Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:44 PM UTC

PDB ID	:	8BD3 / pdb_00008bd3
EMDB ID	:	EMD-15973
Title	:	Cryo-EM structure of the Photosystem II - LHCII supercomplex from Chlorella ohadi
Authors	:	Fadeeva, M.; Klaiman, D.; Caspy, I.; Nelson, N.
Deposited on	:	2022-10-18
Resolution	:	2.73 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

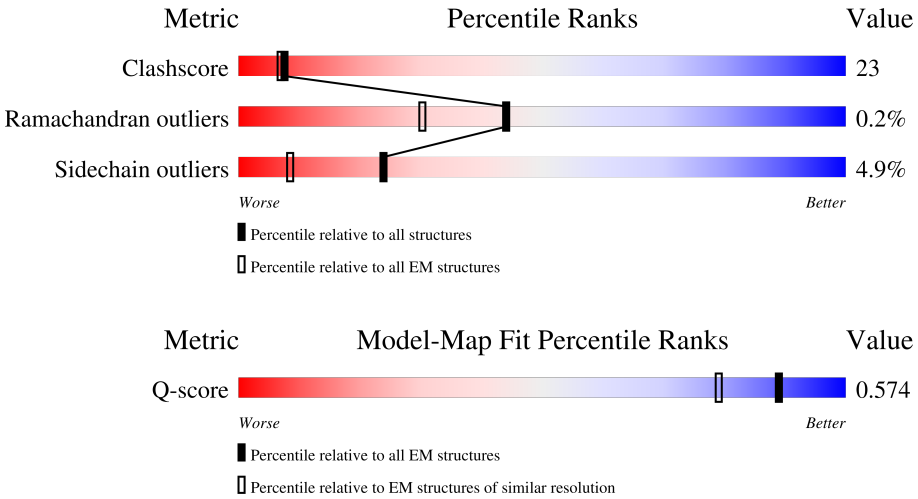
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.73 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	10432 (2.23 - 3.23)

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	214	61% 36% ·
1	7	214	68% 30% ·
2	2	222	· 50% 46% ·
2	4	222	· 44% 50% 6%

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Mol	Chain	Length	Quality of chain
2	9	222	59% 39%
2	G	222	67% 32%
2	g	222	73% 26%
2	q	222	46% 51%
3	3	221	44% 52% 5%
3	5	221	5% 35% 60%
3	8	221	63% 34%
3	N	221	62% 34%
3	n	221	64% 33%
3	p	221	6% 52% 44%
4	0	217	66% 31%
4	6	217	66% 31%
5	A	336	76% 22%
5	a	336	77% 21%
6	B	504	80% 19%
6	b	504	77% 22%
7	C	448	73% 24%
7	c	448	71% 26%
8	D	342	75% 24%
8	d	342	75% 23%
9	E	81	74% 25%
9	e	81	67% 33%
10	F	37	54% 46%
10	f	37	59% 41%
11	H	67	84% 15%

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Mol	Chain	Length	Quality of chain
11	h	67	79% 21%
12	I	34	79% 21%
12	i	34	79% 21%
13	J	38	92% 5%
13	j	38	84% 13%
14	K	37	59% 38%
14	k	37	70% 27%
15	L	37	68% 32%
15	l	37	70% 27%
16	M	57	11% 77% 21%
16	m	57	11% 82% 18%
17	O	240	74% 23%
17	o	240	81% 18%
18	R	236	74% 25%
18	r	236	75% 24%
19	S	257	74% 25%
19	s	257	74% 26%
20	T	30	70% 30%
20	t	30	57% 40%
21	V	32	84% 16%
21	v	32	88% 12%
22	W	60	60% 38%
22	w	60	68% 32%
23	X	37	70% 30%
23	x	37	81% 19%

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Mol	Chain	Length	Quality of chain
24	Y	221	78% 21%
24	y	221	72% 25%
25	Z	62	89% 11%
25	z	62	74% 26%
26	U	144	86% 14%
26	u	144	83% 16%
27	Q1	34	76% 24%
27	q1	34	62% 38%
28	P1	108	88% 12%
28	p1	108	82% 16%
29	F1	188	79% 18%
29	f1	188	80% 20%

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
30	CHL	0	601	X	-	-	-
30	CHL	0	605	X	-	-	-
30	CHL	0	606	X	-	-	-
30	CHL	0	607	X	-	-	-
30	CHL	0	608	X	-	-	-
30	CHL	0	609	X	-	-	-
30	CHL	1	601	X	-	-	-
30	CHL	1	605	X	-	-	-
30	CHL	1	606	X	-	-	-
30	CHL	1	607	X	-	-	-
30	CHL	1	608	X	-	-	-
30	CHL	1	609	X	-	-	-
30	CHL	1	619	X	-	-	-
30	CHL	2	601	X	-	-	-
30	CHL	2	605	X	-	-	-
30	CHL	2	606	X	-	-	-
30	CHL	2	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	2	608	X	-	-	-
30	CHL	3	302	X	-	-	-
30	CHL	3	303	X	-	-	-
30	CHL	3	307	X	-	-	-
30	CHL	3	308	X	-	-	-
30	CHL	3	309	X	-	-	-
30	CHL	3	310	X	-	-	-
30	CHL	4	601	X	-	-	-
30	CHL	4	605	X	-	-	-
30	CHL	4	606	X	-	-	-
30	CHL	4	607	X	-	-	-
30	CHL	4	608	X	-	-	-
30	CHL	4	609	X	-	-	-
30	CHL	5	601	X	-	-	-
30	CHL	5	605	X	-	-	-
30	CHL	5	606	X	-	-	-
30	CHL	5	607	X	-	-	-
30	CHL	5	608	X	-	-	-
30	CHL	5	609	X	-	-	-
30	CHL	6	302	X	-	-	-
30	CHL	6	306	X	-	-	-
30	CHL	6	307	X	-	-	-
30	CHL	6	308	X	-	-	-
30	CHL	6	309	X	-	-	-
30	CHL	6	310	X	-	-	-
30	CHL	7	302	X	-	-	-
30	CHL	7	306	X	-	-	-
30	CHL	7	307	X	-	-	-
30	CHL	7	308	X	-	-	-
30	CHL	7	309	X	-	-	-
30	CHL	7	310	X	-	-	-
30	CHL	7	321	X	-	-	-
30	CHL	8	601	X	-	-	-
30	CHL	8	605	X	-	-	-
30	CHL	8	606	X	-	-	-
30	CHL	8	607	X	-	-	-
30	CHL	8	608	X	-	-	-
30	CHL	9	303	X	-	-	-
30	CHL	9	307	X	-	-	-
30	CHL	9	308	X	-	-	-
30	CHL	9	309	X	-	-	-
30	CHL	9	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	9	311	X	-	-	-
30	CHL	G	601	X	-	-	-
30	CHL	G	605	X	-	-	-
30	CHL	G	606	X	-	-	-
30	CHL	G	607	X	-	-	-
30	CHL	G	608	X	-	-	-
30	CHL	G	623	X	-	-	-
30	CHL	N	301	X	-	-	-
30	CHL	N	302	X	-	-	-
30	CHL	N	306	X	-	-	-
30	CHL	N	307	X	-	-	-
30	CHL	N	308	X	-	-	-
30	CHL	N	309	X	-	-	-
30	CHL	R	308	X	-	-	-
30	CHL	R	309	X	-	-	-
30	CHL	R	310	X	-	-	-
30	CHL	S	302	X	-	-	-
30	CHL	S	307	X	-	-	-
30	CHL	S	308	X	-	-	-
30	CHL	S	309	X	-	-	-
30	CHL	Y	301	X	-	-	-
30	CHL	Y	302	X	-	-	-
30	CHL	Y	306	X	-	-	-
30	CHL	Y	307	X	-	-	-
30	CHL	Y	308	X	-	-	-
30	CHL	Y	309	X	-	-	-
30	CHL	g	302	X	-	-	-
30	CHL	g	306	X	-	-	-
30	CHL	g	307	X	-	-	-
30	CHL	g	308	X	-	-	-
30	CHL	g	309	X	-	-	-
30	CHL	n	301	X	-	-	-
30	CHL	n	302	X	-	-	-
30	CHL	n	306	X	-	-	-
30	CHL	n	307	X	-	-	-
30	CHL	n	308	X	-	-	-
30	CHL	n	309	X	-	-	-
30	CHL	n	310	X	-	-	-
30	CHL	p	601	X	-	-	-
30	CHL	p	605	X	-	-	-
30	CHL	p	606	X	-	-	-
30	CHL	p	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	p	608	X	-	-	-
30	CHL	p	609	X	-	-	-
30	CHL	q	303	X	-	-	-
30	CHL	q	307	X	-	-	-
30	CHL	q	308	X	-	-	-
30	CHL	q	309	X	-	-	-
30	CHL	q	310	X	-	-	-
30	CHL	q	311	X	-	-	-
30	CHL	r	308	X	-	-	-
30	CHL	r	309	X	-	-	-
30	CHL	r	310	X	-	-	-
30	CHL	s	302	X	-	-	-
30	CHL	s	307	X	-	-	-
30	CHL	s	308	X	-	-	-
30	CHL	s	309	X	-	-	-
30	CHL	y	601	X	-	-	-
30	CHL	y	605	X	-	-	-
30	CHL	y	606	X	-	-	-
30	CHL	y	607	X	-	-	-
30	CHL	y	608	X	-	-	-
30	CHL	y	609	X	-	-	-
31	CLA	0	602	X	-	-	-
31	CLA	0	603	X	-	-	-
31	CLA	0	604	X	-	-	-
31	CLA	0	610	X	-	-	-
31	CLA	0	611	X	-	-	-
31	CLA	0	612	X	-	-	-
31	CLA	0	613	X	-	-	-
31	CLA	0	614	X	-	-	-
31	CLA	0	615	X	-	-	-
31	CLA	1	602	X	-	-	-
31	CLA	1	603	X	-	-	-
31	CLA	1	604	X	-	-	-
31	CLA	1	610	X	-	-	-
31	CLA	1	611	X	-	-	-
31	CLA	1	612	X	-	-	-
31	CLA	1	613	X	-	-	-
31	CLA	1	614	X	-	-	-
31	CLA	2	602	X	-	-	-
31	CLA	2	603	X	-	-	-
31	CLA	2	604	X	-	-	-
31	CLA	2	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	2	610	X	-	-	-
31	CLA	2	611	X	-	-	-
31	CLA	2	612	X	-	-	-
31	CLA	2	613	X	-	-	-
31	CLA	3	301	X	-	-	-
31	CLA	3	304	X	-	-	-
31	CLA	3	305	X	-	-	-
31	CLA	3	306	X	-	-	-
31	CLA	3	311	X	-	-	-
31	CLA	3	312	X	-	-	-
31	CLA	3	313	X	-	-	-
31	CLA	3	314	X	-	-	-
31	CLA	3	315	X	-	-	-
31	CLA	3	316	X	-	-	-
31	CLA	4	602	X	-	-	-
31	CLA	4	603	X	-	-	-
31	CLA	4	604	X	-	-	-
31	CLA	4	610	X	-	-	-
31	CLA	4	611	X	-	-	-
31	CLA	4	612	X	-	-	-
31	CLA	4	613	X	-	-	-
31	CLA	4	614	X	-	-	-
31	CLA	5	602	X	-	-	-
31	CLA	5	603	X	-	-	-
31	CLA	5	604	X	-	-	-
31	CLA	5	610	X	-	X	-
31	CLA	5	611	X	-	-	-
31	CLA	5	612	X	-	-	-
31	CLA	5	613	X	-	-	-
31	CLA	5	614	X	-	-	-
31	CLA	5	615	X	-	-	-
31	CLA	6	303	X	-	-	-
31	CLA	6	304	X	-	-	-
31	CLA	6	305	X	-	-	-
31	CLA	6	311	X	-	-	-
31	CLA	6	312	X	-	-	-
31	CLA	6	313	X	-	-	-
31	CLA	6	314	X	-	-	-
31	CLA	6	315	X	-	-	-
31	CLA	6	316	X	-	-	-
31	CLA	7	303	X	-	-	-
31	CLA	7	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	7	305	X	-	-	-
31	CLA	7	311	X	-	-	-
31	CLA	7	312	X	-	-	-
31	CLA	7	313	X	-	-	-
31	CLA	7	314	X	-	-	-
31	CLA	7	315	X	-	-	-
31	CLA	7	316	X	-	-	-
31	CLA	8	602	X	-	-	-
31	CLA	8	603	X	-	-	-
31	CLA	8	604	X	-	-	-
31	CLA	8	609	X	-	-	-
31	CLA	8	610	X	-	-	-
31	CLA	8	611	X	-	-	-
31	CLA	8	612	X	-	-	-
31	CLA	8	613	X	-	-	-
31	CLA	8	614	X	-	-	-
31	CLA	9	304	X	-	-	-
31	CLA	9	305	X	-	-	-
31	CLA	9	306	X	-	-	-
31	CLA	9	312	X	-	-	-
31	CLA	9	313	X	-	-	-
31	CLA	9	314	X	-	-	-
31	CLA	9	315	X	-	-	-
31	CLA	9	316	X	-	-	-
31	CLA	A	405	X	-	-	-
31	CLA	A	406	X	-	-	-
31	CLA	A	407	X	-	-	-
31	CLA	A	409	X	-	-	-
31	CLA	B	601	X	-	-	-
31	CLA	B	602	X	-	-	-
31	CLA	B	603	X	-	-	-
31	CLA	B	604	X	-	-	-
31	CLA	B	605	X	-	-	-
31	CLA	B	606	X	-	-	-
31	CLA	B	607	X	-	-	-
31	CLA	B	608	X	-	-	-
31	CLA	B	609	X	-	-	-
31	CLA	B	610	X	-	-	-
31	CLA	B	611	X	-	-	-
31	CLA	B	612	X	-	-	-
31	CLA	B	613	X	-	-	-
31	CLA	B	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	B	615	X	-	-	-
31	CLA	B	616	X	-	-	-
31	CLA	C	601	X	-	-	-
31	CLA	C	602	X	-	-	-
31	CLA	C	603	X	-	-	-
31	CLA	C	604	X	-	-	-
31	CLA	C	605	X	-	-	-
31	CLA	C	606	X	-	-	-
31	CLA	C	607	X	-	-	-
31	CLA	C	608	X	-	-	-
31	CLA	C	609	X	-	-	-
31	CLA	C	610	X	-	-	-
31	CLA	C	611	X	-	-	-
31	CLA	C	612	X	-	-	-
31	CLA	C	613	X	-	-	-
31	CLA	D	403	X	-	-	-
31	CLA	D	404	X	-	-	-
31	CLA	G	602	X	-	-	-
31	CLA	G	603	X	-	-	-
31	CLA	G	604	X	-	-	-
31	CLA	G	609	X	-	-	-
31	CLA	G	610	X	-	-	-
31	CLA	G	611	X	-	-	-
31	CLA	G	612	X	-	-	-
31	CLA	G	613	X	-	-	-
31	CLA	N	303	X	-	-	-
31	CLA	N	304	X	-	-	-
31	CLA	N	305	X	-	-	-
31	CLA	N	310	X	-	-	-
31	CLA	N	311	X	-	-	-
31	CLA	N	312	X	-	-	-
31	CLA	N	313	X	-	-	-
31	CLA	N	314	X	-	-	-
31	CLA	N	315	X	-	-	-
31	CLA	N	321	X	-	-	-
31	CLA	R	303	X	-	-	-
31	CLA	R	304	X	-	-	-
31	CLA	R	305	X	-	-	-
31	CLA	R	306	X	-	-	-
31	CLA	R	307	X	-	-	-
31	CLA	R	311	X	-	-	-
31	CLA	R	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	R	313	X	-	-	-
31	CLA	R	314	X	-	-	-
31	CLA	R	315	X	-	-	-
31	CLA	R	316	X	-	-	-
31	CLA	S	303	X	-	-	-
31	CLA	S	304	X	-	-	-
31	CLA	S	305	X	-	-	-
31	CLA	S	306	X	-	-	-
31	CLA	S	310	X	-	-	-
31	CLA	S	311	X	-	-	-
31	CLA	S	312	X	-	-	-
31	CLA	S	313	X	-	-	-
31	CLA	S	314	X	-	-	-
31	CLA	S	315	X	-	-	-
31	CLA	S	316	X	-	-	-
31	CLA	Y	303	X	-	-	-
31	CLA	Y	304	X	-	-	-
31	CLA	Y	305	X	-	-	-
31	CLA	Y	310	X	-	-	-
31	CLA	Y	311	X	-	-	-
31	CLA	Y	312	X	-	-	-
31	CLA	Y	313	X	-	-	-
31	CLA	Y	314	X	-	-	-
31	CLA	a	406	X	-	-	-
31	CLA	a	407	X	-	-	-
31	CLA	a	409	X	-	-	-
31	CLA	b	602	X	-	-	-
31	CLA	b	603	X	-	-	-
31	CLA	b	604	X	-	-	-
31	CLA	b	605	X	-	-	-
31	CLA	b	606	X	-	-	-
31	CLA	b	607	X	-	-	-
31	CLA	b	608	X	-	-	-
31	CLA	b	609	X	-	-	-
31	CLA	b	610	X	-	-	-
31	CLA	b	611	X	-	-	-
31	CLA	b	612	X	-	-	-
31	CLA	b	613	X	-	-	-
31	CLA	b	614	X	-	-	-
31	CLA	b	615	X	-	-	-
31	CLA	b	616	X	-	-	-
31	CLA	b	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	c	601	X	-	-	-
31	CLA	c	602	X	-	-	-
31	CLA	c	603	X	-	-	-
31	CLA	c	604	X	-	-	-
31	CLA	c	605	X	-	-	-
31	CLA	c	606	X	-	-	-
31	CLA	c	607	X	-	-	-
31	CLA	c	608	X	-	-	-
31	CLA	c	609	X	-	-	-
31	CLA	c	610	X	-	-	-
31	CLA	c	611	X	-	-	-
31	CLA	c	612	X	-	-	-
31	CLA	c	613	X	-	-	-
31	CLA	d	401	X	-	-	-
31	CLA	d	404	X	-	-	-
31	CLA	d	405	X	-	-	-
31	CLA	g	303	X	-	-	-
31	CLA	g	304	X	-	-	-
31	CLA	g	305	X	-	-	-
31	CLA	g	310	X	-	-	-
31	CLA	g	311	X	-	-	-
31	CLA	g	312	X	-	-	-
31	CLA	g	313	X	-	-	-
31	CLA	g	314	X	-	-	-
31	CLA	n	303	X	-	-	-
31	CLA	n	304	X	-	-	-
31	CLA	n	305	X	-	-	-
31	CLA	n	311	X	-	-	-
31	CLA	n	312	X	-	-	-
31	CLA	n	313	X	-	-	-
31	CLA	n	314	X	-	-	-
31	CLA	n	315	X	-	-	-
31	CLA	n	316	X	-	-	-
31	CLA	p	602	X	-	-	-
31	CLA	p	603	X	-	-	-
31	CLA	p	604	X	-	-	-
31	CLA	p	610	X	-	-	-
31	CLA	p	611	X	-	-	-
31	CLA	p	612	X	-	-	-
31	CLA	p	613	X	-	X	-
31	CLA	p	614	X	-	-	-
31	CLA	p	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	q	304	X	-	-	-
31	CLA	q	305	X	-	-	-
31	CLA	q	306	X	-	-	-
31	CLA	q	312	X	-	X	-
31	CLA	q	313	X	-	-	-
31	CLA	q	314	X	-	-	-
31	CLA	q	315	X	-	-	-
31	CLA	q	316	X	-	-	-
31	CLA	r	303	X	-	-	-
31	CLA	r	304	X	-	-	-
31	CLA	r	305	X	-	-	-
31	CLA	r	306	X	-	-	-
31	CLA	r	307	X	-	-	-
31	CLA	r	311	X	-	-	-
31	CLA	r	312	X	-	-	-
31	CLA	r	313	X	-	-	-
31	CLA	r	314	X	-	-	-
31	CLA	r	315	X	-	-	-
31	CLA	r	316	X	-	-	-
31	CLA	s	303	X	-	-	-
31	CLA	s	304	X	-	-	-
31	CLA	s	305	X	-	-	-
31	CLA	s	306	X	-	-	-
31	CLA	s	310	X	-	-	-
31	CLA	s	311	X	-	-	-
31	CLA	s	312	X	-	-	-
31	CLA	s	313	X	-	-	-
31	CLA	s	314	X	-	-	-
31	CLA	s	315	X	-	-	-
31	CLA	s	316	X	-	-	-
31	CLA	y	602	X	-	-	-
31	CLA	y	603	X	-	-	-
31	CLA	y	604	X	-	-	-
31	CLA	y	610	X	-	-	-
31	CLA	y	611	X	-	-	-
31	CLA	y	612	X	-	-	-
31	CLA	y	613	X	-	-	-
31	CLA	y	614	X	-	-	-
31	CLA	y	615	X	-	-	-
32	LUT	5	616	-	-	X	-
35	RRX	G	614	-	-	X	-
37	XAT	G	620	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
43	BCR	C	615	-	X	-	-
43	BCR	c	614	-	X	-	-
45	DGD	C	620	-	-	X	-
45	DGD	c	619	-	-	X	-
46	BCT	D	402	-	X	-	-

2 Entry composition (i)

There are 49 unique types of molecules in this entry. The entry contains 117990 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, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	214	Total	C	N	O	S	0	0
			1630	1056	265	304	5		
1	7	214	Total	C	N	O	S	0	0
			1630	1056	265	304	5		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	195	LEU	PHE	conflict	UNP A0A2P6TPU9
1	225	GLU	ASP	conflict	UNP A0A2P6TPU9
1	250	ASN	THR	conflict	UNP A0A2P6TPU9
7	195	LEU	PHE	conflict	UNP A0A2P6TPU9
7	225	GLU	ASP	conflict	UNP A0A2P6TPU9
7	250	ASN	THR	conflict	UNP A0A2P6TPU9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	222	Total	C	N	O	S	0	0
			1686	1089	271	321	5		
2	4	222	Total	C	N	O	S	0	0
			1685	1088	271	321	5		
2	G	222	Total	C	N	O	S	0	0
			1686	1089	271	321	5		
2	9	222	Total	C	N	O	S	0	0
			1686	1089	271	321	5		
2	q	222	Total	C	N	O	S	0	0
			1685	1088	271	321	5		
2	g	222	Total	C	N	O	S	0	0
			1686	1089	271	321	5		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	74	THR	SER	conflict	UNP A0A2P6TDA6
4	74	THR	SER	conflict	UNP A0A2P6TDA6
G	74	THR	SER	conflict	UNP A0A2P6TDA6
9	74	THR	SER	conflict	UNP A0A2P6TDA6
q	74	THR	SER	conflict	UNP A0A2P6TDA6
g	74	THR	SER	conflict	UNP A0A2P6TDA6

- Molecule 3 is a protein called Chlorophyll a-b binding of LHCII.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	5	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	N	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	8	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	p	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	n	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		

- Molecule 4 is a protein called Chlorophyll a-b binding of LHCII.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	217	Total	C	N	O	S	0	0
			1657	1070	271	311	5		
4	0	217	Total	C	N	O	S	0	0
			1657	1070	271	311	5		

- Molecule 5 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	336	Total	C	N	O	S	0	0
			2632	1718	431	469	14		
5	a	336	Total	C	N	O	S	0	0
			2632	1718	431	469	14		

- Molecule 6 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	504	Total	C	N	O	S	0	0
			3954	2583	667	692	12		
6	b	504	Total	C	N	O	S	0	0
			3954	2583	667	692	12		

- Molecule 7 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	448	Total	C	N	O	S	0	0
			3482	2280	584	603	15		
7	c	448	Total	C	N	O	S	0	0
			3482	2280	584	603	15		

- Molecule 8 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	342	Total	C	N	O	S	0	0
			2730	1806	449	464	11		
8	d	342	Total	C	N	O	S	0	0
			2730	1806	449	464	11		

- Molecule 9 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	81	Total	C	N	O	0	0
			652	423	106	123		
9	e	81	Total	C	N	O	0	0
			652	423	106	123		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	37	Total	C	N	O	S	0	0
			302	206	49	46	1		
10	f	37	Total	C	N	O	S	0	0
			302	206	49	46	1		

- Molecule 11 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	67	Total	C	N	O	S	0	0
			507	336	73	95	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	h	67	Total 507	C 336	N 73	O 95	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	34	Total 274	C 187	N 41	O 45	S 1	0	0
12	i	34	Total 274	C 187	N 41	O 45	S 1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	J	38	Total 270	C 182	N 42	O 46	0	0
13	j	38	Total 270	C 182	N 42	O 46	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	K	37	Total 295	C 204	N 43	O 48	0	0
14	k	37	Total 295	C 204	N 43	O 48	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	L	37	Total 303	C 203	N 48	O 52	0	0
15	l	37	Total 303	C 203	N 48	O 52	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	57	Total 370	C 242	N 60	O 67	S 1	0	0
16	m	57	Total 370	C 242	N 60	O 67	S 1	0	0

- Molecule 17 is a protein called Chloroplast oxygen-evolving enhancer protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	240	Total	C	N	O	S	0	0
			1789	1134	287	362	6		
17	o	240	Total	C	N	O	S	0	0
			1789	1134	287	362	6		

- Molecule 18 is a protein called Chlorophyll a b binding CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	236	Total	C	N	O	S	0	0
			1818	1148	311	352	7		
18	r	236	Total	C	N	O	S	0	0
			1818	1148	311	352	7		

- Molecule 19 is a protein called Chlorophyll a b-binding CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	257	Total	C	N	O	S	0	0
			1934	1242	323	364	5		
19	s	257	Total	C	N	O	S	0	0
			1934	1242	323	364	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	30	Total	C	N	O	S	0	0
			246	172	36	37	1		
20	t	30	Total	C	N	O	S	0	0
			246	172	36	37	1		

- Molecule 21 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	32	Total	C	N	O	0	0
			233	155	38	40		
21	v	32	Total	C	N	O	0	0
			233	155	38	40		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	60	Total 468	C 301	N 74	O 93	0	0
22	w	60	Total 468	C 301	N 74	O 93	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	37	Total 247	C 156	N 43	O 48	0	0
23	x	37	Total 247	C 156	N 43	O 48	0	0

- Molecule 24 is a protein called Multifunctional fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	221	Total 1688	C 1099	N 270	O 314	S 5	0	0
24	y	221	Total 1688	C 1099	N 270	O 314	S 5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	62	Total 478	C 335	N 68	O 74	S 1	0	0
25	z	62	Total 478	C 335	N 68	O 74	S 1	0	0

- Molecule 26 is a protein called Chloroplast oxygen-evolving enhancer protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	U	144	Total 1122	C 701	N 207	O 214	0	0
26	u	144	Total 1122	C 701	N 207	O 214	0	0

- Molecule 27 is a protein called Chloroplast PsbY.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q1	34	Total 260	C 171	N 44	O 44	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
27	q1	34	Total	C	N	O	S	0	0
			260	171	44	44	1		

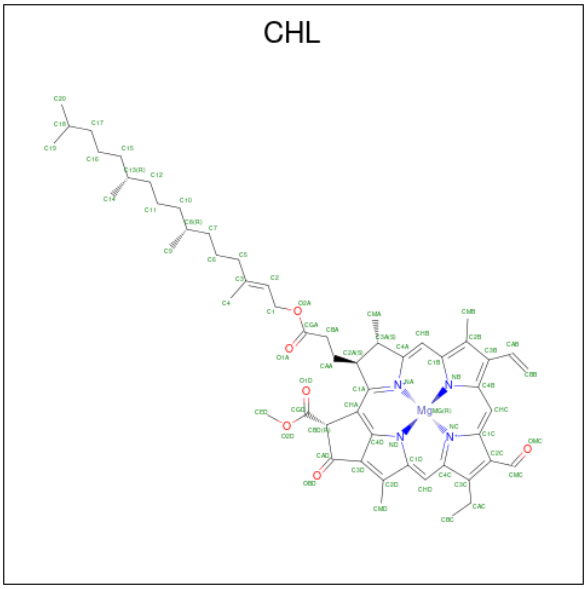
- Molecule 28 is a protein called Chloroplast photosystem II 10 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	P1	108	Total	C	N	O	S	0	0
			820	524	137	157	2		
28	p1	108	Total	C	N	O	S	0	0
			820	524	137	157	2		

- Molecule 29 is a protein called Photosystem II oxygen evolving enhancer 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	F1	188	Total	C	N	O	S	0	0
			1443	918	245	279	1		
29	f1	188	Total	C	N	O	S	0	0
			1443	918	245	279	1		

- Molecule 30 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
30	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
30	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			57	46	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			57	46	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			57	46	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
30	4	1	Total	C	Mg	N	O	0
			57	46	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	G	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
30	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	G	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	G	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
30	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	N	1	Total	C	Mg	N	O	0
			56	45	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
30	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	N	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
30	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	R	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	R	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	R	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
30	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	S	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
30	S	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	S	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
30	Y	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
30	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	Y	1	Total	C	Mg	N	O	0
			59	48	1	4	6	
30	Y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	0	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	0	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
30	0	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
30	0	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	0	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	7	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	7	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
30	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	8	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
30	8	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	9	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
30	9	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
30	9	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	9	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	p	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

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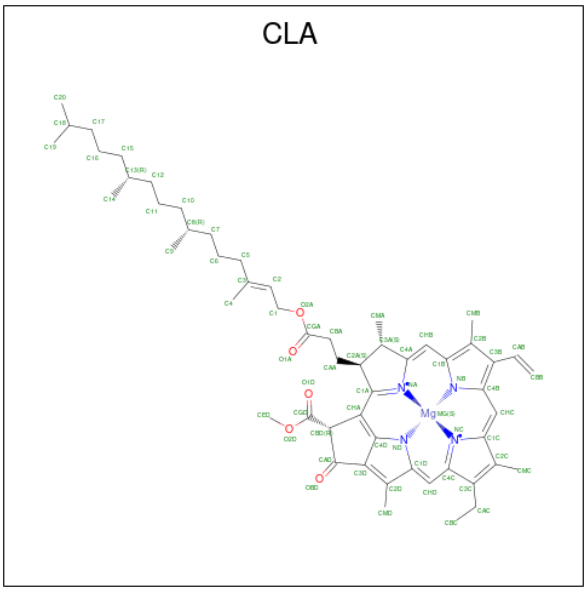
Mol	Chain	Residues	Atoms					AltConf
30	p	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	p	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	p	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	p	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	p	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	q	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	q	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	q	1	Total	C	Mg	N	O	0
			57	46	1	4	6	
30	q	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	q	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	g	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
30	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	g	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	g	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
30	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	n	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	n	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
30	n	1	Total	C	Mg	N	O	0
			63	52	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
30	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	r	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	r	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	r	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
30	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	s	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
30	s	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	s	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			59	48	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 31 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
31	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	1	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	2	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	2	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	C	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	R	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	R	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	R	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
31	R	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
31	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	S	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	S	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	S	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	S	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	Y	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	0	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	8	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	p	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	p	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	p	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	p	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	p	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	p	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	p	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	p	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	q	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
31	q	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
31	q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	d	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	g	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	g	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	n	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	n	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

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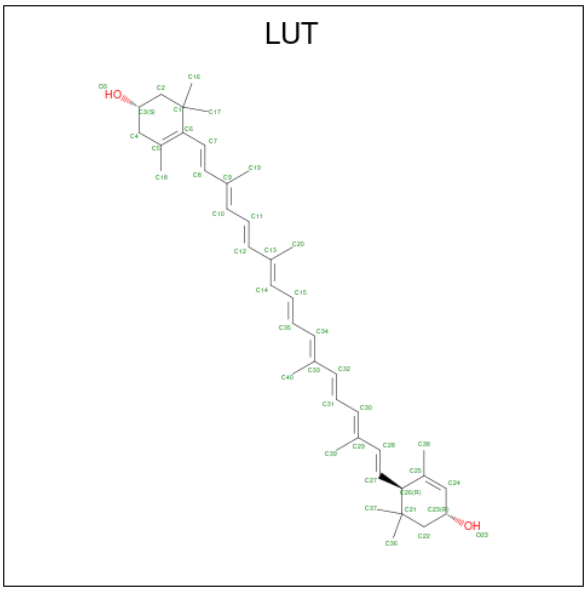
Mol	Chain	Residues	Atoms					AltConf
31	r	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

- Molecule 32 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
32	1	1	Total	C	O	0
			42	40	2	
32	1	1	Total	C	O	0
			42	40	2	
32	2	1	Total	C	O	0
			42	40	2	
32	3	1	Total	C	O	0
			42	40	2	
32	3	1	Total	C	O	0
			42	40	2	
32	4	1	Total	C	O	0
			42	40	2	
32	5	1	Total	C	O	0
			42	40	2	

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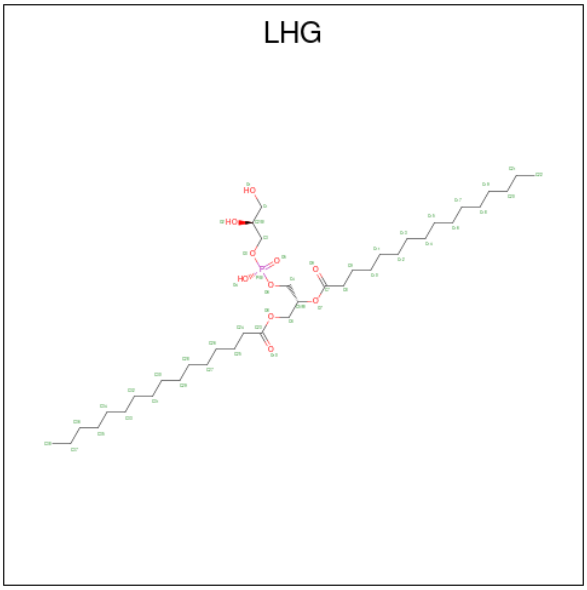
Mol	Chain	Residues	Atoms			AltConf
32	5	1	Total	C	O	0
			42	40	2	
32	6	1	Total	C	O	0
			42	40	2	
32	6	1	Total	C	O	0
			42	40	2	
32	G	1	Total	C	O	0
			42	40	2	
32	N	1	Total	C	O	0
			42	40	2	
32	N	1	Total	C	O	0
			42	40	2	
32	R	1	Total	C	O	0
			42	40	2	
32	S	1	Total	C	O	0
			42	40	2	
32	S	1	Total	C	O	0
			42	40	2	
32	Y	1	Total	C	O	0
			42	40	2	
32	Y	1	Total	C	O	0
			42	40	2	
32	0	1	Total	C	O	0
			42	40	2	
32	0	1	Total	C	O	0
			42	40	2	
32	7	1	Total	C	O	0
			42	40	2	
32	7	1	Total	C	O	0
			42	40	2	
32	8	1	Total	C	O	0
			42	40	2	
32	8	1	Total	C	O	0
			42	40	2	
32	9	1	Total	C	O	0
			42	40	2	
32	p	1	Total	C	O	0
			42	40	2	
32	p	1	Total	C	O	0
			42	40	2	
32	q	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms	AltConf
32	g	1	Total C O 42 40 2	0
32	n	1	Total C O 42 40 2	0
32	n	1	Total C O 42 40 2	0
32	r	1	Total C O 42 40 2	0
32	s	1	Total C O 42 40 2	0
32	s	1	Total C O 42 40 2	0
32	y	1	Total C O 42 40 2	0
32	y	1	Total C O 42 40 2	0

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
33	1	1	Total C O P 35 24 10 1	0
33	2	1	Total C O P 49 38 10 1	0
33	3	1	Total C O P 33 22 10 1	0

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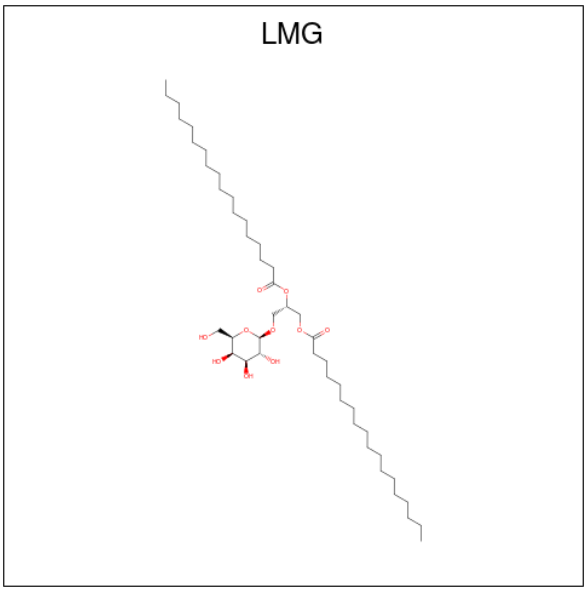
Mol	Chain	Residues	Atoms				AltConf
33	4	1	Total	C	O	P	0
			47	36	10	1	
33	5	1	Total	C	O	P	0
			35	24	10	1	
33	6	1	Total	C	O	P	0
			37	26	10	1	
33	A	1	Total	C	O	P	0
			44	33	10	1	
33	A	1	Total	C	O	P	0
			39	28	10	1	
33	B	1	Total	C	O	P	0
			49	38	10	1	
33	C	1	Total	C	O	P	0
			40	29	10	1	
33	D	1	Total	C	O	P	0
			44	33	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	G	1	Total	C	O	P	0
			44	33	10	1	
33	K	1	Total	C	O	P	0
			36	25	10	1	
33	L	1	Total	C	O	P	0
			49	38	10	1	
33	M	1	Total	C	O	P	0
			41	30	10	1	
33	N	1	Total	C	O	P	0
			49	38	10	1	
33	R	1	Total	C	O	P	0
			38	27	10	1	
33	S	1	Total	C	O	P	0
			41	30	10	1	
33	S	1	Total	C	O	P	0
			44	33	10	1	
33	Y	1	Total	C	O	P	0
			42	31	10	1	
33	0	1	Total	C	O	P	0
			36	25	10	1	
33	7	1	Total	C	O	P	0
			35	24	10	1	
33	8	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
33	9	1	Total	C	O	P	0
			33	22	10	1	
33	p	1	Total	C	O	P	0
			35	24	10	1	
33	q	1	Total	C	O	P	0
			46	35	10	1	
33	a	1	Total	C	O	P	0
			39	28	10	1	
33	b	1	Total	C	O	P	0
			44	33	10	1	
33	b	1	Total	C	O	P	0
			49	38	10	1	
33	c	1	Total	C	O	P	0
			47	36	10	1	
33	d	1	Total	C	O	P	0
			49	38	10	1	
33	e	1	Total	C	O	P	0
			44	33	10	1	
33	g	1	Total	C	O	P	0
			44	33	10	1	
33	j	1	Total	C	O	P	0
			49	38	10	1	
33	l	1	Total	C	O	P	0
			49	38	10	1	
33	n	1	Total	C	O	P	0
			49	38	10	1	
33	r	1	Total	C	O	P	0
			38	27	10	1	
33	s	1	Total	C	O	P	0
			41	30	10	1	
33	s	1	Total	C	O	P	0
			44	33	10	1	
33	t	1	Total	C	O	P	0
			41	30	10	1	
33	y	1	Total	C	O	P	0
			46	35	10	1	
33	z	1	Total	C	O	P	0
			36	25	10	1	
33	F1	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
34	1	1	Total	C	O	0
			38	28	10	
34	2	1	Total	C	O	0
			38	28	10	
34	2	1	Total	C	O	0
			51	41	10	
34	2	1	Total	C	O	0
			40	30	10	
34	3	1	Total	C	O	0
			38	28	10	
34	4	1	Total	C	O	0
			51	41	10	
34	4	1	Total	C	O	0
			40	30	10	
34	5	1	Total	C	O	0
			38	28	10	
34	6	1	Total	C	O	0
			42	32	10	
34	6	1	Total	C	O	0
			39	29	10	
34	6	1	Total	C	O	0
			38	28	10	
34	A	1	Total	C	O	0
			41	31	10	
34	A	1	Total	C	O	0
			38	28	10	
34	A	1	Total	C	O	0
			38	28	10	

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Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			51	41	10	
34	B	1	Total	C	O	0
			38	28	10	
34	B	1	Total	C	O	0
			38	28	10	
34	C	1	Total	C	O	0
			51	41	10	
34	C	1	Total	C	O	0
			38	28	10	
34	C	1	Total	C	O	0
			32	22	10	
34	C	1	Total	C	O	0
			44	34	10	
34	D	1	Total	C	O	0
			46	36	10	
34	D	1	Total	C	O	0
			46	36	10	
34	D	1	Total	C	O	0
			51	41	10	
34	D	1	Total	C	O	0
			48	38	10	
34	G	1	Total	C	O	0
			38	28	10	
34	G	1	Total	C	O	0
			51	41	10	
34	G	1	Total	C	O	0
			40	30	10	
34	I	1	Total	C	O	0
			38	28	10	
34	J	1	Total	C	O	0
			51	41	10	
34	J	1	Total	C	O	0
			38	28	10	
34	N	1	Total	C	O	0
			38	28	10	
34	R	1	Total	C	O	0
			38	28	10	
34	S	1	Total	C	O	0
			41	31	10	
34	W	1	Total	C	O	0
			55	45	10	

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Mol	Chain	Residues	Atoms			AltConf
34	W	1	Total	C	O	0
			38	28	10	
34	W	1	Total	C	O	0
			38	28	10	
34	X	1	Total	C	O	0
			38	28	10	
34	X	1	Total	C	O	0
			38	28	10	
34	Y	1	Total	C	O	0
			38	28	10	
34	0	1	Total	C	O	0
			42	32	10	
34	0	1	Total	C	O	0
			38	28	10	
34	7	1	Total	C	O	0
			39	29	10	
34	7	1	Total	C	O	0
			38	28	10	
34	7	1	Total	C	O	0
			38	28	10	
34	9	1	Total	C	O	0
			51	41	10	
34	9	1	Total	C	O	0
			40	30	10	
34	9	1	Total	C	O	0
			38	28	10	
34	p	1	Total	C	O	0
			38	28	10	
34	q	1	Total	C	O	0
			51	41	10	
34	q	1	Total	C	O	0
			40	30	10	
34	a	1	Total	C	O	0
			38	28	10	
34	a	1	Total	C	O	0
			38	28	10	
34	a	1	Total	C	O	0
			38	28	10	
34	b	1	Total	C	O	0
			45	35	10	
34	b	1	Total	C	O	0
			51	41	10	

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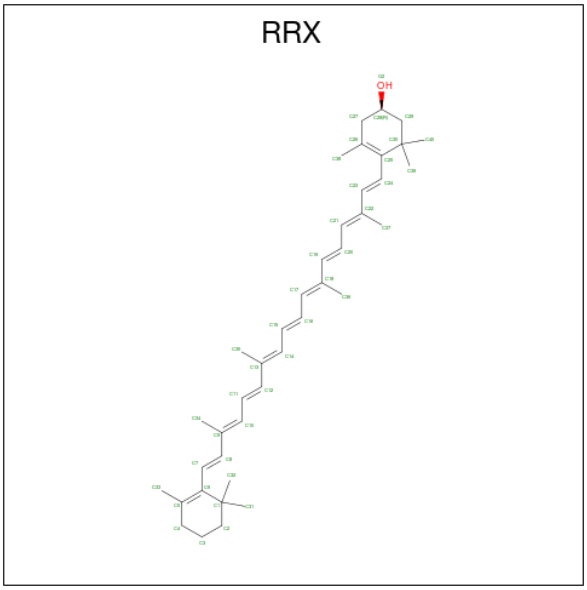
Mol	Chain	Residues	Atoms	AltConf
34	b	1	Total C O 38 28 10	0
34	b	1	Total C O 38 28 10	0
34	b	1	Total C O 46 36 10	0
34	b	1	Total C O 38 28 10	0
34	c	1	Total C O 38 28 10	0
34	c	1	Total C O 38 28 10	0
34	c	1	Total C O 44 34 10	0
34	d	1	Total C O 41 31 10	0
34	d	1	Total C O 51 41 10	0
34	d	1	Total C O 48 38 10	0
34	f	1	Total C O 38 28 10	0
34	g	1	Total C O 38 28 10	0
34	g	1	Total C O 49 39 10	0
34	j	1	Total C O 43 33 10	0
34	k	1	Total C O 48 38 10	0
34	k	1	Total C O 38 28 10	0
34	m	1	Total C O 45 35 10	0
34	n	1	Total C O 38 28 10	0
34	n	1	Total C O 40 30 10	0
34	r	1	Total C O 38 28 10	0
34	s	1	Total C O 41 31 10	0

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Mol	Chain	Residues	Atoms	AltConf
34	w	1	Total C O 48 38 10	0
34	w	1	Total C O 55 45 10	0
34	w	1	Total C O 38 28 10	0
34	w	1	Total C O 38 28 10	0
34	w	1	Total C O 38 28 10	0
34	x	1	Total C O 38 28 10	0
34	y	1	Total C O 38 28 10	0
34	Q1	1	Total C O 38 28 10	0
34	q1	1	Total C O 38 28 10	0

- Molecule 35 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



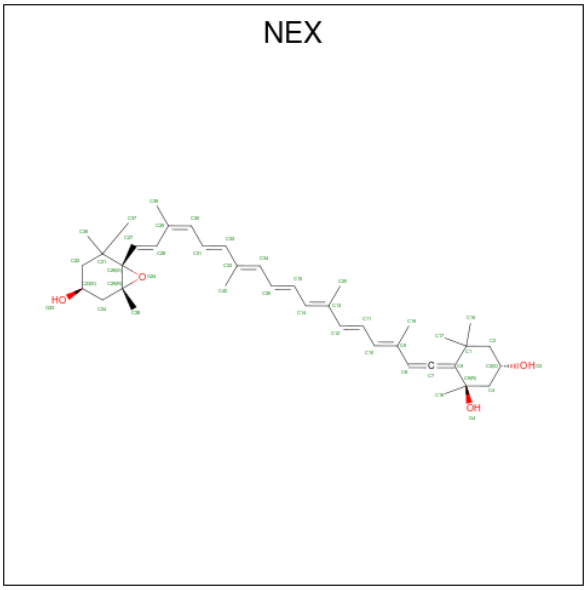
Mol	Chain	Residues	Atoms	AltConf
35	2	1	Total C O 41 40 1	0
35	4	1	Total C O 41 40 1	0

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Mol	Chain	Residues	Atoms	AltConf
35	G	1	Total C O 41 40 1	0
35	9	1	Total C O 41 40 1	0
35	q	1	Total C O 41 40 1	0
35	g	1	Total C O 41 40 1	0

- Molecule 36 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: $C_{40}H_{56}O_4$).



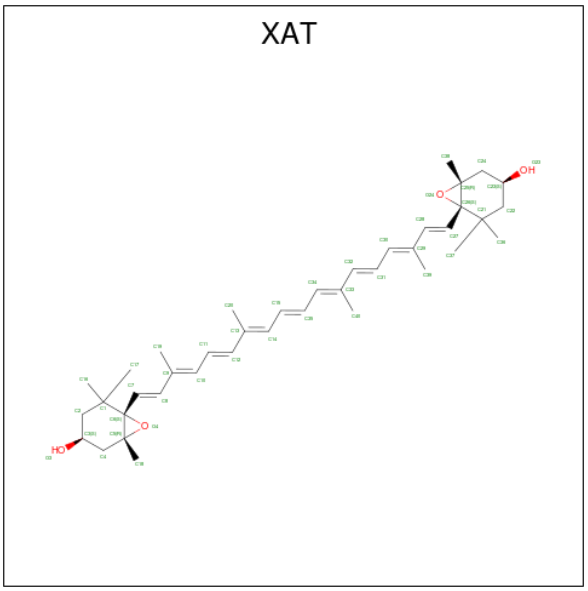
Mol	Chain	Residues	Atoms	AltConf
36	2	1	Total C O 44 40 4	0
36	3	1	Total C O 44 40 4	0
36	4	1	Total C O 44 40 4	0
36	5	1	Total C O 44 40 4	0
36	6	1	Total C O 44 40 4	0
36	G	1	Total C O 44 40 4	0

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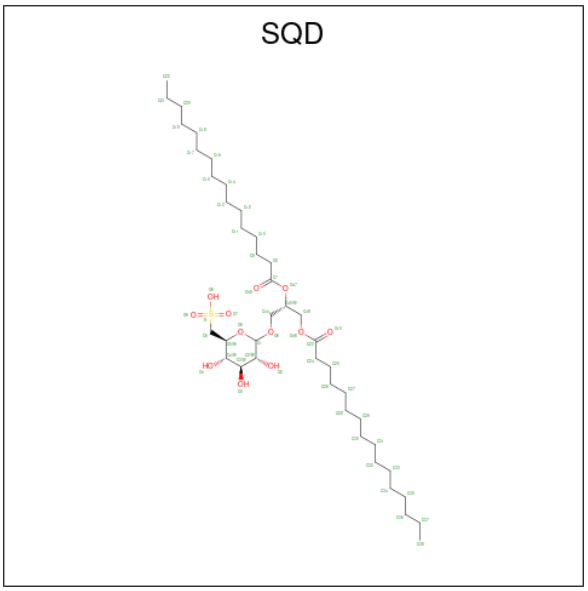
Mol	Chain	Residues	Atoms			AltConf
36	N	1	Total	C	O	0
			44	40	4	
36	R	1	Total	C	O	0
			44	40	4	
36	R	1	Total	C	O	0
			44	40	4	
36	S	1	Total	C	O	0
			44	40	4	
36	Y	1	Total	C	O	0
			44	40	4	
36	0	1	Total	C	O	0
			44	40	4	
36	8	1	Total	C	O	0
			44	40	4	
36	9	1	Total	C	O	0
			44	40	4	
36	p	1	Total	C	O	0
			44	40	4	
36	q	1	Total	C	O	0
			44	40	4	
36	g	1	Total	C	O	0
			44	40	4	
36	n	1	Total	C	O	0
			44	40	4	
36	r	1	Total	C	O	0
			44	40	4	
36	r	1	Total	C	O	0
			44	40	4	
36	s	1	Total	C	O	0
			44	40	4	
36	y	1	Total	C	O	0
			44	40	4	

- Molecule 37 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
37	2	1	Total C O 44 40 4	0
37	4	1	Total C O 44 40 4	0
37	G	1	Total C O 44 40 4	0
37	R	1	Total C O 44 40 4	0
37	9	1	Total C O 44 40 4	0
37	q	1	Total C O 44 40 4	0
37	g	1	Total C O 44 40 4	0
37	r	1	Total C O 44 40 4	0

- Molecule 38 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



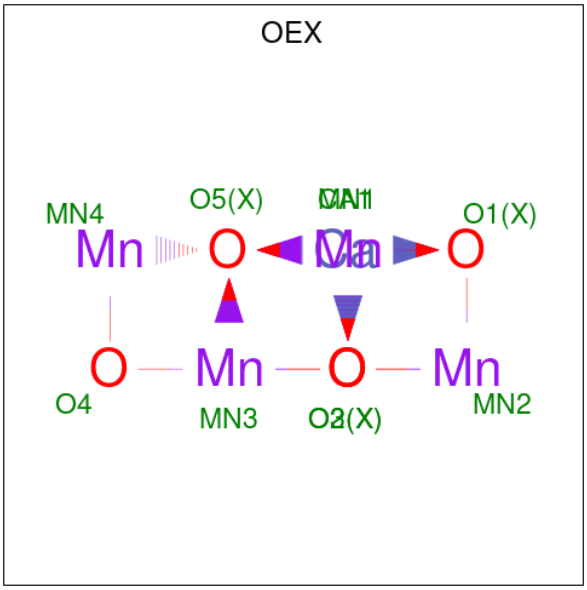
Mol	Chain	Residues	Atoms				AltConf
38	6	1	Total	C	O	S	0
			42	29	12	1	
38	A	1	Total	C	O	S	0
			51	38	12	1	
38	A	1	Total	C	O	S	0
			45	32	12	1	
38	B	1	Total	C	O	S	0
			54	41	12	1	
38	B	1	Total	C	O	S	0
			52	39	12	1	
38	G	1	Total	C	O	S	0
			42	29	12	1	
38	G	1	Total	C	O	S	0
			38	25	12	1	
38	M	1	Total	C	O	S	0
			50	37	12	1	
38	R	1	Total	C	O	S	0
			51	38	12	1	
38	S	1	Total	C	O	S	0
			51	38	12	1	
38	X	1	Total	C	O	S	0
			38	25	12	1	
38	Y	1	Total	C	O	S	0
			42	29	12	1	
38	0	1	Total	C	O	S	0
			42	29	12	1	
38	a	1	Total	C	O	S	0
			48	35	12	1	

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Mol	Chain	Residues	Atoms	AltConf
38	a	1	Total C O S 45 32 12 1	0
38	b	1	Total C O S 54 41 12 1	0
38	b	1	Total C O S 52 39 12 1	0
38	g	1	Total C O S 38 25 12 1	0
38	g	1	Total C O S 42 29 12 1	0
38	m	1	Total C O S 50 37 12 1	0
38	r	1	Total C O S 51 38 12 1	0
38	s	1	Total C O S 51 38 12 1	0
38	x	1	Total C O S 42 29 12 1	0
38	y	1	Total C O S 42 29 12 1	0

- Molecule 39 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

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

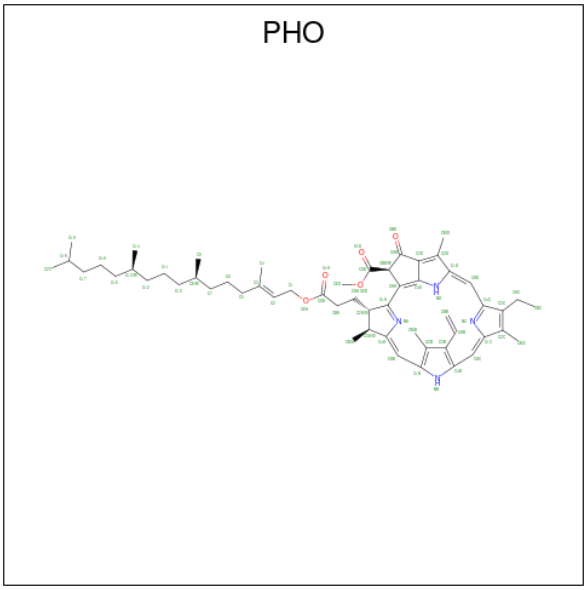
- Molecule 40 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 41 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
41	A	2	Total Cl 2 2	0
41	a	2	Total Cl 2 2	0

- Molecule 42 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



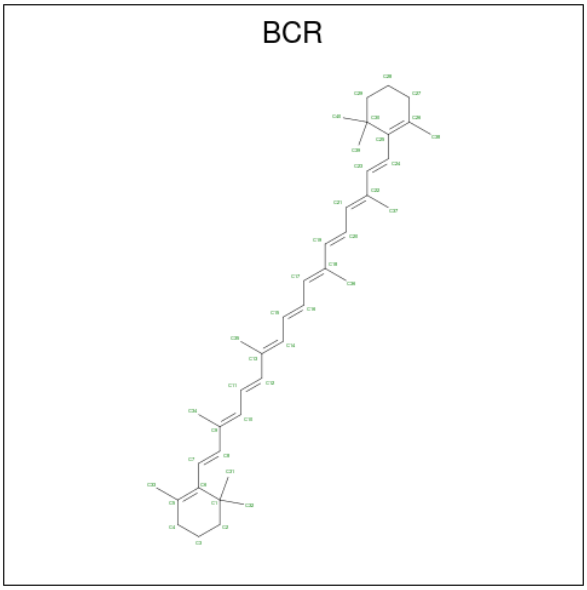
Mol	Chain	Residues	Atoms	AltConf
42	A	1	Total C N O 64 55 4 5	0
42	D	1	Total C N O 64 55 4 5	0

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

- Molecule 43 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



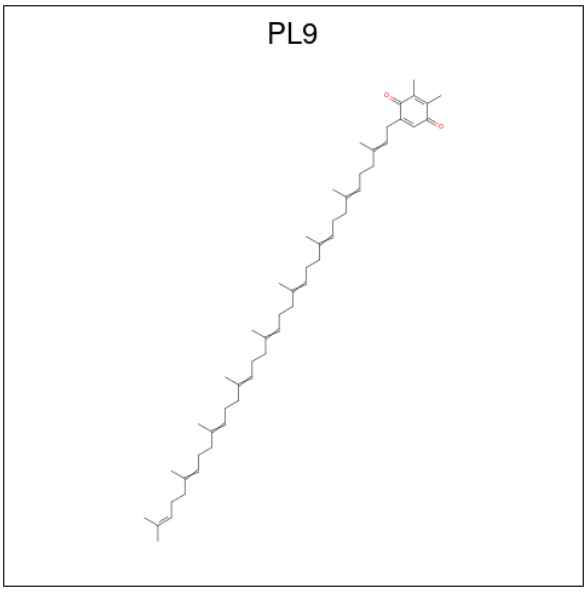
Mol	Chain	Residues	Atoms	AltConf
43	A	1	Total C 40 40	0
43	B	1	Total C 40 40	0
43	B	1	Total C 40 40	0
43	B	1	Total C 40 40	0
43	C	1	Total C 40 40	0
43	C	1	Total C 40 40	0
43	D	1	Total C 40 40	0
43	H	1	Total C 40 40	0
43	T	1	Total C 40 40	0

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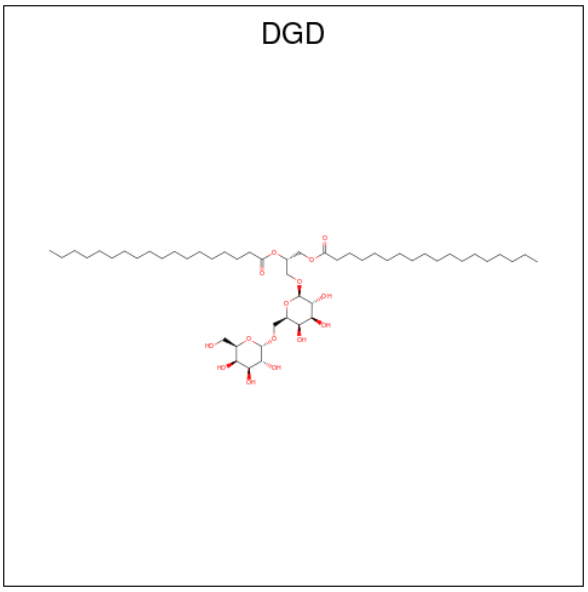
Mol	Chain	Residues	Atoms	AltConf
43	V	1	Total C 40 40	0
43	Z	1	Total C 40 40	0
43	a	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	c	1	Total C 40 40	0
43	c	1	Total C 40 40	0
43	d	1	Total C 40 40	0
43	h	1	Total C 40 40	0
43	t	1	Total C 40 40	0
43	v	1	Total C 40 40	0
43	z	1	Total C 40 40	0

- Molecule 44 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: $C_{53}H_{80}O_2$).



