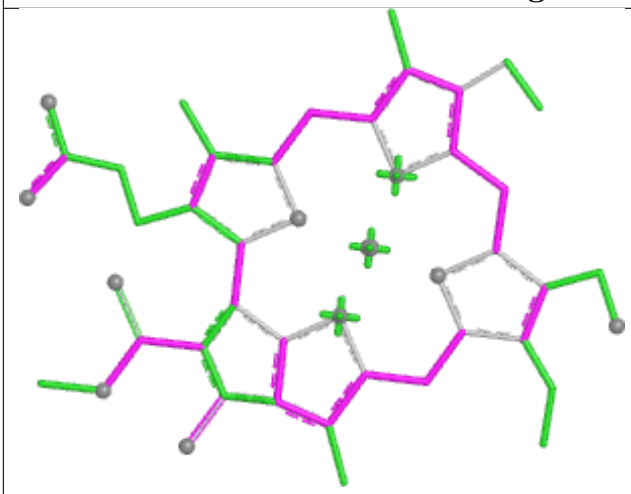


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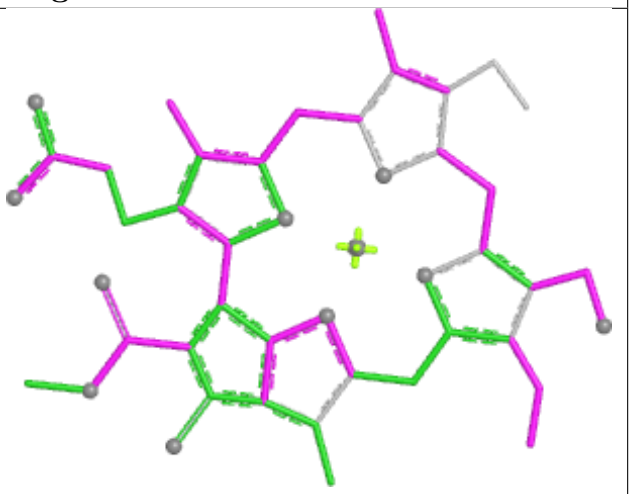


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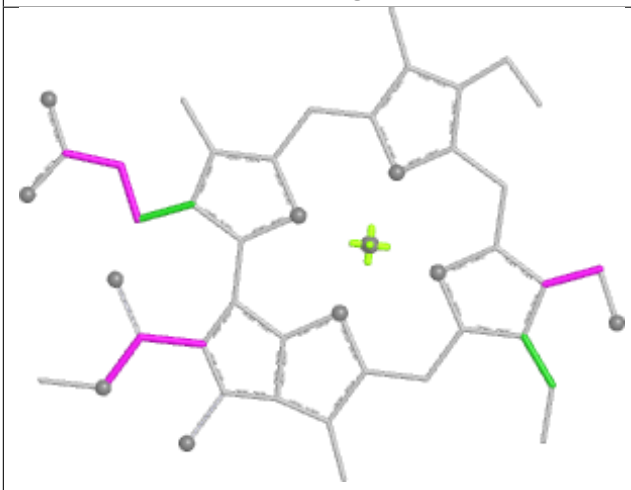
Ligand CHL g 605



Bond lengths



Bond angles

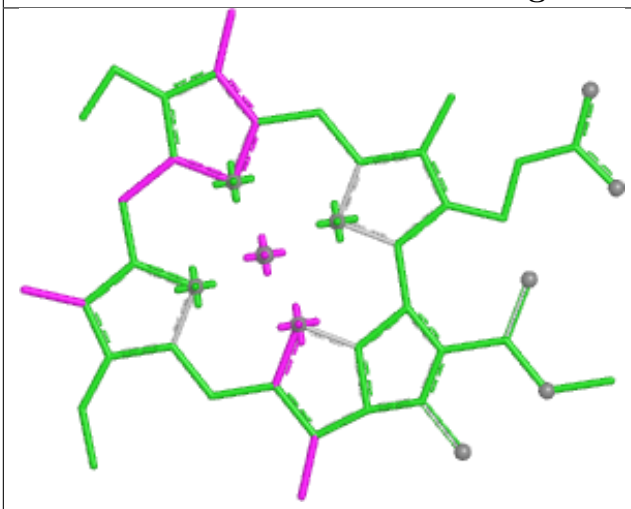


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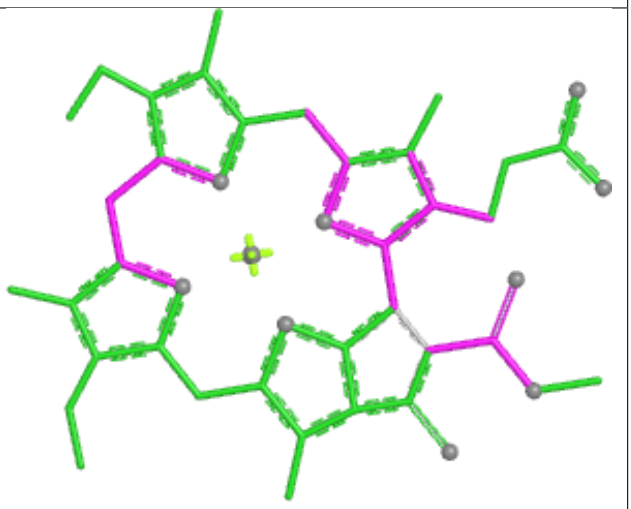


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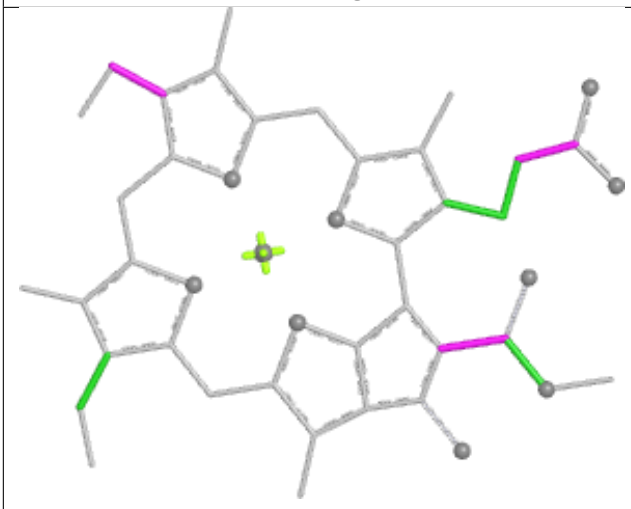
Ligand CLA 1 612



Bond lengths



Bond angles

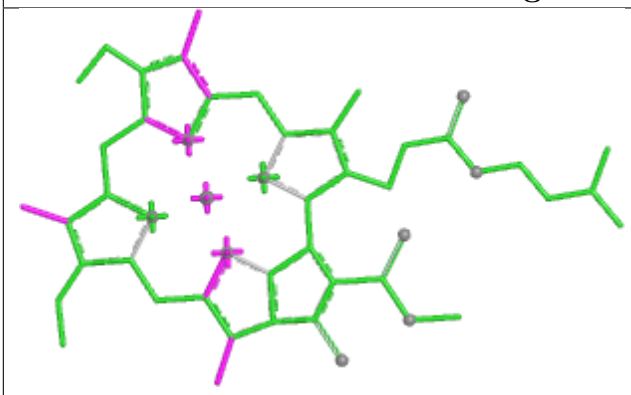


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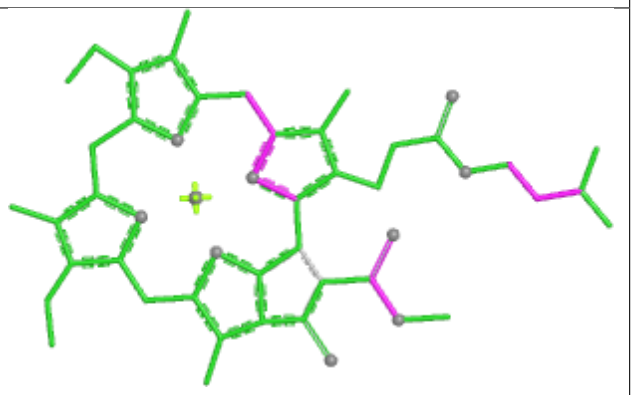


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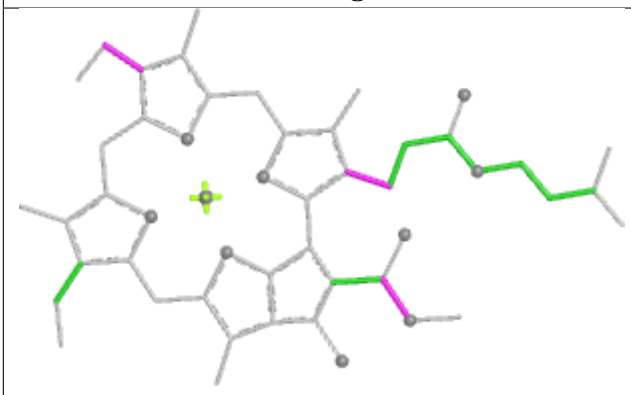
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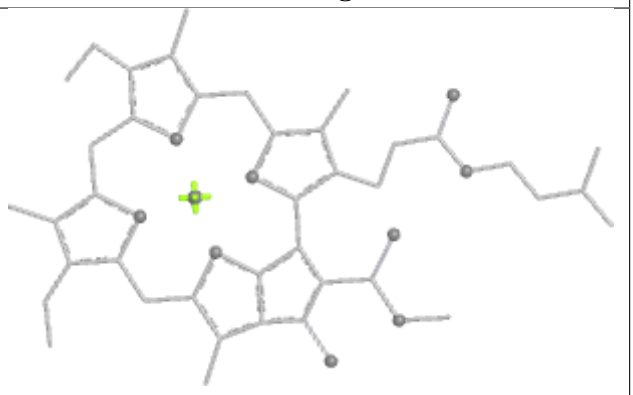
Bond lengths



Bond angles

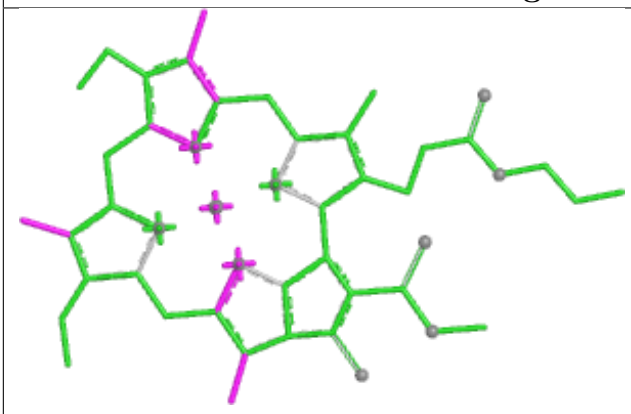


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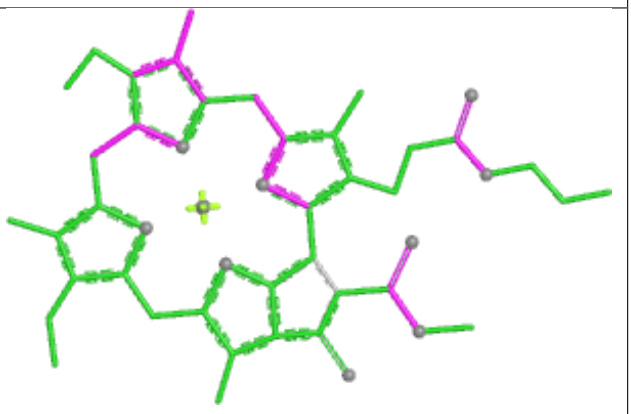


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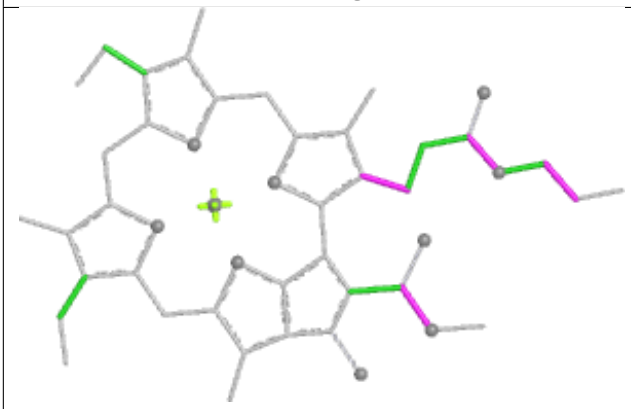
Ligand CLA N 614



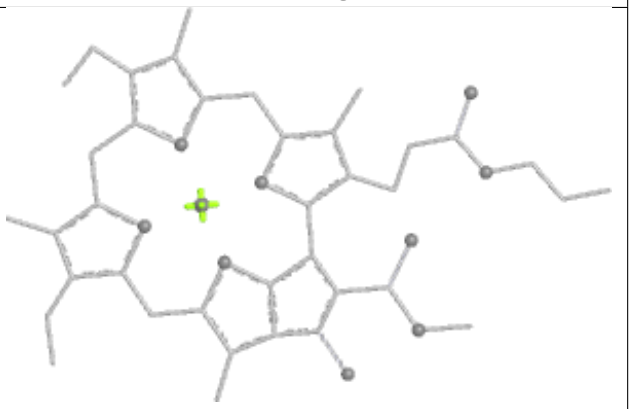
Bond lengths



Bond angles

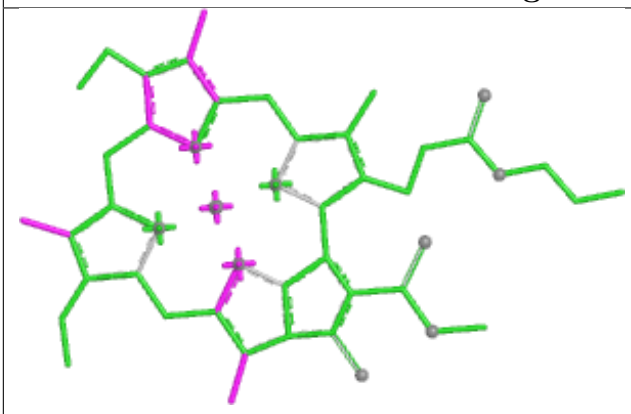


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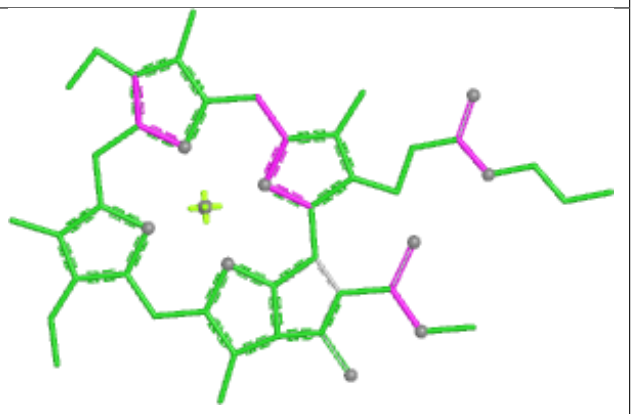


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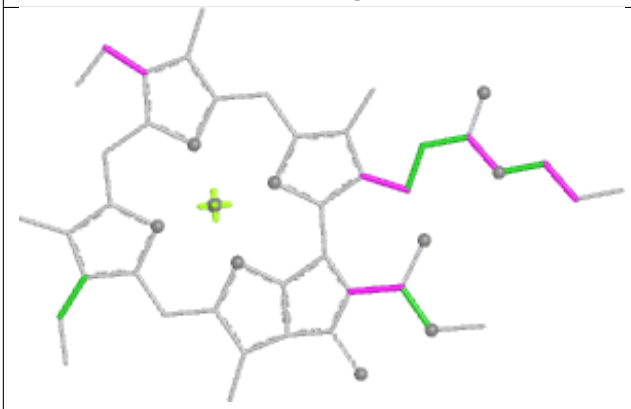
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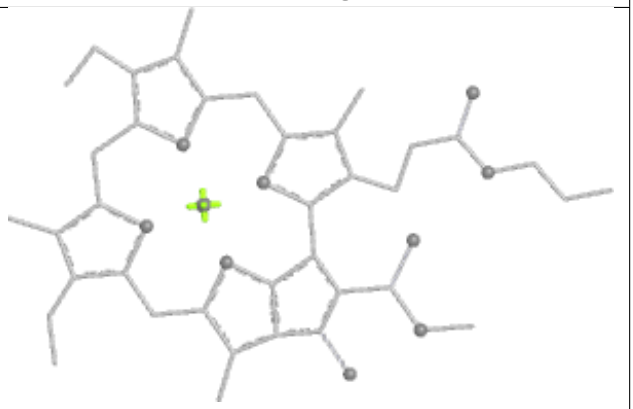
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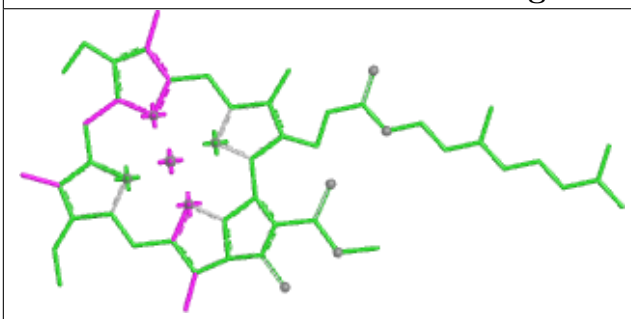


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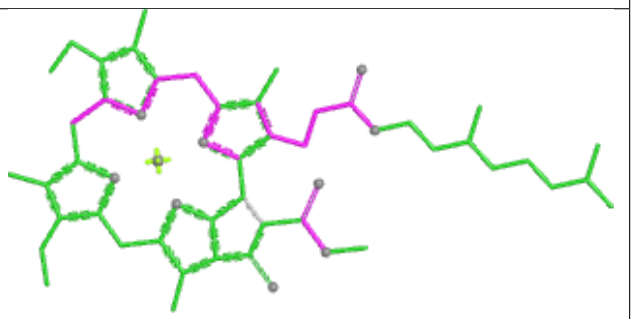


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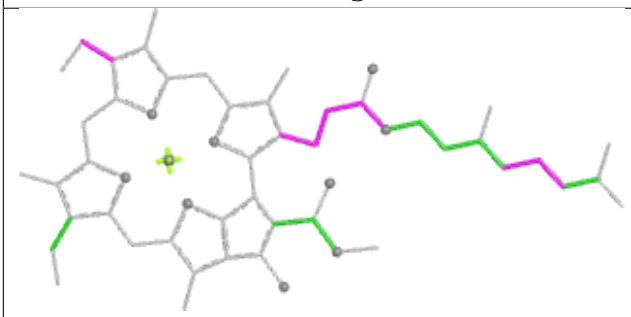
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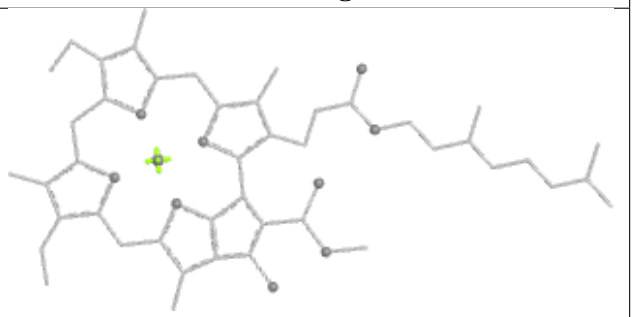
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Bond angles

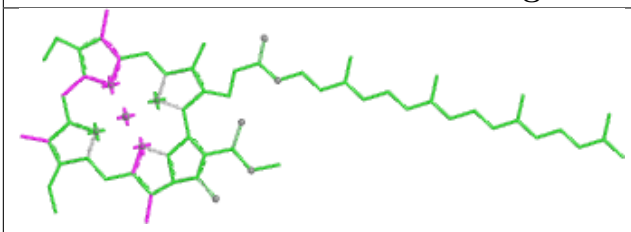


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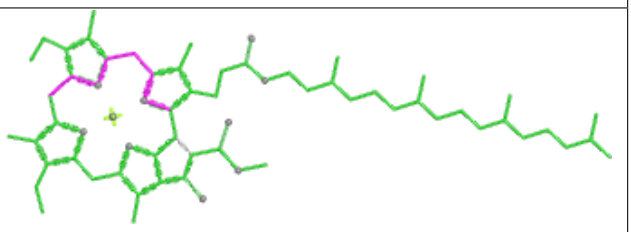


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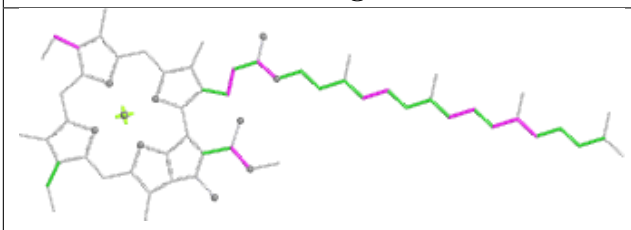
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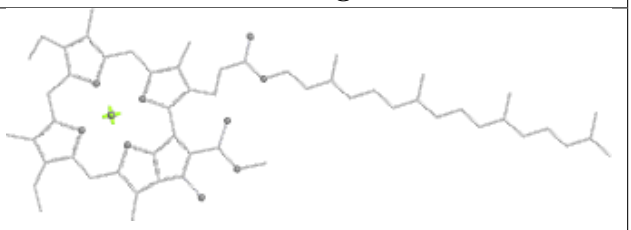
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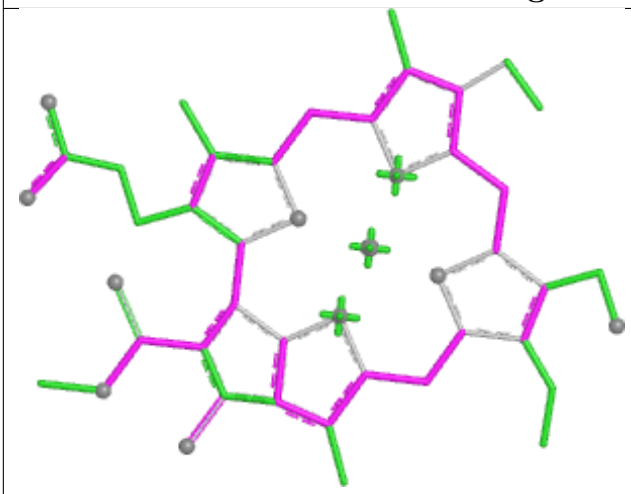


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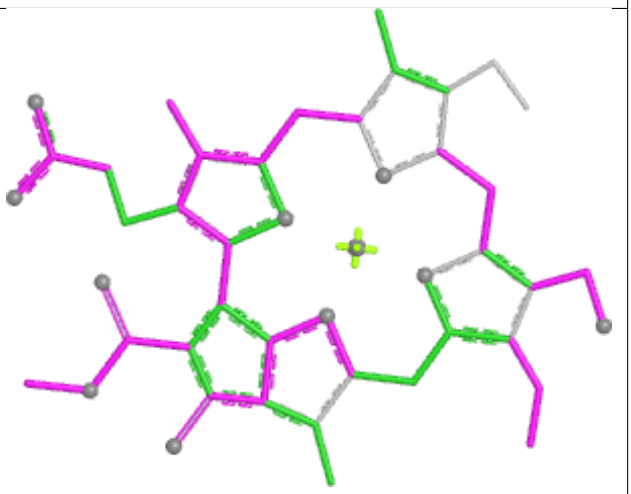


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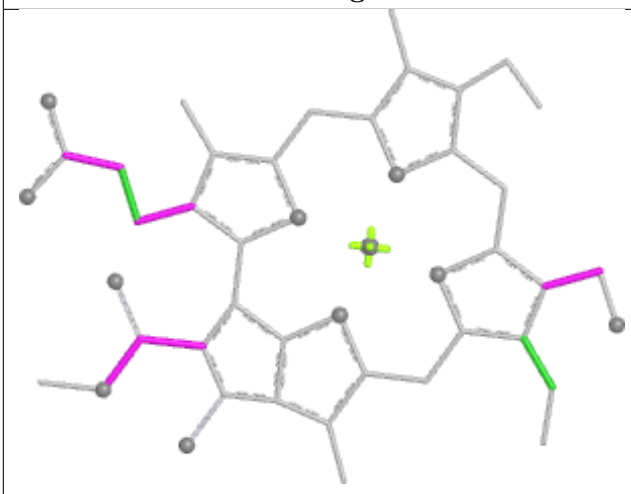
Ligand CHL 8 608



Bond lengths



Bond angles

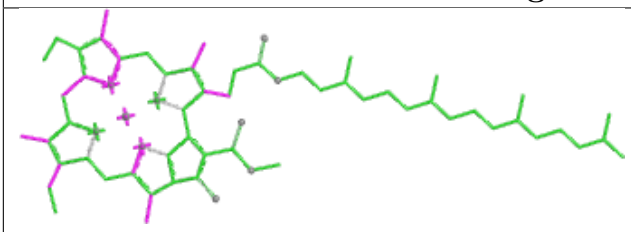


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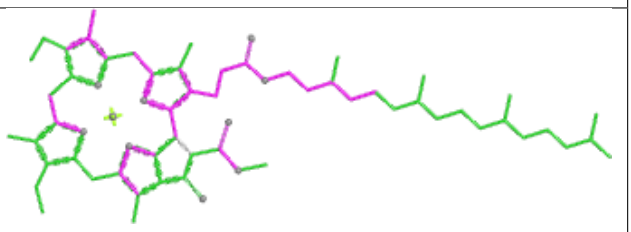


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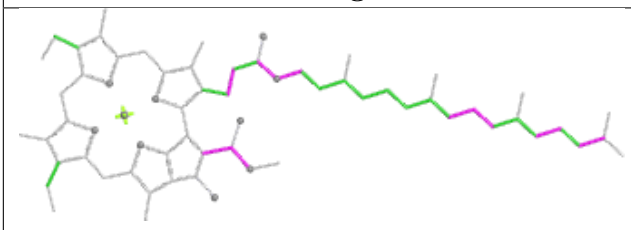
Ligand CLA b 605



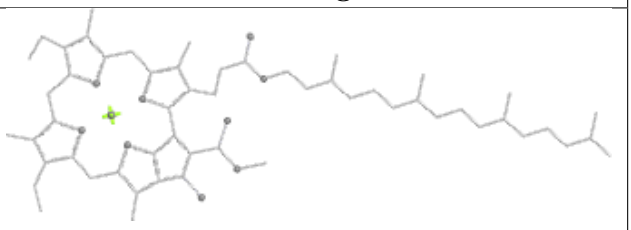
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Bond angles

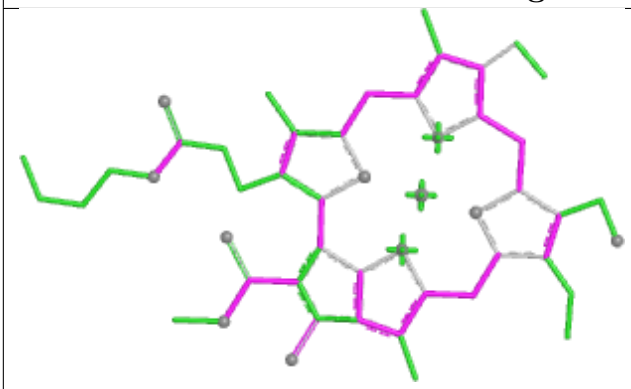


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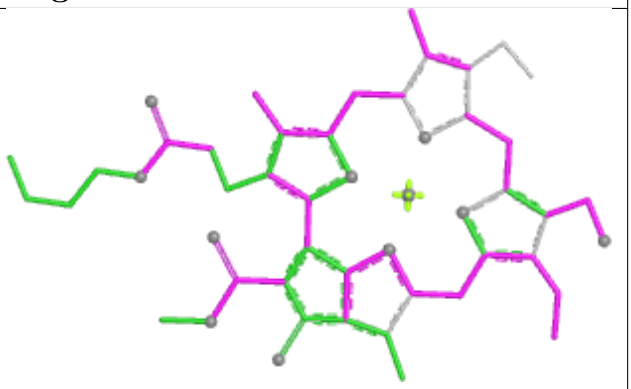


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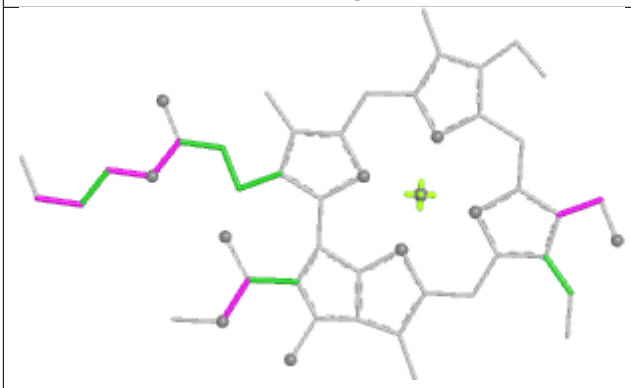
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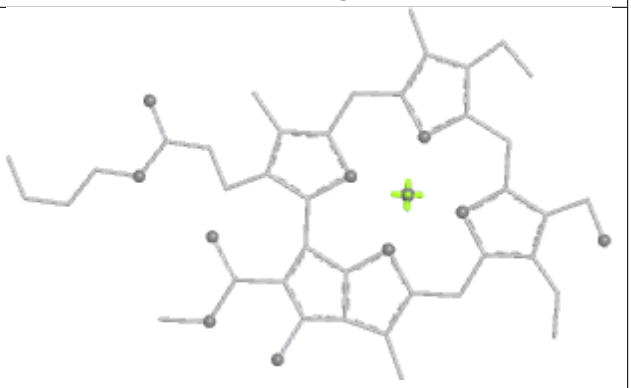
Bond lengths



Bond angles

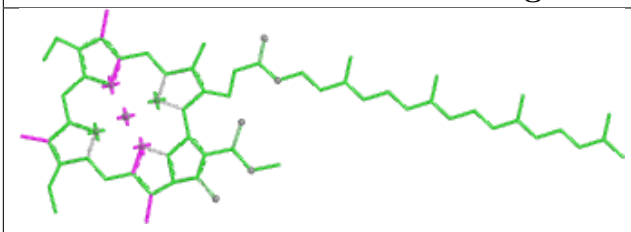


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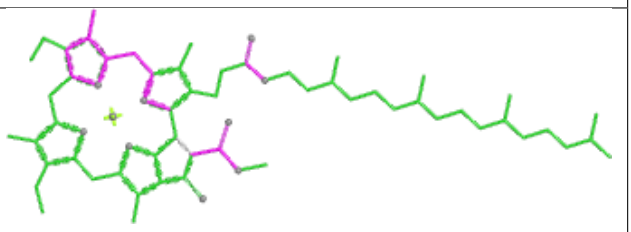


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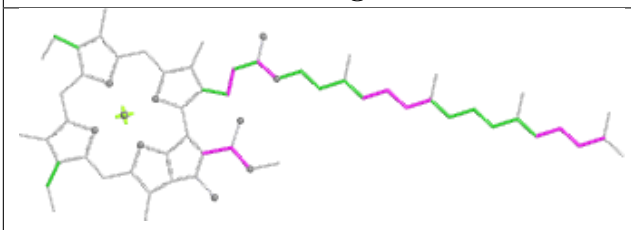
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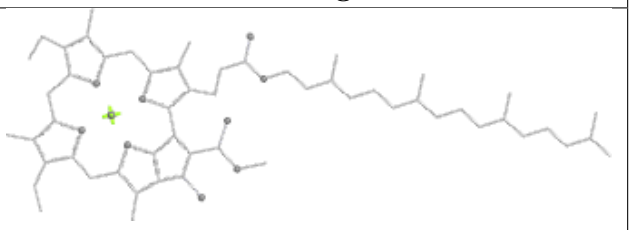
Bond lengths



Bond angles

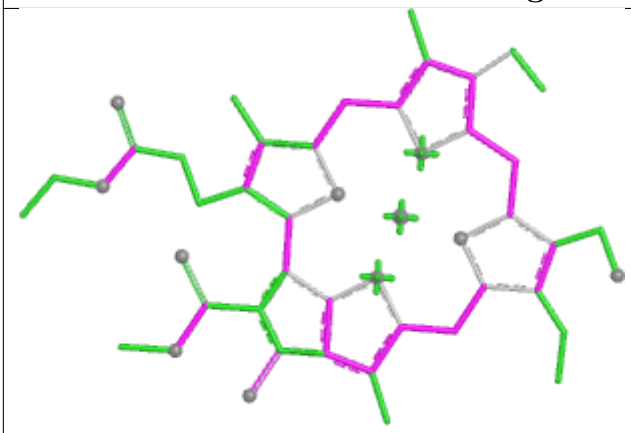


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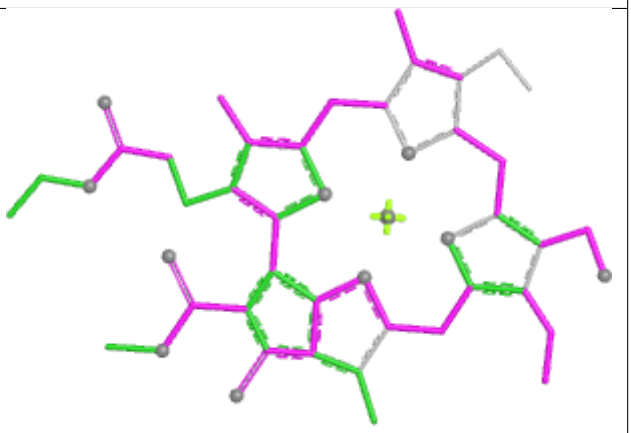


Rings

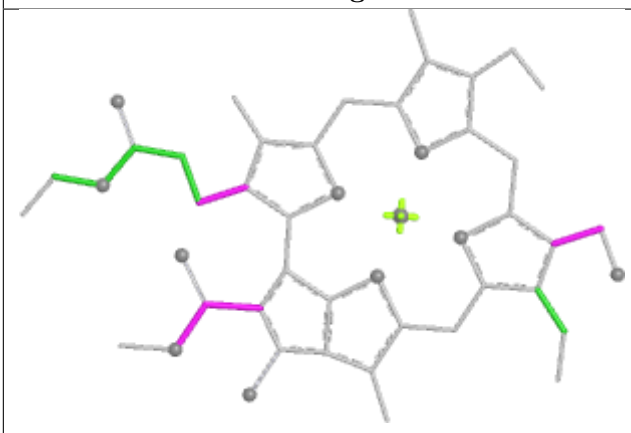
Ligand CHL n 605



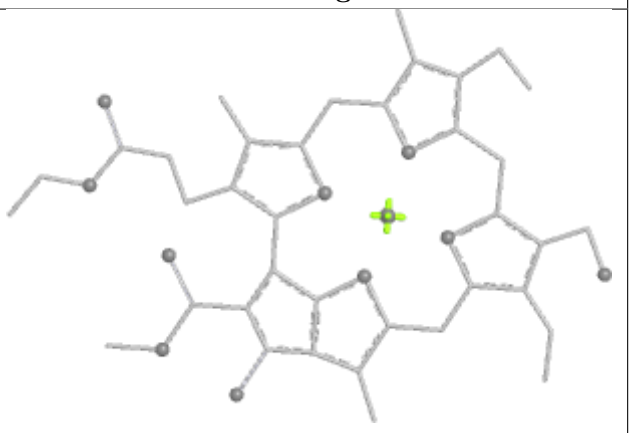
Bond lengths



Bond angles

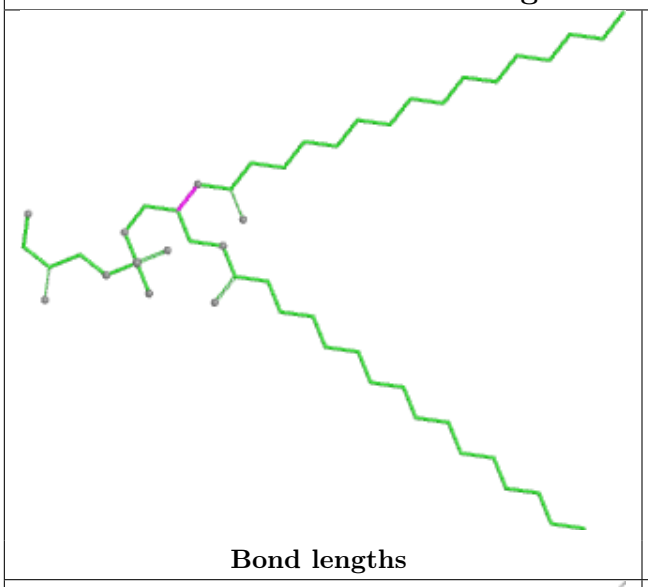


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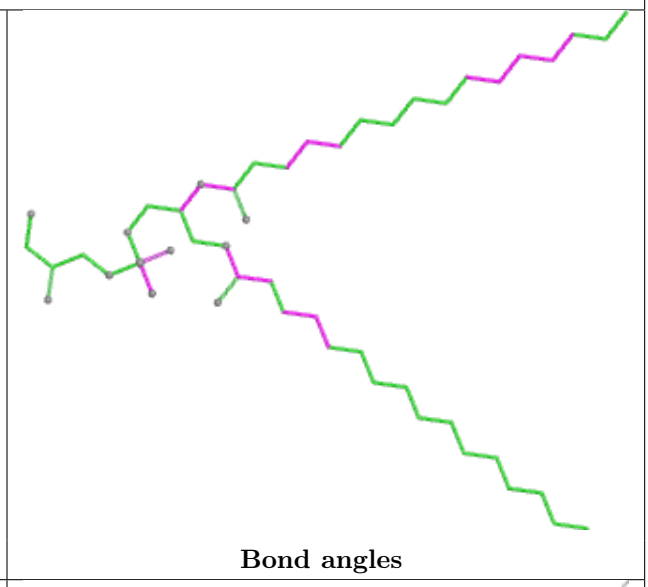


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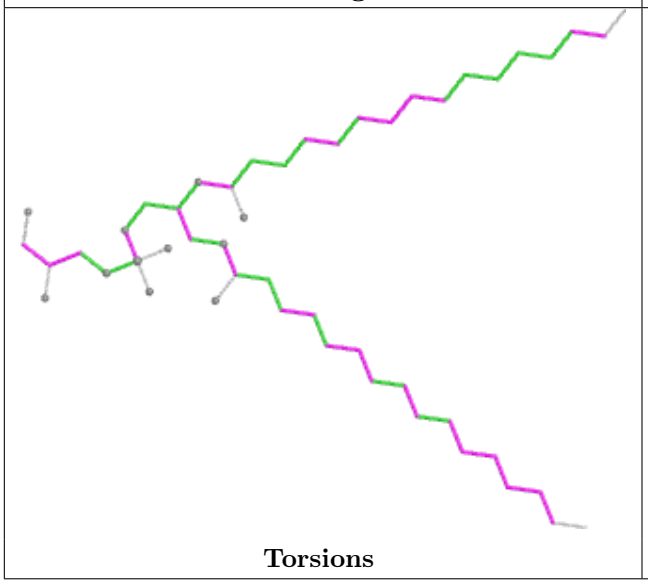
Ligand LHG s 2630



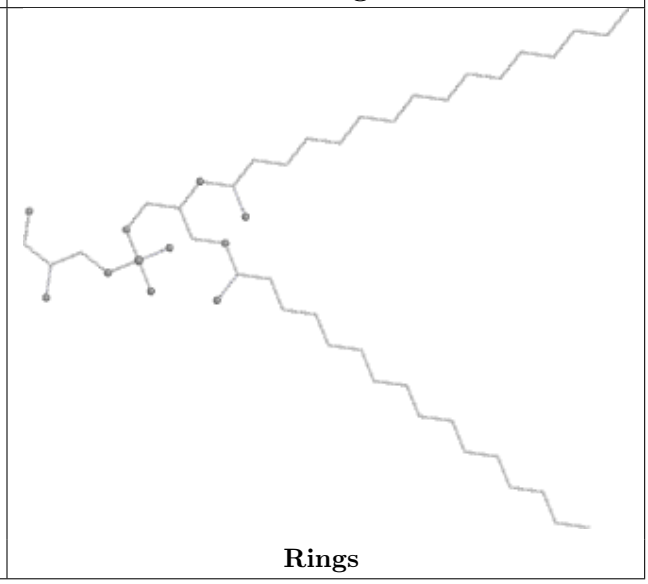
Bond lengths



Bond angles

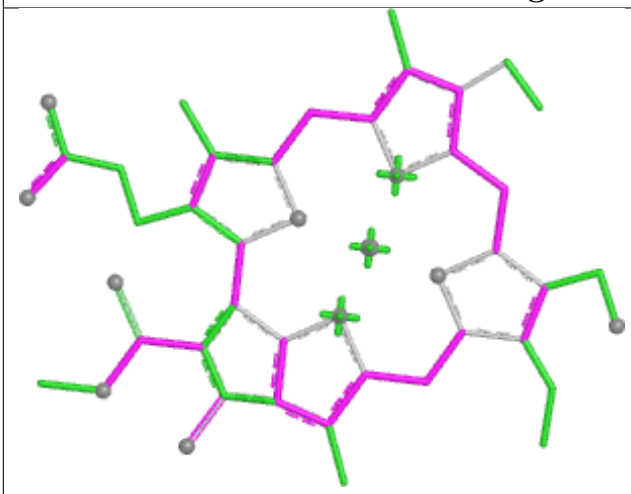


Torsions

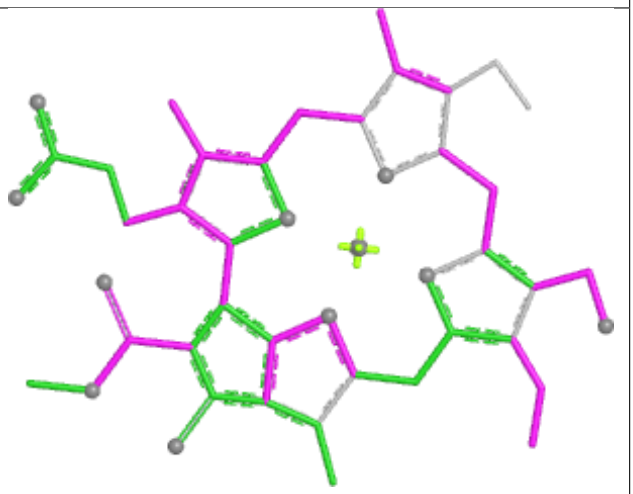


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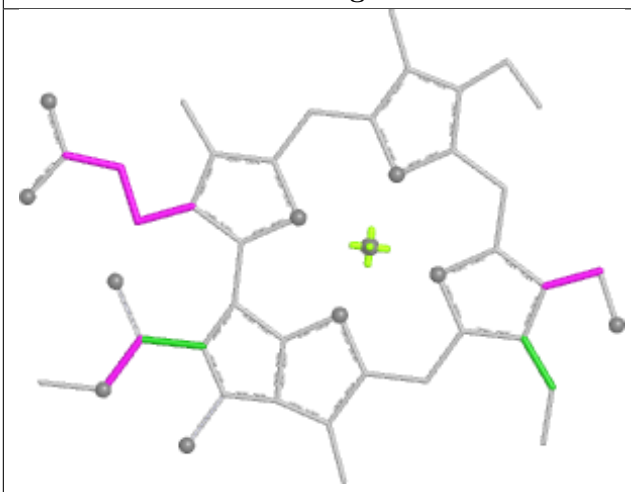
Ligand CHL 2 605