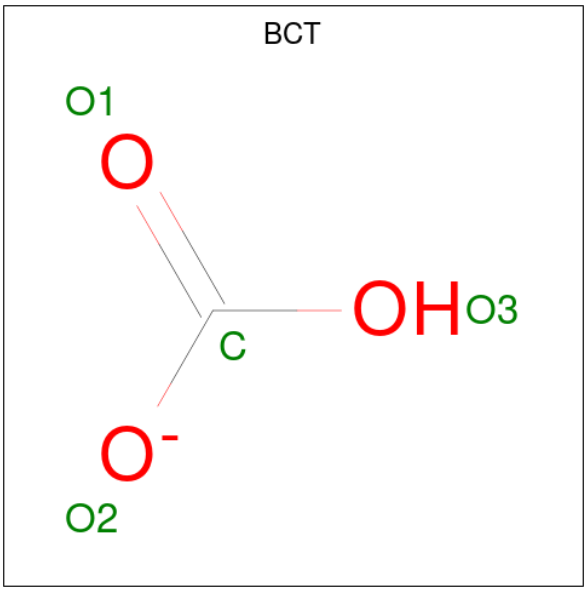
Mol	Chain	Residues	Atoms	AltConf
44	A	1	Total C O 55 53 2	0
44	D	1	Total C O 55 53 2	0
44	a	1	Total C O 55 53 2	0
44	d	1	Total C O 55 53 2	0

- Molecule 45 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



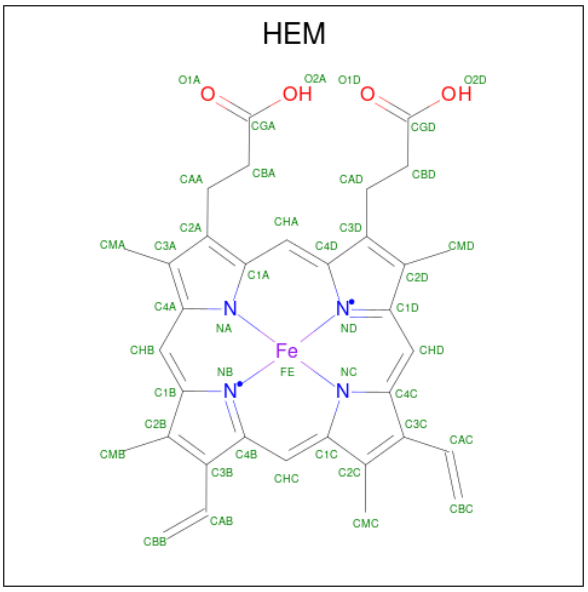
Mol	Chain	Residues	Atoms	AltConf
45	C	1	Total C O 50 35 15	0
45	C	1	Total C O 66 51 15	0
45	C	1	Total C O 66 51 15	0
45	C	1	Total C O 66 51 15	0
45	c	1	Total C O 66 51 15	0
45	c	1	Total C O 62 47 15	0
45	c	1	Total C O 66 51 15	0
45	c	1	Total C O 66 51 15	0

- Molecule 46 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



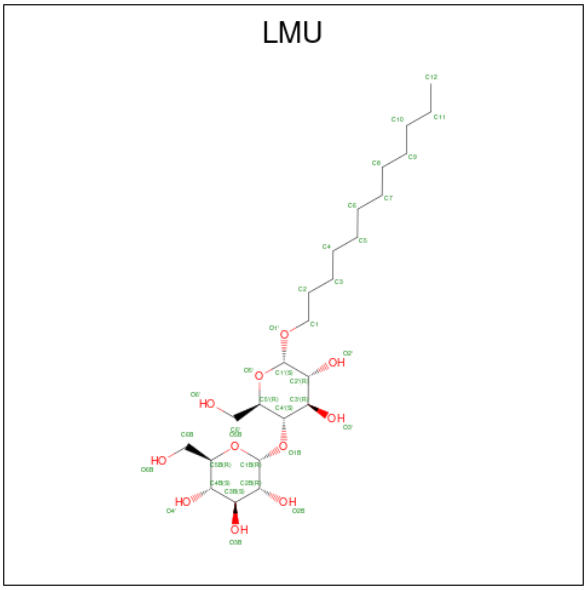
Mol	Chain	Residues	Atoms	AltConf
46	D	1	Total C O 4 1 3	0
46	d	1	Total C O 4 1 3	0

- Molecule 47 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 48 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
48	K	1	Total	C	O	0
			35	24	11	
48	R	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms	AltConf
48	c	1	Total C O 28 17 11	0
48	r	1	Total C O 35 24 11	0

- Molecule 49 is water.

Mol	Chain	Residues	Atoms	AltConf
49	1	3	Total O 3 3	0
49	2	3	Total O 3 3	0
49	3	1	Total O 1 1	0
49	4	1	Total O 1 1	0
49	5	1	Total O 1 1	0
49	6	4	Total O 4 4	0
49	A	21	Total O 21 21	0
49	B	6	Total O 6 6	0
49	C	15	Total O 15 15	0
49	D	12	Total O 12 12	0
49	E	1	Total O 1 1	0
49	G	5	Total O 5 5	0
49	I	1	Total O 1 1	0
49	J	1	Total O 1 1	0
49	N	5	Total O 5 5	0
49	O	6	Total O 6 6	0
49	R	4	Total O 4 4	0

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Mol	Chain	Residues	Atoms	AltConf
49	S	3	Total O 3 3	0
49	T	4	Total O 4 4	0
49	Y	8	Total O 8 8	0
49	0	7	Total O 7 7	0
49	7	6	Total O 6 6	0
49	8	4	Total O 4 4	0
49	9	2	Total O 2 2	0
49	q	1	Total O 1 1	0
49	a	14	Total O 14 14	0
49	b	6	Total O 6 6	0
49	c	15	Total O 15 15	0
49	d	15	Total O 15 15	0
49	e	2	Total O 2 2	0
49	f	1	Total O 1 1	0
49	g	4	Total O 4 4	0
49	j	1	Total O 1 1	0
49	m	2	Total O 2 2	0
49	n	7	Total O 7 7	0
49	o	6	Total O 6 6	0
49	r	4	Total O 4 4	0
49	s	3	Total O 3 3	0

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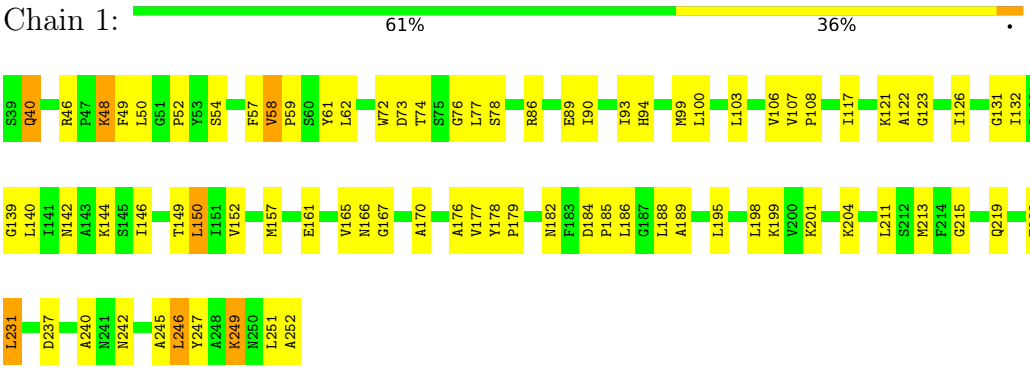
Mol	Chain	Residues	Atoms	AltConf
49	t	2	Total O 2 2	0
49	w	2	Total O 2 2	0
49	y	8	Total O 8 8	0
49	F1	4	Total O 4 4	0
49	f1	3	Total O 3 3	0

3 Residue-property plots (i)

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

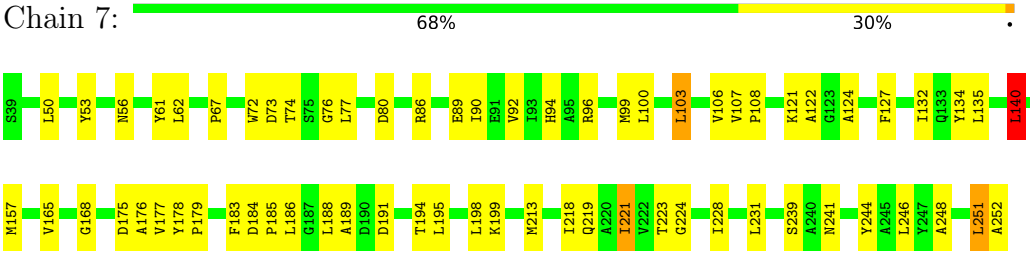
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain 1:



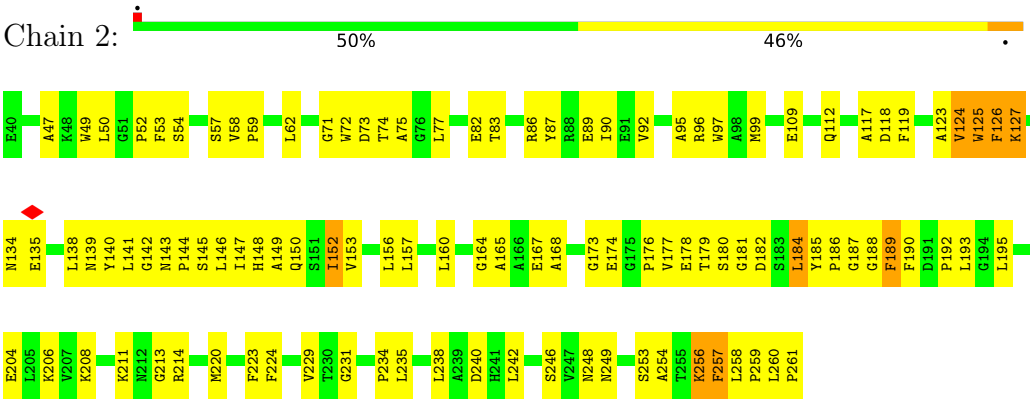
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain 7:



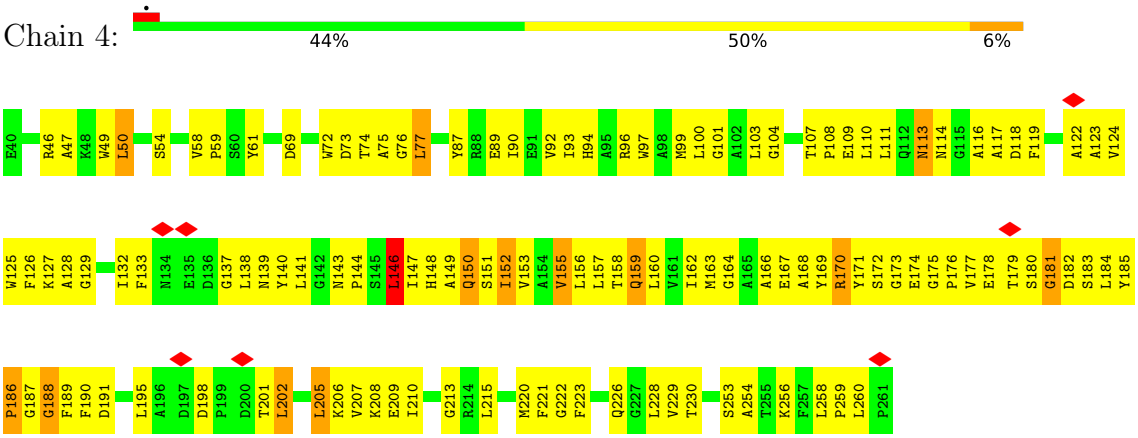
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 2:



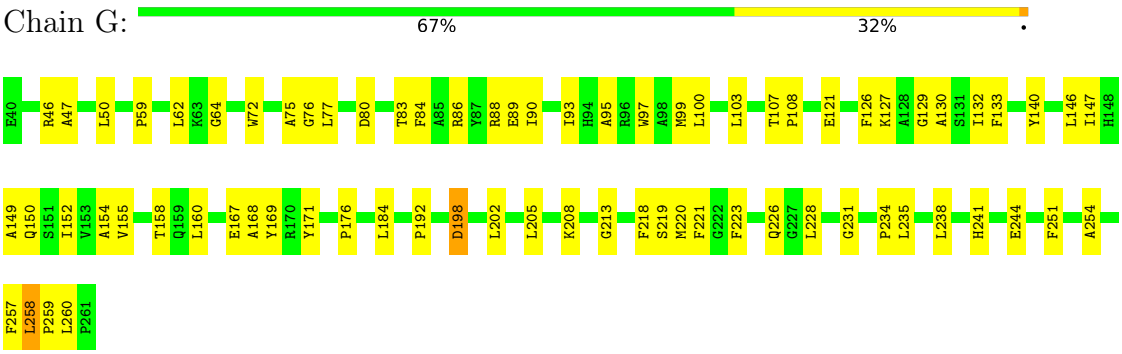
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



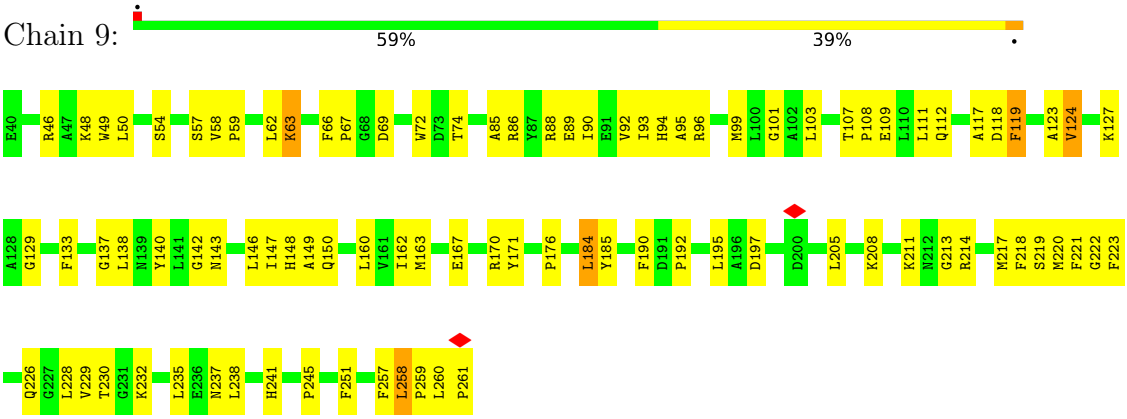
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain G:



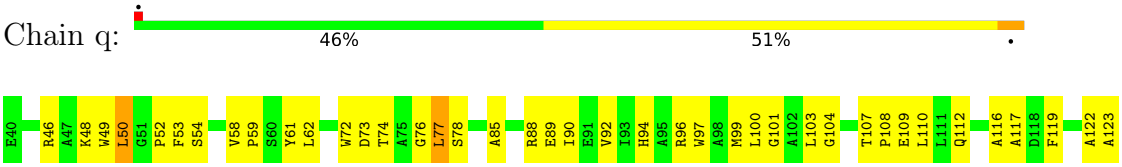
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

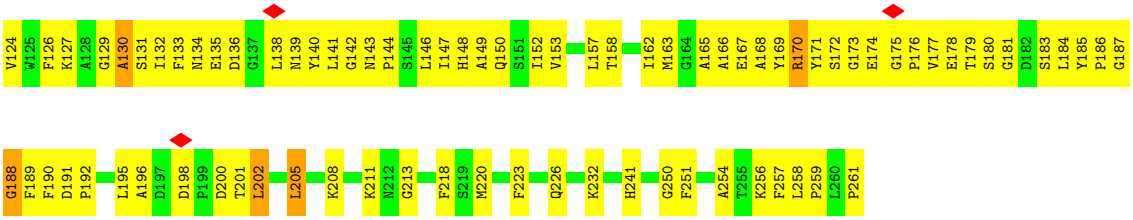
Chain 9:



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

Chain q:

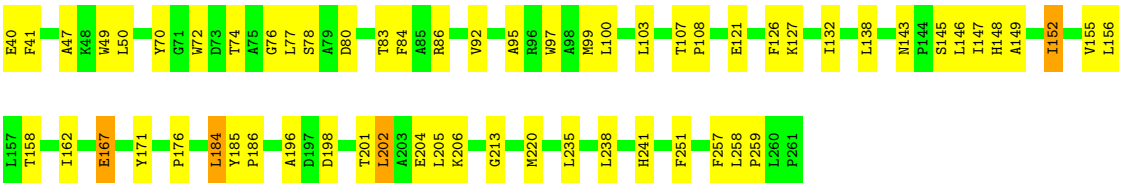




• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain g:

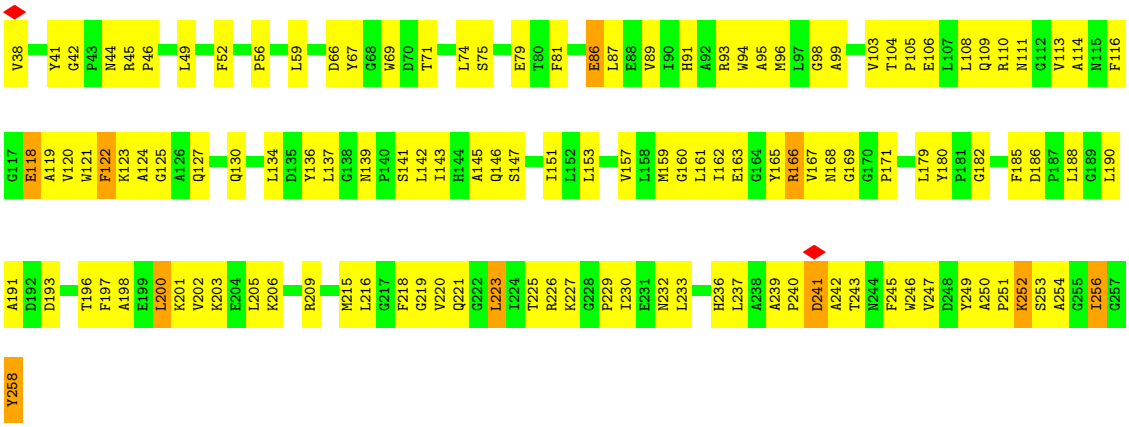




• Molecule 3: Chlorophyll a-b binding of LHCII

Chain 3:

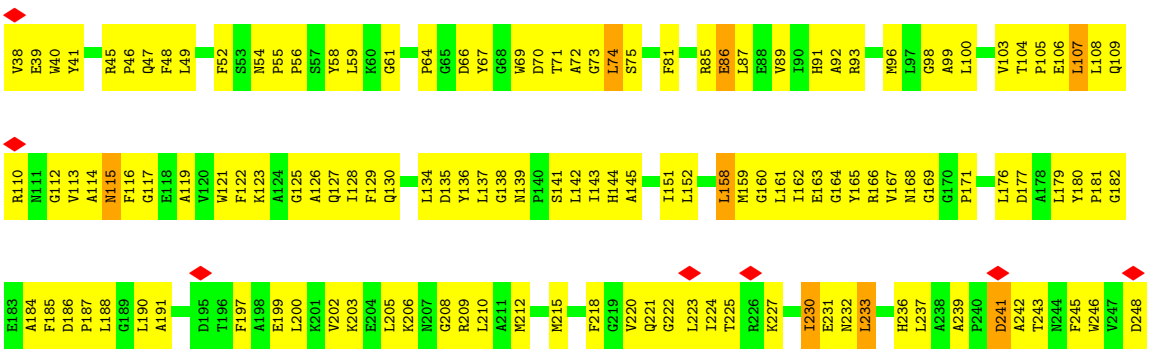




• Molecule 3: Chlorophyll a-b binding of LHCII

Chain 5:

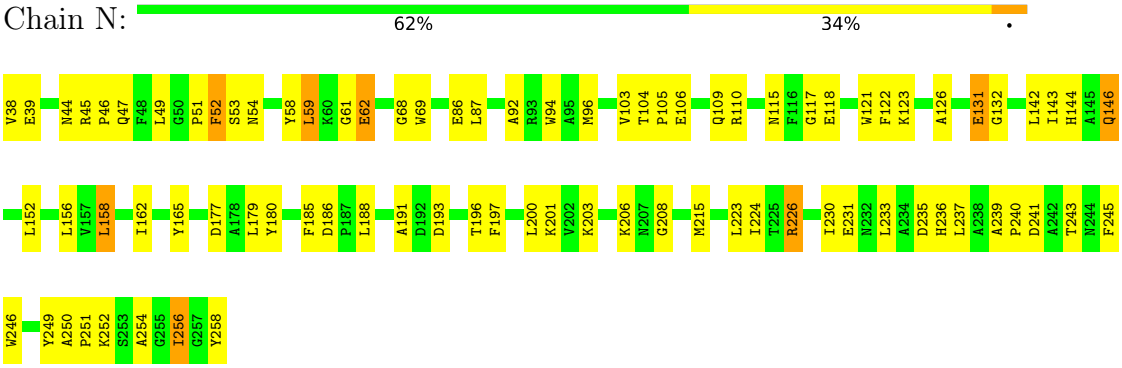






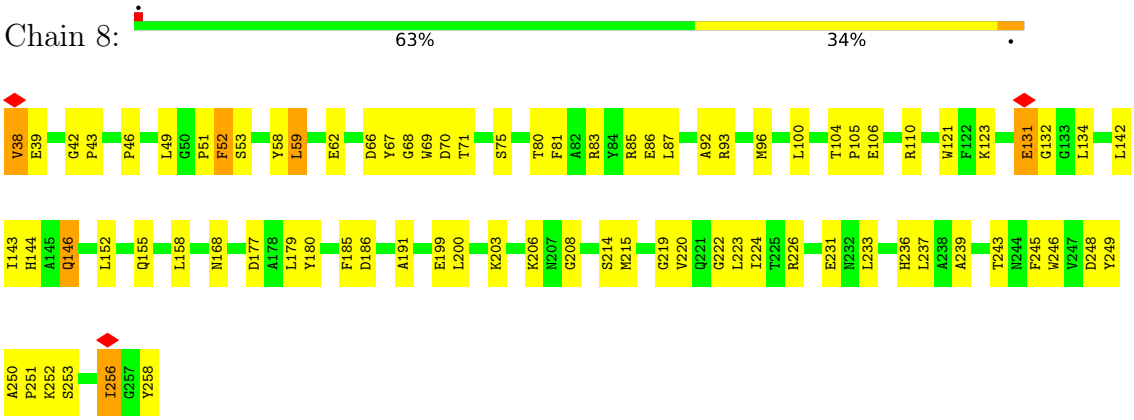
• Molecule 3: Chlorophyll a-b binding of LHCII

Chain N:



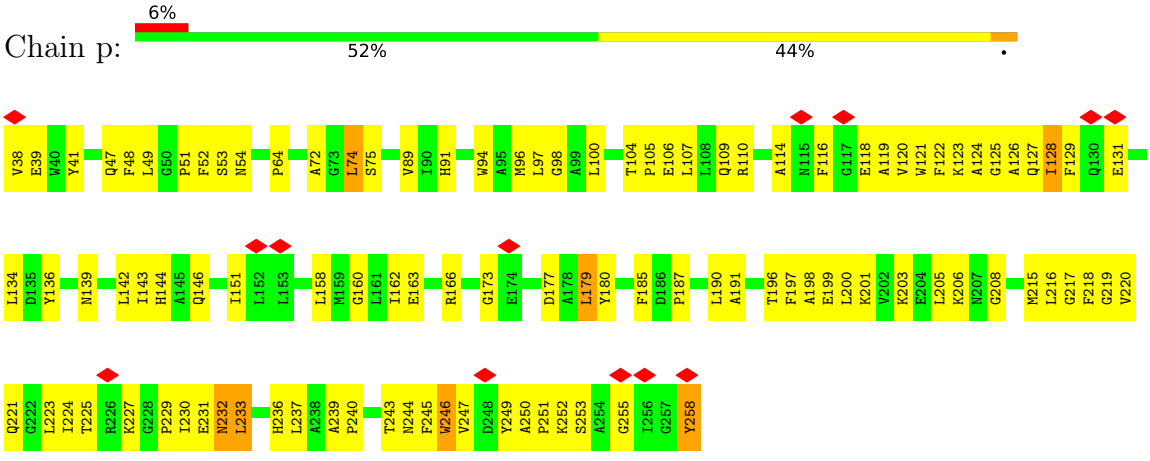
• Molecule 3: Chlorophyll a-b binding of LHCII

Chain 8:



• Molecule 3: Chlorophyll a-b binding of LHCII

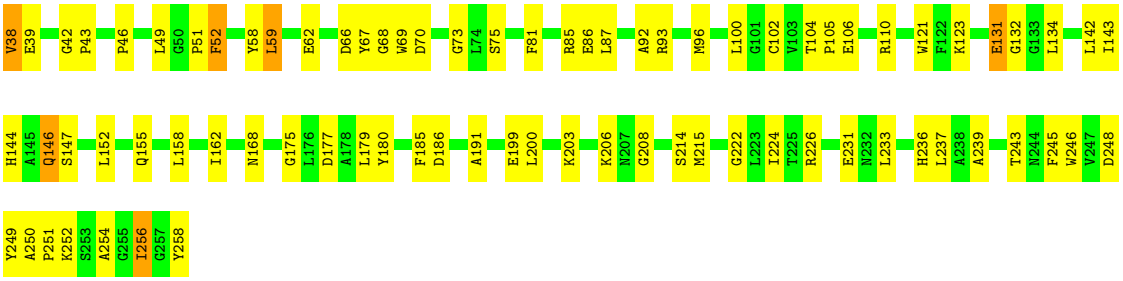
Chain p:



• Molecule 3: Chlorophyll a-b binding of LHCII

Chain n:

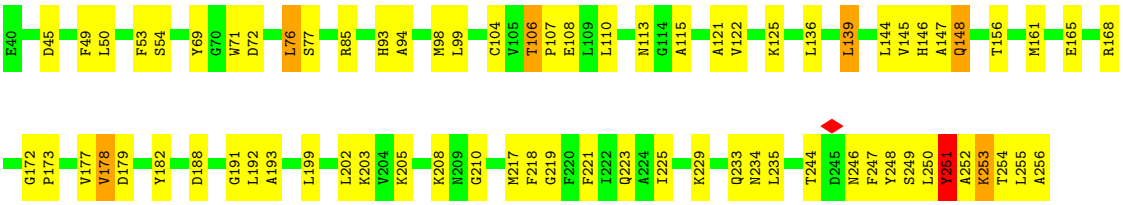




• Molecule 4: Chlorophyll a-b binding of LHCII

Chain 6:

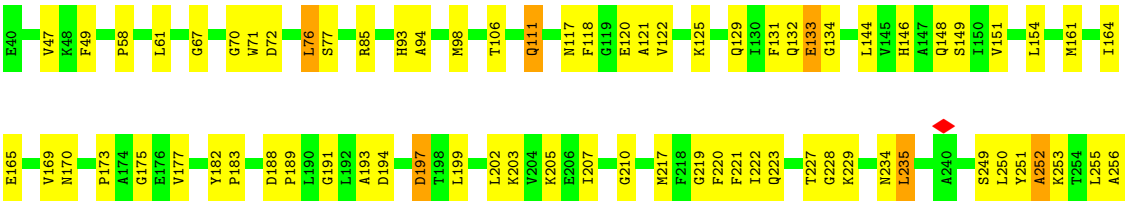




• Molecule 4: Chlorophyll a-b binding of LHCII

Chain 0:

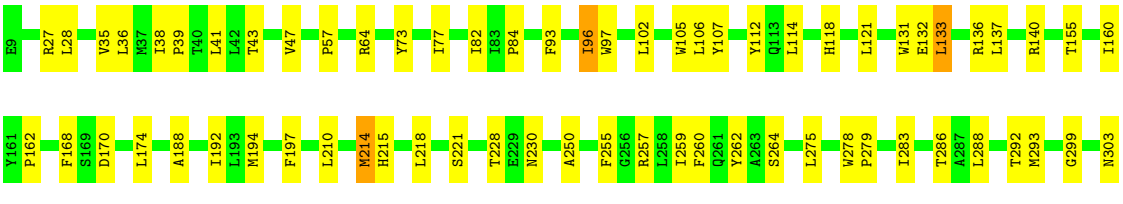




• Molecule 5: Photosystem II protein D1

Chain A:



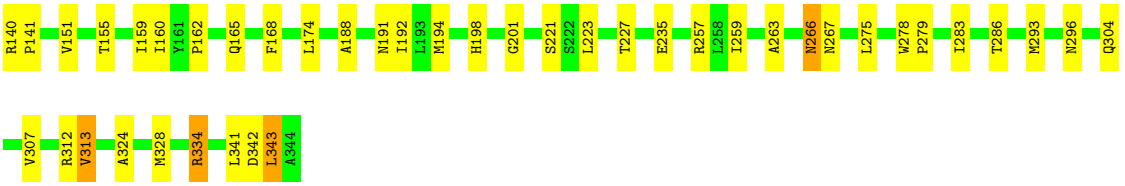


• Molecule 5: Photosystem II protein D1

Chain a:



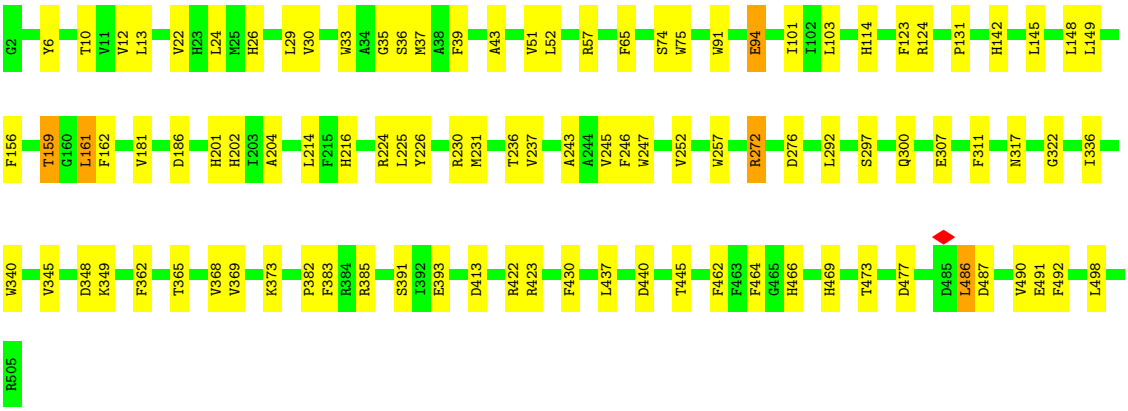




• Molecule 6: Photosystem II CP47 reaction center protein

Chain B:

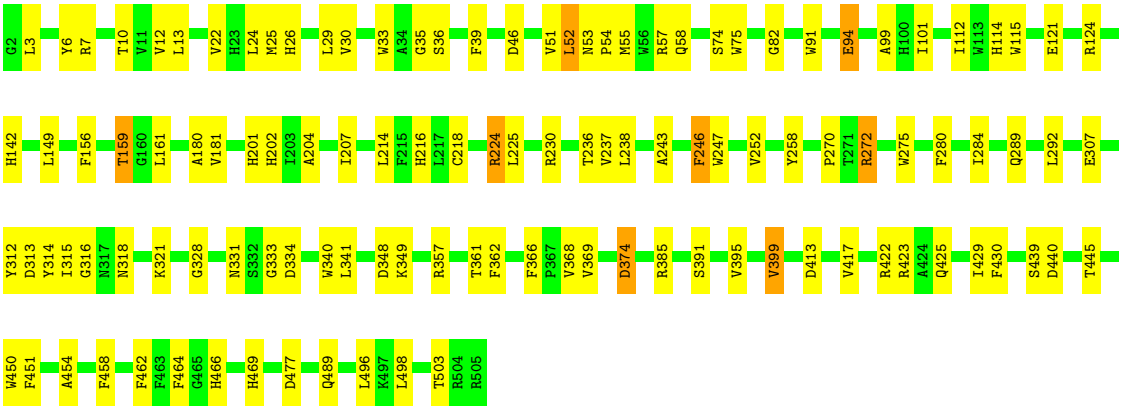




• Molecule 6: Photosystem II CP47 reaction center protein

Chain b:

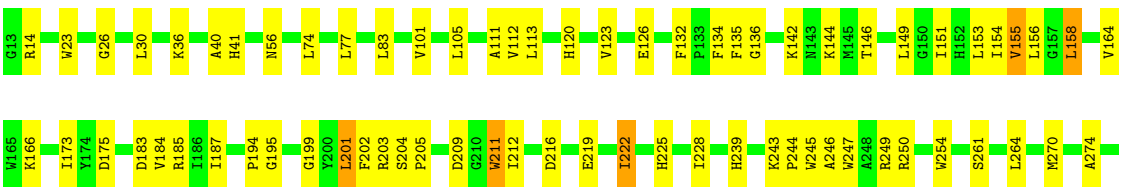


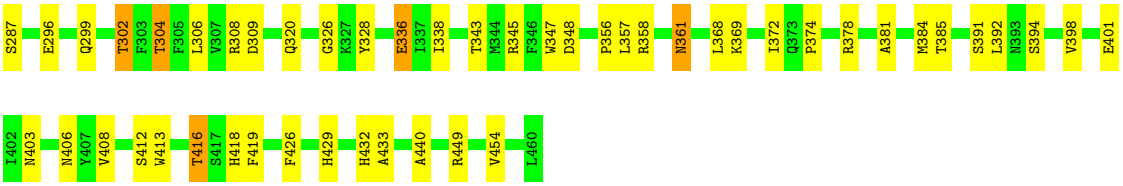


• Molecule 7: Photosystem II CP43 reaction center protein

Chain C:



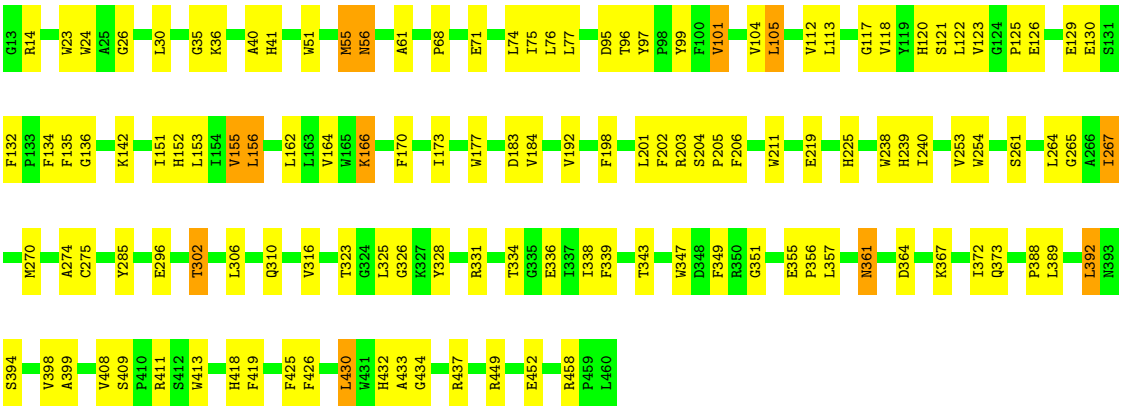




• Molecule 7: Photosystem II CP43 reaction center protein

Chain c:

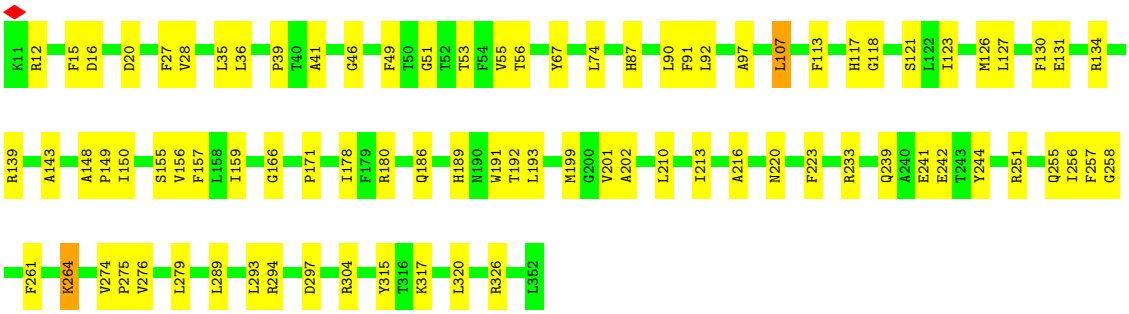




• Molecule 8: Photosystem II D2 protein

Chain D:

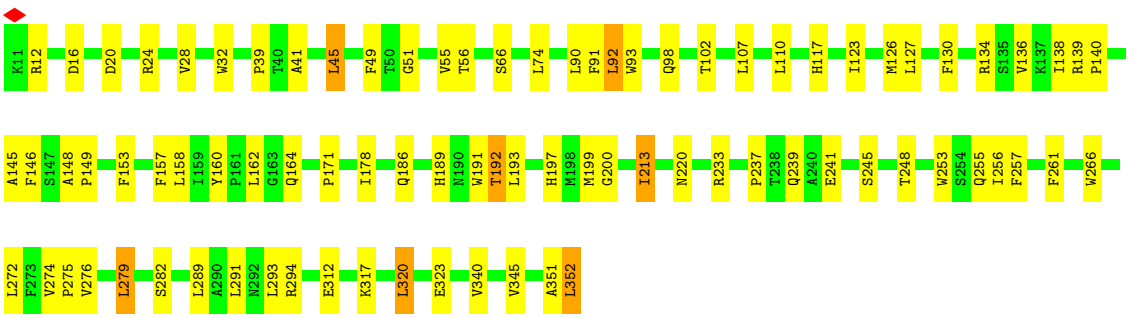




• Molecule 8: Photosystem II D2 protein

Chain d:

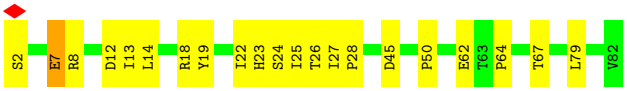




• Molecule 9: Cytochrome b559 subunit alpha

Chain E:

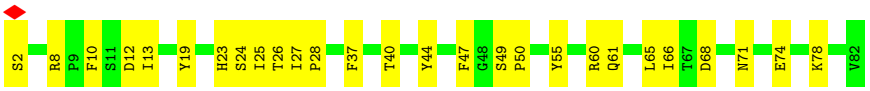




• Molecule 9: Cytochrome b559 subunit alpha

Chain e:





• Molecule 10: Cytochrome b559 subunit beta

Chain F:

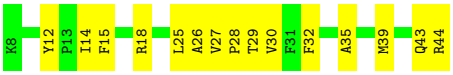




• Molecule 10: Cytochrome b559 subunit beta

Chain f:

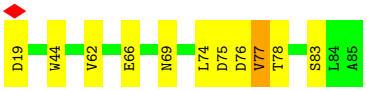




• Molecule 11: Photosystem II reaction center protein H

Chain H:

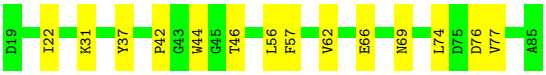




• Molecule 11: Photosystem II reaction center protein H

Chain h:

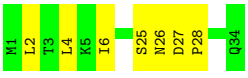




• Molecule 12: Photosystem II reaction center protein I

Chain I:

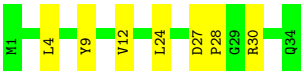




• Molecule 12: Photosystem II reaction center protein I

Chain i:





• Molecule 13: Photosystem II reaction center protein J

Chain J:

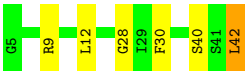




• Molecule 13: Photosystem II reaction center protein J

Chain j:

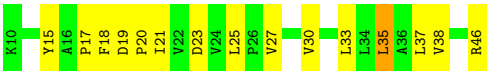




• Molecule 14: Photosystem II reaction center protein K

Chain K:

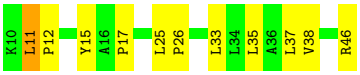




• Molecule 14: Photosystem II reaction center protein K

Chain k:

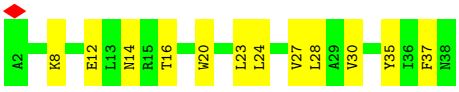




• Molecule 15: Photosystem II reaction center protein L

Chain L:





• Molecule 15: Photosystem II reaction center protein L

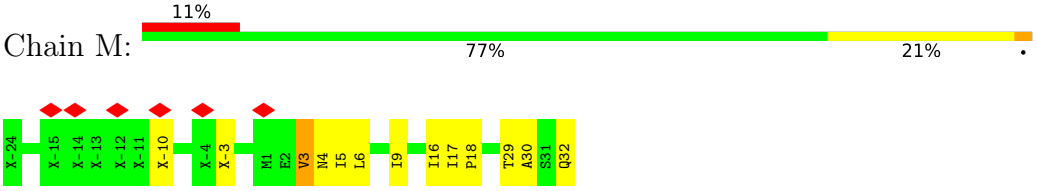
Chain l:





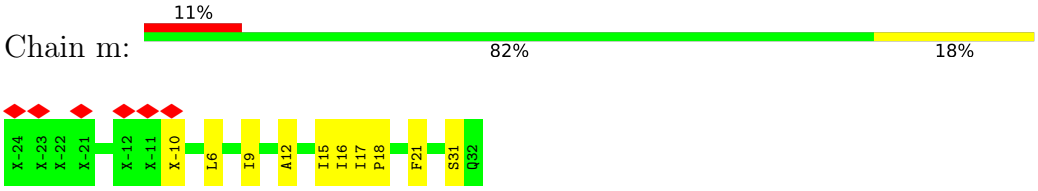
• Molecule 16: Photosystem II reaction center protein M

Chain M:



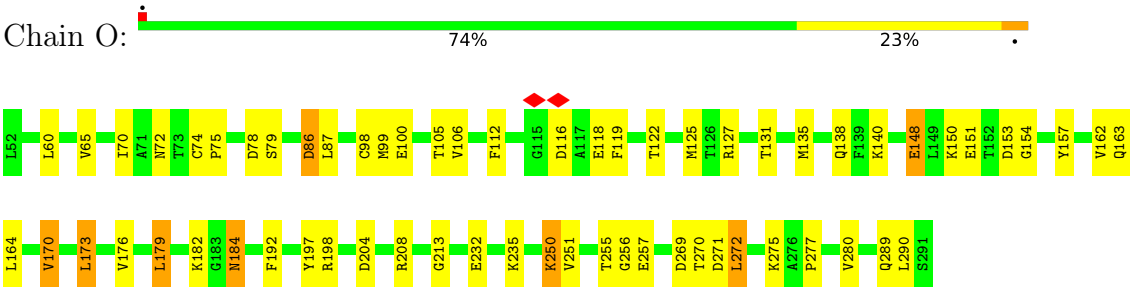
• Molecule 16: Photosystem II reaction center protein M

Chain m:



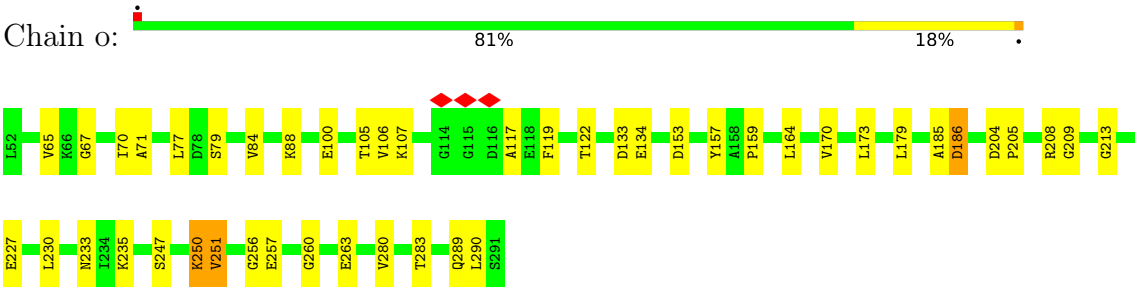
• Molecule 17: Chloroplast oxygen-evolving enhancer protein 1

Chain O:



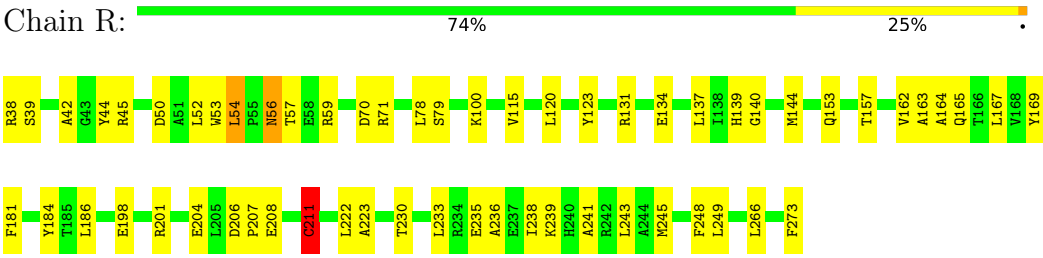
• Molecule 17: Chloroplast oxygen-evolving enhancer protein 1

Chain o:



• Molecule 18: Chlorophyll a b binding CP29

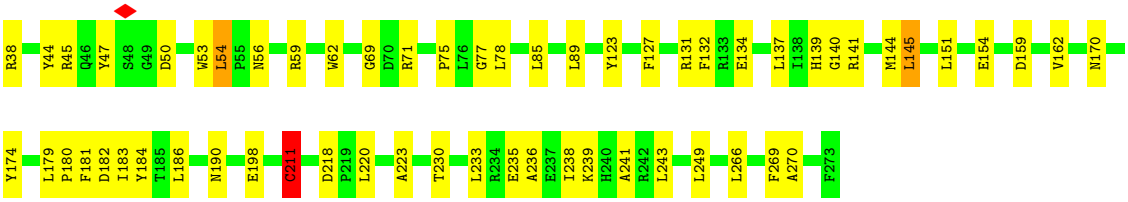
Chain R:



• Molecule 18: Chlorophyll a b binding CP29

Chain r:

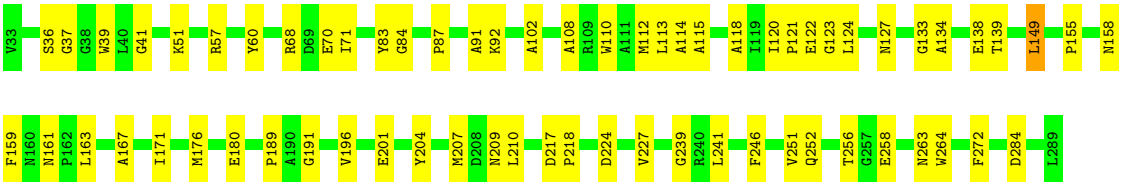




• Molecule 19: Chlorophyll a b-binding CP26

Chain S:

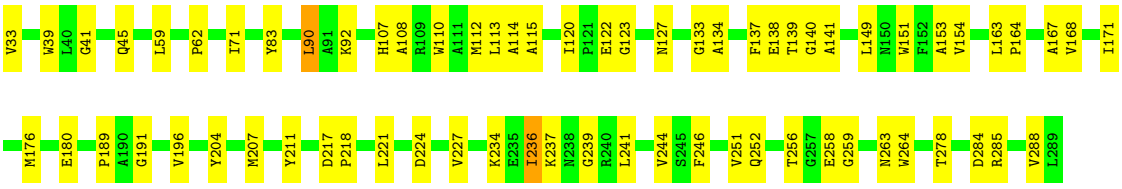




• Molecule 19: Chlorophyll a b-binding CP26

Chain s:





• Molecule 20: Photosystem II reaction center protein T

Chain T:

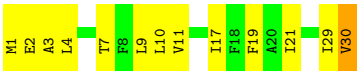




• Molecule 20: Photosystem II reaction center protein T

Chain t:

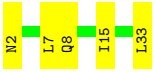




• Molecule 21: Photosystem II reaction center protein Ycf12

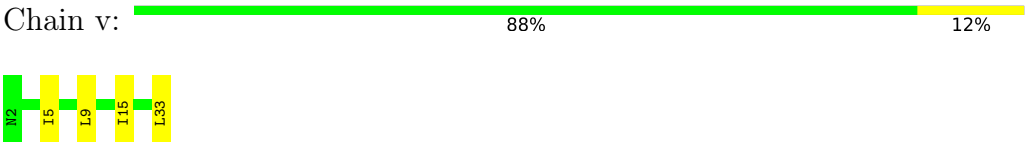
Chain V:





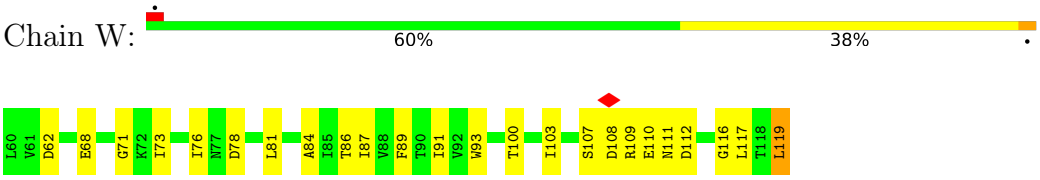
• Molecule 21: Photosystem II reaction center protein Ycf12

Chain v:



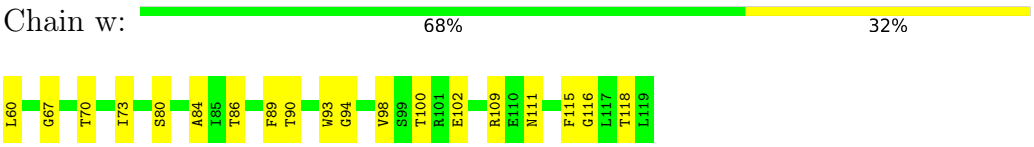
• Molecule 22: Photosystem II reaction center W protein

Chain W:



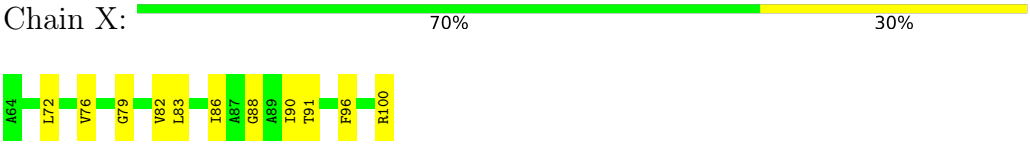
• Molecule 22: Photosystem II reaction center W protein

Chain w:



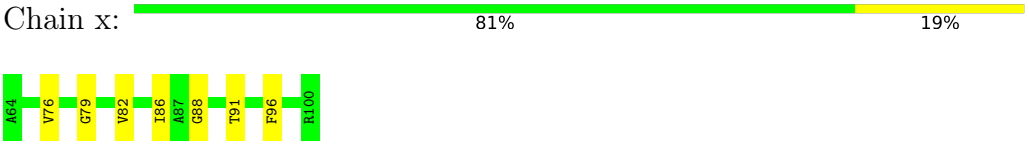
• Molecule 23: Photosystem II reaction center protein X

Chain X:



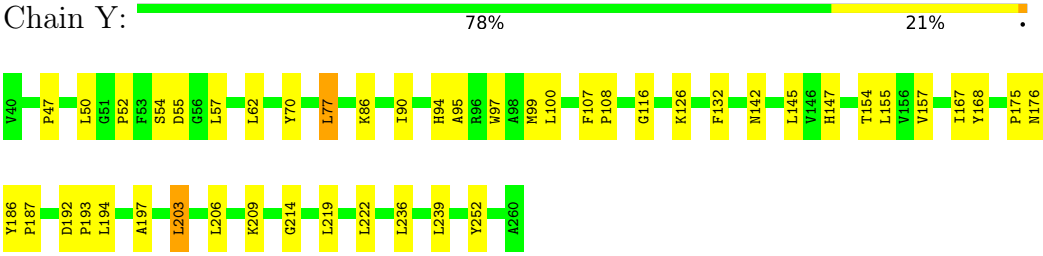
• Molecule 23: Photosystem II reaction center protein X

Chain x:



• Molecule 24: Multifunctional fusion protein

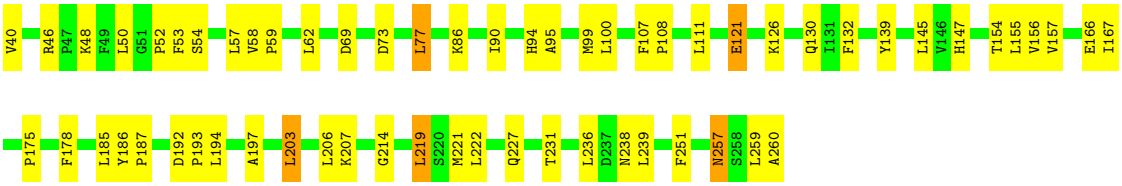
Chain Y:



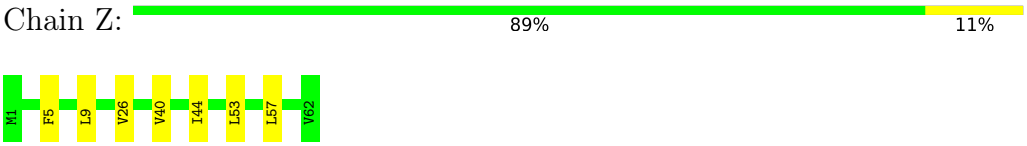
• Molecule 24: Multifunctional fusion protein

Chain y:

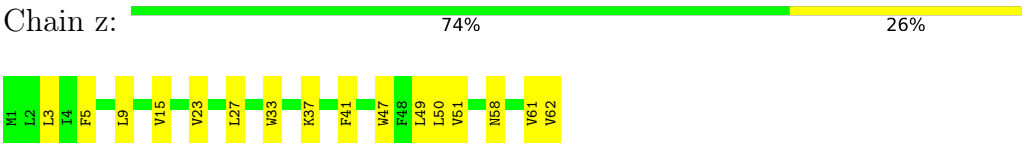




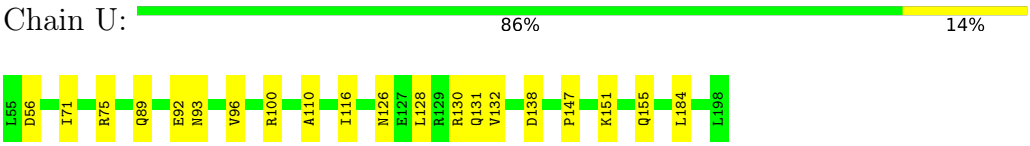
• Molecule 25: Photosystem II reaction center protein Z



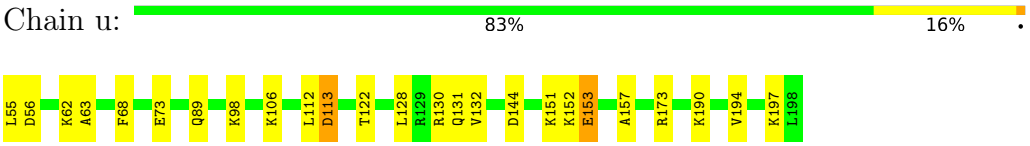
• Molecule 25: Photosystem II reaction center protein Z



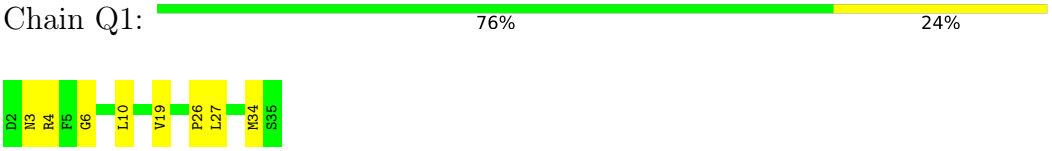
• Molecule 26: Chloroplast oxygen-evolving enhancer protein 3



• Molecule 26: Chloroplast oxygen-evolving enhancer protein 3



• Molecule 27: Chloroplast PsbY

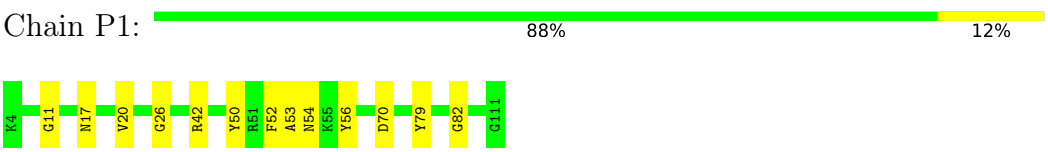


• Molecule 27: Chloroplast PsbY



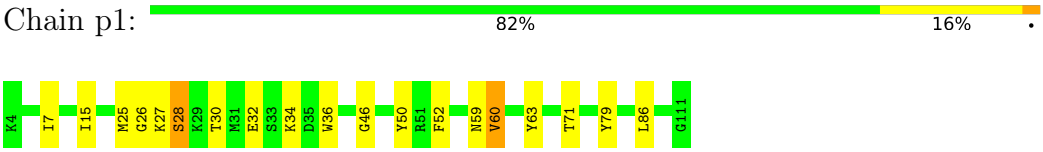
• Molecule 28: Chloroplast photosystem II 10 kDa protein

Chain P1:



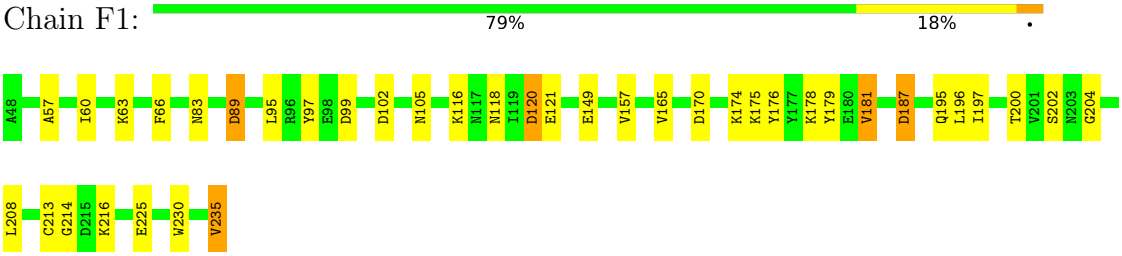
• Molecule 28: Chloroplast photosystem II 10 kDa protein

Chain p1:



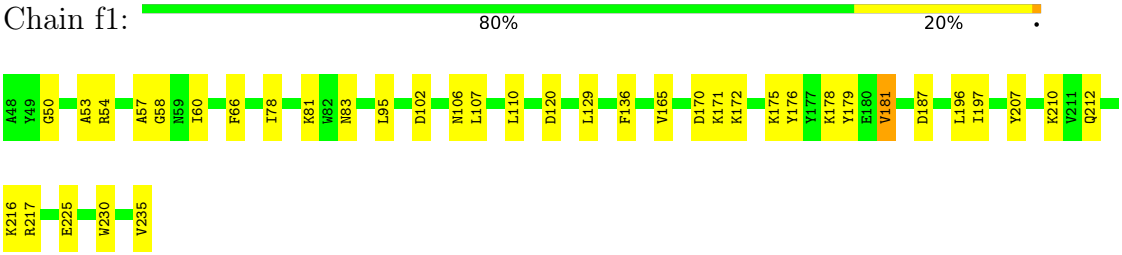
• Molecule 29: Photosystem II oxygen evolving enhancer 2

Chain F1:



• Molecule 29: Photosystem II oxygen evolving enhancer 2

Chain f1:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94893	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	460.8, 460.8, 460.8	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9216, 0.9216, 0.9216	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, LMU, BCT, HEM, PL9, LUT, BCR, DGD, FE2, LHG, CLA, OEX, PHO, CHL, XAT, CL, SQD, NEX, RRX, CSU

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	0.72	1/1675 (0.1%)	0.89	0/2283
1	7	0.68	0/1675	0.88	0/2283
2	2	0.70	0/1734	0.91	1/2359 (0.0%)
2	4	0.76	0/1732	0.98	1/2355 (0.0%)
2	9	0.64	0/1734	0.85	0/2359
2	G	0.50	0/1734	0.66	0/2359
2	g	0.53	0/1734	0.69	0/2359
2	q	0.76	0/1732	0.98	1/2355 (0.0%)
3	3	0.67	0/1734	0.90	1/2362 (0.0%)
3	5	0.90	0/1734	1.14	1/2362 (0.0%)
3	8	0.73	0/1734	0.91	0/2362
3	N	0.72	0/1734	0.92	0/2362
3	n	0.72	0/1734	0.91	0/2362
3	p	0.57	0/1734	0.75	0/2362
4	0	0.42	0/1701	0.60	0/2315
4	6	0.49	0/1701	0.65	0/2315
5	A	0.33	0/2714	0.40	0/3701
5	a	0.38	0/2714	0.47	0/3701
6	B	0.32	0/4085	0.37	0/5564
6	b	0.38	0/4085	0.48	0/5564
7	C	0.35	0/3602	0.42	1/4910 (0.0%)
7	c	0.41	0/3602	0.50	0/4910
8	D	0.42	0/2825	0.53	0/3849
8	d	0.43	0/2825	0.52	0/3849
9	E	0.55	0/670	0.69	0/913
9	e	0.71	0/670	0.87	0/913
10	F	0.71	0/312	0.89	0/426
10	f	0.79	0/312	1.02	0/426
11	H	0.24	0/518	0.30	0/708
11	h	0.24	0/518	0.32	0/708
12	I	0.64	0/282	0.76	0/382

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
12	i	0.60	0/282	0.75	0/382
13	J	0.18	0/276	0.24	0/377
13	j	0.28	0/276	0.30	0/377
14	K	0.27	0/305	0.40	0/420
14	k	0.24	0/305	0.42	0/420
15	L	0.41	0/311	0.53	0/422
15	l	0.42	0/311	0.54	0/422
16	M	0.27	0/248	0.45	0/338
16	m	0.24	0/248	0.39	0/338
17	O	0.36	0/1823	0.48	0/2466
17	o	0.35	0/1823	0.46	0/2466
18	R	0.51	0/1850	0.64	0/2515
18	r	0.60	0/1850	0.75	0/2515
19	S	0.44	0/1985	0.61	0/2711
19	s	0.45	0/1985	0.62	0/2711
20	T	0.25	0/253	0.32	0/343
20	t	0.45	0/253	0.57	0/343
21	V	0.13	0/234	0.28	0/319
21	v	0.13	0/234	0.25	0/319
22	W	0.74	0/477	0.90	0/650
22	w	0.74	0/477	0.91	0/650
23	X	0.55	0/248	0.76	0/339
23	x	0.61	0/248	0.79	0/339
24	Y	0.34	0/1735	0.43	1/2359 (0.0%)
24	y	0.32	0/1735	0.39	0/2359
25	Z	0.19	0/491	0.31	0/672
25	z	0.18	0/491	0.28	0/672
26	U	0.24	0/1132	0.35	0/1521
26	u	0.21	0/1132	0.31	0/1521
27	Q1	0.55	0/265	0.69	0/362
27	q1	0.55	0/265	0.75	0/362
28	P1	0.36	0/835	0.47	0/1127
28	p1	0.34	0/835	0.45	0/1127
29	F1	0.49	0/1473	0.60	0/1991
29	f1	0.57	0/1473	0.68	0/1991
All	All	0.51	1/85454 (0.0%)	0.65	7/116284 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	0	1
18	r	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	58	VAL	N-CA	5.14	1.49	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	126	PHE	CA-CB-CG	6.76	120.56	113.80
3	5	112	GLY	CA-C-O	-5.73	118.32	122.45
3	3	122	PHE	CA-CB-CG	5.68	119.48	113.80
2	q	130	ALA	N-CA-C	-5.51	106.46	114.12
24	Y	55	ASP	N-CA-C	-5.25	108.64	114.62
7	C	211	TRP	CB-CA-C	-5.17	110.60	116.54
2	4	150	GLN	N-CA-C	-5.10	108.81	114.62

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	R	211	CSU	Mainchain
18	r	211	CSU	Mainchain

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	1630	0	1583	90	0
1	7	1630	0	1583	85	0
2	2	1686	0	1616	136	0
2	4	1685	0	1612	187	0
2	9	1686	0	1616	116	0
2	G	1686	0	1616	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	g	1686	0	1616	49	0
2	q	1685	0	1612	161	0
3	3	1686	0	1635	163	0
3	5	1686	0	1635	219	0
3	8	1686	0	1635	86	0
3	N	1686	0	1635	84	0
3	n	1686	0	1635	78	0
3	p	1686	0	1635	146	0
4	0	1657	0	1612	76	0
4	6	1657	0	1612	91	0
5	A	2632	0	2532	62	0
5	a	2632	0	2532	67	0
6	B	3954	0	3823	83	0
6	b	3954	0	3823	98	0
7	C	3482	0	3375	97	0
7	c	3482	0	3375	112	0
8	D	2730	0	2630	73	0
8	d	2730	0	2630	69	0
9	E	652	0	636	20	0
9	e	652	0	636	25	0
10	F	302	0	311	15	0
10	f	302	0	311	16	0
11	H	507	0	520	8	0
11	h	507	0	520	12	0
12	I	274	0	280	6	0
12	i	274	0	280	6	0
13	J	270	0	282	3	0
13	j	270	0	282	7	0
14	K	295	0	311	11	0
14	k	295	0	311	10	0
15	L	303	0	311	10	0
15	l	303	0	311	13	0
16	M	370	0	302	10	0
16	m	370	0	301	7	0
17	O	1789	0	1759	46	0
17	o	1789	0	1759	29	0
18	R	1818	0	1737	59	0
18	r	1818	0	1736	57	0
19	S	1934	0	1879	62	0
19	s	1934	0	1879	67	0
20	T	246	0	262	8	0
20	t	246	0	262	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	V	233	0	263	4	0
21	v	233	0	263	4	0
22	W	468	0	450	26	0
22	w	468	0	450	24	0
23	X	247	0	260	7	0
23	x	247	0	260	5	0
24	Y	1688	0	1637	43	0
24	y	1688	0	1637	56	0
25	Z	478	0	513	5	0
25	z	478	0	513	11	0
26	U	1122	0	1151	16	0
26	u	1122	0	1151	13	0
27	Q1	260	0	269	9	0
27	q1	260	0	269	16	0
28	P1	820	0	834	9	0
28	p1	820	0	834	14	0
29	F1	1443	0	1408	25	0
29	f1	1443	0	1408	34	0
30	0	336	0	282	43	0
30	1	441	0	437	52	0
30	2	270	0	219	43	0
30	3	311	0	236	69	0
30	4	327	0	268	67	0
30	5	305	0	221	58	0
30	6	330	0	275	48	0
30	7	443	0	441	53	0
30	8	296	0	270	34	0
30	9	328	0	269	50	0
30	G	344	0	302	50	0
30	N	346	0	306	52	0
30	R	167	0	138	15	0
30	S	182	0	121	16	0
30	Y	350	0	318	49	0
30	g	278	0	233	34	0
30	n	409	0	366	59	0
30	p	305	0	221	44	0
30	q	326	0	265	60	0
30	r	167	0	138	17	0
30	s	182	0	123	20	0
30	y	353	0	327	42	0
31	0	512	0	481	46	0
31	1	494	0	513	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	2	468	0	451	57	0
31	3	559	0	506	82	0
31	4	435	0	386	66	0
31	5	481	0	410	88	0
31	6	535	0	523	67	0
31	7	545	0	552	69	0
31	8	512	0	489	79	0
31	9	437	0	392	62	0
31	A	239	0	242	22	0
31	B	1024	0	1116	92	0
31	C	818	0	870	61	0
31	D	130	0	144	16	0
31	G	457	0	444	55	0
31	N	566	0	539	95	0
31	R	598	0	536	42	0
31	S	627	0	608	65	0
31	Y	484	0	491	56	0
31	a	190	0	203	20	0
31	b	1024	0	1117	98	0
31	c	826	0	888	72	0
31	d	179	0	183	12	0
31	g	457	0	441	44	0
31	n	512	0	489	86	0
31	p	478	0	408	89	0
31	q	432	0	383	63	0
31	r	598	0	534	46	0
31	s	627	0	606	71	0
31	y	538	0	539	68	0
32	0	84	0	112	12	0
32	1	84	0	112	12	0
32	2	42	0	56	8	0
32	3	84	0	112	24	0
32	4	42	0	56	11	0
32	5	84	0	112	38	0
32	6	84	0	112	19	0
32	7	84	0	112	16	0
32	8	84	0	112	18	0
32	9	42	0	56	15	0
32	G	42	0	56	8	0
32	N	84	0	112	22	0
32	R	42	0	56	3	0
32	S	84	0	112	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	84	0	112	12	0
32	g	42	0	56	8	0
32	n	84	0	112	18	0
32	p	84	0	112	24	0
32	q	42	0	56	12	0
32	r	42	0	56	4	0
32	s	84	0	112	24	0
32	y	84	0	112	16	0
33	0	36	0	42	3	0
33	1	35	0	40	5	0
33	2	49	0	74	4	0
33	3	33	0	36	7	0
33	4	47	0	67	5	0
33	5	35	0	40	9	0
33	6	37	0	44	2	0
33	7	35	0	40	3	0
33	8	49	0	74	4	0
33	9	33	0	36	9	0
33	A	83	0	109	8	0
33	B	49	0	74	6	0
33	C	40	0	53	7	0
33	D	93	0	135	12	0
33	F1	35	0	40	1	0
33	G	44	0	61	15	0
33	K	36	0	42	6	0
33	L	49	0	74	4	0
33	M	41	0	55	1	0
33	N	49	0	74	3	0
33	R	38	0	46	1	0
33	S	85	0	113	11	0
33	Y	42	0	57	4	0
33	a	39	0	48	4	0
33	b	93	0	135	21	0
33	c	47	0	67	8	0
33	d	49	0	74	13	0
33	e	44	0	61	7	0
33	g	44	0	61	12	0
33	j	49	0	74	5	0
33	l	49	0	74	11	0
33	n	49	0	74	3	0
33	p	35	0	40	3	0
33	q	46	0	65	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	r	38	0	46	3	0
33	s	85	0	113	11	0
33	t	41	0	55	1	0
33	y	46	0	65	11	0
33	z	36	0	42	3	0
34	0	80	0	100	13	0
34	1	38	0	46	2	0
34	2	129	0	168	14	0
34	3	38	0	46	13	0
34	4	91	0	122	21	0
34	5	38	0	46	11	0
34	6	119	0	148	21	0
34	7	115	0	140	12	0
34	9	129	0	168	32	0
34	A	117	0	144	9	0
34	B	127	0	164	16	0
34	C	165	0	210	17	0
34	D	191	0	262	16	0
34	G	129	0	168	25	0
34	I	38	0	46	5	0
34	J	89	0	118	5	0
34	N	38	0	46	2	0
34	Q1	38	0	46	14	0
34	R	38	0	46	0	0
34	S	41	0	52	2	0
34	W	131	0	178	15	0
34	X	76	0	92	6	0
34	Y	38	0	46	5	0
34	a	114	0	138	12	0
34	b	256	0	332	21	0
34	c	120	0	150	17	0
34	d	140	0	190	11	0
34	f	38	0	46	1	0
34	g	87	0	114	10	0
34	j	43	0	56	4	0
34	k	86	0	112	5	0
34	m	45	0	60	5	0
34	n	78	0	96	20	0
34	p	38	0	46	5	0
34	q	91	0	122	10	0
34	q1	38	0	46	11	0
34	r	38	0	46	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	s	41	0	52	4	0
34	w	217	0	290	35	0
34	x	38	0	46	5	0
34	y	38	0	44	4	0
35	2	41	0	56	12	0
35	4	41	0	56	17	0
35	9	41	0	56	13	0
35	G	41	0	56	28	0
35	g	41	0	56	3	0
35	q	41	0	56	20	0
36	0	44	0	54	10	0
36	2	44	0	54	6	0
36	3	44	0	54	10	0
36	4	44	0	54	8	0
36	5	44	0	54	16	0
36	6	44	0	54	11	0
36	8	44	0	54	4	0
36	9	44	0	54	9	0
36	G	44	0	54	1	0
36	N	44	0	55	7	0
36	R	88	0	108	15	0
36	S	44	0	54	4	0
36	Y	44	0	54	2	0
36	g	44	0	54	2	0
36	n	44	0	54	2	0
36	p	44	0	54	2	0
36	q	44	0	54	4	0
36	r	88	0	108	9	0
36	s	44	0	54	4	0
36	y	44	0	54	5	0
37	2	44	0	56	11	0
37	4	44	0	56	9	0
37	9	44	0	56	3	0
37	G	44	0	56	22	0
37	R	44	0	56	7	0
37	g	44	0	56	20	0
37	q	44	0	56	16	0
37	r	44	0	56	4	0
38	0	42	0	47	2	0
38	6	42	0	47	4	0
38	A	96	0	121	4	0
38	B	106	0	147	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	G	80	0	86	13	0
38	M	50	0	63	3	0
38	R	51	0	68	6	0
38	S	51	0	68	4	0
38	X	38	0	39	1	0
38	Y	42	0	47	5	0
38	a	93	0	112	8	0
38	b	106	0	147	11	0
38	g	80	0	86	21	0
38	m	50	0	63	2	0
38	r	51	0	68	4	0
38	s	51	0	68	6	0
38	x	42	0	47	3	0
38	y	42	0	47	3	0
39	A	10	0	0	1	0
39	a	10	0	0	0	0
40	A	1	0	0	0	0
40	a	1	0	0	0	0
41	A	2	0	0	1	0
41	a	2	0	0	1	0
42	A	64	0	74	7	0
42	D	64	0	74	9	0
42	a	64	0	74	3	0
42	d	64	0	74	5	0
43	A	40	0	56	3	0
43	B	120	0	168	20	0
43	C	80	0	112	6	0
43	D	40	0	56	13	0
43	H	40	0	56	4	0
43	T	40	0	56	6	0
43	V	40	0	56	1	0
43	Z	40	0	56	3	0
43	a	40	0	56	4	0
43	b	120	0	168	16	0
43	c	80	0	112	15	0
43	d	40	0	56	5	0
43	h	40	0	56	4	0
43	t	40	0	56	13	0
43	v	40	0	56	3	0
43	z	40	0	56	4	0
44	A	55	0	80	5	0
44	D	55	0	80	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	a	55	0	80	9	0
44	d	55	0	80	9	0
45	C	248	0	346	34	0
45	c	260	0	373	51	0
46	D	4	0	0	0	0
46	d	4	0	1	0	0
47	E	43	0	30	10	0
47	e	43	0	30	11	0
48	K	35	0	46	1	0
48	R	35	0	46	8	0
48	c	28	0	29	3	0
48	r	35	0	46	11	0
49	0	7	0	0	0	0
49	1	3	0	0	0	0
49	2	3	0	0	0	0
49	3	1	0	0	0	0
49	4	1	0	0	0	0
49	5	1	0	0	0	0
49	6	4	0	0	0	0
49	7	6	0	0	0	0
49	8	4	0	0	0	0
49	9	2	0	0	0	0
49	A	21	0	0	1	0
49	B	6	0	0	0	0
49	C	15	0	0	1	0
49	D	12	0	0	0	0
49	E	1	0	0	0	0
49	F1	4	0	0	0	0
49	G	5	0	0	0	0
49	I	1	0	0	1	0
49	J	1	0	0	0	0
49	N	5	0	0	0	0
49	O	6	0	0	0	0
49	R	4	0	0	0	0
49	S	3	0	0	0	0
49	T	4	0	0	0	0
49	Y	8	0	0	0	0
49	a	14	0	0	0	0
49	b	6	0	0	0	0
49	c	15	0	0	0	0
49	d	15	0	0	0	0
49	e	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	f	1	0	0	0	0
49	f1	3	0	0	0	0
49	g	4	0	0	0	0
49	j	1	0	0	0	0
49	m	2	0	0	0	0
49	n	7	0	0	0	0
49	o	6	0	0	0	0
49	q	1	0	0	0	0
49	r	4	0	0	0	0
49	s	3	0	0	0	0
49	t	2	0	0	0	0
49	w	2	0	0	0	0
49	y	8	0	0	0	0
All	All	117990	0	117879	5329	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 23.