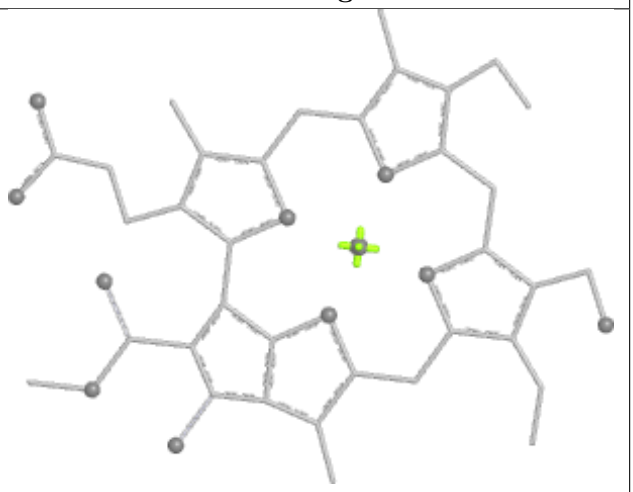
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Bond angles

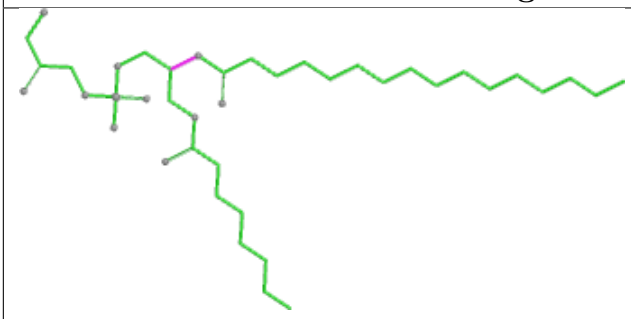


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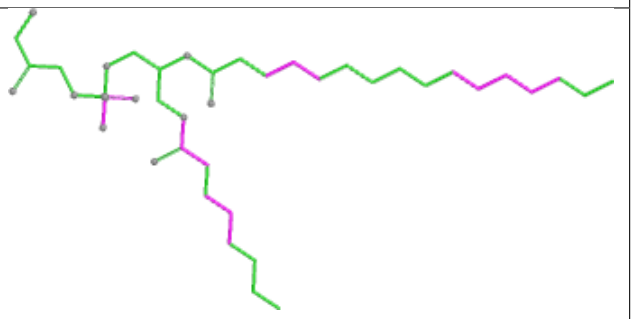


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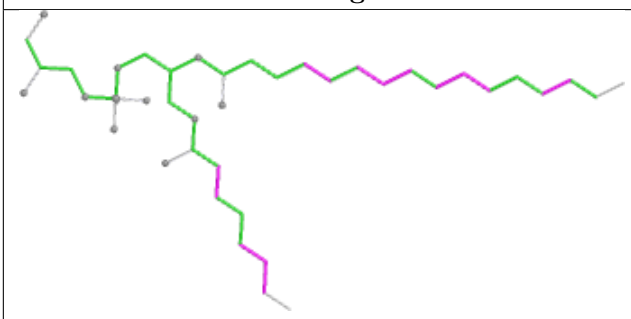
Ligand LHG 1 2630



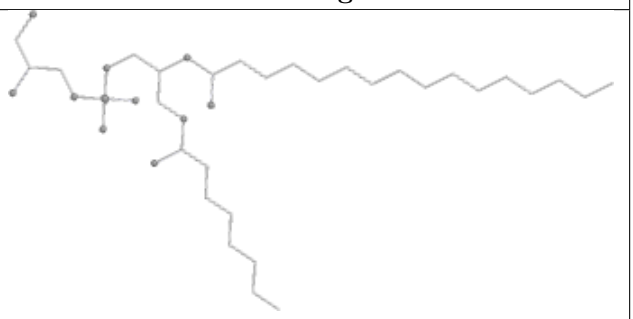
Bond lengths



Bond angles

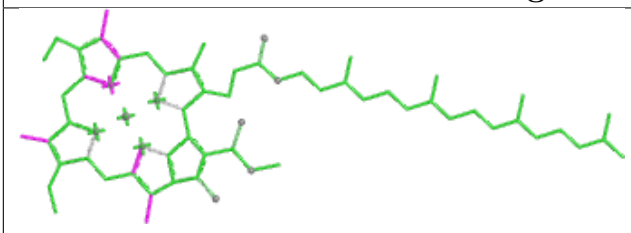


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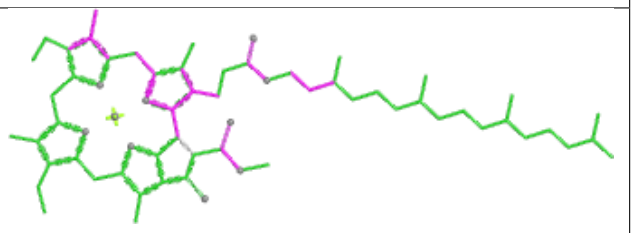


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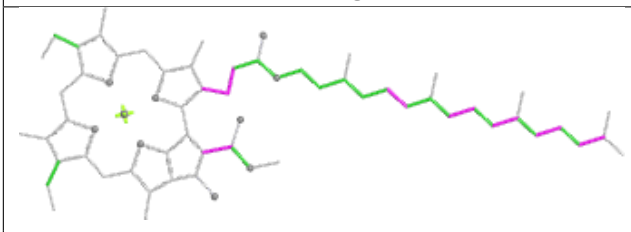
Ligand CLA n 610



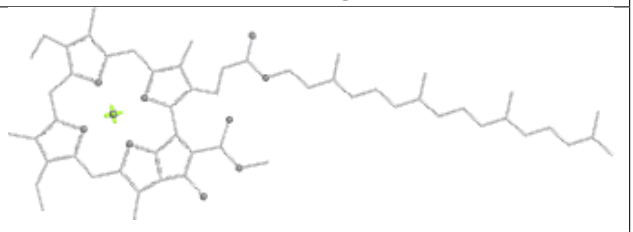
Bond lengths



Bond angles

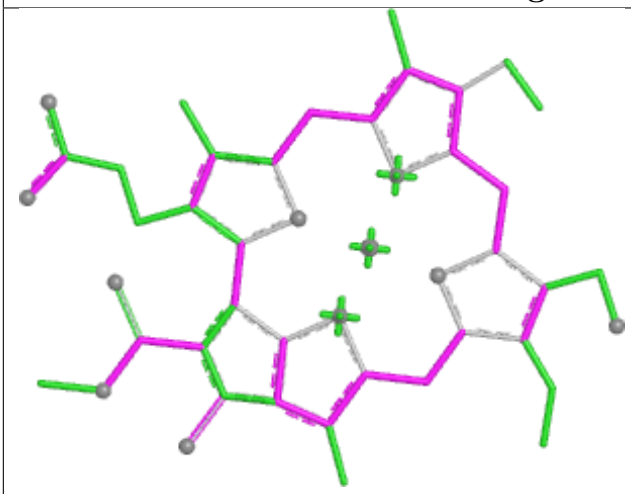


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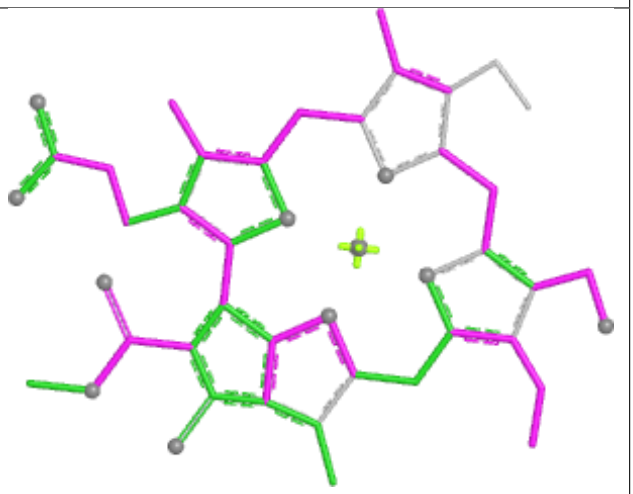


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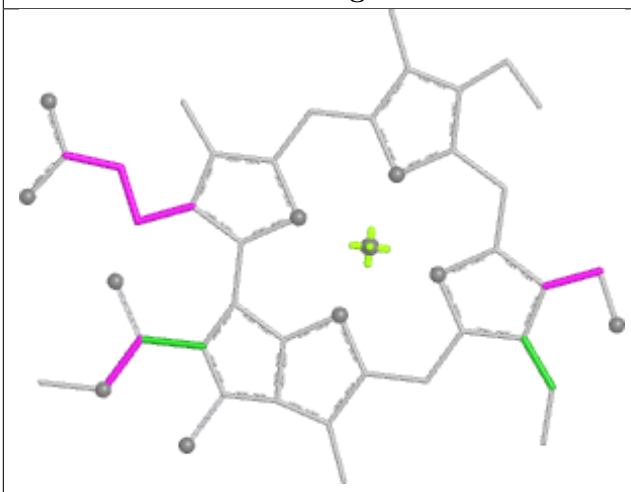
Ligand CHL 8 607



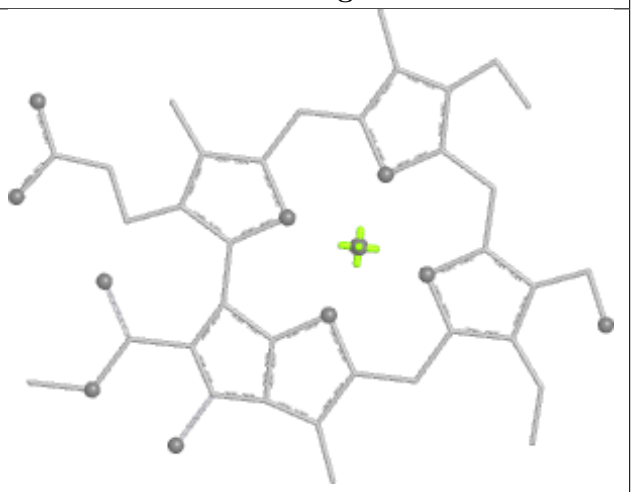
Bond lengths



Bond angles

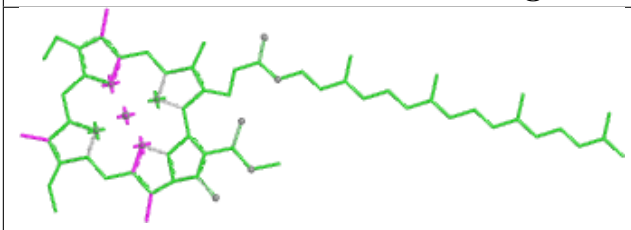


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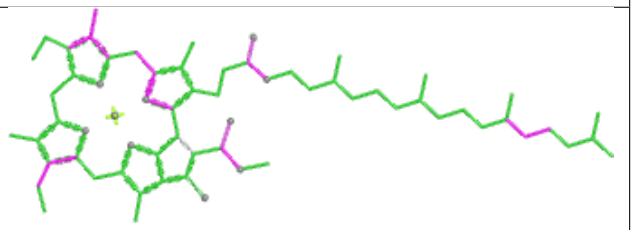


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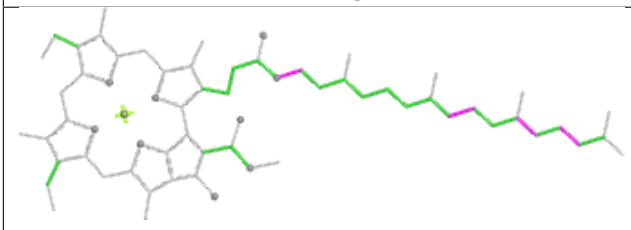
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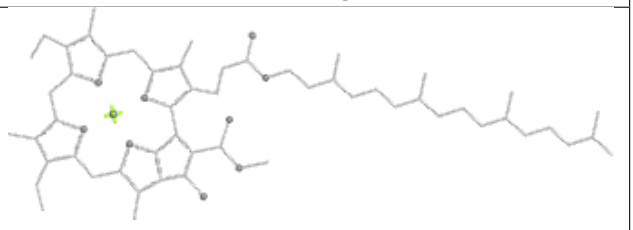
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Bond angles

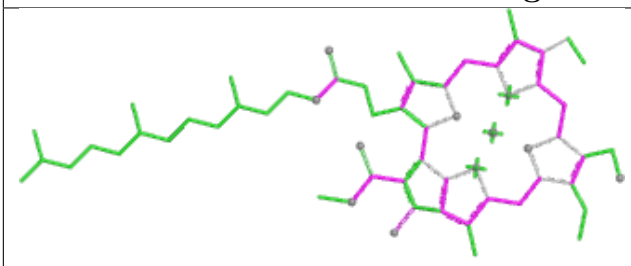


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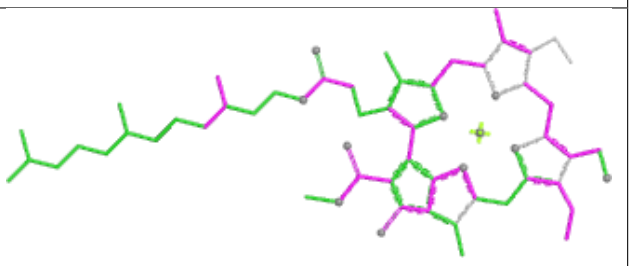


Rings

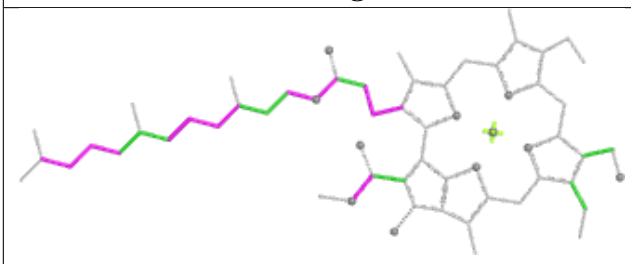
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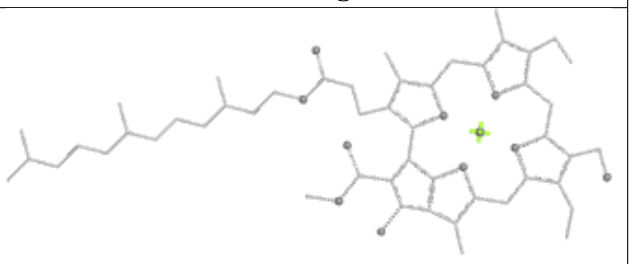
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Bond angles

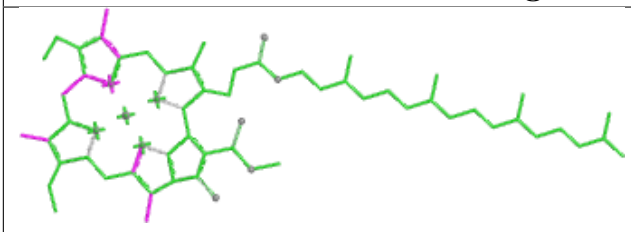


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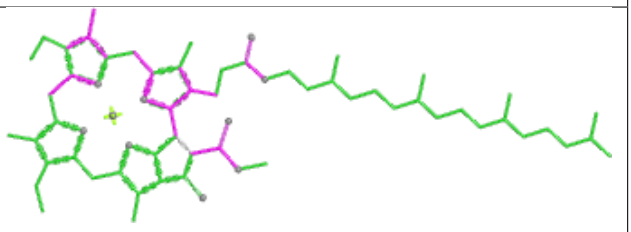


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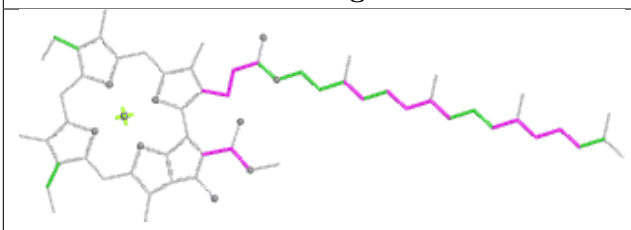
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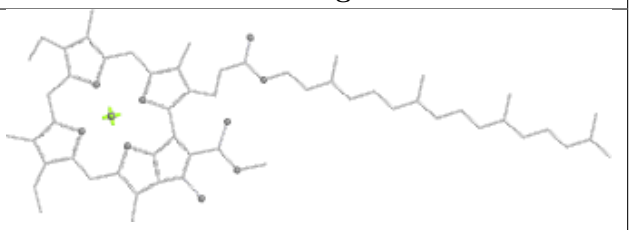
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Bond angles

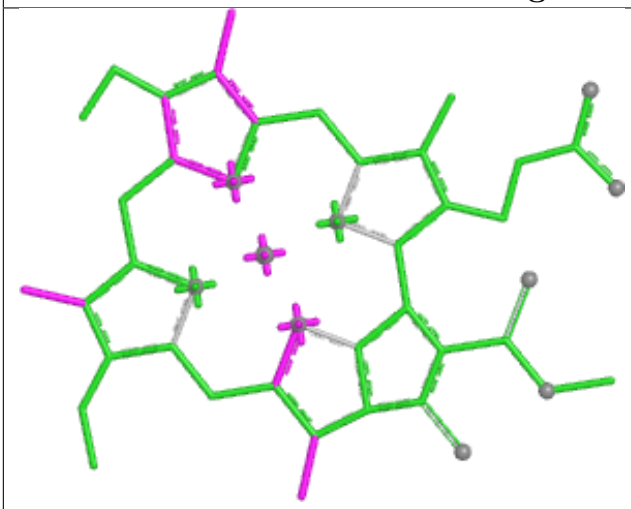


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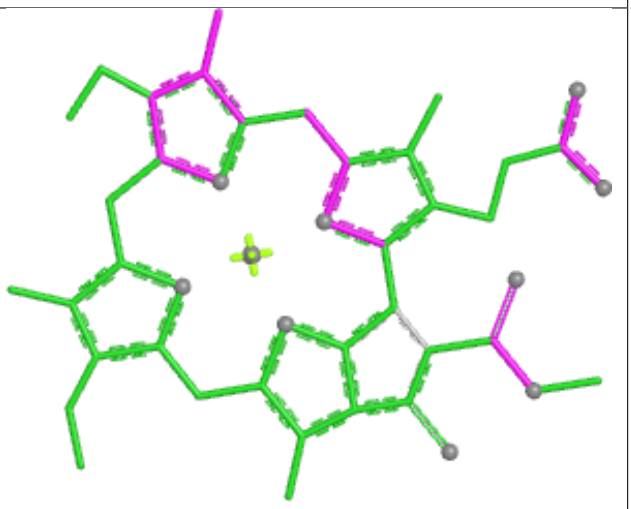


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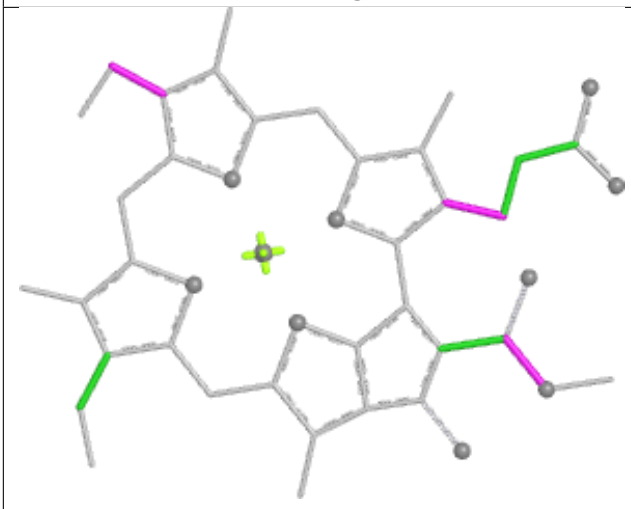
Ligand CLA 5 614



Bond lengths



Bond angles

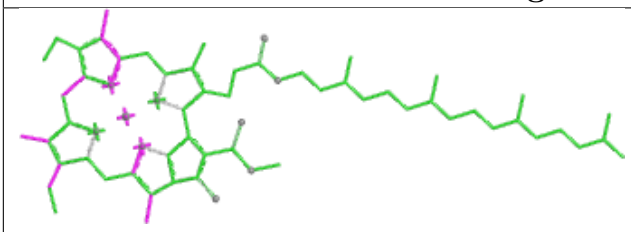


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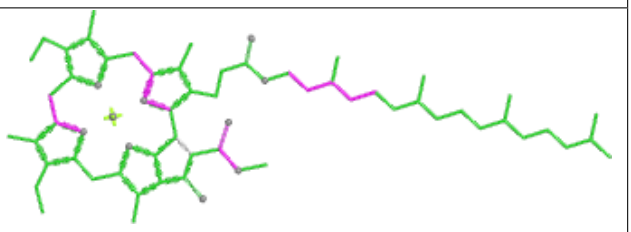


Rings

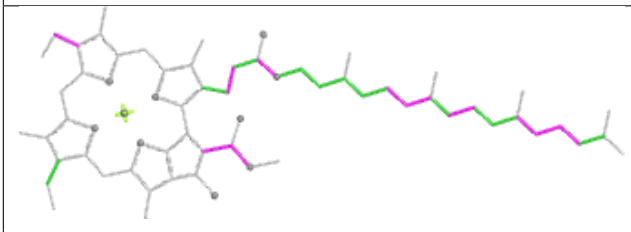
Ligand CLA b 606



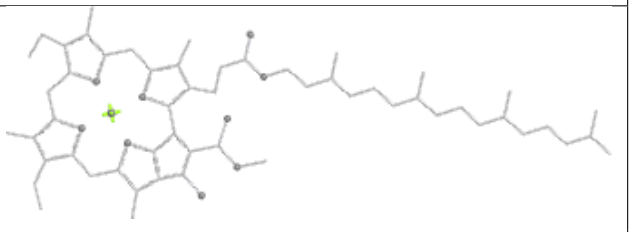
Bond lengths



Bond angles

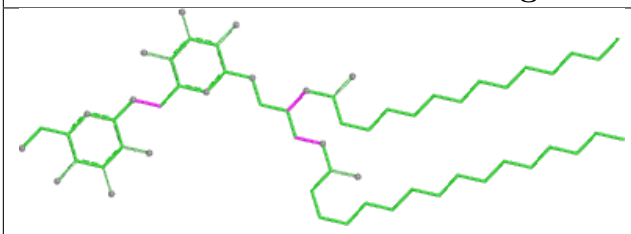


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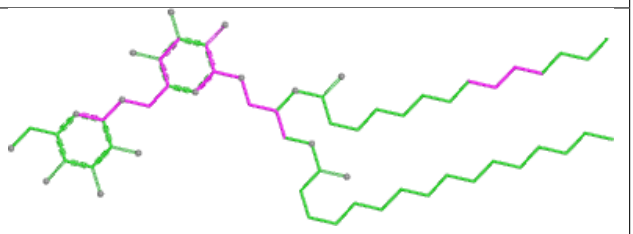


Rings

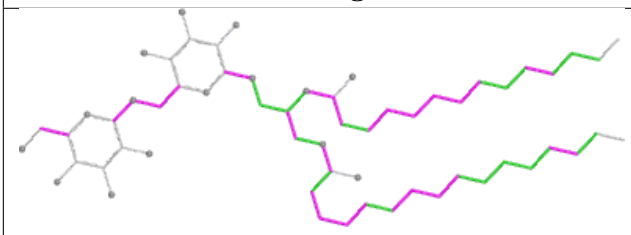
Ligand DGD C 520



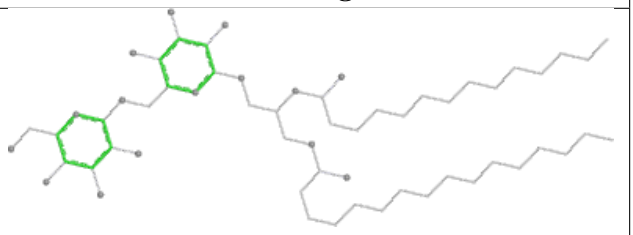
Bond lengths



Bond angles

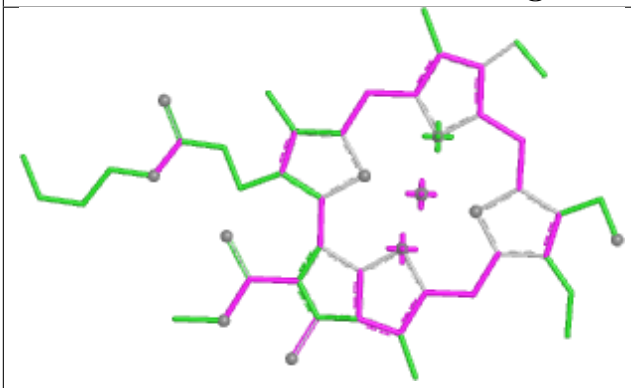


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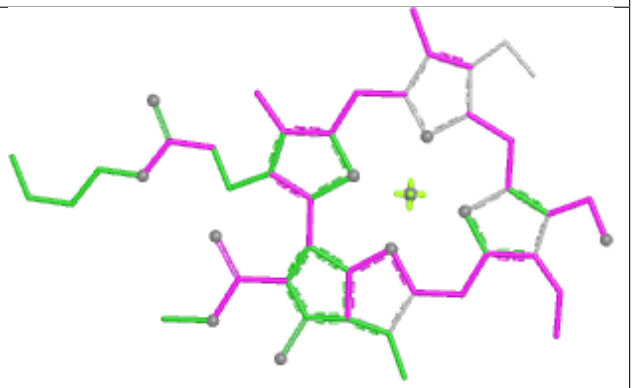


Rings

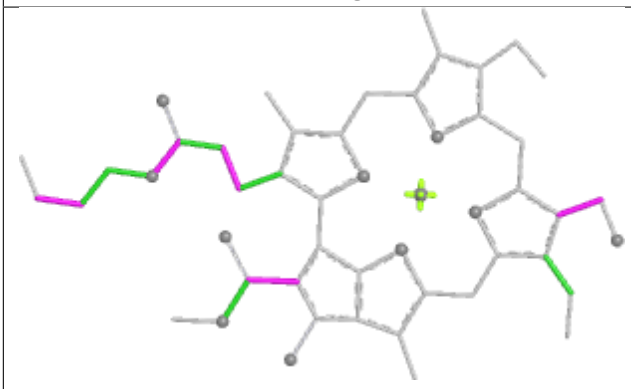
Ligand CHL n 606



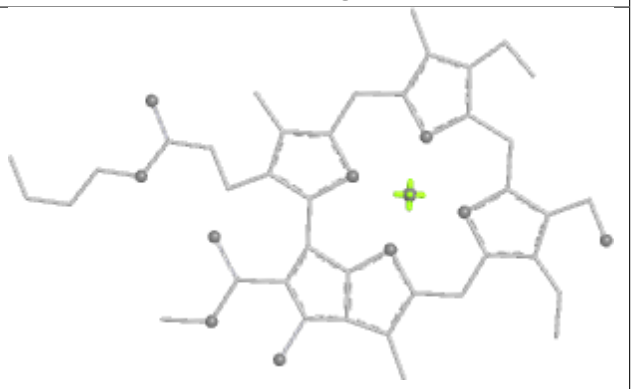
Bond lengths



Bond angles

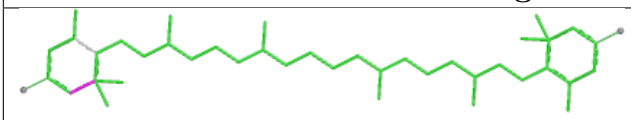


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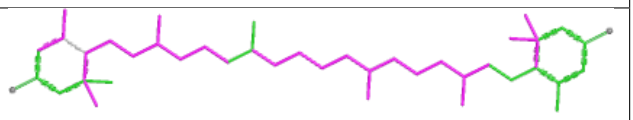


Rings

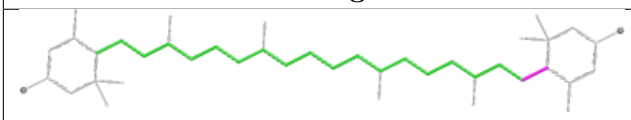
Ligand LUT N 1620



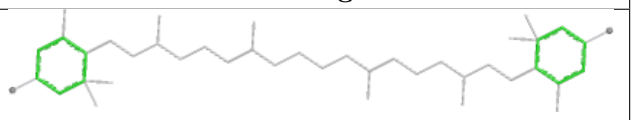
Bond lengths



Bond angles

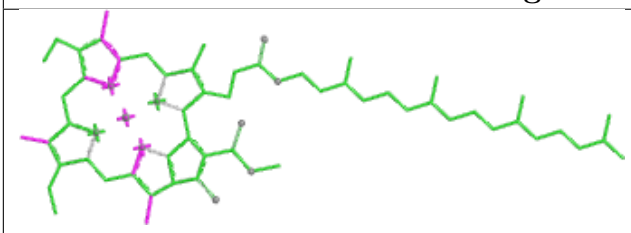


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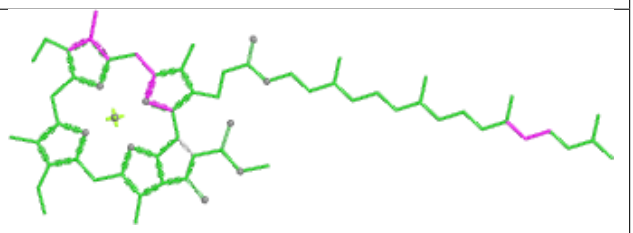


Rings

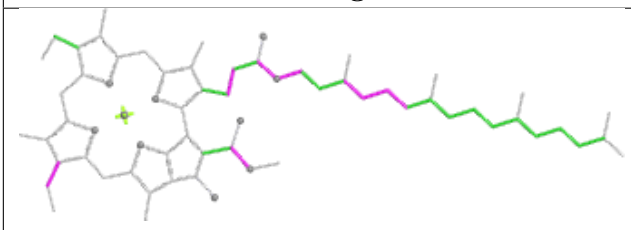
Ligand CLA A 405



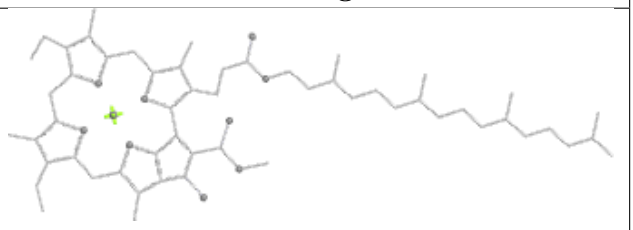
Bond lengths



Bond angles

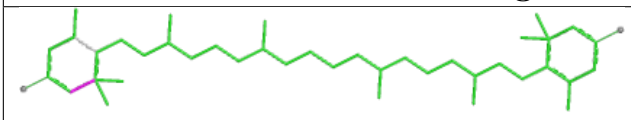


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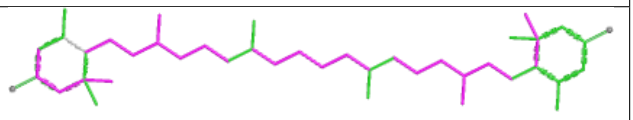


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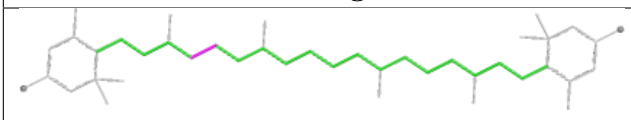
Ligand LUT N 1621



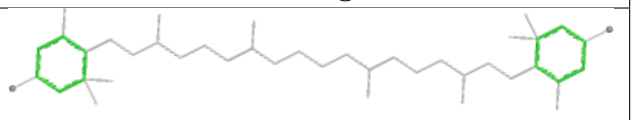
Bond lengths



Bond angles

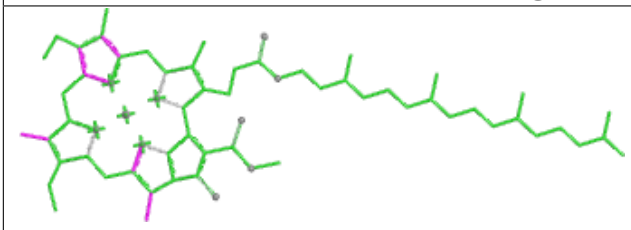


Torsions

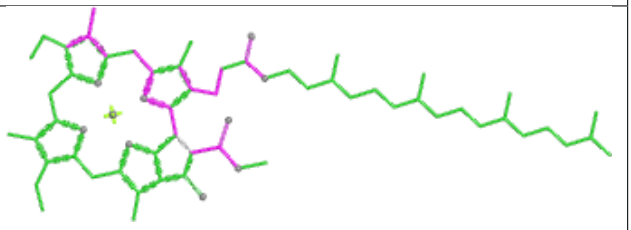


Rings

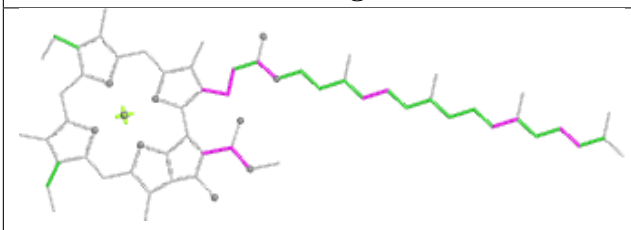
Ligand CLA c 513



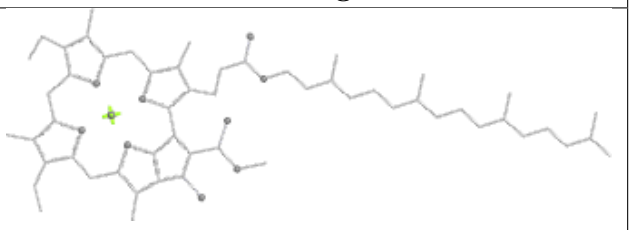
Bond lengths



Bond angles

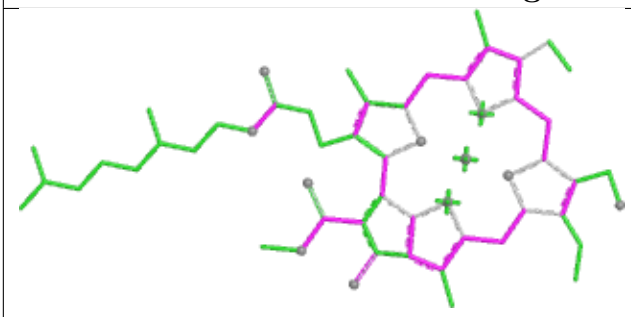


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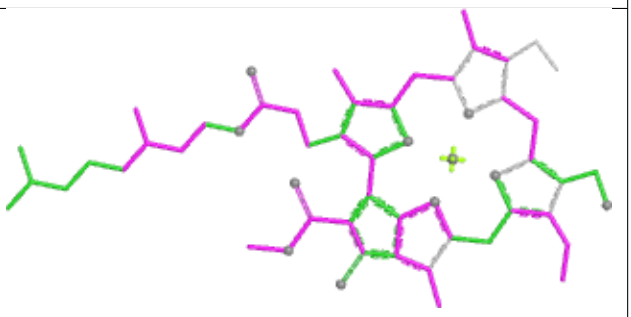


Rings

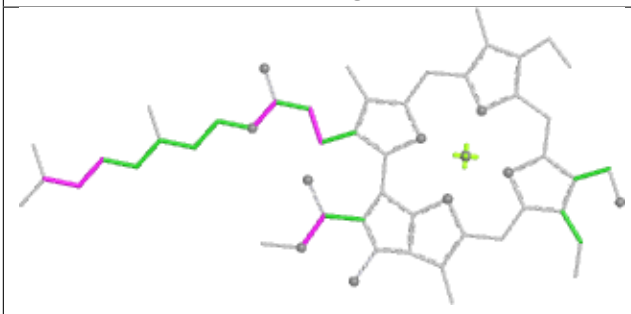
Ligand CHL R 607



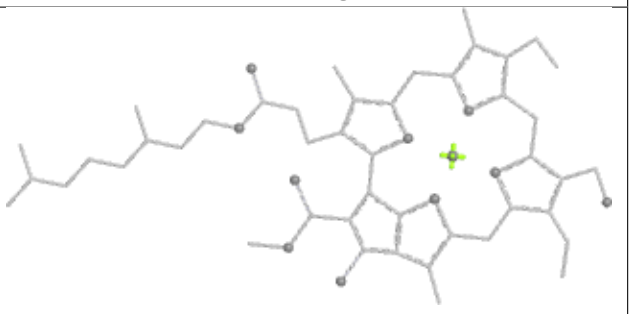
Bond lengths



Bond angles

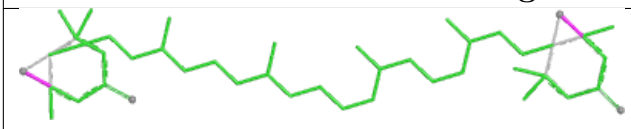


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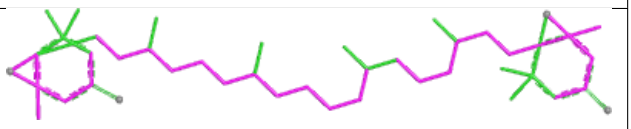


Rings

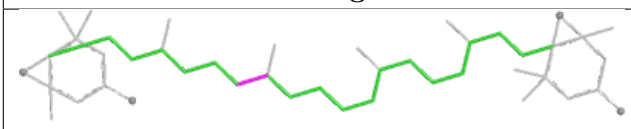
Ligand XAT 5 1622



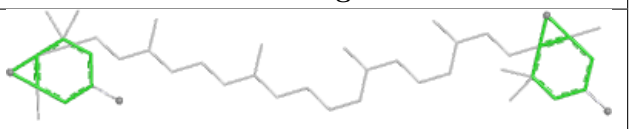
Bond lengths



Bond angles

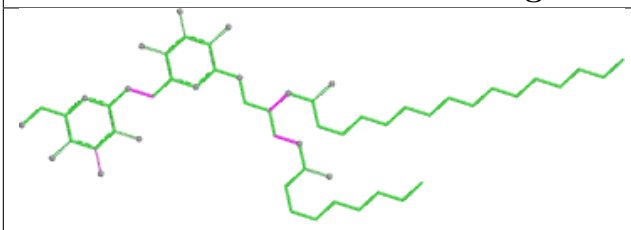


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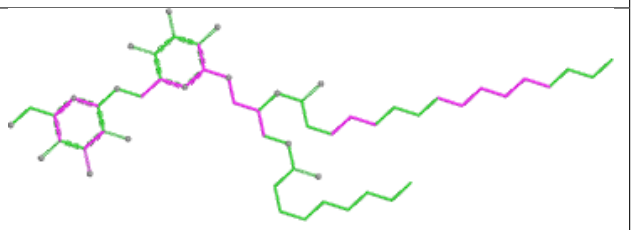


Rings

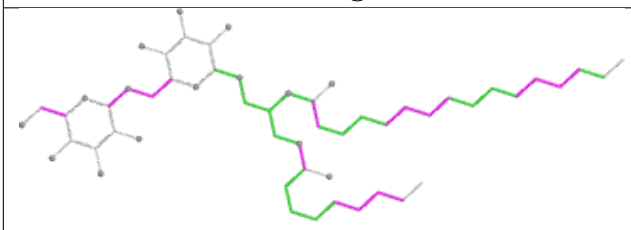
Ligand DGD c 518



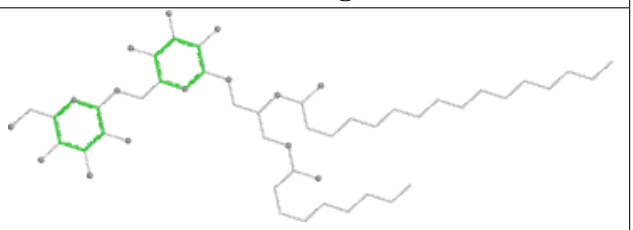
Bond lengths



Bond angles

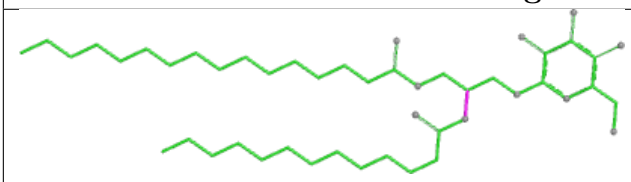


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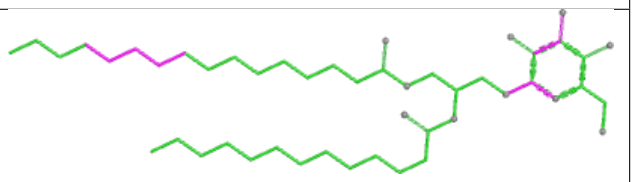