All (5329) 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)
2:4:223:PHE:HE1	35:4:615:RRX:C32	1.41	1.31
2:4:223:PHE:HE1	35:4:615:RRX:H50	1.09	1.17
2:4:223:PHE:CE1	35:4:615:RRX:C32	2.31	1.13
2:G:223:PHE:HE1	35:G:614:RRX:C32	1.61	1.13
38:g:301:SQD:C13	37:g:321:XAT:H362	1.78	1.11
30:9:310:CHL:H42	35:9:317:RRX:H9	1.33	1.11
3:8:53:SER:HA	2:9:171:TYR:HE2	1.11	1.09
3:8:53:SER:HA	2:9:171:TYR:CE2	1.88	1.08
31:N:311:CLA:HHC	31:N:311:CLA:HBB1	1.29	1.07
3:5:171:PRO:HG3	36:5:618:NEX:H8	1.38	1.05
30:1:619:CHL:HBD	30:1:619:CHL:HBA1	1.38	1.04
31:7:311:CLA:H2	32:7:317:LUT:H28	1.39	1.03
19:S:138:GLU:HA	30:S:308:CHL:HED1	1.37	1.03
4:6:110:LEU:CD2	34:6:322:LMG:H331	1.88	1.02
34:0:622:LMG:HC62	34:x:202:LMG:H112	1.37	1.02
2:4:147:ILE:HG12	31:4:604:CLA:H41	1.42	1.01
4:6:217:MET:HG2	32:6:318:LUT:H12	1.43	1.00
33:9:320:LHG:HC92	33:9:320:LHG:H272	1.43	1.00
3:n:147:SER:HB2	34:n:321:LMG:HC4	1.41	0.99
2:4:223:PHE:CE1	35:4:615:RRX:H48	1.96	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2:621:LMG:H172	31:3:301:CLA:H43	1.43	0.98
2:q:176:PRO:HG2	30:q:310:CHL:HBB2	1.42	0.98
37:g:321:XAT:H361	37:g:321:XAT:H28	1.46	0.98
37:9:322:XAT:H28	37:9:322:XAT:H361	1.46	0.97
37:2:619:XAT:H28	37:2:619:XAT:H361	1.46	0.97
3:3:220:VAL:HG21	31:3:314:CLA:HAC2	1.46	0.97
45:c:619:DGD:HA32	45:c:619:DGD:HB21	1.47	0.97
31:G:609:CLA:O2A	35:G:614:RRX:H6	1.63	0.97
4:6:205:LYS:HD3	31:6:313:CLA:HBA1	1.46	0.96
37:G:620:XAT:H28	37:G:620:XAT:H361	1.46	0.96
31:6:304:CLA:HAC2	30:6:308:CHL:H171	1.48	0.96
31:3:306:CLA:H11	36:3:319:NEX:H241	1.46	0.96
37:q:321:XAT:H28	37:q:321:XAT:H361	1.46	0.96
31:g:311:CLA:O1A	38:g:318:SQD:H92	1.66	0.95
2:2:235:LEU:HD22	34:2:618:LMG:HC91	1.47	0.95
37:4:619:XAT:H28	37:4:619:XAT:H361	1.46	0.95
2:G:223:PHE:CE1	35:G:614:RRX:C32	2.50	0.95
2:9:214:ARG:HB3	31:9:304:CLA:HBC3	1.47	0.94
47:e:102:HEM:HHD	47:e:102:HEM:HBC2	1.50	0.94
3:8:236:HIS:HA	3:8:243:THR:HG21	1.49	0.94
3:n:236:HIS:HA	3:n:243:THR:HG21	1.49	0.93
3:5:215:MET:HE2	32:5:617:LUT:H10	1.51	0.93
1:7:244:TYR:HE2	30:7:321:CHL:H41	1.33	0.93
3:3:147:SER:HB2	34:3:321:LMG:H291	1.51	0.93
31:7:311:CLA:H92	32:7:317:LUT:H371	1.52	0.92
2:4:223:PHE:CE1	35:4:615:RRX:H50	1.97	0.92
19:s:90:LEU:HD22	32:s:318:LUT:H221	1.51	0.91
31:6:305:CLA:H61	30:6:307:CHL:HBA1	1.51	0.91
2:q:169:TYR:HD1	2:q:174:GLU:HG3	1.34	0.91
1:7:56:ASN:HB2	3:8:168:ASN:OD1	1.71	0.91
2:9:192:PRO:HD2	35:9:317:RRX:H14	1.52	0.91
3:5:139:ASN:HB3	3:5:142:LEU:HB2	1.50	0.91
47:E:101:HEM:HHD	47:E:101:HEM:HBC2	1.52	0.90
3:3:186:ASP:HA	32:3:317:LUT:H24	1.53	0.90
3:3:252:LYS:HA	3:3:256:ILE:HG23	1.51	0.90
30:q:303:CHL:HED1	33:q:320:LHG:H292	1.53	0.90
31:n:304:CLA:HAC1	30:n:308:CHL:HBB2	1.54	0.90
2:4:146:LEU:HD12	2:4:147:ILE:HD12	1.53	0.89
31:q:305:CLA:HHC	31:q:305:CLA:HBB1	1.52	0.89
1:7:121:LYS:HA	30:7:308:CHL:HED3	1.52	0.89
43:D:405:BCR:H16C	10:F:29:THR:HA	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:122:ALA:HB1	31:7:305:CLA:HED1	1.55	0.88
2:4:146:LEU:HA	30:4:605:CHL:HED3	1.55	0.88
43:B:617:BCR:HC21	34:B:621:LMG:HC91	1.53	0.88
17:O:138:GLN:HG2	17:O:150:LYS:HE3	1.56	0.88
6:b:230:ARG:HH22	38:b:627:SQD:H1	1.38	0.88
31:1:610:CLA:H2	32:1:615:LUT:H28	1.53	0.88
33:C:623:LHG:H251	31:S:312:CLA:HAB	1.55	0.88
31:4:603:CLA:HBB1	31:4:603:CLA:HHC	1.55	0.88
7:c:254:TRP:HB2	22:w:118:THR:HG22	1.55	0.88
2:G:223:PHE:HE1	35:G:614:RRX:H50	1.37	0.88
30:4:608:CHL:HAA1	31:4:610:CLA:HMD1	1.56	0.87
3:8:49:LEU:HD12	2:9:171:TYR:CD2	2.09	0.87
31:b:609:CLA:H142	34:d:410:LMG:C43	2.05	0.87
31:9:305:CLA:HHC	31:9:305:CLA:HBB1	1.56	0.87
2:q:117:ALA:HA	34:q1:101:LMG:H311	1.55	0.87
34:4:620:LMG:H382	3:5:223:LEU:HD11	1.57	0.86
31:1:611:CLA:CAB	38:g:318:SQD:H242	2.05	0.86
34:9:321:LMG:H321	34:9:321:LMG:HC1	1.57	0.86
2:2:214:ARG:HB3	31:2:602:CLA:HBC3	1.56	0.86
1:7:244:TYR:HE2	30:7:321:CHL:C4	1.87	0.85
2:4:101:GLY:HA3	32:4:616:LUT:H10	1.57	0.85
31:9:312:CLA:H72	31:9:314:CLA:HMA2	1.58	0.85
31:6:304:CLA:HMC2	30:6:308:CHL:H121	1.58	0.85
4:6:110:LEU:HD23	34:6:322:LMG:H331	1.56	0.85
31:2:603:CLA:HHC	31:2:603:CLA:HBB1	1.57	0.85
31:9:314:CLA:HHC	31:9:314:CLA:HBB1	1.58	0.85
19:S:155:PRO:HG2	31:S:306:CLA:NB	1.91	0.85
3:5:200:LEU:HA	3:5:203:LYS:HD2	1.57	0.84
2:2:176:PRO:HD2	30:2:607:CHL:HBB2	1.59	0.84
34:q:302:LMG:H132	34:q:302:LMG:HC91	1.56	0.84
30:7:321:CHL:HBB2	31:8:603:CLA:HAC1	1.58	0.84
2:4:143:ASN:HD22	2:4:146:LEU:HD23	1.40	0.84
31:G:612:CLA:C12	37:G:620:XAT:H34	2.06	0.84
4:6:110:LEU:HD21	34:6:322:LMG:H331	1.59	0.84
38:g:301:SQD:C13	37:g:321:XAT:C36	2.56	0.84
31:p:613:CLA:HMB3	32:p:616:LUT:H162	1.60	0.84
30:5:607:CHL:HBA2	4:6:255:LEU:HB2	1.57	0.83
2:q:169:TYR:CD1	2:q:174:GLU:HG3	2.11	0.83
33:l:101:LHG:HC31	33:l:101:LHG:HC62	1.58	0.83
1:7:244:TYR:CE2	30:7:321:CHL:C4	2.61	0.83
4:6:202:LEU:HB3	31:6:311:CLA:CMA	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:163:MET:HE3	30:9:308:CHL:HMB3	1.59	0.83
2:4:155:VAL:HG12	30:4:605:CHL:HAC1	1.60	0.83
3:5:104:THR:HB	3:5:105:PRO:HD3	1.58	0.83
31:s:304:CLA:HHC	31:s:304:CLA:HBB1	1.60	0.83
31:s:311:CLA:H42	31:s:313:CLA:HBA1	1.61	0.83
30:n:308:CHL:H152	30:y:601:CHL:H52	1.60	0.83
34:4:621:LMG:H132	34:4:621:LMG:HC91	1.60	0.83
2:G:223:PHE:CE1	35:G:614:RRX:H48	2.13	0.83
2:9:103:LEU:HB3	31:9:306:CLA:HBC2	1.60	0.83
31:s:305:CLA:H92	30:s:307:CHL:HBA2	1.60	0.82
2:q:258:LEU:HD22	2:q:259:PRO:HD2	1.60	0.82
3:3:159:MET:HE3	30:3:308:CHL:HMB1	1.62	0.82
3:3:239:ALA:HB3	3:3:243:THR:HG22	1.60	0.82
31:G:602:CLA:H91	31:Y:304:CLA:H61	1.62	0.82
19:s:285:ARG:HE	38:s:301:SQD:H3	1.44	0.82
4:0:217:MET:HG2	32:0:617:LUT:H12	1.61	0.82
3:5:136:TYR:HB3	3:5:142:LEU:HB3	1.61	0.82
8:d:98:GLN:HB3	34:d:410:LMG:HC5	1.60	0.81
1:1:149:THR:HG22	30:1:605:CHL:HAC1	1.63	0.81
31:1:611:CLA:HAB	38:g:318:SQD:H242	1.60	0.81
30:y:607:CHL:H102	30:y:609:CHL:H172	1.62	0.81
2:4:137:GLY:HA2	2:4:150:GLN:HG2	1.63	0.81
4:6:217:MET:HE2	32:6:318:LUT:H10	1.61	0.81
3:p:106:GLU:HA	3:p:119:ALA:HB1	1.63	0.81
31:1:610:CLA:H92	32:1:615:LUT:H371	1.61	0.81
3:n:226:ARG:NH2	34:n:322:LMG:HC61	1.96	0.81
4:6:50:LEU:HB3	4:6:54:SER:HB3	1.62	0.80
3:n:226:ARG:HH22	34:n:322:LMG:C6	1.94	0.80
31:G:610:CLA:HAA2	38:G:617:SQD:H441	1.63	0.80
2:q:140:TYR:HB3	2:q:146:LEU:HD23	1.62	0.80
2:G:223:PHE:CE1	35:G:614:RRX:H50	2.14	0.80
24:Y:175:PRO:HG2	38:Y:320:SQD:H441	1.64	0.80
31:8:609:CLA:H52	32:8:615:LUT:H30	1.64	0.80
31:6:311:CLA:H51	32:6:317:LUT:H30	1.63	0.80
31:p:602:CLA:HAC2	33:p:619:LHG:H262	1.61	0.80
38:a:412:SQD:H92	34:a:413:LMG:H111	1.63	0.80
34:b:626:LMG:HC92	38:b:627:SQD:H2	1.64	0.80
45:C:620:DGD:HAV1	34:C:624:LMG:H151	1.62	0.80
2:2:52:PRO:HB2	18:R:42:ALA:HB1	1.64	0.80
7:C:155:VAL:HG12	34:C:621:LMG:H362	1.64	0.80
31:0:614:CLA:HBA2	34:p:620:LMG:H111	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:q:308:CHL:HBB2	30:q:309:CHL:CBB	2.12	0.79
27:Q1:6:GLY:HA3	34:Q1:101:LMG:HC62	1.64	0.79
30:4:609:CHL:HAA2	3:5:71:THR:HG21	1.65	0.79
1:7:56:ASN:CB	3:8:168:ASN:OD1	2.30	0.79
31:8:614:CLA:H11	34:9:302:LMG:HC92	1.64	0.79
31:q:315:CLA:H102	37:q:321:XAT:H34	1.63	0.79
8:d:192:THR:HG23	31:d:404:CLA:HBC2	1.64	0.79
2:9:138:LEU:HD21	31:9:306:CLA:HAA2	1.63	0.79
2:4:179:THR:H	2:4:188:GLY:HA3	1.47	0.79
4:6:188:ASP:HA	32:6:317:LUT:H24	1.65	0.79
3:8:236:HIS:HA	3:8:243:THR:CG2	2.13	0.79
31:b:611:CLA:HHC	31:b:611:CLA:HBB1	1.64	0.79
3:3:159:MET:HE1	36:3:319:NEX:H30	1.63	0.79
31:c:606:CLA:H151	43:c:615:BCR:H363	1.64	0.79
3:n:236:HIS:HA	3:n:243:THR:CG2	2.13	0.79
30:5:608:CHL:HBB2	36:5:618:NEX:H10	1.64	0.79
3:5:252:LYS:HA	3:5:256:ILE:HG23	1.63	0.79
37:G:620:XAT:H362	38:G:624:SQD:C13	2.13	0.79
3:N:245:PHE:HB3	31:N:313:CLA:H11	1.65	0.79
38:g:301:SQD:H92	37:g:321:XAT:H222	1.64	0.79
8:D:192:THR:HG23	31:D:403:CLA:HBC2	1.64	0.78
6:b:142:HIS:HE1	31:b:616:CLA:ND	1.80	0.78
2:4:254:ALA:HA	37:4:619:XAT:H22	1.63	0.78
2:q:103:LEU:HD21	31:q:314:CLA:HBB2	1.65	0.78
31:5:612:CLA:HBB1	31:5:612:CLA:HMB3	1.66	0.78
31:R:304:CLA:HBA1	37:R:318:XAT:H382	1.64	0.78
3:p:54:ASN:H	2:q:171:TYR:HE2	1.29	0.78
18:r:170:ASN:HA	48:r:302:LMU:H2B	1.65	0.78
3:p:247:VAL:HG13	2:q:133:PHE:HE2	1.48	0.78
24:y:126:LYS:HA	30:y:607:CHL:HED3	1.64	0.78
31:4:602:CLA:H61	32:4:616:LUT:H30	1.64	0.78
3:5:86:GLU:HA	3:5:179:LEU:HD11	1.66	0.78
18:R:164:ALA:HB1	31:R:306:CLA:HED1	1.66	0.78
1:7:213:MET:HE2	32:7:318:LUT:H10	1.65	0.78
3:n:59:LEU:HD23	3:n:68:GLY:HA2	1.66	0.78
2:2:220:MET:HE2	32:2:615:LUT:H10	1.66	0.78
1:7:165:VAL:HG11	2:9:57:SER:HB3	1.63	0.78
34:g:322:LMG:H111	30:y:607:CHL:H11	1.66	0.78
1:1:50:LEU:HB2	1:1:54:SER:HB2	1.66	0.78
31:3:306:CLA:H52	30:3:308:CHL:HAA2	1.66	0.77
3:3:191:ALA:HB2	31:3:311:CLA:HAA2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:176:PRO:HD2	30:G:607:CHL:HBB2	1.64	0.77
19:S:189:PRO:HD2	30:S:309:CHL:HBB2	1.66	0.77
1:7:241:ASN:HA	1:7:246:LEU:HD11	1.66	0.77
3:8:59:LEU:HD23	3:8:68:GLY:HA2	1.66	0.77
22:w:80:SER:HB3	34:w:205:LMG:HC4	1.65	0.77
30:N:306:CHL:H171	31:S:315:CLA:HMC3	1.66	0.77
18:R:169:TYR:CE2	48:R:302:LMU:H6D	2.20	0.77
19:s:189:PRO:HD2	30:s:309:CHL:HBB2	1.66	0.77
3:n:226:ARG:NH2	34:n:322:LMG:C6	2.48	0.77
31:1:611:CLA:CAB	38:g:318:SQD:C24	2.63	0.77
45:c:619:DGD:HAW1	45:c:619:DGD:HBE1	1.66	0.77
31:G:612:CLA:H121	37:G:620:XAT:H34	1.67	0.77
30:p:607:CHL:HBD	30:p:607:CHL:HBA1	1.67	0.77
3:3:38:VAL:HA	3:3:42:GLY:HA3	1.66	0.76
7:C:246:ALA:HB1	22:W:111:ASN:ND2	2.00	0.76
31:9:305:CLA:HED2	31:9:305:CLA:H12	1.67	0.76
6:b:230:ARG:NH2	38:b:627:SQD:H1	2.00	0.76
30:0:605:CHL:HBD	30:0:605:CHL:HBA1	1.66	0.76
31:B:611:CLA:H61	31:B:613:CLA:HED3	1.65	0.76
31:8:614:CLA:H2	2:9:228:LEU:HD12	1.66	0.76
3:n:147:SER:CB	34:n:321:LMG:HC4	2.13	0.76
31:4:604:CLA:H43	30:4:606:CHL:CAD	2.16	0.76
30:1:601:CHL:HHC	30:1:601:CHL:HBB1	1.68	0.76
2:4:178:GLU:HG2	2:4:189:PHE:HB3	1.65	0.76
8:d:123:ILE:HD11	34:d:411:LMG:H402	1.66	0.76
31:N:310:CLA:H92	32:N:316:LUT:H371	1.68	0.76
1:7:244:TYR:CE2	30:7:321:CHL:H41	2.18	0.76
3:p:120:VAL:HG23	3:p:123:LYS:HB2	1.66	0.76
30:5:608:CHL:CBB	36:5:618:NEX:H10	2.16	0.76
31:N:312:CLA:HHC	31:N:312:CLA:HBB1	1.67	0.76
2:9:230:THR:HG23	2:9:232:LYS:H	1.51	0.76
3:5:186:ASP:HA	32:5:616:LUT:H24	1.68	0.76
32:S:318:LUT:H371	32:S:318:LUT:H28	1.68	0.76
2:q:178:GLU:HG2	2:q:189:PHE:HD1	1.51	0.76
45:c:619:DGD:HBH1	45:c:619:DGD:HBV2	1.67	0.76
8:D:49:PHE:CG	43:D:405:BCR:H15C	2.21	0.75
30:2:605:CHL:HHC	30:2:605:CHL:HBB1	1.69	0.75
31:7:304:CLA:HAC1	30:7:308:CHL:HBB2	1.66	0.75
30:S:307:CHL:HBB2	30:S:308:CHL:CBB	2.16	0.75
2:2:149:ALA:HA	30:2:605:CHL:CHC	2.17	0.75
31:s:303:CLA:HMB3	31:s:303:CLA:HBB1	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:G:622:LMG:H172	31:N:321:CLA:H43	1.69	0.75
31:g:305:CLA:HBB1	31:g:305:CLA:HMB1	1.68	0.75
48:R:302:LMU:H101	31:R:307:CLA:HED1	1.69	0.75
2:9:162:ILE:HG23	36:9:319:NEX:H15	1.68	0.75
31:n:311:CLA:H52	32:n:317:LUT:H30	1.67	0.75
31:2:609:CLA:H2	35:2:614:RRX:H6	1.66	0.75
2:4:133:PHE:HE1	30:4:607:CHL:HMD3	1.51	0.75
3:5:106:GLU:HB3	3:5:230:ILE:HD11	1.69	0.75
4:6:202:LEU:HB3	31:6:311:CLA:HMA2	1.66	0.75
33:c:622:LHG:H312	33:s:320:LHG:HC92	1.69	0.75
2:2:153:VAL:HA	2:2:156:LEU:HD12	1.69	0.74
3:5:115:ASN:HD22	3:5:115:ASN:H	1.34	0.74
31:b:612:CLA:H8	31:b:614:CLA:H51	1.67	0.74
31:6:315:CLA:HMB1	31:6:315:CLA:HBB1	1.68	0.74
3:p:126:ALA:H	30:p:607:CHL:HED1	1.52	0.74
31:S:303:CLA:HMB3	31:S:303:CLA:HBB1	1.66	0.74
30:q:310:CHL:HHC	30:q:310:CHL:HBB1	1.69	0.74
4:0:202:LEU:HB3	31:0:610:CLA:HMA2	1.67	0.74
2:9:109:GLU:HA	2:9:123:ALA:HB1	1.69	0.74
30:9:303:CHL:HAC1	33:9:320:LHG:HC32	1.68	0.74
30:g:306:CHL:HBB1	30:g:306:CHL:HHC	1.69	0.74
34:w:202:LMG:H211	31:y:612:CLA:H141	1.69	0.74
31:5:610:CLA:H2	32:5:616:LUT:H28	1.69	0.74
31:B:607:CLA:HBB1	31:B:607:CLA:HMB1	1.69	0.74
4:0:164:ILE:HD11	36:0:618:NEX:C34	2.18	0.74
8:d:312:GLU:HG2	17:o:205:PRO:HB3	1.68	0.74
24:y:77:LEU:HD23	31:y:602:CLA:H42	1.70	0.74
6:B:142:HIS:HE1	31:B:615:CLA:ND	1.85	0.74
24:Y:50:LEU:HB2	24:Y:54:SER:HB3	1.68	0.74
6:b:216:HIS:HE1	31:b:610:CLA:C1A	2.01	0.74
34:d:410:LMG:H402	23:x:79:GLY:HA2	1.68	0.74
30:6:306:CHL:HHC	30:6:306:CHL:HBB1	1.69	0.74
7:C:245:TRP:HB3	45:C:620:DGD:HD2	1.68	0.74
31:N:311:CLA:HHC	31:N:311:CLA:CBB	2.13	0.74
2:9:223:PHE:CZ	35:9:317:RRX:H48	2.23	0.74
33:g:319:LHG:H282	37:g:321:XAT:C33	2.17	0.74
31:c:603:CLA:H203	31:c:610:CLA:HAB	1.69	0.74
4:0:205:LYS:HG3	31:0:611:CLA:HED2	1.69	0.74
31:g:310:CLA:HBA1	35:g:315:RRX:H18	1.70	0.74
31:7:311:CLA:HMB3	31:7:311:CLA:HBB1	1.70	0.73
31:2:609:CLA:H12	31:2:609:CLA:H3A	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:247:PHE:HB2	31:6:314:CLA:CAD	2.18	0.73
3:N:110:ARG:HH21	3:N:231:GLU:HA	1.53	0.73
3:p:225:THR:HB	3:p:249:TYR:CE2	2.24	0.73
3:3:236:HIS:HB2	31:3:314:CLA:HAA2	1.70	0.73
2:4:177:VAL:HA	2:4:189:PHE:HD2	1.54	0.73
3:5:185:PHE:HA	30:5:608:CHL:H2	1.70	0.73
41:A:403:CL:CL	8:D:317:LYS:NZ	2.57	0.73
31:S:311:CLA:H42	31:S:313:CLA:HBA1	1.68	0.73
31:8:611:CLA:HBB1	31:8:611:CLA:HMB3	1.70	0.73
31:b:611:CLA:H102	31:b:616:CLA:HAA1	1.71	0.73
31:n:305:CLA:H152	31:s:306:CLA:CHB	2.19	0.73
2:4:228:LEU:HD21	34:4:621:LMG:H341	1.70	0.73
31:4:603:CLA:HMC3	32:4:616:LUT:H191	1.69	0.73
3:5:236:HIS:HA	3:5:243:THR:OG1	1.88	0.73
3:N:245:PHE:HB2	31:N:313:CLA:CAD	2.18	0.73
24:Y:77:LEU:HD23	31:Y:303:CLA:H42	1.69	0.73
31:p:612:CLA:HHC	31:p:612:CLA:HBB1	1.70	0.73
2:4:152:ILE:H	2:4:152:ILE:HD12	1.54	0.73
31:N:305:CLA:H121	31:S:306:CLA:H3A	1.69	0.73
31:p:611:CLA:H43	31:p:612:CLA:HMD2	1.68	0.73
3:n:226:ARG:HH22	34:n:322:LMG:HC61	1.54	0.73
3:3:215:MET:HE2	32:3:318:LUT:H10	1.71	0.73
3:p:245:PHE:HZ	30:q:309:CHL:H11	1.52	0.73
4:0:202:LEU:HB3	31:0:610:CLA:CMA	2.18	0.73
31:7:305:CLA:HMA2	30:7:307:CHL:C3C	2.19	0.73
30:p:605:CHL:HHC	30:p:605:CHL:HBB1	1.69	0.73
31:7:313:CLA:HBB1	31:7:313:CLA:HHC	1.71	0.73
31:s:303:CLA:H61	32:s:318:LUT:H28	1.70	0.73
3:3:245:PHE:HB3	31:3:314:CLA:H11	1.71	0.72
33:D:408:LHG:H312	20:T:21:ILE:HD11	1.71	0.72
33:G:618:LHG:C6	37:G:620:XAT:H382	2.18	0.72
31:Y:310:CLA:HBB1	31:Y:310:CLA:HMB3	1.71	0.72
3:8:215:MET:HE2	32:8:616:LUT:H10	1.70	0.72
3:p:191:ALA:HB2	3:p:200:LEU:HD12	1.71	0.72
30:q:307:CHL:HHC	30:q:307:CHL:HBB1	1.70	0.72
45:c:619:DGD:HBG3	32:y:616:LUT:H193	1.70	0.72
8:d:56:THR:HG21	9:e:50:PRO:HD3	1.71	0.72
30:3:303:CHL:HHC	30:3:303:CHL:HBB1	1.71	0.72
7:C:83:LEU:O	7:C:166:LYS:NZ	2.22	0.72
30:G:605:CHL:HHC	30:G:605:CHL:HBB1	1.70	0.72
31:b:614:CLA:H43	33:b:625:LHG:H371	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:b:629:LMG:H302	30:r:309:CHL:H42	1.70	0.72
30:6:309:CHL:HHC	30:6:309:CHL:HBB1	1.71	0.72
31:7:305:CLA:HBB1	31:7:305:CLA:HMB3	1.70	0.72
5:a:38:ILE:HG23	34:a:401:LMG:H362	1.72	0.72
5:a:141:PRO:O	8:d:220:ASN:ND2	2.23	0.72
1:7:77:LEU:HD23	31:7:303:CLA:H42	1.70	0.72
31:n:303:CLA:H61	32:n:318:LUT:H30	1.71	0.72
31:5:602:CLA:HBB1	31:5:602:CLA:HMB3	1.72	0.72
30:R:309:CHL:HHC	30:R:309:CHL:HBB1	1.71	0.72
3:8:87:LEU:HD13	31:8:603:CLA:HBA1	1.71	0.72
1:7:178:TYR:HB3	31:7:311:CLA:HED3	1.70	0.72
2:q:176:PRO:CG	30:q:310:CHL:HBB2	2.18	0.72
31:n:313:CLA:HBB1	31:n:313:CLA:HMB3	1.70	0.72
30:2:607:CHL:HHC	30:2:607:CHL:HBB1	1.72	0.72
5:A:192:ILE:HG13	5:A:293:MET:HE1	1.72	0.72
30:N:306:CHL:HHC	30:N:306:CHL:HBB1	1.72	0.72
4:0:149:SER:HB2	34:0:622:LMG:HC92	1.72	0.72
45:c:617:DGD:HBW2	45:c:618:DGD:HAG2	1.70	0.72
31:7:316:CLA:HBD	31:7:316:CLA:HBA1	1.72	0.72
3:n:87:LEU:HD13	31:n:304:CLA:HBA1	1.72	0.72
31:b:613:CLA:HMB1	31:b:613:CLA:HBB1	1.72	0.72
34:b:629:LMG:H342	30:r:309:CHL:H61	1.71	0.72
31:1:603:CLA:HAC1	30:1:607:CHL:HBB2	1.71	0.71
2:2:259:PRO:HA	34:2:620:LMG:HC5	1.72	0.71
30:4:605:CHL:HBB1	30:4:605:CHL:HHC	1.71	0.71
31:5:610:CLA:H52	32:5:616:LUT:H30	1.72	0.71
31:N:304:CLA:HAC1	30:Y:301:CHL:HBB2	1.70	0.71
34:n:321:LMG:H311	34:n:321:LMG:H151	1.72	0.71
2:4:177:VAL:HA	2:4:189:PHE:CD2	2.25	0.71
3:5:191:ALA:HB2	31:5:610:CLA:HAA2	1.72	0.71
30:G:607:CHL:HBB1	30:G:607:CHL:HHC	1.72	0.71
30:7:302:CHL:HHC	30:7:302:CHL:HBB1	1.72	0.71
3:8:96:MET:SD	31:8:609:CLA:HAB	2.31	0.71
31:b:616:CLA:H2	31:b:617:CLA:HBB2	1.73	0.71
30:5:605:CHL:HHC	30:5:605:CHL:HBB1	1.70	0.71
31:9:314:CLA:CHC	35:9:317:RRX:H37	2.19	0.71
31:q:313:CLA:C3C	33:q:320:LHG:HC61	2.21	0.71
2:g:155:VAL:HG12	30:g:306:CHL:HAC1	1.72	0.71
34:4:621:LMG:HC91	34:4:621:LMG:C13	2.21	0.71
30:N:302:CHL:HBB1	30:N:302:CHL:HHC	1.73	0.71
3:p:223:LEU:HD11	34:q:301:LMG:H382	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:p:244:ASN:HB3	3:p:246:TRP:HD1	1.55	0.71
24:Y:154:THR:HG22	30:Y:306:CHL:HAC1	1.72	0.71
4:0:170:ASN:HD22	2:q:53:PHE:HA	1.56	0.71
2:q:119:PHE:HB3	2:q:122:ALA:HB3	1.73	0.71
3:n:215:MET:HE2	32:n:318:LUT:H10	1.72	0.71
30:0:601:CHL:HBB1	30:0:601:CHL:HHC	1.73	0.71
31:3:311:CLA:H52	32:3:317:LUT:H30	1.71	0.71
31:4:610:CLA:H72	35:4:615:RRX:H25	1.72	0.71
31:5:610:CLA:H2	32:5:616:LUT:H26	1.72	0.71
8:d:145:ALA:HB2	8:d:272:LEU:HD11	1.71	0.71
3:3:104:THR:HB	3:3:105:PRO:HD3	1.73	0.71
2:4:59:PRO:HA	4:6:85:ARG:HH22	1.56	0.71
2:4:171:TYR:HE2	3:5:54:ASN:H	1.39	0.71
3:5:123:LYS:HA	30:5:607:CHL:HED3	1.72	0.71
3:N:233:LEU:HD13	31:N:314:CLA:HBC2	1.71	0.71
34:q1:101:LMG:H132	34:q1:101:LMG:H352	1.73	0.71
30:1:619:CHL:HBA1	30:1:619:CHL:CBD	2.17	0.71
30:p:608:CHL:HHC	30:p:608:CHL:HBB1	1.71	0.71
31:p:614:CLA:HHC	31:p:614:CLA:HBB1	1.73	0.71
34:n:322:LMG:H321	31:y:615:CLA:H61	1.73	0.71
18:r:184:TYR:HA	48:r:302:LMU:H31	1.70	0.71
1:1:195:LEU:HG	1:1:199:LYS:HE2	1.71	0.71
33:G:618:LHG:H281	37:G:620:XAT:C32	2.21	0.71
30:S:307:CHL:HHC	30:S:307:CHL:HBB1	1.72	0.71
34:c:624:LMG:H341	33:y:619:LHG:H101	1.71	0.71
8:d:126:MET:HG3	8:d:146:PHE:HD2	1.56	0.71
30:n:302:CHL:HHC	30:n:302:CHL:HBB1	1.72	0.71
30:4:608:CHL:HBB1	30:4:608:CHL:HHC	1.71	0.70
3:N:47:GLN:HG3	3:N:53:SER:HB2	1.73	0.70
3:8:246:TRP:HH2	30:9:309:CHL:H62	1.54	0.70
30:9:303:CHL:HBB1	30:9:303:CHL:HHC	1.72	0.70
16:m:31:SER:HA	38:m:101:SQD:H2	1.73	0.70
24:y:197:ALA:HB1	24:y:203:LEU:HG	1.72	0.70
30:2:608:CHL:HHC	30:2:608:CHL:HBB1	1.73	0.70
30:4:609:CHL:HHC	30:4:609:CHL:HBB1	1.72	0.70
3:5:151:ILE:HD13	30:5:605:CHL:HAC1	1.72	0.70
30:5:601:CHL:HHC	30:5:601:CHL:HBB1	1.72	0.70
30:7:310:CHL:HAA2	2:9:74:THR:HG21	1.72	0.70
32:p:617:LUT:H363	31:q:305:CLA:HED3	1.73	0.70
30:r:309:CHL:HHC	30:r:309:CHL:HBB1	1.72	0.70
3:5:106:GLU:HB3	3:5:230:ILE:CD1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:609:CHL:HAA2	2:q:74:THR:HG21	1.73	0.70
2:G:260:LEU:H	34:G:621:LMG:HC61	1.57	0.70
30:Y:309:CHL:HHC	30:Y:309:CHL:HBB1	1.73	0.70
30:0:609:CHL:HHC	30:0:609:CHL:HBB1	1.73	0.70
30:g:308:CHL:HHC	30:g:308:CHL:HBB1	1.72	0.70
19:s:241:LEU:HD21	31:s:313:CLA:HBC2	1.72	0.70
43:B:617:BCR:HC22	34:B:621:LMG:H292	1.73	0.70
31:2:603:CLA:HED2	31:2:603:CLA:H12	1.73	0.70
30:3:307:CHL:HHC	30:3:307:CHL:HBB1	1.72	0.70
30:8:601:CHL:HBB1	30:8:601:CHL:HHC	1.72	0.70
30:q:310:CHL:H42	35:q:317:RRX:H9	1.73	0.70
31:q:312:CLA:H2	35:q:317:RRX:C40	2.21	0.70
34:D:411:LMG:H402	23:X:79:GLY:HA2	1.72	0.70
3:N:87:LEU:HD13	31:N:304:CLA:HBA1	1.73	0.70
3:8:53:SER:CA	2:9:171:TYR:HE2	1.98	0.70
2:9:211:LYS:HE3	33:9:320:LHG:HC61	1.73	0.70
9:e:55:TYR:O	9:e:60:ARG:NH2	2.24	0.70
30:3:307:CHL:HBB2	34:3:321:LMG:H322	1.74	0.70
4:6:205:LYS:HD3	31:6:313:CLA:CBA	2.22	0.70
31:C:603:CLA:H203	31:C:610:CLA:HAB	1.74	0.70
3:N:59:LEU:HD23	3:N:68:GLY:HA2	1.74	0.70
30:0:607:CHL:HHC	30:0:607:CHL:HBB1	1.74	0.70
30:6:308:CHL:H122	30:6:308:CHL:HMB3	1.72	0.70
31:B:610:CLA:HHC	31:B:610:CLA:HBB1	1.72	0.70
3:N:252:LYS:HA	3:N:256:ILE:HG23	1.73	0.70
18:R:139:HIS:HD2	37:R:318:XAT:H15	1.56	0.70
31:R:304:CLA:CAB	37:R:318:XAT:H32	2.22	0.70
31:8:614:CLA:HBB1	31:8:614:CLA:HMB3	1.74	0.70
30:5:609:CHL:HHC	30:5:609:CHL:HBB1	1.74	0.70
31:B:611:CLA:HMB1	31:B:611:CLA:HBB1	1.72	0.70
31:8:602:CLA:H61	32:8:616:LUT:H30	1.73	0.70
6:b:53:ASN:HD21	6:b:331:ASN:HD21	1.39	0.70
19:s:207:MET:HE3	30:s:309:CHL:HBC3	1.71	0.70
30:s:307:CHL:HHC	30:s:307:CHL:HBB1	1.72	0.70
2:2:130:ALA:H	30:3:302:CHL:HED1	1.56	0.69
2:4:117:ALA:H	34:Q1:101:LMG:H121	1.57	0.69
3:5:72:ALA:HB3	3:5:74:LEU:HD21	1.74	0.69
3:8:186:ASP:HA	32:8:615:LUT:H24	1.74	0.69
31:5:615:CLA:HBD	31:5:615:CLA:HBA1	1.74	0.69
31:C:606:CLA:H41	34:W:201:LMG:H331	1.73	0.69
2:q:122:ALA:HB1	31:q:306:CLA:HED2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:q:303:CHL:HHC	30:q:303:CHL:HBB1	1.74	0.69
3:n:186:ASP:HA	32:n:317:LUT:H24	1.74	0.69
30:9:308:CHL:HHC	30:9:308:CHL:HBB1	1.74	0.69
2:q:223:PHE:CD1	35:q:317:RRX:H48	2.27	0.69
34:2:621:LMG:H132	34:2:621:LMG:HC91	1.73	0.69
3:5:225:THR:HG23	3:5:227:LYS:H	1.57	0.69
30:6:302:CHL:HBB1	30:6:302:CHL:HHC	1.74	0.69
3:p:180:TYR:HB3	31:p:610:CLA:HED3	1.73	0.69
2:q:132:ILE:HB	2:q:138:LEU:HD12	1.74	0.69
31:q:312:CLA:H2	35:q:317:RRX:H6	1.73	0.69
10:f:14:ILE:HD11	27:q1:26:PRO:HB2	1.73	0.69
3:3:96:MET:SD	31:3:311:CLA:HAB	2.32	0.69
6:B:216:HIS:HE1	31:B:609:CLA:C1A	2.04	0.69
31:B:615:CLA:H2	31:B:616:CLA:HBB2	1.75	0.69
19:S:207:MET:HE3	30:S:309:CHL:HBC3	1.75	0.69
22:W:119:LEU:HD21	28:P1:42:ARG:HG2	1.74	0.69
31:8:614:CLA:H42	34:9:302:LMG:H112	1.73	0.69
3:p:220:VAL:HG11	31:p:613:CLA:HAC2	1.75	0.69
30:1:605:CHL:HBB1	30:1:605:CHL:HHC	1.73	0.69
2:2:133:PHE:HE2	30:3:302:CHL:HMD3	1.56	0.69
30:3:302:CHL:HBB1	30:3:302:CHL:HHC	1.74	0.69
3:5:251:PRO:HG2	3:5:252:LYS:HD2	1.75	0.69
31:5:615:CLA:HBA1	31:5:615:CLA:CHA	2.22	0.69
45:C:620:DGD:HBH2	45:C:620:DGD:HBV2	1.73	0.69
3:5:158:LEU:HG	36:5:618:NEX:H15	1.75	0.69
33:D:407:LHG:HC91	33:L:101:LHG:HC81	1.74	0.69
2:q:254:ALA:HA	37:q:321:XAT:H22	1.75	0.69
30:g:309:CHL:HHC	30:g:309:CHL:HBB1	1.74	0.69
30:y:608:CHL:HHC	30:y:608:CHL:HBB1	1.73	0.69
31:1:604:CLA:HMA2	30:1:606:CHL:HBC3	1.72	0.69
30:4:601:CHL:HHC	30:4:601:CHL:HBB1	1.75	0.69
30:5:609:CHL:HMB2	30:6:302:CHL:HHB	1.75	0.69
31:6:316:CLA:HBB1	31:6:316:CLA:HMB3	1.75	0.69
8:D:186:GLN:HB2	31:D:403:CLA:HBC1	1.75	0.69
30:7:306:CHL:HBB1	30:7:306:CHL:HHC	1.74	0.69
2:g:205:LEU:HB3	31:g:310:CLA:HMA2	1.74	0.69
34:w:202:LMG:H182	34:w:202:LMG:H431	1.73	0.69
3:3:110:ARG:HH11	3:3:230:ILE:HG22	1.58	0.69
1:1:213:MET:HE2	32:1:616:LUT:H10	1.74	0.69
30:4:607:CHL:HAA2	3:5:253:SER:HB2	1.75	0.69
45:C:620:DGD:HBN2	31:Y:311:CLA:H142	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:140:LYS:HB2	17:O:148:GLU:HG3	1.75	0.69
30:q:311:CHL:HBB1	30:q:311:CHL:HHC	1.74	0.69
4:6:115:ALA:O	34:6:321:LMG:HC2	1.93	0.68
34:7:322:LMG:H291	34:7:322:LMG:H332	1.74	0.68
2:q:196:ALA:HB2	31:q:312:CLA:HAA2	1.74	0.68
45:c:617:DGD:HBH1	45:c:618:DGD:HAT1	1.74	0.68
3:n:96:MET:SD	31:n:311:CLA:HAB	2.33	0.68
30:y:609:CHL:HHC	30:y:609:CHL:HBB1	1.74	0.68
34:6:321:LMG:H111	34:6:322:LMG:H111	1.76	0.68
19:S:241:LEU:HD21	31:S:313:CLA:HBC2	1.75	0.68
5:a:267:ASN:HD22	38:a:411:SQD:H3	1.58	0.68
34:q1:101:LMG:H312	34:q1:101:LMG:C10	2.23	0.68
1:1:107:VAL:HB	1:1:108:PRO:HD3	1.73	0.68
31:3:306:CLA:H92	30:3:308:CHL:HBA2	1.74	0.68
5:A:188:ALA:HB2	5:A:328:MET:HB2	1.76	0.68
30:g:302:CHL:H161	33:g:319:LHG:H372	1.73	0.68
1:1:251:LEU:HB3	30:1:619:CHL:HBA2	1.74	0.68
3:5:143:ILE:HA	30:5:605:CHL:C4D	2.23	0.68
6:B:365:THR:HG22	8:D:326:ARG:HH21	1.57	0.68
45:C:620:DGD:HBV2	31:Y:311:CLA:H51	1.76	0.68
2:4:149:ALA:HA	30:4:605:CHL:CHC	2.24	0.68
3:5:246:TRP:O	3:5:251:PRO:HD3	1.94	0.68
42:D:401:PHO:H3A	31:D:403:CLA:H142	1.76	0.68
3:p:206:LYS:HD3	31:p:611:CLA:O1D	1.93	0.68
24:y:50:LEU:HB2	24:y:54:SER:HB3	1.74	0.68
2:2:59:PRO:HG2	2:2:73:ASP:HB3	1.76	0.68
3:N:96:MET:SD	31:N:310:CLA:HAB	2.33	0.68
24:Y:116:GLY:HA3	34:Y:319:LMG:HC3	1.75	0.68
30:7:309:CHL:HHC	30:7:309:CHL:HBB1	1.76	0.68
30:9:309:CHL:C4B	30:9:309:CHL:H43	2.24	0.68
3:p:200:LEU:HA	3:p:203:LYS:HD2	1.75	0.68
2:2:165:ALA:HB3	36:2:616:NEX:H203	1.74	0.68
2:2:223:PHE:HE1	35:2:614:RRX:H48	1.58	0.68
31:6:305:CLA:HBB1	31:6:305:CLA:HMB3	1.74	0.68
31:G:609:CLA:H72	35:G:614:RRX:C21	2.24	0.68
31:N:310:CLA:H2	32:N:316:LUT:H28	1.76	0.68
30:Y:308:CHL:HHC	30:Y:308:CHL:HBB1	1.76	0.68
31:p:602:CLA:H11	32:p:617:LUT:H373	1.76	0.68
30:0:607:CHL:H12	2:q:259:PRO:HD3	1.74	0.68
19:S:176:MET:HE2	19:S:176:MET:HA	1.76	0.68
24:y:175:PRO:HD2	30:y:608:CHL:HBB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:p1:34:LYS:HG2	28:p1:46:GLY:HA2	1.75	0.68
4:0:125:LYS:HE2	2:q:258:LEU:HD11	1.76	0.68
17:O:99:MET:SD	17:O:176:VAL:HG11	2.34	0.67
5:a:133:LEU:HD12	8:d:256:ILE:HG12	1.76	0.67
19:s:176:MET:HE2	19:s:176:MET:HA	1.75	0.67
30:y:606:CHL:HHC	30:y:606:CHL:HBB1	1.76	0.67
30:2:601:CHL:HHC	30:2:601:CHL:HBB1	1.74	0.67
36:Y:317:NEX:H402	38:Y:320:SQD:H162	1.75	0.67
1:7:74:THR:O	3:8:83:ARG:NE	2.26	0.67
30:9:310:CHL:HHC	30:9:310:CHL:HBB1	1.76	0.67
3:p:245:PHE:HB2	31:p:613:CLA:CAD	2.24	0.67
3:n:252:LYS:HA	3:n:256:ILE:HG23	1.76	0.67
30:1:609:CHL:HHC	30:1:609:CHL:HBB1	1.76	0.67
4:6:253:LYS:HD2	4:6:254:THR:N	2.10	0.67
31:N:305:CLA:H191	31:S:306:CLA:ND	2.10	0.67
4:0:205:LYS:HD3	31:0:612:CLA:HBA1	1.74	0.67
3:p:91:HIS:HE1	31:p:603:CLA:ND	1.91	0.67
6:b:29:LEU:HD11	43:b:618:BCR:H19C	1.75	0.67
31:B:612:CLA:HMB1	31:B:612:CLA:HBB1	1.75	0.67
45:C:620:DGD:HAV2	33:Y:318:LHG:H361	1.76	0.67
33:c:622:LHG:H242	31:s:312:CLA:HAB	1.76	0.67
2:4:152:ILE:O	2:4:156:LEU:HG	1.95	0.67
3:5:220:VAL:HG21	31:5:613:CLA:HAC2	1.77	0.67
31:g:312:CLA:HBB1	31:g:312:CLA:HMB3	1.76	0.67
31:5:610:CLA:H12	31:5:610:CLA:H3A	1.77	0.67
30:G:608:CHL:HBB1	30:G:608:CHL:HHC	1.76	0.67
30:Y:307:CHL:HHC	30:Y:307:CHL:HBB1	1.76	0.67
30:p:607:CHL:HHC	30:p:607:CHL:HBB1	1.76	0.67
1:1:185:PRO:HD2	32:1:615:LUT:H23	1.77	0.67
4:6:172:GLY:O	18:R:56:ASN:ND2	2.28	0.67
30:6:310:CHL:HHC	30:6:310:CHL:HBB1	1.77	0.67
5:A:140:ARG:HH22	33:A:417:LHG:HC41	1.58	0.67
2:9:86:ARG:NH1	2:9:86:ARG:HA	2.10	0.67
3:p:52:PHE:CG	2:q:168:ALA:HB1	2.29	0.67
3:p:198:ALA:HA	3:p:201:LYS:HD3	1.76	0.67
3:8:252:LYS:HA	3:8:256:ILE:HG23	1.76	0.67
30:9:307:CHL:HHC	30:9:307:CHL:HBB1	1.75	0.67
3:p:225:THR:HB	3:p:249:TYR:HE2	1.60	0.67
6:b:216:HIS:HE1	31:b:610:CLA:NA	1.90	0.67
7:c:357:LEU:HD21	7:c:372:ILE:HG12	1.77	0.67
30:1:608:CHL:HHC	30:1:608:CHL:HBB1	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:606:CHL:HBB1	30:4:606:CHL:HMB1	1.76	0.67
44:A:416:PL9:H453	8:D:39:PRO:HA	1.76	0.67
30:G:601:CHL:HHC	30:G:601:CHL:HBB1	1.76	0.67
31:Y:304:CLA:CAD	30:Y:309:CHL:H2	2.24	0.67
1:7:106:VAL:HG13	1:7:228:ILE:HD11	1.76	0.67
31:p:610:CLA:H52	32:p:616:LUT:H28	1.76	0.67
30:g:302:CHL:HHC	30:g:302:CHL:HBB1	1.75	0.67
3:3:95:ALA:HA	32:3:318:LUT:H11	1.77	0.67
30:6:308:CHL:HHC	30:6:308:CHL:HBB1	1.76	0.67
3:N:200:LEU:HB3	31:N:310:CLA:HMA2	1.76	0.67
31:9:304:CLA:H102	32:9:318:LUT:H371	1.76	0.67
5:a:188:ALA:HB2	5:a:328:MET:HB2	1.76	0.67
2:g:258:LEU:HD22	2:g:259:PRO:HD2	1.76	0.67
2:4:73:ASP:HA	32:4:616:LUT:H24	1.78	0.66
30:Y:301:CHL:H93	30:Y:302:CHL:H8	1.77	0.66
1:7:107:VAL:HB	1:7:108:PRO:HD3	1.76	0.66
2:9:190:PHE:HE2	30:9:310:CHL:NA	1.93	0.66
31:9:304:CLA:HBC2	31:9:304:CLA:HMC1	1.76	0.66
3:p:215:MET:HA	3:p:218:PHE:CD2	2.30	0.66
2:4:117:ALA:HA	34:Q1:101:LMG:H351	1.75	0.66
38:B:620:SQD:H372	43:t:101:BCR:H362	1.75	0.66
30:R:308:CHL:HBB1	30:R:308:CHL:HHC	1.78	0.66
35:2:614:RRX:H55	34:2:618:LMG:H322	1.76	0.66
33:G:618:LHG:H362	37:G:620:XAT:H12	1.77	0.66
5:a:41:LEU:HD22	42:a:408:PHO:H61	1.77	0.66
45:c:617:DGD:HA22	34:k:101:LMG:H351	1.77	0.66
3:5:164:GLY:O	3:5:167:VAL:HG22	1.96	0.66
38:B:623:SQD:H351	23:X:83:LEU:HD21	1.78	0.66
15:L:8:LYS:HZ2	15:L:8:LYS:HB3	1.60	0.66
30:N:309:CHL:H52	30:Y:302:CHL:H51	1.77	0.66
30:7:310:CHL:HHC	30:7:310:CHL:HBB1	1.76	0.66
3:8:110:ARG:HH21	3:8:231:GLU:HA	1.61	0.66
13:j:40:SER:O	13:j:42:LEU:HD22	1.96	0.66
3:n:92:ALA:HB1	3:n:208:GLY:HA3	1.78	0.66
4:0:183:PRO:HD2	31:0:610:CLA:OBD	1.94	0.66
30:p:609:CHL:HBB1	30:p:609:CHL:HHC	1.76	0.66
22:w:86:THR:HG21	34:w:202:LMG:H221	1.77	0.66
2:4:223:PHE:CZ	35:4:615:RRX:H48	2.30	0.66
30:5:607:CHL:HHC	30:5:607:CHL:HBB1	1.76	0.66
30:0:608:CHL:HHC	30:0:608:CHL:HBB1	1.77	0.66
3:8:92:ALA:HB1	3:8:208:GLY:HA3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:p:89:VAL:HG21	3:p:179:LEU:HD11	1.78	0.66
27:q1:3:ASN:HD22	34:q1:101:LMG:HC72	1.60	0.66
4:6:156:THR:HG21	30:6:307:CHL:HED3	1.78	0.66
34:6:321:LMG:O2	18:R:273:PHE:HB3	1.96	0.66
4:0:255:LEU:HD12	31:0:615:CLA:HED1	1.78	0.66
30:8:605:CHL:HHC	30:8:605:CHL:HBB1	1.78	0.66
2:4:208:LYS:HG3	31:4:611:CLA:HED2	1.78	0.66
3:5:110:ARG:HH12	3:5:231:GLU:CD	2.04	0.66
3:5:227:LYS:HB2	3:5:232:ASN:HD21	1.61	0.66
5:A:255:PHE:HD2	5:A:264:SER:HB3	1.61	0.66
8:D:233:ARG:HH21	28:P1:26:GLY:HA2	1.60	0.66
33:G:618:LHG:HC61	37:G:620:XAT:H382	1.76	0.66
34:W:202:LMG:H371	31:Y:311:CLA:H171	1.77	0.66
31:c:606:CLA:H52	34:w:202:LMG:H331	1.77	0.66
19:s:163:LEU:HD21	19:s:171:ILE:HD12	1.78	0.66
29:F1:187:ASP:N	29:F1:187:ASP:OD1	2.29	0.66
1:1:186:LEU:HD12	32:1:615:LUT:H222	1.78	0.66
31:3:315:CLA:H2	31:3:315:CLA:HBA2	1.77	0.66
30:4:605:CHL:HHD	30:4:606:CHL:HED2	1.77	0.66
30:4:607:CHL:H11	3:5:250:ALA:HA	1.77	0.66
33:A:417:LHG:HC2	31:C:608:CLA:HED2	1.78	0.66
2:G:220:MET:HE2	32:G:615:LUT:H10	1.75	0.66
1:7:107:VAL:HG21	31:7:305:CLA:HAC2	1.78	0.66
2:9:220:MET:HE2	32:9:318:LUT:H10	1.78	0.66
6:b:12:VAL:HG23	31:b:613:CLA:HMC2	1.78	0.66
31:n:314:CLA:H13	33:n:320:LHG:H321	1.78	0.66
6:B:162:PHE:CE1	48:R:302:LMU:H1'	2.31	0.66
31:N:310:CLA:H52	32:N:316:LUT:H30	1.78	0.66
31:8:609:CLA:H2	32:8:615:LUT:H28	1.77	0.66
33:q:320:LHG:HC92	37:q:321:XAT:H393	1.77	0.66
30:s:308:CHL:HBB2	31:s:310:CLA:HBC3	1.76	0.66
30:y:607:CHL:HHC	30:y:607:CHL:HBB1	1.78	0.66
2:4:133:PHE:CE1	30:4:607:CHL:HMD3	2.32	0.65
2:4:223:PHE:CE1	35:4:615:RRX:C31	2.79	0.65
32:5:617:LUT:H12	32:5:617:LUT:H191	1.77	0.65
1:7:53:TYR:HA	3:8:168:ASN:HD22	1.60	0.65
30:7:307:CHL:HBB1	30:7:307:CHL:HHC	1.78	0.65
31:2:613:CLA:H62	31:2:613:CLA:NB	2.11	0.65
2:4:229:VAL:HG13	2:4:256:LYS:HZ2	1.61	0.65
8:D:123:ILE:HD11	34:D:412:LMG:H402	1.79	0.65
2:G:99:MET:SD	31:G:609:CLA:HAB	2.36	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:0:164:ILE:HD11	36:0:618:NEX:C35	2.27	0.65
31:9:304:CLA:HBC1	33:9:320:LHG:H262	1.77	0.65
1:1:178:TYR:HB3	31:1:610:CLA:HED3	1.78	0.65
30:1:606:CHL:HBB1	30:1:606:CHL:HHC	1.77	0.65
30:1:607:CHL:H12	2:2:259:PRO:HD3	1.78	0.65
2:2:192:PRO:HD2	35:2:614:RRX:H14	1.78	0.65
30:4:607:CHL:HBB1	30:4:607:CHL:HHC	1.77	0.65
38:A:411:SQD:H352	31:C:608:CLA:H72	1.79	0.65
2:G:223:PHE:HE1	35:G:614:RRX:H48	1.44	0.65
3:N:224:ILE:HD12	3:N:258:TYR:HE2	1.60	0.65
31:N:304:CLA:H2	31:N:304:CLA:HMA1	1.78	0.65
31:n:311:CLA:H2	32:n:317:LUT:H28	1.77	0.65
31:4:613:CLA:H12	31:4:614:CLA:HED2	1.79	0.65
3:5:253:SER:HA	3:5:258:TYR:CE1	2.31	0.65
31:Y:305:CLA:HMA3	30:Y:307:CHL:C2C	2.26	0.65
2:9:218:PHE:HE1	31:9:315:CLA:HAB	1.60	0.65
2:g:176:PRO:HD2	30:g:308:CHL:HBB2	1.78	0.65
19:s:137:PHE:HE1	19:s:259:GLY:HA2	1.61	0.65
2:4:258:LEU:HD22	2:4:259:PRO:HD2	1.78	0.65
30:0:607:CHL:HED3	2:q:258:LEU:HD23	1.77	0.65
7:c:204:SER:HB3	34:w:201:LMG:HC72	1.79	0.65
19:s:123:GLY:O	19:s:127:ASN:ND2	2.27	0.65
22:w:93:TRP:CZ2	34:w:202:LMG:H131	2.32	0.65
34:w:202:LMG:H252	31:y:612:CLA:H162	1.79	0.65
3:8:131:GLU:OE1	3:8:132:GLY:N	2.30	0.65
31:8:612:CLA:H13	33:8:618:LHG:H321	1.78	0.65
7:c:202:PHE:CZ	31:c:606:CLA:H13	2.31	0.65
3:5:115:ASN:HD22	3:5:115:ASN:N	1.94	0.65
4:6:202:LEU:HB3	31:6:311:CLA:HMA1	1.77	0.65
30:7:308:CHL:HBB1	30:7:308:CHL:HMB3	1.78	0.65
33:q:320:LHG:HC5	37:q:321:XAT:H382	1.77	0.65
33:b:628:LHG:H251	33:b:628:LHG:H132	1.78	0.65
30:n:306:CHL:HHC	30:n:306:CHL:HBB1	1.78	0.65
31:s:316:CLA:HBB1	31:s:316:CLA:HHC	1.79	0.65
31:y:610:CLA:H52	32:y:616:LUT:H30	1.76	0.65
30:3:302:CHL:H52	30:3:302:CHL:H93	1.78	0.65
30:G:606:CHL:HBB1	30:G:606:CHL:HHC	1.79	0.65
18:R:236:ALA:HB2	31:R:313:CLA:HED2	1.76	0.65
31:8:604:CLA:H92	30:8:606:CHL:HBA2	1.78	0.65
2:9:112:GLN:HA	2:9:117:ALA:HA	1.77	0.65
3:n:233:LEU:HD13	31:n:315:CLA:HBC2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:112:MET:SD	31:s:311:CLA:HAB	2.36	0.65
30:3:309:CHL:HHC	30:3:309:CHL:HBB1	1.79	0.65
3:5:64:PRO:HB2	3:5:205:LEU:HD12	1.79	0.65
30:5:606:CHL:HMB1	30:5:606:CHL:HBB1	1.79	0.65
45:C:617:DGD:HA42	34:J:101:LMG:H381	1.78	0.65
31:0:614:CLA:C4B	31:0:614:CLA:H71	2.27	0.65
31:7:304:CLA:HBB1	31:7:304:CLA:HHC	1.78	0.65
3:p:163:GLU:HG3	30:p:609:CHL:C4B	2.27	0.65
2:2:238:LEU:HD13	34:2:618:LMG:HC92	1.79	0.65
31:B:606:CLA:H72	43:B:619:BCR:H342	1.79	0.65
31:n:316:CLA:H11	34:n:322:LMG:C9	2.27	0.65
31:1:612:CLA:HMD2	38:g:301:SQD:H251	1.79	0.64
6:B:124:ARG:NH1	11:H:19:ASP:O	2.29	0.64
31:y:604:CLA:HMA3	30:y:606:CHL:C2C	2.27	0.64
33:B:624:LHG:H122	30:R:309:CHL:HBA2	1.77	0.64
9:E:14:LEU:HD11	34:J:102:LMG:H372	1.79	0.64
22:W:86:THR:HG21	34:W:201:LMG:H221	1.79	0.64
4:0:98:MET:SD	31:0:610:CLA:HAB	2.37	0.64
2:9:221:PHE:HB2	32:9:318:LUT:H401	1.79	0.64
2:2:125:TRP:CG	2:2:126:PHE:H	2.15	0.64
2:2:144:PRO:O	2:2:148:HIS:HB2	1.97	0.64
3:3:38:VAL:HA	3:3:42:GLY:CA	2.27	0.64
30:3:308:CHL:CBB	32:3:318:LUT:H161	2.27	0.64
19:S:112:MET:SD	31:S:311:CLA:HAB	2.38	0.64
4:0:125:LYS:HA	30:0:607:CHL:HED2	1.78	0.64
31:8:604:CLA:HMA3	30:8:606:CHL:C2C	2.27	0.64
3:p:185:PHE:HZ	30:p:608:CHL:NB	1.95	0.64
3:p:199:GLU:HG2	3:p:203:LYS:HE2	1.79	0.64
31:q:312:CLA:HBA1	35:q:317:RRX:C40	2.27	0.64
3:n:110:ARG:HH21	3:n:231:GLU:HA	1.61	0.64
38:s:301:SQD:H282	31:s:315:CLA:HAA2	1.78	0.64
22:w:80:SER:HB2	34:w:205:LMG:H302	1.79	0.64
29:f1:197:ILE:C	29:f1:230:TRP:HE1	2.04	0.64
2:2:126:PHE:CD2	2:2:127:LYS:HG3	2.32	0.64
2:4:92:VAL:HB	2:4:184:LEU:HD11	1.78	0.64
2:4:163:MET:HE2	30:4:606:CHL:HMA3	1.79	0.64
9:e:8:ARG:HD3	9:e:13:ILE:HG12	1.79	0.64
31:3:313:CLA:HHC	31:3:313:CLA:HBB1	1.79	0.64
2:4:124:VAL:HB	2:4:127:LYS:HB3	1.79	0.64
3:5:185:PHE:HB3	31:5:610:CLA:HMD3	1.78	0.64
31:B:607:CLA:C4A	31:B:607:CLA:HBA2	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:5:608:CHL:H12	32:5:616:LUT:H383	1.78	0.64
31:5:615:CLA:HBA1	31:5:615:CLA:CBD	2.27	0.64
10:F:14:ILE:HD11	27:Q1:26:PRO:HB2	1.79	0.64
3:N:86:GLU:HA	3:N:179:LEU:HD11	1.78	0.64
9:e:25:ILE:HD12	27:q1:18:TRP:CD1	2.32	0.64
31:y:610:CLA:H62	31:y:612:CLA:HMA2	1.79	0.64
31:1:611:CLA:C3B	38:g:318:SQD:H241	2.28	0.64
3:3:258:TYR:CE2	31:3:316:CLA:HHD	2.32	0.64
2:4:157:LEU:HA	2:4:160:LEU:HD12	1.79	0.64
37:4:619:XAT:H163	34:4:620:LMG:H172	1.80	0.64
30:Y:302:CHL:HBB1	30:Y:302:CHL:HMB3	1.80	0.64
4:0:76:LEU:HD23	31:0:602:CLA:H42	1.80	0.64
2:9:86:ARG:HA	2:9:86:ARG:HH11	1.62	0.64
2:g:72:TRP:CZ2	30:g:302:CHL:HBA1	2.32	0.64
19:s:218:PRO:HD2	32:s:317:LUT:H23	1.80	0.64
2:2:186:PRO:HG3	30:2:607:CHL:CHD	2.28	0.64
30:3:307:CHL:CBB	34:3:321:LMG:H322	2.27	0.64
7:C:368:LEU:HA	7:C:372:ILE:HD11	1.77	0.64
31:S:305:CLA:H171	31:S:305:CLA:H141	1.79	0.64
2:9:129:GLY:H	30:9:309:CHL:HED1	1.63	0.64
3:n:131:GLU:OE1	3:n:132:GLY:N	2.30	0.64
2:2:149:ALA:HA	30:2:605:CHL:C1C	2.28	0.64
2:2:223:PHE:HE1	35:2:614:RRX:C32	2.10	0.64
3:3:185:PHE:HZ	30:3:309:CHL:NB	1.95	0.64
31:G:609:CLA:H102	35:G:614:RRX:H26	1.80	0.64
30:Y:301:CHL:HBB1	30:Y:301:CHL:HMB1	1.79	0.64
4:0:111:GLN:HG3	4:0:121:ALA:HB2	1.80	0.64
30:n:301:CHL:HHC	30:n:301:CHL:HBB1	1.79	0.64
30:n:308:CHL:HMB1	30:n:308:CHL:HBB1	1.80	0.64
19:s:204:TYR:HA	19:s:207:MET:HE2	1.79	0.64
30:y:601:CHL:HBB1	30:y:601:CHL:HMB1	1.80	0.64
3:3:134:LEU:HD21	31:3:306:CLA:HAA2	1.79	0.64
3:5:177:ASP:HB3	3:5:180:TYR:O	1.98	0.64
3:5:245:PHE:HB2	31:5:613:CLA:CAD	2.27	0.64
5:A:133:LEU:HD12	8:D:256:ILE:HG12	1.78	0.64
6:B:464:PHE:HD2	31:B:611:CLA:HAC2	1.63	0.64
19:S:217:ASP:HA	32:S:317:LUT:H24	1.79	0.64
30:Y:301:CHL:H121	30:Y:301:CHL:H91	1.80	0.64
8:d:257:PHE:HE2	33:d:408:LHG:H112	1.63	0.64
29:F1:170:ASP:HB2	29:F1:176:TYR:HE1	1.63	0.64
1:1:249:LYS:H	1:1:249:LYS:HD2	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:125:GLY:HA2	30:5:606:CHL:HAC2	1.80	0.63
5:A:341:LEU:HB3	5:A:343:LEU:HD13	1.80	0.63
30:G:606:CHL:HBB2	30:N:301:CHL:HBB1	1.80	0.63
1:7:186:LEU:HD12	32:7:317:LUT:H222	1.80	0.63
30:9:309:CHL:HHC	30:9:309:CHL:HBB1	1.80	0.63
6:b:413:ASP:N	6:b:413:ASP:OD1	2.31	0.63
7:c:302:THR:HG21	7:c:343:THR:HG21	1.79	0.63
8:d:233:ARG:HH21	28:p1:26:GLY:HA2	1.63	0.63
33:d:408:LHG:HC91	15:l:20:TRP:HZ2	1.63	0.63
31:n:305:CLA:HMA3	30:n:307:CHL:C2C	2.28	0.63
2:2:112:GLN:HB3	2:2:119:PHE:HD2	1.63	0.63
3:8:233:LEU:HD13	31:8:613:CLA:HBC2	1.80	0.63
15:l:27:VAL:HG11	33:l:101:LHG:H201	1.79	0.63
31:Y:310:CLA:H2	32:Y:315:LUT:H28	1.81	0.63
1:7:176:ALA:HB2	18:r:38:ARG:HH21	1.63	0.63
31:p:602:CLA:H111	32:p:617:LUT:H361	1.80	0.63
31:q:312:CLA:HBA1	35:q:317:RRX:H7	1.81	0.63
3:n:86:GLU:HA	3:n:179:LEU:HD11	1.79	0.63
31:y:612:CLA:HHC	31:y:612:CLA:HBB1	1.80	0.63
1:1:121:LYS:HA	30:1:607:CHL:HED2	1.79	0.63
30:G:606:CHL:HBB2	30:N:301:CHL:CBB	2.28	0.63
3:p:110:ARG:HH22	3:p:230:ILE:HG21	1.63	0.63
44:a:414:PL9:H102	44:a:414:PL9:HC2	1.81	0.63
18:r:236:ALA:HB2	31:r:313:CLA:HED2	1.80	0.63
34:Q1:101:LMG:H161	34:Q1:101:LMG:H372	1.80	0.63
30:2:606:CHL:HMB1	30:2:606:CHL:HBB1	1.80	0.63
3:3:122:PHE:CD1	3:3:123:LYS:HG3	2.33	0.63
30:5:608:CHL:HMB1	30:5:608:CHL:HBB1	1.81	0.63
34:B:625:LMG:H372	30:R:309:CHL:C10	2.29	0.63
10:F:43:GLN:HB3	29:F1:57:ALA:HB3	1.79	0.63
31:G:603:CLA:H2	31:G:603:CLA:HMA3	1.81	0.63
34:G:621:LMG:H411	30:N:309:CHL:H161	1.81	0.63
12:I:26:ASN:ND2	49:I:201:HOH:O	2.30	0.63
2:9:226:GLN:O	2:9:230:THR:HG22	1.99	0.63
34:9:321:LMG:HC1	34:9:321:LMG:H292	1.81	0.63
3:p:143:ILE:HA	30:p:605:CHL:C4D	2.28	0.63
31:p:611:CLA:HAA1	31:p:612:CLA:OBD	1.99	0.63
7:c:112:VAL:HG12	33:s:322:LHG:H342	1.80	0.63
33:d:408:LHG:H312	20:t:21:ILE:HD11	1.79	0.63
3:5:203:LYS:HG3	31:5:611:CLA:HED2	1.78	0.63
34:5:620:LMG:HC62	31:6:315:CLA:CMA	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:8:614:CLA:CHC	34:9:302:LMG:H362	2.27	0.63
3:p:151:ILE:HG22	30:p:605:CHL:HAC1	1.80	0.63
3:p:247:VAL:HG13	2:q:133:PHE:CE2	2.30	0.63
31:q:312:CLA:C2	35:q:317:RRX:H6	2.29	0.63
30:g:307:CHL:HHC	30:g:307:CHL:HBB1	1.79	0.63
2:2:86:ARG:HA	2:2:86:ARG:HH11	1.62	0.63
3:3:245:PHE:HB2	31:3:314:CLA:CAD	2.28	0.63
2:4:144:PRO:O	2:4:148:HIS:HB2	1.98	0.63
31:4:610:CLA:H2	35:4:615:RRX:H6	1.81	0.63
6:B:423:ARG:NH2	6:B:430:PHE:O	2.31	0.63
10:F:20:LEU:HD11	34:X:203:LMG:H292	1.79	0.63
30:N:307:CHL:HBB2	30:Y:301:CHL:HAB	1.81	0.63
3:p:233:LEU:HA	31:p:613:CLA:CMA	2.28	0.63
34:d:411:LMG:O10	11:h:69:ASN:ND2	2.32	0.63
2:g:235:LEU:HD22	34:g:320:LMG:HC91	1.81	0.63
19:s:217:ASP:HA	32:s:317:LUT:H24	1.81	0.63
1:1:99:MET:SD	31:1:610:CLA:HAB	2.39	0.63
30:3:302:CHL:HMA2	31:3:316:CLA:C3B	2.28	0.63
30:7:307:CHL:HBB2	30:7:308:CHL:HAB	1.80	0.63
3:p:136:TYR:HB3	3:p:142:LEU:HB3	1.81	0.63
31:c:613:CLA:HBA1	31:c:613:CLA:HBD	1.80	0.63
3:p:197:PHE:CE2	3:p:201:LYS:HD2	2.33	0.63
30:p:605:CHL:CBB	34:p:620:LMG:H321	2.28	0.63
30:q:308:CHL:HAA2	30:q:308:CHL:HBD	1.81	0.63
30:q:309:CHL:C4B	30:q:309:CHL:H102	2.29	0.63
5:a:118:HIS:HE1	31:a:409:CLA:C4D	2.12	0.63
31:c:611:CLA:H42	21:v:33:LEU:HA	1.79	0.63
3:n:254:ALA:HB3	30:n:301:CHL:HED3	1.81	0.63
30:n:307:CHL:H52	31:s:313:CLA:H102	1.81	0.63
31:y:603:CLA:HMA1	31:y:603:CLA:H2	1.81	0.63
30:3:310:CHL:HMB3	30:3:310:CHL:HBB1	1.80	0.62
30:N:301:CHL:HBB1	30:N:301:CHL:HHC	1.79	0.62
31:Y:310:CLA:H62	31:Y:312:CLA:HMA2	1.80	0.62
3:n:203:LYS:HD3	31:n:313:CLA:HAA2	1.81	0.62
31:n:315:CLA:HBA1	31:n:315:CLA:CHA	2.28	0.62
30:r:309:CHL:HBD	30:r:309:CHL:HAA1	1.81	0.62
24:y:186:TYR:HB3	31:y:610:CLA:HED3	1.81	0.62
31:y:613:CLA:H93	33:y:619:LHG:H152	1.80	0.62
30:3:303:CHL:HAC1	33:3:320:LHG:HC32	1.81	0.62
2:4:132:ILE:HA	2:4:138:LEU:HB2	1.81	0.62
2:4:147:ILE:CG1	31:4:604:CLA:H41	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:86:GLU:HA	3:8:179:LEU:HD11	1.79	0.62
31:8:613:CLA:CHA	31:8:613:CLA:HBA1	2.28	0.62
2:9:185:TYR:HB3	31:9:312:CLA:HED3	1.80	0.62
31:q:306:CLA:H62	36:q:319:NEX:H373	1.80	0.62
31:c:603:CLA:H161	31:c:610:CLA:HBB2	1.80	0.62
19:s:256:THR:HG23	19:s:258:GLU:H	1.62	0.62
24:y:192:ASP:HA	32:y:616:LUT:H24	1.79	0.62
3:3:246:TRP:O	3:3:251:PRO:HD3	1.99	0.62
4:6:106:THR:OG1	4:6:107:PRO:HD3	1.99	0.62
6:B:272:ARG:NH1	6:B:276:ASP:OD2	2.33	0.62
6:B:322:GLY:HA3	6:B:445:THR:HG23	1.80	0.62
45:C:620:DGD:HBH2	31:Y:311:CLA:H51	1.81	0.62
33:G:618:LHG:HC62	37:G:620:XAT:H382	1.80	0.62
31:c:605:CLA:H201	45:c:616:DGD:HAN1	1.81	0.62
4:6:235:LEU:HD23	32:6:317:LUT:H163	1.80	0.62
43:B:618:BCR:HC41	34:B:621:LMG:H331	1.81	0.62
8:D:117:HIS:HE1	31:D:404:CLA:C4D	2.13	0.62
30:8:607:CHL:HBB1	30:8:607:CHL:HMB3	1.81	0.62
1:1:122:ALA:HB1	31:1:604:CLA:HED1	1.80	0.62
30:1:607:CHL:HBB1	30:1:607:CHL:HMB3	1.80	0.62
31:1:611:CLA:H2	31:1:612:CLA:OBD	1.98	0.62
2:2:118:ASP:HB3	2:2:142:GLY:HA3	1.82	0.62
30:3:308:CHL:HBB1	32:3:318:LUT:H161	1.80	0.62
2:4:132:ILE:HB	2:4:138:LEU:HD12	1.80	0.62
31:N:305:CLA:HMA3	30:N:307:CHL:C2C	2.29	0.62
8:d:186:GLN:HB2	31:d:404:CLA:HBC1	1.82	0.62
43:C:614:BCR:H11C	38:S:301:SQD:H281	1.81	0.62
2:G:231:GLY:HA2	31:N:315:CLA:HMA2	1.82	0.62
31:N:314:CLA:CHA	31:N:314:CLA:HBA1	2.29	0.62
5:A:118:HIS:HE1	31:A:409:CLA:C4D	2.13	0.62
6:B:382:PRO:HG2	6:B:385:ARG:HG2	1.81	0.62
7:C:264:LEU:HD21	31:C:608:CLA:HAB	1.80	0.62
30:S:308:CHL:HHC	30:S:308:CHL:HBB1	1.80	0.62
1:7:252:ALA:HB2	30:7:321:CHL:HAA2	1.80	0.62
3:p:245:PHE:CD1	3:p:249:TYR:HB2	2.34	0.62
30:p:606:CHL:HMB1	30:p:606:CHL:HBB1	1.81	0.62
30:p:608:CHL:HBD	30:p:608:CHL:HAA1	1.82	0.62
31:r:305:CLA:HBC1	31:r:311:CLA:CBC	2.30	0.62
19:s:138:GLU:HA	30:s:308:CHL:CED	2.30	0.62
2:2:47:ALA:HB1	30:2:601:CHL:HBC1	1.82	0.62
2:4:180:SER:O	2:4:181:GLY:C	2.41	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:50:LEU:CB	4:6:54:SER:HB3	2.30	0.62
24:Y:175:PRO:HD2	30:Y:308:CHL:HBB2	1.81	0.62
44:d:407:PL9:H502	20:t:10:LEU:HD13	1.82	0.62
31:n:305:CLA:H92	30:n:307:CHL:HBA2	1.79	0.62
2:4:143:ASN:ND2	2:4:146:LEU:HD23	2.15	0.62
2:4:205:LEU:HD11	31:4:610:CLA:H43	1.82	0.62
2:4:229:VAL:HG13	2:4:256:LYS:NZ	2.14	0.62
31:G:604:CLA:H2	30:G:606:CHL:HBD	1.80	0.62
31:0:610:CLA:H2	32:0:616:LUT:H28	1.82	0.62
3:8:203:LYS:HD3	31:8:611:CLA:HAA2	1.81	0.62
2:9:137:GLY:HA3	2:9:150:GLN:HG2	1.81	0.62
3:p:225:THR:CG2	31:p:613:CLA:HED2	2.29	0.62
31:q:304:CLA:H61	32:q:318:LUT:H28	1.81	0.62
45:c:619:DGD:HBT2	31:y:611:CLA:HBC3	1.82	0.62
30:3:307:CHL:C1C	34:3:321:LMG:H371	2.29	0.62
2:G:155:VAL:HG12	30:G:605:CHL:HAC1	1.81	0.62
38:g:301:SQD:H92	37:g:321:XAT:C22	2.30	0.62
30:r:308:CHL:HHC	30:r:308:CHL:HBB1	1.82	0.62
24:y:154:THR:HG22	30:y:605:CHL:HAC1	1.82	0.62
30:1:605:CHL:C4A	34:6:321:LMG:H302	2.30	0.61
3:5:237:LEU:HD21	31:5:614:CLA:HMC3	1.81	0.61
30:5:606:CHL:CBB	30:5:609:CHL:HBC1	2.29	0.61
4:6:208:LYS:NZ	33:6:320:LHG:O5	2.33	0.61
7:C:203:ARG:HG2	7:C:209:ASP:HB3	1.82	0.61
31:R:304:CLA:CBB	37:R:318:XAT:H32	2.30	0.61
30:7:321:CHL:HBB1	30:7:321:CHL:HMB3	1.80	0.61
3:8:180:TYR:HB3	31:8:609:CLA:HED3	1.81	0.61
2:9:72:TRP:CE3	32:9:318:LUT:H383	2.35	0.61
30:9:310:CHL:HMB1	36:9:319:NEX:C12	2.30	0.61
30:p:601:CHL:HHC	30:p:601:CHL:HBB1	1.82	0.61
2:g:171:TYR:CD2	3:n:49:LEU:HD12	2.35	0.61
30:3:308:CHL:HBB1	30:3:308:CHL:HHC	1.82	0.61
2:4:205:LEU:HB3	31:4:610:CLA:HMA2	1.82	0.61
30:5:607:CHL:HED1	4:6:256:ALA:HA	1.82	0.61
3:p:225:THR:HG21	31:p:613:CLA:HED2	1.80	0.61
1:1:251:LEU:CB	30:1:619:CHL:HBA2	2.31	0.61
30:1:619:CHL:HBD	30:1:619:CHL:CBA	2.24	0.61
2:4:59:PRO:HB3	2:4:61:TYR:CZ	2.34	0.61
31:B:612:CLA:H171	31:B:613:CLA:HBB2	1.81	0.61
31:C:601:CLA:H192	31:C:607:CLA:H152	1.82	0.61
11:h:42:PRO:HG3	18:r:85:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:n:304:CLA:HAC1	30:n:308:CHL:CBB	2.29	0.61
19:s:122:GLU:HA	19:s:134:ALA:HB1	1.83	0.61
2:2:133:PHE:HE1	3:3:247:VAL:HG22	1.65	0.61
31:4:602:CLA:H2	31:4:602:CLA:CHB	2.31	0.61
3:5:246:TRP:HA	3:5:250:ALA:HB3	1.82	0.61
18:R:139:HIS:CD2	37:R:318:XAT:H15	2.36	0.61
34:9:301:LMG:H411	34:9:301:LMG:H372	1.82	0.61
2:q:147:ILE:HG22	2:q:149:ALA:HB2	1.82	0.61
2:q:173:GLY:HA2	30:q:310:CHL:HMC	1.82	0.61
6:b:91:TRP:CD2	31:b:607:CLA:HBA2	2.36	0.61
24:y:99:MET:SD	31:y:610:CLA:HAB	2.41	0.61
30:y:607:CHL:C10	30:y:609:CHL:H172	2.31	0.61
31:2:610:CLA:H61	31:2:611:CLA:C4D	2.30	0.61
2:9:190:PHE:HB3	30:9:310:CHL:H11	1.83	0.61
2:g:99:MET:SD	31:g:310:CLA:HAB	2.40	0.61
31:y:613:CLA:H18	31:y:614:CLA:O1A	2.01	0.61
3:3:191:ALA:HB1	3:3:197:PHE:CD1	2.35	0.61
2:4:139:ASN:HB3	2:4:143:ASN:O	2.01	0.61
30:4:601:CHL:HED1	33:4:618:LHG:H292	1.83	0.61
30:5:607:CHL:HBD	30:5:607:CHL:HBA1	1.81	0.61
44:A:416:PL9:H33	10:F:25:LEU:HD21	1.82	0.61
34:G:622:LMG:H132	34:G:622:LMG:HC91	1.82	0.61
30:G:623:CHL:H93	30:Y:309:CHL:H193	1.81	0.61
31:N:304:CLA:HMD2	30:N:309:CHL:H2	1.81	0.61
30:N:308:CHL:HMB1	30:N:308:CHL:HBB1	1.81	0.61
17:O:269:ASP:O	17:O:275:LYS:NZ	2.34	0.61
30:7:302:CHL:C1D	33:7:319:LHG:HC81	2.31	0.61
31:a:409:CLA:H101	34:w:201:LMG:H142	1.82	0.61
18:r:44:TYR:HB2	36:r:301:NEX:O3	2.01	0.61
34:5:620:LMG:C6	31:6:315:CLA:HMA2	2.31	0.61
19:s:171:ILE:HG21	30:s:307:CHL:HED3	1.82	0.61
2:4:187:GLY:O	2:4:188:GLY:C	2.43	0.61
31:4:604:CLA:NA	36:4:617:NEX:H242	2.14	0.61
31:S:303:CLA:H203	31:S:304:CLA:HBB1	1.83	0.61
2:q:186:PRO:HG3	30:q:310:CHL:HBC2	1.82	0.61
30:s:308:CHL:HHC	30:s:308:CHL:HBB1	1.83	0.61
43:t:101:BCR:H382	43:t:101:BCR:H23C	1.82	0.61
3:3:143:ILE:HA	30:3:307:CHL:C4D	2.30	0.61
3:3:188:LEU:HD12	32:3:317:LUT:H222	1.83	0.61
3:5:45:ARG:HB2	3:5:46:PRO:HD2	1.82	0.61
5:A:215:HIS:HA	44:A:416:PL9:HC2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:S:301:SQD:H302	31:S:315:CLA:HBD	1.83	0.61
30:7:309:CHL:HBD	30:7:309:CHL:HAA1	1.82	0.61
31:c:606:CLA:H41	34:w:202:LMG:H331	1.83	0.61
30:n:307:CHL:HHC	30:n:307:CHL:HBB1	1.83	0.61
29:f1:66:PHE:CZ	29:f1:225:GLU:HA	2.36	0.61
30:1:619:CHL:CBB	30:3:308:CHL:HBB2	2.31	0.61
30:3:309:CHL:HAA1	30:3:309:CHL:HBD	1.83	0.61
2:4:183:SER:O	30:4:608:CHL:HMD1	2.01	0.61
5:A:303:ASN:O	7:C:403:ASN:ND2	2.29	0.61
31:0:604:CLA:H52	30:0:606:CHL:HBA1	1.83	0.61
30:0:605:CHL:O2D	30:0:605:CHL:H2A	2.01	0.61
1:7:189:ALA:HB1	1:7:195:LEU:HD13	1.82	0.61
3:8:69:TRP:O	32:8:616:LUT:H24	2.01	0.61
42:d:402:PHO:H72	31:d:404:CLA:H111	1.82	0.61
30:n:309:CHL:HMB1	30:n:309:CHL:HBB1	1.82	0.61
31:y:603:CLA:ND	30:y:609:CHL:H8	2.16	0.61
3:N:38:VAL:HG13	3:N:44:ASN:HB2	1.83	0.60
31:7:304:CLA:HED2	31:7:304:CLA:H12	1.82	0.60
30:8:601:CHL:HED1	33:8:618:LHG:H292	1.83	0.60
2:q:185:TYR:HA	31:q:312:CLA:O1D	2.00	0.60
7:c:253:VAL:HG21	7:c:437:ARG:HG2	1.83	0.60
31:Y:310:CLA:H52	32:Y:315:LUT:H30	1.83	0.60
31:q:312:CLA:H72	35:q:317:RRX:H25	1.82	0.60
2:2:90:ILE:HG21	31:2:603:CLA:HAA2	1.82	0.60
31:2:604:CLA:HMA2	30:2:606:CHL:C3C	2.30	0.60
3:5:107:LEU:HD22	3:5:230:ILE:HD13	1.83	0.60
34:C:624:LMG:H111	33:Y:318:LHG:HC31	1.83	0.60
30:N:308:CHL:H12	32:N:316:LUT:H383	1.83	0.60
5:a:334:ARG:HD3	8:d:320:LEU:HD23	1.83	0.60
31:a:409:CLA:HMA2	45:c:616:DGD:HBH1	1.82	0.60
3:n:147:SER:HB2	34:n:321:LMG:C4	2.25	0.60
17:o:256:GLY:O	17:o:290:LEU:N	2.30	0.60
30:y:608:CHL:H2	32:y:616:LUT:H383	1.84	0.60
2:2:95:ALA:HB1	2:2:213:GLY:HA3	1.82	0.60
2:2:185:TYR:HA	31:2:609:CLA:O1D	2.01	0.60
3:3:103:VAL:HG13	3:3:230:ILE:HD11	1.83	0.60
30:6:307:CHL:HBB1	30:6:307:CHL:HMB1	1.83	0.60
30:6:309:CHL:HMA2	36:6:319:NEX:H30	1.83	0.60
3:N:215:MET:HG3	32:N:317:LUT:H12	1.83	0.60
31:b:612:CLA:HMB1	31:b:612:CLA:HBB1	1.83	0.60
45:c:619:DGD:HA32	45:c:619:DGD:C2B	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:173:GLY:HA2	30:2:607:CHL:HBC1	1.83	0.60
3:5:224:ILE:HG23	3:5:258:TYR:CE2	2.36	0.60
31:5:610:CLA:H122	31:5:612:CLA:HMB2	1.83	0.60
2:G:59:PRO:HD2	2:G:62:LEU:HD12	1.84	0.60
17:O:106:VAL:HG22	17:O:280:VAL:HG22	1.83	0.60
4:0:93:HIS:HE1	31:0:603:CLA:C4D	2.14	0.60
3:p:123:LYS:HA	30:p:607:CHL:HED2	1.83	0.60
3:p:250:ALA:HB3	3:p:251:PRO:HD3	1.84	0.60
2:q:196:ALA:HB1	2:q:202:LEU:HG	1.84	0.60
8:d:117:HIS:HE1	31:d:405:CLA:ND	1.99	0.60
17:o:263:GLU:HG3	17:o:283:THR:HG22	1.81	0.60
31:y:603:CLA:CAD	30:y:609:CHL:H2	2.32	0.60
31:1:611:CLA:HBA1	38:g:301:SQD:H462	1.83	0.60
30:N:309:CHL:HMB1	30:N:309:CHL:HBB1	1.84	0.60
30:Y:306:CHL:HHC	30:Y:306:CHL:HBB1	1.83	0.60
19:s:39:TRP:HE1	34:s:321:LMG:HC4	1.66	0.60
31:S:305:CLA:H92	30:S:307:CHL:HBA2	1.83	0.60
30:9:308:CHL:HBB2	30:9:309:CHL:CBB	2.31	0.60
30:q:308:CHL:HMB1	30:q:308:CHL:HBB1	1.83	0.60
33:d:408:LHG:HC91	15:l:20:TRP:CZ2	2.36	0.60
31:y:610:CLA:H2	32:y:616:LUT:H28	1.81	0.60
28:P1:50:TYR:CZ	28:P1:52:PHE:HB2	2.36	0.60
6:B:12:VAL:HG23	31:B:612:CLA:HMC2	1.83	0.60
31:D:404:CLA:H43	23:X:76:VAL:HA	1.83	0.60
2:9:241:HIS:CG	31:9:315:CLA:HAA2	2.37	0.60
31:b:604:CLA:HMB2	31:b:604:CLA:H51	1.83	0.60
14:k:17:PRO:HB2	33:z:102:LHG:H241	1.84	0.60
36:r:319:NEX:H161	38:r:322:SQD:H92	1.84	0.60
6:B:159:THR:HG22	6:B:161:LEU:H	1.67	0.60
18:R:52:LEU:HD23	18:R:57:THR:HG23	1.83	0.60
2:9:218:PHE:CE1	31:9:315:CLA:HAB	2.36	0.60
31:q:312:CLA:H92	31:q:314:CLA:HMA1	1.83	0.60
2:g:143:ASN:OD1	2:g:145:SER:OG	2.20	0.60
30:n:310:CHL:HBB1	30:n:310:CHL:HMB1	1.84	0.60
3:5:75:SER:HB3	3:5:81:PHE:CD1	2.37	0.60
4:6:122:VAL:HG23	4:6:125:LYS:HB2	1.84	0.60
2:G:219:SER:OG	35:G:614:RRX:H45	2.02	0.60
31:G:609:CLA:O2A	35:G:614:RRX:C40	2.44	0.60
30:N:309:CHL:HBA2	30:Y:302:CHL:H12	1.84	0.60
33:S:320:LHG:H111	33:S:320:LHG:H321	1.84	0.60
31:0:611:CLA:H12	38:0:621:SQD:O10	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:0:620:LMG:H341	30:7:306:CHL:CHA	2.31	0.60
1:7:244:TYR:CE2	30:7:321:CHL:H43	2.37	0.60
6:b:496:LEU:HB2	6:b:503:THR:HB	1.84	0.60
45:c:619:DGD:HAG1	31:y:614:CLA:H51	1.84	0.60
33:d:408:LHG:H191	20:t:17:ILE:HD11	1.84	0.60
2:g:72:TRP:CE3	32:g:316:LUT:H383	2.37	0.60
31:r:305:CLA:HBC1	31:r:311:CLA:HBC2	1.83	0.60
30:r:308:CHL:HBB2	30:r:309:CHL:HMB2	1.82	0.60
30:3:309:CHL:H42	32:3:317:LUT:H383	1.82	0.59
30:4:607:CHL:H102	30:4:607:CHL:C4B	2.32	0.59
7:C:249:ARG:NH2	22:W:111:ASN:O	2.35	0.59
30:G:623:CHL:HHC	30:G:623:CHL:HBB1	1.82	0.59
3:n:69:TRP:O	32:n:318:LUT:H24	2.01	0.59
34:n:322:LMG:H141	31:y:615:CLA:H42	1.84	0.59
31:y:604:CLA:H61	36:y:618:NEX:H23	1.84	0.59
39:A:401:OEX:O4	7:C:345:ARG:NH2	2.36	0.59
31:B:613:CLA:H43	33:D:407:LHG:H362	1.85	0.59
3:8:185:PHE:HA	30:8:607:CHL:H43	1.84	0.59
31:q:312:CLA:HAA1	31:q:312:CLA:HED2	1.83	0.59
7:c:264:LEU:HD21	31:c:608:CLA:HAB	1.84	0.59
18:r:144:MET:SD	31:r:312:CLA:HAB	2.42	0.59
4:6:205:LYS:HG3	31:6:312:CLA:HED2	1.83	0.59
31:N:313:CLA:H172	31:N:314:CLA:C1D	2.32	0.59
4:0:193:ALA:HB1	4:0:199:LEU:HD13	1.84	0.59
4:0:251:TYR:O	4:0:253:LYS:N	2.35	0.59
4:0:255:LEU:HB2	30:p:607:CHL:HBA2	1.84	0.59
31:p:615:CLA:HBC3	34:q:302:LMG:H321	1.84	0.59
31:b:608:CLA:H203	15:l:36:ILE:HG13	1.82	0.59
2:2:168:ALA:HB1	3:3:52:PHE:CG	2.36	0.59
19:S:41:GLY:HA3	24:Y:52:PRO:HB2	1.85	0.59
30:S:309:CHL:HHC	30:S:309:CHL:HBB1	1.83	0.59
4:0:169:VAL:HG21	2:q:50:LEU:HD23	1.84	0.59
31:9:312:CLA:HBA1	35:9:317:RRX:H7	1.84	0.59
3:p:236:HIS:HA	3:p:243:THR:HG21	1.85	0.59
6:b:25:MET:HG2	43:b:618:BCR:H23C	1.85	0.59
33:b:625:LHG:H302	33:b:625:LHG:H251	1.84	0.59
7:c:30:LEU:HD21	31:c:611:CLA:H2A	1.82	0.59
9:e:26:THR:HB	47:e:102:HEM:HAB	1.82	0.59
28:p1:28:SER:O	28:p1:32:GLU:HG2	2.02	0.59
1:1:107:VAL:HG21	31:1:604:CLA:HAC2	1.83	0.59
3:3:145:ALA:HA	30:3:307:CHL:C1C	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:163:GLU:HG3	30:3:310:CHL:C4B	2.32	0.59
3:5:206:LYS:HD3	31:5:611:CLA:O1D	2.02	0.59
30:N:307:CHL:HHC	30:N:307:CHL:HBB1	1.84	0.59
30:n:302:CHL:HED1	33:n:320:LHG:H292	1.83	0.59
17:o:204:ASP:HB3	17:o:235:LYS:HE3	1.84	0.59
31:5:611:CLA:H12	31:5:612:CLA:OBD	2.02	0.59
31:p:610:CLA:H2	32:p:616:LUT:C25	2.32	0.59
3:n:236:HIS:CA	3:n:243:THR:HG21	2.28	0.59
30:y:605:CHL:HHC	30:y:605:CHL:HBB1	1.84	0.59
3:3:165:TYR:HA	3:3:169:GLY:O	2.03	0.59
2:G:72:TRP:CZ2	30:G:601:CHL:HBA1	2.37	0.59
43:H:101:BCR:H21C	34:X:202:LMG:H311	1.83	0.59
22:w:90:THR:HG21	34:w:202:LMG:H261	1.84	0.59
2:2:231:GLY:HA2	31:3:316:CLA:HMA3	1.85	0.59
30:2:608:CHL:HAA2	3:3:71:THR:HG21	1.85	0.59
2:4:75:ALA:HB3	2:4:77:LEU:CD2	2.33	0.59
3:5:250:ALA:N	3:5:251:PRO:HD2	2.18	0.59
30:5:606:CHL:HBA1	36:5:618:NEX:C32	2.33	0.59
34:D:409:LMG:H142	34:D:409:LMG:H292	1.84	0.59
31:Y:304:CLA:C1B	30:Y:309:CHL:H121	2.33	0.59
30:0:607:CHL:HBB2	30:0:609:CHL:HBC1	1.84	0.59
18:r:50:ASP:HB3	18:r:59:ARG:HH21	1.67	0.59
2:4:156:LEU:O	2:4:160:LEU:HG	2.03	0.59
30:5:608:CHL:HBD	30:5:608:CHL:HAA1	1.85	0.59
7:C:134:PHE:HA	34:C:621:LMG:HC4	1.83	0.59
18:R:139:HIS:HE1	31:R:305:CLA:C4D	2.16	0.59
30:8:601:CHL:H93	2:9:160:LEU:HD21	1.85	0.59
31:c:612:CLA:HBB2	34:c:620:LMG:H312	1.84	0.59
29:f1:197:ILE:HG12	29:f1:210:LYS:HG3	1.84	0.59
1:1:167:GLY:N	18:R:38:ARG:HB3	2.18	0.59
2:2:187:GLY:HA3	31:2:609:CLA:HED2	1.85	0.59
2:4:77:LEU:HD22	2:4:77:LEU:H	1.67	0.59
2:4:100:LEU:HB3	31:4:604:CLA:HAB	1.84	0.59
3:5:143:ILE:HA	30:5:605:CHL:ND	2.18	0.59
4:6:108:GLU:HA	4:6:121:ALA:HB1	1.85	0.59
8:D:189:HIS:HA	8:D:294:ARG:HD2	1.85	0.59
35:G:614:RRX:H55	34:G:619:LMG:H322	1.85	0.59
31:R:307:CLA:HBA1	31:R:316:CLA:H172	1.84	0.59
19:S:155:PRO:HG3	31:S:306:CLA:NA	2.18	0.59
30:8:606:CHL:HHC	30:8:606:CHL:HBB1	1.83	0.59
30:q:307:CHL:HAA1	30:q:307:CHL:HBD	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:c:619:DGD:HD1	31:y:611:CLA:HBA1	1.85	0.59
9:e:10:PHE:CZ	10:f:18:ARG:HD3	2.37	0.59
34:g:322:LMG:H411	34:g:322:LMG:H372	1.85	0.59
36:s:319:NEX:H193	36:s:319:NEX:H161	1.83	0.59
1:1:166:ASN:ND2	2:2:53:PHE:HA	2.18	0.58
31:4:610:CLA:HMB3	31:4:610:CLA:HBB1	1.84	0.58
30:5:607:CHL:HMA2	4:6:256:ALA:O	2.03	0.58
7:C:247:TRP:CZ2	45:C:620:DGD:HA21	2.38	0.58
31:C:604:CLA:HMB1	31:C:604:CLA:HBB1	1.85	0.58
19:S:138:GLU:HA	30:S:308:CHL:CED	2.23	0.58
31:Y:304:CLA:H2	31:Y:304:CLA:HMA3	1.83	0.58
30:7:321:CHL:HAA1	30:7:321:CHL:HBD	1.84	0.58
30:1:601:CHL:HMB3	30:3:310:CHL:HBB1	1.84	0.58
2:2:202:LEU:HG	2:2:206:LYS:HE3	1.84	0.58
3:3:122:PHE:HE1	3:3:123:LYS:HE2	1.68	0.58
31:B:604:CLA:HBB1	31:B:604:CLA:HMB1	1.86	0.58
31:N:314:CLA:HBC1	32:N:316:LUT:H162	1.85	0.58
31:8:603:CLA:HMD2	30:8:608:CHL:H2	1.85	0.58
2:9:163:MET:HE1	36:9:319:NEX:H30	1.85	0.58
2:9:257:PHE:CB	34:9:301:LMG:H152	2.32	0.58
30:9:303:CHL:HAA2	30:9:303:CHL:HBD	1.84	0.58
1:1:165:VAL:HG11	2:2:57:SER:HB3	1.85	0.58
2:2:133:PHE:HE2	30:3:302:CHL:CMD	2.16	0.58
3:5:70:ASP:HB2	31:5:602:CLA:HBA2	1.85	0.58
6:B:204:ALA:CB	31:B:602:CLA:HAB	2.33	0.58
31:N:310:CLA:HBB1	31:N:310:CLA:HMB3	1.85	0.58
24:Y:99:MET:SD	31:Y:310:CLA:HAB	2.43	0.58
4:0:235:LEU:HB2	32:0:616:LUT:H22	1.84	0.58
2:2:253:SER:O	2:2:256:LYS:HG3	2.03	0.58
31:4:610:CLA:HBB1	31:4:612:CLA:H3A	1.85	0.58
30:6:308:CHL:HAA2	30:6:308:CHL:HBD	1.85	0.58
30:G:606:CHL:HMB1	30:G:608:CHL:HMC	1.85	0.58
4:0:221:PHE:CD1	30:0:607:CHL:H71	2.39	0.58
2:9:245:PRO:HG2	31:9:316:CLA:HMB2	1.85	0.58
2:q:149:ALA:HA	30:q:307:CHL:CHC	2.34	0.58
2:q:177:VAL:HG22	2:q:189:PHE:CE2	2.38	0.58
7:c:23:TRP:HD1	48:c:623:LMU:H6'1	1.68	0.58
2:g:259:PRO:HD3	30:y:607:CHL:H12	1.83	0.58
31:g:304:CLA:C4D	30:g:309:CHL:H71	2.34	0.58
2:2:86:ARG:HA	2:2:86:ARG:NH1	2.19	0.58
30:R:310:CHL:HHC	30:R:310:CHL:HBB1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:100:THR:OG1	34:W:201:LMG:HC5	2.02	0.58
30:7:306:CHL:HBA2	31:r:315:CLA:HMA3	1.86	0.58
31:8:614:CLA:H43	2:9:257:PHE:CE1	2.38	0.58
9:e:8:ARG:HE	9:e:12:ASP:CG	2.11	0.58
2:g:138:LEU:HD11	30:g:307:CHL:HAC1	1.84	0.58
30:s:309:CHL:HBB1	30:s:309:CHL:HHC	1.86	0.58
24:y:48:LYS:HD3	24:y:58:VAL:HG21	1.85	0.58
2:2:125:TRP:CG	2:2:126:PHE:N	2.71	0.58
31:5:604:CLA:HMA3	30:5:606:CHL:C2C	2.34	0.58
31:G:610:CLA:C1C	38:G:617:SQD:H142	2.34	0.58
30:N:308:CHL:HMB3	36:N:318:NEX:H35	1.85	0.58
26:U:100:ARG:NH2	26:U:138:ASP:OD1	2.36	0.58
30:0:608:CHL:HMA3	36:0:618:NEX:H402	1.84	0.58
30:7:308:CHL:O1A	2:9:259:PRO:HD2	2.03	0.58
31:b:612:CLA:H152	31:b:614:CLA:O1D	2.03	0.58
43:d:406:BCR:H20C	34:d:409:LMG:H301	1.83	0.58
31:p:613:CLA:H12	31:p:614:CLA:HMD2	1.86	0.58
2:q:169:TYR:HD1	2:q:174:GLU:CG	2.10	0.58
19:s:264:TRP:HB2	32:s:317:LUT:H22	1.86	0.58
3:3:122:PHE:HD1	3:3:123:LYS:HG3	1.68	0.58
2:4:139:ASN:HA	2:4:148:HIS:H	1.67	0.58
2:4:170:ARG:HA	30:4:608:CHL:C4C	2.33	0.58
3:5:110:ARG:NH1	3:5:230:ILE:HB	2.19	0.58
6:B:145:LEU:HB3	31:B:604:CLA:H161	1.85	0.58
3:N:226:ARG:NH2	31:N:321:CLA:H3A	2.19	0.58
31:N:305:CLA:H101	31:S:306:CLA:CMA	2.34	0.58
19:S:155:PRO:CG	31:S:306:CLA:NB	2.66	0.58
2:q:59:PRO:HB3	2:q:61:TYR:CZ	2.39	0.58
38:b:627:SQD:H91	8:d:130:PHE:HB3	1.86	0.58
31:1:611:CLA:H52	31:1:612:CLA:C3D	2.34	0.58
2:4:179:THR:HB	2:4:188:GLY:HA2	1.86	0.58
34:5:620:LMG:HC62	31:6:315:CLA:HMA1	1.86	0.58
34:5:620:LMG:H302	34:5:620:LMG:H342	1.85	0.58
38:6:301:SQD:H462	31:6:312:CLA:HHB	1.86	0.58
31:6:305:CLA:HMA3	30:6:307:CHL:C2C	2.34	0.58
9:E:8:ARG:HD3	9:E:13:ILE:HG12	1.85	0.58
2:G:223:PHE:CE1	35:G:614:RRX:C31	2.86	0.58
3:N:246:TRP:O	3:N:251:PRO:HD3	2.03	0.58
33:a:415:LHG:HC2	31:c:608:CLA:HED2	1.84	0.58
45:c:619:DGD:HBE1	45:c:619:DGD:CCA	2.33	0.58
2:g:149:ALA:HA	30:g:306:CHL:CHC	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:g:307:CHL:HBB2	30:n:301:CHL:CBB	2.34	0.58
33:g:319:LHG:H312	37:g:321:XAT:C35	2.33	0.58
30:n:306:CHL:H191	31:s:313:CLA:HAC1	1.85	0.58
5:A:317:TRP:CZ3	8:D:180:ARG:HD2	2.39	0.58
31:A:406:CLA:CHA	31:A:406:CLA:HBA1	2.34	0.58
30:9:310:CHL:HMB3	36:9:319:NEX:H14	1.85	0.58
31:9:314:CLA:C1C	35:9:317:RRX:H37	2.34	0.58
3:p:232:ASN:HB3	31:p:613:CLA:O2D	2.04	0.58
7:c:192:VAL:HG22	34:n:321:LMG:H131	1.85	0.58
30:n:308:CHL:HAA1	30:n:308:CHL:HBD	1.84	0.58
31:n:315:CLA:H2A	31:n:315:CLA:HED3	1.86	0.58
30:r:310:CHL:HHC	30:r:310:CHL:HBB1	1.85	0.58
2:4:147:ILE:HD11	31:4:604:CLA:H51	1.86	0.57
31:7:311:CLA:H52	32:7:317:LUT:H30	1.86	0.57
3:p:236:HIS:HB2	31:p:613:CLA:HAA2	1.86	0.57
31:g:313:CLA:H191	24:y:156:VAL:HG23	1.84	0.57
31:1:611:CLA:HAB	38:g:318:SQD:C24	2.32	0.57
3:3:200:LEU:HA	3:3:203:LYS:HD2	1.86	0.57
3:5:236:HIS:ND1	31:5:613:CLA:HAA2	2.19	0.57
4:6:93:HIS:HE1	31:6:304:CLA:C4D	2.16	0.57
6:B:336:ILE:HD13	16:m:-10:UNK:HA	1.86	0.57
11:H:62:VAL:O	11:H:66:GLU:HG2	2.03	0.57
3:p:118:GLU:OE1	3:p:127:GLN:NE2	2.37	0.57
3:p:125:GLY:HA3	30:p:607:CHL:C3D	2.34	0.57
2:q:223:PHE:CE1	35:q:317:RRX:H48	2.39	0.57
2:g:238:LEU:HD23	34:g:320:LMG:HC92	1.86	0.57
31:n:305:CLA:HMB1	31:n:305:CLA:HBB1	1.86	0.57
31:n:315:CLA:HBC1	32:n:317:LUT:H162	1.86	0.57
31:s:303:CLA:H172	31:s:303:CLA:H141	1.86	0.57
34:Q1:101:LMG:O7	34:Q1:101:LMG:HC1	2.04	0.57
6:B:114:HIS:HE1	31:B:616:CLA:C1D	2.17	0.57
2:G:257:PHE:CE1	31:N:315:CLA:H12	2.40	0.57
3:N:186:ASP:HA	32:N:316:LUT:H24	1.86	0.57
31:N:304:CLA:HED2	31:N:304:CLA:H12	1.84	0.57
18:R:140:GLY:HA3	18:R:241:ALA:HB1	1.86	0.57
34:0:620:LMG:H331	34:7:301:LMG:H161	1.85	0.57
1:7:198:LEU:HB3	31:7:311:CLA:HMA2	1.86	0.57
3:p:255:GLY:H	31:p:615:CLA:HMA3	1.69	0.57
2:q:77:LEU:HD23	31:q:304:CLA:H42	1.85	0.57
7:c:201:LEU:HD13	31:c:606:CLA:H141	1.86	0.57
2:g:103:LEU:HD13	31:g:312:CLA:HBB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:n:316:CLA:H11	34:n:322:LMG:HC92	1.86	0.57
29:f1:170:ASP:HB2	29:f1:176:TYR:HE1	1.69	0.57
4:6:106:THR:HG22	34:6:322:LMG:C36	2.34	0.57
31:6:305:CLA:HBA1	30:6:307:CHL:CHD	2.35	0.57
5:A:47:VAL:HG11	5:A:114:LEU:HD22	1.87	0.57
43:B:618:BCR:H19C	38:B:620:SQD:H223	1.85	0.57
8:D:244:TYR:OH	8:D:264:LYS:HD2	2.04	0.57
30:9:311:CHL:HMB1	30:9:311:CHL:HBB1	1.87	0.57
3:p:247:VAL:HG22	2:q:133:PHE:CD2	2.40	0.57
2:q:167:GLU:HG3	30:q:311:CHL:C4B	2.34	0.57
5:a:266:ASN:HD22	5:a:266:ASN:H	1.50	0.57
31:c:612:CLA:HBB1	31:c:612:CLA:HMB3	1.85	0.57
31:g:304:CLA:H2	31:g:304:CLA:HED2	1.84	0.57
31:n:304:CLA:HMD2	30:n:310:CHL:H2	1.85	0.57
31:2:602:CLA:HBC1	33:2:617:LHG:H252	1.86	0.57
3:5:218:PHE:CZ	32:5:616:LUT:H8	2.40	0.57
6:B:156:PHE:HZ	33:B:624:LHG:H282	1.68	0.57
19:S:120:ILE:HD11	31:S:311:CLA:H193	1.86	0.57
24:Y:206:LEU:HD23	24:Y:209:LYS:HD2	1.86	0.57
34:0:622:LMG:HC72	34:0:622:LMG:O10	2.05	0.57
1:7:198:LEU:HB3	31:7:311:CLA:CMA	2.35	0.57
31:7:315:CLA:HBA1	31:7:315:CLA:CHA	2.32	0.57
31:9:305:CLA:HHC	31:9:305:CLA:CBB	2.33	0.57
3:p:106:GLU:OE2	3:p:231:GLU:HG3	2.05	0.57
31:p:611:CLA:H92	31:p:612:CLA:HED1	1.86	0.57
45:c:619:DGD:HD5	31:y:611:CLA:HMA2	1.86	0.57
3:n:110:ARG:NH2	3:n:231:GLU:HA	2.19	0.57
31:n:305:CLA:H152	31:s:306:CLA:C4A	2.35	0.57
17:o:133:ASP:OD1	17:o:134:GLU:N	2.37	0.57
22:w:93:TRP:CE2	34:w:202:LMG:H131	2.40	0.57
24:y:221:MET:HE2	32:y:617:LUT:H10	1.84	0.57
30:y:607:CHL:H121	30:y:609:CHL:H152	1.86	0.57
29:F1:116:LYS:O	29:F1:204:GLY:HA2	2.04	0.57
2:2:140:TYR:HB3	2:2:146:LEU:HB3	1.87	0.57
33:A:417:LHG:O3	33:A:417:LHG:O1	2.16	0.57
6:B:74:SER:OG	6:B:94:GLU:OE2	2.22	0.57
8:D:216:ALA:O	8:D:220:ASN:ND2	2.27	0.57
38:G:617:SQD:H251	31:7:312:CLA:HAB	1.86	0.57
30:G:623:CHL:CBB	30:Y:307:CHL:HBB2	2.34	0.57
20:T:15:GLY:HA3	38:b:621:SQD:H321	1.86	0.57
8:d:189:HIS:HA	8:d:294:ARG:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f1:196:LEU:HB3	29:f1:230:TRP:CD2	2.40	0.57
31:4:604:CLA:CHB	36:4:617:NEX:H383	2.34	0.57
31:C:611:CLA:H42	21:V:33:LEU:HA	1.86	0.57
2:G:254:ALA:HA	37:G:620:XAT:H172	1.86	0.57
30:N:307:CHL:H92	36:N:318:NEX:H202	1.85	0.57
31:7:316:CLA:HBB2	3:8:121:TRP:CZ2	2.40	0.57
2:9:149:ALA:HA	30:9:307:CHL:CHC	2.35	0.57
3:p:162:ILE:HD13	30:p:608:CHL:HMA2	1.86	0.57
31:p:613:CLA:H51	31:p:613:CLA:C4B	2.34	0.57
31:q:313:CLA:C1C	38:x:201:SQD:H142	2.34	0.57
31:n:304:CLA:H43	24:y:77:LEU:HD21	1.86	0.57
31:r:303:CLA:HBD	33:r:320:LHG:HC82	1.86	0.57
30:4:601:CHL:CMC	37:4:619:XAT:H23	2.35	0.57
31:5:613:CLA:ND	31:5:613:CLA:H52	2.20	0.57
32:5:617:LUT:H191	32:5:617:LUT:C12	2.34	0.57
5:A:292:THR:HG22	7:C:416:THR:HG23	1.85	0.57
31:G:609:CLA:H52	35:G:614:RRX:H25	1.85	0.57
24:Y:186:TYR:HB3	31:Y:310:CLA:HED3	1.86	0.57
24:Y:194:LEU:HD12	32:Y:315:LUT:H222	1.85	0.57
34:0:620:LMG:H341	30:7:306:CHL:C4D	2.34	0.57
1:7:145:SER:HB2	34:7:301:LMG:HC5	1.87	0.57
31:7:316:CLA:H2	34:9:301:LMG:HC72	1.85	0.57
2:9:241:HIS:HB2	31:9:315:CLA:HAA2	1.86	0.57
2:g:80:ASP:HB3	2:g:83:THR:HG22	1.86	0.57
17:o:100:GLU:OE2	22:w:60:LEU:N	2.38	0.57
24:y:94:HIS:HE1	31:y:603:CLA:C4D	2.18	0.57
2:2:140:TYR:CD1	2:2:141:LEU:HG	2.40	0.57
31:0:614:CLA:H91	34:p:620:LMG:H131	1.86	0.57
2:q:89:GLU:HA	2:q:184:LEU:HD21	1.86	0.57
2:q:139:ASN:CG	2:q:144:PRO:HA	2.30	0.57
2:q:175:GLY:N	2:q:176:PRO:HD2	2.20	0.57
6:b:374:ASP:OD1	6:b:374:ASP:N	2.37	0.57
7:c:113:LEU:HD13	43:c:614:BCR:H19C	1.85	0.57
2:4:195:LEU:HB2	31:4:610:CLA:O1A	2.04	0.57
3:5:87:LEU:HD13	31:5:603:CLA:HBA1	1.87	0.57
6:B:162:PHE:CD1	48:R:302:LMU:H1'	2.39	0.57
34:B:625:LMG:H342	30:R:309:CHL:H42	1.86	0.57
34:C:624:LMG:H162	33:Y:318:LHG:HC92	1.87	0.57
42:D:401:PHO:H72	31:D:403:CLA:H111	1.87	0.57
34:G:622:LMG:H112	31:N:315:CLA:H11	1.87	0.57
3:N:191:ALA:HB2	31:N:310:CLA:HAA2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:0:173:PRO:HB3	18:r:54:LEU:HG	1.87	0.57
3:p:142:LEU:HA	30:p:605:CHL:HED3	1.86	0.57
31:q:305:CLA:HHC	31:q:305:CLA:CBB	2.32	0.57
31:c:606:CLA:H8	43:c:615:BCR:H12C	1.85	0.57
45:c:619:DGD:HAS1	33:y:619:LHG:H332	1.86	0.57
30:g:308:CHL:HBD	30:g:308:CHL:HAA1	1.86	0.57
17:o:257:GLU:HG2	17:o:289:GLN:HG2	1.87	0.57
19:s:41:GLY:HA3	24:y:52:PRO:HB2	1.85	0.57
34:3:321:LMG:O6	34:3:321:LMG:HC92	2.05	0.56
3:5:107:LEU:HD22	3:5:230:ILE:CD1	2.35	0.56
7:C:306:LEU:HD12	7:C:328:TYR:HB3	1.87	0.56
2:G:149:ALA:HA	30:G:605:CHL:CHC	2.35	0.56
34:G:622:LMG:H141	31:N:315:CLA:H71	1.86	0.56
19:S:252:GLN:HE21	19:S:263:ASN:HD22	1.53	0.56
24:Y:192:ASP:HA	32:Y:315:LUT:H24	1.87	0.56
3:8:223:LEU:HD21	34:9:302:LMG:H172	1.87	0.56
2:q:220:MET:HE2	32:q:318:LUT:H10	1.87	0.56
31:b:605:CLA:HBB1	31:b:605:CLA:HMB1	1.87	0.56
45:c:618:DGD:HE4	13:j:42:LEU:HD21	1.86	0.56
9:e:26:THR:HB	47:e:102:HEM:CAB	2.35	0.56
2:2:59:PRO:HD2	2:2:62:LEU:HD12	1.87	0.56
3:5:224:ILE:HG23	3:5:258:TYR:CD2	2.40	0.56
3:5:255:GLY:H	31:5:615:CLA:H2A	1.70	0.56
45:C:620:DGD:HB22	45:C:620:DGD:HG11	1.86	0.56
34:D:412:LMG:O10	11:H:69:ASN:ND2	2.37	0.56
3:N:235:ASP:C	3:N:243:THR:HG21	2.30	0.56
19:S:272:PHE:HD1	38:S:301:SQD:H461	1.70	0.56
1:7:124:ALA:HB2	30:7:308:CHL:HED2	1.87	0.56
30:8:608:CHL:HMB1	30:8:608:CHL:HBB1	1.87	0.56
3:p:196:THR:O	3:p:200:LEU:HG	2.05	0.56
31:p:613:CLA:H41	31:p:613:CLA:H72	1.86	0.56
31:p:614:CLA:NC	31:p:614:CLA:H51	2.20	0.56
14:k:46:ARG:NH2	21:v:33:LEU:O	2.38	0.56
19:s:252:GLN:HE21	19:s:263:ASN:HD22	1.53	0.56
2:2:208:LYS:HD3	31:2:611:CLA:HAA2	1.87	0.56
31:2:609:CLA:HBA1	35:2:614:RRX:H7	1.85	0.56
30:4:606:CHL:HBB2	30:4:607:CHL:CBB	2.35	0.56
3:5:74:LEU:HD22	3:5:74:LEU:H	1.70	0.56
34:6:321:LMG:H111	34:6:322:LMG:C11	2.35	0.56
31:A:405:CLA:H122	42:A:408:PHO:H3A	1.88	0.56
31:B:611:CLA:C3B	31:B:613:CLA:HMA2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:26:GLY:HA3	31:C:611:CLA:HMD2	1.88	0.56
33:G:618:LHG:HC61	37:G:620:XAT:C38	2.34	0.56
37:G:620:XAT:O23	38:G:624:SQD:H81	2.05	0.56
3:N:58:TYR:CD1	3:N:59:LEU:HD13	2.40	0.56
31:N:305:CLA:H112	31:S:306:CLA:HHB	1.86	0.56
17:O:235:LYS:HD3	17:O:272:LEU:HD23	1.87	0.56
18:R:144:MET:SD	31:R:312:CLA:HAB	2.45	0.56
30:R:308:CHL:HBB2	30:R:309:CHL:HMB2	1.85	0.56
6:b:24:LEU:HD21	31:b:617:CLA:CAB	2.35	0.56
3:n:185:PHE:HA	30:n:309:CHL:H43	1.87	0.56
31:r:305:CLA:H2	31:r:305:CLA:HED2	1.86	0.56
22:w:89:PHE:CD2	34:w:202:LMG:H432	2.41	0.56
34:w:203:LMG:H122	34:w:203:LMG:HC91	1.87	0.56
34:w:205:LMG:O9	34:w:205:LMG:HC91	2.06	0.56
26:u:144:ASP:HA	26:u:151:LYS:HE3	1.87	0.56
30:2:605:CHL:HAA1	30:2:605:CHL:HBD	1.87	0.56
2:4:182:ASP:OD2	2:4:185:TYR:HB2	2.06	0.56
31:4:603:CLA:HHC	31:4:603:CLA:CBB	2.33	0.56
7:C:326:GLY:HA2	17:O:157:TYR:OH	2.06	0.56
30:G:623:CHL:HED2	24:Y:126:LYS:HA	1.87	0.56
6:b:114:HIS:HE1	31:b:617:CLA:C1D	2.19	0.56
9:e:24:SER:O	9:e:28:PRO:HG2	2.06	0.56
2:2:130:ALA:HA	2:2:133:PHE:HD2	1.70	0.56
2:2:132:ILE:HG23	2:2:152:ILE:HD12	1.87	0.56
31:3:314:CLA:C4C	31:3:314:CLA:H62	2.35	0.56
31:4:604:CLA:O2A	36:4:617:NEX:H241	2.05	0.56
3:5:209:ARG:HB2	33:5:619:LHG:H262	1.88	0.56
6:B:237:VAL:HG22	31:B:610:CLA:HBC2	1.87	0.56
7:C:432:HIS:HE1	31:C:608:CLA:NA	1.99	0.56
3:N:223:LEU:HD21	31:N:321:CLA:H41	1.86	0.56
30:N:307:CHL:H41	30:N:307:CHL:H72	1.88	0.56
31:8:609:CLA:H92	32:8:615:LUT:H371	1.87	0.56
3:p:232:ASN:HB3	31:p:613:CLA:CED	2.36	0.56
2:q:162:ILE:HG22	36:q:319:NEX:H34	1.86	0.56
30:q:303:CHL:HBC1	33:q:320:LHG:C3	2.36	0.56
5:a:77:ILE:HD13	15:l:30:VAL:HG13	1.86	0.56
30:g:306:CHL:HBA1	30:g:306:CHL:CHA	2.34	0.56
31:s:304:CLA:HHC	31:s:304:CLA:CBB	2.34	0.56
31:4:602:CLA:HMB2	31:4:602:CLA:H52	1.86	0.56
31:5:602:CLA:H11	32:5:617:LUT:H26	1.86	0.56
33:5:619:LHG:HC62	33:5:619:LHG:O5	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:6:322:LMG:H301	34:6:322:LMG:HC92	1.85	0.56
7:C:356:PRO:HB3	26:U:130:ARG:HB2	1.88	0.56
3:N:69:TRP:O	32:N:317:LUT:H24	2.06	0.56
3:N:226:ARG:HH22	31:N:321:CLA:H3A	1.70	0.56
30:N:307:CHL:HBB2	30:Y:301:CHL:CAB	2.34	0.56
17:O:148:GLU:HB3	17:O:182:LYS:HG3	1.87	0.56
1:7:178:TYR:CZ	1:7:199:LYS:HE3	2.40	0.56
3:8:38:VAL:HG11	3:8:43:PRO:HD2	1.88	0.56
2:q:97:TRP:CE2	30:q:310:CHL:HED3	2.41	0.56
2:q:172:SER:O	2:q:174:GLU:HG2	2.06	0.56
34:b:624:LMG:H321	34:b:624:LMG:H361	1.87	0.56
8:d:55:VAL:O	8:d:66:SER:HB3	2.06	0.56
3:n:46:PRO:HB2	30:n:302:CHL:CBC	2.36	0.56
17:o:105:THR:HB	17:o:119:PHE:HB3	1.87	0.56
29:f1:78:ILE:HD11	29:f1:95:LEU:HD21	1.88	0.56
3:3:87:LEU:HD13	31:3:305:CLA:HBA1	1.88	0.56
3:3:159:MET:CE	36:3:319:NEX:H30	2.34	0.56
3:3:258:TYR:CD1	3:3:258:TYR:C	2.83	0.56
2:4:254:ALA:O	37:4:619:XAT:H42	2.06	0.56
2:4:258:LEU:HD21	4:6:125:LYS:HG3	1.87	0.56
3:N:92:ALA:HB1	3:N:208:GLY:HA3	1.86	0.56
3:N:254:ALA:HB3	30:N:301:CHL:HED3	1.87	0.56
19:S:91:ALA:HB2	31:S:303:CLA:HBA1	1.87	0.56
31:S:313:CLA:H92	31:S:313:CLA:H41	1.88	0.56
22:W:86:THR:CG2	34:W:201:LMG:H221	2.35	0.56
1:7:76:GLY:HA3	3:8:80:THR:HA	1.87	0.56
1:7:90:ILE:HG21	31:7:304:CLA:HAA2	1.87	0.56
3:8:46:PRO:HB2	30:8:601:CHL:CBC	2.36	0.56
43:c:615:BCR:H332	12:i:24:LEU:HD21	1.88	0.56
3:n:46:PRO:HB2	30:n:302:CHL:HBC1	1.88	0.56
30:s:307:CHL:HBD	30:s:307:CHL:HAA2	1.88	0.56
31:1:611:CLA:HBB1	31:1:611:CLA:HHC	1.88	0.56
3:3:252:LYS:CA	3:3:256:ILE:HG23	2.30	0.56
31:4:610:CLA:H2	35:4:615:RRX:C40	2.35	0.56
30:5:608:CHL:HMB1	36:5:618:NEX:H14	1.88	0.56
5:A:41:LEU:HD22	42:A:408:PHO:H61	1.88	0.56
7:C:429:HIS:CE1	31:C:605:CLA:ND	2.73	0.56
8:D:12:ARG:NH1	8:D:20:ASP:OD2	2.39	0.56
30:G:601:CHL:H13	33:G:618:LHG:H371	1.87	0.56
18:R:186:LEU:HD13	30:R:308:CHL:HMD1	1.88	0.56
2:9:107:THR:OG1	31:9:306:CLA:HBC3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:p:221:GLN:HB2	31:p:613:CLA:CED	2.36	0.56
3:p:245:PHE:CZ	30:q:309:CHL:H11	2.37	0.56
2:q:205:LEU:HB3	31:q:312:CLA:HMA2	1.88	0.56
44:a:414:PL9:H261	33:e:101:LHG:H361	1.88	0.56
31:b:615:CLA:H161	34:b:622:LMG:H411	1.87	0.56
31:c:613:CLA:H13	33:c:622:LHG:H171	1.88	0.56
13:j:28:GLY:HA3	34:j:101:LMG:H321	1.87	0.56
30:n:308:CHL:O1A	24:y:259:LEU:HD12	2.05	0.56
31:2:602:CLA:H8	32:2:615:LUT:H371	1.87	0.56
3:3:67:TYR:HB2	31:3:304:CLA:HMD1	1.87	0.56
3:3:146:GLN:HB2	30:3:307:CHL:CBB	2.36	0.56
30:4:607:CHL:H102	30:4:607:CHL:CHC	2.36	0.56
3:5:40:TRP:HH2	33:5:619:LHG:O4	1.89	0.56
3:5:72:ALA:HB3	3:5:74:LEU:CD2	2.36	0.56
17:O:79:SER:O	17:O:250:LYS:NZ	2.37	0.56
3:8:110:ARG:NH2	3:8:231:GLU:HA	2.19	0.56
31:9:312:CLA:H2	35:9:317:RRX:H8	1.87	0.56
3:p:89:VAL:HG22	3:p:205:LEU:HD21	1.88	0.56
5:a:133:LEU:HD22	5:a:137:LEU:HG	1.88	0.56
31:c:606:CLA:H51	31:c:607:CLA:H192	1.88	0.56
31:2:610:CLA:CGA	38:6:301:SQD:H441	2.35	0.56
2:4:93:ILE:HG23	2:4:170:ARG:HH21	1.70	0.56
7:C:432:HIS:HE1	31:C:608:CLA:C1A	2.19	0.56
47:E:101:HEM:HMC2	10:F:30:VAL:HG21	1.88	0.56
18:R:59:ARG:NH1	18:R:70:ASP:OD1	2.39	0.56
19:S:83:TYR:HB2	31:S:303:CLA:HMD1	1.88	0.56
3:8:46:PRO:HB2	30:8:601:CHL:HBC1	1.88	0.56
30:8:607:CHL:HAA1	30:8:607:CHL:HBD	1.87	0.56
31:9:305:CLA:HMA3	31:9:305:CLA:H2	1.88	0.56
31:p:602:CLA:H42	32:p:617:LUT:H371	1.88	0.56
30:p:606:CHL:CBB	30:p:609:CHL:HBC1	2.36	0.56
6:b:334:ASP:N	6:b:334:ASP:OD1	2.36	0.56
31:g:305:CLA:H52	30:g:307:CHL:HAA2	1.87	0.56
22:w:109:ARG:HH21	22:w:115:PHE:HA	1.71	0.56
28:p1:30:THR:HG22	28:p1:36:TRP:CD1	2.41	0.56
31:1:610:CLA:HMB2	31:1:612:CLA:HBA2	1.88	0.55
2:4:139:ASN:OD1	2:4:148:HIS:HA	2.06	0.55
2:4:253:SER:HB2	2:4:256:LYS:HD3	1.88	0.55
3:5:168:ASN:ND2	4:6:53:PHE:HA	2.22	0.55
3:5:225:THR:O	3:5:227:LYS:HG3	2.06	0.55
3:5:252:LYS:HB3	3:5:258:TYR:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:304:GLN:HG2	5:A:313:VAL:HG21	1.88	0.55
2:G:103:LEU:HD13	31:G:611:CLA:HBB2	1.87	0.55
3:N:200:LEU:HB3	31:N:310:CLA:CMA	2.35	0.55
19:S:256:THR:HG23	19:S:258:GLU:H	1.71	0.55
30:0:605:CHL:HHC	30:0:605:CHL:HBB1	1.88	0.55
3:8:199:GLU:OE2	3:8:203:LYS:HE3	2.06	0.55
5:a:296:ASN:HB3	7:c:389:LEU:HA	1.87	0.55
6:b:423:ARG:NH2	6:b:430:PHE:O	2.39	0.55
47:e:102:HEM:HBD2	47:e:102:HEM:HHA	1.87	0.55
30:n:309:CHL:HBD	30:n:309:CHL:HAA1	1.88	0.55
28:p1:59:ASN:N	28:p1:59:ASN:OD1	2.39	0.55
2:2:139:ASN:HB3	2:2:143:ASN:O	2.07	0.55
3:3:182:GLY:HA2	3:3:186:ASP:HB2	1.88	0.55
3:3:200:LEU:HD22	31:3:311:CLA:HHB	1.88	0.55
4:6:250:LEU:O	4:6:251:TYR:C	2.49	0.55
31:6:314:CLA:ND	31:6:314:CLA:H2	2.21	0.55
7:C:394:SER:HA	7:C:408:VAL:HG23	1.88	0.55
8:D:257:PHE:CE1	33:D:408:LHG:H331	2.41	0.55
18:R:201:ARG:NH1	31:R:311:CLA:O1D	2.32	0.55
5:a:342:ASP:HB2	8:d:352:LEU:HG	1.88	0.55
44:a:414:PL9:H353	33:e:101:LHG:H322	1.87	0.55
7:c:356:PRO:HB3	26:u:130:ARG:HB2	1.88	0.55
34:c:624:LMG:H311	33:y:619:LHG:HC92	1.88	0.55
18:r:123:TYR:CD2	18:r:131:ARG:HG3	2.42	0.55
19:s:224:ASP:HB3	19:s:227:VAL:HB	1.89	0.55
31:s:312:CLA:C4C	33:s:320:LHG:HC62	2.37	0.55
1:1:231:LEU:HG	32:1:615:LUT:H163	1.89	0.55
3:3:246:TRP:HA	3:3:250:ALA:CB	2.36	0.55
2:4:126:PHE:CE1	31:5:615:CLA:HMA3	2.41	0.55
19:S:204:TYR:HA	19:S:207:MET:HE2	1.87	0.55
30:0:607:CHL:C1	2:q:259:PRO:HD3	2.35	0.55
7:c:75:ILE:HG13	7:c:76:LEU:HD12	1.87	0.55
7:c:432:HIS:HE1	31:c:608:CLA:C1A	2.19	0.55
9:e:68:ASP:OD2	9:e:71:ASN:ND2	2.39	0.55
20:t:4:LEU:HG	33:t:102:LHG:H282	1.87	0.55
2:2:127:LYS:HG2	3:3:254:ALA:O	2.06	0.55
30:2:601:CHL:HBC1	33:2:617:LHG:HC31	1.88	0.55
34:5:620:LMG:O10	34:5:620:LMG:H361	2.07	0.55
7:c:123:VAL:HG21	25:z:27:LEU:HD22	1.88	0.55
30:2:606:CHL:CBB	30:2:608:CHL:HBC1	2.36	0.55
3:3:240:PRO:HB2	31:3:315:CLA:CHB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:205:LEU:CD1	31:4:610:CLA:H43	2.36	0.55
2:4:208:LYS:HD3	31:4:612:CLA:O1A	2.05	0.55
34:G:621:LMG:H351	3:N:223:LEU:HD22	1.88	0.55
19:S:138:GLU:CA	30:S:308:CHL:HED1	2.25	0.55