Rings

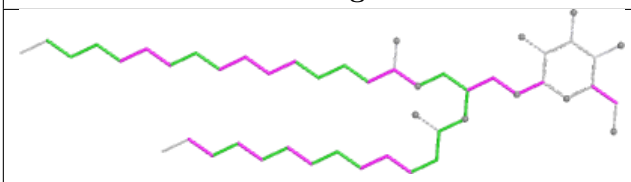
Ligand LMG a 413



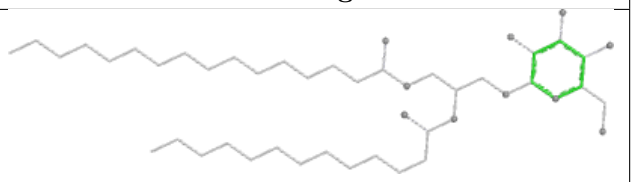
Bond lengths



Bond angles

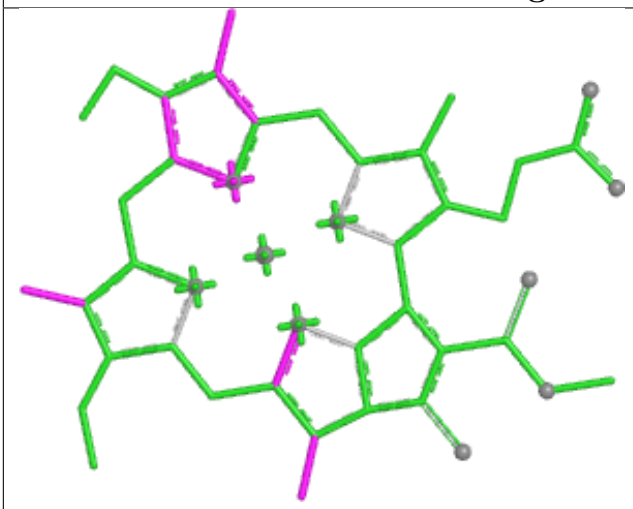


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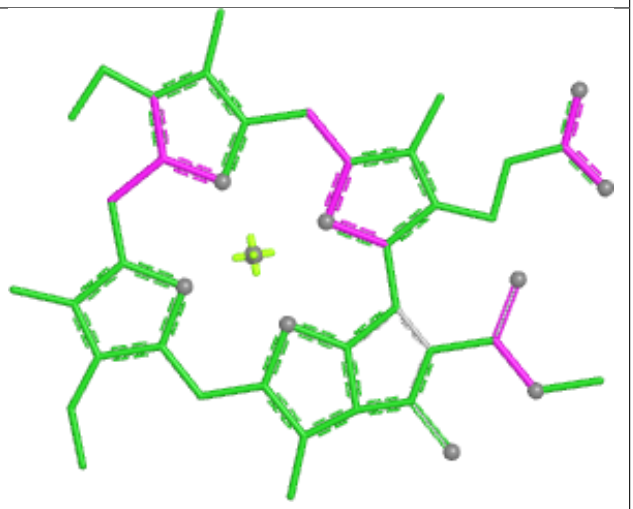


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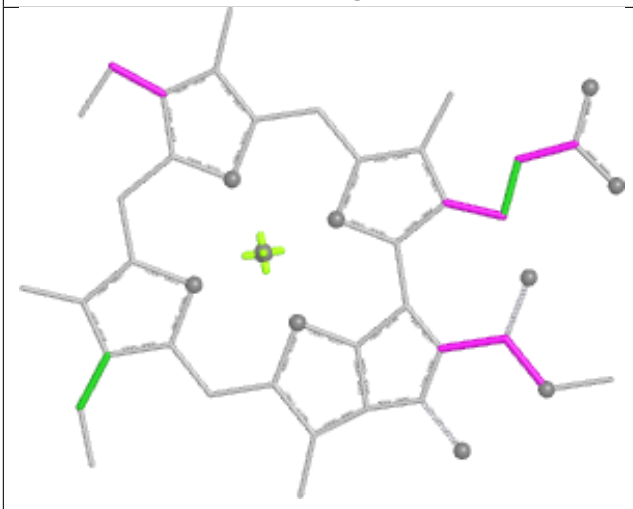
Ligand CLA 8 611



Bond lengths



Bond angles

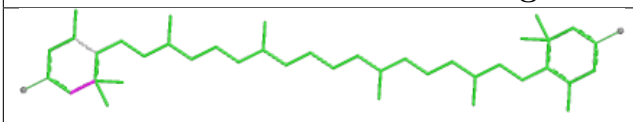


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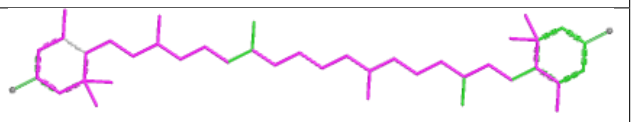


Rings

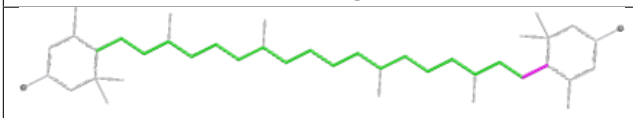
Ligand LUT 3 1620



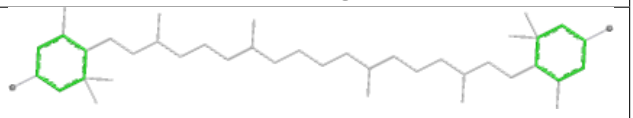
Bond lengths



Bond angles

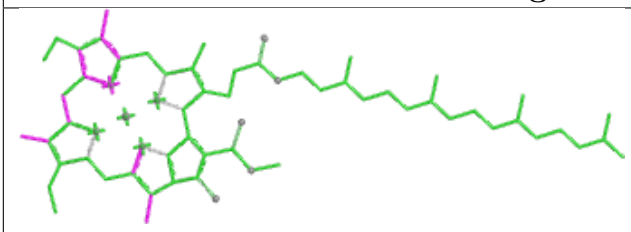


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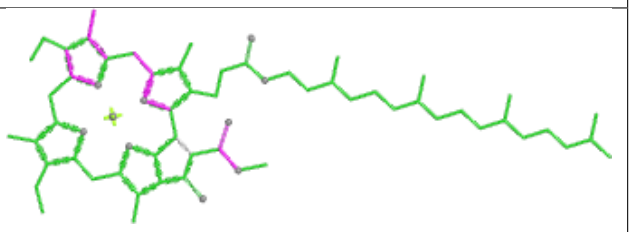


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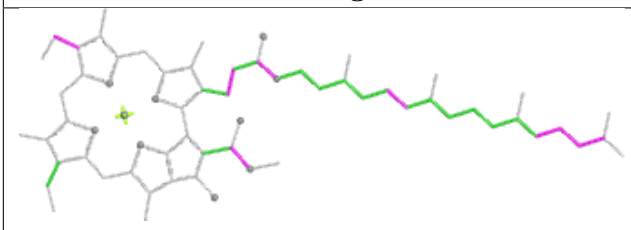
Ligand CLA c 503



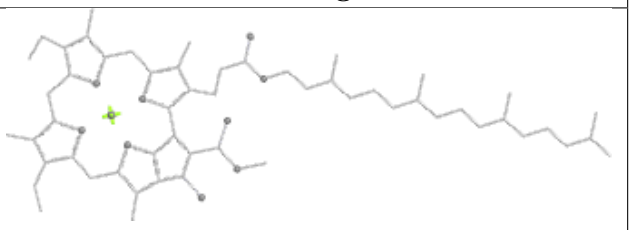
Bond lengths



Bond angles



Torsions

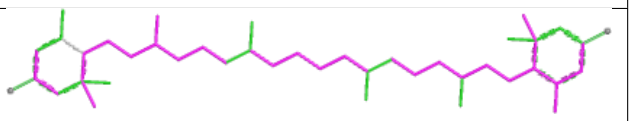


Rings

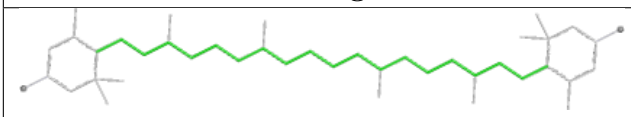
Ligand LUT 6 1621



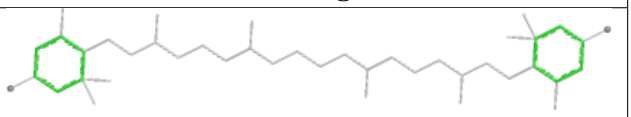
Bond lengths



Bond angles

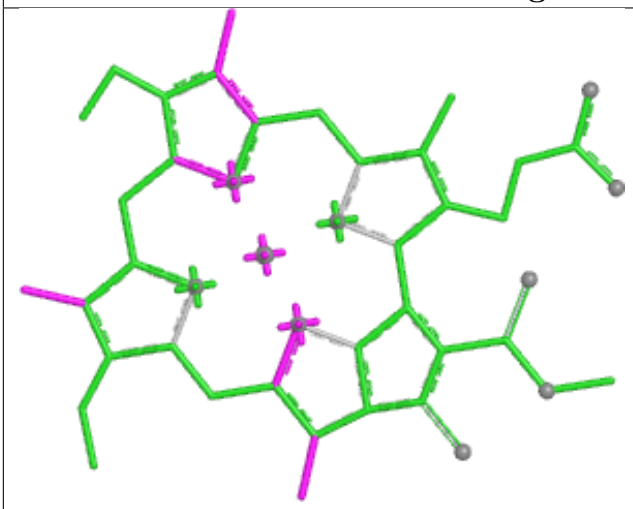


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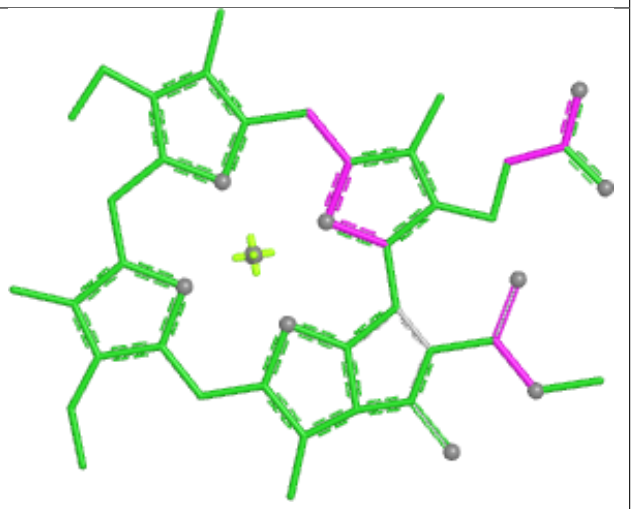


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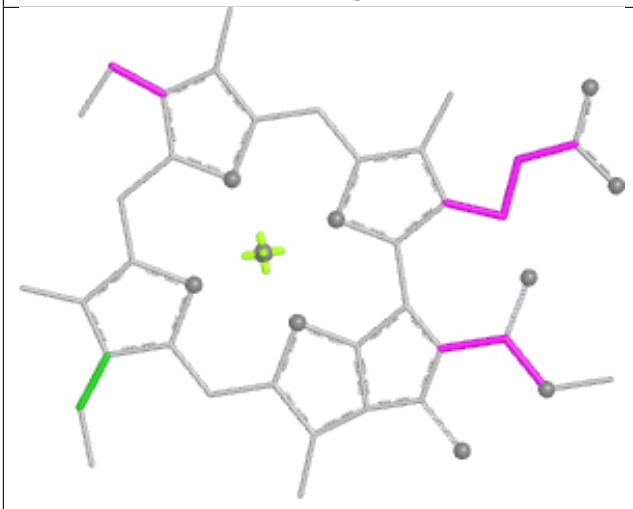
Ligand CLA 3 604



Bond lengths



Bond angles

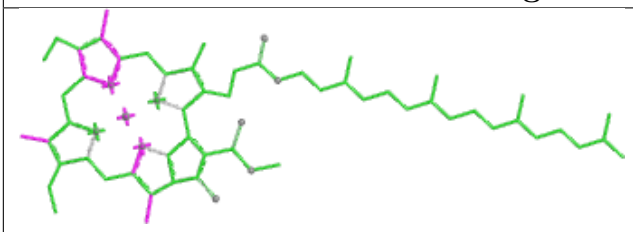


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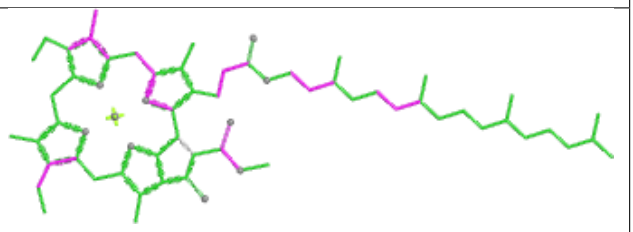


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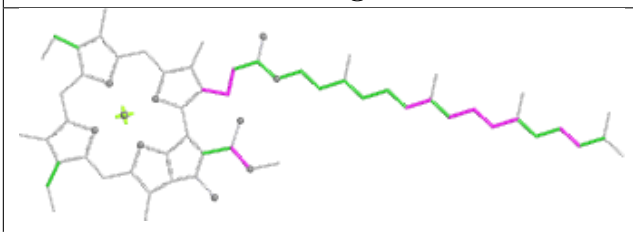
Ligand CLA G 602



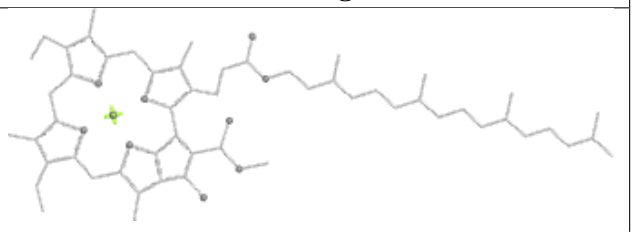
Bond lengths



Bond angles

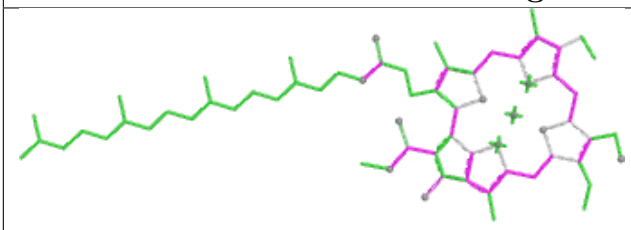


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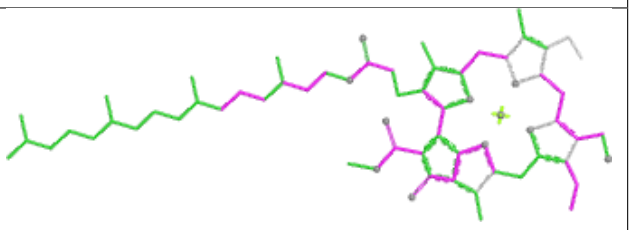


Rings

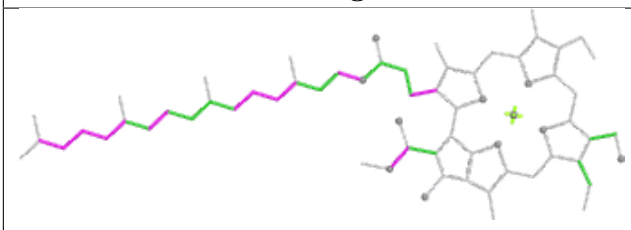
Ligand CHL n 608



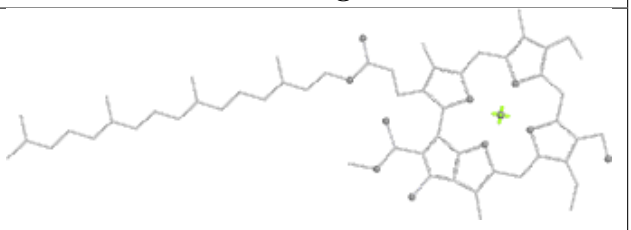
Bond lengths



Bond angles

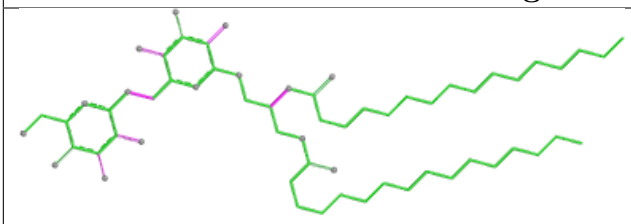


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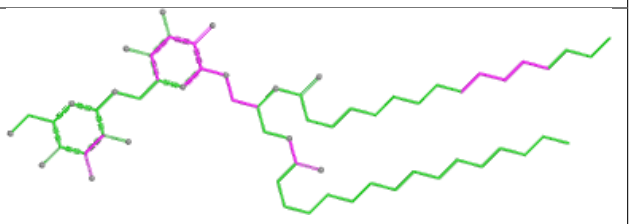


Rings

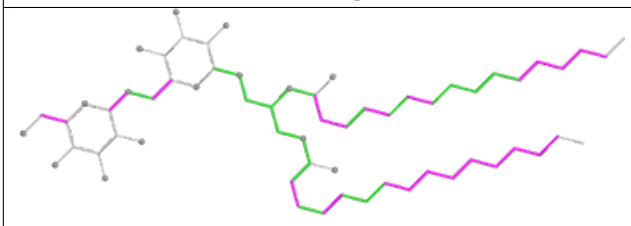
Ligand DGD h 102



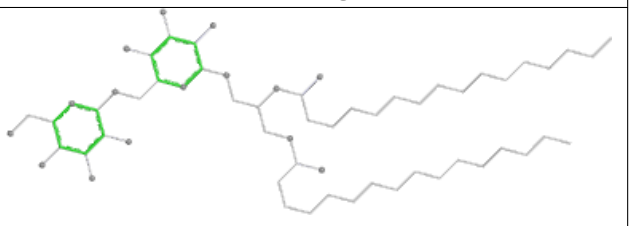
Bond lengths



Bond angles

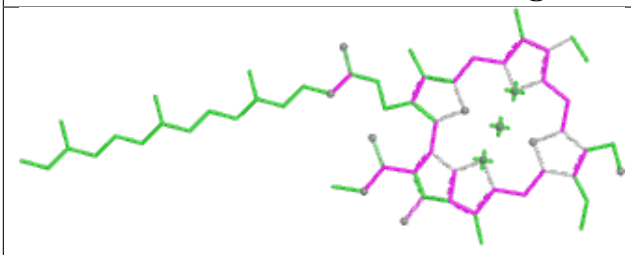


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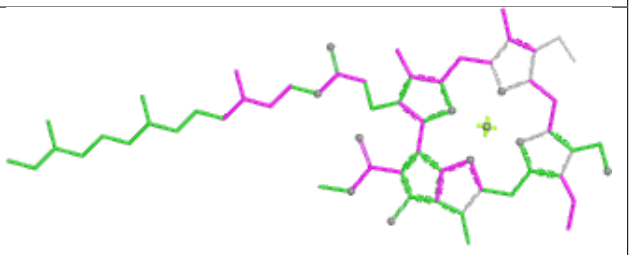


Rings

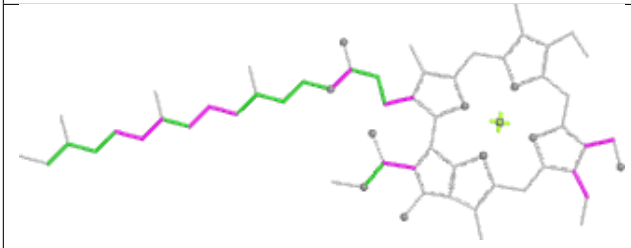
Ligand CHL 5 609



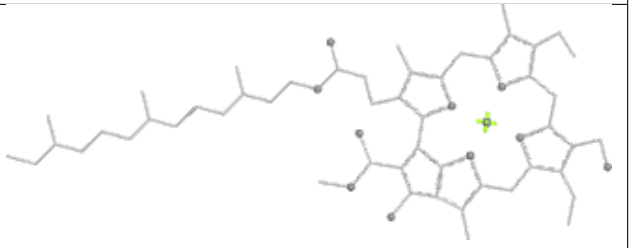
Bond lengths



Bond angles

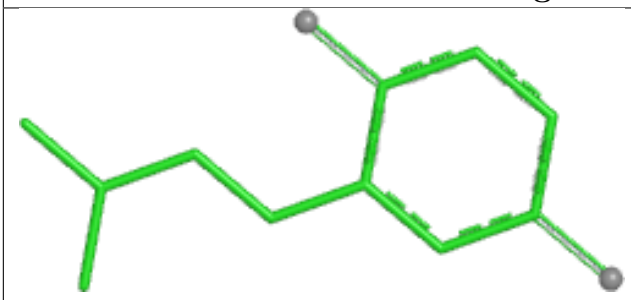


Torsions

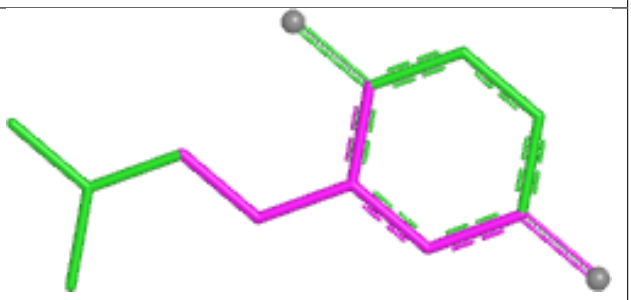


Rings

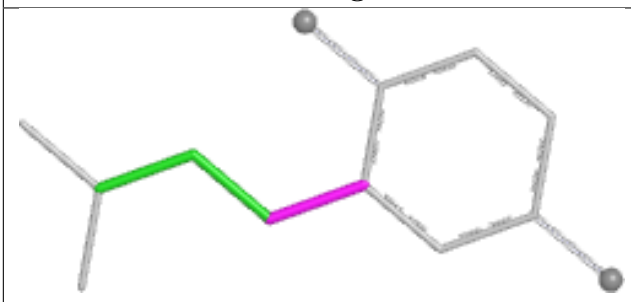
Ligand PL9 a 414



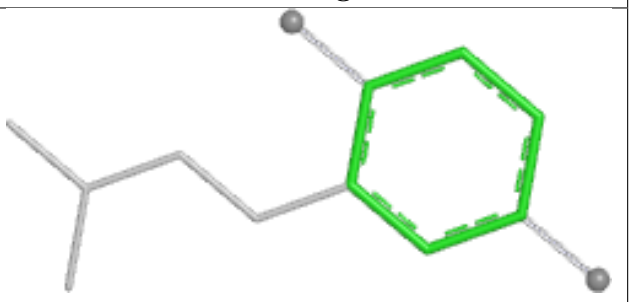
Bond lengths



Bond angles

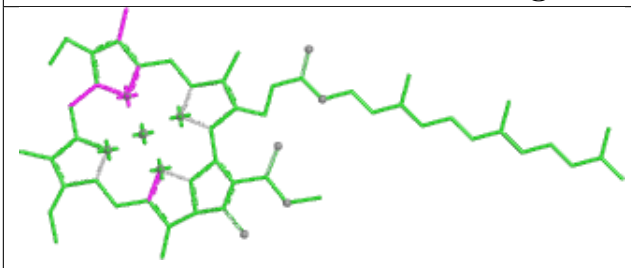


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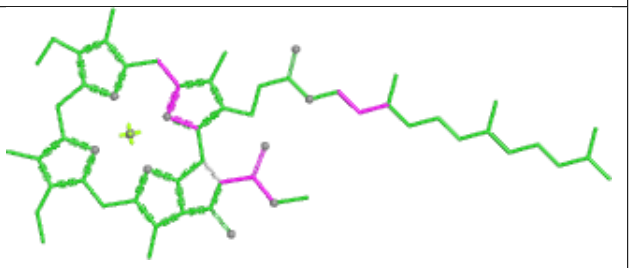


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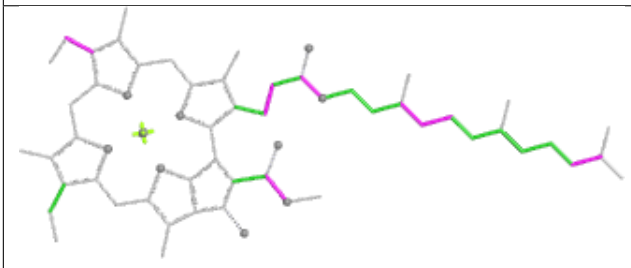
Ligand CLA r 613



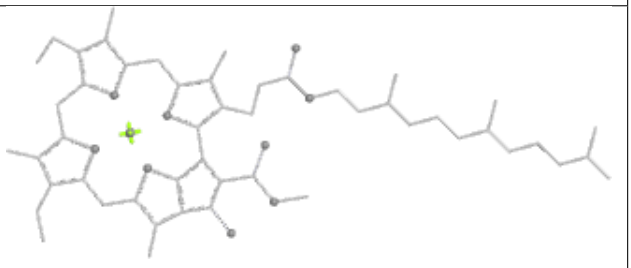
Bond lengths



Bond angles

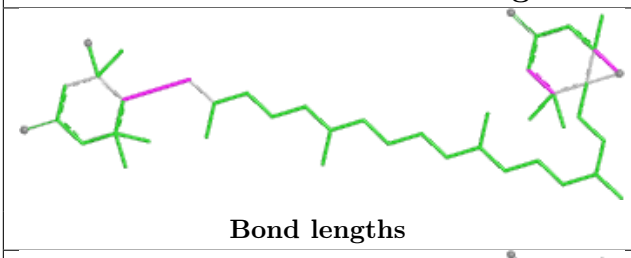


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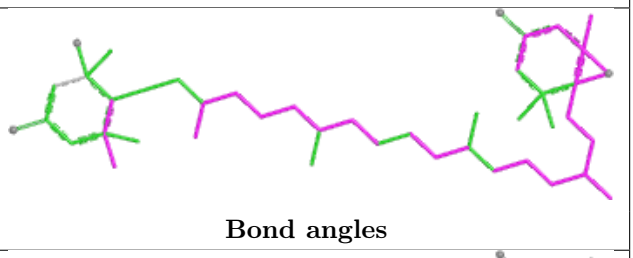


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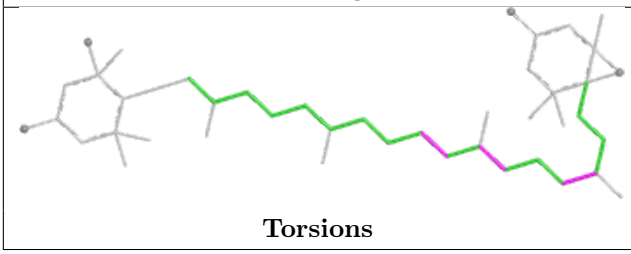
Ligand NEX N 1623



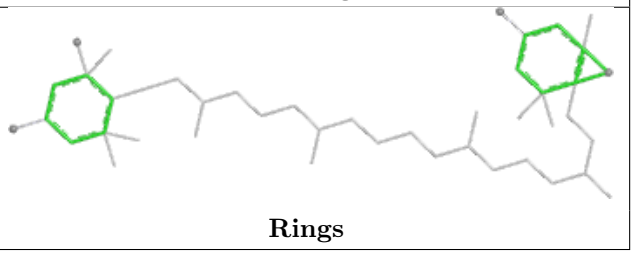
Bond lengths



Bond angles

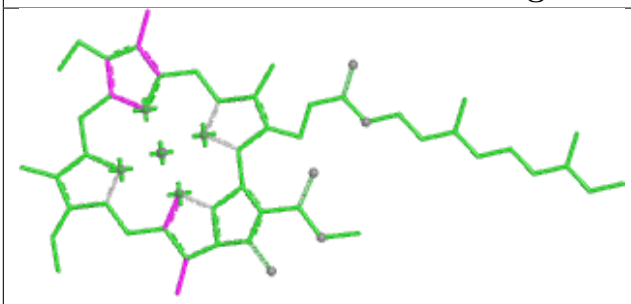


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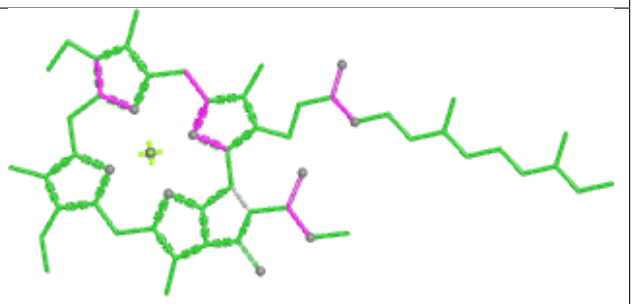


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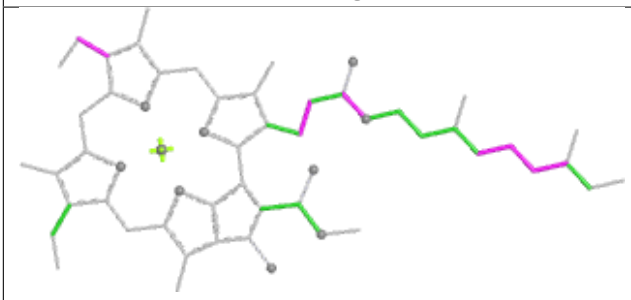
Ligand CLA S 611



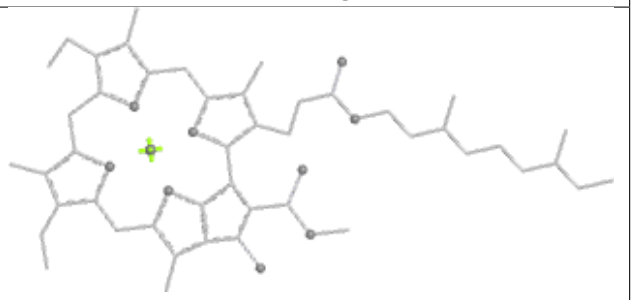
Bond lengths



Bond angles

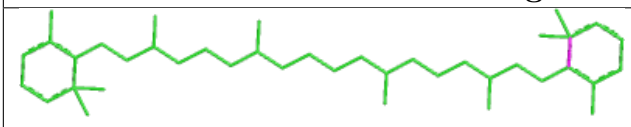


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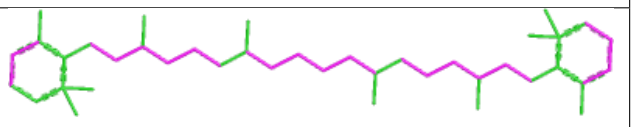


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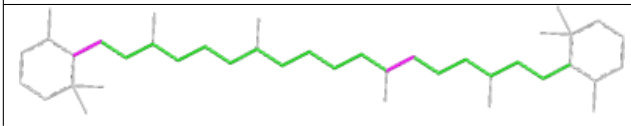
Ligand BCR b 618



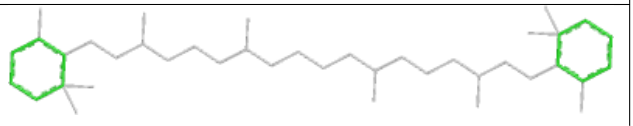
Bond lengths



Bond angles

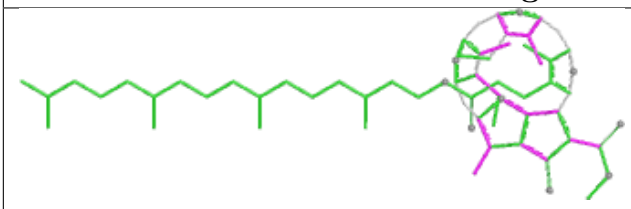


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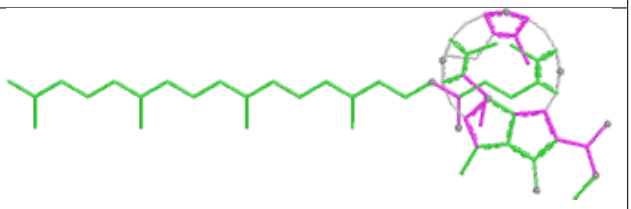


Rings

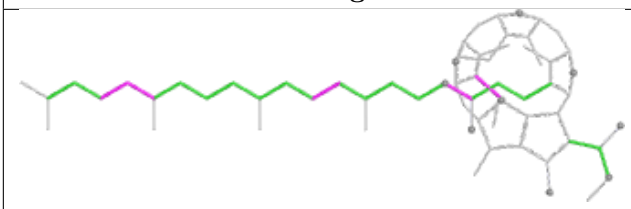
Ligand PHO A 408



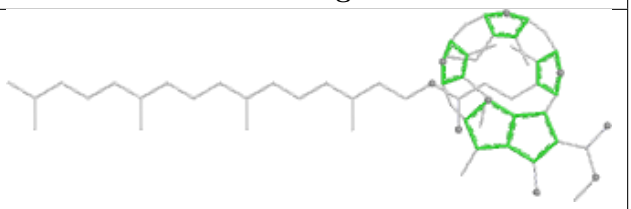
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Bond angles

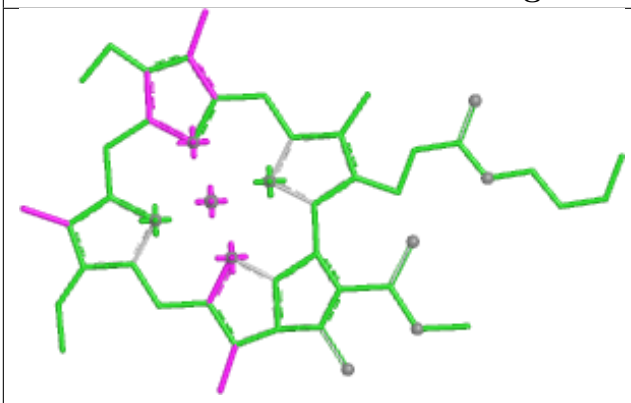


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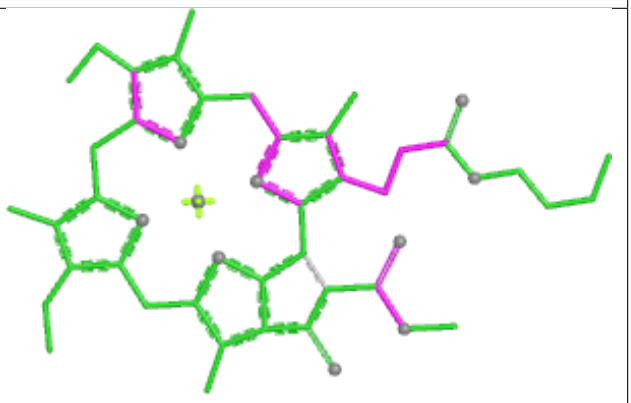


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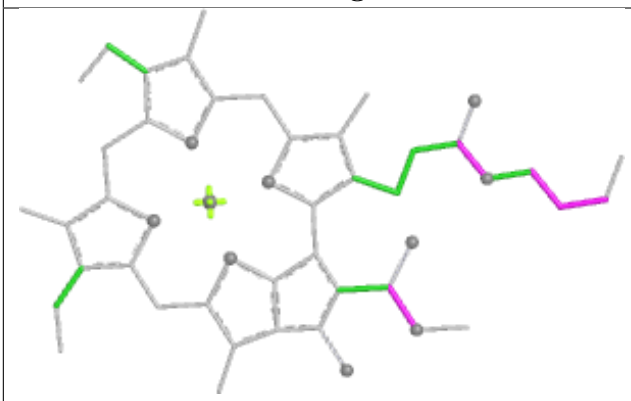
Ligand CLA R 612



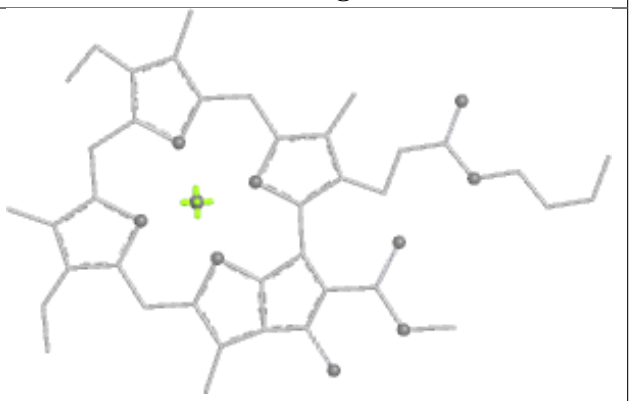
Bond lengths



Bond angles

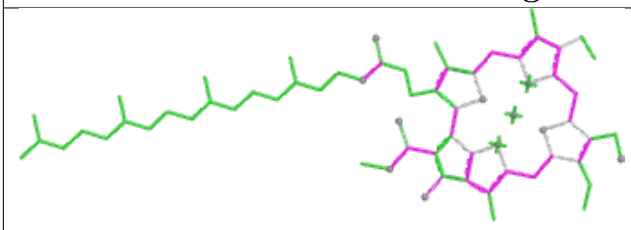


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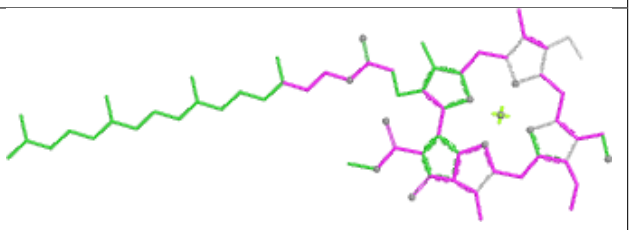


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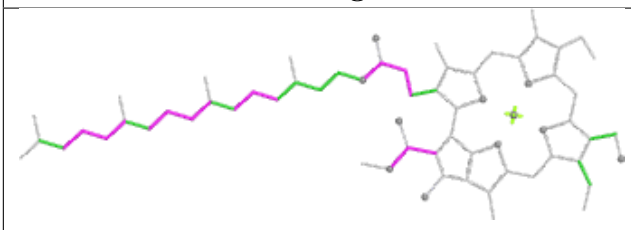
Ligand CHL N 601



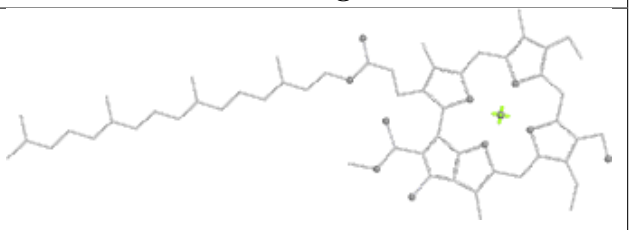
Bond lengths



Bond angles

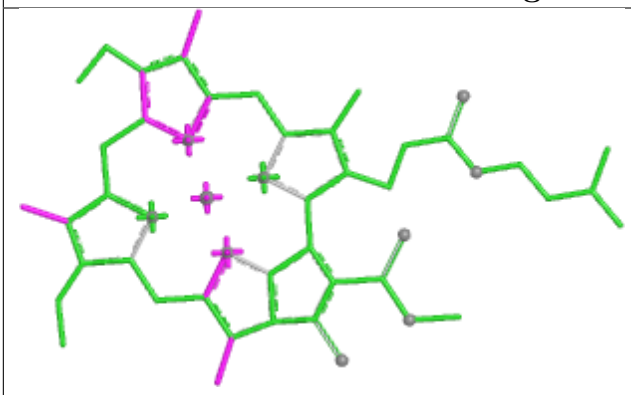


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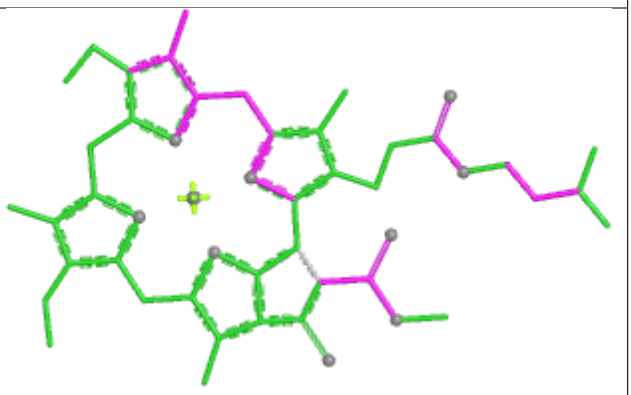


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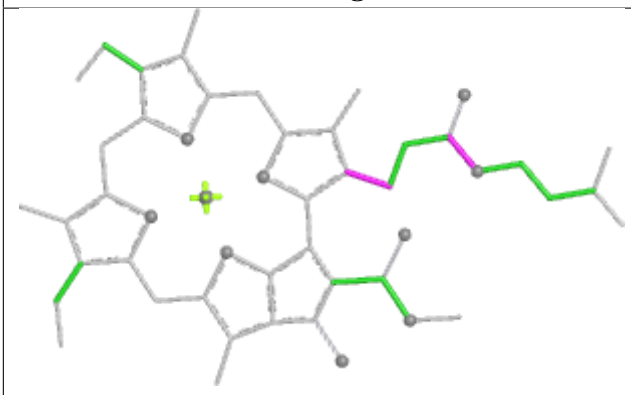
Ligand CLA N 604



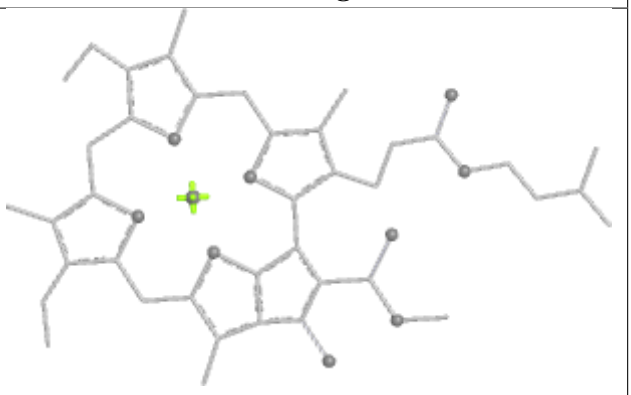
Bond lengths



Bond angles

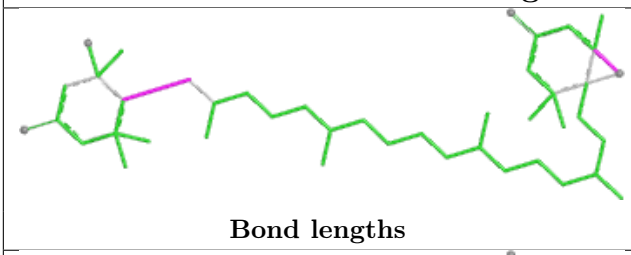


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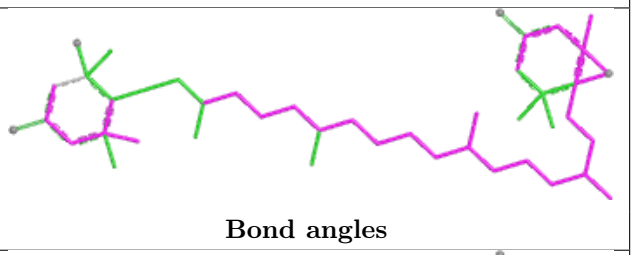


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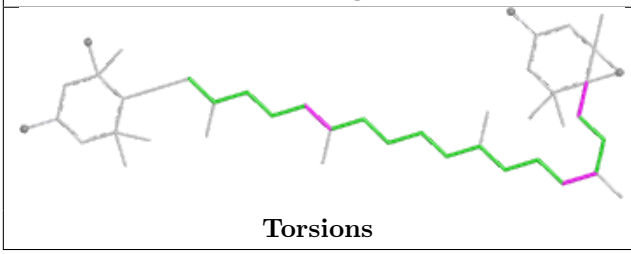
Ligand NEX R 623