31:7:304:CLA:HAC1	30:7:308:CHL:CBB	2.35	0.55
31:g:312:CLA:HAB	34:g:320:LMG:H361	1.89	0.55
31:n:311:CLA:H12	31:n:311:CLA:CHB	2.37	0.55
18:r:218:ASP:HA	32:r:317:LUT:H24	1.89	0.55
31:s:314:CLA:HMA1	32:s:317:LUT:H162	1.88	0.55
38:x:201:SQD:H45	38:x:201:SQD:O5	2.07	0.55
30:1:606:CHL:O2A	36:R:301:NEX:H31	2.06	0.55
5:A:334:ARG:HD3	8:D:320:LEU:HD23	1.88	0.55
7:C:111:ALA:HB1	33:S:322:LHG:H383	1.89	0.55
7:C:185:ARG:NH1	7:C:219:GLU:OE2	2.36	0.55
7:C:381:ALA:HB1	26:U:75:ARG:HG3	1.87	0.55
3:N:146:GLN:HB2	30:N:306:CHL:CBB	2.37	0.55
2:q:59:PRO:HG2	2:q:73:ASP:HB3	1.89	0.55
31:b:608:CLA:HBB1	31:b:608:CLA:HMB1	1.89	0.55
32:g:316:LUT:H28	32:g:316:LUT:H361	1.86	0.55
3:3:120:VAL:HG23	3:3:123:LYS:HB2	1.88	0.55
2:4:140:TYR:HD1	2:4:146:LEU:HG	1.70	0.55
3:5:227:LYS:HB2	3:5:232:ASN:ND2	2.20	0.55
31:8:612:CLA:H172	31:8:613:CLA:C1D	2.37	0.55
3:p:246:TRP:CD1	3:p:246:TRP:H	2.23	0.55
2:q:250:GLY:HA3	37:q:321:XAT:H193	1.89	0.55
34:c:624:LMG:H292	30:y:601:CHL:HAC1	1.89	0.55
31:n:311:CLA:H92	32:n:317:LUT:H371	1.88	0.55
3:3:38:VAL:HA	3:3:42:GLY:H	1.72	0.55
31:4:611:CLA:C4C	33:4:618:LHG:HC62	2.37	0.55
3:5:99:ALA:HB1	32:5:616:LUT:H12	1.89	0.55
9:E:26:THR:HB	47:E:101:HEM:HAB	1.89	0.55
30:0:605:CHL:HED3	31:r:315:CLA:O1A	2.07	0.55
1:7:62:LEU:HD11	1:7:73:ASP:HB2	1.89	0.55
1:7:134:TYR:O	1:7:140:LEU:HD12	2.07	0.55
31:8:613:CLA:HBC1	32:8:615:LUT:H162	1.87	0.55
3:p:191:ALA:HB3	31:p:610:CLA:HAA2	1.89	0.55
2:q:258:LEU:O	34:q:301:LMG:HC4	2.07	0.55
31:a:407:CLA:HBA1	31:a:407:CLA:CHA	2.36	0.55
31:a:409:CLA:H12	34:w:201:LMG:H112	1.87	0.55
3:n:250:ALA:N	3:n:251:PRO:HD2	2.21	0.55
19:s:252:GLN:O	19:s:256:THR:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:610:CLA:HMA3	38:6:301:SQD:H5	1.89	0.55
30:3:302:CHL:HBD	30:3:302:CHL:HAA1	1.88	0.55
2:4:132:ILE:HG13	2:4:152:ILE:HG13	1.89	0.55
3:5:89:VAL:HG21	3:5:179:LEU:HD13	1.89	0.55
15:L:27:VAL:HG11	33:L:101:LHG:H182	1.88	0.55
24:Y:178:PHE:HA	38:Y:320:SQD:H2	1.89	0.55
31:Y:313:CLA:H121	33:Y:318:LHG:H332	1.89	0.55
4:0:133:GLU:OE1	4:0:134:GLY:N	2.40	0.55
3:8:250:ALA:N	3:8:251:PRO:HD2	2.21	0.55
7:c:452:GLU:OE2	8:d:248:THR:OG1	2.25	0.55
2:2:179:THR:C	2:2:181:GLY:H	2.15	0.55
31:5:604:CLA:H43	30:5:606:CHL:HAA2	1.88	0.55
31:A:409:CLA:H12	34:A:412:LMG:H121	1.88	0.55
30:0:608:CHL:CMA	36:0:618:NEX:H30	2.37	0.55
1:7:157:MET:HB3	30:7:310:CHL:CBB	2.36	0.55
30:8:606:CHL:HAA2	30:8:606:CHL:HBD	1.89	0.55
5:a:28:LEU:HB2	34:a:401:LMG:H292	1.88	0.55
7:c:162:LEU:HD22	31:c:602:CLA:H202	1.89	0.55
33:g:319:LHG:H371	37:g:321:XAT:H10	1.89	0.55
3:n:38:VAL:HG11	3:n:43:PRO:HD2	1.88	0.55
3:n:199:GLU:OE2	3:n:203:LYS:HE3	2.06	0.55
31:n:316:CLA:H11	34:n:322:LMG:HC91	1.88	0.55
30:y:607:CHL:H143	30:y:609:CHL:H112	1.89	0.55
2:2:89:GLU:HA	2:2:184:LEU:HD11	1.90	0.54
3:3:159:MET:HE3	30:3:308:CHL:CMB	2.36	0.54
31:3:313:CLA:HHC	31:3:313:CLA:CBB	2.37	0.54
31:3:314:CLA:H8	31:3:314:CLA:C1C	2.37	0.54
2:4:254:ALA:HB1	37:4:619:XAT:H183	1.89	0.54
3:5:81:PHE:CZ	3:5:85:ARG:HD3	2.41	0.54
3:5:167:VAL:HG21	4:6:50:LEU:HD23	1.89	0.54
31:5:614:CLA:HBA2	31:5:614:CLA:CHA	2.37	0.54
5:A:160:ILE:HG12	7:C:419:PHE:CZ	2.42	0.54
33:G:618:LHG:C6	37:G:620:XAT:C38	2.85	0.54
30:0:607:CHL:HAA2	30:0:607:CHL:HBD	1.88	0.54
1:7:127:PHE:HZ	2:9:251:PHE:HB3	1.73	0.54
2:q:158:THR:O	2:q:162:ILE:HG12	2.06	0.54
6:b:161:LEU:O	48:r:302:LMU:H6E	2.07	0.54
29:F1:66:PHE:CZ	29:F1:225:GLU:HA	2.42	0.54
1:1:94:HIS:HE1	31:1:603:CLA:C4D	2.20	0.54
3:5:161:LEU:CD1	36:5:618:NEX:H11	2.38	0.54
30:5:606:CHL:HBB2	30:5:607:CHL:CBB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:229:LYS:HB2	4:6:234:ASN:OD1	2.07	0.54
6:B:35:GLY:HA3	6:B:101:ILE:HG12	1.89	0.54
7:C:202:PHE:HB2	22:W:73:ILE:HG23	1.89	0.54
31:0:604:CLA:HMA2	30:0:606:CHL:C3C	2.38	0.54
31:8:604:CLA:O1A	36:8:617:NEX:H241	2.07	0.54
2:9:109:GLU:OE2	2:9:235:LEU:HB2	2.07	0.54
3:p:203:LYS:HG3	31:p:611:CLA:HED2	1.88	0.54
31:p:610:CLA:C2	32:p:616:LUT:H26	2.37	0.54
5:a:54:ALA:HB2	5:a:72:LEU:HD12	1.88	0.54
6:b:348:ASP:OD1	6:b:349:LYS:N	2.38	0.54
45:c:617:DGD:HB32	34:j:101:LMG:H142	1.89	0.54
8:d:117:HIS:HE1	31:d:405:CLA:C4D	2.20	0.54
8:d:213:ILE:HG21	44:d:407:PL9:HC8	1.89	0.54
3:n:200:LEU:HB3	31:n:311:CLA:HMA2	1.89	0.54
34:2:618:LMG:O8	34:2:618:LMG:H122	2.07	0.54
3:3:143:ILE:HA	30:3:307:CHL:CHA	2.38	0.54
3:5:96:MET:SD	31:5:610:CLA:HAB	2.47	0.54
3:5:249:TYR:HA	3:5:252:LYS:HD3	1.89	0.54
4:6:110:LEU:CD2	34:6:322:LMG:C33	2.77	0.54
6:B:224:ARG:NH1	34:D:410:LMG:O3	2.41	0.54
2:G:80:ASP:HB3	2:G:83:THR:HG22	1.87	0.54
3:N:236:HIS:HA	3:N:243:THR:CG2	2.38	0.54
17:O:198:ARG:HB2	17:O:272:LEU:HD13	1.89	0.54
19:S:252:GLN:O	19:S:256:THR:HG22	2.07	0.54
22:W:109:ARG:HH22	22:W:116:GLY:H	1.55	0.54
30:0:607:CHL:HAA1	37:q:321:XAT:H41	1.88	0.54
3:p:122:PHE:CD2	3:p:123:LYS:HG2	2.42	0.54
6:b:35:GLY:HA3	6:b:101:ILE:HG12	1.87	0.54
3:n:168:ASN:HD22	24:y:53:PHE:HA	1.72	0.54
3:n:180:TYR:HB3	31:n:311:CLA:HED3	1.88	0.54
31:n:311:CLA:HBB1	31:n:311:CLA:HMB3	1.88	0.54
19:s:138:GLU:HA	30:s:308:CHL:HED2	1.89	0.54
2:4:228:LEU:HD22	34:4:621:LMG:H322	1.88	0.54
9:E:13:ILE:HG21	47:E:101:HEM:HAD2	1.88	0.54
2:G:127:LYS:HA	30:N:301:CHL:HED2	1.89	0.54
14:K:18:PHE:CE1	33:K:102:LHG:H242	2.43	0.54
3:N:246:TRP:HD1	31:N:314:CLA:HED2	1.72	0.54
31:N:312:CLA:HHC	31:N:312:CLA:CBB	2.36	0.54
17:O:232:GLU:O	17:O:235:LYS:NZ	2.40	0.54
33:S:322:LHG:H282	25:Z:44:ILE:HG21	1.90	0.54
31:9:312:CLA:H2	35:9:317:RRX:C40	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:314:CLA:O2A	31:9:314:CLA:H2A	2.07	0.54
3:p:139:ASN:HB3	3:p:142:LEU:HB2	1.88	0.54
6:b:204:ALA:CB	31:b:603:CLA:HAB	2.38	0.54
6:b:422:ARG:O	6:b:425:GLN:HG2	2.08	0.54
7:c:270:MET:HE1	31:c:607:CLA:H11	1.89	0.54
47:e:102:HEM:HMB1	27:q1:19:VAL:HG21	1.88	0.54
2:2:97:TRP:CE2	30:2:607:CHL:HED2	2.42	0.54
2:2:167:GLU:HG3	30:2:608:CHL:C4B	2.38	0.54
31:2:613:CLA:HED2	37:2:619:XAT:H202	1.89	0.54
3:3:99:ALA:HB1	32:3:317:LUT:H12	1.90	0.54
2:4:75:ALA:HB3	2:4:77:LEU:HD21	1.89	0.54
30:4:607:CHL:C4A	30:4:607:CHL:HBA2	2.38	0.54
3:5:187:PRO:HD2	32:5:616:LUT:C24	2.38	0.54
31:5:603:CLA:HBC1	30:5:609:CHL:HAC2	1.90	0.54
4:6:99:LEU:HB3	31:6:305:CLA:HAB	1.90	0.54
31:6:314:CLA:H2	31:6:314:CLA:C4D	2.37	0.54
31:B:609:CLA:HMA3	31:B:610:CLA:C1C	2.38	0.54
8:D:41:ALA:HB1	42:D:401:PHO:H42	1.89	0.54
34:J:101:LMG:HC91	34:J:101:LMG:H121	1.88	0.54
3:8:200:LEU:HB3	31:8:609:CLA:HMA2	1.88	0.54
34:9:321:LMG:H321	34:9:321:LMG:HC8	1.89	0.54
3:p:240:PRO:HG3	31:p:614:CLA:HMB3	1.89	0.54
31:q:314:CLA:HAB	35:q:317:RRX:C14	2.38	0.54
5:a:10:SER:HA	22:w:102:GLU:OE1	2.08	0.54
6:b:156:PHE:HZ	33:b:628:LHG:H282	1.72	0.54
6:b:275:TRP:HB3	6:b:318:ASN:HD22	1.72	0.54
38:b:627:SQD:H151	8:d:127:LEU:HD13	1.89	0.54
18:r:223:ALA:HB3	31:r:312:CLA:HAA2	1.89	0.54
19:s:151:TRP:NE1	36:s:319:NEX:O23	2.30	0.54
24:y:219:LEU:HD12	33:y:619:LHG:H271	1.89	0.54
3:3:49:LEU:HB3	3:3:52:PHE:O	2.06	0.54
6:B:247:TRP:HB2	31:B:608:CLA:HBC1	1.90	0.54
31:B:610:CLA:HHC	31:B:610:CLA:CBB	2.37	0.54
7:C:74:LEU:HD13	7:C:77:LEU:HD22	1.89	0.54
30:N:306:CHL:H193	31:S:315:CLA:HBC3	1.90	0.54
18:R:174:TYR:HD2	31:R:306:CLA:HBA1	1.73	0.54
1:7:94:HIS:HE1	31:7:304:CLA:C4D	2.20	0.54
7:c:325:LEU:HD23	17:o:159:PRO:HG2	1.89	0.54
3:n:246:TRP:O	3:n:251:PRO:HD3	2.08	0.54
31:n:304:CLA:HED2	31:n:304:CLA:H2	1.90	0.54
24:y:206:LEU:HB3	31:y:610:CLA:CMA	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:B:614:CLA:HMB3	31:B:614:CLA:HBB1	1.90	0.54
2:G:133:PHE:CE2	2:G:152:ILE:HG12	2.43	0.54
2:G:152:ILE:HD12	2:G:152:ILE:H	1.72	0.54
3:N:121:TRP:CH2	31:N:321:CLA:HBB2	2.42	0.54
4:0:188:ASP:HA	32:0:616:LUT:H24	1.88	0.54
1:7:77:LEU:HD21	31:8:603:CLA:H43	1.89	0.54
31:8:612:CLA:H192	31:8:613:CLA:C4C	2.38	0.54
3:p:49:LEU:HD12	2:q:171:TYR:CD2	2.42	0.54
30:p:606:CHL:HAA2	30:p:606:CHL:HBD	1.88	0.54
6:b:30:VAL:HG13	31:b:614:CLA:HMC2	1.89	0.54
43:c:614:BCR:H12C	38:s:301:SQD:H311	1.89	0.54
14:k:38:VAL:HG21	43:v:101:BCR:H19C	1.88	0.54
3:3:109:GLN:HA	3:3:114:ALA:O	2.07	0.54
31:A:405:CLA:H152	42:A:408:PHO:H11	1.89	0.54
31:A:406:CLA:HMB1	31:A:406:CLA:HBB1	1.90	0.54
6:B:75:TRP:HB2	6:B:94:GLU:HG3	1.90	0.54
6:B:413:ASP:N	6:B:413:ASP:OD1	2.41	0.54
31:N:305:CLA:HMA3	30:N:307:CHL:C3C	2.38	0.54
4:0:125:LYS:HG2	2:q:258:LEU:HD21	1.89	0.54
1:7:184:ASP:HA	32:7:317:LUT:H24	1.90	0.54
3:8:246:TRP:O	3:8:251:PRO:HD3	2.08	0.54
31:b:606:CLA:HMA3	31:b:607:CLA:H3A	1.90	0.54
33:b:628:LHG:H152	30:r:309:CHL:HBA2	1.88	0.54
31:c:612:CLA:CBB	34:c:620:LMG:H312	2.38	0.54
31:n:305:CLA:H121	31:s:306:CLA:H3A	1.90	0.54
31:n:311:CLA:H52	32:n:317:LUT:C30	2.37	0.54
34:w:202:LMG:C21	31:y:612:CLA:H141	2.38	0.54
31:y:604:CLA:HBB1	31:y:604:CLA:HMB3	1.89	0.54
4:6:202:LEU:CB	31:6:311:CLA:HMA2	2.37	0.54
5:A:221:SER:HA	8:D:139:ARG:HB2	1.89	0.54
2:G:198:ASP:N	2:G:198:ASP:OD1	2.32	0.54
3:N:250:ALA:N	3:N:251:PRO:HD2	2.23	0.54
31:N:313:CLA:H2	31:N:313:CLA:C4D	2.38	0.54
31:N:313:CLA:H192	31:N:314:CLA:C4C	2.38	0.54
1:7:134:TYR:CD2	1:7:135:LEU:HG	2.43	0.54
31:8:609:CLA:H52	32:8:615:LUT:C30	2.37	0.54
31:8:612:CLA:H202	31:8:613:CLA:CGA	2.38	0.54
3:p:215:MET:HA	3:p:218:PHE:HD2	1.72	0.54
5:a:82:ILE:HB	5:a:174:LEU:HB2	1.89	0.54
7:c:239:HIS:HE1	31:c:606:CLA:C1A	2.19	0.54
31:3:311:CLA:CBB	32:3:317:LUT:H32	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:4:620:LMG:H322	31:6:316:CLA:NC	2.22	0.54
3:5:221:GLN:O	3:5:225:THR:HG22	2.07	0.54
43:B:617:BCR:HC22	34:B:621:LMG:H321	1.88	0.54
2:G:150:GLN:HB2	30:G:605:CHL:CBB	2.37	0.54
2:G:228:LEU:HD11	34:G:622:LMG:H361	1.90	0.54
16:M:4:ASN:C	16:M:6:LEU:H	2.15	0.54
16:M:6:LEU:HD12	16:M:9:ILE:HD12	1.91	0.54
22:W:109:ARG:NH2	22:W:116:GLY:H	2.06	0.54
1:7:239:SER:OG	34:7:322:LMG:HC62	2.07	0.54
3:p:139:ASN:OD1	3:p:142:LEU:N	2.41	0.54
38:a:412:SQD:H262	34:a:413:LMG:H312	1.89	0.54
2:g:220:MET:HE2	32:g:316:LUT:H10	1.90	0.54
31:g:313:CLA:HBB1	31:g:313:CLA:HMB3	1.88	0.54
3:n:86:GLU:HA	3:n:179:LEU:HD21	1.90	0.54
18:r:137:LEU:HD12	18:r:211:CSU:HB2	1.89	0.54
31:r:311:CLA:HMA2	31:r:316:CLA:HHD	1.90	0.54
20:t:11:VAL:HG23	43:t:101:BCR:H14C	1.89	0.54
24:y:206:LEU:HB3	31:y:610:CLA:HMA2	1.89	0.54
30:y:606:CHL:HBB2	30:y:607:CHL:CBB	2.38	0.54
31:y:613:CLA:H111	33:y:619:LHG:H311	1.88	0.54
30:1:606:CHL:HAA2	30:1:606:CHL:HBD	1.90	0.53
3:3:109:GLN:HB2	3:3:116:PHE:HD1	1.72	0.53
3:3:223:LEU:HD23	31:3:301:CLA:C1B	2.38	0.53
3:5:39:GLU:O	3:5:45:ARG:HA	2.08	0.53
31:G:610:CLA:H3A	38:G:617:SQD:H441	1.90	0.53
18:R:169:TYR:OH	48:R:302:LMU:H4'	2.08	0.53
31:8:604:CLA:HMB1	31:8:604:CLA:HBB1	1.90	0.53
3:p:245:PHE:C	3:p:247:VAL:H	2.16	0.53
34:q:302:LMG:H132	34:q:302:LMG:C9	2.33	0.53
38:b:627:SQD:H5	8:d:134:ARG:HE	1.73	0.53
7:c:334:THR:OG1	7:c:336:GLU:OE1	2.25	0.53
18:r:69:GLY:HA2	18:r:71:ARG:NH2	2.23	0.53
3:5:92:ALA:HB1	3:5:208:GLY:HA3	1.89	0.53
31:B:614:CLA:H62	43:B:617:BCR:H20C	1.90	0.53
30:N:307:CHL:HMB1	30:N:309:CHL:HMC	1.90	0.53
31:7:315:CLA:C8	31:7:315:CLA:H2	2.38	0.53
31:p:610:CLA:H2	32:p:616:LUT:H26	1.91	0.53
31:p:614:CLA:HHC	31:p:614:CLA:CBB	2.37	0.53
2:q:109:GLU:HA	2:q:123:ALA:HB1	1.90	0.53
2:q:175:GLY:O	2:q:176:PRO:C	2.50	0.53
7:c:425:PHE:HA	31:c:608:CLA:HMC2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:c:619:DGD:HAV2	33:y:619:LHG:H351	1.90	0.53
8:d:266:TRP:HH2	33:l:101:LHG:H102	1.72	0.53
1:1:117:ILE:HD11	1:1:122:ALA:HA	1.90	0.53
1:1:189:ALA:HB1	1:1:195:LEU:HD13	1.90	0.53
2:2:229:VAL:HG22	2:2:257:PHE:CZ	2.43	0.53
3:3:118:GLU:HG2	3:3:124:ALA:HA	1.89	0.53
3:3:121:TRP:CH2	31:3:301:CLA:HBB2	2.43	0.53
45:C:617:DGD:HAS2	45:C:618:DGD:HAV2	1.90	0.53
34:C:624:LMG:H142	31:Y:311:CLA:HAB	1.90	0.53
22:W:93:TRP:CZ2	34:W:201:LMG:H112	2.43	0.53
30:7:321:CHL:CBB	31:8:603:CLA:HAC1	2.32	0.53
2:q:177:VAL:HA	2:q:189:PHE:CD1	2.43	0.53
2:q:178:GLU:HG2	2:q:189:PHE:CD1	2.38	0.53
5:a:106:LEU:HD11	43:a:410:BCR:H402	1.89	0.53
45:c:619:DGD:HE1	31:y:611:CLA:HMA2	1.90	0.53
2:g:76:GLY:HA3	24:y:86:LYS:HD2	1.88	0.53
26:u:56:ASP:OD1	26:u:56:ASP:N	2.42	0.53
1:1:139:GLY:HA2	1:1:142:ASN:HD21	1.73	0.53
30:2:607:CHL:H2	35:2:614:RRX:H12	1.89	0.53
31:3:304:CLA:H62	31:3:305:CLA:HMA3	1.89	0.53
2:4:147:ILE:HG23	30:4:605:CHL:C1D	2.39	0.53
3:5:249:TYR:HB3	3:5:258:TYR:CD2	2.44	0.53
3:5:254:ALA:O	3:5:256:ILE:HG22	2.08	0.53
31:5:603:CLA:H43	4:6:76:LEU:HD21	1.90	0.53
6:B:114:HIS:HE1	31:B:616:CLA:ND	2.01	0.53
2:G:205:LEU:HD23	2:G:208:LYS:HD2	1.89	0.53
2:G:251:PHE:HB3	24:Y:132:PHE:HZ	1.73	0.53
31:8:614:CLA:C4D	34:9:302:LMG:H292	2.39	0.53
31:p:612:CLA:HHC	31:p:612:CLA:CBB	2.36	0.53
9:e:13:ILE:HG21	47:e:102:HEM:HAD2	1.91	0.53
30:n:307:CHL:HAA2	30:n:307:CHL:HBD	1.89	0.53
30:n:308:CHL:HAA2	24:y:260:ALA:HB2	1.90	0.53
22:w:67:GLY:O	34:w:201:LMG:O5	2.25	0.53
31:1:611:CLA:H8	31:1:612:CLA:ND	2.22	0.53
2:4:170:ARG:HA	30:4:608:CHL:C3C	2.39	0.53
34:4:620:LMG:O7	34:4:621:LMG:H121	2.09	0.53
31:C:606:CLA:H52	34:W:201:LMG:H352	1.91	0.53
47:E:101:HEM:HBD2	47:E:101:HEM:HHA	1.90	0.53
31:N:314:CLA:HBA1	31:N:314:CLA:HBD	1.90	0.53
31:7:316:CLA:CHC	30:7:321:CHL:HMA2	2.38	0.53
3:8:86:GLU:HA	3:8:179:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:245:PHE:HB2	31:8:612:CLA:CAD	2.38	0.53
3:p:98:GLY:HA2	32:p:617:LUT:H181	1.89	0.53
8:d:136:VAL:HG12	8:d:138:ILE:HG23	1.90	0.53
48:r:302:LMU:H52	31:r:307:CLA:HAB	1.90	0.53
43:T:101:BCR:HC8	43:b:618:BCR:H341	1.90	0.53
31:7:316:CLA:C4D	34:9:301:LMG:H301	2.37	0.53
31:8:613:CLA:HMB1	31:8:613:CLA:HBB1	1.89	0.53
30:9:309:CHL:HAA1	30:9:309:CHL:HBD	1.91	0.53
3:p:240:PRO:HB2	31:p:614:CLA:CHB	2.38	0.53
30:p:606:CHL:HBB2	30:p:607:CHL:CBB	2.39	0.53
31:b:603:CLA:HBD	31:b:603:CLA:HBA2	1.91	0.53
34:c:621:LMG:H111	34:c:621:LMG:H292	1.91	0.53
26:u:112:LEU:HD21	26:u:128:LEU:HD13	1.89	0.53
34:Q1:101:LMG:HC71	34:Q1:101:LMG:O2	2.08	0.53
29:F1:178:LYS:HB3	29:F1:230:TRP:CZ2	2.43	0.53
31:2:602:CLA:HMC1	32:2:615:LUT:C32	2.38	0.53
3:3:109:GLN:HB2	3:3:116:PHE:CD1	2.43	0.53
3:3:216:LEU:HD23	31:3:305:CLA:HBB2	1.91	0.53
2:4:158:THR:HG21	30:4:606:CHL:HED3	1.90	0.53
7:C:175:ASP:OD2	7:C:185:ARG:NH2	2.22	0.53
12:I:25:SER:HB3	22:W:103:ILE:HD13	1.91	0.53
31:R:311:CLA:HMA2	31:R:316:CLA:HHD	1.90	0.53
24:Y:157:VAL:HG11	30:Y:307:CHL:HED2	1.91	0.53
30:9:310:CHL:CMB	36:9:319:NEX:H14	2.39	0.53
6:b:30:VAL:HG12	31:b:606:CLA:HHD	1.91	0.53
43:b:618:BCR:HC32	16:m:6:LEU:HB3	1.90	0.53
7:c:238:TRP:HA	34:c:624:LMG:H141	1.91	0.53
45:c:619:DGD:HAN2	45:c:619:DGD:HBE2	1.89	0.53
27:q1:6:GLY:HA3	34:q1:101:LMG:HC4	1.89	0.53
30:1:606:CHL:HBB2	30:1:607:CHL:HAB	1.90	0.53
2:2:99:MET:SD	31:2:609:CLA:HAB	2.48	0.53
31:2:610:CLA:H2	31:2:611:CLA:HMD2	1.90	0.53
3:5:188:LEU:HD12	32:5:616:LUT:H222	1.89	0.53
3:5:252:LYS:HA	3:5:256:ILE:CG2	2.36	0.53
38:M:102:SQD:H112	31:b:615:CLA:H42	1.90	0.53
19:S:102:ALA:HA	19:S:210:LEU:HD11	1.90	0.53
31:Y:303:CLA:H101	32:Y:316:LUT:H371	1.91	0.53
2:9:49:TRP:CE2	2:9:50:LEU:HG	2.44	0.53
34:9:321:LMG:H112	34:9:321:LMG:H322	1.91	0.53
2:q:135:GLU:O	2:q:136:ASP:C	2.52	0.53
5:a:84:PRO:HA	5:a:112:TYR:CG	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:a:414:PL9:H453	8:d:39:PRO:HA	1.91	0.53
6:b:114:HIS:HE1	31:b:617:CLA:ND	2.04	0.53
6:b:161:LEU:HD22	33:b:628:LHG:H242	1.91	0.53
9:e:44:TYR:HE2	29:f1:53:ALA:HB2	1.74	0.53
31:g:305:CLA:HMA3	30:g:307:CHL:C2C	2.38	0.53
3:n:245:PHE:HB2	31:n:314:CLA:CAD	2.38	0.53
19:s:278:THR:HG22	38:s:301:SQD:H1	1.89	0.53
2:2:229:VAL:HA	2:2:257:PHE:HZ	1.73	0.53
31:2:609:CLA:H3A	31:2:609:CLA:C1	2.38	0.53
2:4:49:TRP:HE3	30:4:601:CHL:HAA1	1.72	0.53
7:C:144:LYS:HD3	34:C:621:LMG:HC61	1.91	0.53
31:G:604:CLA:HBB1	31:G:604:CLA:HMB3	1.91	0.53
4:0:67:GLY:HA3	4:0:207:ILE:HG21	1.91	0.53
3:8:236:HIS:CA	3:8:243:THR:HG21	2.29	0.53
31:9:313:CLA:C4D	31:9:314:CLA:HMD3	2.38	0.53
34:9:321:LMG:H292	34:9:321:LMG:C1	2.39	0.53
2:q:97:TRP:CD1	30:q:311:CHL:HMD3	2.44	0.53
2:q:107:THR:N	2:q:108:PRO:HD2	2.24	0.53
7:c:166:LYS:HA	7:c:170:PHE:HB2	1.91	0.53
13:j:28:GLY:HA2	34:j:101:LMG:H171	1.91	0.53
3:n:233:LEU:HD22	32:n:317:LUT:H163	1.91	0.53
31:n:314:CLA:H172	31:n:315:CLA:C1D	2.39	0.53
18:r:123:TYR:OH	18:r:134:GLU:OE1	2.21	0.53
31:y:610:CLA:H62	31:y:612:CLA:CMA	2.38	0.53
31:1:603:CLA:HAC2	30:1:607:CHL:H193	1.91	0.53
3:5:40:TRP:CE3	3:5:46:PRO:HG3	2.44	0.53
30:G:623:CHL:H121	30:Y:309:CHL:H112	1.91	0.53
24:Y:94:HIS:HE1	31:Y:304:CLA:C4D	2.22	0.53
30:7:308:CHL:HMB1	30:7:308:CHL:H101	1.91	0.53
2:9:140:TYR:HB2	2:9:147:ILE:HD12	1.91	0.53
31:9:304:CLA:H52	32:9:318:LUT:H28	1.91	0.53
30:9:308:CHL:HAA2	30:9:308:CHL:HBD	1.91	0.53
3:p:125:GLY:O	3:p:128:ILE:HG22	2.09	0.53
31:p:614:CLA:H2	31:p:614:CLA:HBA2	1.91	0.53
5:a:283:ILE:HA	5:a:286:THR:HG22	1.91	0.53
31:1:614:CLA:HBA1	31:1:614:CLA:CHA	2.32	0.52
5:A:84:PRO:HA	5:A:112:TYR:CG	2.44	0.52
8:D:46:GLY:HA2	43:D:405:BCR:H11C	1.90	0.52
31:G:612:CLA:C11	37:G:620:XAT:H34	2.39	0.52
38:G:617:SQD:H61	38:G:617:SQD:O6	2.09	0.52
31:7:316:CLA:C4C	34:9:301:LMG:H341	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:7:321:CHL:HMC	3:8:155:GLN:OE1	2.09	0.52
30:9:310:CHL:HAB	36:9:319:NEX:H10	1.90	0.52
31:b:610:CLA:HMA3	31:b:611:CLA:C1C	2.39	0.52
43:b:619:BCR:HC41	34:b:622:LMG:H322	1.90	0.52
20:t:3:ALA:O	20:t:7:THR:HG23	2.08	0.52
22:w:86:THR:CG2	34:w:202:LMG:H221	2.39	0.52
1:1:198:LEU:HB3	31:1:610:CLA:CMA	2.39	0.52
34:3:321:LMG:C10	34:3:321:LMG:H141	2.39	0.52
6:B:39:PHE:CD1	34:m:102:LMG:HC92	2.44	0.52
6:B:216:HIS:HE1	31:B:609:CLA:NA	1.96	0.52
3:N:123:LYS:HA	30:Y:301:CHL:HED3	1.91	0.52
4:0:164:ILE:CD1	36:0:618:NEX:C34	2.88	0.52
3:p:89:VAL:HB	3:p:179:LEU:HD21	1.92	0.52
3:p:120:VAL:CG2	3:p:123:LYS:HB2	2.36	0.52
30:q:309:CHL:H8	30:q:309:CHL:C1C	2.39	0.52
31:b:612:CLA:C3B	31:b:614:CLA:HMA2	2.39	0.52
7:c:118:VAL:HG12	25:z:27:LEU:HD12	1.91	0.52
30:g:302:CHL:H11	30:y:609:CHL:C1B	2.39	0.52
18:r:139:HIS:HE1	31:r:305:CLA:C4D	2.22	0.52
18:r:223:ALA:HB1	18:r:230:THR:HG23	1.92	0.52
31:S:305:CLA:H52	30:S:307:CHL:HBA2	1.90	0.52
31:8:603:CLA:H2	31:8:603:CLA:HED2	1.91	0.52
7:c:68:PRO:HG2	7:c:71:GLU:HG3	1.91	0.52
45:c:619:DGD:O3E	34:c:624:LMG:HC5	2.10	0.52
8:d:239:GLN:OE1	28:p1:50:TYR:OH	2.23	0.52
34:s:321:LMG:O5	34:s:321:LMG:O4	2.23	0.52
31:y:604:CLA:HMA3	30:y:606:CHL:C3C	2.40	0.52
31:2:603:CLA:HHC	31:2:603:CLA:CBB	2.33	0.52
3:3:147:SER:HB2	34:3:321:LMG:H321	1.91	0.52
4:6:98:MET:SD	31:6:311:CLA:HAB	2.49	0.52
31:C:606:CLA:H92	31:C:607:CLA:H193	1.92	0.52
33:S:322:LHG:H161	33:S:322:LHG:H262	1.92	0.52
4:0:131:PHE:HZ	2:q:251:PHE:HB3	1.75	0.52
2:q:165:ALA:O	2:q:168:ALA:N	2.42	0.52
33:g:319:LHG:H312	37:g:321:XAT:C34	2.40	0.52
3:n:155:GLN:OE1	30:n:308:CHL:HMC	2.09	0.52
30:1:609:CHL:HAA2	2:2:74:THR:HG21	1.91	0.52
3:3:165:TYR:HB3	30:3:309:CHL:CMC	2.39	0.52
3:5:163:GLU:O	3:5:167:VAL:HG13	2.10	0.52
31:B:615:CLA:H2	31:B:616:CLA:CBB	2.39	0.52
7:C:320:GLN:HG2	17:O:157:TYR:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:604:CLA:HMA3	30:G:606:CHL:C3C	2.39	0.52
3:N:142:LEU:O	3:N:144:HIS:N	2.41	0.52
24:Y:90:ILE:HG21	31:Y:304:CLA:HAA2	1.91	0.52
31:8:602:CLA:H92	31:9:305:CLA:H52	1.90	0.52
5:a:93:PHE:HZ	31:a:409:CLA:HAA1	1.75	0.52
3:n:175:GLY:HA3	19:s:33:VAL:HA	1.91	0.52
31:r:306:CLA:CHA	31:r:306:CLA:HBA1	2.38	0.52
3:3:143:ILE:HD12	3:3:145:ALA:H	1.74	0.52
30:5:605:CHL:HAA1	30:5:605:CHL:HBD	1.91	0.52
34:A:412:LMG:HC72	7:C:204:SER:HB2	1.90	0.52
7:C:195:GLY:HA3	34:W:203:LMG:HC2	1.91	0.52
31:C:613:CLA:HBA1	31:C:613:CLA:HBD	1.90	0.52
8:D:148:ALA:HB2	8:D:276:VAL:HG13	1.90	0.52
36:N:318:NEX:H10	19:S:39:TRP:CZ3	2.44	0.52
3:8:233:LEU:HD22	32:8:615:LUT:H163	1.91	0.52
30:8:606:CHL:HMB2	30:8:608:CHL:HMC	1.91	0.52
3:p:233:LEU:HA	31:p:613:CLA:HMA3	1.91	0.52
6:b:53:ASN:HD21	6:b:331:ASN:ND2	2.05	0.52
31:n:314:CLA:H71	31:n:315:CLA:HMD3	1.92	0.52
2:2:185:TYR:HB3	31:2:609:CLA:HED3	1.91	0.52
30:4:607:CHL:HBB2	30:4:609:CHL:HBC1	1.91	0.52
4:6:193:ALA:HB1	4:6:199:LEU:HD13	1.92	0.52
31:6:311:CLA:H51	32:6:317:LUT:C30	2.37	0.52
38:A:413:SQD:H441	6:b:75:TRP:CE2	2.45	0.52
2:G:90:ILE:HG21	31:G:603:CLA:HAA2	1.91	0.52
2:9:176:PRO:HD2	30:9:310:CHL:HBB2	1.91	0.52
31:q:313:CLA:C4D	31:q:314:CLA:HMD3	2.39	0.52
5:a:50:ILE:HD12	34:m:102:LMG:H161	1.91	0.52
31:d:405:CLA:CHA	31:d:405:CLA:HBA1	2.40	0.52
31:g:305:CLA:HMA3	30:g:307:CHL:C3C	2.40	0.52
4:6:173:PRO:HB3	18:R:54:LEU:HG	1.92	0.52
31:6:304:CLA:HHC	31:6:304:CLA:HBB1	1.90	0.52
9:E:24:SER:O	9:E:28:PRO:HG2	2.10	0.52
31:G:609:CLA:HBA1	35:G:614:RRX:H7	1.91	0.52
3:N:246:TRP:O	3:N:250:ALA:HB3	2.09	0.52
18:R:120:LEU:O	31:R:316:CLA:ND	2.42	0.52
4:0:122:VAL:HG23	4:0:125:LYS:HB2	1.92	0.52
2:9:59:PRO:HD2	2:9:62:LEU:HD12	1.91	0.52
3:p:218:PHE:CD1	3:p:229:PRO:HB3	2.44	0.52
31:b:615:CLA:H171	43:b:618:BCR:C12	2.40	0.52
7:c:205:PRO:HD3	34:w:201:LMG:H332	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:c:617:DGD:HBG1	43:d:406:BCR:H402	1.91	0.52
31:y:604:CLA:H91	34:y:620:LMG:H372	1.91	0.52
1:1:179:PRO:HD2	31:1:610:CLA:OBD	2.09	0.52
31:1:612:CLA:CMD	38:g:301:SQD:H251	2.40	0.52
2:2:164:GLY:HA2	30:2:608:CHL:CAB	2.40	0.52
31:5:603:CLA:H2	31:5:603:CLA:H2A	1.92	0.52
5:A:64:ARG:O	17:O:198:ARG:NH2	2.42	0.52
7:C:41:HIS:CD2	31:C:609:CLA:NA	2.77	0.52
2:G:95:ALA:HB1	2:G:213:GLY:HA3	1.91	0.52
2:G:221:PHE:CD2	31:G:612:CLA:HAC1	2.43	0.52
3:N:240:PRO:HG3	31:N:314:CLA:HMB2	1.91	0.52
31:N:313:CLA:H122	31:N:314:CLA:HMD3	1.92	0.52
31:0:610:CLA:H51	32:0:616:LUT:H30	1.90	0.52
2:q:140:TYR:CE2	31:q:306:CLA:H2	2.44	0.52
5:a:131:TRP:CH2	31:c:605:CLA:HAA2	2.45	0.52
9:e:74:GLU:O	9:e:78:LYS:HG2	2.10	0.52
18:r:174:TYR:CD1	31:r:306:CLA:H2	2.45	0.52
26:u:113:ASP:N	26:u:113:ASP:OD1	2.38	0.52
29:F1:196:LEU:HB3	29:F1:230:TRP:CD2	2.45	0.52
29:f1:129:LEU:HD11	29:f1:136:PHE:HZ	1.75	0.52
3:3:219:GLY:HA2	31:3:301:CLA:HBB2	1.90	0.52
3:3:239:ALA:HB1	3:3:242:ALA:HB3	1.92	0.52
2:4:122:ALA:O	2:4:128:ALA:HB2	2.10	0.52
2:4:169:TYR:HB3	2:4:174:GLU:HG3	1.92	0.52
3:5:222:GLY:O	31:6:316:CLA:HMB3	2.09	0.52
42:A:408:PHO:H202	44:D:406:PL9:H453	1.92	0.52
2:G:76:GLY:N	24:Y:86:LYS:HD2	2.25	0.52
3:N:131:GLU:OE1	3:N:132:GLY:N	2.41	0.52
3:N:239:ALA:O	3:N:243:THR:HG22	2.10	0.52
1:7:86:ARG:HD3	2:9:74:THR:O	2.10	0.52
30:7:307:CHL:HBB2	30:7:308:CHL:CAB	2.40	0.52
31:8:612:CLA:H71	31:8:613:CLA:HMD3	1.91	0.52
3:p:218:PHE:HD1	3:p:229:PRO:HB3	1.75	0.52
5:a:192:ILE:HG13	5:a:293:MET:HE1	1.92	0.52
6:b:454:ALA:HB2	34:b:622:LMG:H181	1.91	0.52
34:b:601:LMG:H371	43:b:619:BCR:H371	1.91	0.52
31:b:615:CLA:HBB1	31:b:615:CLA:HMB3	1.91	0.52
30:r:309:CHL:HAA1	30:r:309:CHL:CBD	2.40	0.52
29:F1:105:ASN:HD22	29:F1:213:CYS:HA	1.75	0.52
1:1:59:PRO:HG2	1:1:62:LEU:HD12	1.91	0.51
1:1:78:SER:OG	31:1:602:CLA:O1A	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:165:VAL:CG1	2:2:57:SER:HB3	2.40	0.51
1:1:245:ALA:HB3	1:1:246:LEU:HD13	1.91	0.51
2:2:238:LEU:O	2:2:242:LEU:HG	2.09	0.51
3:3:253:SER:OG	30:3:302:CHL:HBA1	2.10	0.51
32:3:318:LUT:H191	32:3:318:LUT:C12	2.40	0.51
2:4:206:LYS:O	2:4:209:GLU:HB3	2.10	0.51
3:5:45:ARG:HG3	3:5:66:ASP:O	2.11	0.51
3:5:89:VAL:HG22	3:5:205:LEU:HD21	1.91	0.51
4:6:161:MET:HE3	36:6:319:NEX:H31	1.92	0.51
4:6:229:LYS:HB3	4:6:233:GLN:HG2	1.91	0.51
6:B:91:TRP:HE1	34:B:622:LMG:HC91	1.74	0.51
8:D:304:ARG:NH1	16:M:-3:UNK:O	2.43	0.51
2:G:235:LEU:HD22	34:G:619:LMG:HC91	1.91	0.51
33:M:101:LHG:HC62	20:T:1:MET:HB2	1.92	0.51
31:Y:305:CLA:HBB1	31:Y:305:CLA:HMB3	1.92	0.51
31:8:614:CLA:H43	2:9:257:PHE:CD1	2.45	0.51
2:9:49:TRP:CE3	30:9:303:CHL:HAA1	2.45	0.51
2:9:147:ILE:HA	30:9:307:CHL:C4D	2.40	0.51
3:p:187:PRO:HD2	32:p:616:LUT:H23	1.93	0.51
3:p:245:PHE:C	3:p:247:VAL:N	2.68	0.51
30:p:607:CHL:HBA1	30:p:607:CHL:CBD	2.40	0.51
31:p:610:CLA:H12	31:p:610:CLA:H3A	1.92	0.51
6:b:247:TRP:HB2	31:b:609:CLA:HBC1	1.92	0.51
9:e:2:SER:OG	28:p1:63:TYR:O	2.27	0.51
9:e:27:ILE:HB	9:e:28:PRO:HD3	1.92	0.51
1:1:49:PHE:HD2	30:1:601:CHL:HAA1	1.74	0.51
31:1:611:CLA:H101	31:1:612:CLA:NB	2.25	0.51
2:2:146:LEU:HD23	30:2:605:CHL:HED3	1.92	0.51
3:3:215:MET:HE2	32:3:318:LUT:C10	2.39	0.51
3:3:227:LYS:HB2	3:3:232:ASN:OD1	2.10	0.51
3:5:145:ALA:HA	30:5:605:CHL:CHC	2.40	0.51
45:C:620:DGD:HBW1	31:Y:312:CLA:HBC3	1.92	0.51
9:E:26:THR:HB	47:E:101:HEM:CAB	2.40	0.51
3:N:58:TYR:HD1	3:N:59:LEU:HD13	1.74	0.51
31:N:314:CLA:C2	31:N:314:CLA:HAA2	2.40	0.51
18:R:184:TYR:CE1	48:R:302:LMU:H21	2.46	0.51
31:S:311:CLA:H51	32:S:317:LUT:H373	1.93	0.51
33:S:320:LHG:H282	33:S:320:LHG:HC92	1.91	0.51
24:Y:100:LEU:HB3	31:Y:305:CLA:HAB	1.91	0.51
31:Y:310:CLA:H62	31:Y:312:CLA:CMA	2.39	0.51
30:7:308:CHL:H101	30:7:308:CHL:CMB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:63:LYS:NZ	2:9:63:LYS:HB2	2.25	0.51
31:p:604:CLA:NB	36:p:618:NEX:H242	2.25	0.51
31:p:613:CLA:CGA	31:p:613:CLA:C1A	2.88	0.51
5:a:307:VAL:HG23	10:f:44:ARG:HD2	1.91	0.51
43:b:618:BCR:H12C	34:b:622:LMG:H421	1.91	0.51
18:r:75:PRO:HD2	37:r:318:XAT:H242	1.92	0.51
18:r:233:LEU:HB3	31:r:312:CLA:HMA2	1.93	0.51
1:1:73:ASP:HA	32:1:616:LUT:H24	1.92	0.51
30:5:606:CHL:HAB	32:5:617:LUT:H161	1.93	0.51
30:6:308:CHL:HBB2	30:6:310:CHL:HBC1	1.92	0.51
7:C:239:HIS:HE1	31:C:606:CLA:C1A	2.23	0.51
8:D:279:LEU:HD11	42:D:401:PHO:HMC3	1.92	0.51
2:G:257:PHE:CE1	31:N:315:CLA:H43	2.45	0.51
17:O:72:ASN:O	17:O:131:THR:HG21	2.10	0.51
4:0:222:ILE:HG13	31:0:613:CLA:HAC2	1.93	0.51
33:p:619:LHG:O10	33:p:619:LHG:H272	2.11	0.51
2:q:100:LEU:HG	31:q:312:CLA:HMC3	1.92	0.51
45:c:616:DGD:HAH1	45:c:616:DGD:HA82	1.91	0.51
38:g:301:SQD:C9	37:g:321:XAT:H222	2.36	0.51
31:g:311:CLA:HMA2	38:g:318:SQD:H61	1.92	0.51
2:4:163:MET:HE3	30:4:606:CHL:HMB3	1.93	0.51
2:4:186:PRO:HD2	31:4:610:CLA:OBD	2.10	0.51
4:6:248:TYR:HA	4:6:252:ALA:HB2	1.93	0.51
2:G:130:ALA:HA	2:G:133:PHE:HD1	1.75	0.51
34:I:101:LMG:H322	22:W:84:ALA:HA	1.92	0.51
31:7:304:CLA:HHC	31:7:304:CLA:CBB	2.40	0.51
3:p:216:LEU:HB2	32:p:617:LUT:H402	1.93	0.51
31:p:614:CLA:O1A	2:q:157:LEU:HD21	2.11	0.51
2:q:72:TRP:O	32:q:318:LUT:H24	2.10	0.51
6:b:399:VAL:HG23	6:b:417:VAL:HG22	1.90	0.51
33:b:625:LHG:HC91	33:l:101:LHG:HC81	1.92	0.51
30:n:301:CHL:HMA3	31:n:316:CLA:CAB	2.40	0.51
30:n:310:CHL:HBA2	30:y:601:CHL:H12	1.92	0.51
22:w:86:THR:HG23	34:w:202:LMG:H442	1.91	0.51
3:3:200:LEU:HB3	31:3:311:CLA:HMA2	1.92	0.51
3:5:136:TYR:HD1	3:5:142:LEU:HD13	1.75	0.51
8:D:193:LEU:O	15:L:35:TYR:OH	2.24	0.51
2:G:171:TYR:CD2	3:N:49:LEU:HD12	2.45	0.51
30:S:307:CHL:HAA2	30:S:307:CHL:HBD	1.93	0.51
31:8:602:CLA:H61	32:8:616:LUT:H28	1.91	0.51
31:8:609:CLA:H8	32:8:615:LUT:C30	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:195:LEU:HB2	31:9:312:CLA:O1A	2.10	0.51
3:p:232:ASN:HB3	31:p:613:CLA:HED1	1.92	0.51
31:q:306:CLA:H2A	31:q:306:CLA:HED3	1.92	0.51
30:q:308:CHL:CBB	30:q:309:CHL:CBB	2.87	0.51
5:a:28:LEU:HB2	34:a:401:LMG:C29	2.40	0.51
7:c:26:GLY:HA3	31:c:611:CLA:HMD2	1.92	0.51
44:d:407:PL9:H421	33:d:408:LHG:H222	1.92	0.51
3:n:146:GLN:HB2	30:n:306:CHL:CBB	2.41	0.51
31:n:314:CLA:H202	31:n:315:CLA:CGA	2.40	0.51
3:3:118:GLU:HB3	3:3:124:ALA:HA	1.92	0.51
3:3:136:TYR:CD1	3:3:137:LEU:HG	2.45	0.51
3:3:162:ILE:HD11	36:3:319:NEX:C34	2.40	0.51
3:3:246:TRP:HZ3	30:3:302:CHL:CHD	2.24	0.51
2:4:103:LEU:HG	35:4:615:RRX:H28	1.92	0.51
3:5:143:ILE:N	30:5:605:CHL:O1D	2.43	0.51
3:5:161:LEU:HD13	36:5:618:NEX:H11	1.93	0.51
30:5:601:CHL:HBD	30:5:601:CHL:HAA1	1.92	0.51
43:B:617:BCR:H383	38:B:620:SQD:H121	1.91	0.51
31:C:603:CLA:H161	31:C:610:CLA:HBB2	1.93	0.51
9:E:45:ASP:OD2	27:Q1:4:ARG:NH2	2.38	0.51
30:G:606:CHL:HBB1	32:G:615:LUT:H161	1.92	0.51
30:G:623:CHL:H171	31:Y:304:CLA:HAC2	1.91	0.51
31:N:310:CLA:H62	31:N:312:CLA:HMA3	1.93	0.51
19:S:158:ASN:OD1	19:S:159:PHE:N	2.40	0.51
31:0:615:CLA:C1C	34:q:301:LMG:H341	2.40	0.51
3:p:109:GLN:HB3	3:p:110:ARG:HD3	1.92	0.51
6:b:464:PHE:CZ	33:b:625:LHG:H252	2.46	0.51
7:c:151:ILE:HG12	34:c:620:LMG:H322	1.93	0.51
45:c:619:DGD:C1D	31:y:611:CLA:HBA1	2.40	0.51
2:g:121:GLU:HB3	2:g:127:LYS:HE2	1.93	0.51
31:n:314:CLA:H192	31:n:315:CLA:C4C	2.39	0.51
18:r:62:TRP:CZ2	18:r:77:GLY:HA2	2.46	0.51
30:s:307:CHL:HBB2	30:s:308:CHL:CBB	2.41	0.51
22:w:100:THR:OG1	34:w:202:LMG:HC5	2.10	0.51
34:q1:101:LMG:H152	34:q1:101:LMG:H361	1.93	0.51
28:p1:34:LYS:HG2	28:p1:46:GLY:CA	2.40	0.51
31:3:315:CLA:H62	31:3:315:CLA:NB	2.26	0.51
3:5:86:GLU:HA	3:5:179:LEU:HD21	1.93	0.51
31:B:614:CLA:H72	38:m:101:SQD:H141	1.93	0.51
38:B:620:SQD:H192	38:B:620:SQD:H362	1.92	0.51
7:C:302:THR:HG21	7:C:343:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:449:ARG:NH2	8:D:241:GLU:HB2	2.26	0.51
33:D:408:LHG:H271	15:L:23:LEU:HD22	1.93	0.51
31:N:313:CLA:HBB1	32:N:316:LUT:H8	1.92	0.51
1:7:90:ILE:HD13	31:7:304:CLA:HBA1	1.92	0.51
1:7:134:TYR:CE1	31:7:305:CLA:H2	2.46	0.51
1:7:179:PRO:HD2	31:7:311:CLA:OBD	2.10	0.51
2:9:54:SER:O	2:9:58:VAL:HG23	2.10	0.51
2:q:179:THR:H	2:q:189:PHE:HB2	1.76	0.51
34:g:322:LMG:H292	31:y:615:CLA:HBD	1.93	0.51
30:1:607:CHL:C1	2:2:259:PRO:HD3	2.41	0.51
2:2:153:VAL:O	2:2:157:LEU:HG	2.10	0.51
3:3:165:TYR:HB3	30:3:309:CHL:C2C	2.40	0.51
3:3:225:THR:O	3:3:227:LYS:HD3	2.11	0.51
2:4:140:TYR:CD1	2:4:146:LEU:HG	2.45	0.51
3:5:176:LEU:HB3	3:5:181:PRO:HA	1.93	0.51
5:A:57:PRO:HD3	5:A:73:TYR:CE2	2.46	0.51
33:A:415:LHG:H152	33:A:415:LHG:H101	1.92	0.51
7:C:146:THR:HG21	7:C:244:PRO:HD3	1.91	0.51
8:D:91:PHE:CE1	31:D:404:CLA:HAA1	2.46	0.51
3:8:146:GLN:HB2	30:8:605:CHL:CBB	2.41	0.51
2:9:260:LEU:HD12	34:9:301:LMG:HC62	1.92	0.51
2:q:186:PRO:O	31:q:312:CLA:HED3	2.11	0.51
2:g:205:LEU:HB3	31:g:310:CLA:CMA	2.39	0.51
31:g:311:CLA:HBD	31:g:311:CLA:HBA1	1.92	0.51
33:l:101:LHG:H251	33:l:101:LHG:HC91	1.92	0.51
1:1:106:VAL:HG13	1:1:228:ILE:HD11	1.92	0.51
31:3:305:CLA:HBD	31:3:305:CLA:HBA2	1.92	0.51
2:4:132:ILE:HD13	30:4:606:CHL:HMD3	1.91	0.51
31:4:613:CLA:HBB1	31:4:613:CLA:HHC	1.92	0.51
3:5:91:HIS:HE1	31:5:603:CLA:ND	2.08	0.51
3:5:158:LEU:HA	36:5:618:NEX:H201	1.91	0.51
31:5:610:CLA:O2A	32:5:616:LUT:H221	2.10	0.51
30:6:307:CHL:CBB	30:6:310:CHL:HBC1	2.41	0.51
7:C:136:GLY:O	7:C:144:LYS:NZ	2.39	0.51
2:G:126:PHE:HB2	30:N:301:CHL:HMA3	1.92	0.51
30:G:606:CHL:CBB	32:G:615:LUT:H161	2.41	0.51
3:N:197:PHE:CZ	3:N:201:LYS:HD3	2.46	0.51
24:Y:239:LEU:HD22	32:Y:315:LUT:H163	1.91	0.51
3:p:200:LEU:HB2	31:p:610:CLA:HMA2	1.91	0.51
3:p:243:THR:O	3:p:244:ASN:C	2.53	0.51
2:q:143:ASN:HB3	2:q:146:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c:602:CLA:H62	31:c:603:CLA:NB	2.26	0.51
18:r:183:ILE:CG2	48:r:302:LMU:H3'	2.40	0.51
24:y:166:GLU:HG3	30:y:609:CHL:C4B	2.41	0.51
27:q1:4:ARG:NH1	29:f1:50:GLY:HA2	2.26	0.51
1:1:231:LEU:HD21	31:1:614:CLA:HMC2	1.92	0.51
31:3:306:CLA:HBB1	32:3:318:LUT:H8	1.93	0.51
2:4:61:TYR:OH	2:4:76:GLY:HA2	2.11	0.51
3:5:64:PRO:HB2	3:5:205:LEU:CD1	2.41	0.51
4:6:182:TYR:HB3	31:6:311:CLA:HED3	1.92	0.51
5:A:82:ILE:HB	5:A:174:LEU:HB2	1.91	0.51
7:C:413:TRP:CD1	31:C:604:CLA:HMA2	2.46	0.51
34:C:622:LMG:HC92	34:N:320:LMG:HC4	1.92	0.51
31:G:603:CLA:C1C	30:G:608:CHL:H111	2.41	0.51
19:S:246:PHE:CZ	32:S:318:LUT:H10	2.46	0.51
26:U:56:ASP:OD1	26:U:56:ASP:N	2.43	0.51
4:0:229:LYS:HE3	4:0:234:ASN:ND2	2.26	0.51
1:7:73:ASP:HA	32:7:318:LUT:H24	1.93	0.51
31:9:306:CLA:H12	30:9:308:CHL:CAD	2.41	0.51
2:q:143:ASN:HD22	34:q1:101:LMG:H362	1.76	0.51
6:b:466:HIS:HE1	31:b:609:CLA:C4D	2.23	0.51
31:g:313:CLA:H172	31:g:314:CLA:HBD	1.92	0.51
17:o:107:LYS:NZ	17:o:117:ALA:O	2.44	0.51
31:s:314:CLA:H91	33:s:320:LHG:H301	1.93	0.51
34:4:620:LMG:H112	34:4:621:LMG:H122	1.93	0.50
31:B:606:CLA:H61	43:B:619:BCR:H311	1.91	0.50
2:G:192:PRO:HD2	35:G:614:RRX:H14	1.94	0.50
15:L:24:LEU:O	15:L:28:LEU:HB2	2.12	0.50
30:Y:301:CHL:H161	30:Y:302:CHL:H52	1.93	0.50
31:q:306:CLA:HMA3	30:q:308:CHL:C2C	2.41	0.50
7:c:432:HIS:HE1	31:c:608:CLA:NA	2.04	0.50
31:c:613:CLA:HMC2	43:c:614:BCR:H20C	1.93	0.50
15:l:21:GLY:O	15:l:25:ILE:HG12	2.12	0.50
3:5:203:LYS:HD3	31:5:612:CLA:CGA	2.41	0.50
5:A:278:TRP:HB3	5:A:279:PRO:HD3	1.91	0.50
6:B:462:PHE:HA	31:B:611:CLA:HMC2	1.92	0.50
38:B:620:SQD:H372	43:t:101:BCR:C36	2.39	0.50
14:K:17:PRO:HB2	33:K:102:LHG:H241	1.92	0.50
17:O:122:THR:HG22	17:O:164:LEU:HD23	1.93	0.50
19:S:224:ASP:HB3	19:S:227:VAL:HB	1.93	0.50
30:0:608:CHL:HAA1	30:0:608:CHL:HBD	1.94	0.50
34:0:620:LMG:H122	34:7:301:LMG:HC91	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:8:601:CHL:HED2	33:8:618:LHG:H122	1.92	0.50
2:9:49:TRP:CZ3	30:9:303:CHL:HAA1	2.45	0.50
3:p:109:GLN:HA	3:p:114:ALA:HB3	1.92	0.50
34:b:629:LMG:H112	34:r:321:LMG:H291	1.91	0.50
8:d:199:MET:HG2	44:d:407:PL9:H321	1.93	0.50
43:t:101:BCR:H23C	43:t:101:BCR:C38	2.41	0.50
1:1:224:GLY:HA3	2:2:261:PRO:HA	1.92	0.50
31:1:611:CLA:CAB	38:g:318:SQD:H241	2.37	0.50
31:2:610:CLA:H61	31:2:611:CLA:C3D	2.41	0.50
3:3:38:VAL:HA	3:3:42:GLY:N	2.25	0.50
30:3:309:CHL:HMB2	36:3:319:NEX:H14	1.94	0.50
7:C:154:ILE:HG22	34:C:621:LMG:H361	1.93	0.50
43:D:405:BCR:H373	10:F:33:LEU:HD21	1.93	0.50
2:G:86:ARG:NE	2:G:86:ARG:HA	2.26	0.50
30:G:601:CHL:HED3	33:G:618:LHG:H291	1.93	0.50
16:M:17:ILE:HB	16:M:18:PRO:HD3	1.92	0.50
30:N:301:CHL:HMA2	31:N:315:CLA:C3B	2.41	0.50
31:N:314:CLA:HBA1	31:N:314:CLA:CBD	2.41	0.50
31:R:306:CLA:HBA1	31:R:306:CLA:CHA	2.40	0.50
19:S:87:PRO:HD2	32:S:318:LUT:H23	1.93	0.50
1:7:231:LEU:HB2	32:7:317:LUT:H22	1.93	0.50
31:8:603:CLA:HBC1	30:8:608:CHL:HAC2	1.92	0.50
2:9:108:PRO:HB2	2:9:123:ALA:HA	1.93	0.50
30:q:303:CHL:ND	33:q:320:LHG:HC81	2.26	0.50
31:a:409:CLA:HMA2	45:c:616:DGD:CDB	2.41	0.50
8:d:291:LEU:HB2	8:d:293:LEU:HD23	1.92	0.50
30:n:302:CHL:HED2	33:n:320:LHG:H122	1.92	0.50
31:n:304:CLA:HBC1	30:n:310:CHL:HAC2	1.91	0.50
18:r:71:ARG:HD2	31:r:303:CLA:HED3	1.93	0.50
29:F1:197:ILE:C	29:F1:230:TRP:HE1	2.19	0.50
3:3:94:TRP:CE2	30:3:309:CHL:HED3	2.46	0.50
3:5:116:PHE:CZ	3:5:137:LEU:HD23	2.47	0.50
3:5:151:ILE:CD1	30:5:605:CHL:HAC1	2.41	0.50
3:5:162:ILE:HD11	36:5:618:NEX:C34	2.41	0.50
5:A:210:LEU:HD23	5:A:214:MET:HG3	1.92	0.50
31:B:605:CLA:HMA3	31:B:606:CLA:H3A	1.94	0.50
7:C:36:LYS:HE2	7:C:126:GLU:HG3	1.93	0.50
2:G:47:ALA:HB1	30:G:601:CHL:HBC1	1.93	0.50
31:G:603:CLA:HBB1	31:G:603:CLA:HHC	1.94	0.50
19:S:123:GLY:O	19:S:127:ASN:ND2	2.28	0.50
24:Y:90:ILE:HD13	31:Y:304:CLA:HBA1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:142:ASN:HD22	34:Y:319:LMG:H292	1.76	0.50
30:Y:301:CHL:H121	30:Y:301:CHL:C9	2.41	0.50
1:7:80:ASP:OD1	1:7:80:ASP:N	2.41	0.50
30:7:307:CHL:O2A	36:r:301:NEX:H403	2.11	0.50
31:p:613:CLA:HMB2	31:p:613:CLA:H43	1.93	0.50
5:a:15:ALA:O	5:a:19:GLU:HG2	2.11	0.50
30:n:308:CHL:H2	30:y:601:CHL:H152	1.93	0.50
2:2:178:GLU:HB3	2:2:188:GLY:C	2.36	0.50
34:3:321:LMG:H332	34:3:321:LMG:HC72	1.93	0.50
3:5:69:TRP:HZ3	31:5:602:CLA:HBC2	1.75	0.50
31:5:604:CLA:CHB	36:5:618:NEX:H383	2.41	0.50
43:D:405:BCR:H21C	34:D:409:LMG:H361	1.92	0.50
31:N:310:CLA:H8	32:N:316:LUT:C30	2.42	0.50
17:O:105:THR:HB	17:O:119:PHE:HB3	1.94	0.50
19:S:133:GLY:O	19:S:139:THR:HG22	2.11	0.50
30:0:606:CHL:CBB	30:0:609:CHL:HBC1	2.42	0.50
30:0:608:CHL:HMB1	36:0:618:NEX:H401	1.93	0.50
2:9:208:LYS:HG3	31:9:313:CLA:HED2	1.94	0.50
2:q:166:ALA:HB1	30:q:310:CHL:CHB	2.42	0.50
31:b:609:CLA:HMB1	31:b:609:CLA:HBB1	1.93	0.50
7:c:198:PHE:HD2	7:c:202:PHE:HE2	1.59	0.50
7:c:302:THR:HG21	7:c:339:PHE:HB3	1.92	0.50
7:c:413:TRP:CD1	31:c:604:CLA:HMA2	2.47	0.50
17:o:84:VAL:HG21	17:o:185:ALA:HB1	1.94	0.50
31:y:603:CLA:C3D	30:y:609:CHL:H2	2.42	0.50
1:1:219:GLN:HG2	31:1:613:CLA:C1D	2.41	0.50
2:2:156:LEU:O	2:2:160:LEU:HG	2.11	0.50
3:3:106:GLU:HA	3:3:119:ALA:HB1	1.93	0.50
3:3:196:THR:O	3:3:200:LEU:HB2	2.12	0.50
3:5:233:LEU:HB2	32:5:616:LUT:H22	1.94	0.50
3:5:252:LYS:HD2	3:5:252:LYS:N	2.26	0.50
31:B:614:CLA:H122	34:B:621:LMG:H422	1.94	0.50
31:G:609:CLA:CGA	35:G:614:RRX:H6	2.40	0.50
34:G:622:LMG:H151	31:N:321:CLA:C1	2.41	0.50
31:Y:304:CLA:NB	30:Y:309:CHL:H121	2.26	0.50
4:0:223:GLN:HG2	31:0:613:CLA:C1D	2.41	0.50
3:8:253:SER:HB2	30:9:309:CHL:CAA	2.42	0.50
3:p:246:TRP:HA	3:p:250:ALA:HB2	1.92	0.50
33:c:622:LHG:H241	33:s:320:LHG:HC2	1.93	0.50
33:d:408:LHG:HC62	15:l:16:THR:OG1	2.12	0.50
31:s:311:CLA:H51	32:s:317:LUT:H373	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:y:621:SQD:H81	38:y:621:SQD:O10	2.10	0.50
3:5:40:TRP:O	3:5:45:ARG:HB2	2.12	0.50
3:5:93:ARG:HA	3:5:96:MET:HE3	1.93	0.50
3:5:220:VAL:O	3:5:224:ILE:HG13	2.11	0.50
43:D:405:BCR:H383	34:D:409:LMG:H182	1.93	0.50
31:7:316:CLA:C1C	34:9:301:LMG:H361	2.42	0.50
3:8:142:LEU:O	3:8:144:HIS:N	2.44	0.50
31:9:313:CLA:CHD	33:9:320:LHG:HC62	2.42	0.50
3:p:94:TRP:HB3	32:p:617:LUT:H191	1.94	0.50
3:p:203:LYS:CG	31:p:611:CLA:HED2	2.42	0.50
2:q:143:ASN:HB2	34:q1:101:LMG:H362	1.94	0.50
31:b:611:CLA:HHC	31:b:611:CLA:CBB	2.36	0.50
16:m:17:ILE:HB	16:m:18:PRO:HD3	1.94	0.50
1:1:152:VAL:HG11	30:1:606:CHL:HED2	1.93	0.50
1:1:252:ALA:HA	31:3:301:CLA:CHB	2.42	0.50
2:2:173:GLY:HA2	30:2:607:CHL:CBC	2.42	0.50
2:2:256:LYS:HD3	2:2:257:PHE:CZ	2.47	0.50
3:3:42:GLY:O	3:3:45:ARG:HG3	2.11	0.50
2:4:202:LEU:HD13	2:4:206:LYS:HG3	1.93	0.50
2:4:205:LEU:HB3	31:4:610:CLA:CMA	2.41	0.50
30:4:607:CHL:H42	3:5:245:PHE:HE2	1.75	0.50
30:6:307:CHL:HMC	32:6:318:LUT:H163	1.93	0.50
30:G:601:CHL:H11	30:Y:309:CHL:CHB	2.42	0.50
3:N:39:GLU:O	3:N:46:PRO:HD3	2.12	0.50
3:N:62:GLU:CD	3:N:62:GLU:H	2.20	0.50
3:N:188:LEU:HD12	32:N:316:LUT:H222	1.93	0.50
3:N:224:ILE:HD12	3:N:258:TYR:CE2	2.45	0.50
31:N:305:CLA:H92	30:N:307:CHL:HBA2	1.93	0.50
18:R:131:ARG:NH2	31:R:305:CLA:O1A	2.45	0.50
31:S:303:CLA:H91	32:S:318:LUT:H363	1.93	0.50
31:0:615:CLA:HMC3	30:p:607:CHL:HHB	1.93	0.50
1:7:89:GLU:HG3	1:7:177:VAL:HG22	1.93	0.50
31:8:612:CLA:H151	31:8:613:CLA:C2D	2.41	0.50
31:9:314:CLA:HHC	31:9:314:CLA:CBB	2.35	0.50
3:p:224:ILE:HG22	3:p:249:TYR:CD2	2.46	0.50
31:p:610:CLA:H12	31:p:610:CLA:C4A	2.42	0.50
7:c:51:TRP:CE2	7:c:55:MET:HG3	2.47	0.50
8:d:193:LEU:O	15:l:35:TYR:OH	2.26	0.50
10:f:27:VAL:N	10:f:28:PRO:HD2	2.25	0.50
33:j:102:LHG:H262	21:v:9:LEU:HD11	1.93	0.50
34:k:102:LMG:HC61	28:p1:15:ILE:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:x:96:PHE:CZ	27:q1:34:MET:HG3	2.46	0.50
1:1:195:LEU:O	1:1:199:LYS:HG3	2.11	0.50
31:2:604:CLA:NA	36:2:616:NEX:H242	2.27	0.50
3:5:127:GLN:HA	3:5:130:GLN:HG3	1.93	0.50
5:A:312:ARG:NH1	29:F1:83:ASN:OD1	2.44	0.50
30:G:623:CHL:H111	30:Y:309:CHL:H172	1.94	0.50
12:I:28:PRO:HB3	22:W:117:LEU:HD12	1.93	0.50
31:S:305:CLA:H161	31:S:316:CLA:HMB2	1.93	0.50
3:8:233:LEU:O	3:8:237:LEU:HG	2.12	0.50
30:8:608:CHL:HAA1	30:8:608:CHL:HBD	1.94	0.50
30:p:605:CHL:HAA1	30:p:605:CHL:HBD	1.94	0.50
31:q:304:CLA:H61	32:q:318:LUT:C28	2.41	0.50
43:b:618:BCR:H383	38:b:621:SQD:H91	1.94	0.50
45:c:619:DGD:HBT2	45:c:619:DGD:HBF2	1.92	0.50
34:c:620:LMG:H162	34:c:620:LMG:H342	1.94	0.50
34:g:322:LMG:O9	34:g:322:LMG:HC1	2.11	0.50
31:s:311:CLA:O2A	32:s:317:LUT:H26	2.12	0.50
3:3:46:PRO:HB2	30:3:303:CHL:HBC1	1.93	0.49
2:4:47:ALA:HB1	30:4:601:CHL:CBC	2.42	0.49
2:4:147:ILE:HG22	2:4:149:ALA:HB2	1.94	0.49
3:5:180:TYR:HB3	31:5:610:CLA:HED3	1.93	0.49
43:B:618:BCR:H382	43:t:101:BCR:H361	1.94	0.49
26:U:116:ILE:HD12	26:U:184:LEU:HD22	1.94	0.49
2:q:61:TYR:OH	2:q:76:GLY:HA2	2.12	0.49
5:a:267:ASN:ND2	38:a:411:SQD:H3	2.24	0.49
10:f:43:GLN:HB3	29:f1:57:ALA:HB3	1.94	0.49
48:r:302:LMU:H22	31:r:307:CLA:CAB	2.42	0.49
29:f1:216:LYS:HZ2	29:f1:217:ARG:HH12	1.60	0.49
2:2:176:PRO:HB3	36:2:616:NEX:H163	1.93	0.49
31:3:301:CLA:H72	31:3:316:CLA:HAC1	1.93	0.49
2:4:156:LEU:HD22	3:5:246:TRP:CH2	2.47	0.49
3:5:224:ILE:HD11	31:5:615:CLA:HBC1	1.92	0.49
30:5:606:CHL:HAA2	30:5:606:CHL:HBD	1.94	0.49
30:5:607:CHL:CED	4:6:256:ALA:HA	2.43	0.49
10:F:27:VAL:N	10:F:28:PRO:HD2	2.27	0.49
13:J:6:THR:HG23	28:P1:79:TYR:HB3	1.92	0.49
3:N:206:LYS:HE3	33:N:319:LHG:HC62	1.94	0.49
17:O:271:ASP:HB2	17:O:275:LYS:HE3	1.95	0.49
24:Y:193:PRO:HD2	32:Y:315:LUT:H23	1.94	0.49
31:0:611:CLA:H2	31:0:612:CLA:OBD	2.12	0.49
31:g:310:CLA:H52	35:g:315:RRX:H25	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f1:207:TYR:HB2	29:f1:235:VAL:HG21	1.95	0.49
1:1:90:ILE:HG21	31:1:603:CLA:HAA2	1.94	0.49
2:4:125:TRP:CE2	2:4:126:PHE:HD2	2.30	0.49
3:5:188:LEU:HB2	3:5:190:LEU:HD13	1.94	0.49
3:5:200:LEU:HB3	31:5:610:CLA:HMA1	1.94	0.49
4:6:148:GLN:HB2	30:6:306:CHL:CBB	2.42	0.49
4:6:192:LEU:HD12	31:6:311:CLA:O2A	2.13	0.49
30:6:309:CHL:HAA1	30:6:309:CHL:HBD	1.93	0.49
5:A:43:THR:O	5:A:47:VAL:HG12	2.12	0.49
5:A:283:ILE:HA	5:A:286:THR:HG22	1.94	0.49
30:G:601:CHL:H192	30:G:623:CHL:CHB	2.42	0.49
31:7:311:CLA:H8	32:7:317:LUT:C30	2.42	0.49
2:9:214:ARG:HA	2:9:217:MET:HE2	1.93	0.49
2:9:257:PHE:HB2	34:9:301:LMG:H152	1.94	0.49
30:9:307:CHL:HBD	30:9:307:CHL:HAA1	1.94	0.49
3:p:72:ALA:HA	2:q:90:ILE:HD11	1.94	0.49
31:q:313:CLA:HBD	31:q:314:CLA:OBD	2.12	0.49
5:a:223:LEU:HD12	8:d:139:ARG:NH1	2.28	0.49
6:b:54:PRO:HD2	6:b:57:ARG:HB2	1.92	0.49
34:d:409:LMG:H112	13:j:30:PHE:HB3	1.92	0.49
31:g:312:CLA:HMC3	35:g:315:RRX:H44	1.93	0.49
15:l:27:VAL:HG21	33:l:101:LHG:H182	1.93	0.49
34:w:205:LMG:H312	34:w:205:LMG:O10	2.12	0.49
1:1:166:ASN:C	18:R:38:ARG:HB3	2.38	0.49
2:2:138:LEU:HD13	30:2:606:CHL:HMD3	1.94	0.49
30:3:307:CHL:HAA1	30:3:307:CHL:HBD	1.93	0.49
34:3:321:LMG:HC71	34:3:321:LMG:O10	2.12	0.49
2:4:113:ASN:C	2:4:113:ASN:HD22	2.21	0.49
3:5:126:ALA:HA	3:5:129:PHE:HD2	1.76	0.49
31:6:314:CLA:NC	31:6:314:CLA:H51	2.27	0.49
2:G:257:PHE:CD2	34:G:621:LMG:H162	2.47	0.49
3:N:104:THR:HB	3:N:105:PRO:HD3	1.95	0.49
31:S:305:CLA:HMA3	30:S:307:CHL:C4C	2.42	0.49
30:8:601:CHL:H71	2:9:160:LEU:HD23	1.95	0.49
30:8:605:CHL:H141	30:8:605:CHL:H18	1.94	0.49
30:8:606:CHL:OMC	32:8:616:LUT:H163	2.13	0.49
2:9:90:ILE:HG21	31:9:305:CLA:HAA2	1.93	0.49
3:p:97:LEU:HB3	31:p:604:CLA:HAB	1.93	0.49
5:a:162:PRO:HB3	5:a:168:PHE:HA	1.94	0.49
30:n:307:CHL:HMB2	30:n:310:CHL:HMC	1.94	0.49
48:r:302:LMU:H82	31:r:307:CLA:C1B	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:91:HIS:HE1	31:3:305:CLA:C4D	2.25	0.49
2:4:260:LEU:HB2	34:4:620:LMG:O5	2.12	0.49
3:5:100:LEU:HA	3:5:103:VAL:HG22	1.95	0.49
3:5:159:MET:HG3	30:5:609:CHL:CMC	2.42	0.49
31:5:610:CLA:C4D	32:5:616:LUT:H382	2.42	0.49
31:A:406:CLA:H203	42:A:408:PHO:H91	1.93	0.49
8:D:16:ASP:OD1	34:D:410:LMG:O3	2.30	0.49
3:N:103:VAL:HB	3:N:230:ILE:HD11	1.95	0.49
17:O:257:GLU:HG2	17:O:289:GLN:HG2	1.95	0.49
30:8:601:CHL:HAA2	30:8:601:CHL:HBD	1.95	0.49
31:8:603:CLA:HBC2	30:8:608:CHL:HHD	1.94	0.49
31:8:612:CLA:H172	31:8:613:CLA:C4D	2.42	0.49
3:p:124:ALA:O	3:p:127:GLN:HG2	2.12	0.49
42:a:408:PHO:H202	44:d:407:PL9:H453	1.95	0.49
8:d:41:ALA:HB1	42:d:402:PHO:H42	1.94	0.49
3:n:142:LEU:O	3:n:144:HIS:N	2.44	0.49
30:n:301:CHL:HMA3	31:n:316:CLA:C3B	2.42	0.49
31:n:305:CLA:H201	31:s:305:CLA:HBC1	1.94	0.49
36:y:618:NEX:H161	36:y:618:NEX:H193	1.93	0.49
34:Q1:101:LMG:HC1	34:Q1:101:LMG:C10	2.42	0.49
2:2:72:TRP:H	31:2:602:CLA:CAD	2.26	0.49
3:3:143:ILE:HG22	30:3:307:CHL:C3D	2.42	0.49
30:5:607:CHL:HBA1	30:5:607:CHL:CHA	2.42	0.49
31:A:406:CLA:H172	44:D:406:PL9:H512	1.94	0.49
7:C:264:LEU:HD21	31:C:608:CLA:CAB	2.42	0.49
8:D:27:PHE:HB2	9:E:7:GLU:HG3	1.93	0.49
3:N:106:GLU:O	3:N:110:ARG:HG2	2.12	0.49
31:Y:304:CLA:H2	31:Y:304:CLA:CMA	2.43	0.49
4:0:249:SER:H	3:p:129:PHE:HE1	1.59	0.49
30:7:308:CHL:HED1	2:9:258:LEU:CD1	2.43	0.49
30:7:310:CHL:HAA1	30:7:310:CHL:HBD	1.95	0.49
2:9:94:HIS:CD2	32:9:318:LUT:H15	2.47	0.49
2:q:177:VAL:HG23	30:q:310:CHL:HBB1	1.94	0.49
5:a:341:LEU:HB3	5:a:343:LEU:HD13	1.93	0.49
7:c:41:HIS:CD2	31:c:609:CLA:NA	2.81	0.49
7:c:364:ASP:HB2	7:c:367:LYS:HB2	1.95	0.49
11:h:76:ASP:N	11:h:76:ASP:OD1	2.40	0.49
3:n:233:LEU:O	3:n:237:LEU:HG	2.12	0.49
30:n:306:CHL:H18	30:n:306:CHL:H141	1.94	0.49
30:2:607:CHL:C2	35:2:614:RRX:H12	2.42	0.49
31:2:610:CLA:HBA1	38:6:301:SQD:H1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:162:ILE:HD11	36:3:319:NEX:C35	2.42	0.49
2:4:147:ILE:HA	30:4:605:CHL:C4D	2.43	0.49
34:4:620:LMG:H112	34:4:621:LMG:C12	2.43	0.49
3:5:221:GLN:C	3:5:225:THR:HG22	2.37	0.49
31:5:613:CLA:C2	31:5:613:CLA:HBA2	2.42	0.49
31:6:303:CLA:HED2	31:6:303:CLA:H2A	1.95	0.49
31:B:608:CLA:HBB1	31:B:608:CLA:HMB3	1.94	0.49
33:D:408:LHG:HC91	15:L:20:TRP:HZ2	1.78	0.49
30:G:623:CHL:H171	31:Y:304:CLA:CAC	2.43	0.49
30:N:302:CHL:HAA2	30:N:302:CHL:HBD	1.93	0.49
31:Y:312:CLA:HHC	31:Y:312:CLA:HBB1	1.94	0.49
4:0:228:GLY:HA3	2:q:261:PRO:HG3	1.93	0.49
1:7:134:TYR:HB3	1:7:140:LEU:HD12	1.94	0.49
3:8:251:PRO:HB3	2:9:133:PHE:CD2	2.48	0.49
2:9:146:LEU:HA	30:9:307:CHL:HED3	1.95	0.49
3:p:162:ILE:HD11	36:p:618:NEX:C34	2.42	0.49
2:q:130:ALA:CB	30:q:309:CHL:HED1	2.42	0.49
5:a:160:ILE:HG12	7:c:419:PHE:CZ	2.48	0.49
5:a:283:ILE:HG13	42:a:408:PHO:HBC3	1.94	0.49
2:g:257:PHE:CE1	31:n:316:CLA:H43	2.46	0.49
3:n:123:LYS:HA	30:n:308:CHL:HED3	1.94	0.49
18:r:183:ILE:HG22	48:r:302:LMU:H3'	1.95	0.49
48:r:302:LMU:H52	31:r:307:CLA:CAB	2.43	0.49
31:1:602:CLA:H43	31:1:602:CLA:HMB2	1.94	0.49
30:1:619:CHL:HHC	30:1:619:CHL:HBB1	1.95	0.49
2:2:125:TRP:CH2	2:2:224:PHE:HD1	2.30	0.49
2:2:182:ASP:OD2	2:2:185:TYR:HB2	2.12	0.49
30:4:605:CHL:HBD	30:4:605:CHL:HAA1	1.95	0.49
31:6:303:CLA:H52	32:6:318:LUT:H30	1.94	0.49
38:A:413:SQD:O9	49:A:501:HOH:O	2.20	0.49
6:B:348:ASP:OD1	6:B:349:LYS:N	2.46	0.49
6:B:469:HIS:HE1	31:B:611:CLA:NA	2.07	0.49
31:C:608:CLA:HBC3	31:C:610:CLA:H71	1.93	0.49
9:E:19:TYR:HE2	47:E:101:HEM:C3D	2.30	0.49
19:S:246:PHE:CE2	32:S:318:LUT:H10	2.46	0.49
31:0:614:CLA:CBA	34:p:620:LMG:H111	2.40	0.49
3:8:58:TYR:CD2	3:8:59:LEU:HD13	2.48	0.49
31:8:604:CLA:HMA3	30:8:606:CHL:C3C	2.43	0.49
2:9:205:LEU:HD13	31:9:312:CLA:H12	1.95	0.49
8:d:55:VAL:HG21	8:d:110:LEU:HD22	1.93	0.49
31:g:313:CLA:H201	24:y:156:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:o:204:ASP:OD1	17:o:208:ARG:N	2.46	0.49
2:2:130:ALA:H	30:3:302:CHL:CED	2.24	0.49
2:4:133:PHE:HZ	3:5:246:TRP:HB3	1.78	0.49
3:5:46:PRO:HB2	3:5:67:TYR:CE2	2.48	0.49
30:5:607:CHL:HBA1	30:5:607:CHL:CBD	2.43	0.49
6:B:33:TRP:HD1	43:t:101:BCR:H332	1.78	0.49
30:G:605:CHL:HBA1	30:G:605:CHL:CHA	2.42	0.49
3:N:224:ILE:HG23	3:N:258:TYR:CE2	2.47	0.49
17:O:125:MET:HE3	17:O:163:GLN:HB2	1.94	0.49
19:S:113:LEU:HB3	31:S:305:CLA:HAB	1.95	0.49
24:Y:95:ALA:HB1	24:Y:214:GLY:HA3	1.95	0.49
3:8:71:THR:CB	30:9:311:CHL:HAA2	2.43	0.49
31:8:603:CLA:CAD	30:8:608:CHL:H11	2.43	0.49
3:n:58:TYR:CD2	3:n:59:LEU:HD13	2.47	0.49
30:n:306:CHL:H201	31:s:313:CLA:HMC2	1.94	0.49
19:s:246:PHE:CZ	32:s:318:LUT:H10	2.48	0.49
31:s:303:CLA:H72	32:s:318:LUT:H30	1.94	0.49
22:w:73:ILE:HG13	34:w:204:LMG:HC61	1.93	0.49
22:w:84:ALA:HA	34:w:205:LMG:H341	1.94	0.49
1:1:198:LEU:HB3	31:1:610:CLA:HMA2	1.95	0.49
34:2:621:LMG:O7	34:2:621:LMG:HC1	2.13	0.49
3:3:104:THR:OG1	31:3:306:CLA:HBC3	2.13	0.49
3:3:118:GLU:CG	3:3:124:ALA:HA	2.42	0.49
31:4:610:CLA:HBA1	35:4:615:RRX:H7	1.95	0.49
3:5:171:PRO:HB3	36:5:618:NEX:H181	1.95	0.49
30:5:607:CHL:H2A	30:5:607:CHL:O2D	2.13	0.49
31:A:406:CLA:H141	31:A:406:CLA:H161	1.65	0.49
7:C:270:MET:HG2	31:C:601:CLA:H72	1.95	0.49
7:C:304:THR:HG21	7:C:384:MET:HE1	1.95	0.49
45:C:618:DGD:HBF1	34:D:409:LMG:H191	1.95	0.49
31:G:603:CLA:C2	31:G:603:CLA:HED2	2.42	0.49
31:R:305:CLA:HBC1	31:R:311:CLA:CBC	2.43	0.49
4:0:144:LEU:O	4:0:146:HIS:N	2.46	0.49
3:p:219:GLY:O	3:p:223:LEU:HG	2.13	0.49
30:q:309:CHL:H102	30:q:309:CHL:NB	2.28	0.49
10:f:12:TYR:OH	28:p1:71:THR:O	2.28	0.49
2:g:146:LEU:O	2:g:148:HIS:N	2.46	0.49
31:n:311:CLA:H8	32:n:317:LUT:C30	2.42	0.49
1:1:132:ILE:HD12	30:1:606:CHL:HMD3	1.95	0.48
30:1:605:CHL:CHA	34:6:321:LMG:H341	2.43	0.48
30:1:608:CHL:HBD	30:1:608:CHL:HAA1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:603:CLA:H72	31:3:305:CLA:H92	1.95	0.48
2:4:90:ILE:HG21	31:4:603:CLA:HAA2	1.94	0.48
2:4:175:GLY:N	2:4:176:PRO:HD2	2.27	0.48
31:5:603:CLA:H2	31:5:603:CLA:HMA3	1.95	0.48
44:A:416:PL9:H222	42:D:401:PHO:HMA2	1.95	0.48
6:B:29:LEU:HD11	43:B:617:BCR:H19C	1.95	0.48
6:B:487:ASP:O	6:B:491:GLU:HG3	2.12	0.48
7:C:194:PRO:HG3	31:Y:314:CLA:HMB1	1.94	0.48
8:D:223:PHE:HE2	8:D:242:GLU:HG3	1.77	0.48
43:D:405:BCR:H272	34:D:409:LMG:H241	1.95	0.48
2:G:258:LEU:HD23	2:G:259:PRO:HD2	1.94	0.48
34:G:622:LMG:H171	31:N:315:CLA:H92	1.95	0.48
17:O:162:VAL:HG23	17:O:170:VAL:HG13	1.95	0.48
4:0:199:LEU:HD11	4:0:203:LYS:HZ2	1.78	0.48
30:0:605:CHL:HAA1	31:r:315:CLA:HMD3	1.95	0.48
3:p:206:LYS:HE3	33:p:619:LHG:O8	2.12	0.48
31:c:613:CLA:H72	33:c:622:LHG:H281	1.95	0.48
2:g:77:LEU:HD13	31:g:303:CLA:H42	1.94	0.48
11:h:62:VAL:O	11:h:66:GLU:HG2	2.12	0.48
18:r:186:LEU:HD13	30:r:308:CHL:HMD1	1.94	0.48
19:s:236:ILE:HD12	19:s:237:LYS:HG3	1.95	0.48
34:w:205:LMG:H292	34:w:205:LMG:HC5	1.95	0.48
29:F1:170:ASP:HB2	29:F1:176:TYR:CE1	2.46	0.48
29:F1:200:THR:HB	29:F1:235:VAL:HG11	1.95	0.48
31:4:610:CLA:H72	35:4:615:RRX:C21	2.42	0.48
3:5:107:LEU:HD13	3:5:110:ARG:HD3	1.95	0.48
3:5:218:PHE:HZ	32:5:616:LUT:H8	1.77	0.48
31:5:614:CLA:CED	31:5:614:CLA:H2A	2.44	0.48
4:6:125:LYS:HA	30:6:308:CHL:HED2	1.94	0.48
5:A:308:ASP:OD1	5:A:312:ARG:N	2.47	0.48
31:A:409:CLA:H41	31:A:409:CLA:H62	1.55	0.48
6:B:216:HIS:HE1	31:B:609:CLA:CHA	2.26	0.48
8:D:239:GLN:HA	28:P1:56:TYR:CZ	2.48	0.48
31:G:612:CLA:CMA	35:G:614:RRX:H4	2.42	0.48
31:G:612:CLA:H112	37:G:620:XAT:H34	1.94	0.48
12:I:6:ILE:HG21	34:I:101:LMG:HC91	1.94	0.48
17:O:176:VAL:O	17:O:179:LEU:HB2	2.12	0.48
19:S:37:GLY:H	34:S:321:LMG:HC61	1.77	0.48
3:p:197:PHE:HE1	31:p:610:CLA:H2A	1.78	0.48
2:q:85:ALA:HA	2:q:88:ARG:NH1	2.28	0.48
30:q:309:CHL:H101	30:q:309:CHL:H61	1.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:a:121:LEU:HD23	31:a:409:CLA:HMB2	1.95	0.48
5:a:278:TRP:HB3	5:a:279:PRO:HD3	1.94	0.48
6:b:99:ALA:HB1	31:b:607:CLA:H62	1.94	0.48
6:b:156:PHE:CZ	33:b:628:LHG:H282	2.47	0.48
31:c:604:CLA:HAC2	14:k:26:PRO:O	2.13	0.48
8:d:91:PHE:CE1	31:d:405:CLA:HAA1	2.48	0.48
2:g:186:PRO:HG3	30:g:308:CHL:HBC2	1.95	0.48
24:y:193:PRO:HD2	32:y:616:LUT:H23	1.95	0.48
3:3:205:LEU:O	3:3:209:ARG:N	2.31	0.48
3:3:215:MET:HA	3:3:218:PHE:CD2	2.49	0.48
3:3:245:PHE:O	3:3:246:TRP:HB2	2.13	0.48
3:5:117:GLY:HA3	3:5:130:GLN:HE22	1.78	0.48
3:5:125:GLY:O	3:5:128:ILE:HG22	2.12	0.48
31:5:602:CLA:H92	31:5:602:CLA:H61	1.65	0.48
4:6:235:LEU:HB2	32:6:317:LUT:H22	1.94	0.48
30:6:307:CHL:H3A	36:6:319:NEX:C31	2.43	0.48
7:C:287:SER:OG	7:C:296:GLU:OE1	2.31	0.48
9:E:7:GLU:HB2	10:F:18:ARG:NH2	2.28	0.48
34:G:621:LMG:H411	34:G:621:LMG:H372	1.95	0.48
30:N:309:CHL:HAA1	30:N:309:CHL:HBD	1.96	0.48
18:R:165:GLN:HG2	37:R:318:XAT:H21	1.95	0.48
30:7:321:CHL:HED3	3:8:123:LYS:HA	1.94	0.48
3:p:221:GLN:HE22	32:p:616:LUT:H41	1.79	0.48
31:p:602:CLA:HED2	31:p:602:CLA:H2A	1.95	0.48
2:q:78:SER:OG	31:q:304:CLA:HAA2	2.12	0.48
31:b:613:CLA:HBB1	31:b:613:CLA:CMB	2.43	0.48
7:c:142:LYS:HE3	7:c:254:TRP:CD1	2.49	0.48
7:c:240:ILE:HG21	34:c:620:LMG:H121	1.94	0.48
7:c:334:THR:HG21	17:o:67:GLY:HA2	1.95	0.48
7:c:351:GLY:O	7:c:355:GLU:HG2	2.14	0.48
33:g:319:LHG:H142	33:g:319:LHG:H241	1.95	0.48
24:y:145:LEU:O	24:y:147:HIS:N	2.45	0.48
3:5:236:HIS:CG	31:5:613:CLA:HAA2	2.49	0.48
31:6:311:CLA:H51	32:6:317:LUT:C28	2.44	0.48
5:A:259:ILE:HG22	5:A:260:PHE:CD2	2.49	0.48
2:G:130:ALA:HA	2:G:133:PHE:CD1	2.48	0.48
2:G:259:PRO:HA	34:G:621:LMG:HC4	1.95	0.48
31:G:609:CLA:HBA1	35:G:614:RRX:C40	2.42	0.48
31:G:610:CLA:HAA2	38:G:617:SQD:C44	2.40	0.48
31:N:311:CLA:HBB1	31:N:311:CLA:CHC	2.19	0.48
31:S:314:CLA:H141	31:S:314:CLA:H202	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:p:110:ARG:NH2	3:p:230:ILE:HG21	2.29	0.48
6:b:464:PHE:HD2	31:b:612:CLA:HAC2	1.78	0.48
34:g:322:LMG:H322	31:y:615:CLA:ND	2.28	0.48
30:n:301:CHL:HBD	30:n:301:CHL:HAA1	1.95	0.48
24:y:100:LEU:HB3	31:y:604:CLA:HAB	1.95	0.48
34:q1:101:LMG:HC8	34:q1:101:LMG:HC1	1.50	0.48
1:1:117:ILE:CD1	1:1:122:ALA:HA	2.43	0.48
30:2:606:CHL:HBB1	30:2:608:CHL:HBC1	1.94	0.48
31:3:301:CLA:H72	31:3:316:CLA:CAC	2.43	0.48
45:C:620:DGD:HB32	31:Y:311:CLA:C1B	2.43	0.48
3:N:165:TYR:OH	19:S:39:TRP:O	2.26	0.48
18:R:223:ALA:HB1	18:R:230:THR:HG23	1.95	0.48
36:R:319:NEX:H181	36:R:319:NEX:H193	1.95	0.48
19:S:264:TRP:HB2	32:S:317:LUT:H22	1.96	0.48
31:7:303:CLA:H61	32:7:318:LUT:H28	1.95	0.48
3:8:70:ASP:OD2	3:8:75:SER:OG	2.30	0.48
5:a:118:HIS:CE1	31:a:409:CLA:C4D	2.96	0.48
5:a:140:ARG:HH22	33:a:415:LHG:HC41	1.78	0.48
6:b:224:ARG:HG2	11:h:44:TRP:CE2	2.49	0.48
7:c:306:LEU:HD12	7:c:328:TYR:HB3	1.95	0.48
30:g:307:CHL:HBB2	30:n:301:CHL:HBB1	1.95	0.48
1:1:89:GLU:HG3	1:1:177:VAL:HG22	1.95	0.48
1:1:131:GLY:HA3	1:1:144:LYS:HG2	1.96	0.48
1:1:184:ASP:HA	32:1:615:LUT:H24	1.95	0.48
2:2:72:TRP:CZ3	30:2:601:CHL:HBD	2.49	0.48
2:2:125:TRP:O	2:2:126:PHE:C	2.56	0.48
3:3:252:LYS:O	3:3:258:TYR:HB3	2.13	0.48
31:3:312:CLA:C3C	33:3:320:LHG:HC62	2.43	0.48
2:4:149:ALA:HA	30:4:605:CHL:C1C	2.44	0.48
3:5:41:TYR:CZ	3:5:202:VAL:HG23	2.48	0.48
33:5:619:LHG:O10	33:5:619:LHG:H291	2.13	0.48
30:6:306:CHL:HAA1	30:6:306:CHL:HBD	1.95	0.48
31:6:314:CLA:HMB1	31:6:315:CLA:CBC	2.43	0.48
34:6:321:LMG:HC71	18:R:273:PHE:CG	2.49	0.48
6:B:204:ALA:HB3	31:B:602:CLA:HAB	1.95	0.48
33:B:624:LHG:H321	33:B:624:LHG:H291	1.56	0.48
31:G:603:CLA:ND	30:G:608:CHL:H8	2.28	0.48
3:N:200:LEU:HD12	3:N:203:LYS:HD2	1.94	0.48
18:R:223:ALA:HB3	31:R:312:CLA:HAA2	1.94	0.48
31:R:306:CLA:C1C	36:R:319:NEX:H222	2.44	0.48
19:S:167:ALA:O	19:S:171:ILE:HG13	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:15:ILE:O	43:V:101:BCR:H14C	2.14	0.48
24:Y:252:TYR:CD1	31:Y:314:CLA:HED2	2.48	0.48
31:Y:305:CLA:HMA3	30:Y:307:CHL:C3C	2.44	0.48
31:0:610:CLA:H91	31:0:610:CLA:H111	1.60	0.48
3:8:214:SER:HB2	32:8:615:LUT:H8	1.95	0.48
2:9:111:LEU:HB2	2:9:119:PHE:HE1	1.79	0.48
5:a:304:GLN:HG2	5:a:313:VAL:HG21	1.94	0.48
31:a:409:CLA:H42	12:i:9:TYR:CE2	2.48	0.48
7:c:155:VAL:HG12	34:c:620:LMG:H371	1.95	0.48
8:d:157:PHE:CE2	8:d:171:PRO:HG2	2.49	0.48
30:g:302:CHL:H121	30:g:302:CHL:H93	1.95	0.48
33:g:319:LHG:H282	37:g:321:XAT:C32	2.43	0.48
34:g:322:LMG:H361	31:y:615:CLA:C1C	2.43	0.48
31:n:315:CLA:HMB1	31:n:315:CLA:HBB1	1.96	0.48
31:s:303:CLA:C6	32:s:318:LUT:H28	2.42	0.48
28:P1:53:ALA:O	28:P1:54:ASN:HB3	2.13	0.48
29:f1:136:PHE:CE1	29:f1:181:VAL:HG11	2.49	0.48
1:1:157:MET:HB3	30:1:609:CHL:CBB	2.43	0.48
1:1:198:LEU:CB	31:1:610:CLA:HMA2	2.44	0.48
31:2:602:CLA:H62	32:2:615:LUT:H28	1.96	0.48
3:3:246:TRP:HA	3:3:250:ALA:HB2	1.95	0.48
30:4:606:CHL:CBB	30:4:609:CHL:HBC1	2.43	0.48
3:5:61:GLY:HA2	3:5:66:ASP:HB3	1.94	0.48
3:5:253:SER:HA	3:5:258:TYR:HE1	1.79	0.48
6:B:149:LEU:HD11	34:B:622:LMG:H342	1.95	0.48
31:C:608:CLA:H161	45:C:618:DGD:HAH1	1.95	0.48
45:C:620:DGD:HA22	45:C:620:DGD:HG12	1.58	0.48
31:N:305:CLA:H112	31:S:306:CLA:CHB	2.43	0.48
36:R:301:NEX:H192	36:R:301:NEX:H183	1.95	0.48
31:R:303:CLA:HBD	33:R:320:LHG:HC82	1.96	0.48
31:p:615:CLA:CGA	34:q:302:LMG:HC2	2.44	0.48
31:b:612:CLA:H2	31:b:612:CLA:H61	1.62	0.48
7:c:225:HIS:HE1	31:c:601:CLA:NA	2.12	0.48
7:c:285:TYR:O	7:c:411:ARG:NH2	2.43	0.48
31:c:610:CLA:H161	31:c:610:CLA:H202	1.69	0.48
30:n:307:CHL:OMC	32:n:318:LUT:H163	2.13	0.48
31:s:303:CLA:H12	31:s:303:CLA:HBA2	1.56	0.48
30:y:607:CHL:HAA2	30:y:607:CHL:HBD	1.96	0.48
29:f1:196:LEU:HB3	29:f1:230:TRP:CG	2.49	0.48
30:1:601:CHL:CHD	33:1:617:LHG:HC82	2.44	0.48
2:4:119:PHE:CE2	2:4:141:LEU:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:607:CHL:CHD	3:5:246:TRP:HZ3	2.27	0.48
6:B:103:LEU:HD21	31:B:605:CLA:HMC3	1.95	0.48
31:B:603:CLA:H41	31:B:603:CLA:H61	1.46	0.48
38:B:620:SQD:H2	38:B:620:SQD:H441	1.46	0.48
38:B:623:SQD:H91	8:D:130:PHE:HB3	1.96	0.48
31:N:314:CLA:HBC1	32:N:316:LUT:C16	2.43	0.48
17:O:184:ASN:H	17:O:184:ASN:HD22	1.62	0.48
30:R:310:CHL:CBB	38:R:322:SQD:H91	2.43	0.48
30:S:302:CHL:HBB1	30:S:302:CHL:HMB3	1.96	0.48
1:7:165:VAL:CG1	2:9:57:SER:HB3	2.40	0.48
31:8:612:CLA:C1A	31:8:612:CLA:CGA	2.92	0.48
3:p:41:TYR:OH	3:p:64:PRO:HB3	2.13	0.48
34:q:302:LMG:H152	34:q:302:LMG:O9	2.13	0.48
6:b:6:TYR:O	31:b:612:CLA:HBD	2.14	0.48
6:b:216:HIS:HE1	31:b:610:CLA:CHA	2.26	0.48
43:d:406:BCR:H363	10:f:32:PHE:HB3	1.96	0.48
9:e:19:TYR:HE2	47:e:102:HEM:C3D	2.32	0.48
3:n:214:SER:HB2	32:n:317:LUT:H8	1.95	0.48
31:n:314:CLA:CGA	31:n:314:CLA:C1A	2.92	0.48
18:r:53:TRP:CE3	18:r:54:LEU:HD13	2.49	0.48
19:s:141:ALA:H	30:s:308:CHL:HED1	1.78	0.48
29:f1:66:PHE:HZ	29:f1:225:GLU:HA	1.78	0.48
29:f1:165:VAL:HG12	29:f1:179:TYR:HD1	1.79	0.48
31:3:315:CLA:HBA2	31:3:315:CLA:C2	2.43	0.48
2:4:207:VAL:C	2:4:209:GLU:N	2.71	0.48
3:5:200:LEU:HD23	3:5:203:LYS:CD	2.44	0.48
4:6:193:ALA:HB2	31:6:311:CLA:HAA2	1.96	0.48
9:E:27:ILE:HB	9:E:28:PRO:HD3	1.94	0.48
1:7:56:ASN:CG	3:8:168:ASN:OD1	2.57	0.48
31:p:615:CLA:HHC	31:p:615:CLA:HBB1	1.96	0.48
2:q:103:LEU:HD12	35:q:317:RRX:H30	1.95	0.48
2:q:208:LYS:HD3	31:q:314:CLA:HAA2	1.95	0.48
7:c:129:GLU:HA	7:c:136:GLY:HA3	1.96	0.48
45:c:617:DGD:HB61	45:c:617:DGD:HB92	1.71	0.48
8:d:153:PHE:CE1	42:d:402:PHO:H91	2.49	0.48
2:g:241:HIS:HB2	31:g:313:CLA:HAA2	1.95	0.48
31:n:314:CLA:H172	31:n:315:CLA:C4D	2.44	0.48
19:s:112:MET:HG3	19:s:239:GLY:HA2	1.94	0.48
30:1:608:CHL:O1A	31:1:610:CLA:HMD1	2.14	0.48
2:2:50:LEU:HB2	2:2:54:SER:HB3	1.96	0.48
31:3:306:CLA:C1C	36:3:319:NEX:H222	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:97:TRP:CD1	30:4:609:CHL:HMD2	2.49	0.48
3:5:104:THR:O	3:5:108:LEU:HG	2.14	0.48
3:5:199:GLU:HG3	3:5:200:LEU:N	2.29	0.48
6:B:466:HIS:HE1	31:B:608:CLA:C4D	2.27	0.48
2:G:238:LEU:HD21	34:G:619:LMG:H161	1.96	0.48
30:G:601:CHL:H62	30:G:601:CHL:H41	1.64	0.48
3:N:245:PHE:HB3	31:N:313:CLA:C1	2.42	0.48
31:R:306:CLA:CHC	36:R:319:NEX:H222	2.44	0.48
31:8:614:CLA:HED2	34:9:302:LMG:O4	2.14	0.48
2:9:72:TRP:O	32:9:318:LUT:H24	2.13	0.48
2:9:85:ALA:HA	2:9:88:ARG:NH1	2.29	0.48
2:9:222:GLY:O	2:9:226:GLN:HG3	2.13	0.48
31:9:305:CLA:H2	31:9:305:CLA:H61	1.68	0.48
32:p:617:LUT:H35	32:p:617:LUT:H401	1.40	0.48
2:q:208:LYS:HD3	31:q:314:CLA:HBD	1.96	0.48
47:e:102:HEM:HMC2	10:f:30:VAL:HG21	1.95	0.48
30:n:302:CHL:HAA2	30:n:302:CHL:HBD	1.95	0.48
31:y:610:CLA:H8	32:y:616:LUT:C30	2.44	0.48
31:2:604:CLA:O1A	31:2:604:CLA:H3A	2.14	0.47
31:2:609:CLA:H71	31:2:611:CLA:HMA2	1.96	0.47
31:3:314:CLA:H62	31:3:314:CLA:NC	2.28	0.47
31:4:603:CLA:HED3	32:5:617:LUT:H372	1.96	0.47
4:6:173:PRO:HB2	30:6:309:CHL:HBB2	1.96	0.47
31:B:601:CLA:C2B	34:X:202:LMG:H342	2.44	0.47
18:R:78:LEU:HD13	31:R:304:CLA:H42	1.96	0.47
19:S:191:GLY:HA3	31:S:316:CLA:C2D	2.44	0.47
31:Y:314:CLA:H2	31:Y:314:CLA:H62	1.63	0.47
31:0:614:CLA:H2	31:0:614:CLA:NA	2.29	0.47
3:8:191:ALA:HB2	31:8:609:CLA:HAA2	1.96	0.47
31:8:604:CLA:CHA	31:8:604:CLA:HBA1	2.41	0.47
30:9:303:CHL:HHD	33:9:320:LHG:HC41	1.96	0.47
31:9:304:CLA:H62	31:9:304:CLA:H41	1.67	0.47
31:9:312:CLA:H72	31:9:314:CLA:CMA	2.36	0.47
3:p:47:GLN:HB3	3:p:53:SER:OG	2.14	0.47
8:d:200:GLY:HA3	8:d:282:SER:OG	2.13	0.47
9:e:13:ILE:HD13	47:e:102:HEM:HBD1	1.96	0.47
31:n:316:CLA:HAC1	31:y:615:CLA:H62	1.96	0.47
17:o:106:VAL:HB	17:o:164:LEU:HD21	1.95	0.47
17:o:208:ARG:HD2	17:o:233:ASN:HA	1.96	0.47
3:3:139:ASN:HB3	3:3:142:LEU:HG	1.96	0.47
3:3:171:PRO:HG2	30:3:309:CHL:HBB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:3:301:CLA:H41	31:3:301:CLA:H93	1.96	0.47
2:4:220:MET:SD	2:4:223:PHE:HD2	2.37	0.47
34:4:620:LMG:C38	3:5:223:LEU:HD11	2.38	0.47
3:5:96:MET:HE3	31:5:610:CLA:HMC2	1.95	0.47
31:5:603:CLA:HED3	32:6:318:LUT:H372	1.95	0.47
38:B:620:SQD:H361	20:t:19:PHE:HE1	1.80	0.47
12:I:2:LEU:HD21	22:W:78:ASP:OD2	2.14	0.47
3:N:109:GLN:HE22	3:N:115:ASN:ND2	2.11	0.47
3:N:185:PHE:O	32:N:316:LUT:H24	2.14	0.47
4:0:255:LEU:CB	30:p:607:CHL:HBA2	2.44	0.47
2:9:226:GLN:HG2	31:9:315:CLA:C1D	2.43	0.47
3:p:158:LEU:HD11	30:p:606:CHL:HED3	1.95	0.47
31:c:606:CLA:H111	31:c:606:CLA:H152	1.54	0.47
31:n:303:CLA:H61	32:n:318:LUT:H28	1.95	0.47
31:n:316:CLA:C1	34:n:322:LMG:HC92	2.44	0.47
31:1:603:CLA:HAC1	30:1:607:CHL:CBB	2.40	0.47
2:2:109:GLU:OE2	2:2:235:LEU:HB2	2.14	0.47
30:3:303:CHL:HAC2	33:3:320:LHG:HC41	1.96	0.47
30:4:601:CHL:HED3	31:4:602:CLA:HBC1	1.96	0.47
31:4:602:CLA:H102	31:4:603:CLA:HMB1	1.95	0.47
3:5:109:GLN:HA	3:5:114:ALA:HB3	1.97	0.47
4:6:178:VAL:HG23	4:6:179:ASP:H	1.80	0.47
6:B:26:HIS:CE1	31:B:612:CLA:HMA2	2.49	0.47
7:C:151:ILE:HG23	34:C:621:LMG:H342	1.95	0.47
31:C:613:CLA:H72	33:C:623:LHG:H291	1.95	0.47
8:D:239:GLN:HG3	8:D:241:GLU:CD	2.39	0.47
18:R:38:ARG:HD2	18:R:38:ARG:N	2.29	0.47
34:Y:319:LMG:H321	18:r:181:PHE:CE1	2.49	0.47
1:7:223:THR:HG21	31:7:314:CLA:O1D	2.15	0.47
31:9:304:CLA:H2	32:9:318:LUT:H26	1.96	0.47
3:p:203:LYS:HD3	31:p:612:CLA:HAA2	1.96	0.47
2:q:99:MET:HG3	2:q:213:GLY:HA2	1.96	0.47
31:a:407:CLA:HMA2	44:d:407:PL9:H402	1.96	0.47
6:b:29:LEU:HD13	31:b:614:CLA:HMD2	1.96	0.47
6:b:462:PHE:HA	31:b:612:CLA:HMC2	1.96	0.47
2:g:47:ALA:HB1	30:g:302:CHL:HBC1	1.95	0.47
31:g:313:CLA:H171	37:g:321:XAT:H201	1.96	0.47
13:j:40:SER:C	13:j:42:LEU:H	2.22	0.47
31:n:305:CLA:HMA3	30:n:307:CHL:C3C	2.45	0.47
31:n:314:CLA:H151	31:n:315:CLA:C2D	2.43	0.47
31:r:305:CLA:HED2	31:r:305:CLA:H2A	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:y:606:CHL:CBB	32:y:617:LUT:H161	2.45	0.47
1:1:211:LEU:HD23	33:1:617:LHG:H291	1.95	0.47
31:1:602:CLA:H92	31:1:603:CLA:HMA1	1.95	0.47
31:3:312:CLA:C4C	33:3:320:LHG:HC62	2.43	0.47
3:5:38:VAL:HG22	3:5:41:TYR:HD2	1.78	0.47
31:6:305:CLA:HBA1	30:6:307:CHL:C1D	2.44	0.47
42:A:408:PHO:H112	42:A:408:PHO:H93	1.68	0.47
6:B:65:PHE:HE1	31:B:604:CLA:HED2	1.80	0.47
7:C:23:TRP:HD1	48:K:101:LMU:H6'1	1.80	0.47
7:C:401:GLU:OE1	49:C:701:HOH:O	2.20	0.47
38:G:624:SQD:H91	31:7:312:CLA:H42	1.96	0.47
19:S:122:GLU:HA	19:S:134:ALA:HB1	1.96	0.47
31:S:313:CLA:HBC1	31:S:314:CLA:H201	1.96	0.47
31:S:314:CLA:H143	33:S:320:LHG:H331	1.96	0.47
23:X:88:GLY:O	23:X:91:THR:HG22	2.15	0.47
4:0:58:PRO:HB2	4:0:61:LEU:HB2	1.97	0.47
4:0:165:GLU:HG3	30:0:609:CHL:C4B	2.43	0.47
4:0:252:ALA:N	4:0:255:LEU:HD13	2.29	0.47
36:0:618:NEX:H173	18:r:53:TRP:HH2	1.80	0.47
1:7:185:PRO:HD2	32:7:317:LUT:H23	1.96	0.47
31:7:316:CLA:H52	34:9:301:LMG:HC72	1.96	0.47
2:9:94:HIS:HD2	32:9:318:LUT:H15	1.79	0.47
2:9:124:VAL:HG11	2:9:127:LYS:HE3	1.95	0.47
2:9:143:ASN:HB3	2:9:146:LEU:HG	1.96	0.47
31:9:305:CLA:HED2	31:9:305:CLA:C1	2.40	0.47
2:q:101:GLY:HA2	32:q:318:LUT:H181	1.97	0.47
31:a:409:CLA:HMA3	45:c:616:DGD:HBW1	1.96	0.47
7:c:394:SER:HA	7:c:408:VAL:HG23	1.95	0.47
8:d:145:ALA:CB	8:d:272:LEU:HD11	2.44	0.47
18:r:45:ARG:HD2	18:r:47:TYR:OH	2.15	0.47
30:s:302:CHL:HBB1	30:s:302:CHL:HMB1	1.96	0.47
30:s:307:CHL:CMC	32:s:318:LUT:H163	2.44	0.47
24:y:257:ASN:N	24:y:257:ASN:OD1	2.47	0.47
29:F1:118:ASN:HB2	29:F1:121:GLU:HG3	1.95	0.47
2:2:47:ALA:HB1	30:2:601:CHL:CBC	2.44	0.47
2:2:125:TRP:HH2	2:2:224:PHE:HD1	1.61	0.47
3:3:233:LEU:HB2	32:3:317:LUT:H22	1.96	0.47
34:3:321:LMG:HC71	34:3:321:LMG:H312	1.97	0.47
2:4:94:HIS:HE1	31:4:603:CLA:C4D	2.28	0.47
2:4:223:PHE:CE1	35:4:615:RRX:H52	2.49	0.47
3:5:258:TYR:OH	31:5:615:CLA:HBC3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:6:314:CLA:C4B	31:6:314:CLA:H62	2.43	0.47
43:A:410:BCR:H351	43:A:410:BCR:H15C	1.65	0.47
6:B:36:SER:OG	43:B:618:BCR:H362	2.14	0.47
7:C:216:ASP:OD1	7:C:216:ASP:N	2.47	0.47
45:C:620:DGD:HBF1	45:C:620:DGD:HBG2	1.97	0.47
2:G:171:TYR:HE2	3:N:54:ASN:H	1.62	0.47
30:G:623:CHL:HAA2	30:G:623:CHL:HBD	1.95	0.47
31:S:303:CLA:H8	31:S:303:CLA:H122	1.35	0.47
31:8:604:CLA:NB	36:8:617:NEX:H242	2.30	0.47
3:p:245:PHE:CE1	3:p:249:TYR:HB2	2.49	0.47
2:q:130:ALA:HB2	30:q:309:CHL:HED1	1.97	0.47
2:q:130:ALA:O	2:q:134:ASN:N	2.47	0.47
6:b:385:ARG:NH1	17:o:213:GLY:O	2.38	0.47
8:d:20:ASP:O	8:d:24:ARG:HG3	2.15	0.47
19:s:140:GLY:HA3	30:s:308:CHL:C3D	2.44	0.47
33:s:322:LHG:H262	33:s:322:LHG:H161	1.96	0.47
34:x:202:LMG:H301	34:x:202:LMG:H332	1.62	0.47
26:u:153:GLU:OE1	26:u:197:LYS:NZ	2.47	0.47
29:F1:89:ASP:N	29:F1:89:ASP:OD1	2.47	0.47
2:2:234:PRO:HB3	35:2:614:RRX:H50	1.95	0.47
31:2:613:CLA:HMB1	31:2:613:CLA:HBB1	1.95	0.47
3:3:258:TYR:OH	31:3:316:CLA:HAC1	2.14	0.47
2:4:230:THR:HG21	31:4:613:CLA:O1D	2.15	0.47
31:4:604:CLA:C1C	36:4:617:NEX:H362	2.45	0.47
34:4:620:LMG:H141	30:6:308:CHL:C2	2.45	0.47
7:C:225:HIS:HE1	31:C:601:CLA:NA	2.12	0.47
2:G:223:PHE:HE1	35:G:614:RRX:C31	2.26	0.47
31:G:604:CLA:C1C	36:G:616:NEX:H222	2.44	0.47
13:J:6:THR:HG22	28:P1:82:GLY:HA2	1.96	0.47
34:W:201:LMG:H151	34:W:201:LMG:H122	1.56	0.47
1:7:157:MET:HG2	30:7:310:CHL:CMC	2.44	0.47
34:7:322:LMG:H341	34:7:322:LMG:H122	1.95	0.47
31:8:613:CLA:HBA1	31:8:613:CLA:HBD	1.95	0.47
3:p:253:SER:OG	30:q:309:CHL:HAA1	2.15	0.47
30:q:309:CHL:H102	30:q:309:CHL:CHC	2.45	0.47
6:b:237:VAL:HG22	31:b:611:CLA:HBC2	1.96	0.47
7:c:74:LEU:HD13	7:c:77:LEU:HD22	1.95	0.47
7:c:373:GLN:HG2	26:u:131:GLN:HA	1.97	0.47
8:d:351:ALA:N	29:f1:187:ASP:O	2.46	0.47
30:g:307:CHL:HAA2	30:g:307:CHL:HBD	1.97	0.47
34:r:321:LMG:H121	34:x:202:LMG:O7	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:y:178:PHE:CZ	38:y:621:SQD:H92	2.50	0.47
29:f1:54:ARG:HB3	29:f1:57:ALA:HB2	1.97	0.47
1:1:86:ARG:O	1:1:90:ILE:HG13	2.15	0.47
1:1:247:TYR:O	1:1:251:LEU:HD13	2.13	0.47
34:2:621:LMG:HC2	31:3:316:CLA:O2A	2.15	0.47
3:3:111:ASN:HB2	3:3:113:VAL:HG23	1.96	0.47
3:3:116:PHE:C	3:3:118:GLU:H	2.23	0.47
3:3:245:PHE:HB3	31:3:314:CLA:C1	2.43	0.47
2:4:222:GLY:O	2:4:226:GLN:HG3	2.15	0.47
31:4:614:CLA:H41	31:4:614:CLA:H61	1.68	0.47
3:5:47:GLN:NE2	3:5:55:PRO:HG3	2.29	0.47
31:5:603:CLA:HBC2	30:5:609:CHL:HHD	1.95	0.47
4:6:69:TYR:HE2	30:6:302:CHL:HBC2	1.79	0.47
4:6:115:ALA:HB2	34:6:322:LMG:O10	2.14	0.47
4:6:217:MET:CG	32:6:318:LUT:H12	2.29	0.47
31:6:304:CLA:HHC	31:6:304:CLA:CBB	2.44	0.47
7:C:358:ARG:O	26:U:126:ASN:ND2	2.47	0.47
45:C:620:DGD:HAF2	31:Y:311:CLA:HBB2	1.96	0.47
8:D:148:ALA:HB1	8:D:279:LEU:HB2	1.97	0.47
8:D:191:TRP:CE3	8:D:289:LEU:HD11	2.50	0.47
2:G:234:PRO:HB3	35:G:614:RRX:H50	1.97	0.47
30:G:606:CHL:HBD	30:G:606:CHL:HAA2	1.97	0.47
38:G:617:SQD:C32	33:7:319:LHG:C9	2.92	0.47
30:N:306:CHL:H122	32:S:317:LUT:C17	2.45	0.47
31:N:313:CLA:C1A	31:N:313:CLA:CGA	2.93	0.47
17:O:204:ASP:OD1	17:O:208:ARG:N	2.41	0.47
18:R:139:HIS:CE1	31:R:305:CLA:C4D	2.96	0.47
19:S:284:ASP:OD1	19:S:284:ASP:N	2.47	0.47
1:7:218:ILE:HD12	31:7:314:CLA:HAC2	1.96	0.47
31:8:603:CLA:HBA2	31:8:603:CLA:H12	1.59	0.47
31:8:609:CLA:H3A	31:8:609:CLA:HBA2	1.50	0.47
33:8:618:LHG:H271	33:8:618:LHG:H242	1.75	0.47
2:9:167:GLU:HG3	30:9:311:CHL:C4B	2.44	0.47
3:p:118:GLU:H	3:p:127:GLN:HE22	1.60	0.47
2:q:52:PRO:HD2	30:q:303:CHL:CBB	2.45	0.47
5:a:151:VAL:O	5:a:155:THR:HG23	2.15	0.47
5:a:312:ARG:NH1	29:f1:83:ASN:OD1	2.48	0.47
6:b:207:ILE:CD1	33:b:628:LHG:H201	2.45	0.47
31:b:603:CLA:H41	31:b:603:CLA:H61	1.41	0.47
31:b:609:CLA:H152	31:b:610:CLA:H172	1.97	0.47
7:c:14:ARG:HA	7:c:14:ARG:HE	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:d:404:CLA:H62	31:d:404:CLA:H41	1.47	0.47
14:k:17:PRO:HB2	33:z:102:LHG:HC61	1.96	0.47
15:l:30:VAL:HG22	20:t:9:LEU:HB3	1.97	0.47
3:n:177:ASP:HB3	3:n:180:TYR:O	2.15	0.47
17:o:106:VAL:HG22	17:o:280:VAL:HG22	1.95	0.47
31:s:316:CLA:CHA	31:s:316:CLA:HBA1	2.45	0.47
24:y:157:VAL:HG11	30:y:606:CHL:HED2	1.95	0.47
31:y:613:CLA:H18	31:y:614:CLA:CGA	2.44	0.47
28:P1:17:ASN:HD22	28:P1:20:VAL:HG23	1.80	0.47
1:1:198:LEU:HD23	1:1:201:LYS:HD2	1.97	0.47
2:2:92:VAL:HB	2:2:184:LEU:HD21	1.95	0.47
31:2:604:CLA:CHB	36:2:616:NEX:H383	2.45	0.47
31:3:301:CLA:H93	31:3:301:CLA:H62	1.65	0.47
2:4:129:GLY:HA3	30:4:607:CHL:CGD	2.45	0.47
4:6:106:THR:HG21	31:6:305:CLA:HAC2	1.96	0.47
6:B:123:PHE:O	6:B:131:PRO:HA	2.15	0.47
6:B:201:HIS:HE1	31:B:602:CLA:C1D	2.14	0.47
7:C:120:HIS:HE1	31:C:613:CLA:NA	2.11	0.47
34:D:409:LMG:H152	34:D:409:LMG:H181	1.78	0.47
3:N:162:ILE:HD11	36:N:318:NEX:C34	2.45	0.47
17:O:270:THR:HG22	17:O:277:PRO:HB3	1.97	0.47
4:0:189:PRO:HA	18:r:47:TYR:OH	2.14	0.47
31:0:610:CLA:H41	31:0:612:CLA:HMA2	1.97	0.47
31:8:610:CLA:HHC	31:8:610:CLA:HBB1	1.97	0.47
31:8:612:CLA:NC	31:8:612:CLA:H51	2.30	0.47
3:p:166:ARG:HG3	30:p:608:CHL:CHD	2.45	0.47
31:p:613:CLA:C3B	32:p:616:LUT:H183	2.45	0.47
2:q:226:GLN:HG2	31:q:315:CLA:C1D	2.45	0.47
30:q:309:CHL:HHC	30:q:309:CHL:HBB1	1.97	0.47
5:a:259:ILE:HD13	44:a:414:PL9:H18	1.96	0.47
6:b:112:ILE:HG12	43:b:618:BCR:H272	1.97	0.47
31:c:607:CLA:H112	43:c:615:BCR:H362	1.97	0.47
43:d:406:BCR:H19C	10:f:29:THR:HG23	1.96	0.47
31:g:313:CLA:H122	31:g:313:CLA:H8	1.63	0.47
11:h:56:LEU:HB3	43:h:101:BCR:H14C	1.97	0.47
3:n:224:ILE:HD12	3:n:258:TYR:OH	2.14	0.47
2:2:211:LYS:NZ	33:2:617:LHG:O5	2.48	0.47
2:2:258:LEU:HD22	2:2:260:LEU:HD12	1.96	0.47
3:3:69:TRP:CG	3:3:69:TRP:O	2.68	0.47
34:A:414:LMG:HC71	34:A:414:LMG:HC2	1.62	0.47
31:B:606:CLA:H193	43:B:619:BCR:H363	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:D:401:PHO:H71	42:D:401:PHO:H112	1.55	0.47
18:R:204:GLU:OE1	18:R:206:ASP:N	2.48	0.47
19:S:180:GLU:HG3	31:S:310:CLA:C4B	2.45	0.47
31:9:306:CLA:H8	31:9:306:CLA:H51	1.36	0.47
3:p:136:TYR:CE1	31:p:604:CLA:H2	2.49	0.47
3:p:227:LYS:HB2	3:p:232:ASN:OD1	2.15	0.47
6:b:36:SER:OG	43:b:619:BCR:H362	2.15	0.47
6:b:333:GLY:O	6:b:439:SER:HB3	2.15	0.47
31:b:614:CLA:H62	31:b:614:CLA:H41	1.56	0.47
7:c:36:LYS:NZ	7:c:121:SER:O	2.47	0.47
31:c:601:CLA:H203	31:c:607:CLA:H152	1.96	0.47
45:c:619:DGD:HE1	31:y:611:CLA:CMA	2.44	0.47
11:h:57:PHE:HB2	43:h:101:BCR:H12C	1.97	0.47
24:y:90:ILE:HG21	31:y:603:CLA:HAA2	1.97	0.47
31:1:611:CLA:HHC	31:1:611:CLA:CBB	2.44	0.47
30:1:619:CHL:HED3	3:3:123:LYS:HA	1.96	0.47
30:3:302:CHL:CGA	30:3:302:CHL:C1A	2.93	0.47
31:3:306:CLA:HMA2	30:3:308:CHL:C3C	2.45	0.47
31:5:602:CLA:HED2	31:5:602:CLA:H2A	1.95	0.47
4:6:93:HIS:CE1	31:6:304:CLA:C4D	2.97	0.47
4:6:246:ASN:HB2	31:6:314:CLA:O1A	2.15	0.47
30:6:307:CHL:O2D	30:6:307:CHL:HBA2	2.15	0.47
31:6:312:CLA:NB	33:6:320:LHG:O4	2.48	0.47
31:B:602:CLA:HBD	31:B:602:CLA:HBA2	1.97	0.47
31:B:610:CLA:C2	31:B:610:CLA:H72	2.45	0.47
38:B:623:SQD:H223	38:B:623:SQD:H341	1.95	0.47
8:D:157:PHE:CE2	8:D:171:PRO:HG2	2.50	0.47
2:G:218:PHE:CE1	31:G:612:CLA:HMC1	2.50	0.47
36:N:318:NEX:H161	36:N:318:NEX:H192	1.96	0.47
18:R:233:LEU:HB3	31:R:312:CLA:HMA2	1.97	0.47
31:R:305:CLA:HED2	31:R:305:CLA:H2A	1.97	0.47
4:0:72:ASP:HA	32:0:617:LUT:H24	1.97	0.47
3:p:54:ASN:N	2:q:171:TYR:HE2	2.06	0.47
3:p:75:SER:OG	31:p:602:CLA:O1A	2.21	0.47
5:a:101:SER:HA	34:a:413:LMG:HC61	1.97	0.47
7:c:36:LYS:HE2	7:c:126:GLU:HG3	1.97	0.47
7:c:101:VAL:HG21	38:s:301:SQD:H462	1.97	0.47
31:c:612:CLA:CBB	33:c:622:LHG:H102	2.45	0.47
3:n:134:LEU:HD21	31:n:305:CLA:HAA1	1.97	0.47
30:n:306:CHL:C2	19:s:120:ILE:HA	2.44	0.47
30:n:308:CHL:H122	30:n:310:CHL:CMC	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:n:314:CLA:NC	31:n:314:CLA:H51	2.30	0.47
36:r:301:NEX:H161	36:r:301:NEX:H193	1.97	0.47
22:w:67:GLY:O	22:w:70:THR:OG1	2.26	0.47
25:z:61:VAL:HG13	25:z:62:VAL:HG23	1.97	0.47
1:1:90:ILE:HD13	31:1:603:CLA:HBA1	1.97	0.46
2:2:240:ASP:HB3	2:2:248:ASN:HD22	1.80	0.46
32:2:615:LUT:H35	32:2:615:LUT:H401	1.38	0.46
3:3:86:GLU:HA	3:3:179:LEU:HD11	1.97	0.46
3:3:221:GLN:HE21	3:3:232:ASN:HD22	1.63	0.46
2:4:118:ASP:HB3	34:Q1:101:LMG:C38	2.44	0.46
3:5:110:ARG:CZ	3:5:230:ILE:HB	2.45	0.46
5:A:106:LEU:HD11	43:A:410:BCR:H402	1.97	0.46
33:A:415:LHG:H162	34:A:418:LMG:H151	1.97	0.46
7:C:244:PRO:HA	31:C:606:CLA:HED3	1.96	0.46
34:G:622:LMG:H151	31:N:321:CLA:H11	1.97	0.46
11:H:74:LEU:HB2	11:H:77:VAL:HG22	1.97	0.46
34:J:101:LMG:H331	34:J:101:LMG:H161	1.97	0.46
48:R:302:LMU:O2'	48:R:302:LMU:H5'	2.15	0.46
1:7:132:ILE:HD12	30:7:307:CHL:HMD1	1.97	0.46
3:8:177:ASP:HB3	3:8:180:TYR:O	2.15	0.46
2:9:118:ASP:HB3	2:9:142:GLY:HA3	1.96	0.46
2:9:127:LYS:HA	30:9:309:CHL:HED3	1.96	0.46
2:9:218:PHE:CD1	33:9:320:LHG:H301	2.50	0.46
3:p:94:TRP:CE2	30:p:608:CHL:HED2	2.50	0.46
3:p:249:TYR:CD1	3:p:258:TYR:CD1	3.03	0.46
31:p:610:CLA:HMB1	31:p:610:CLA:HBB1	1.96	0.46
2:q:49:TRP:CD1	2:q:49:TRP:H	2.33	0.46
2:q:94:HIS:HE1	31:q:305:CLA:C4D	2.28	0.46
2:q:177:VAL:HG22	2:q:189:PHE:CD2	2.50	0.46
5:a:46:SER:O	5:a:50:ILE:HG12	2.15	0.46
6:b:315:ILE:HG12	6:b:321:LYS:HG3	1.97	0.46
31:b:614:CLA:HBB1	31:b:614:CLA:HMB1	1.96	0.46
34:b:626:LMG:H121	8:d:32:TRP:CD1	2.50	0.46
10:f:15:PHE:CD2	27:q1:27:LEU:HD13	2.49	0.46
31:n:312:CLA:HHC	31:n:312:CLA:HBB1	1.97	0.46
19:s:114:ALA:HA	32:s:318:LUT:C18	2.45	0.46
31:s:304:CLA:HED2	31:s:304:CLA:H2A	1.96	0.46
30:1:601:CHL:HHC	30:1:601:CHL:CBB	2.43	0.46
31:1:612:CLA:HBB1	31:1:612:CLA:HHC	1.98	0.46
33:1:617:LHG:H281	33:1:617:LHG:H242	1.97	0.46
2:2:256:LYS:HD3	2:2:257:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:172:SER:HA	3:5:54:ASN:OD1	2.15	0.46
3:5:115:ASN:N	3:5:115:ASN:ND2	2.63	0.46
3:5:241:ASP:OD1	3:5:241:ASP:N	2.47	0.46
31:5:602:CLA:CHA	31:5:602:CLA:HBA1	2.45	0.46