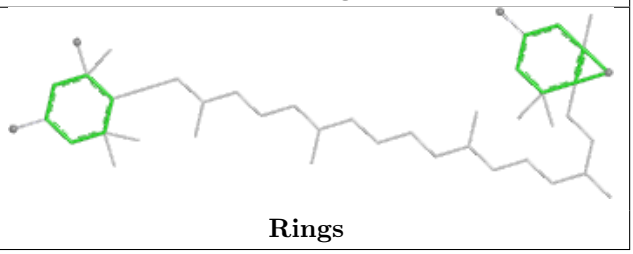
Bond lengths



Bond angles

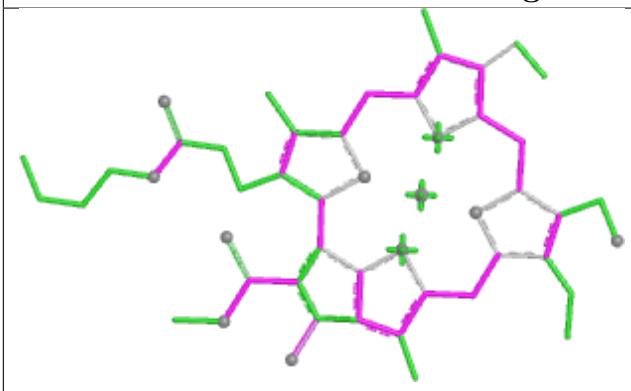


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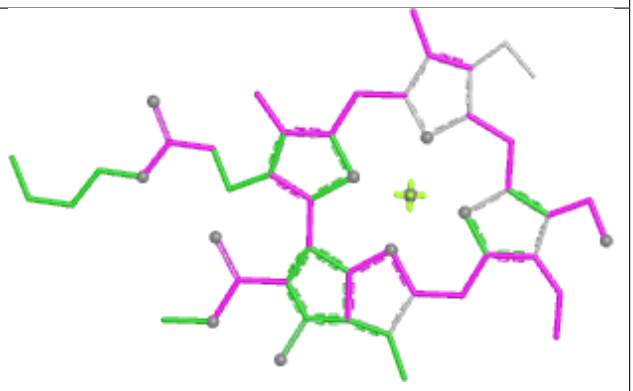


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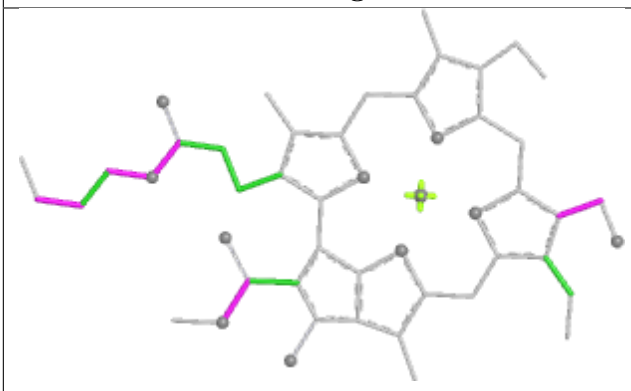
Ligand CHL G 606



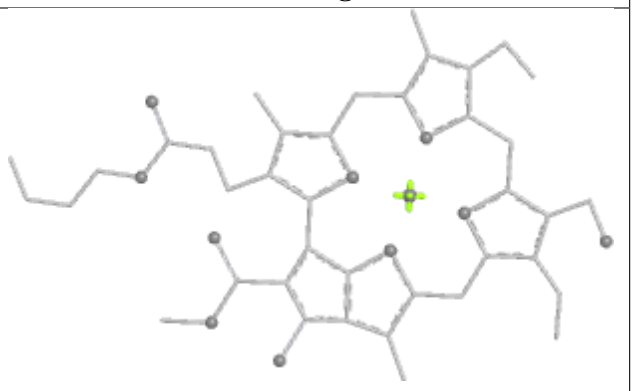
Bond lengths



Bond angles

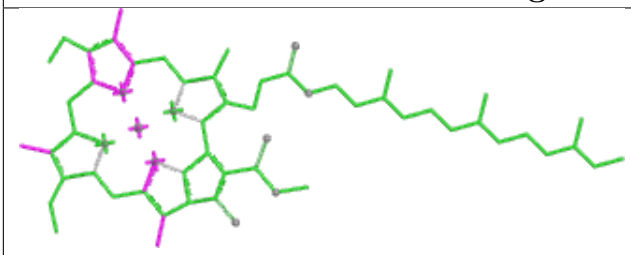


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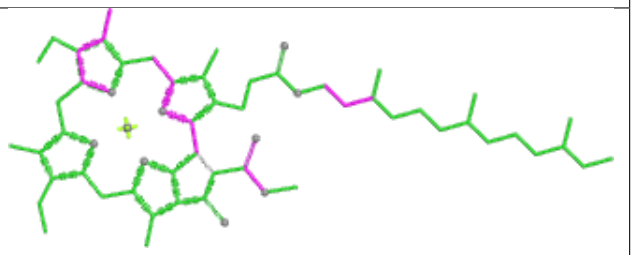


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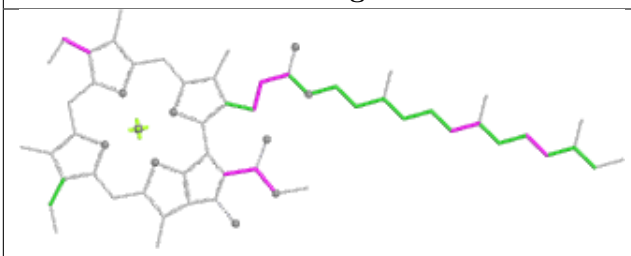
Ligand CLA 1 602



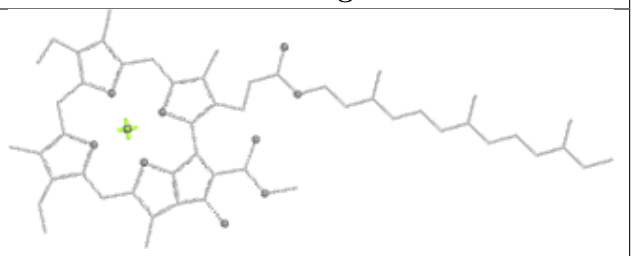
Bond lengths



Bond angles

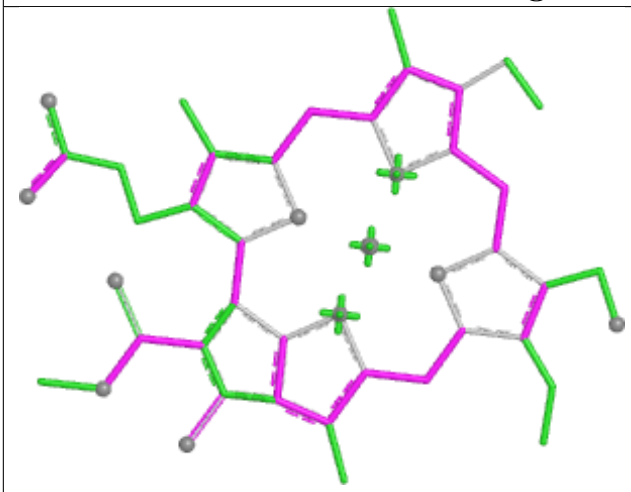


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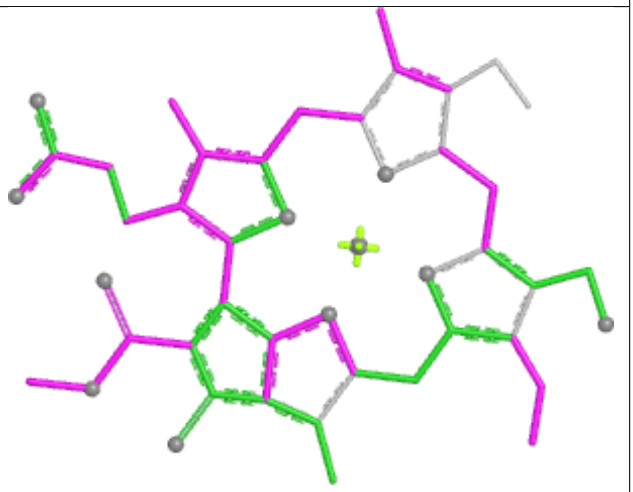


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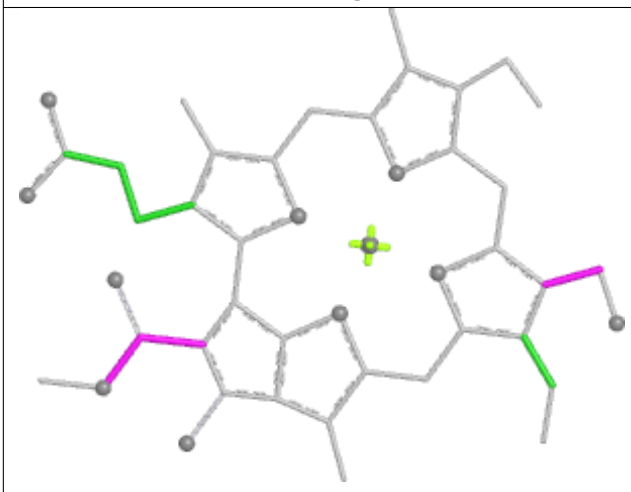
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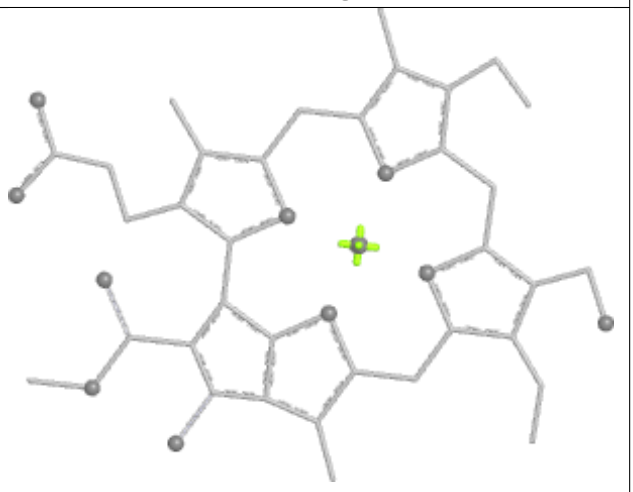
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Bond angles

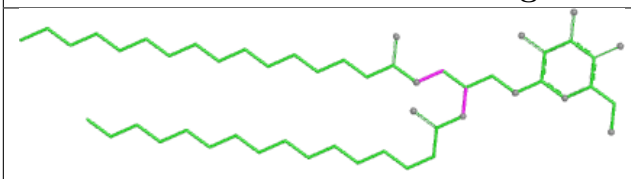


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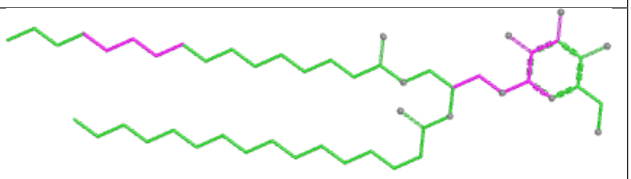


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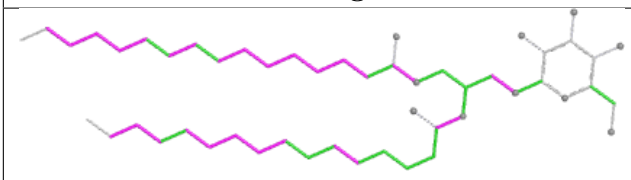
Ligand LMG B 622



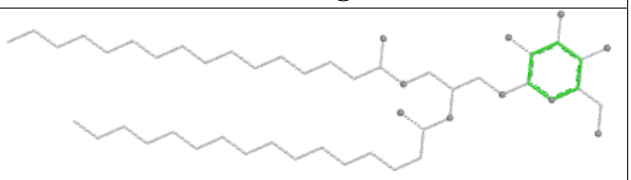
Bond lengths



Bond angles

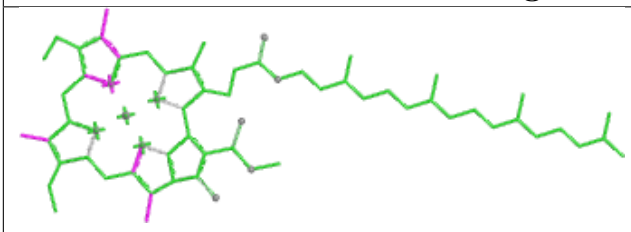


Torsions

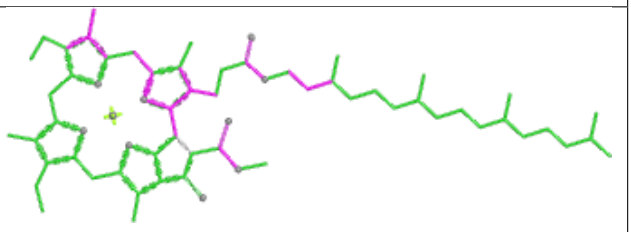


Rings

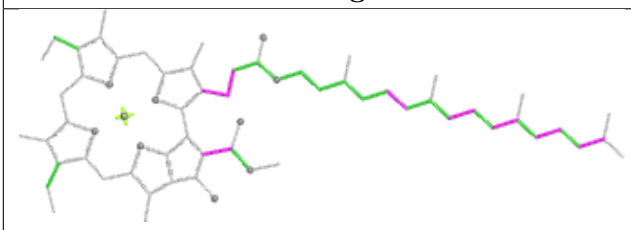
Ligand CLA N 610



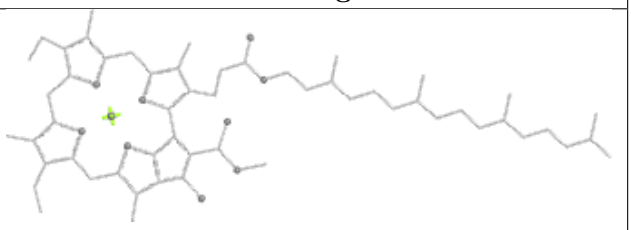
Bond lengths



Bond angles

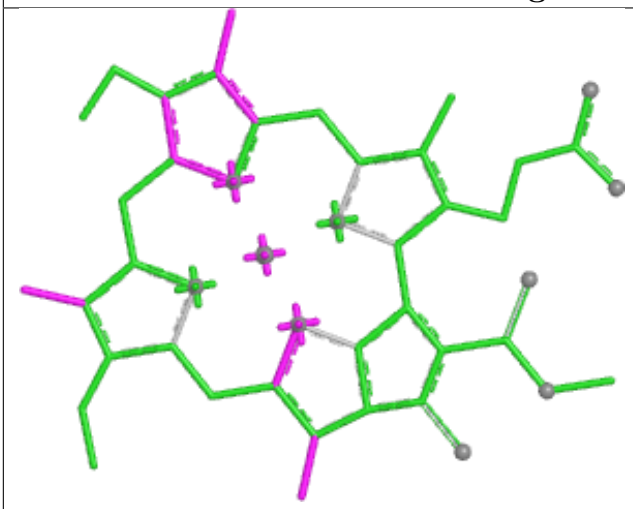


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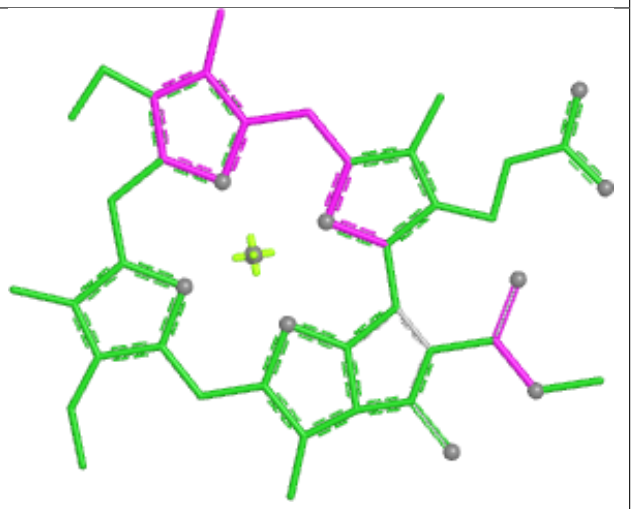


Rings

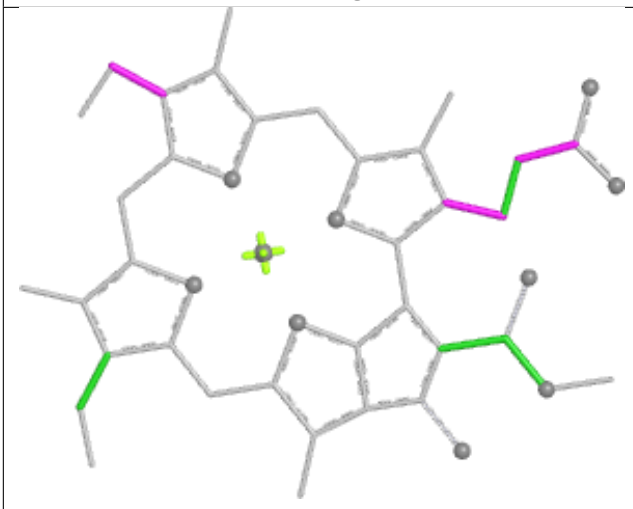
Ligand CLA 8 610



Bond lengths



Bond angles

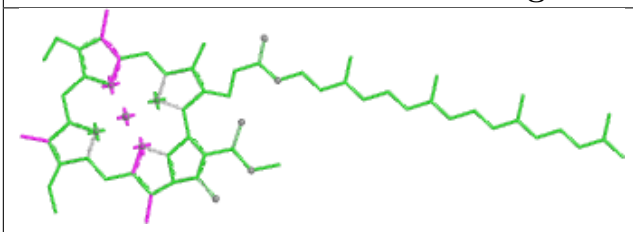


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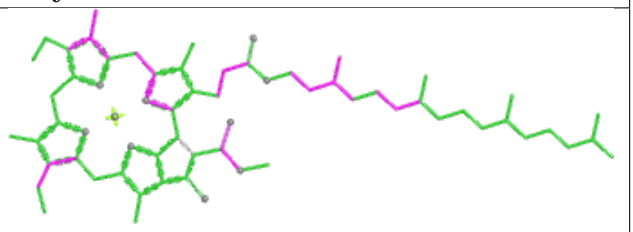


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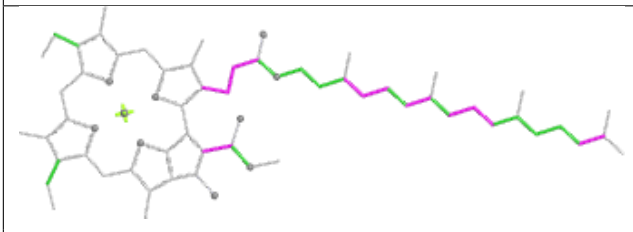
Ligand CLA y 602



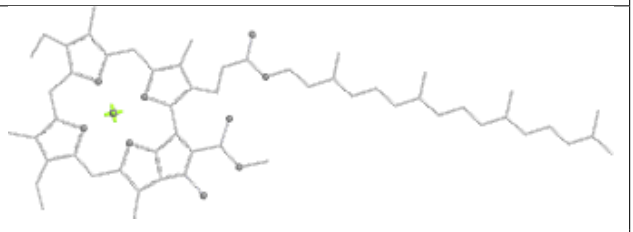
Bond lengths



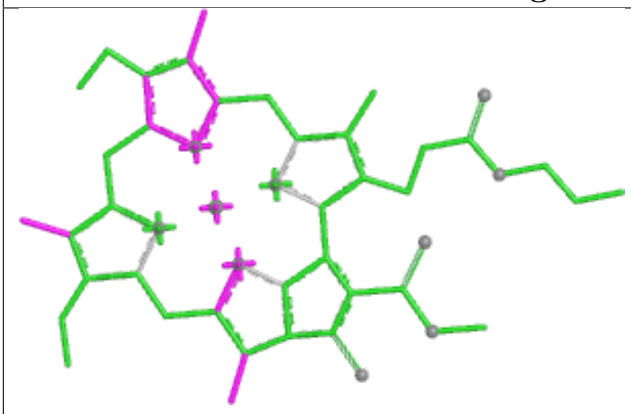
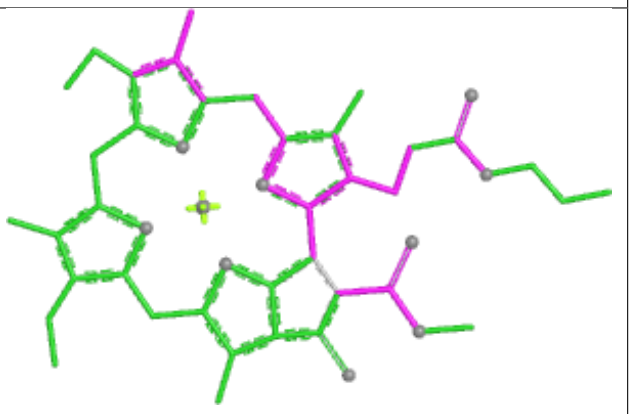
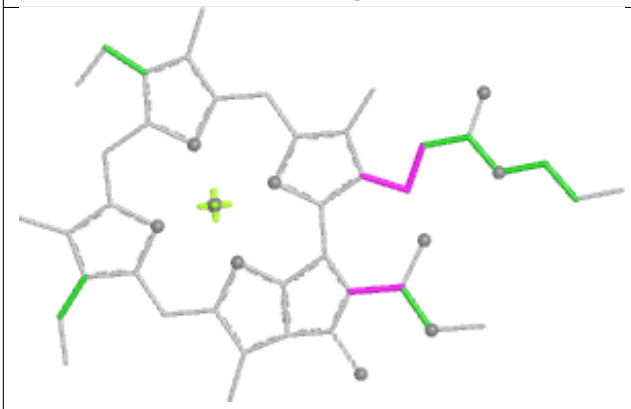
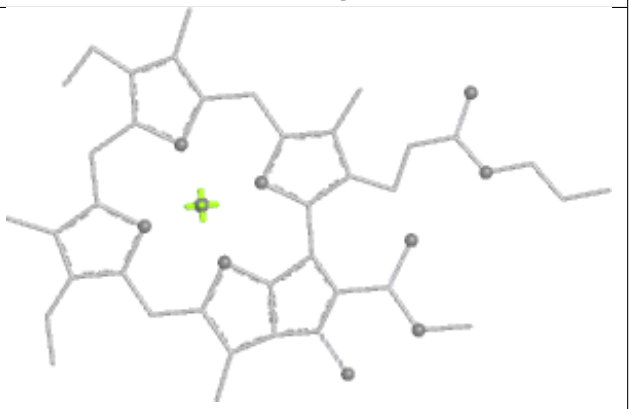
Bond angles

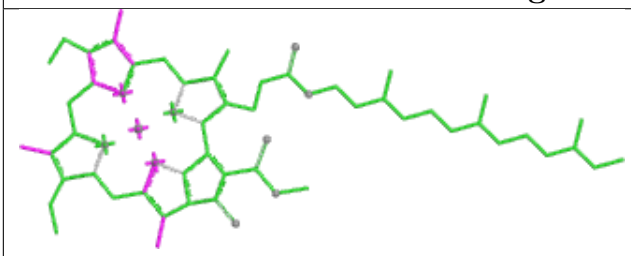
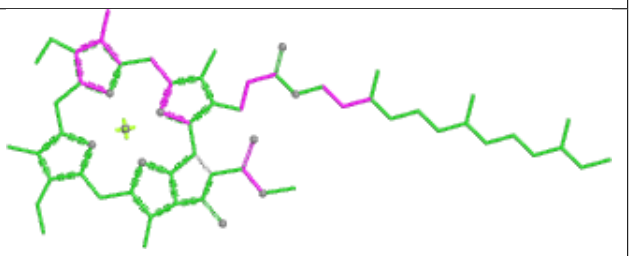
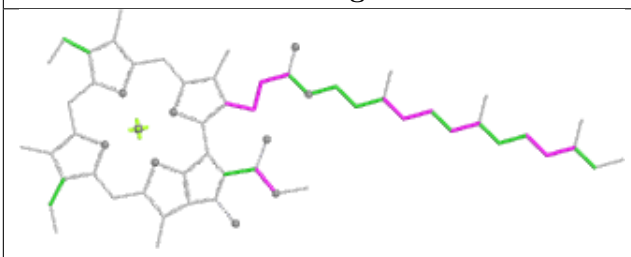
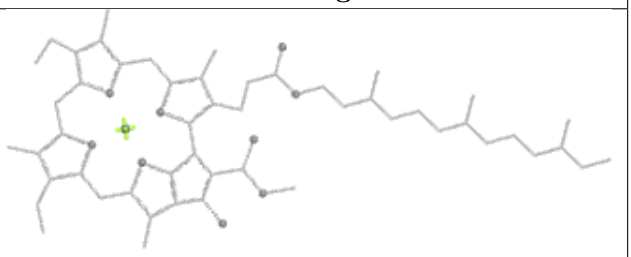


Torsions

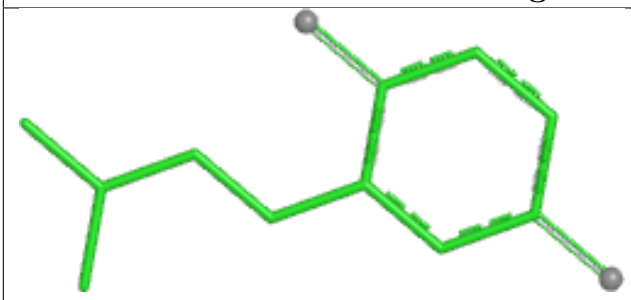


Rings

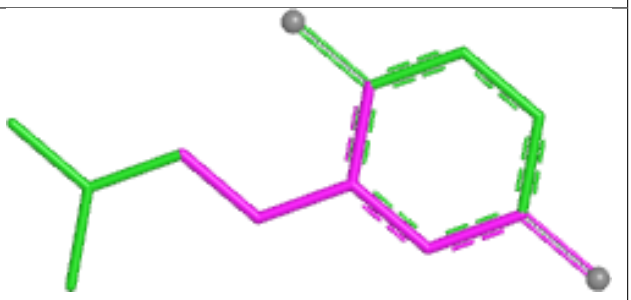
Ligand CLA r 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

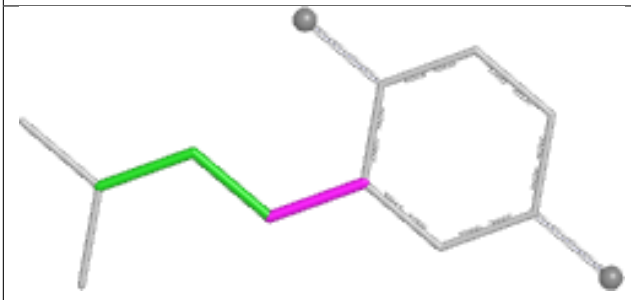
Ligand PL9 A 414



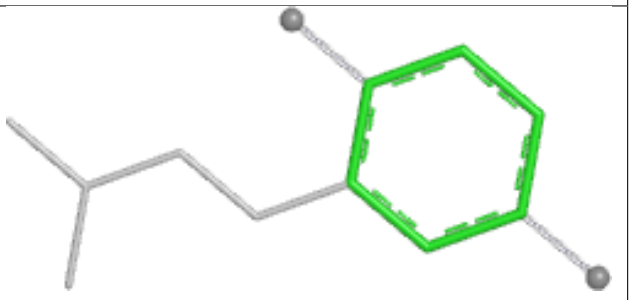
Bond lengths



Bond angles

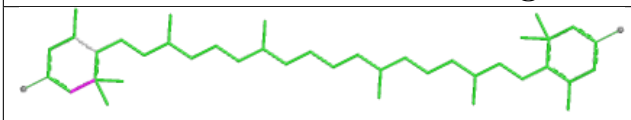


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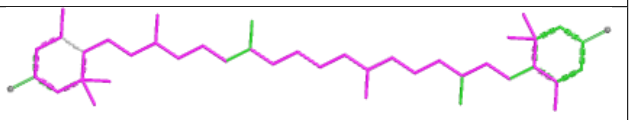


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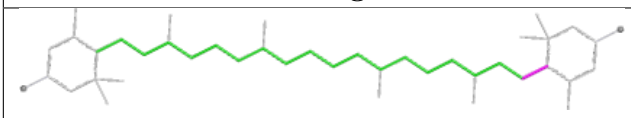
Ligand LUT 7 1620



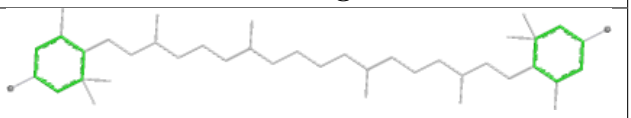
Bond lengths



Bond angles

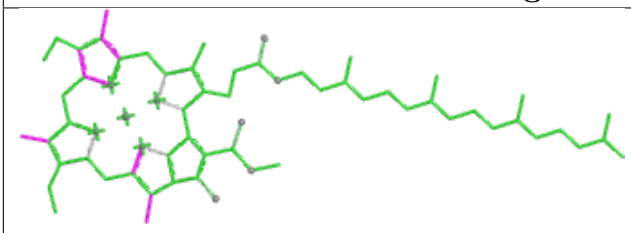


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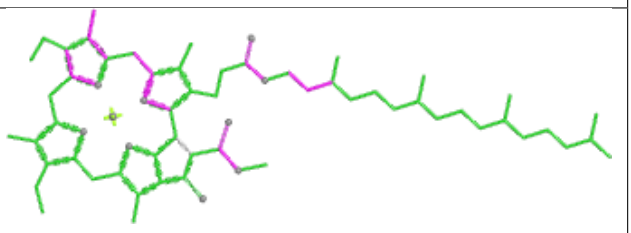


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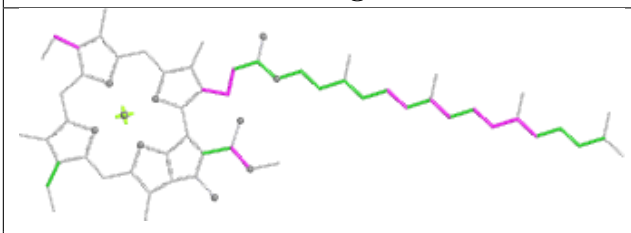
Ligand CLA R 610



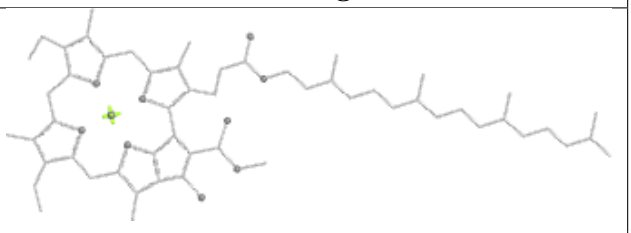
Bond lengths



Bond angles

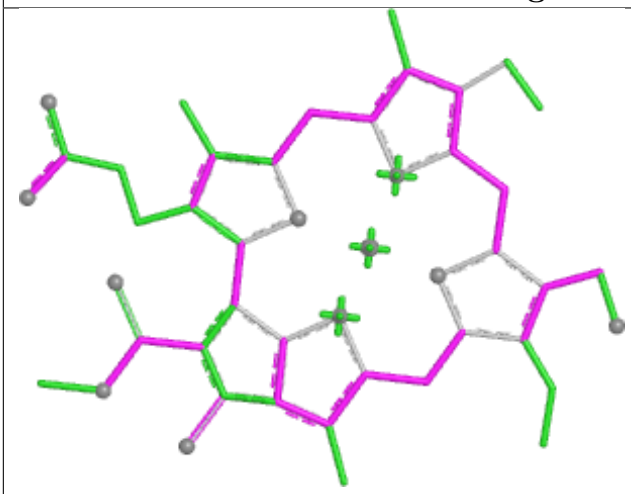


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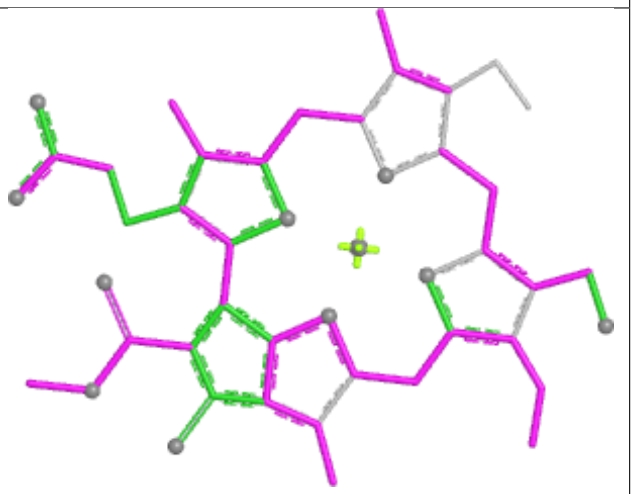


Rings

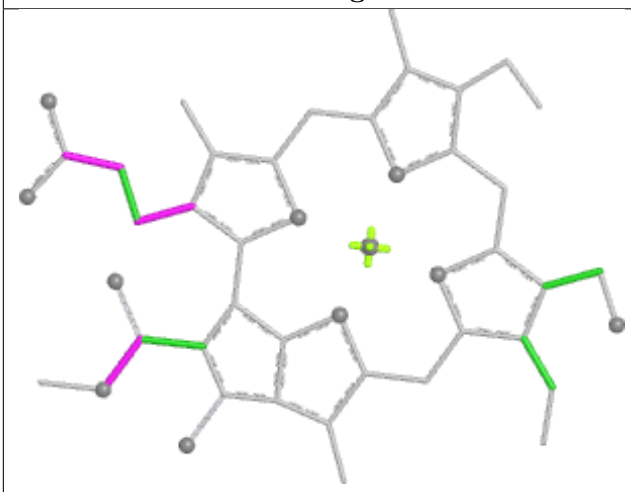
Ligand CHL 6 601



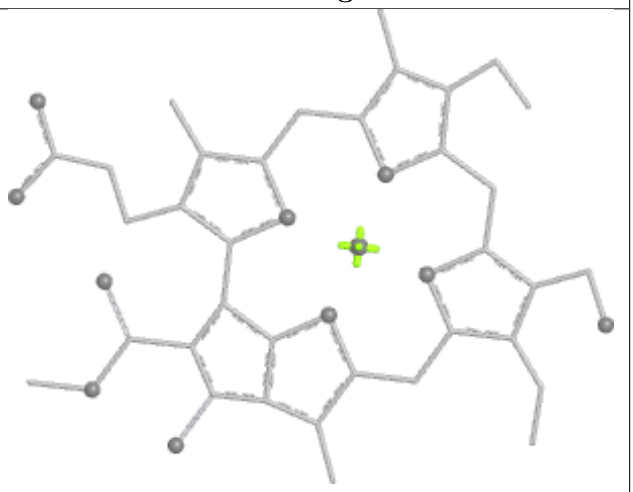
Bond lengths



Bond angles

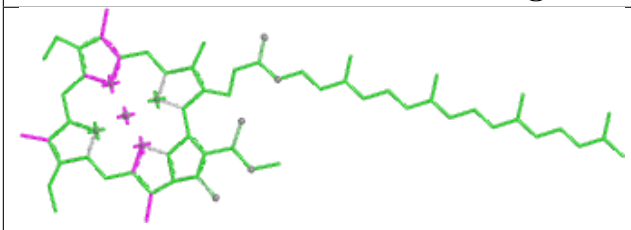


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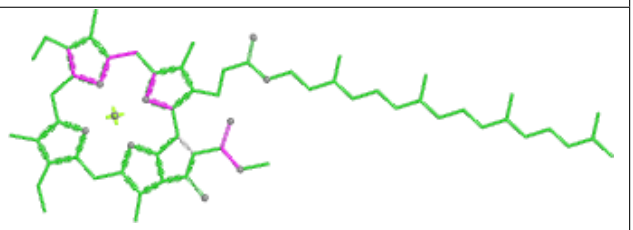


Rings

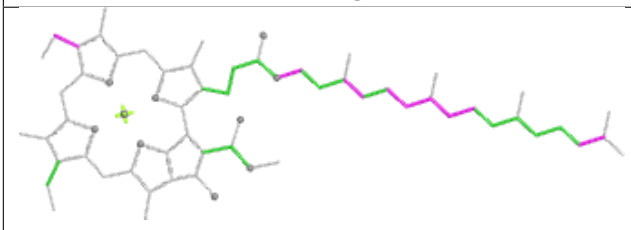
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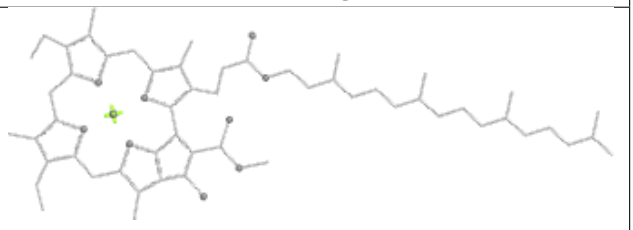
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Bond angles

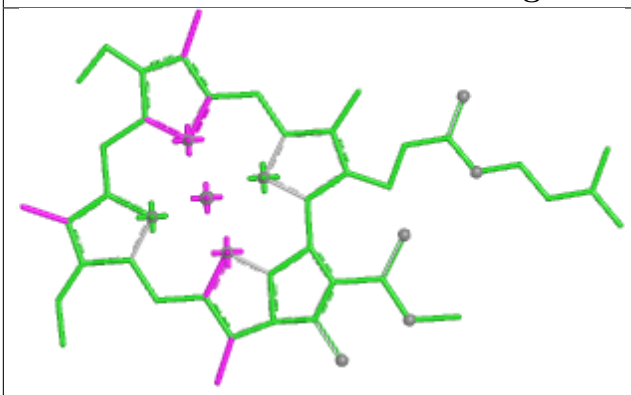


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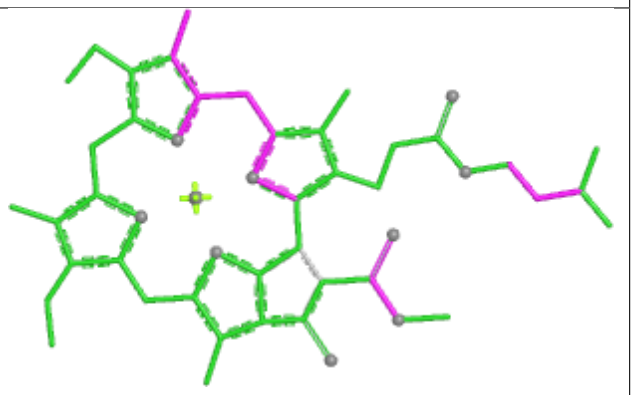


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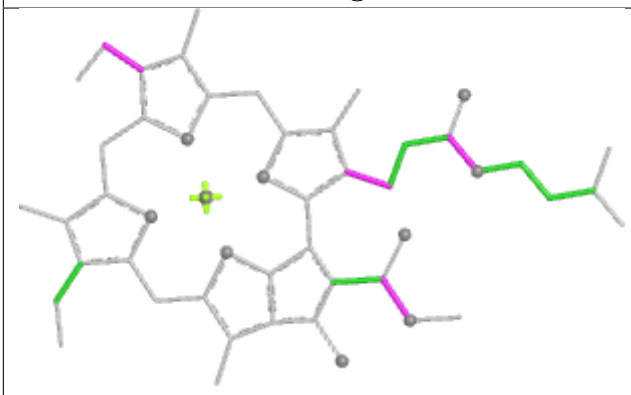
Ligand CLA G 604



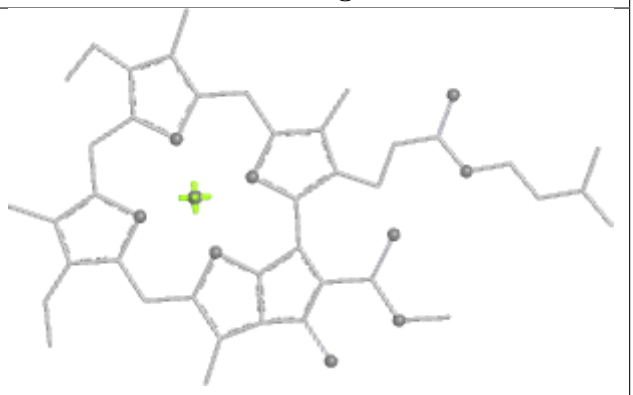
Bond lengths



Bond angles

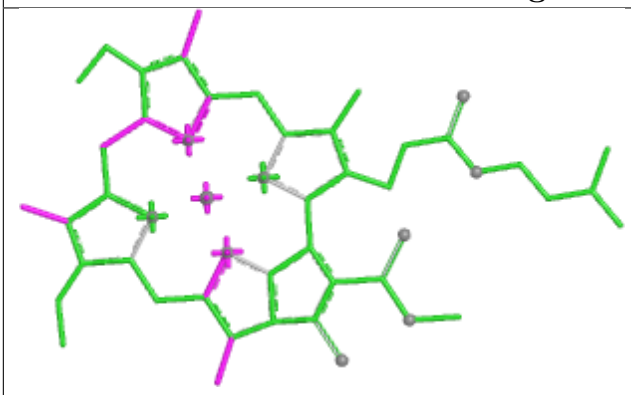


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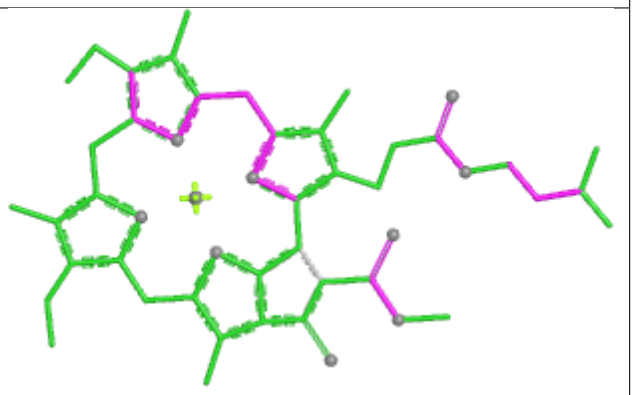


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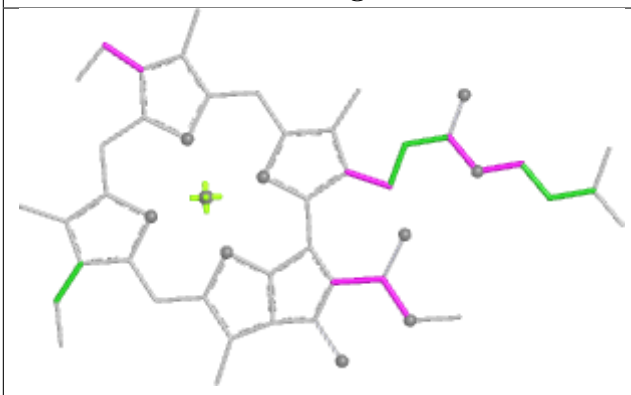
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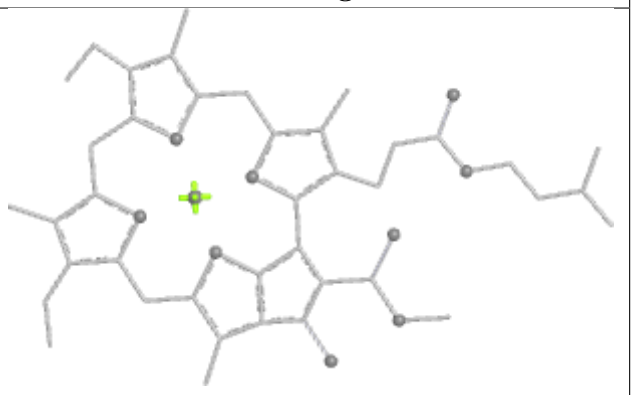
Bond lengths



Bond angles

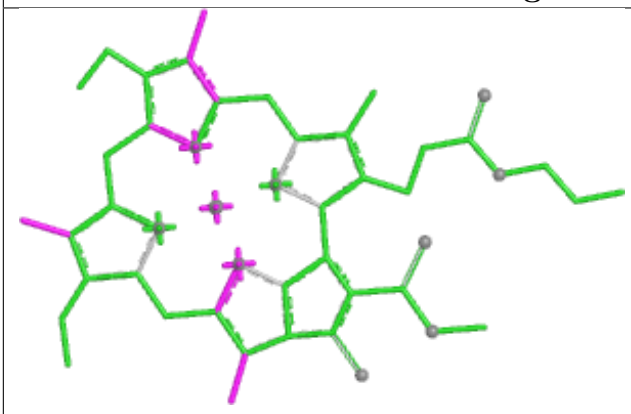


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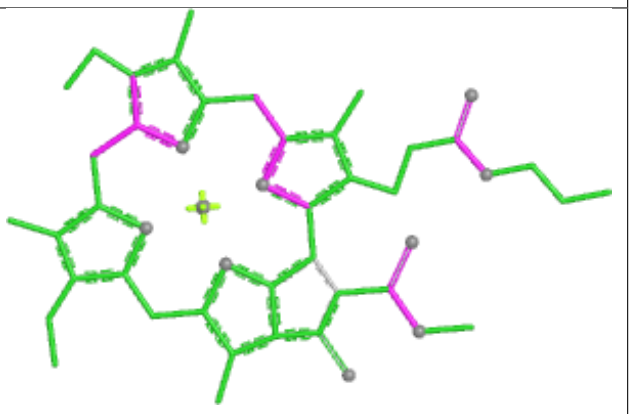


Rings

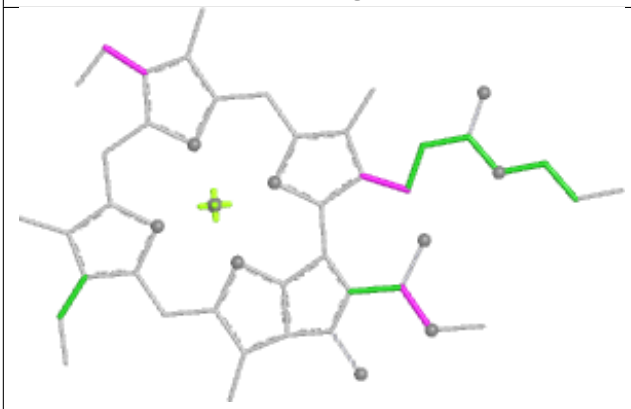
Ligand CLA Y 614



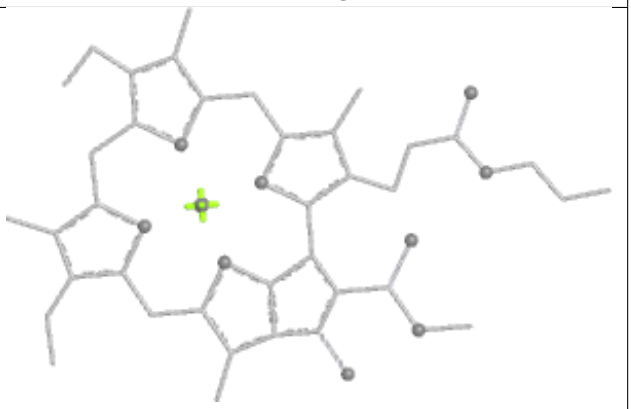
Bond lengths



Bond angles

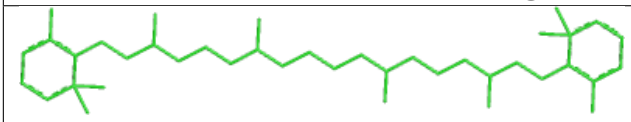


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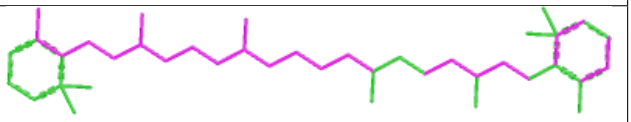


Rings

Ligand BCR C 516



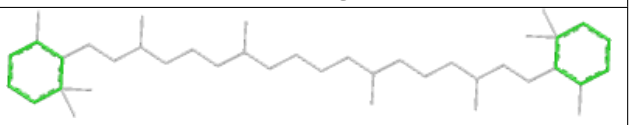
Bond lengths



Bond angles

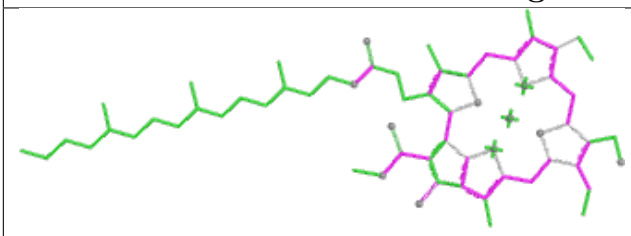


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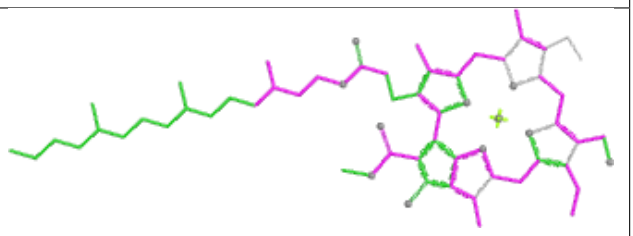


Rings

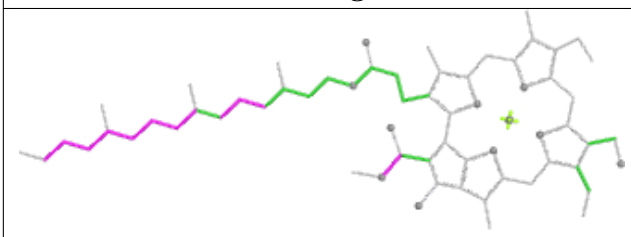
Ligand CHL 7 601



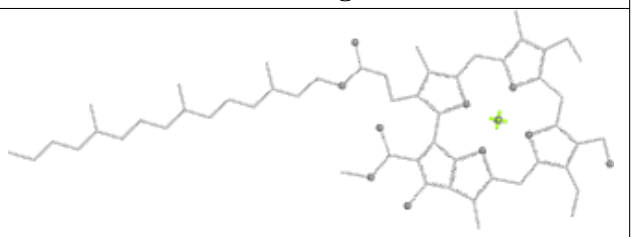
Bond lengths



Bond angles

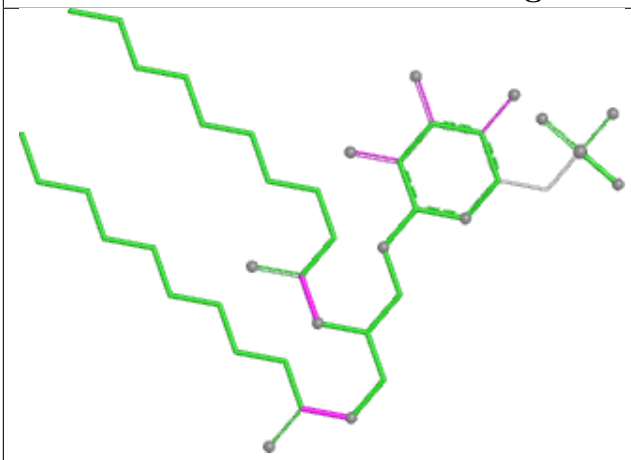


Torsions

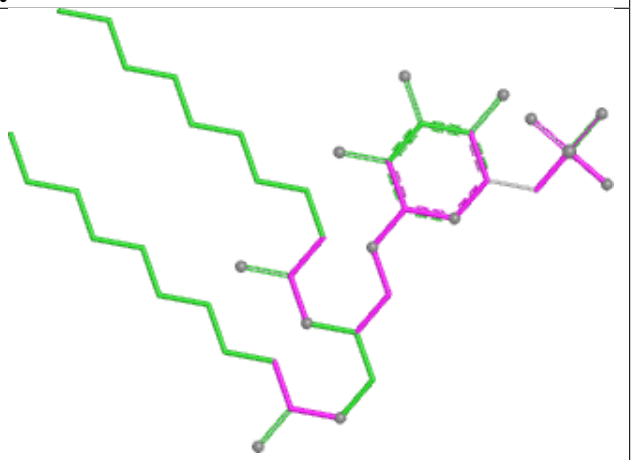


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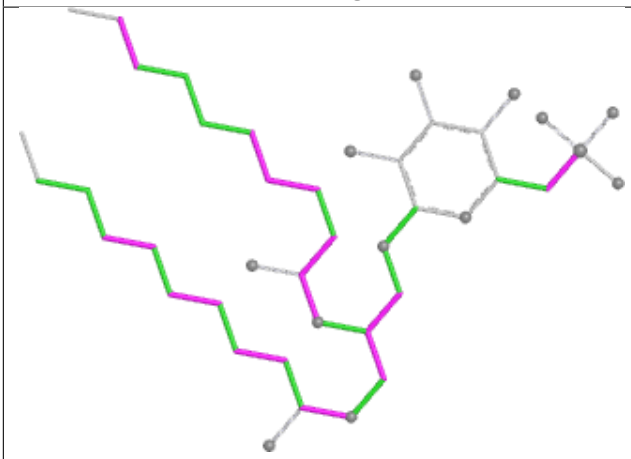
Ligand SQD B 623



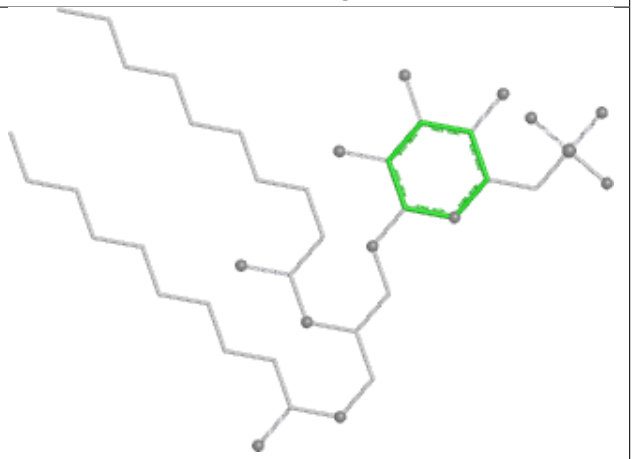
Bond lengths



Bond angles

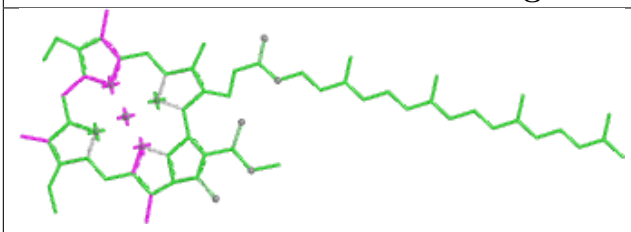


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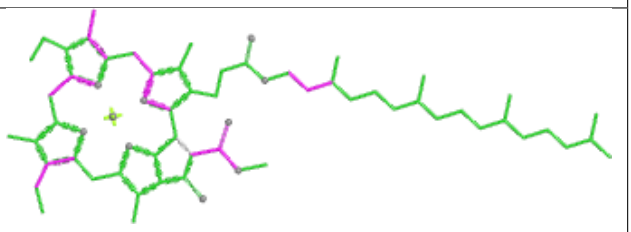


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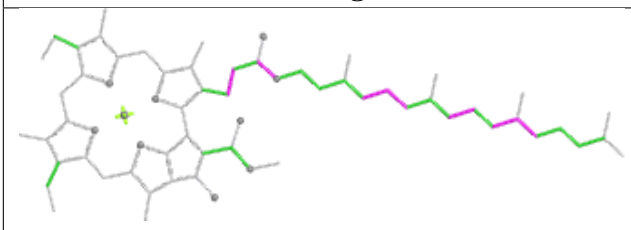
Ligand CLA Y 613



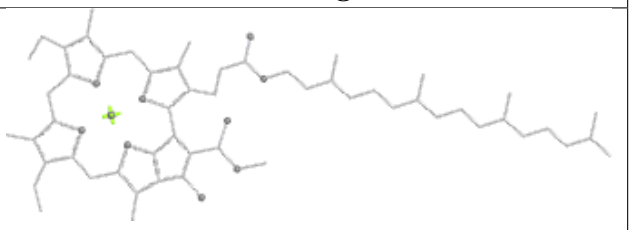
Bond lengths



Bond angles



Torsions

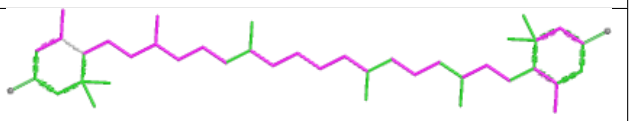


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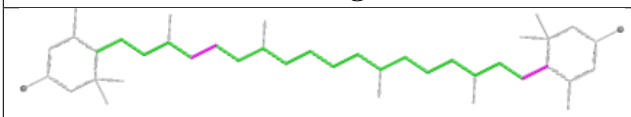
Ligand LUT 7 1621



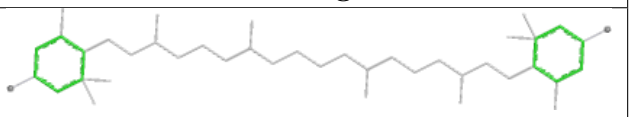
Bond lengths



Bond angles

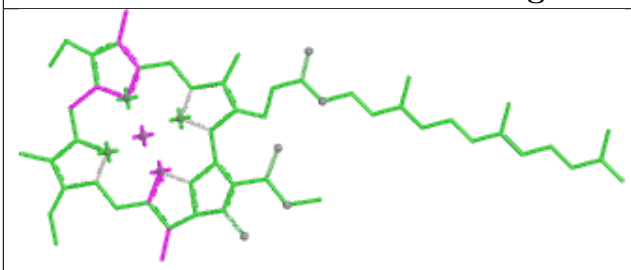


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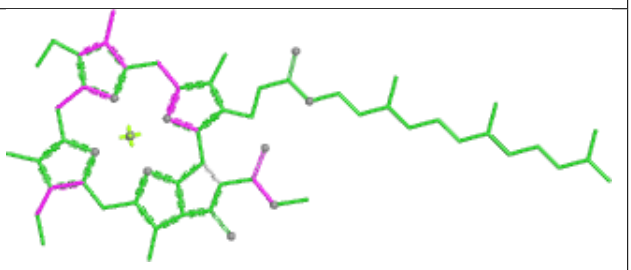


Rings

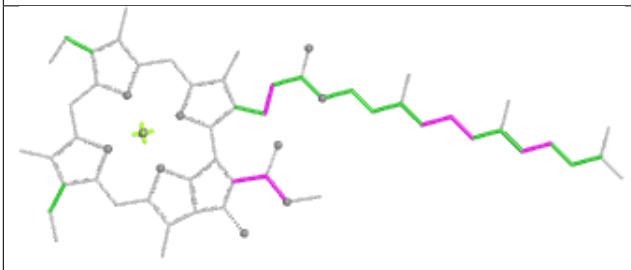
Ligand CLA n 613



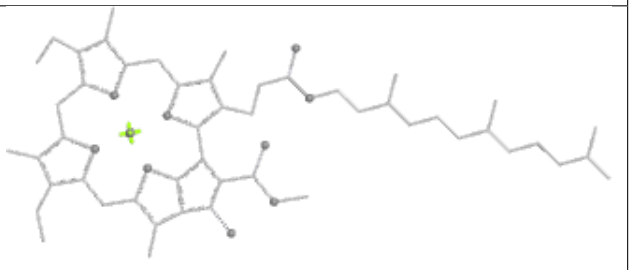
Bond lengths



Bond angles

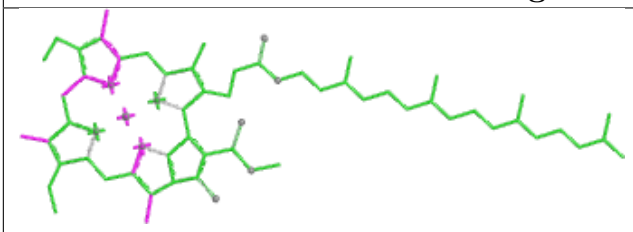


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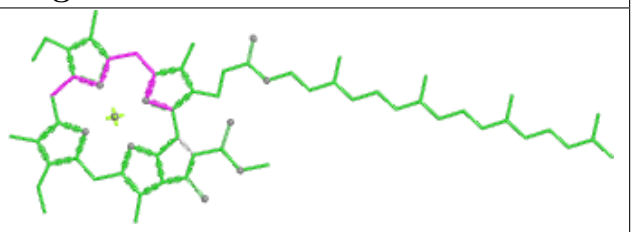


Rings

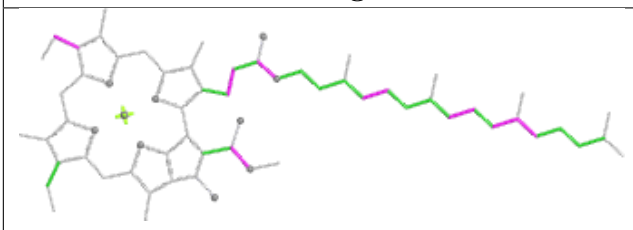
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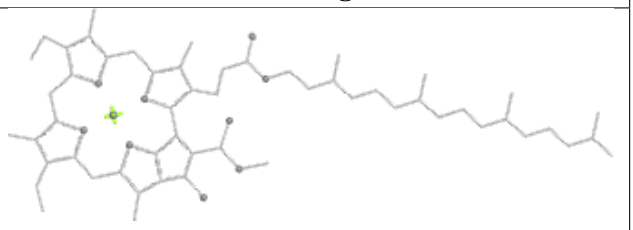
Bond lengths



Bond angles

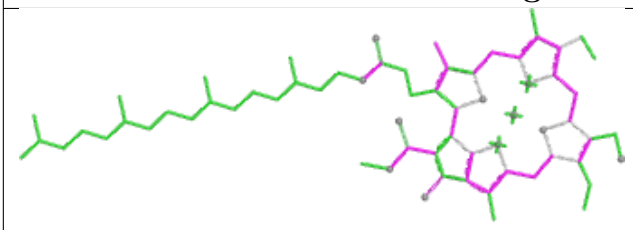


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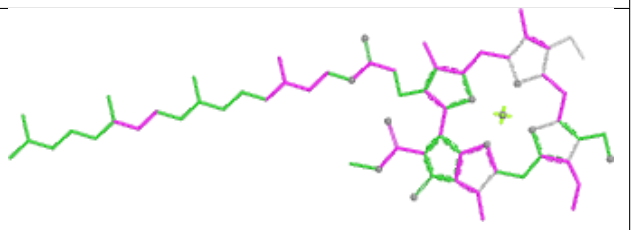


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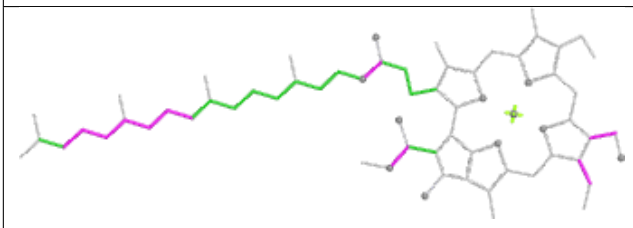
Ligand CHL Y 609



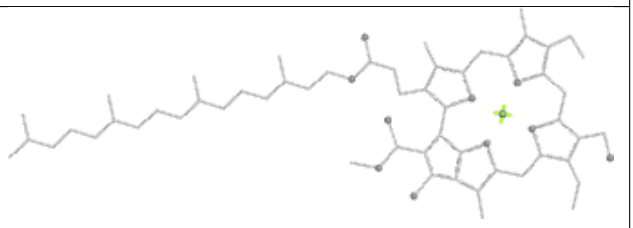
Bond lengths



Bond angles

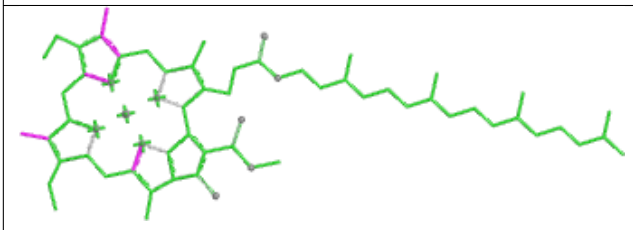


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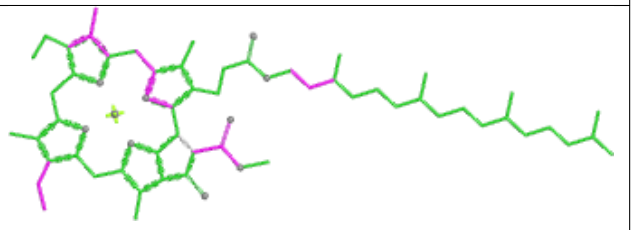


Rings

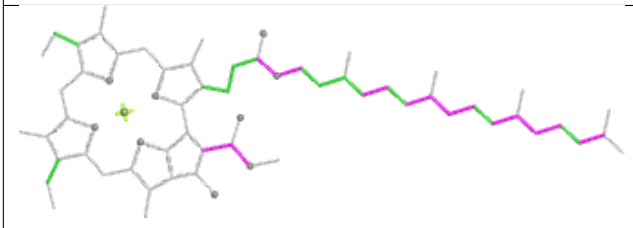
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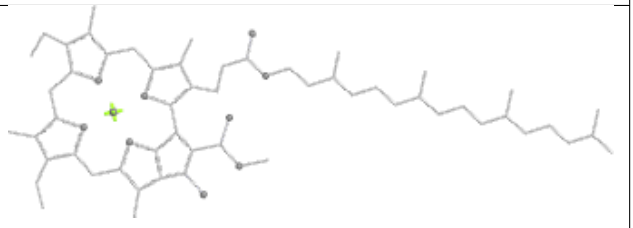
Bond lengths



Bond angles

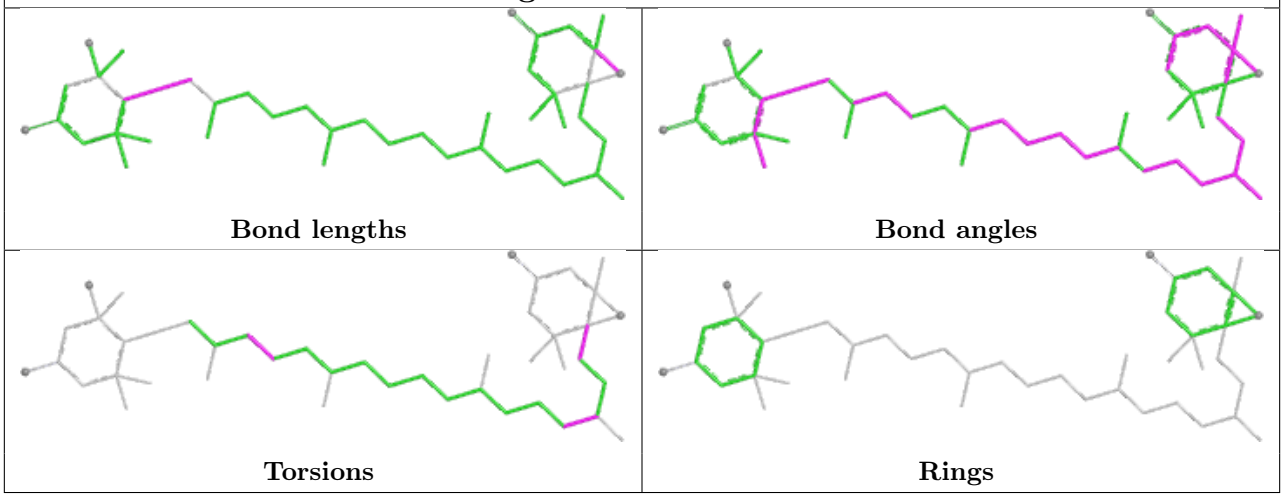


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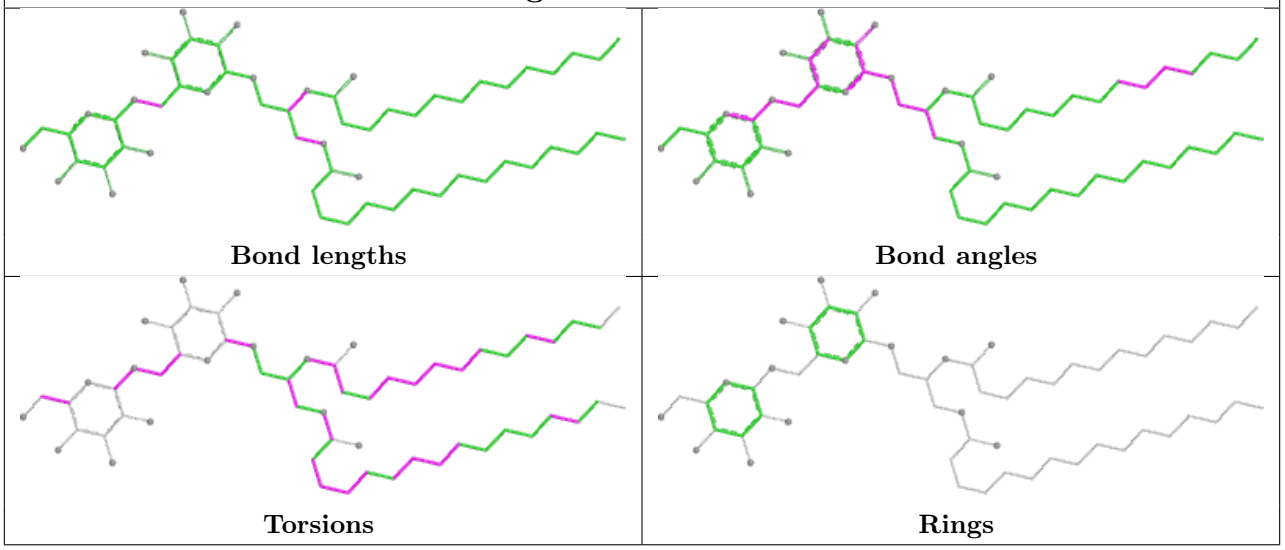


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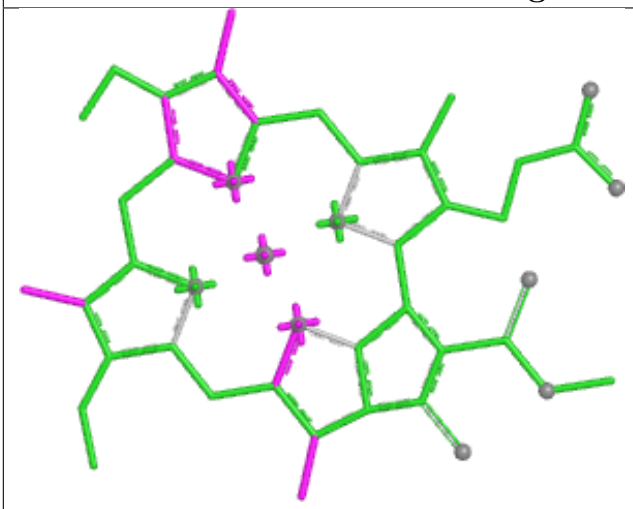
Ligand NEX 6 1623



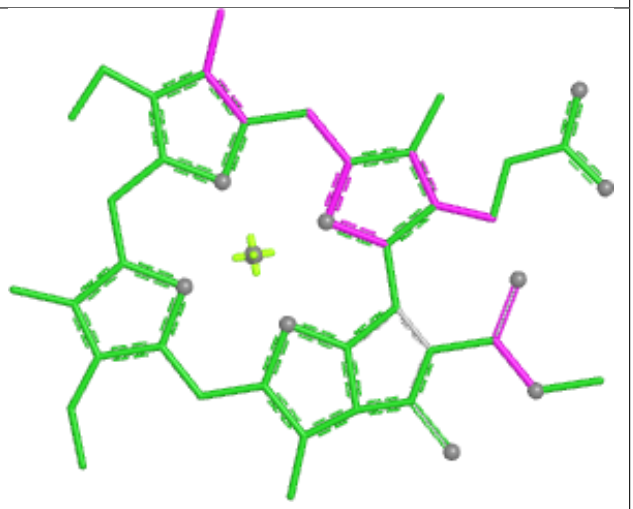
Ligand DGD c 520



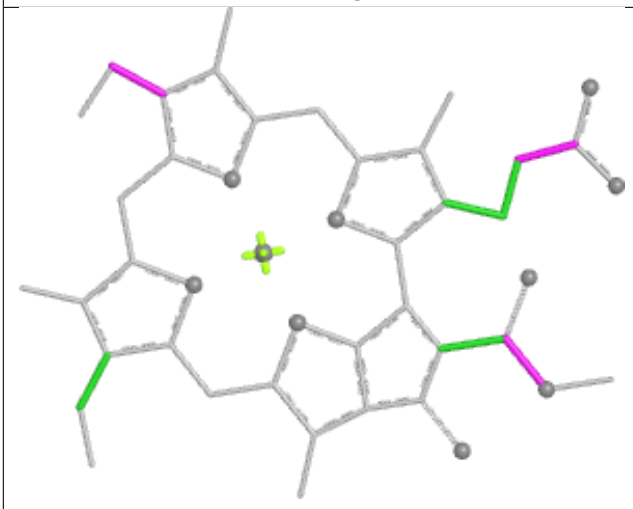
Ligand CLA 4 603



Bond lengths



Bond angles

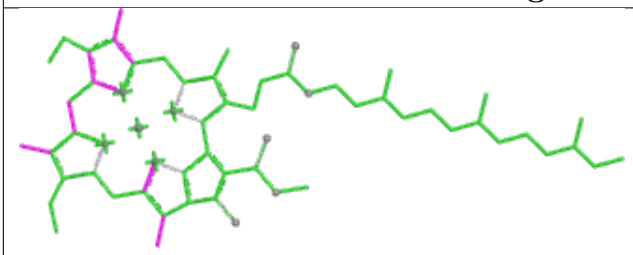


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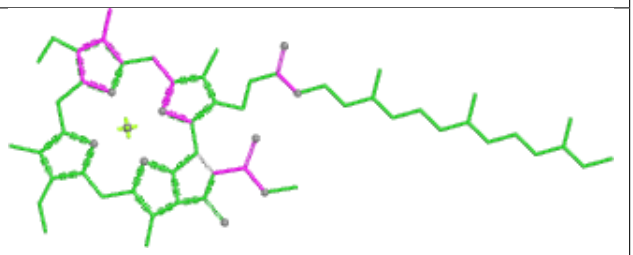


Rings

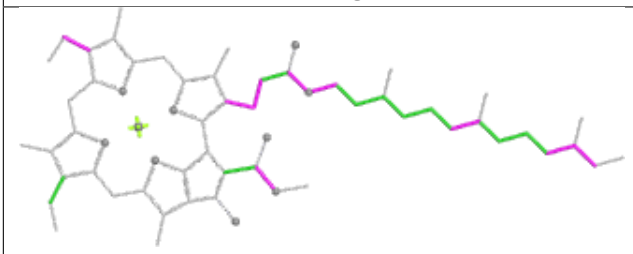
Ligand CLA S 602



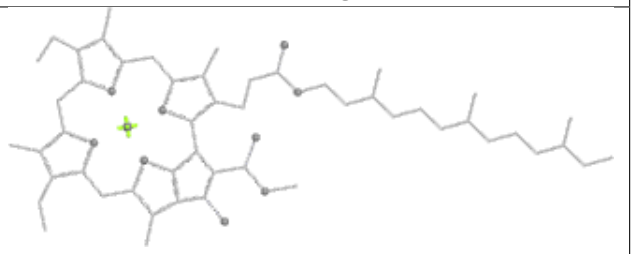
Bond lengths



Bond angles

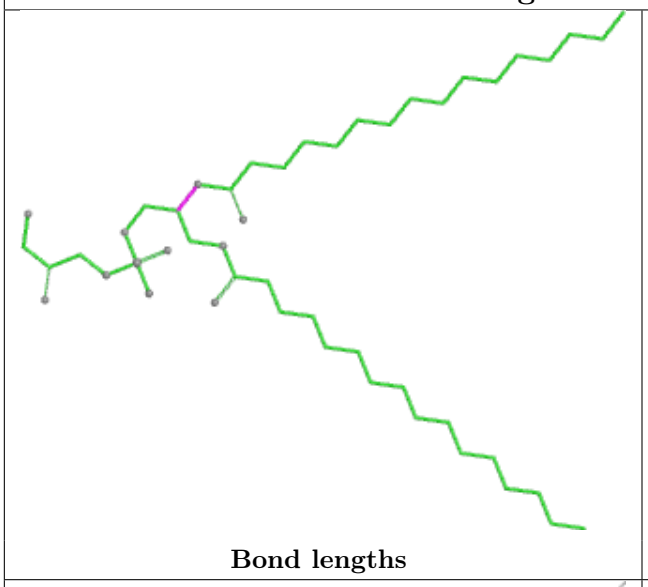


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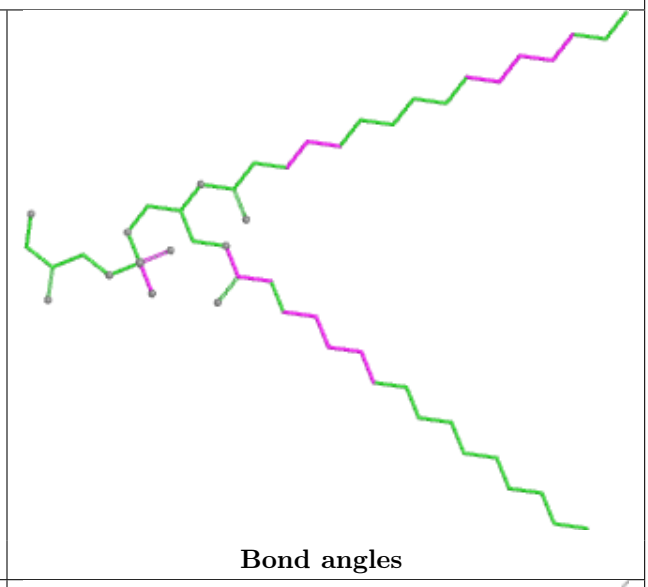


Rings

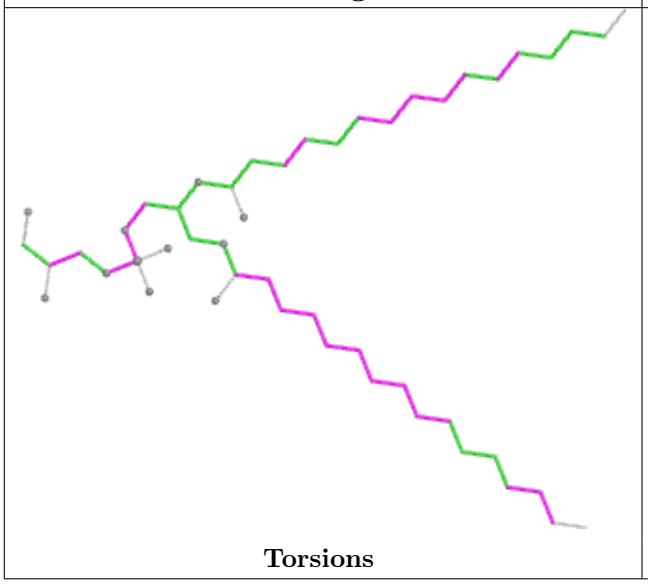
Ligand LHG n 2630



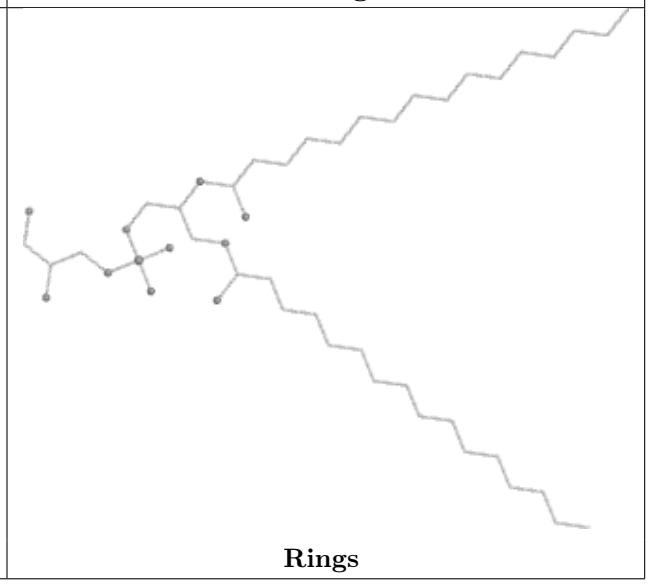
Bond lengths



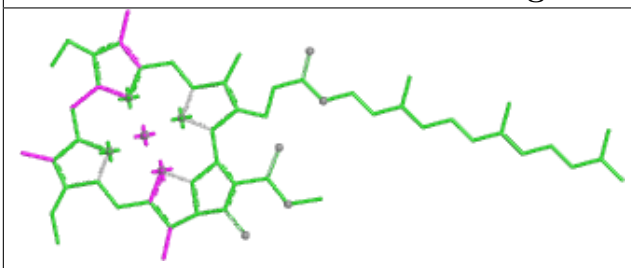
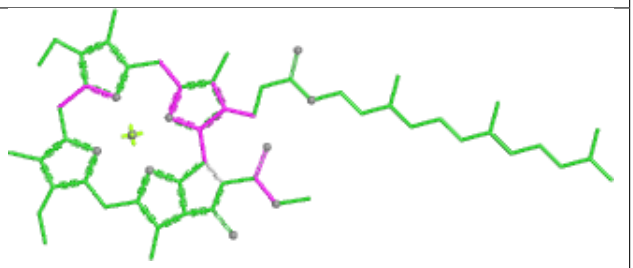
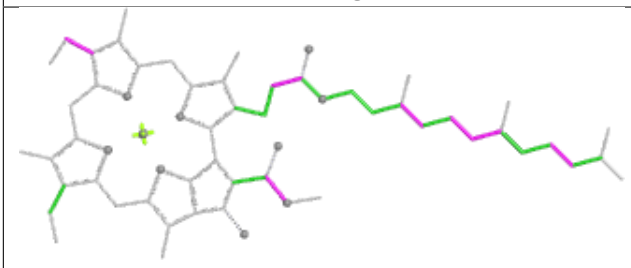
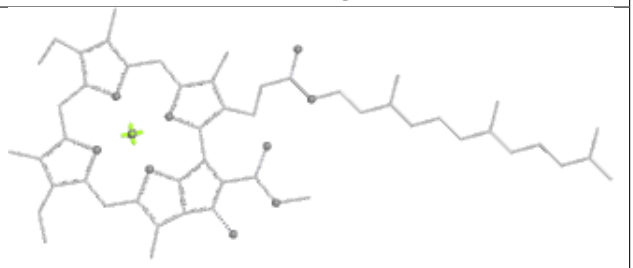
Bond angles

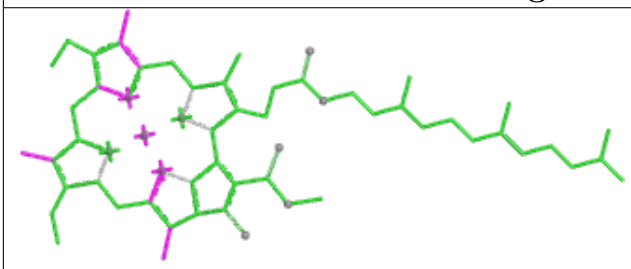
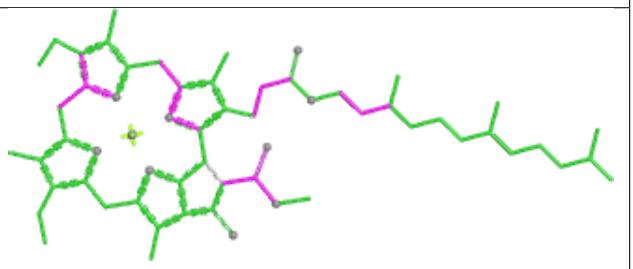
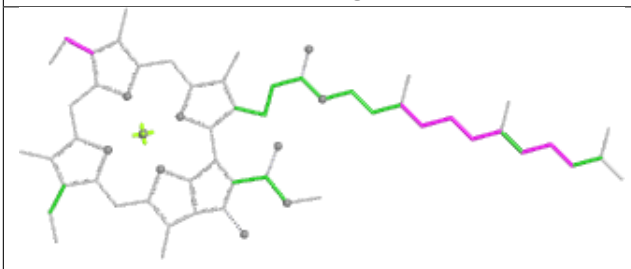
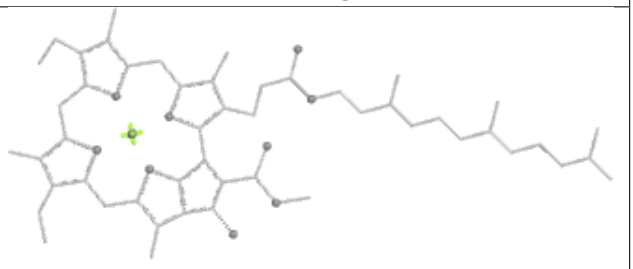


Torsions

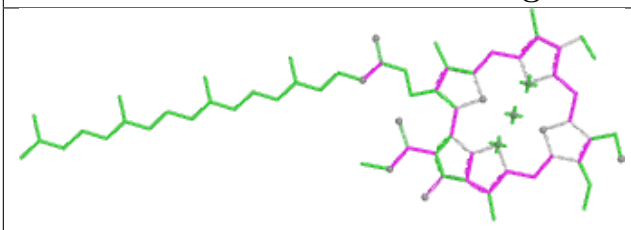


Rings

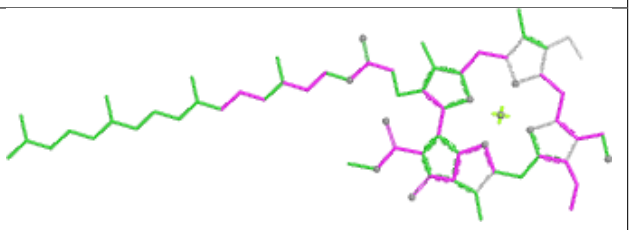
Ligand CLA n 612	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA a 410	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

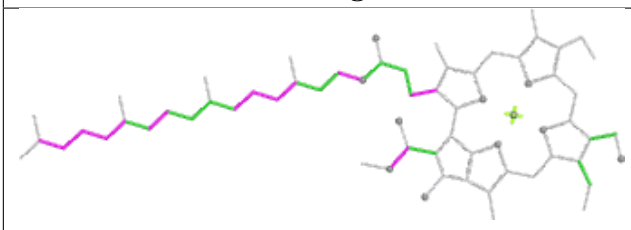
Ligand CHL N 608



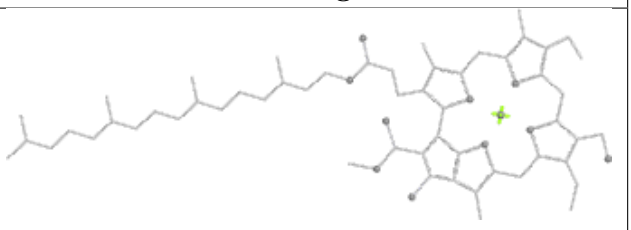
Bond lengths



Bond angles

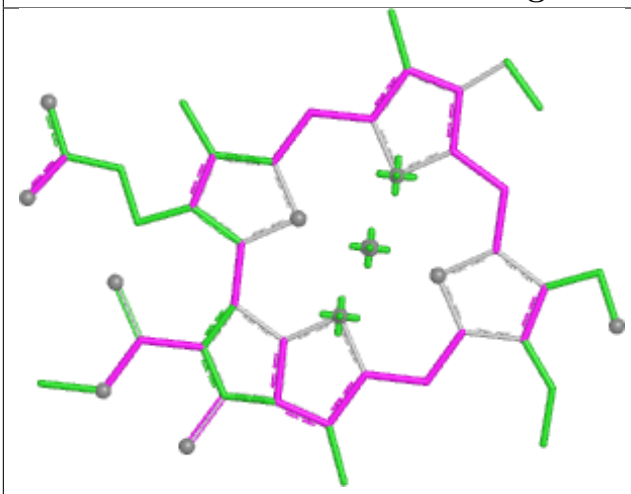


Torsions

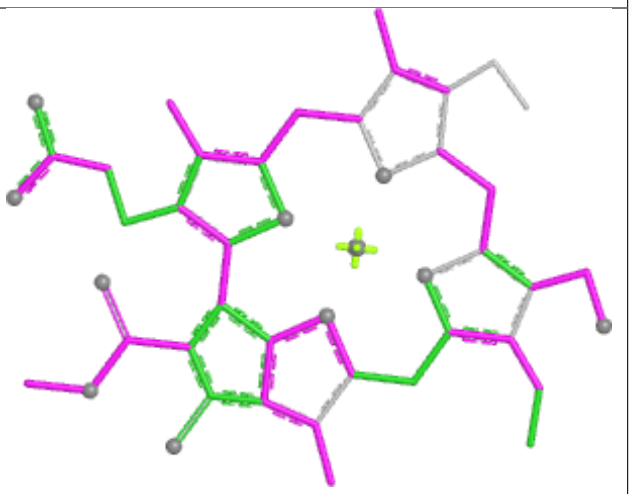


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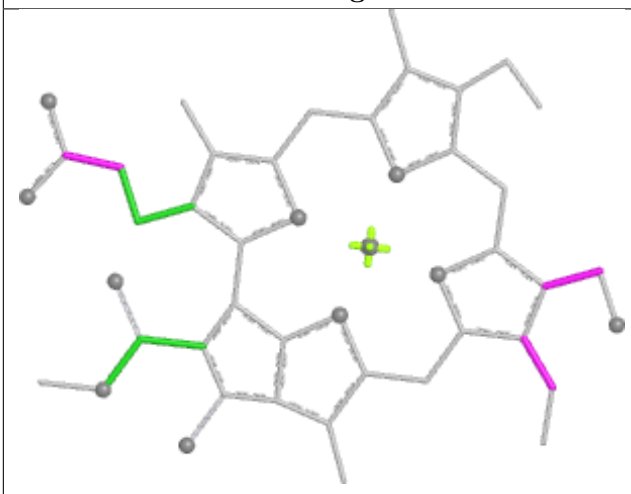
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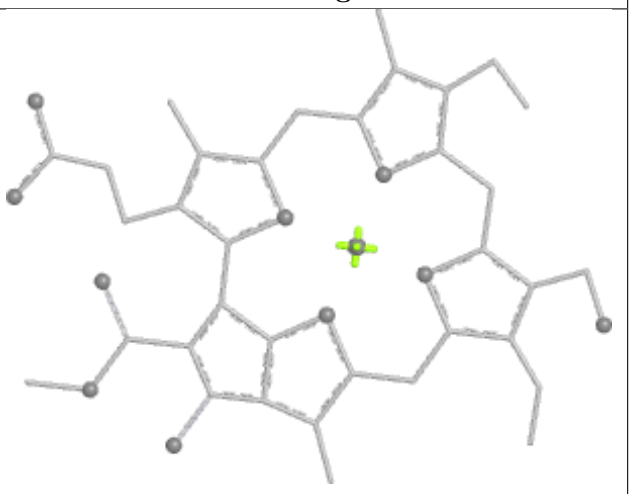
Bond lengths



Bond angles

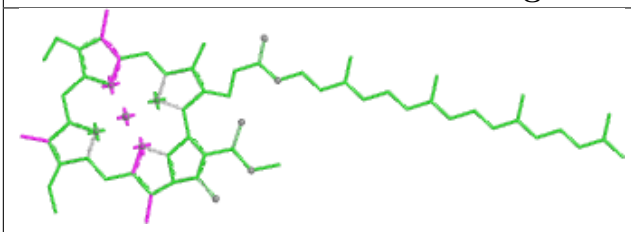


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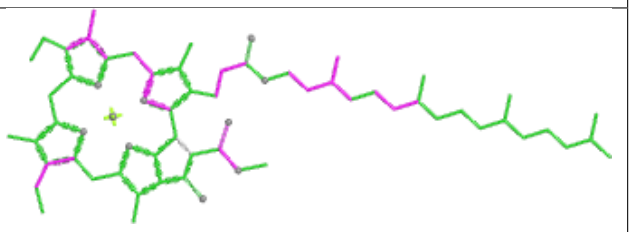


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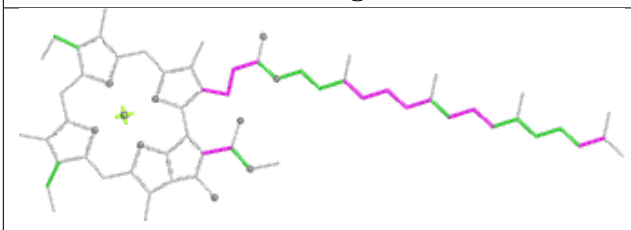
Ligand CLA Y 602



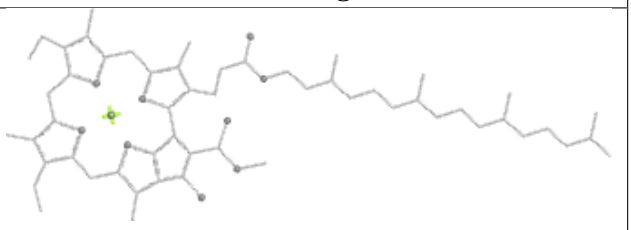
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Bond angles

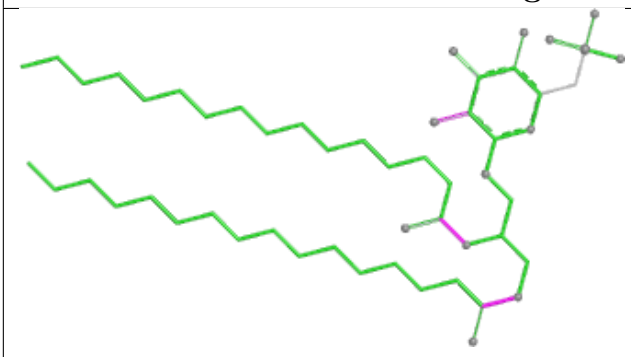


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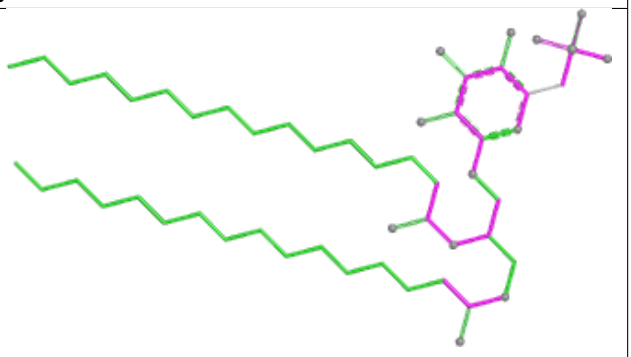


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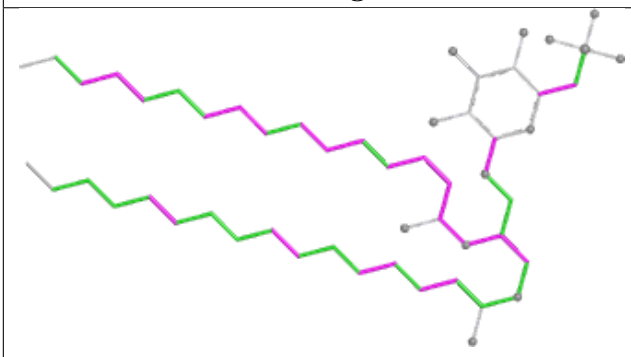
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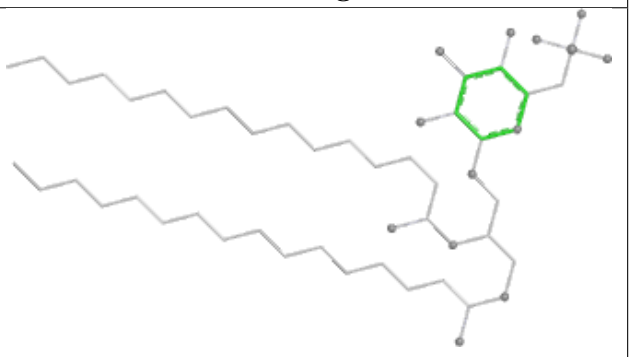
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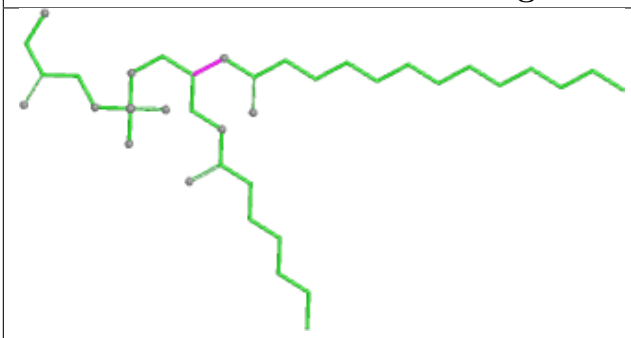


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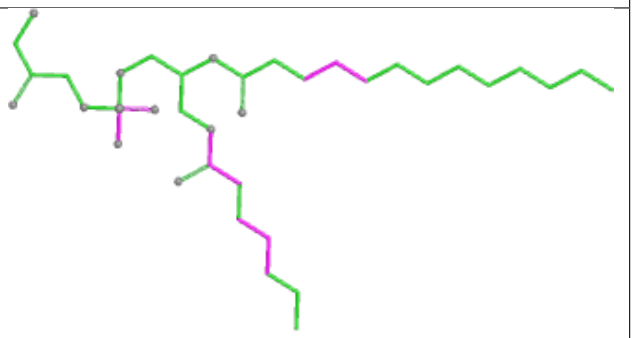


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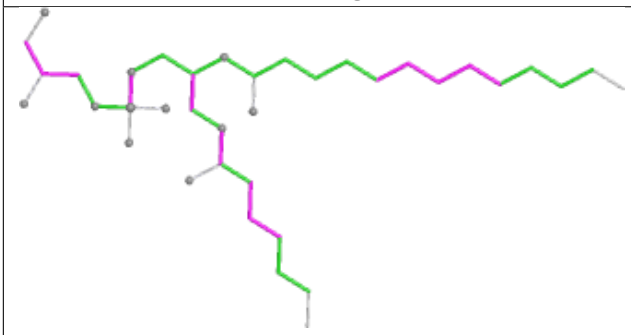
Ligand LHG 2 2630



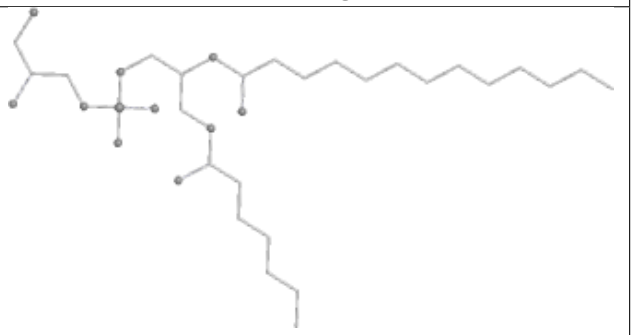
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Bond angles

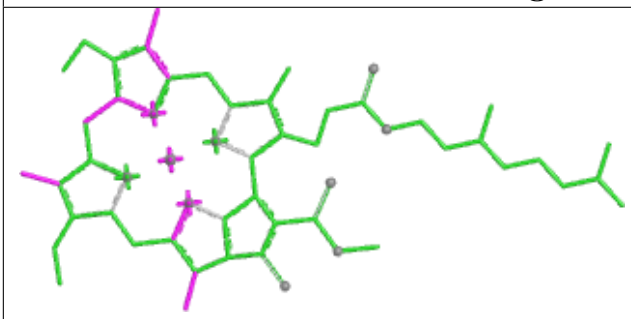


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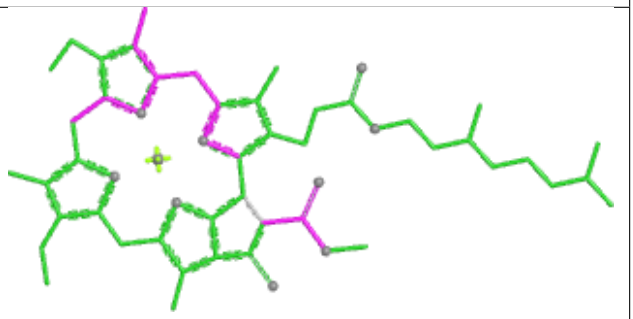


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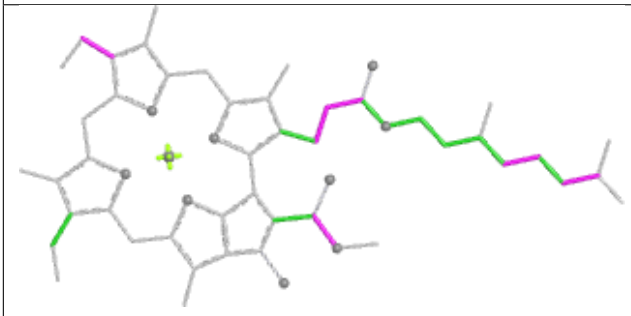
Ligand CLA 5 613



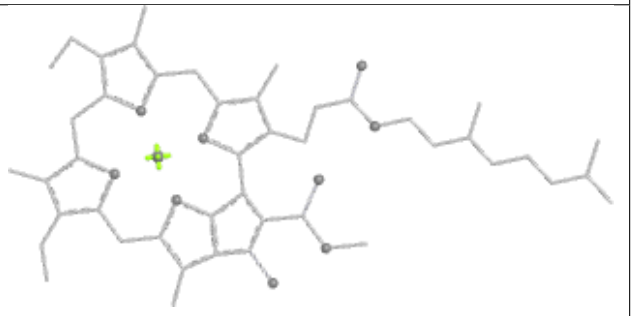
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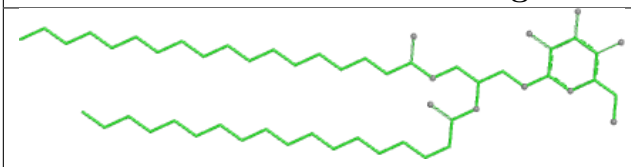


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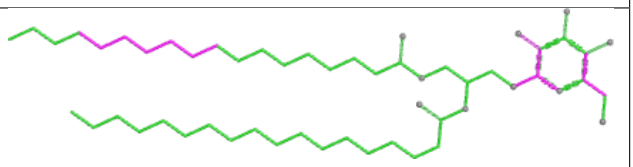


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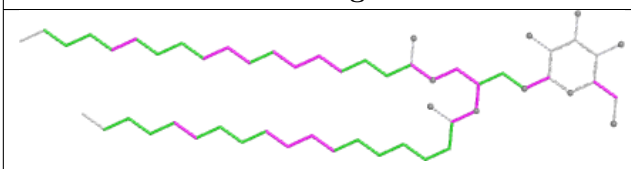
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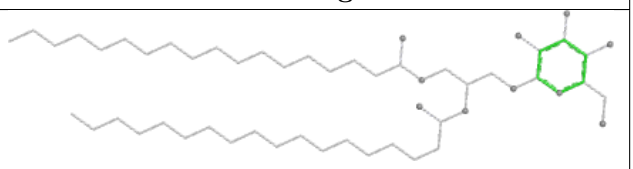
Bond lengths



Bond angles

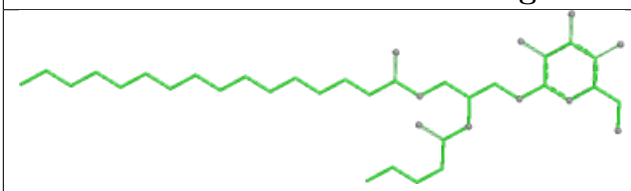


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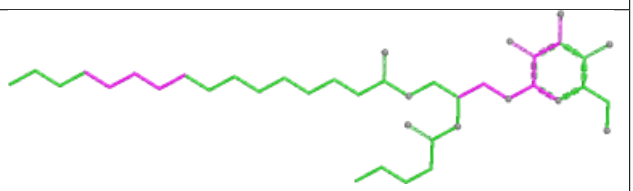


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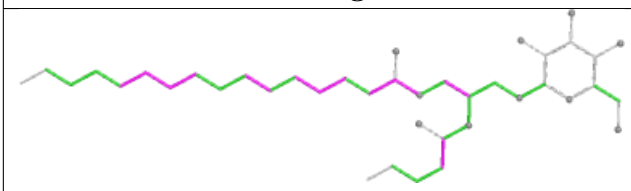
Ligand LMG A 415



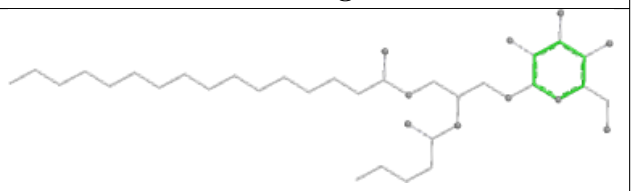
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Bond angles

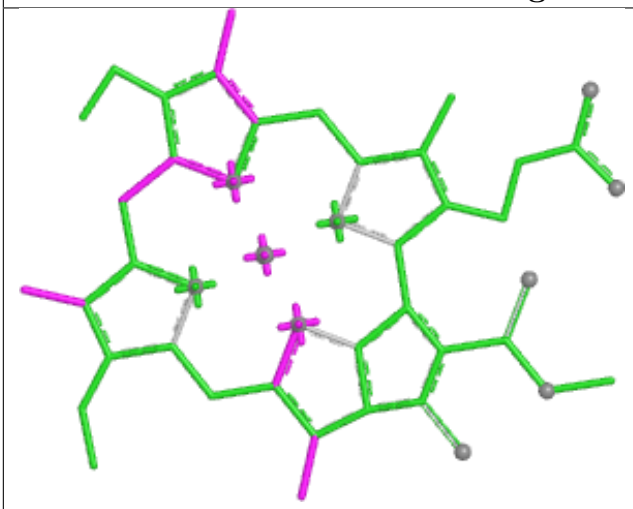


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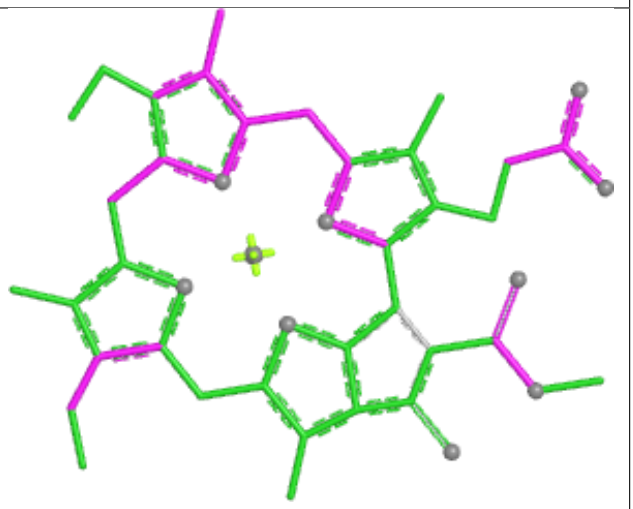


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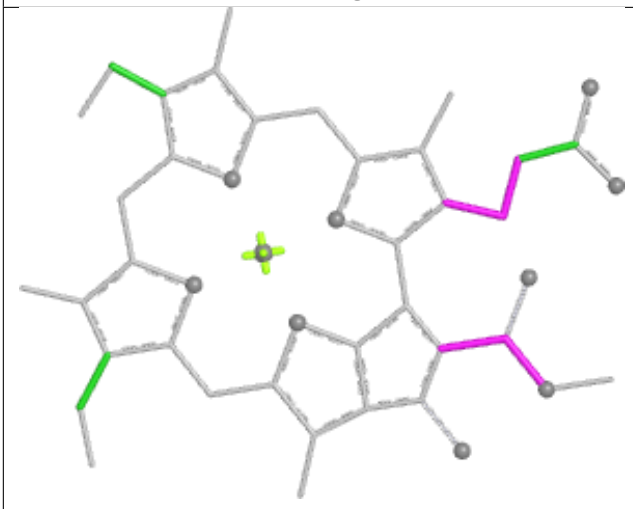
Ligand CLA 2 604



Bond lengths



Bond angles

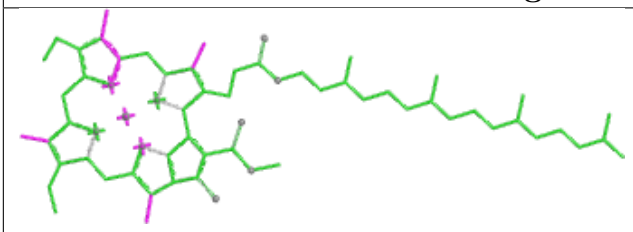


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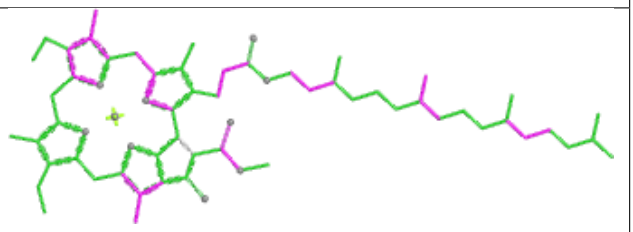


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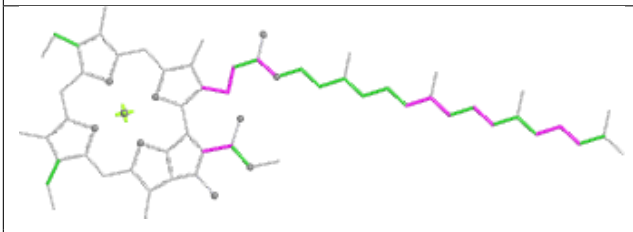
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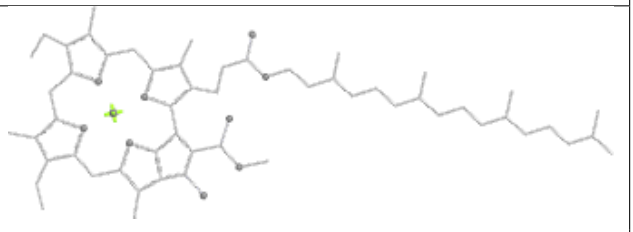
Bond lengths



Bond angles

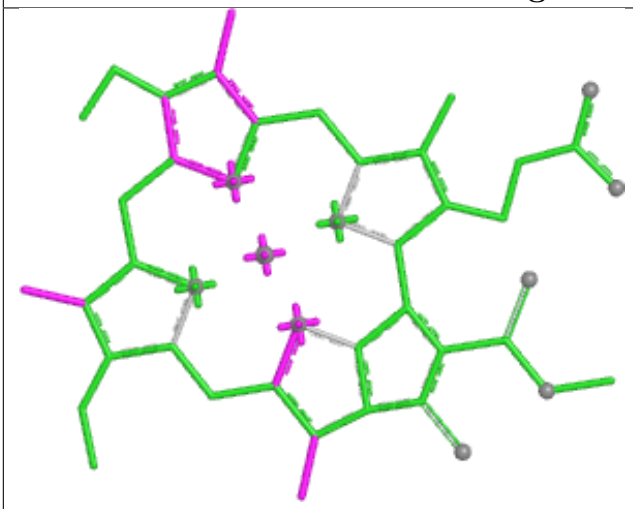


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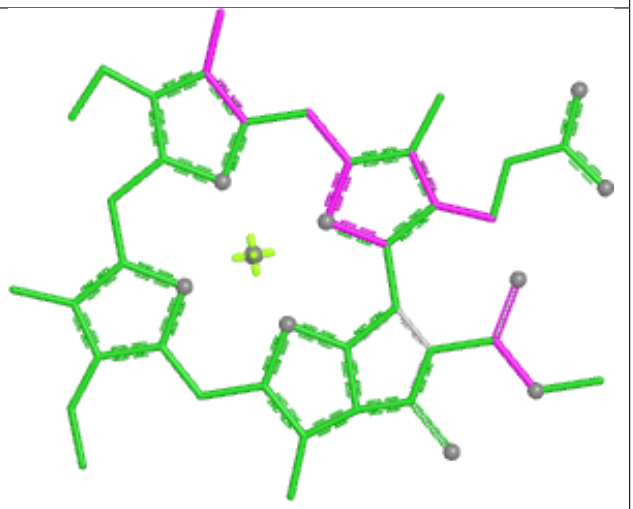


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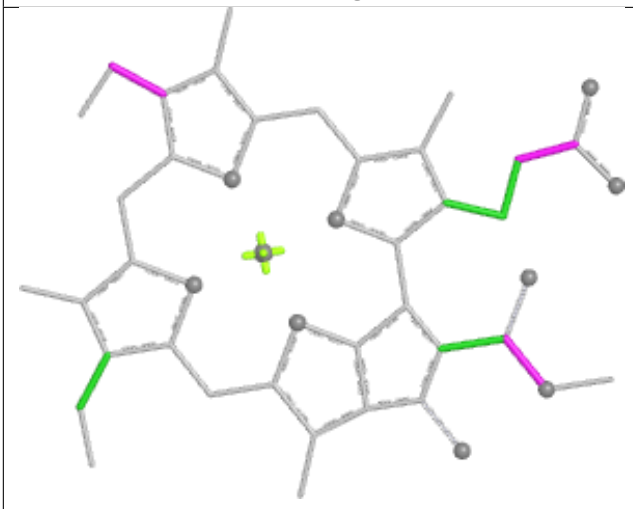
Ligand CLA 8 603



Bond lengths



Bond angles

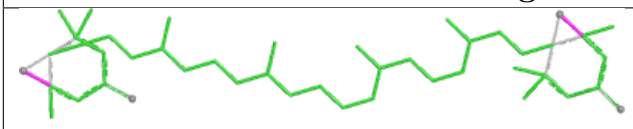


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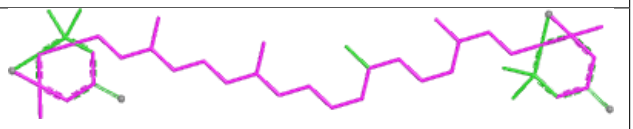


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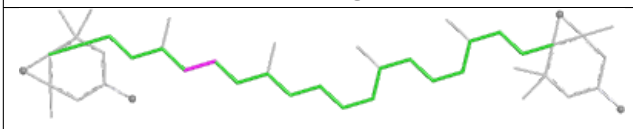
Ligand XAT 3 1622



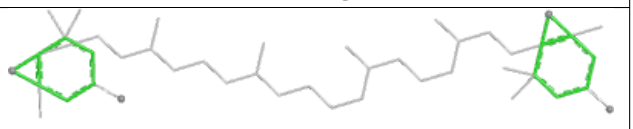
Bond lengths



Bond angles

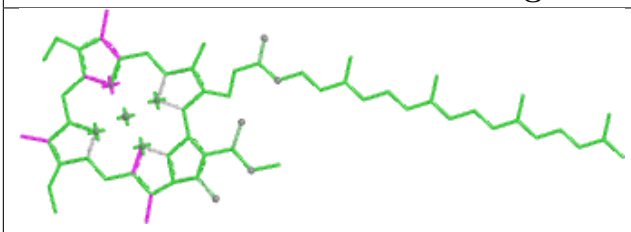


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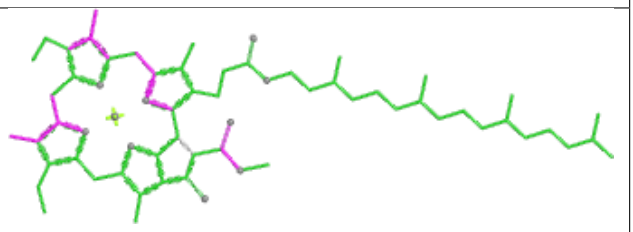


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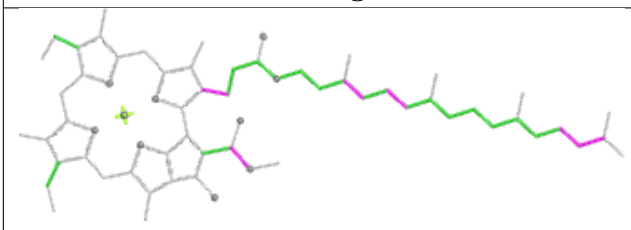
Ligand CLA C 508



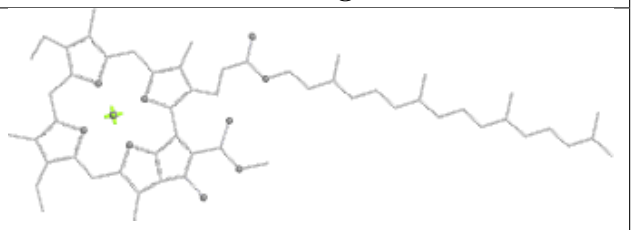
Bond lengths



Bond angles

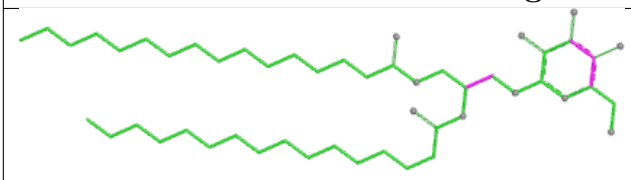


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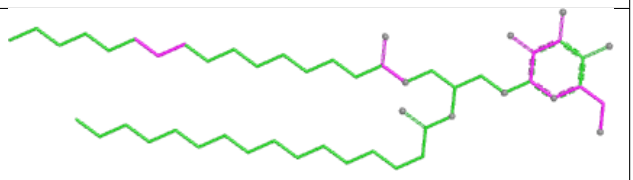


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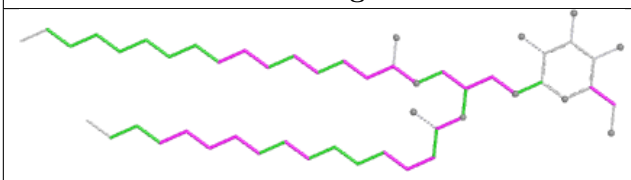
Ligand LMG z 101



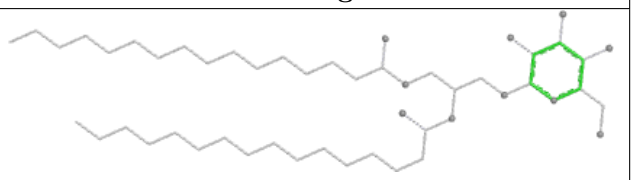
Bond lengths



Bond angles



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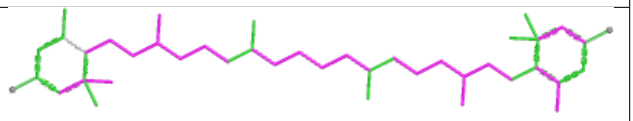


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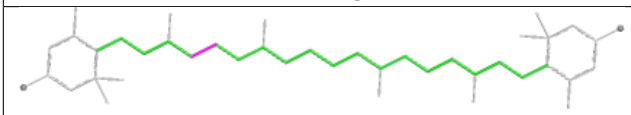
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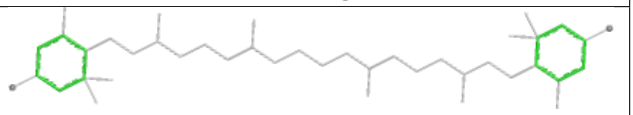
Bond lengths



Bond angles

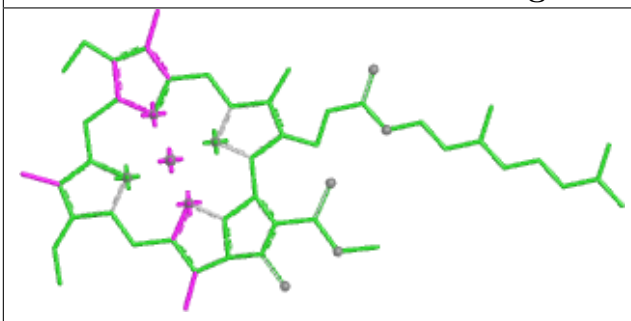


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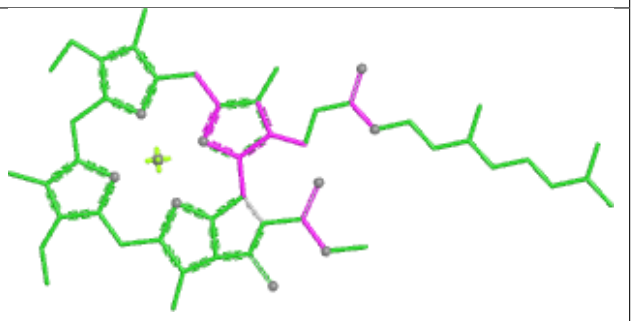


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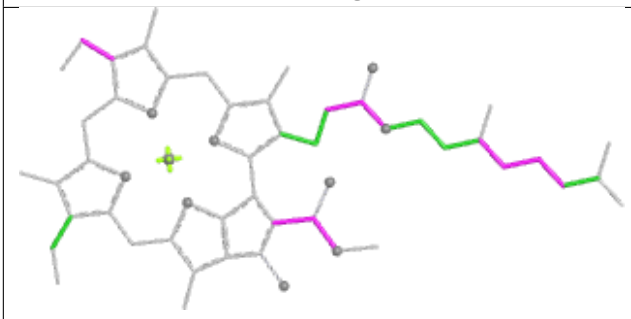
Ligand CLA 6 603



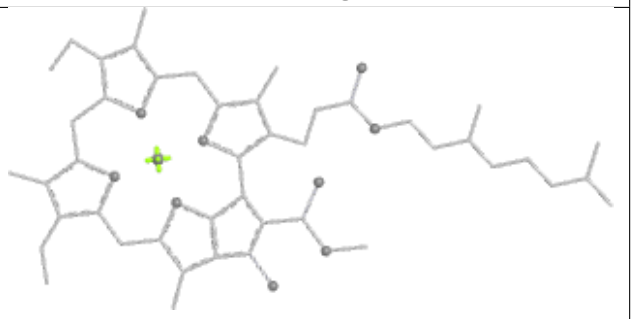
Bond lengths



Bond angles

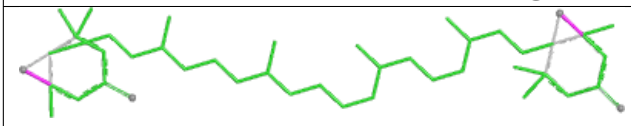


Torsions

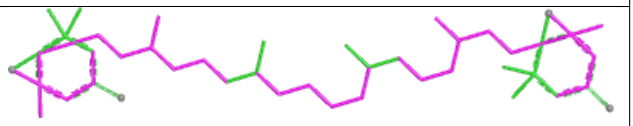


Rings

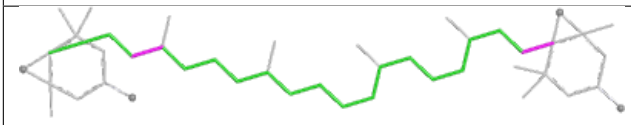
Ligand XAT 4 622



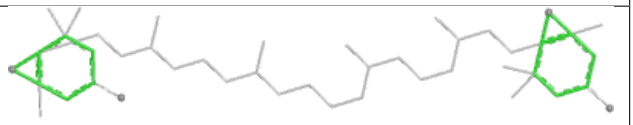
Bond lengths



Bond angles

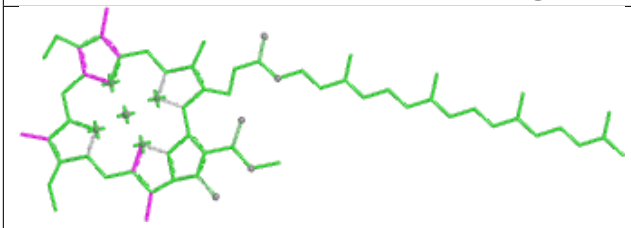


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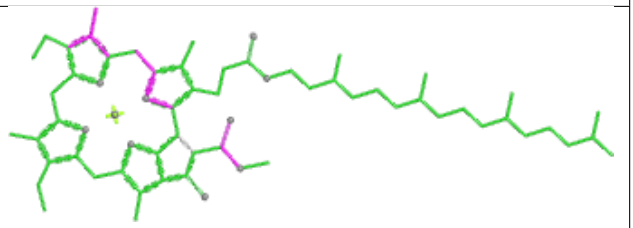


Rings

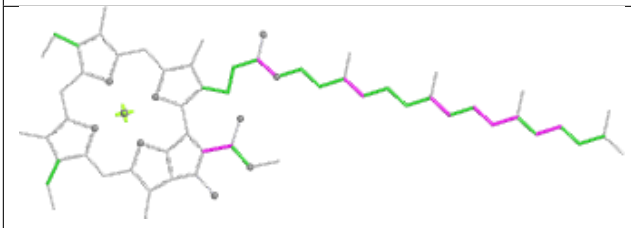
Ligand CLA c 504



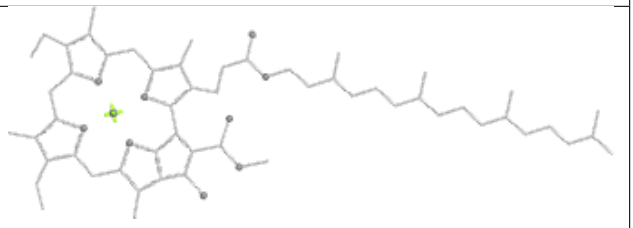
Bond lengths



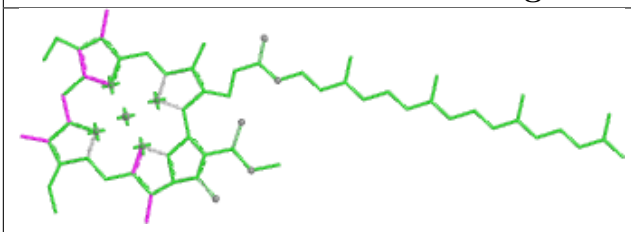
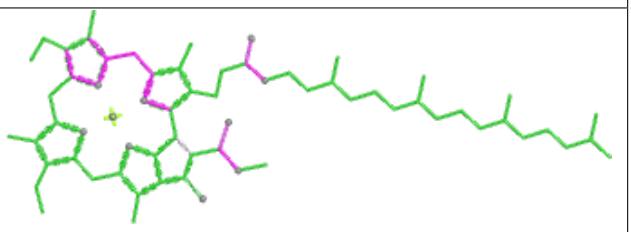
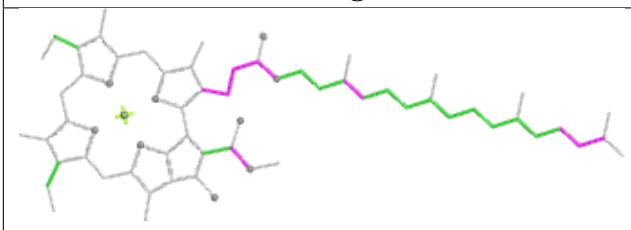
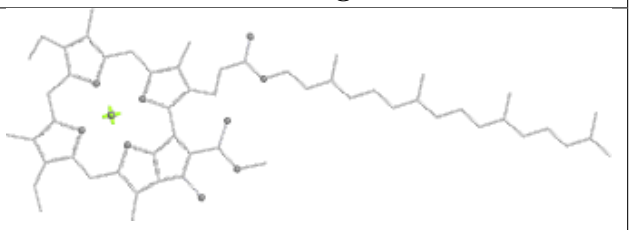
Bond angles

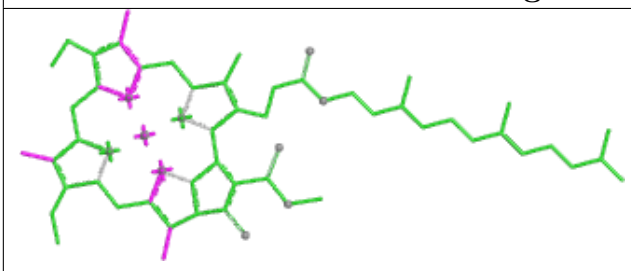
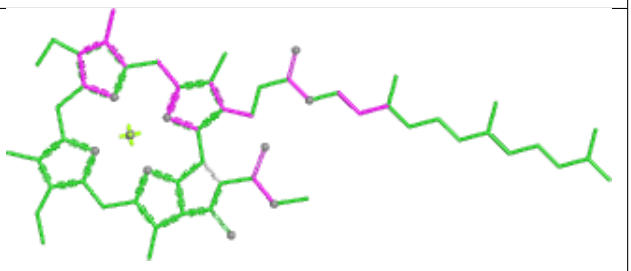
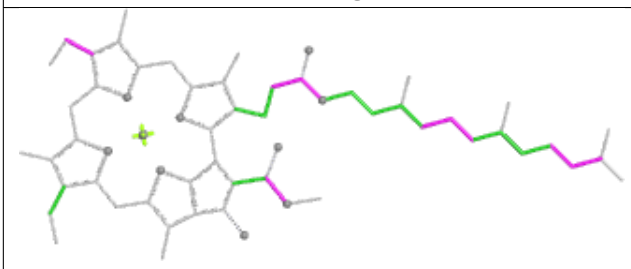
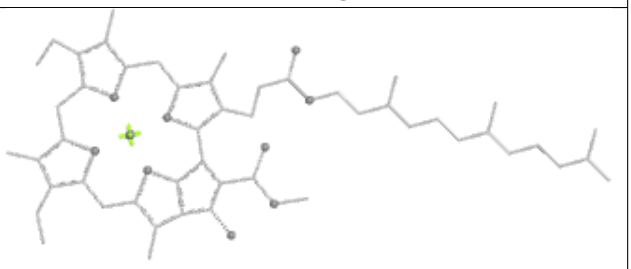


Torsions

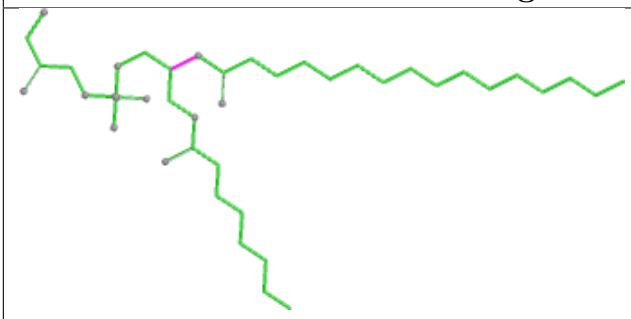


Rings

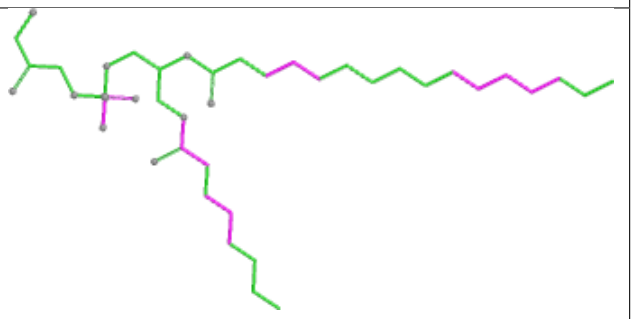
Ligand CLA C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA R 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

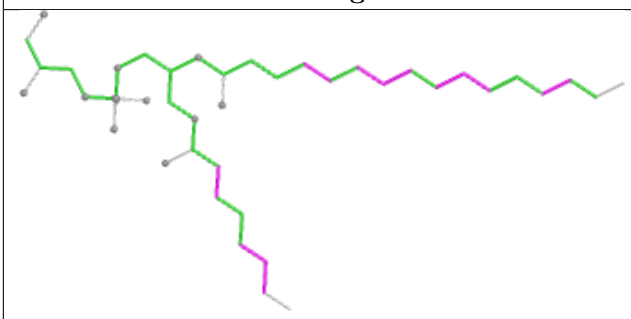
Ligand LHG 5 2630



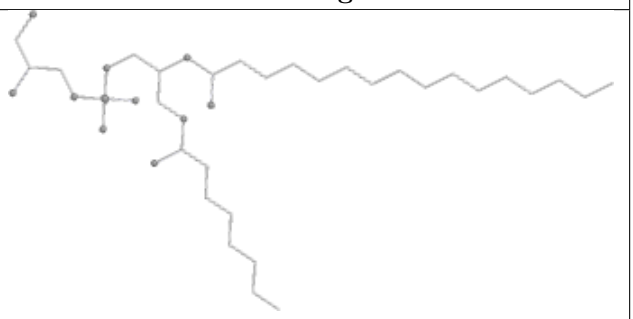
Bond lengths



Bond angles

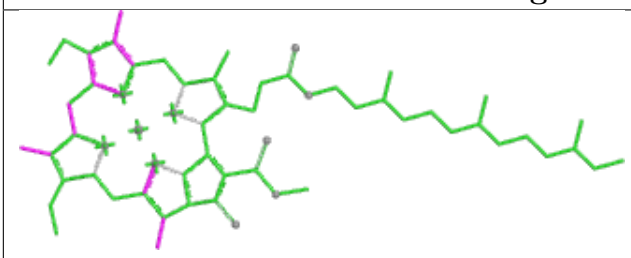


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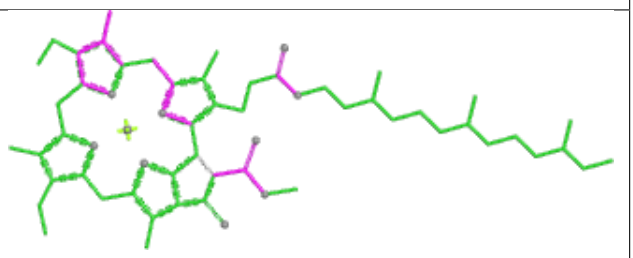


Rings

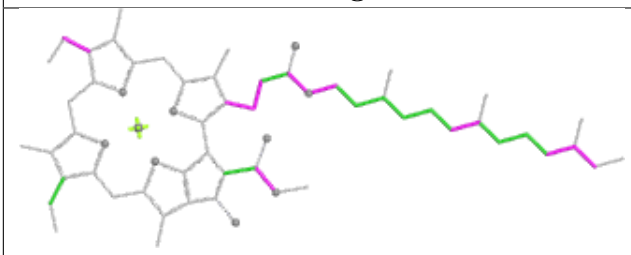
Ligand CLA s 602



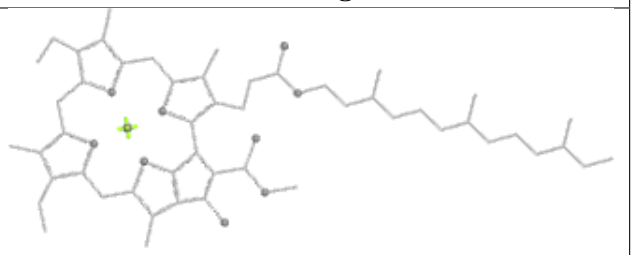
Bond lengths



Bond angles

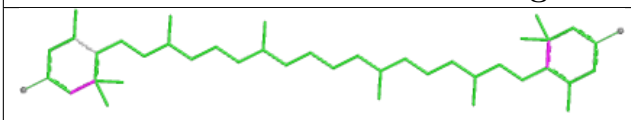


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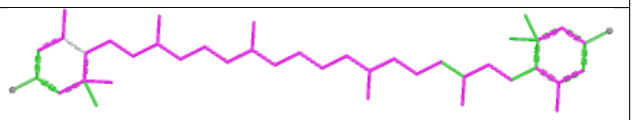


Rings

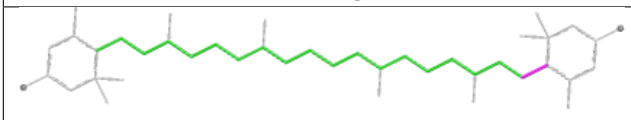
Ligand LUT r 620



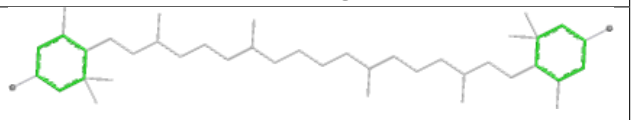
Bond lengths



Bond angles

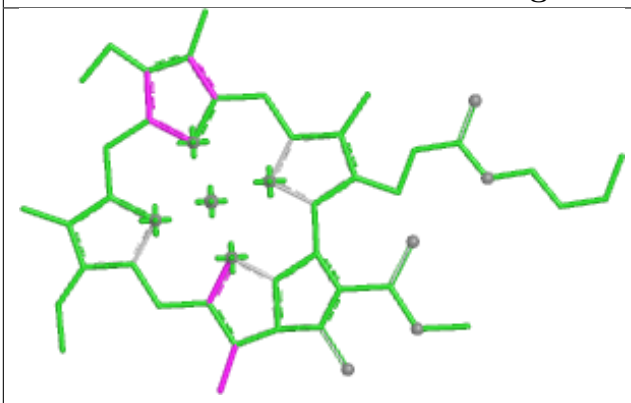


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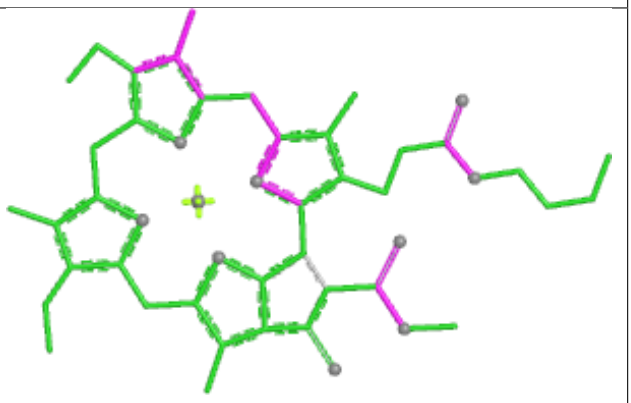


Rings

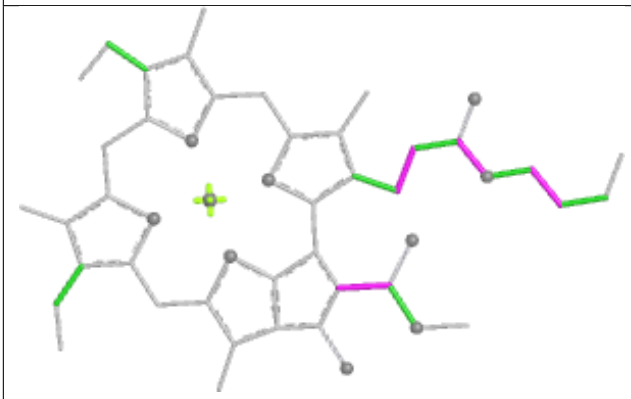
Ligand CLA s 614



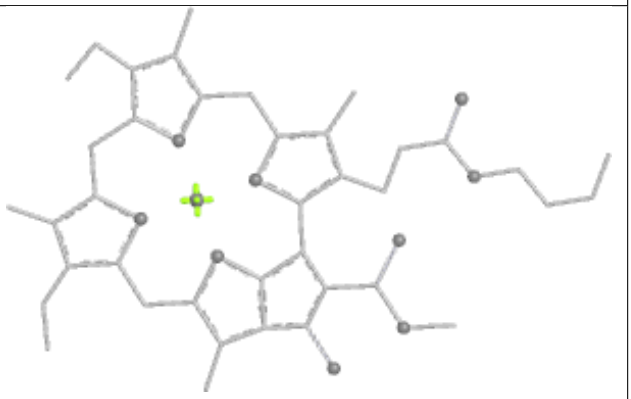
Bond lengths



Bond angles

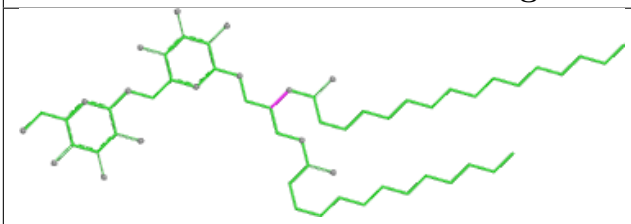


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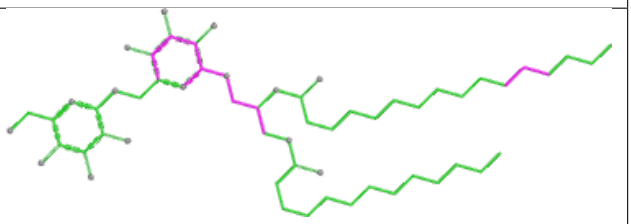


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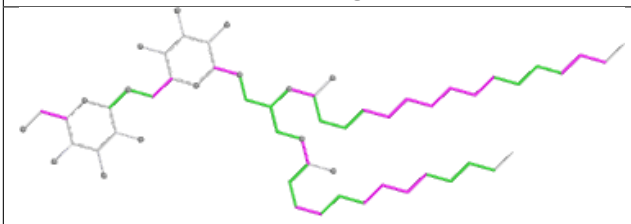
Ligand DGD B 626



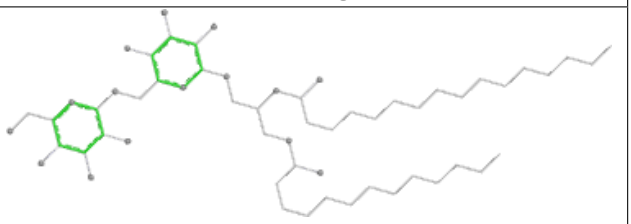
Bond lengths



Bond angles

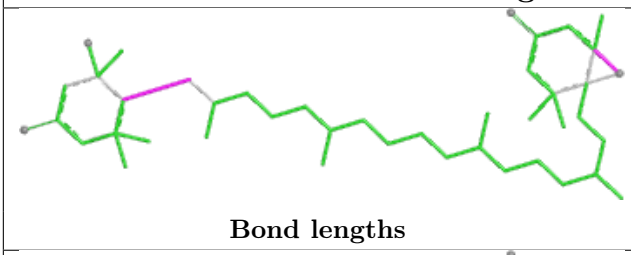


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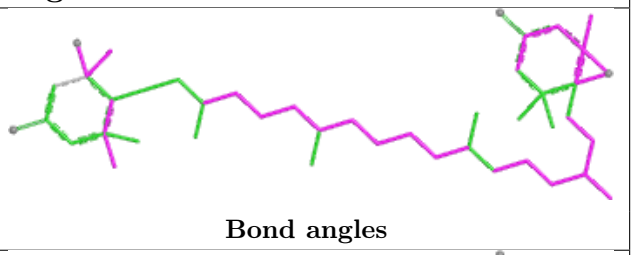


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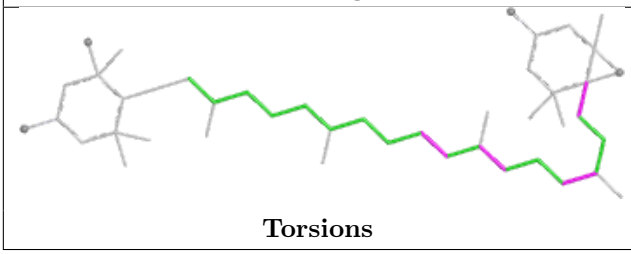
Ligand NEX g 1623



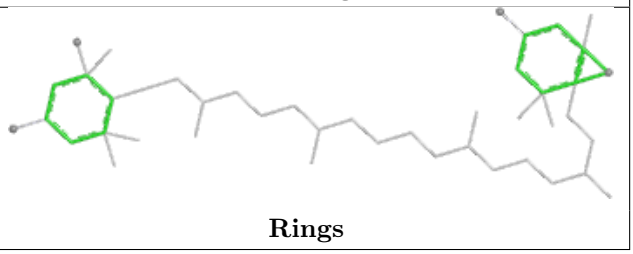
Bond lengths



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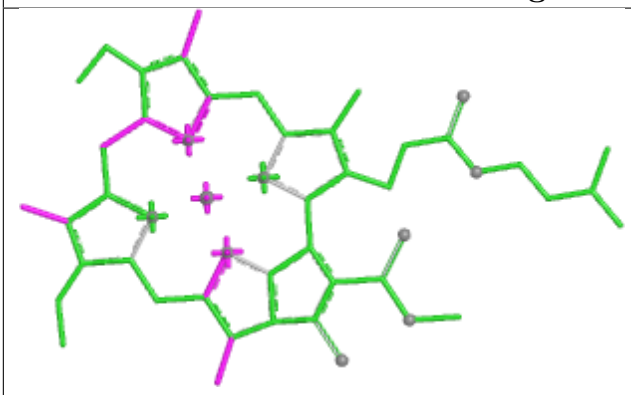


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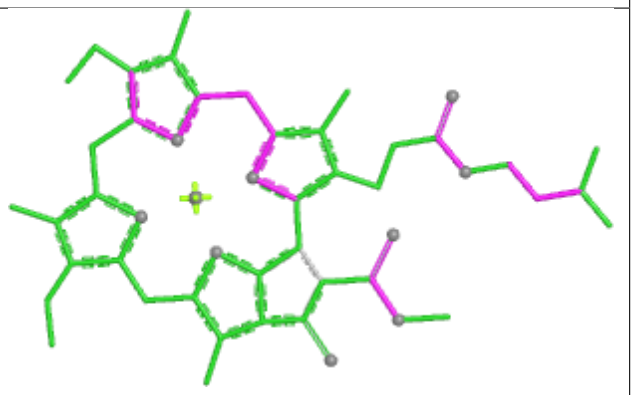


Rings

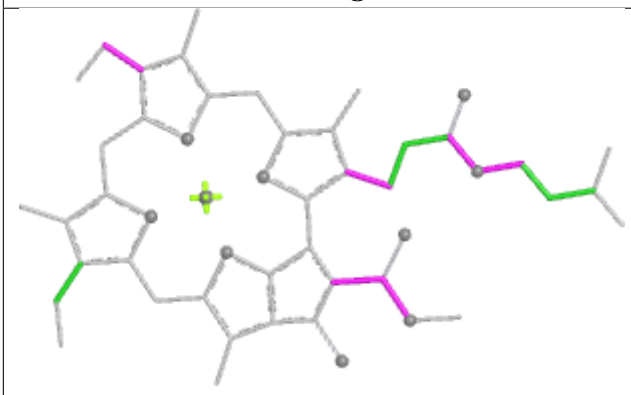
Ligand CLA 5 604



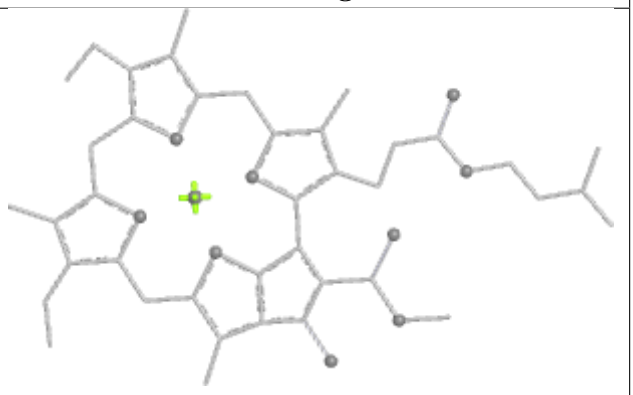
Bond lengths



Bond angles

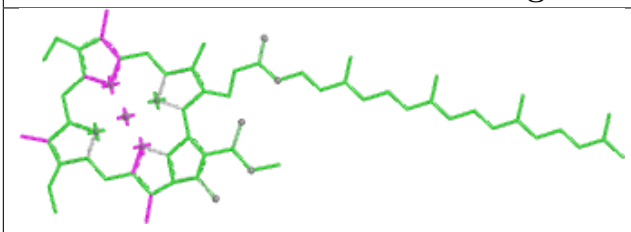


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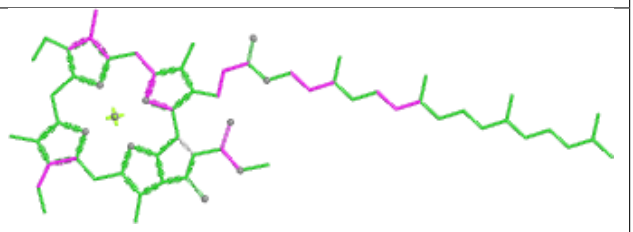


Rings

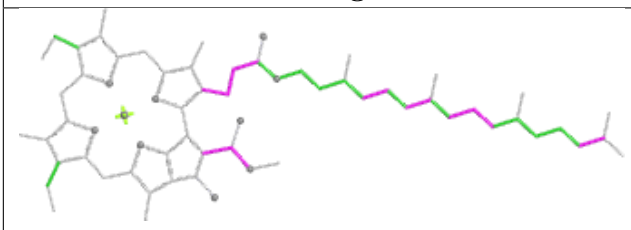
Ligand CLA n 602



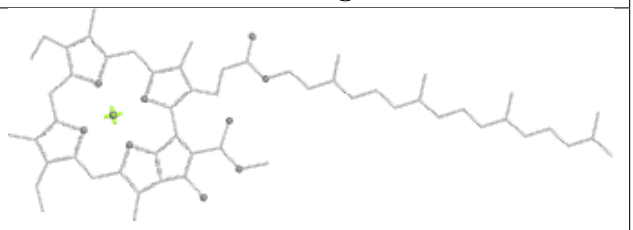
Bond lengths



Bond angles

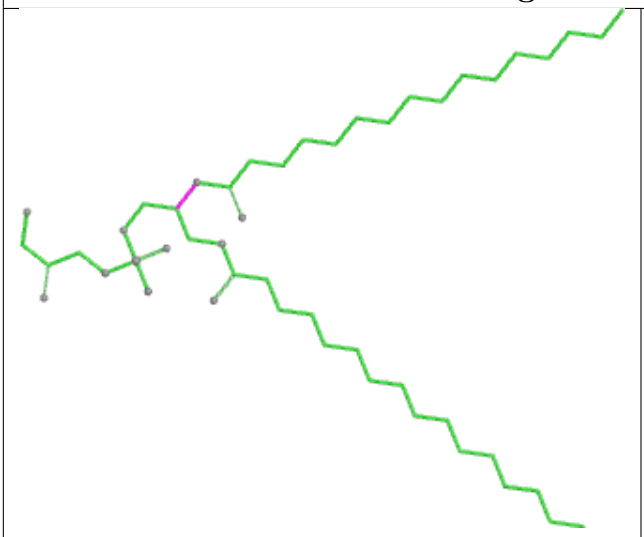


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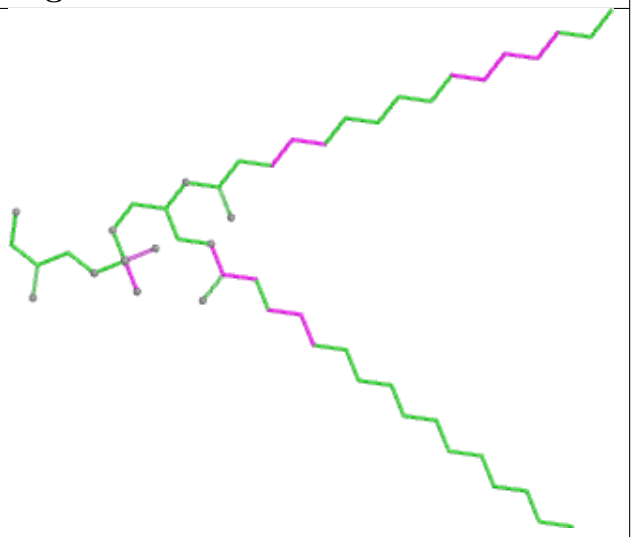


Rings

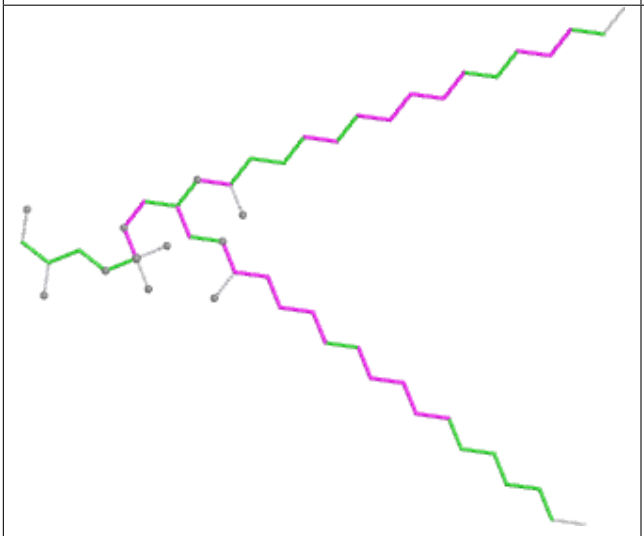
Ligand LHG g 2630



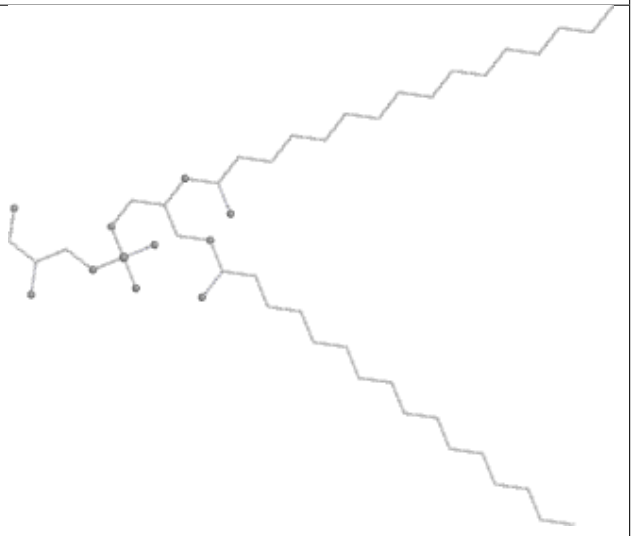
Bond lengths



Bond angles

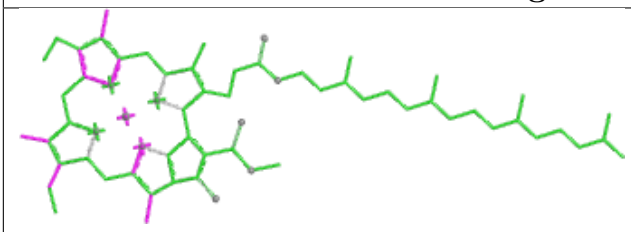


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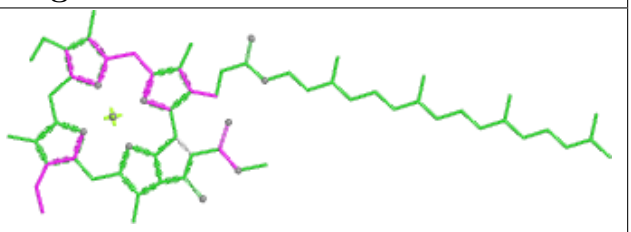


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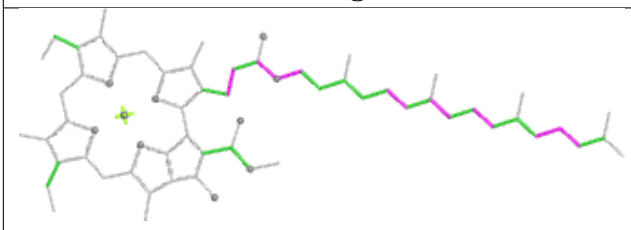
Ligand CLA g 603



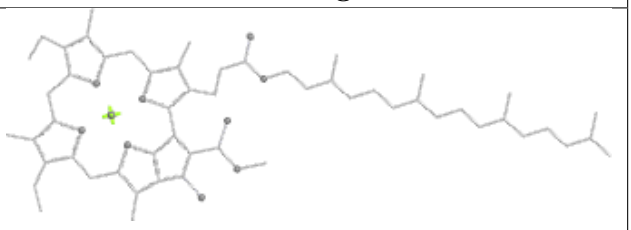
Bond lengths



Bond angles

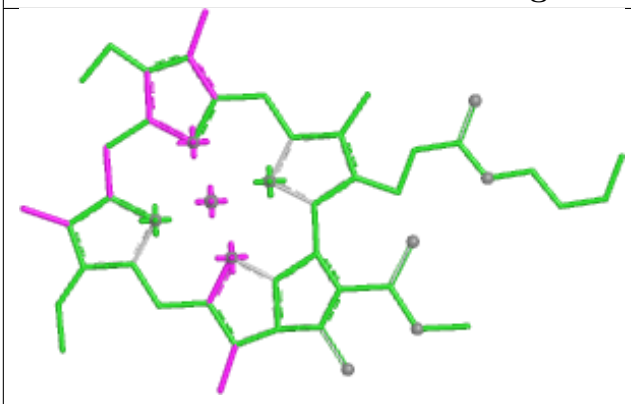


Torsions

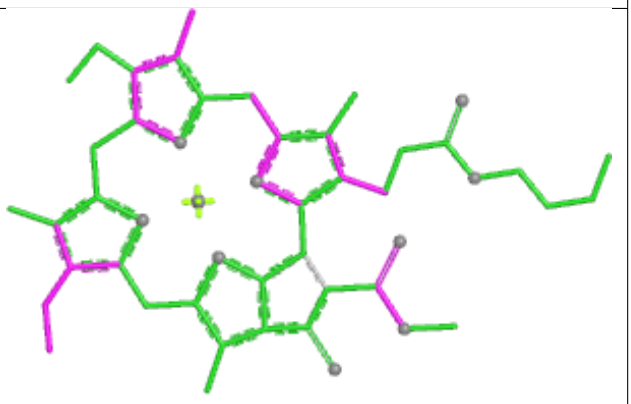


Rings

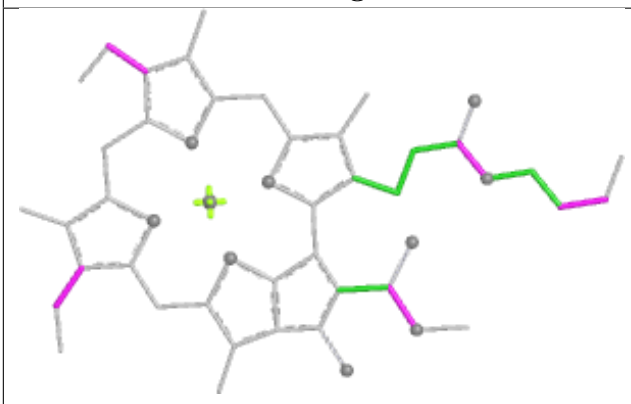
Ligand CLA r 601



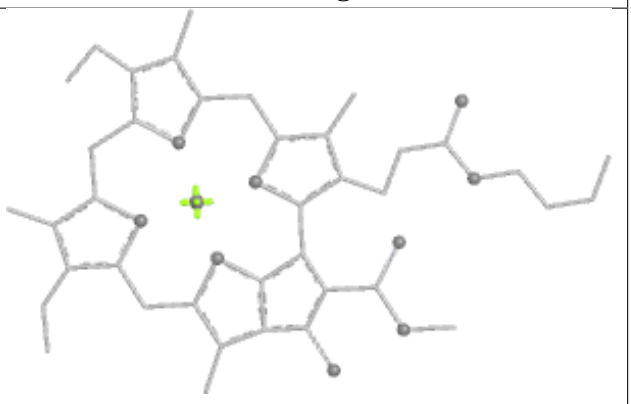
Bond lengths



Bond angles

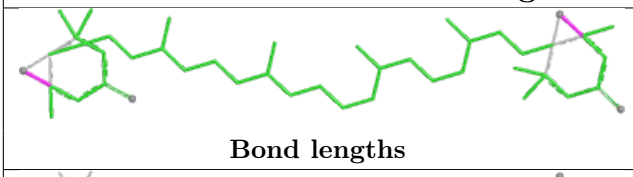


Torsions

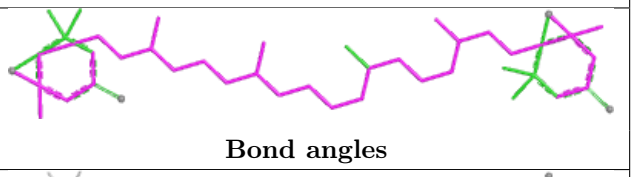


Rings

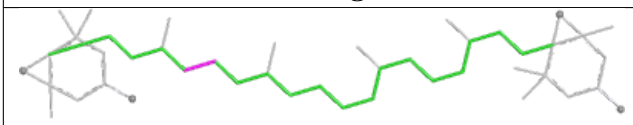
Ligand XAT 7 1622



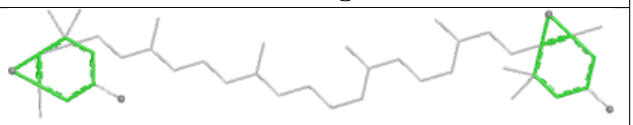
Bond lengths



Bond angles

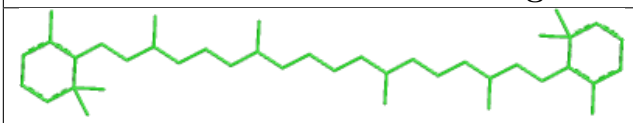


Torsions

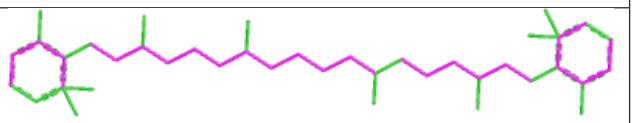


Rings

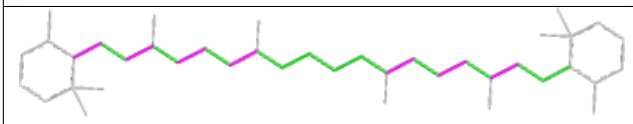
Ligand BCR 4 623



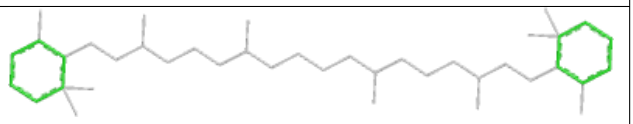
Bond lengths



Bond angles

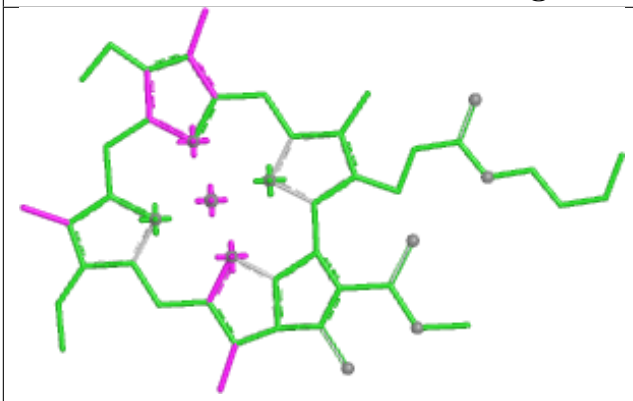


Torsions

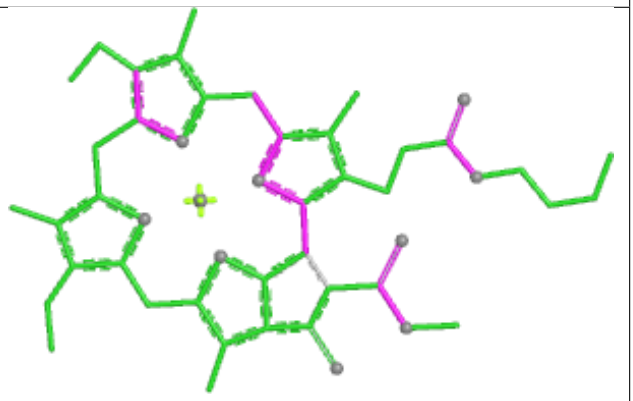


Rings

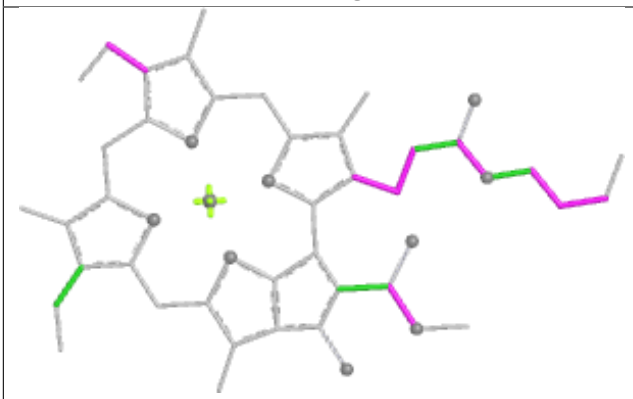
Ligand CLA r 611



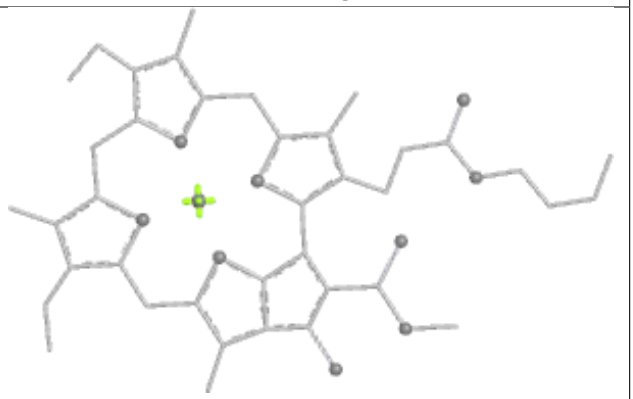
Bond lengths



Bond angles

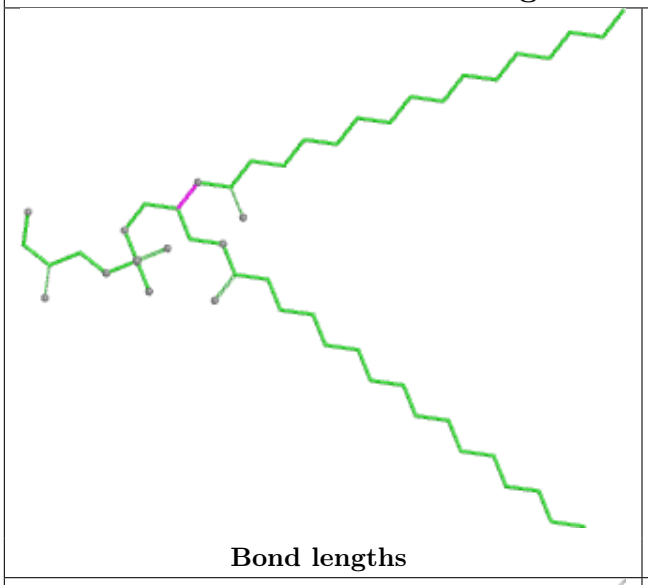


Torsions

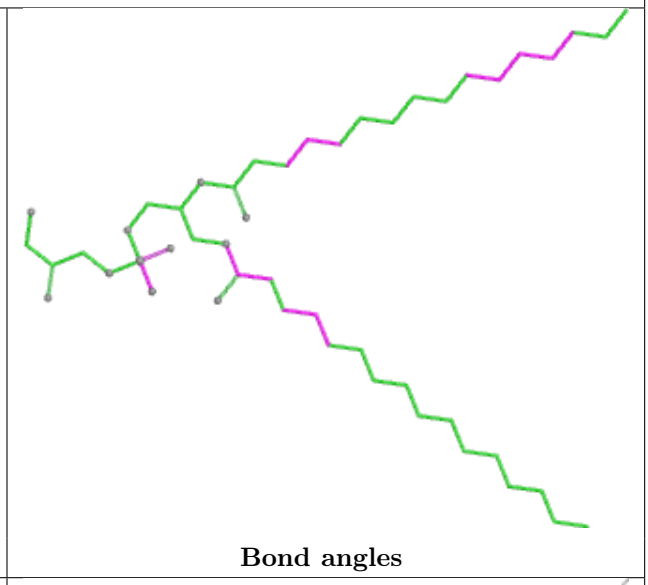


Rings

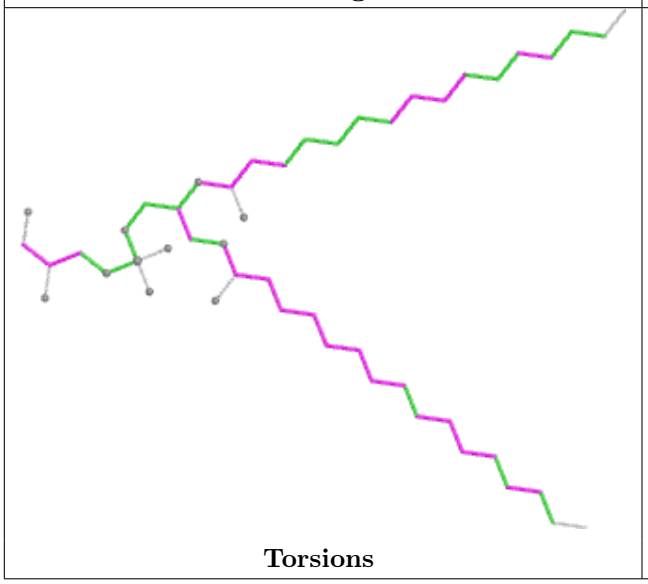
Ligand LHG c 2630



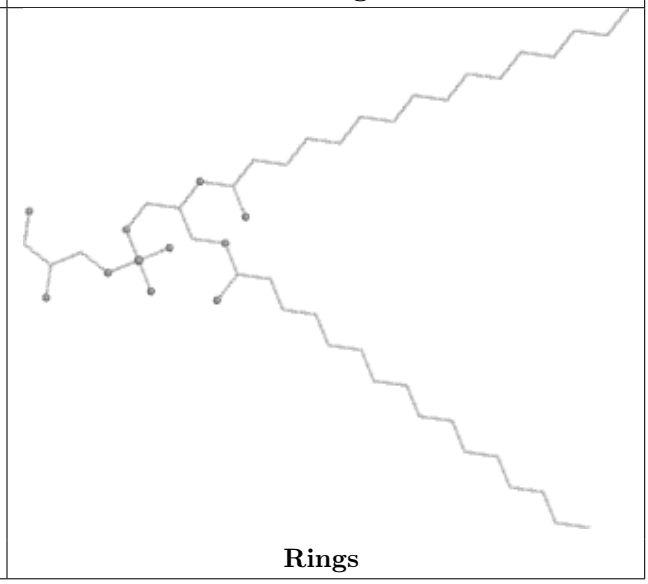
Bond lengths



Bond angles

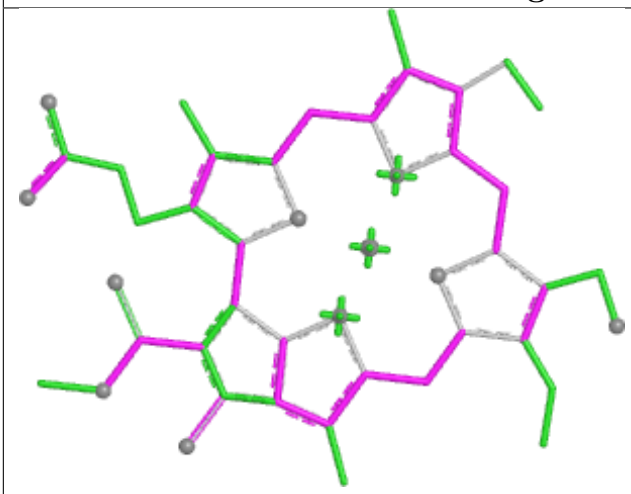


Torsions

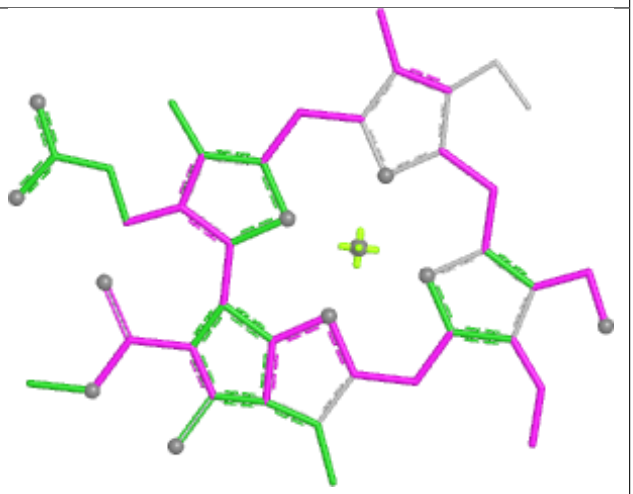


Rings

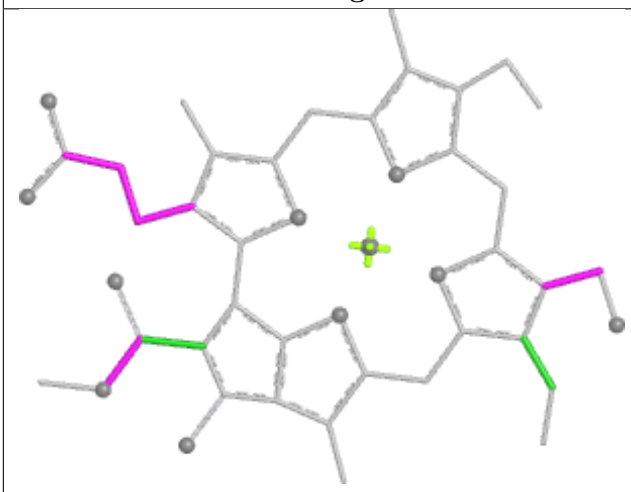
Ligand CHL 7 605



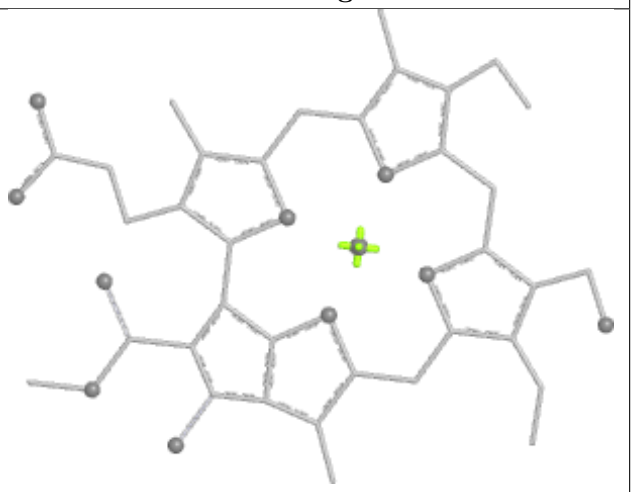
Bond lengths



Bond angles

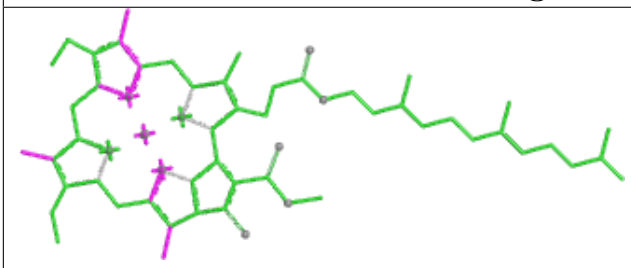


Torsions

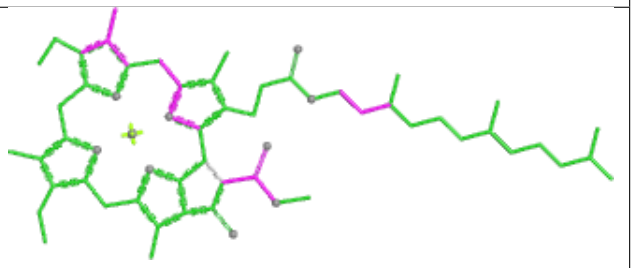


Rings

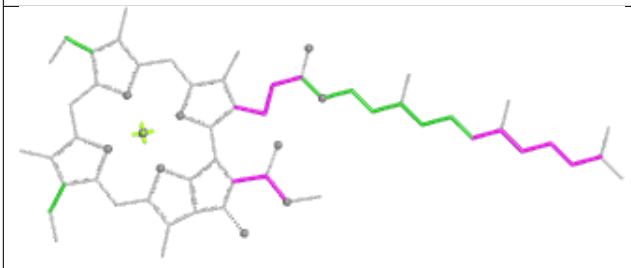
Ligand CLA 3 602



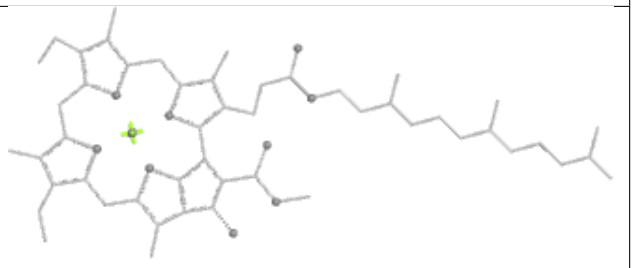
Bond lengths



Bond angles

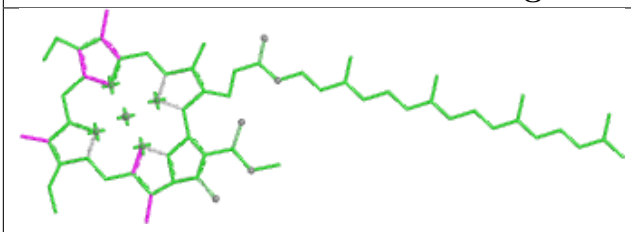


Torsions

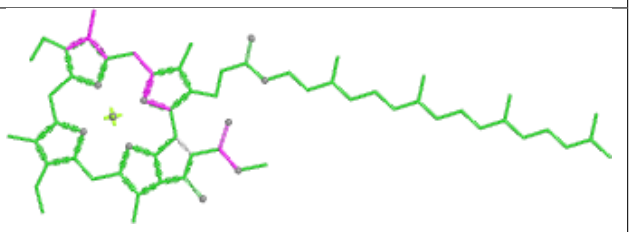


Rings

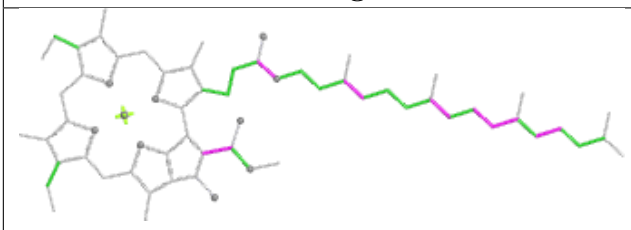
Ligand CLA C 504



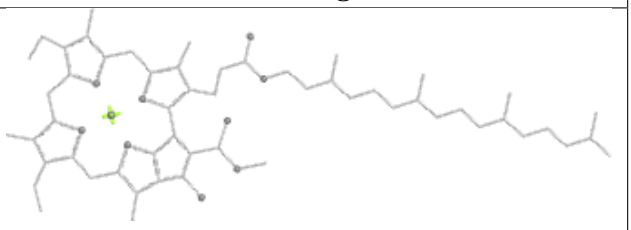
Bond lengths



Bond angles

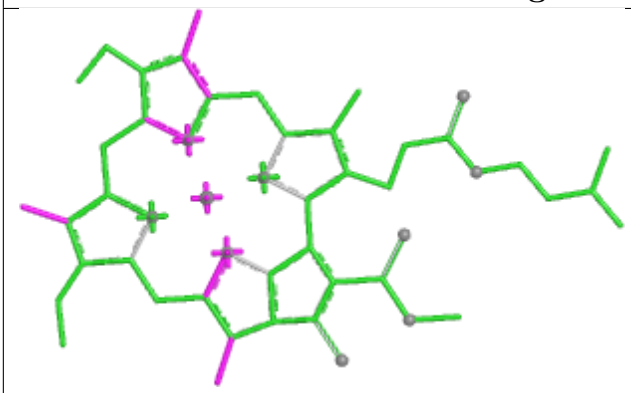


Torsions

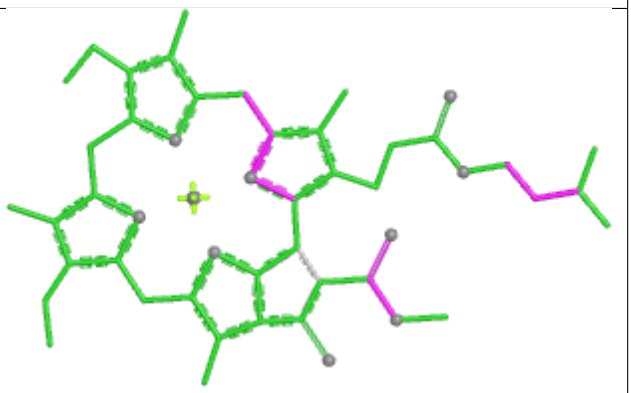


Rings

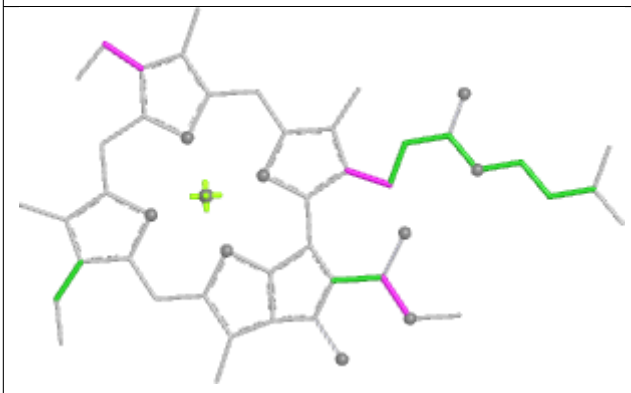
Ligand CLA a 407



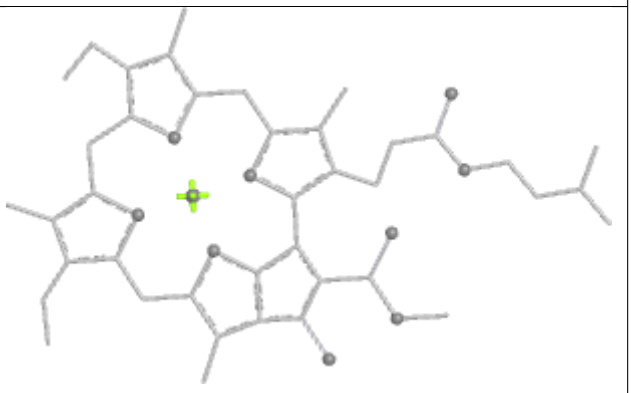
Bond lengths



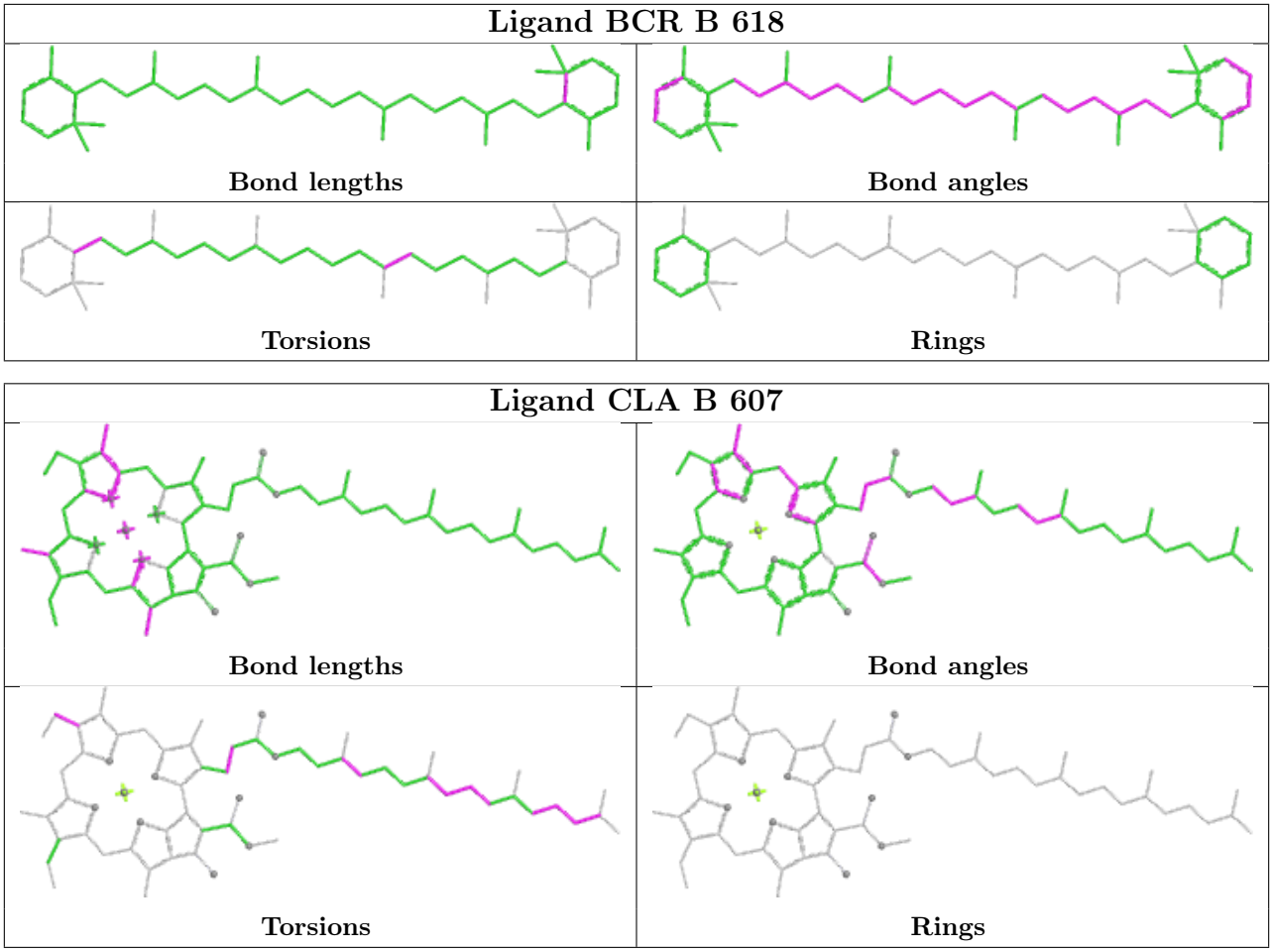
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

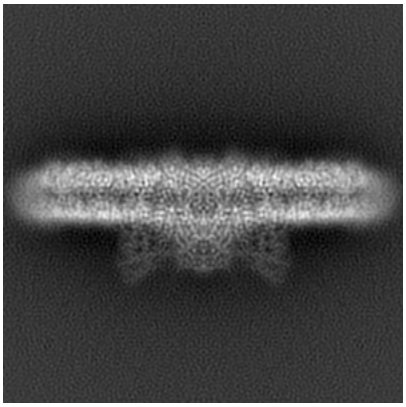
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6742. These allow visual inspection of the internal detail of the map and identification of artifacts.

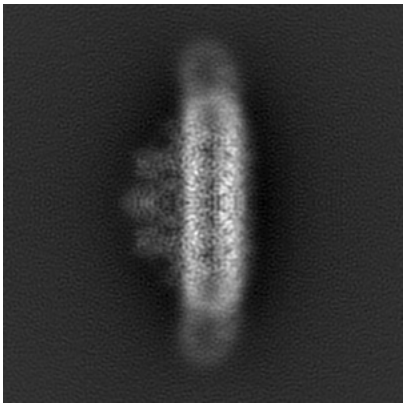
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

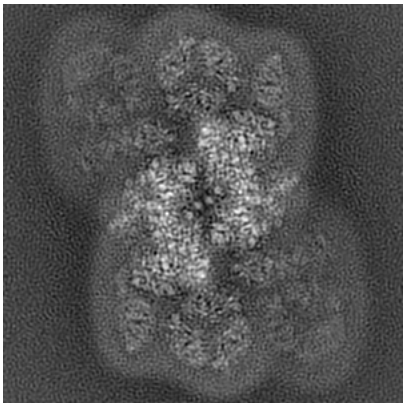
6.1.1 Primary map



X



Y

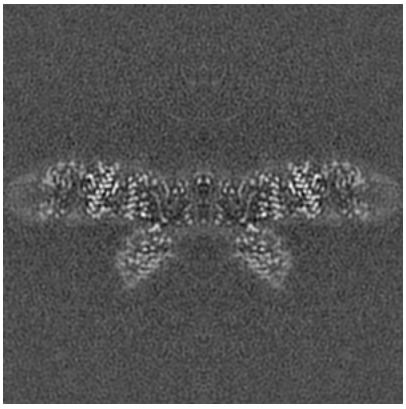


Z

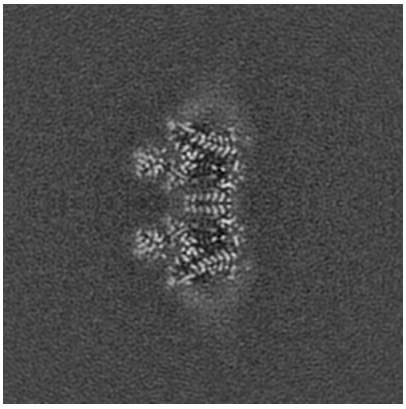
The images above show the map projected in three orthogonal directions.

6.2 Central slices

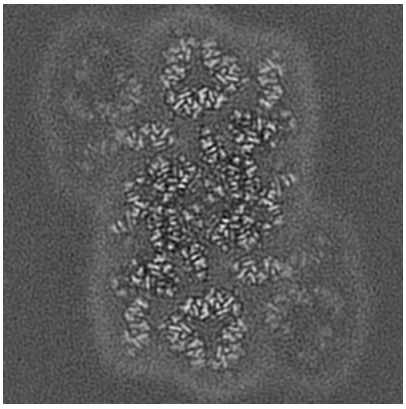
6.2.1 Primary map



X Index: 150



Y Index: 150

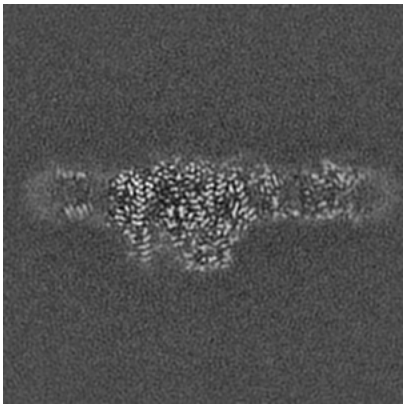


Z Index: 150

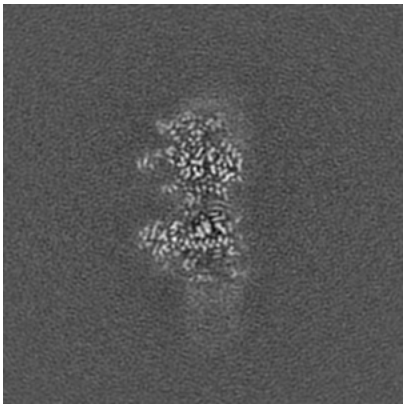
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

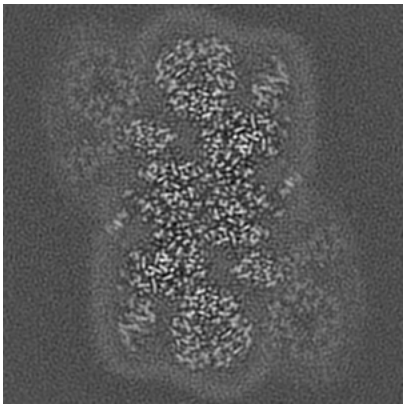
6.3.1 Primary map



X Index: 122



Y Index: 162

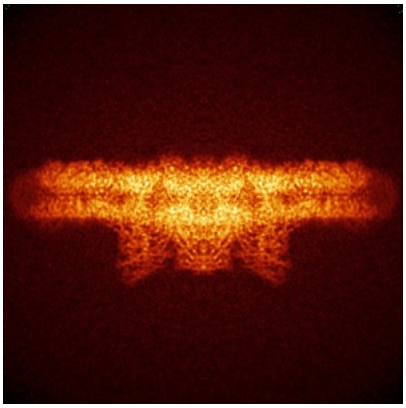


Z Index: 164

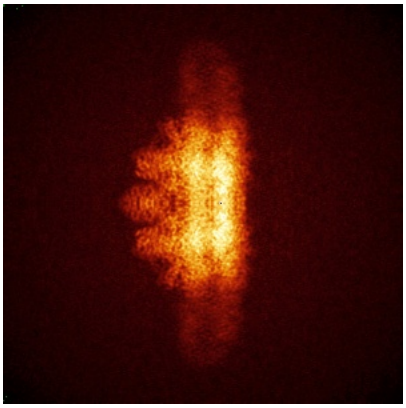
The images above show the largest variance slices of the map in three orthogonal directions.

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

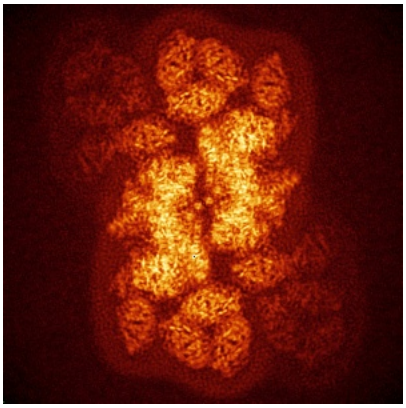
6.4.1 Primary map



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)

This section was not generated.

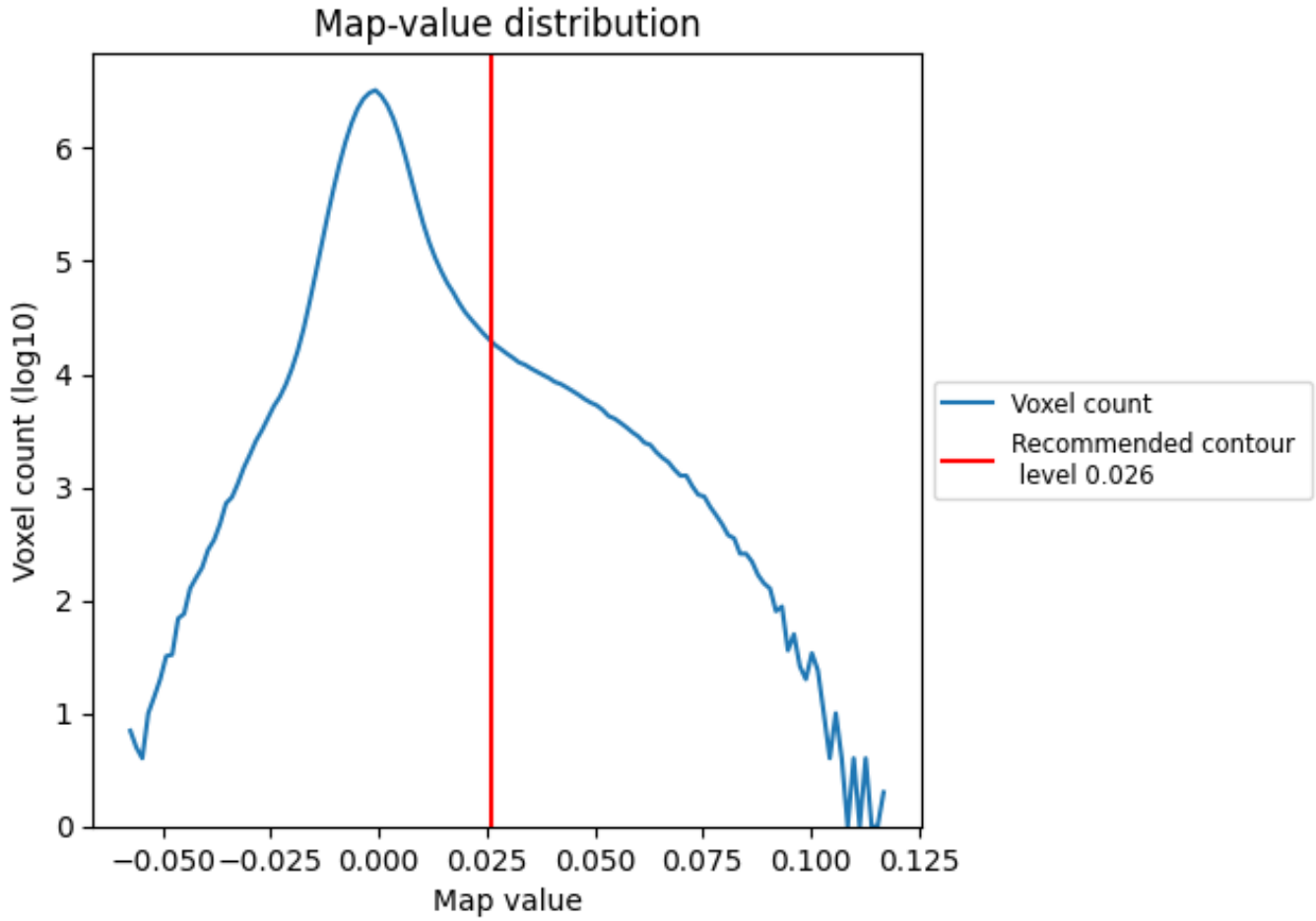
6.6 Mask visualisation (i)

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

7 Map analysis

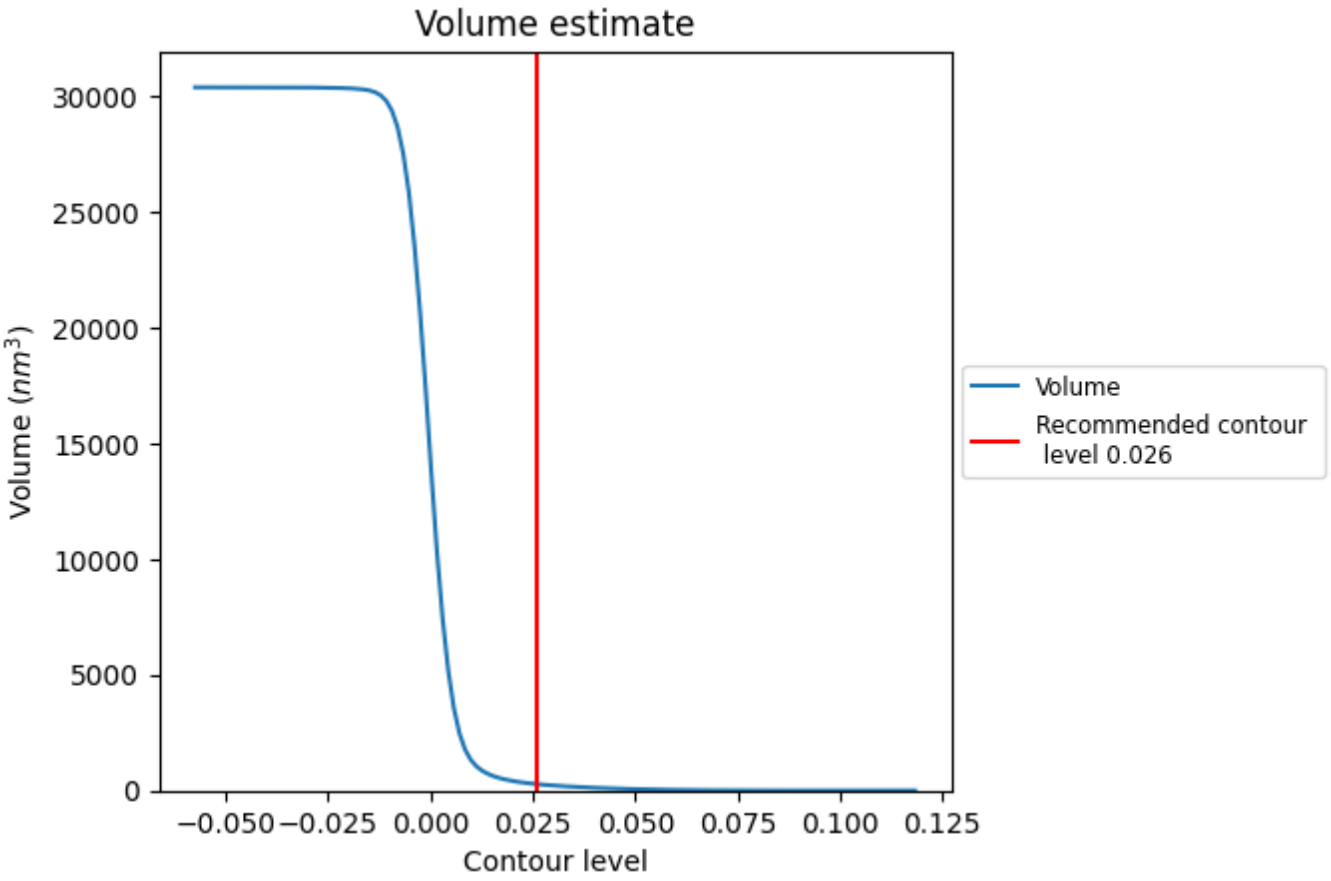
This section contains the results of statistical analysis of the map.

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.

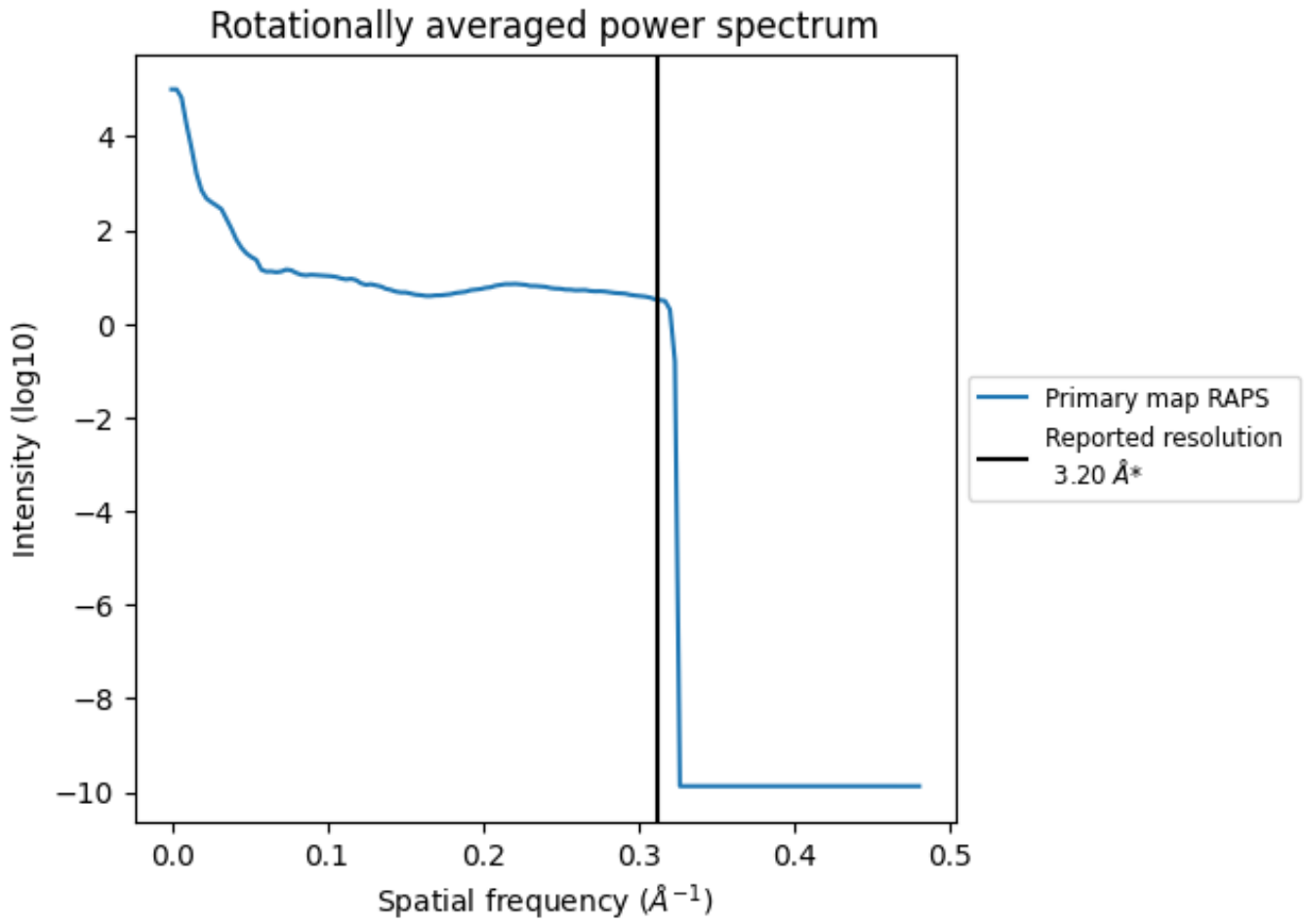
7.2 Volume estimate



The volume at the recommended contour level is 276 nm^3; this corresponds to an approximate mass of 249 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 0.312 $Å^{-1}$

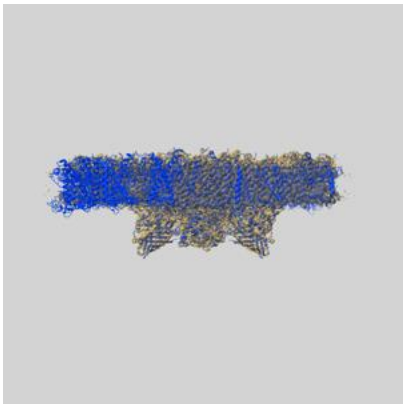
8 Fourier-Shell correlation

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

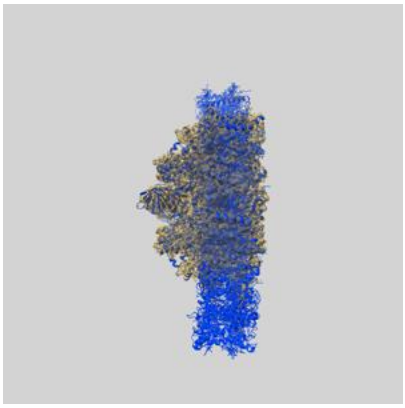
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6742 and PDB model 5XNM. Per-residue inclusion information can be found in section 3 on page 48.

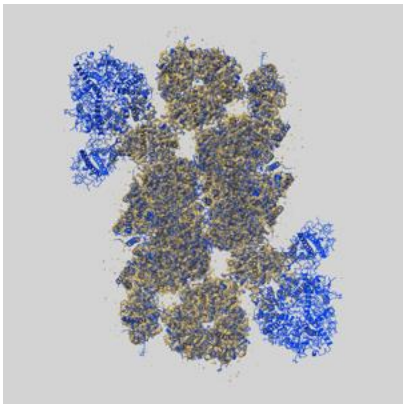
9.1 Map-model overlay



X



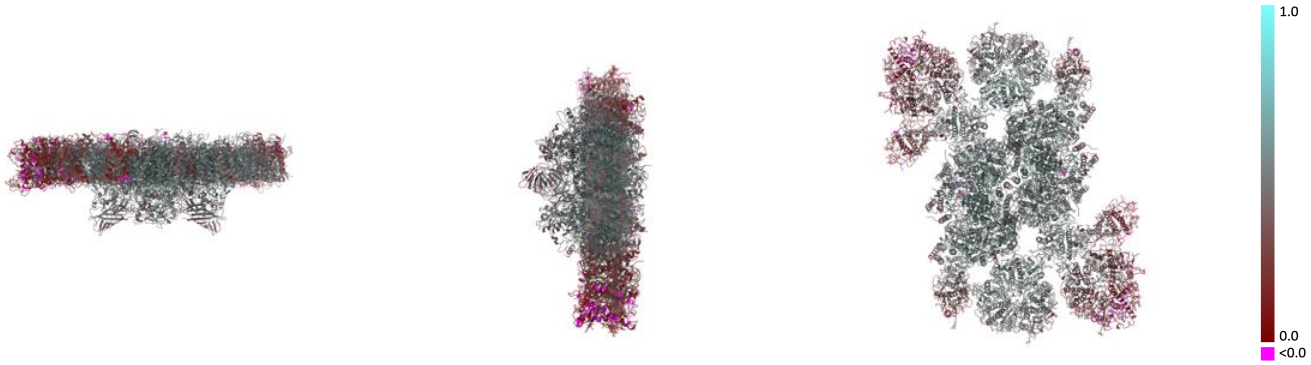
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026 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)



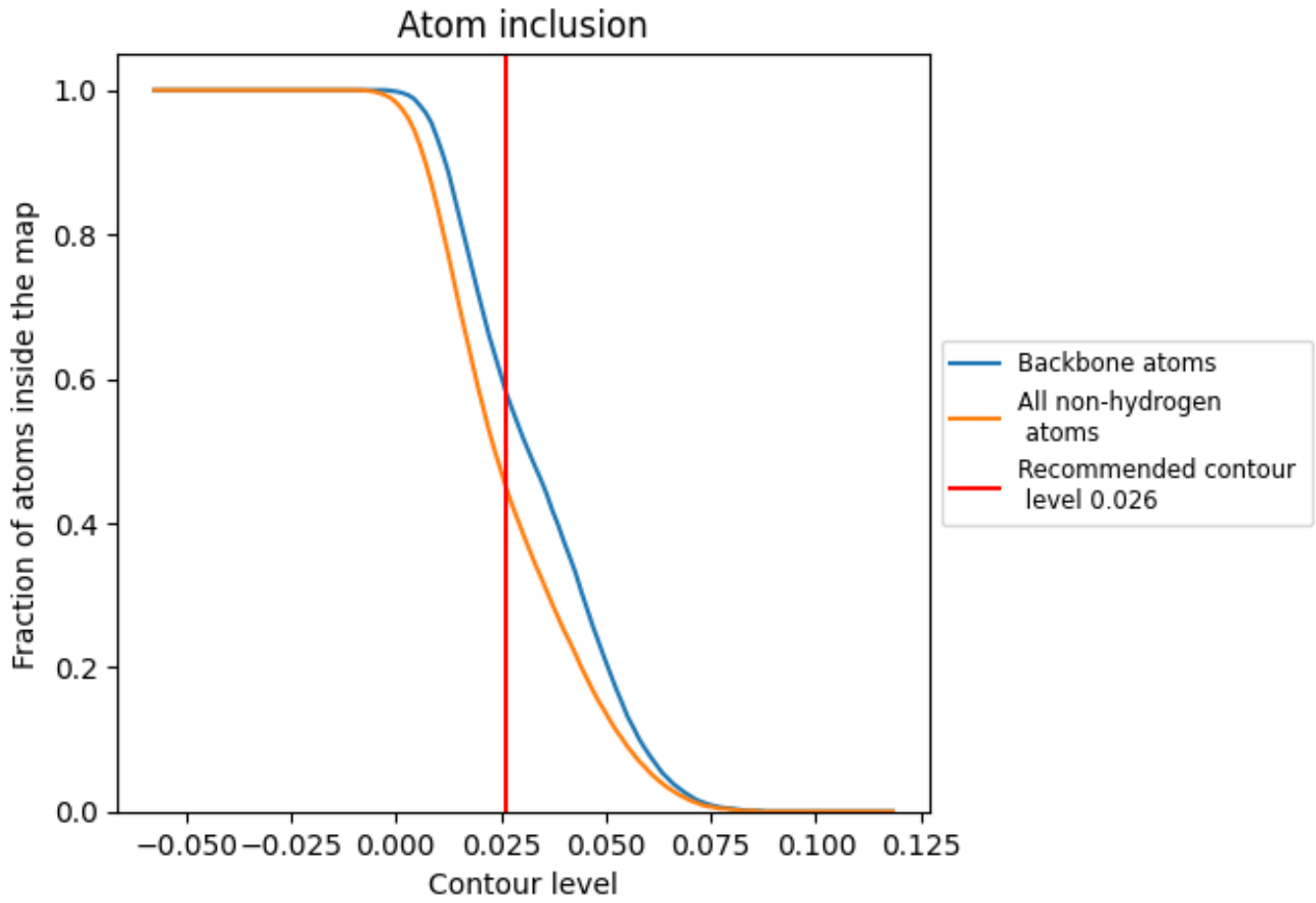
X Y Z

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)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 45% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4540	0.4380
1	0.0860	0.2990
2	0.0030	0.1580
3	0.0400	0.2970
4	0.0390	0.2450
5	0.0870	0.2990
6	0.0030	0.1560
7	0.0390	0.2950
8	0.0390	0.2440
A	0.6450	0.5320
B	0.6120	0.5170
C	0.5920	0.5110
D	0.6600	0.5410
E	0.4810	0.4190
F	0.5240	0.4390
G	0.5320	0.4690
H	0.5590	0.5160
I	0.6670	0.5430
J	0.0910	0.3730
K	0.5830	0.4850
L	0.5940	0.5140
M	0.4780	0.4670
N	0.5510	0.4770
O	0.4200	0.4010
R	0.5310	0.4820
S	0.4280	0.3750
T	0.5100	0.5200
U	0.3420	0.4140
W	0.5760	0.4860
X	0.4200	0.4390
Y	0.6590	0.5350
Z	0.3880	0.4010
a	0.6480	0.5320
b	0.6150	0.5180
c	0.5940	0.5110



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Chain	Atom inclusion	Q-score
d	0.6580	0.5400
e	0.4760	0.4190
f	0.5200	0.4380
g	0.5310	0.4630
h	0.5540	0.5110
i	0.6850	0.5440
j	0.0950	0.3710
k	0.5890	0.4840
l	0.5940	0.5190
m	0.4670	0.4620
n	0.5490	0.4720
o	0.4200	0.4030
r	0.5260	0.4830
s	0.4280	0.3740
t	0.5070	0.5170
u	0.3480	0.4170
w	0.5790	0.4920
x	0.4270	0.4410
y	0.6610	0.5320
z	0.3880	0.3920