4:6:49:PHE:CE2	4:6:50:LEU:HD13	2.49	0.46
7:C:149:LEU:O	7:C:153:LEU:HB2	2.15	0.46
45:C:620:DGD:HD2	45:C:620:DGD:HG31	1.64	0.46
2:G:223:PHE:CZ	35:G:614:RRX:H48	2.48	0.46
31:G:603:CLA:HMC2	30:G:608:CHL:H13	1.97	0.46
17:O:179:LEU:HD23	17:O:192:PHE:HB3	1.98	0.46
32:S:318:LUT:H35	32:S:318:LUT:H401	1.76	0.46
20:T:29:ILE:HG22	20:T:30:VAL:HG22	1.97	0.46
4:0:47:VAL:HB	30:0:601:CHL:CBC	2.45	0.46
4:0:169:VAL:HG21	2:q:50:LEU:CD2	2.46	0.46
30:0:609:CHL:HMB3	30:q:303:CHL:HHB	1.96	0.46
2:9:170:ARG:HA	30:9:310:CHL:C3C	2.44	0.46
31:9:315:CLA:C1A	31:9:315:CLA:CGA	2.93	0.46
3:p:134:LEU:HD13	30:p:606:CHL:HHD	1.96	0.46
2:q:187:GLY:O	2:q:188:GLY:C	2.59	0.46
2:q:188:GLY:O	2:q:189:PHE:C	2.59	0.46
33:q:320:LHG:H291	33:q:320:LHG:H261	1.58	0.46
41:a:404:CL:CL	8:d:317:LYS:HE2	2.51	0.46
31:b:609:CLA:HBA2	31:b:609:CLA:H3A	1.60	0.46
45:c:616:DGD:HBV2	34:w:201:LMG:H122	1.96	0.46
2:g:146:LEU:HD23	30:g:306:CHL:HED2	1.97	0.46
33:g:319:LHG:C6	37:g:321:XAT:H382	2.46	0.46
3:n:38:VAL:HG12	3:n:42:GLY:HA3	1.97	0.46
3:n:104:THR:HB	3:n:105:PRO:HD3	1.97	0.46
31:n:305:CLA:H101	31:s:306:CLA:CMA	2.45	0.46
17:o:209:GLY:HA2	17:o:235:LYS:HD2	1.97	0.46
19:s:90:LEU:HD23	31:s:303:CLA:H42	1.98	0.46
31:s:305:CLA:H92	31:s:305:CLA:H61	1.69	0.46
34:Q1:101:LMG:H362	34:Q1:101:LMG:H151	1.97	0.46
31:2:610:CLA:C4D	31:2:611:CLA:HMD3	2.45	0.46
3:3:79:GLU:OE1	3:3:79:GLU:N	2.46	0.46
2:4:153:VAL:O	2:4:157:LEU:HD13	2.14	0.46
2:4:164:GLY:HA2	30:4:609:CHL:CAB	2.45	0.46
31:4:602:CLA:HAC2	33:4:618:LHG:H252	1.97	0.46
3:5:246:TRP:H	3:5:246:TRP:CD1	2.33	0.46
30:6:308:CHL:H41	30:6:308:CHL:H101	1.96	0.46
44:A:416:PL9:H451	44:A:416:PL9:H471	1.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:B:619:BCR:H382	34:a:401:LMG:H151	1.97	0.46
31:G:610:CLA:H61	31:G:610:CLA:H41	1.62	0.46
33:K:102:LHG:HC82	33:K:102:LHG:HC5	1.66	0.46
30:N:307:CHL:OMC	32:N:317:LUT:H163	2.15	0.46
1:7:168:GLY:HA2	18:r:44:TYR:CE1	2.50	0.46
31:7:305:CLA:HBB1	31:7:305:CLA:CMB	2.44	0.46
30:q:303:CHL:C1D	33:q:320:LHG:HC81	2.45	0.46
44:a:414:PL9:H321	10:f:25:LEU:HD21	1.97	0.46
6:b:53:ASN:OD1	6:b:58:GLN:NE2	2.48	0.46
6:b:243:ALA:HA	6:b:246:PHE:CD2	2.51	0.46
31:b:612:CLA:HBB1	31:b:612:CLA:CMB	2.45	0.46
45:c:619:DGD:CIA	31:y:614:CLA:H51	2.45	0.46
38:g:301:SQD:H462	38:g:301:SQD:H242	1.60	0.46
30:g:302:CHL:HED3	33:g:319:LHG:H292	1.96	0.46
33:j:102:LHG:HC31	29:f1:58:GLY:HA2	1.98	0.46
3:n:70:ASP:OD2	3:n:75:SER:OG	2.30	0.46
30:n:306:CHL:H142	32:s:317:LUT:H171	1.96	0.46
31:r:304:CLA:H93	31:r:304:CLA:H62	1.72	0.46
34:y:620:LMG:H332	34:y:620:LMG:H361	1.81	0.46
26:u:63:ALA:O	26:u:68:PHE:HB2	2.15	0.46
29:F1:118:ASN:HB3	29:F1:120:ASP:OD1	2.16	0.46
30:1:601:CHL:HHB	30:3:310:CHL:HMB3	1.96	0.46
2:4:74:THR:HG21	30:6:310:CHL:HBA1	1.98	0.46
34:4:621:LMG:H171	34:4:621:LMG:H142	1.69	0.46
36:6:319:NEX:H161	36:6:319:NEX:H193	1.97	0.46
7:C:406:ASN:HD21	45:C:617:DGD:HD4	1.81	0.46
7:C:412:SER:O	7:C:416:THR:HB	2.15	0.46
31:C:613:CLA:H11	43:C:614:BCR:H381	1.98	0.46
34:C:624:LMG:H322	34:C:624:LMG:H291	1.75	0.46
8:D:202:ALA:HB2	44:D:406:PL9:H353	1.98	0.46
10:F:15:PHE:CD2	27:Q1:27:LEU:HD13	2.51	0.46
3:N:180:TYR:HB3	31:N:310:CLA:HED3	1.96	0.46
31:N:305:CLA:CHA	31:N:305:CLA:HBA1	2.39	0.46
17:O:112:PHE:HZ	6:b:82:GLY:HA3	1.79	0.46
31:S:313:CLA:HBB1	31:S:313:CLA:HMB3	1.96	0.46
31:0:614:CLA:H92	31:0:614:CLA:H62	1.76	0.46
36:0:618:NEX:H161	36:0:618:NEX:H193	1.97	0.46
31:7:311:CLA:H41	31:7:311:CLA:H61	1.61	0.46
31:q:312:CLA:ND	35:q:317:RRX:H11	2.30	0.46
7:c:105:LEU:HD23	38:s:301:SQD:H141	1.97	0.46
2:2:124:VAL:O	2:2:125:TRP:C	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:132:ILE:HG13	2:2:152:ILE:HD13	1.96	0.46
2:2:195:LEU:HB2	31:2:609:CLA:O1A	2.16	0.46
31:2:609:CLA:H62	31:2:609:CLA:H41	1.75	0.46
36:2:616:NEX:H171	36:2:616:NEX:H193	1.97	0.46
37:2:619:XAT:H31	37:2:619:XAT:H391	1.77	0.46
2:4:49:TRP:CD1	2:4:49:TRP:H	2.34	0.46
2:4:139:ASN:CG	2:4:144:PRO:HA	2.41	0.46
30:4:606:CHL:HAA2	30:4:606:CHL:HBD	1.98	0.46
8:D:113:PHE:CZ	43:D:405:BCR:HC22	2.50	0.46
31:N:303:CLA:H72	32:N:317:LUT:H30	1.97	0.46
31:Y:310:CLA:H92	31:Y:310:CLA:H61	1.65	0.46
4:0:151:VAL:O	4:0:154:LEU:N	2.49	0.46
31:7:305:CLA:H61	31:7:305:CLA:H92	1.61	0.46
31:7:316:CLA:CHC	34:9:301:LMG:H361	2.45	0.46
3:p:118:GLU:N	3:p:127:GLN:HE22	2.14	0.46
3:p:142:LEU:O	3:p:144:HIS:N	2.49	0.46
31:p:610:CLA:H92	32:p:616:LUT:C28	2.46	0.46
2:q:110:LEU:HD23	2:q:110:LEU:C	2.40	0.46
38:b:627:SQD:H341	38:b:627:SQD:H202	1.98	0.46
33:b:628:LHG:H182	31:r:316:CLA:H202	1.96	0.46
7:c:40:ALA:HB2	31:c:611:CLA:HMA2	1.98	0.46
45:c:618:DGD:HA91	45:c:618:DGD:HA62	1.60	0.46
30:y:601:CHL:H41	30:y:601:CHL:H61	1.72	0.46
1:1:48:LYS:HG2	1:1:54:SER:OG	2.16	0.46
30:1:605:CHL:HAA2	30:1:605:CHL:HBD	1.97	0.46
34:1:618:LMG:H351	36:R:301:NEX:H402	1.98	0.46
31:2:609:CLA:HMB2	31:2:611:CLA:HBA2	1.96	0.46
3:3:66:ASP:HA	31:3:304:CLA:O1D	2.15	0.46
31:5:613:CLA:HBA1	31:5:614:CLA:C2D	2.46	0.46
34:5:620:LMG:C6	31:6:315:CLA:CMA	2.93	0.46
4:6:208:LYS:HE2	31:6:312:CLA:O1D	2.15	0.46
4:6:221:PHE:O	4:6:225:ILE:HG13	2.15	0.46
6:B:237:VAL:CG2	31:B:610:CLA:HBC2	2.45	0.46
6:B:464:PHE:CZ	33:D:407:LHG:H261	2.51	0.46
31:B:606:CLA:H91	31:B:606:CLA:H111	1.69	0.46
43:B:618:BCR:H363	43:t:101:BCR:H341	1.97	0.46
34:B:625:LMG:H342	30:R:309:CHL:C4	2.44	0.46
8:D:46:GLY:CA	43:D:405:BCR:H11C	2.45	0.46
31:G:604:CLA:H3A	31:G:604:CLA:HBA2	1.36	0.46
33:G:618:LHG:H362	37:G:620:XAT:C12	2.44	0.46
34:G:622:LMG:HC91	34:G:622:LMG:C13	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:145:LEU:HD11	34:Y:319:LMG:H322	1.98	0.46
26:U:130:ARG:C	26:U:132:VAL:H	2.23	0.46
31:0:614:CLA:H71	31:0:614:CLA:C3B	2.45	0.46
3:8:38:VAL:HG12	3:8:42:GLY:HA3	1.98	0.46
2:q:101:GLY:HA2	32:q:318:LUT:C18	2.46	0.46
5:a:221:SER:HA	8:d:139:ARG:HB2	1.98	0.46
6:b:159:THR:O	6:b:180:ALA:HB1	2.15	0.46
31:b:605:CLA:HBA1	31:b:613:CLA:H152	1.98	0.46
31:b:612:CLA:O2A	33:b:625:LHG:H381	2.16	0.46
8:d:93:TRP:HB3	34:d:410:LMG:HC92	1.98	0.46
31:d:405:CLA:H43	23:x:76:VAL:HA	1.98	0.46
31:n:312:CLA:HHC	31:n:312:CLA:CBB	2.46	0.46
19:s:163:LEU:HD23	19:s:168:VAL:HG22	1.96	0.46
31:y:613:CLA:H93	31:y:613:CLA:H112	1.62	0.46
29:f1:120:ASP:HB3	29:f1:175:LYS:NZ	2.31	0.46
1:1:123:GLY:O	1:1:126:ILE:HG22	2.16	0.46
31:1:610:CLA:C2	32:1:615:LUT:H28	2.37	0.46
2:2:146:LEU:O	2:2:148:HIS:N	2.45	0.46
30:2:605:CHL:HHC	30:2:605:CHL:CBB	2.44	0.46
3:5:115:ASN:ND2	3:5:138:GLY:HA3	2.31	0.46
31:6:304:CLA:CMA	31:6:304:CLA:H2	2.46	0.46
33:A:415:LHG:H251	33:A:415:LHG:H142	1.98	0.46
6:B:186:ASP:OD1	6:B:186:ASP:N	2.49	0.46
31:C:613:CLA:HBB1	31:C:613:CLA:HMB3	1.97	0.46
2:G:147:ILE:HG23	30:G:605:CHL:C1D	2.46	0.46
31:G:603:CLA:H52	31:G:603:CLA:H8	1.47	0.46
30:G:605:CHL:HHC	30:G:605:CHL:CBB	2.44	0.46
18:R:245:MET:SD	31:R:304:CLA:HAB	2.56	0.46
19:S:121:PRO:HA	19:S:124:LEU:HD12	1.98	0.46
1:7:140:LEU:HD13	31:7:305:CLA:H91	1.97	0.46
1:7:244:TYR:HA	1:7:248:ALA:HB2	1.96	0.46
31:8:613:CLA:HBA1	31:8:613:CLA:CBD	2.46	0.46
3:p:104:THR:HB	3:p:105:PRO:HD3	1.98	0.46
31:p:613:CLA:C2	31:p:614:CLA:HMD2	2.45	0.46
2:q:50:LEU:HD12	2:q:50:LEU:HA	1.80	0.46
2:q:169:TYR:HB2	30:q:310:CHL:CHC	2.46	0.46
5:a:60:ILE:HD12	5:a:84:PRO:HD2	1.98	0.46
6:b:258:TYR:OH	8:d:162:LEU:O	2.24	0.46
2:g:259:PRO:HD3	30:y:607:CHL:C1	2.46	0.46
33:l:101:LHG:H122	33:l:101:LHG:HC92	1.53	0.46
3:n:143:ILE:HA	30:n:306:CHL:C4D	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:n:162:ILE:HD11	36:n:319:NEX:C34	2.45	0.46
31:n:313:CLA:HBB1	31:n:313:CLA:CMB	2.45	0.46
31:s:303:CLA:H112	31:s:303:CLA:H152	1.53	0.46
29:f1:107:LEU:C	29:f1:107:LEU:HD12	2.41	0.46
3:3:89:VAL:HG22	3:3:205:LEU:HD21	1.97	0.46
30:3:302:CHL:H71	30:3:302:CHL:CHC	2.46	0.46
32:3:318:LUT:H15	32:3:318:LUT:H201	1.71	0.46
3:5:49:LEU:HA	30:5:601:CHL:C4B	2.46	0.46
34:5:620:LMG:HC62	31:6:315:CLA:HMA2	1.95	0.46
31:6:316:CLA:HBB1	31:6:316:CLA:CMB	2.45	0.46
5:A:131:TRP:CH2	31:C:605:CLA:HAA2	2.51	0.46
31:A:406:CLA:H121	31:A:406:CLA:HMA3	1.98	0.46
6:B:311:PHE:O	6:B:317:ASN:ND2	2.47	0.46
6:B:385:ARG:NH1	17:O:213:GLY:O	2.43	0.46
7:C:374:PRO:O	7:C:378:ARG:HG3	2.16	0.46
9:E:13:ILE:HD13	47:E:101:HEM:HBD1	1.96	0.46
14:K:18:PHE:CD1	33:K:102:LHG:H261	2.51	0.46
31:N:313:CLA:H172	31:N:314:CLA:ND	2.31	0.46
32:R:317:LUT:H35	32:R:317:LUT:H401	1.41	0.46
36:S:319:NEX:H161	36:S:319:NEX:H193	1.98	0.46
24:Y:176:ASN:HB2	38:Y:320:SQD:O3	2.15	0.46
4:0:72:ASP:OD2	4:0:77:SER:OG	2.29	0.46
32:7:317:LUT:H11	32:7:317:LUT:H191	1.81	0.46
3:8:143:ILE:HA	30:8:605:CHL:C4D	2.46	0.46
3:8:239:ALA:O	3:8:243:THR:HG22	2.16	0.46
31:9:314:CLA:HMC3	35:9:317:RRX:H44	1.97	0.46
3:p:245:PHE:O	3:p:247:VAL:N	2.48	0.46
2:q:85:ALA:O	2:q:89:GLU:HG3	2.15	0.46
5:a:159:ILE:HG23	45:c:616:DGD:HB61	1.98	0.46
6:b:314:TYR:CE2	6:b:316:GLY:HA3	2.51	0.46
33:b:628:LHG:H321	33:b:628:LHG:H291	1.40	0.46
7:c:23:TRP:CD1	48:c:623:LMU:H6'1	2.50	0.46
7:c:270:MET:HG2	31:c:601:CLA:H72	1.98	0.46
44:d:407:PL9:H513	33:d:408:LHG:H221	1.96	0.46
3:n:239:ALA:O	3:n:243:THR:HG22	2.16	0.46
30:r:308:CHL:HMB2	31:r:311:CLA:HMC1	1.98	0.46
33:s:322:LHG:H311	33:s:322:LHG:H282	1.56	0.46
29:F1:174:LYS:HE3	29:F1:200:THR:HG21	1.97	0.46
1:1:215:GLY:O	1:1:219:GLN:HG3	2.15	0.46
3:3:118:GLU:HG2	3:3:123:LYS:O	2.16	0.46
3:5:239:ALA:HB1	3:5:242:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:C:617:DGD:HAF2	45:C:618:DGD:HAF2	1.97	0.46
11:H:75:ASP:OD1	11:H:75:ASP:N	2.48	0.46
3:N:126:ALA:HB2	30:Y:301:CHL:HED2	1.98	0.46
30:S:302:CHL:C1D	33:S:320:LHG:HC82	2.46	0.46
31:S:303:CLA:H92	31:S:303:CLA:H62	1.64	0.46
24:Y:192:ASP:OD1	32:Y:315:LUT:O23	2.23	0.46
31:0:603:CLA:H3A	31:0:603:CLA:HBA1	1.56	0.46
34:0:620:LMG:H142	34:7:301:LMG:H301	1.97	0.46
3:8:104:THR:HB	3:8:105:PRO:HD3	1.98	0.46
3:8:134:LEU:HD21	31:8:604:CLA:HAA1	1.97	0.46
3:8:219:GLY:HA3	34:9:301:LMG:H392	1.98	0.46
2:q:201:THR:O	2:q:205:LEU:HB2	2.15	0.46
34:a:416:LMG:H132	48:c:623:LMU:O2'	2.16	0.46
6:b:26:HIS:CE1	31:b:613:CLA:HMA2	2.51	0.46
33:b:628:LHG:H171	31:r:316:CLA:C20	2.45	0.46
8:d:117:HIS:CE1	31:d:405:CLA:C4D	2.99	0.46
8:d:237:PRO:HD3	28:p1:60:VAL:HG12	1.98	0.46
31:n:304:CLA:CAD	30:n:310:CHL:H11	2.46	0.46
31:n:305:CLA:H202	31:s:306:CLA:CHA	2.46	0.46
17:o:227:GLU:HA	17:o:230:LEU:HD12	1.97	0.46
31:r:304:CLA:H102	31:r:305:CLA:CMB	2.45	0.46
20:t:29:ILE:HG22	20:t:30:VAL:HG13	1.98	0.46
29:F1:165:VAL:HG13	29:F1:179:TYR:CE1	2.50	0.46
3:3:56:PRO:HG2	3:3:59:LEU:HB2	1.97	0.46
2:4:72:TRP:O	32:4:616:LUT:H24	2.16	0.46
3:5:190:LEU:HB2	31:5:610:CLA:O2A	2.16	0.46
3:5:239:ALA:CB	3:5:242:ALA:HB3	2.45	0.46
31:5:610:CLA:H12	31:5:610:CLA:C3A	2.45	0.46
33:5:619:LHG:HC62	33:5:619:LHG:P	2.56	0.46
5:A:307:VAL:HG23	10:F:44:ARG:HD2	1.97	0.46
31:B:605:CLA:H91	31:B:605:CLA:H111	1.72	0.46
38:B:623:SQD:H242	34:D:410:LMG:H311	1.98	0.46
7:C:304:THR:HG23	26:U:71:ILE:HG21	1.98	0.46
7:C:454:VAL:HG13	8:D:251:ARG:HD2	1.97	0.46
31:C:607:CLA:H3A	31:C:607:CLA:HBA1	1.74	0.46
47:E:101:HEM:CAC	10:F:26:ALA:HB1	2.46	0.46
34:G:621:LMG:H311	31:N:321:CLA:H42	1.98	0.46
16:M:16:ILE:HG23	38:M:102:SQD:H191	1.98	0.46
17:O:135:MET:HA	17:O:154:GLY:HA3	1.98	0.46
18:R:115:VAL:HG23	18:R:207:PRO:HG3	1.97	0.46
18:R:238:ILE:HD12	18:R:239:LYS:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:S:306:CLA:O1D	31:S:306:CLA:H2A	2.16	0.46
30:Y:301:CHL:HBD	30:Y:301:CHL:HAA1	1.97	0.46
4:0:202:LEU:HB3	31:0:610:CLA:HMA1	1.96	0.46
3:p:122:PHE:O	30:p:607:CHL:HMA3	2.15	0.46
3:p:126:ALA:HA	3:p:129:PHE:HD2	1.81	0.46
3:p:220:VAL:CG1	31:p:613:CLA:HAC2	2.44	0.46
2:q:103:LEU:HD12	35:q:317:RRX:C36	2.45	0.46
45:c:619:DGD:HAN2	45:c:619:DGD:CBB	2.46	0.46
47:e:102:HEM:CMB	27:q1:19:VAL:HG21	2.46	0.46
31:g:305:CLA:HBA2	31:g:305:CLA:H3A	1.26	0.46
30:g:306:CHL:HHC	30:g:306:CHL:CBB	2.44	0.46
31:n:311:CLA:H171	31:s:306:CLA:HBB2	1.97	0.46
30:r:310:CHL:HBA1	38:r:322:SQD:H301	1.97	0.46
43:t:101:BCR:H361	43:t:101:BCR:H20C	1.62	0.46
31:2:602:CLA:CGA	32:2:615:LUT:H24	2.46	0.45
31:3:305:CLA:HMC3	32:3:318:LUT:H12	1.97	0.45
31:4:602:CLA:H122	31:4:602:CLA:H8	1.76	0.45
31:6:311:CLA:HBB1	31:6:311:CLA:HMB1	1.98	0.45
5:A:118:HIS:CE1	31:A:409:CLA:C4D	2.98	0.45
5:A:170:ASP:OD2	7:C:345:ARG:NH1	2.47	0.45
34:A:418:LMG:H321	34:A:418:LMG:H292	1.72	0.45
6:B:149:LEU:HD13	31:B:604:CLA:H202	1.98	0.45
6:B:202:HIS:HE1	31:B:603:CLA:NA	2.12	0.45
6:B:466:HIS:CE1	31:B:608:CLA:C4D	2.99	0.45
31:B:606:CLA:H161	31:B:616:CLA:H111	1.98	0.45
7:C:384:MET:HE1	26:U:75:ARG:HH11	1.81	0.45
31:G:602:CLA:H2	31:G:602:CLA:C1B	2.47	0.45
19:S:115:ALA:HB1	32:S:317:LUT:H12	1.98	0.45
19:S:241:LEU:HD21	31:S:313:CLA:CBC	2.46	0.45
31:S:311:CLA:O2A	32:S:317:LUT:H26	2.17	0.45
4:0:111:GLN:OE1	4:0:117:ASN:ND2	2.46	0.45
31:7:316:CLA:HBB1	31:7:316:CLA:HMB3	1.98	0.45
31:8:611:CLA:HBB1	31:8:611:CLA:CMB	2.45	0.45
36:8:617:NEX:H171	36:8:617:NEX:H192	1.98	0.45
2:9:66:PHE:HB3	2:9:67:PRO:HD2	1.99	0.45
31:9:306:CLA:C3B	32:9:318:LUT:H183	2.45	0.45
30:9:310:CHL:HAA1	30:9:310:CHL:HBD	1.97	0.45
2:q:46:ARG:NH2	2:q:62:LEU:O	2.50	0.45
2:q:177:VAL:HA	2:q:189:PHE:CG	2.51	0.45
2:q:211:LYS:HD3	31:q:313:CLA:O1D	2.16	0.45
31:q:313:CLA:CAC	33:q:320:LHG:HC61	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:a:132:GLU:O	5:a:136:ARG:HG2	2.16	0.45
6:b:341:LEU:HD22	6:b:429:ILE:HG22	1.97	0.45
8:d:148:ALA:HB2	8:d:276:VAL:HG13	1.97	0.45
8:d:261:PHE:CZ	33:d:408:LHG:HC81	2.51	0.45
8:d:261:PHE:CE2	33:d:408:LHG:HC81	2.51	0.45
31:g:305:CLA:O1A	36:g:317:NEX:H241	2.16	0.45
3:n:39:GLU:O	3:n:46:PRO:HD3	2.16	0.45
17:o:186:ASP:N	17:o:186:ASP:OD1	2.48	0.45
31:s:303:CLA:H12	31:s:303:CLA:H3A	1.98	0.45
34:x:202:LMG:HC8	34:x:202:LMG:H111	1.45	0.45
31:y:612:CLA:H2	31:y:612:CLA:HMA3	1.98	0.45
2:2:238:LEU:HD13	34:2:618:LMG:C9	2.46	0.45
2:4:157:LEU:HD11	31:5:614:CLA:O1A	2.16	0.45
2:4:171:TYR:HE2	3:5:54:ASN:N	2.12	0.45
3:5:108:LEU:HB2	3:5:116:PHE:HE2	1.81	0.45
31:5:611:CLA:HHC	31:5:611:CLA:HBB1	1.97	0.45
31:A:406:CLA:H52	44:D:406:PL9:H151	1.98	0.45
43:B:619:BCR:HC41	34:B:622:LMG:H141	1.97	0.45
31:C:604:CLA:H42	45:C:617:DGD:HB61	1.98	0.45
3:N:131:GLU:CD	3:N:132:GLY:H	2.23	0.45
31:N:304:CLA:H8	31:N:304:CLA:H51	1.38	0.45
31:N:305:CLA:H101	31:S:306:CLA:HMA2	1.98	0.45
18:R:79:SER:OG	31:R:304:CLA:O1A	2.21	0.45
36:R:319:NEX:H10	38:R:322:SQD:H132	1.97	0.45
23:X:86:ILE:O	23:X:90:ILE:HG12	2.16	0.45
30:Y:301:CHL:C1C	30:Y:301:CHL:H51	2.45	0.45
30:0:601:CHL:HAA2	30:0:601:CHL:HBD	1.98	0.45
30:7:307:CHL:HAA2	30:7:307:CHL:HBD	1.97	0.45
2:9:72:TRP:CD2	32:9:318:LUT:H383	2.51	0.45
2:9:86:ARG:HH22	30:9:311:CHL:HED1	1.81	0.45
30:9:308:CHL:HBB2	30:9:309:CHL:HBB1	1.97	0.45
3:p:105:PRO:HA	3:p:116:PHE:CE2	2.52	0.45
6:b:218:CYS:SG	31:r:316:CLA:HBA1	2.56	0.45
31:b:615:CLA:H151	31:b:615:CLA:H18	1.74	0.45
2:g:127:LYS:HA	30:n:301:CHL:HED2	1.98	0.45
3:n:121:TRP:CH2	31:y:615:CLA:HBB2	2.52	0.45
19:s:180:GLU:HG3	31:s:310:CLA:C4B	2.47	0.45
28:P1:11:GLY:HA2	28:P1:70:ASP:HB2	1.97	0.45
3:3:200:LEU:HD21	31:3:313:CLA:O1A	2.15	0.45
3:5:49:LEU:HB2	3:5:52:PHE:O	2.17	0.45
31:5:611:CLA:HHC	31:5:611:CLA:CBB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:445:THR:HG21	8:D:293:LEU:HD13	1.98	0.45
19:S:218:PRO:HD2	32:S:317:LUT:H23	1.97	0.45
32:S:318:LUT:H31	32:S:318:LUT:H391	1.74	0.45
30:Y:301:CHL:H122	30:Y:302:CHL:H61	1.99	0.45
30:0:606:CHL:HMB1	30:0:606:CHL:HBB1	1.98	0.45
1:7:191:ASP:OD2	1:7:194:THR:HG23	2.17	0.45
1:7:221:ILE:HD12	1:7:221:ILE:HA	1.80	0.45
31:7:312:CLA:H2	31:7:312:CLA:H62	1.72	0.45
3:p:74:LEU:HD21	31:q:305:CLA:H12	1.97	0.45
31:q:313:CLA:C2C	38:x:201:SQD:H142	2.46	0.45
31:q:315:CLA:C10	37:q:321:XAT:H34	2.41	0.45
6:b:450:TRP:NE1	31:b:608:CLA:HBA1	2.32	0.45
31:b:616:CLA:H52	31:b:617:CLA:HBB1	1.97	0.45
33:b:628:LHG:H132	33:b:628:LHG:C25	2.46	0.45
30:g:309:CHL:H41	31:n:303:CLA:H161	1.99	0.45
31:n:316:CLA:C1C	34:n:322:LMG:H331	2.47	0.45
19:s:234:LYS:HD3	31:s:313:CLA:HAA2	1.97	0.45
24:y:239:LEU:HB2	32:y:616:LUT:H22	1.98	0.45
1:1:137:ILE:HB	1:1:140:LEU:HD23	1.99	0.45
2:2:82:GLU:O	2:2:86:ARG:HG2	2.16	0.45
30:2:606:CHL:HAA2	30:2:606:CHL:HBD	1.98	0.45
31:3:312:CLA:H2	31:3:313:CLA:OBD	2.17	0.45
34:5:620:LMG:HC8	34:5:620:LMG:C36	2.47	0.45
30:6:309:CHL:HMA1	36:6:319:NEX:H402	1.98	0.45
32:6:317:LUT:H35	32:6:317:LUT:H401	1.81	0.45
31:B:603:CLA:HAB	31:B:605:CLA:H18	1.99	0.45
7:C:135:PHE:HA	31:C:612:CLA:HMC1	1.98	0.45
31:C:612:CLA:HBB1	33:C:623:LHG:H102	1.99	0.45
8:D:97:ALA:HB2	8:D:107:LEU:HD22	1.99	0.45
31:D:403:CLA:HBA2	31:D:403:CLA:H3A	1.78	0.45
2:G:46:ARG:HD3	2:G:64:GLY:HA3	1.98	0.45
31:R:316:CLA:C4B	31:R:316:CLA:H52	2.47	0.45
1:7:224:GLY:O	2:9:261:PRO:HG3	2.17	0.45
31:q:312:CLA:HBA1	35:q:317:RRX:H6	1.96	0.45
31:q:313:CLA:CMB	33:q:320:LHG:HC11	2.46	0.45
31:q:315:CLA:CGA	31:q:315:CLA:C1A	2.95	0.45
33:a:415:LHG:H251	33:a:415:LHG:H301	1.97	0.45
6:b:201:HIS:HE1	31:b:603:CLA:C1D	2.18	0.45
6:b:466:HIS:CE1	31:b:609:CLA:C4D	2.99	0.45
7:c:202:PHE:HZ	31:c:606:CLA:H13	1.80	0.45
31:g:313:CLA:H121	31:g:313:CLA:H162	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:102:LHG:H332	33:j:102:LHG:H362	1.83	0.45
31:n:315:CLA:HBA1	31:n:315:CLA:HBD	1.97	0.45
31:1:610:CLA:H62	31:1:612:CLA:HMA2	1.99	0.45
31:2:604:CLA:HED2	31:2:604:CLA:H2A	1.97	0.45
5:A:162:PRO:HB3	5:A:168:PHE:HA	1.98	0.45
5:A:262:TYR:HB3	33:A:415:LHG:HC92	1.99	0.45
5:A:288:LEU:O	5:A:292:THR:HG23	2.16	0.45
31:A:405:CLA:H3A	31:A:405:CLA:HBA1	1.71	0.45
6:B:6:TYR:O	31:B:611:CLA:HBD	2.17	0.45
31:C:602:CLA:H71	31:C:612:CLA:H42	1.98	0.45
31:C:606:CLA:H43	43:C:615:BCR:H332	1.97	0.45
8:D:126:MET:HE3	8:D:143:ALA:O	2.16	0.45
9:E:18:ARG:NH1	27:Q1:26:PRO:HG3	2.31	0.45
9:E:22:ILE:HG23	27:Q1:19:VAL:HG22	1.97	0.45
31:N:304:CLA:HBC1	30:N:309:CHL:HAC2	1.97	0.45
31:0:610:CLA:H92	32:0:616:LUT:H371	1.98	0.45
3:p:129:PHE:HE2	30:p:607:CHL:HMD1	1.81	0.45
43:a:410:BCR:H21C	43:a:410:BCR:H361	1.99	0.45
6:b:477:ASP:N	6:b:477:ASP:OD1	2.48	0.45
7:c:296:GLU:HG3	7:c:349:PHE:CZ	2.51	0.45
8:d:253:TRP:CG	44:d:407:PL9:HC71	2.52	0.45
42:d:402:PHO:H2	42:d:402:PHO:H61	1.61	0.45
18:r:140:GLY:HA3	18:r:241:ALA:HB1	1.97	0.45
19:s:164:PRO:HD2	19:s:167:ALA:HB3	1.97	0.45
2:2:90:ILE:HD13	31:2:603:CLA:HBA1	1.98	0.45
30:3:308:CHL:HMB2	30:3:310:CHL:OMC	2.17	0.45
3:5:48:PHE:N	3:5:67:TYR:HB3	2.32	0.45
3:5:215:MET:HE2	32:5:617:LUT:C10	2.35	0.45
3:5:237:LEU:HD22	31:5:614:CLA:HBB1	1.97	0.45
31:6:305:CLA:H3A	31:6:305:CLA:HBA2	1.47	0.45
5:A:118:HIS:HE1	31:A:409:CLA:ND	2.12	0.45
31:B:612:CLA:H61	31:B:612:CLA:H102	1.83	0.45
31:C:606:CLA:H112	31:C:606:CLA:H72	1.52	0.45
2:G:86:ARG:O	2:G:90:ILE:HG13	2.17	0.45
31:G:610:CLA:HBD	31:G:610:CLA:HBA1	1.98	0.45
3:N:117:GLY:O	3:N:118:GLU:HG3	2.16	0.45
17:O:256:GLY:O	17:O:290:LEU:N	2.50	0.45
22:W:93:TRP:CZ2	34:W:201:LMG:C11	3.00	0.45
24:Y:97:TRP:CE2	30:Y:308:CHL:HED3	2.52	0.45
1:7:176:ALA:HB2	18:r:38:ARG:NH2	2.29	0.45
1:7:219:GLN:HG2	31:7:314:CLA:C1D	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:q:305:CLA:HBC1	30:q:311:CHL:CBC	2.45	0.45
9:e:10:PHE:N	33:e:101:LHG:O5	2.44	0.45
2:g:196:ALA:HB1	2:g:202:LEU:HG	1.98	0.45
31:g:303:CLA:H2	31:g:303:CLA:O1A	2.16	0.45
31:n:316:CLA:H42	34:n:322:LMG:H121	1.99	0.45
18:r:238:ILE:HD12	18:r:239:LYS:N	2.31	0.45
19:s:138:GLU:HA	30:s:308:CHL:HED1	1.99	0.45
1:1:223:THR:HG21	31:1:613:CLA:O1D	2.16	0.45
3:3:245:PHE:HD2	3:3:246:TRP:CD1	2.34	0.45
30:3:307:CHL:C2C	34:3:321:LMG:H371	2.47	0.45
2:4:104:GLY:HA3	32:4:616:LUT:H183	1.98	0.45
31:4:604:CLA:HMA1	32:4:616:LUT:H3	1.98	0.45
30:5:606:CHL:HMC	32:5:617:LUT:H163	1.98	0.45
31:5:610:CLA:H52	32:5:616:LUT:H28	1.99	0.45
7:C:40:ALA:HB2	31:C:611:CLA:HMA2	1.98	0.45
31:G:603:CLA:HHC	31:G:603:CLA:CBB	2.46	0.45
30:Y:308:CHL:HMB3	38:Y:320:SQD:H262	1.99	0.45
31:8:612:CLA:H172	31:8:613:CLA:ND	2.32	0.45
34:a:416:LMG:H122	33:e:101:LHG:HC81	1.99	0.45
7:c:183:ASP:OD1	7:c:184:VAL:N	2.45	0.45
45:c:617:DGD:HB71	45:c:617:DGD:HB42	1.82	0.45
31:n:304:CLA:HBC2	30:n:310:CHL:HHD	1.97	0.45
22:w:89:PHE:CZ	34:w:202:LMG:H371	2.52	0.45
31:y:615:CLA:HBA2	31:y:615:CLA:H3A	1.41	0.45
30:2:606:CHL:HAB	32:2:615:LUT:H161	1.99	0.45
3:3:142:LEU:HA	30:3:307:CHL:HED2	1.99	0.45
30:4:607:CHL:H101	30:4:607:CHL:H61	1.50	0.45
30:4:607:CHL:CAA	3:5:253:SER:HB2	2.46	0.45
5:A:133:LEU:HD22	5:A:137:LEU:HG	1.99	0.45
8:D:239:GLN:OE1	8:D:241:GLU:HG2	2.16	0.45
2:G:97:TRP:CE2	30:G:607:CHL:HED2	2.52	0.45
30:N:307:CHL:HAA2	30:N:307:CHL:HBD	1.97	0.45
17:O:74:CYS:HB2	17:O:98:CYS:SG	2.57	0.45
18:R:71:ARG:NH2	18:R:235:GLU:OE2	2.22	0.45
36:R:319:NEX:C10	38:R:322:SQD:H132	2.47	0.45
20:T:21:ILE:HD12	43:T:101:BCR:H402	1.99	0.45
24:Y:70:TYR:HE2	30:Y:302:CHL:HBC2	1.81	0.45
30:0:607:CHL:H61	30:0:607:CHL:HMA3	1.99	0.45
1:7:103:LEU:HB3	31:7:305:CLA:HMC1	1.99	0.45
31:7:312:CLA:H8	31:7:313:CLA:C4D	2.47	0.45
43:a:410:BCR:H371	43:a:410:BCR:H24C	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:b:204:ALA:HB3	31:b:603:CLA:HAB	1.99	0.45
31:c:612:CLA:H61	31:c:612:CLA:H41	1.82	0.45
2:g:132:ILE:HG21	2:g:152:ILE:HG12	1.98	0.45
18:r:180:PRO:HG2	18:r:181:PHE:CE2	2.52	0.45
19:s:83:TYR:HB2	31:s:303:CLA:HMD1	1.99	0.45
33:s:322:LHG:H251	25:z:41:PHE:CD1	2.52	0.45
22:w:89:PHE:CE2	34:w:202:LMG:H422	2.52	0.45
1:1:40:GLN:O	1:1:46:ARG:HA	2.17	0.45
1:1:72:TRP:HD1	1:1:74:THR:HG23	1.81	0.45
1:1:204:LYS:HE3	33:1:617:LHG:HC61	1.98	0.45
30:1:609:CHL:HBD	30:1:609:CHL:HAA1	1.99	0.45
31:1:610:CLA:H62	31:1:612:CLA:CMA	2.47	0.45
2:2:147:ILE:HA	30:2:605:CHL:C4D	2.46	0.45
3:3:237:LEU:HD11	31:3:315:CLA:HMC3	1.99	0.45
2:4:138:LEU:HD13	30:4:606:CHL:CMD	2.47	0.45
2:4:166:ALA:HA	2:4:169:TYR:CD2	2.52	0.45
31:4:610:CLA:H41	31:4:610:CLA:H61	1.55	0.45
32:4:616:LUT:H35	32:4:616:LUT:H401	1.87	0.45
4:6:94:ALA:HB1	4:6:210:GLY:HA3	1.98	0.45
31:B:611:CLA:H152	31:B:613:CLA:O1D	2.17	0.45
45:C:620:DGD:HBV1	34:W:201:LMG:H142	1.99	0.45
8:D:51:GLY:HA2	8:D:55:VAL:HB	1.98	0.45
8:D:199:MET:HG2	44:D:406:PL9:H321	1.99	0.45
43:D:405:BCR:H321	43:D:405:BCR:HC8	1.98	0.45
43:D:405:BCR:H363	10:F:32:PHE:HB3	1.97	0.45
33:G:618:LHG:H281	37:G:620:XAT:C31	2.46	0.45
33:L:101:LHG:H101	33:L:101:LHG:H132	1.75	0.45
3:N:233:LEU:HD22	32:N:316:LUT:H163	1.99	0.45
30:N:306:CHL:H12	19:S:123:GLY:HA3	1.99	0.45
17:O:122:THR:HB	17:O:162:VAL:HB	1.99	0.45
36:R:301:NEX:H15	36:R:301:NEX:H201	1.88	0.45
30:R:308:CHL:HAA2	30:R:308:CHL:HBD	1.98	0.45
30:Y:307:CHL:HAA2	30:Y:307:CHL:HBD	1.98	0.45
31:0:610:CLA:H41	31:0:610:CLA:H61	1.54	0.45
31:0:610:CLA:H3A	31:0:610:CLA:HBA2	1.35	0.45
2:9:69:ASP:HA	31:9:304:CLA:O1D	2.16	0.45
30:9:308:CHL:C1C	30:9:309:CHL:HBC2	2.47	0.45
37:9:322:XAT:H31	37:9:322:XAT:H391	1.77	0.45
31:p:610:CLA:H12	31:p:610:CLA:C3A	2.47	0.45
2:q:198:ASP:HB3	2:q:201:THR:OG1	2.17	0.45
31:q:306:CLA:H92	31:q:306:CLA:H61	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:q:309:CHL:O1A	30:q:309:CHL:C2	2.64	0.45
5:a:201:GLY:HA3	5:a:286:THR:HB	1.99	0.45
38:a:412:SQD:H121	34:a:413:LMG:H291	1.99	0.45
6:b:270:PRO:HG3	6:b:312:TYR:CD1	2.52	0.45
33:b:625:LHG:H101	33:b:625:LHG:H352	1.99	0.45
33:b:625:LHG:H341	33:b:625:LHG:H311	1.54	0.45
7:c:156:LEU:HD11	31:c:609:CLA:H61	1.99	0.45
7:c:240:ILE:CG2	34:c:620:LMG:H121	2.46	0.45
7:c:326:GLY:HA2	17:o:157:TYR:OH	2.17	0.45
31:c:610:CLA:H12	31:c:610:CLA:HBA2	1.76	0.45
45:c:618:DGD:HB51	34:d:409:LMG:H121	1.98	0.45
2:g:95:ALA:HB1	2:g:213:GLY:HA3	1.98	0.45
30:n:310:CHL:HBD	30:n:310:CHL:HAA1	1.98	0.45
19:s:113:LEU:HB3	31:s:305:CLA:HAB	1.99	0.45
24:y:203:LEU:HD22	24:y:207:LYS:HE3	1.99	0.45
29:f1:170:ASP:HB2	29:f1:176:TYR:CE1	2.51	0.45
1:1:100:LEU:HB3	31:1:604:CLA:HAB	1.99	0.45
1:1:219:GLN:OE1	32:1:615:LUT:H42	2.17	0.45
31:1:604:CLA:HMA2	30:1:606:CHL:CBC	2.43	0.45
2:2:139:ASN:ND2	2:2:144:PRO:HA	2.32	0.45
31:2:613:CLA:HED2	37:2:619:XAT:C20	2.47	0.45
30:3:302:CHL:O1A	30:3:302:CHL:C2	2.65	0.45
3:5:69:TRP:CD1	32:5:617:LUT:H24	2.52	0.45
3:5:158:LEU:HA	36:5:618:NEX:C20	2.46	0.45
3:5:215:MET:HA	3:5:218:PHE:CD2	2.52	0.45
31:B:609:CLA:H2	31:B:609:CLA:H62	1.77	0.45
31:B:612:CLA:HBB1	31:B:612:CLA:CMB	2.44	0.45
8:D:126:MET:SD	8:D:150:ILE:HD12	2.57	0.45
9:E:8:ARG:HE	9:E:12:ASP:CG	2.24	0.45
3:N:122:PHE:CB	31:N:321:CLA:HAB	2.47	0.45
31:N:313:CLA:HHB	31:N:314:CLA:HBC3	1.98	0.45
17:O:86:ASP:OD1	17:O:86:ASP:N	2.49	0.45
34:7:322:LMG:H291	34:7:322:LMG:H111	1.98	0.45
31:8:610:CLA:HHC	31:8:610:CLA:CBB	2.46	0.45
2:9:197:ASP:N	2:9:197:ASP:OD1	2.49	0.45
31:9:312:CLA:C8	35:9:317:RRX:H25	2.47	0.45
3:p:177:ASP:HB3	3:p:180:TYR:O	2.17	0.45
3:p:233:LEU:O	3:p:237:LEU:HG	2.17	0.45
30:p:606:CHL:HBB1	30:p:609:CHL:HBC1	1.99	0.45
31:p:613:CLA:HED3	31:p:613:CLA:CHA	2.46	0.45
31:p:615:CLA:H3A	31:p:615:CLA:HBA2	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:89:GLU:HA	2:q:184:LEU:HD11	1.99	0.45
31:n:314:CLA:H152	31:n:314:CLA:H193	1.99	0.45
19:s:107:HIS:HE1	31:s:304:CLA:C4D	2.30	0.45
31:s:303:CLA:H61	32:s:318:LUT:H26	1.99	0.45
29:F1:174:LYS:NZ	29:F1:202:SER:HB2	2.32	0.45
33:2:617:LHG:HC82	37:2:619:XAT:H381	1.98	0.44
3:5:200:LEU:HD23	3:5:203:LYS:HD2	1.98	0.44
30:5:606:CHL:HBB1	30:5:609:CHL:HBC1	1.99	0.44
30:5:608:CHL:CMB	36:5:618:NEX:H14	2.47	0.44
30:6:310:CHL:HBD	30:6:310:CHL:HAA1	1.99	0.44
5:A:140:ARG:HB2	8:D:220:ASN:HA	2.00	0.44
6:B:486:LEU:O	6:B:490:VAL:HG23	2.17	0.44
7:C:30:LEU:HD21	31:C:611:CLA:H2A	1.98	0.44
7:C:183:ASP:OD1	7:C:184:VAL:N	2.47	0.44
31:C:605:CLA:CMD	31:C:607:CLA:HAB	2.47	0.44
34:C:621:LMG:HC71	34:C:621:LMG:HC2	1.73	0.44
34:G:622:LMG:C17	31:N:321:CLA:H43	2.43	0.44
31:N:321:CLA:HMC2	30:Y:301:CHL:HHB	1.99	0.44
31:S:312:CLA:H192	31:S:313:CLA:HBB2	1.98	0.44
4:0:93:HIS:CE1	31:0:603:CLA:C4D	2.98	0.44
4:0:144:LEU:HG	18:r:269:PHE:HE1	1.82	0.44
30:0:607:CHL:CAA	37:q:321:XAT:H41	2.46	0.44
34:9:302:LMG:HC2	34:9:302:LMG:HC72	1.72	0.44
31:p:602:CLA:H92	31:p:602:CLA:H61	1.68	0.44
2:q:149:ALA:HA	30:q:307:CHL:C1C	2.47	0.44
6:b:3:LEU:HD22	6:b:7:ARG:HB2	1.98	0.44
6:b:275:TRP:CD1	6:b:361:THR:HG23	2.52	0.44
31:b:610:CLA:H42	38:b:627:SQD:H261	1.98	0.44
34:b:622:LMG:H151	34:b:622:LMG:H182	1.76	0.44
31:c:602:CLA:H71	31:c:612:CLA:H42	1.99	0.44
2:g:76:GLY:CA	24:y:86:LYS:HD2	2.47	0.44
38:g:301:SQD:H442	31:g:311:CLA:HMB1	1.98	0.44
32:g:316:LUT:H31	32:g:316:LUT:H391	1.64	0.44
33:l:101:LHG:H331	16:m:21:PHE:CD2	2.52	0.44
3:n:87:LEU:CD1	31:n:304:CLA:HBA1	2.44	0.44
37:r:318:XAT:H15	37:r:318:XAT:H201	1.78	0.44
1:1:188:LEU:CD1	32:1:615:LUT:H221	2.47	0.44
2:2:96:ARG:HA	2:2:99:MET:HE3	2.00	0.44
2:2:134:ASN:O	2:2:135:GLU:C	2.60	0.44
2:2:138:LEU:HD11	30:2:606:CHL:HAC1	1.99	0.44
3:3:98:GLY:HA3	32:3:318:LUT:C10	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:185:PHE:HA	30:3:309:CHL:C2	2.46	0.44
31:3:315:CLA:HHC	31:3:315:CLA:CBB	2.47	0.44
2:4:75:ALA:HB3	2:4:77:LEU:HD22	1.99	0.44
34:4:621:LMG:HC92	34:4:621:LMG:HC2	2.00	0.44
31:6:305:CLA:HBB1	31:6:305:CLA:CMB	2.46	0.44
30:6:308:CHL:H41	30:6:308:CHL:H62	1.62	0.44
5:A:132:GLU:O	5:A:136:ARG:HG2	2.17	0.44
31:A:405:CLA:H72	31:A:405:CLA:H111	1.85	0.44
6:B:43:ALA:HA	34:m:102:LMG:HC2	1.99	0.44
31:B:608:CLA:H3A	31:B:608:CLA:HBA2	1.67	0.44
31:B:615:CLA:H122	31:B:615:CLA:H162	1.67	0.44
31:C:604:CLA:CAD	45:C:617:DGD:HB21	2.47	0.44
33:G:618:LHG:H301	37:G:620:XAT:C40	2.47	0.44
3:N:226:ARG:HH22	31:N:321:CLA:HBA1	1.83	0.44
17:O:78:ASP:OD1	17:O:79:SER:N	2.46	0.44
31:S:304:CLA:HBB1	31:S:304:CLA:CMB	2.47	0.44
22:W:107:SER:O	22:W:108:ASP:HB2	2.18	0.44
4:0:220:PHE:HE1	32:0:616:LUT:H41	1.82	0.44
31:p:615:CLA:HHC	31:p:615:CLA:CBB	2.47	0.44
2:q:163:MET:CE	30:q:308:CHL:HMA3	2.47	0.44
2:q:226:GLN:NE2	35:q:317:RRX:H50	2.33	0.44
30:q:311:CHL:HBD	30:q:311:CHL:HAA1	1.98	0.44
31:b:610:CLA:C4	38:b:627:SQD:H261	2.47	0.44
7:c:130:GLU:H	7:c:130:GLU:CD	2.25	0.44
7:c:452:GLU:OE2	8:d:245:SER:OG	2.34	0.44
30:g:309:CHL:HAA1	30:g:309:CHL:HBD	1.99	0.44
31:n:305:CLA:CHA	31:n:305:CLA:HBA1	2.40	0.44
34:n:322:LMG:O9	34:n:322:LMG:H142	2.17	0.44
26:u:73:GLU:OE2	26:u:89:GLN:NE2	2.51	0.44
31:2:609:CLA:H72	35:2:614:RRX:H25	1.99	0.44
2:4:167:GLU:HG3	30:4:609:CHL:C4B	2.47	0.44
2:4:253:SER:HB2	2:4:256:LYS:HZ2	1.83	0.44
31:5:613:CLA:H52	31:5:613:CLA:NC	2.31	0.44
31:6:311:CLA:H52	31:6:311:CLA:H8	1.47	0.44
31:D:404:CLA:H62	31:D:404:CLA:H41	1.41	0.44
2:G:259:PRO:HD3	30:G:623:CHL:H12	1.98	0.44
30:N:306:CHL:HAA2	30:N:306:CHL:HBD	1.98	0.44
31:S:303:CLA:H203	31:S:304:CLA:CBB	2.46	0.44
31:S:311:CLA:H161	31:S:311:CLA:H122	1.71	0.44
4:0:182:TYR:CE2	4:0:203:LYS:HE3	2.53	0.44
1:7:67:PRO:HG3	1:7:199:LYS:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:251:LEU:CD2	30:7:321:CHL:O1A	2.66	0.44
31:7:305:CLA:HMA2	30:7:307:CHL:C2C	2.47	0.44
30:9:303:CHL:C4D	33:9:320:LHG:HC91	2.48	0.44
31:b:602:CLA:HBA2	31:b:602:CLA:H3A	1.58	0.44
7:c:206:PHE:HZ	45:c:616:DGD:HBW2	1.81	0.44
43:c:615:BCR:H20C	43:c:615:BCR:H361	1.74	0.44
31:g:312:CLA:HBB1	31:g:312:CLA:CMB	2.44	0.44
15:l:25:ILE:HG22	16:m:15:ILE:HD13	1.99	0.44
31:s:312:CLA:C3C	33:s:320:LHG:HC62	2.48	0.44
34:w:202:LMG:H111	31:y:611:CLA:H11	1.98	0.44
30:y:606:CHL:HAA2	30:y:606:CHL:HBD	1.98	0.44
2:2:145:SER:O	30:2:605:CHL:H2A	2.18	0.44
31:2:603:CLA:HED3	32:3:318:LUT:H372	1.99	0.44
3:3:185:PHE:HA	30:3:309:CHL:H2	2.00	0.44
3:3:193:ASP:HB2	3:3:196:THR:OG1	2.18	0.44
2:4:169:TYR:CD1	2:4:174:GLU:HG3	2.53	0.44
3:5:48:PHE:HD2	30:5:601:CHL:HBA1	1.82	0.44
3:5:56:PRO:HD2	3:5:59:LEU:HB2	2.00	0.44
3:5:135:ASP:HB3	3:5:139:ASN:O	2.17	0.44
31:B:611:CLA:H193	31:B:611:CLA:H162	1.75	0.44
34:C:622:LMG:HC8	34:N:320:LMG:O10	2.17	0.44
2:G:168:ALA:HB1	3:N:52:PHE:CG	2.52	0.44
31:G:609:CLA:H122	35:G:614:RRX:H22	1.99	0.44
32:G:615:LUT:H28	32:G:615:LUT:H361	1.98	0.44
17:O:106:VAL:HB	17:O:164:LEU:HD21	1.99	0.44
19:S:39:TRP:HE1	34:S:321:LMG:HC3	1.82	0.44
22:W:110:GLU:O	22:W:112:ASP:N	2.45	0.44
1:7:178:TYR:CE2	1:7:199:LYS:HE3	2.52	0.44
31:7:305:CLA:HMA2	30:7:307:CHL:HBC3	1.99	0.44
3:8:100:LEU:HD13	31:8:611:CLA:HBB2	1.99	0.44
3:p:144:HIS:CE1	3:p:146:GLN:HE22	2.35	0.44
2:q:138:LEU:HD21	31:q:306:CLA:HAA1	1.99	0.44
33:q:320:LHG:HC5	37:q:321:XAT:C38	2.46	0.44
34:b:601:LMG:H311	34:b:601:LMG:H141	2.00	0.44
3:n:106:GLU:O	3:n:110:ARG:HG2	2.17	0.44
31:s:303:CLA:CAB	32:s:318:LUT:H32	2.47	0.44
34:w:202:LMG:H211	31:y:612:CLA:C14	2.43	0.44
30:y:606:CHL:HBB1	32:y:617:LUT:H161	1.99	0.44
29:f1:178:LYS:HB3	29:f1:230:TRP:CZ2	2.53	0.44
3:3:125:GLY:HA2	30:3:308:CHL:HAC2	1.99	0.44
2:4:93:ILE:HG22	2:4:97:TRP:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:158:THR:HG21	30:4:606:CHL:CED	2.47	0.44
2:4:179:THR:HB	2:4:188:GLY:CA	2.48	0.44
2:4:202:LEU:O	2:4:206:LYS:N	2.50	0.44
2:4:228:LEU:HD11	34:4:621:LMG:H361	1.98	0.44
3:5:110:ARG:HH22	3:5:231:GLU:HA	1.82	0.44
5:A:107:TYR:CG	17:O:125:MET:HG3	2.53	0.44
6:B:26:HIS:O	6:B:30:VAL:HG23	2.17	0.44
6:B:33:TRP:CD1	43:t:101:BCR:H332	2.52	0.44
2:G:107:THR:HB	2:G:108:PRO:HD3	1.99	0.44
2:G:221:PHE:CE2	31:G:612:CLA:HAC1	2.52	0.44
15:L:30:VAL:HG22	20:T:9:LEU:HB3	1.99	0.44
31:N:304:CLA:HAC1	30:Y:301:CHL:CBB	2.42	0.44
36:S:319:NEX:H35	36:S:319:NEX:H401	1.87	0.44
3:8:39:GLU:O	3:8:46:PRO:HD3	2.16	0.44
31:p:613:CLA:HAA1	31:p:613:CLA:HBD	1.99	0.44
2:q:100:LEU:HB3	31:q:306:CLA:HAB	1.99	0.44
7:c:274:ALA:HB2	31:c:602:CLA:HMD1	2.00	0.44
8:d:45:LEU:HD12	8:d:49:PHE:HE2	1.82	0.44
2:g:86:ARG:HG3	3:n:73:GLY:HA3	1.98	0.44
31:n:304:CLA:HBA2	31:n:304:CLA:H12	1.60	0.44
18:r:71:ARG:NH2	18:r:235:GLU:OE2	2.31	0.44
32:r:317:LUT:H15	32:r:317:LUT:H201	1.90	0.44
31:y:613:CLA:H62	31:y:613:CLA:C1C	2.48	0.44
27:q1:15:VAL:O	27:q1:19:VAL:HG23	2.18	0.44
2:2:235:LEU:HD13	34:2:618:LMG:HC72	2.00	0.44
30:2:608:CHL:HMB3	30:3:303:CHL:HHB	1.99	0.44
2:4:180:SER:O	2:4:182:ASP:N	2.51	0.44
3:5:105:PRO:HA	3:5:116:PHE:CE2	2.52	0.44
4:6:251:TYR:HB2	4:6:252:ALA:H	1.56	0.44
6:B:492:PHE:HB2	9:E:2:SER:O	2.17	0.44
31:B:611:CLA:H112	31:B:611:CLA:H72	1.64	0.44
33:B:624:LHG:H251	33:B:624:LHG:H132	1.98	0.44
8:D:67:TYR:O	34:D:409:LMG:O5	2.26	0.44
8:D:239:GLN:HG3	8:D:241:GLU:OE2	2.16	0.44
3:N:158:LEU:HG	36:N:318:NEX:H15	1.98	0.44
18:R:208:GLU:HA	18:R:211:CSU:OD2	2.18	0.44
31:R:305:CLA:HBC1	31:R:311:CLA:HBC2	1.99	0.44
31:0:610:CLA:H12	31:0:610:CLA:CHB	2.47	0.44
30:7:321:CHL:H122	30:8:608:CHL:CMC	2.47	0.44
3:8:246:TRP:O	2:9:133:PHE:CZ	2.71	0.44
3:p:250:ALA:C	3:p:252:LYS:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:a:49:ILE:HG21	34:m:102:LMG:H381	2.00	0.44
5:a:267:ASN:HD22	38:a:411:SQD:C3	2.29	0.44
6:b:328:GLY:HA3	34:b:622:LMG:HC5	1.98	0.44
33:d:408:LHG:H311	33:d:408:LHG:H341	1.76	0.44
2:g:251:PHE:HB3	24:y:132:PHE:HZ	1.81	0.44
12:i:27:ASP:N	12:i:28:PRO:CD	2.81	0.44
14:k:38:VAL:HG23	43:v:101:BCR:H21C	1.99	0.44
16:m:12:ALA:O	16:m:16:ILE:HG12	2.18	0.44
17:o:153:ASP:N	17:o:153:ASP:OD1	2.51	0.44
30:r:309:CHL:H62	30:r:309:CHL:H41	1.79	0.44
31:r:315:CLA:HBA2	31:r:315:CLA:H3A	1.36	0.44
19:s:251:VAL:HG21	31:s:314:CLA:HAC2	2.00	0.44
19:s:264:TRP:CD1	32:s:317:LUT:H163	2.53	0.44
20:t:21:ILE:HD12	43:t:101:BCR:H401	2.00	0.44
34:y:620:LMG:O9	34:y:620:LMG:H162	2.18	0.44
1:1:237:ASP:HB3	1:1:240:ALA:HB3	1.98	0.44
2:2:54:SER:O	2:2:58:VAL:HG23	2.18	0.44
2:2:90:ILE:HG23	30:2:608:CHL:OBD	2.18	0.44
2:2:132:ILE:HB	2:2:138:LEU:HD12	1.99	0.44
2:2:138:LEU:CD1	30:2:606:CHL:HHD	2.48	0.44
31:2:603:CLA:HBC1	30:2:608:CHL:CBC	2.48	0.44
3:3:236:HIS:CB	31:3:314:CLA:HAA2	2.44	0.44
31:3:306:CLA:H92	36:3:319:NEX:H403	1.99	0.44
2:4:186:PRO:HB2	2:4:190:PHE:CD1	2.53	0.44
3:5:98:GLY:HA2	32:5:617:LUT:H181	2.00	0.44
3:5:190:LEU:HB2	31:5:610:CLA:CGA	2.47	0.44
3:5:210:LEU:HA	33:5:619:LHG:H301	1.99	0.44
31:B:614:CLA:HBB1	31:B:614:CLA:CMB	2.48	0.44
38:B:623:SQD:H151	8:D:127:LEU:HD13	1.99	0.44
33:D:408:LHG:H362	43:T:101:BCR:H281	2.00	0.44
2:G:84:PHE:O	2:G:88:ARG:HG3	2.17	0.44
2:G:154:ALA:O	2:G:158:THR:OG1	2.30	0.44
31:G:610:CLA:H2	31:G:611:CLA:OBD	2.17	0.44
31:N:310:CLA:HBA2	31:N:310:CLA:H3A	1.41	0.44
32:N:317:LUT:H15	32:N:317:LUT:H201	1.85	0.44
19:S:149:LEU:HG	31:S:305:CLA:HED1	1.99	0.44
24:Y:107:PHE:HB3	24:Y:108:PRO:HD3	2.00	0.44
30:Y:307:CHL:CBB	32:Y:316:LUT:H161	2.48	0.44
31:8:612:CLA:H151	31:8:613:CLA:CMD	2.47	0.44
31:8:614:CLA:C4	34:9:302:LMG:H112	2.46	0.44
2:q:72:TRP:CE3	32:q:318:LUT:H383	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:401:LMG:H111	34:a:401:LMG:HC8	1.39	0.44
6:b:6:TYR:HB2	33:b:625:LHG:H382	2.00	0.44
8:d:51:GLY:HA2	8:d:55:VAL:HB	1.98	0.44
9:e:23:HIS:HA	9:e:26:THR:OG1	2.18	0.44
31:g:314:CLA:HAA2	31:g:314:CLA:H12	2.00	0.44
34:m:102:LMG:H311	34:m:102:LMG:H342	1.75	0.44
31:n:315:CLA:HBA1	31:n:315:CLA:CBD	2.47	0.44
34:n:321:LMG:O1	34:n:321:LMG:HC61	2.18	0.44
18:r:269:PHE:CD1	31:r:315:CLA:HAA2	2.53	0.44
31:s:305:CLA:CHC	36:s:319:NEX:H362	2.48	0.44
22:w:116:GLY:O	22:w:118:THR:HG23	2.18	0.44
1:1:86:ARG:HA	1:1:86:ARG:HE	1.83	0.44
3:3:186:ASP:HA	32:3:317:LUT:C24	2.36	0.44
2:4:96:ARG:HA	2:4:99:MET:HE3	2.00	0.44
2:4:195:LEU:HB2	31:4:610:CLA:CGA	2.47	0.44
2:4:253:SER:HB2	2:4:256:LYS:NZ	2.33	0.44
30:4:607:CHL:H42	3:5:245:PHE:CE2	2.53	0.44
31:5:610:CLA:C5	32:5:616:LUT:H30	2.45	0.44
4:6:244:THR:O	4:6:249:SER:HB2	2.18	0.44
30:6:308:CHL:H101	30:6:308:CHL:H62	1.75	0.44
45:C:618:DGD:HE4	13:J:42:LEU:HD11	1.99	0.44
34:C:621:LMG:HC8	34:C:621:LMG:H111	1.58	0.44
8:D:210:LEU:HA	8:D:213:ILE:HG22	2.00	0.44
14:K:27:VAL:O	14:K:30:VAL:HG12	2.18	0.44
3:N:235:ASP:O	3:N:243:THR:HG21	2.18	0.44
30:N:308:CHL:HAA1	30:N:308:CHL:HBD	2.00	0.44
31:N:313:CLA:H13	33:N:319:LHG:H321	1.99	0.44
18:R:174:TYR:HD2	31:R:306:CLA:CBA	2.30	0.44
31:R:305:CLA:H143	31:R:305:CLA:H111	1.78	0.44
30:R:309:CHL:HHC	30:R:309:CHL:CBB	2.46	0.44
32:R:317:LUT:H393	32:R:317:LUT:H27	1.84	0.44
19:S:264:TRP:CD1	32:S:317:LUT:H163	2.53	0.44
31:S:312:CLA:H92	31:S:312:CLA:H61	1.67	0.44
31:Y:303:CLA:H93	31:Y:304:CLA:HMB1	2.00	0.44
30:0:607:CHL:HAA1	37:q:321:XAT:C4	2.48	0.44
3:8:223:LEU:CD2	34:9:302:LMG:H172	2.47	0.44
3:p:131:GLU:H	3:p:131:GLU:CD	2.26	0.44
2:q:99:MET:HB2	31:q:312:CLA:HMC2	2.00	0.44
30:q:309:CHL:HBB2	30:q:311:CHL:HBC1	2.00	0.44
30:q:310:CHL:HHC	30:q:310:CHL:CBB	2.44	0.44
31:q:312:CLA:H2	35:q:317:RRX:H8	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:b:272:ARG:HA	6:b:318:ASN:ND2	2.33	0.44
6:b:458:PHE:HB3	31:b:605:CLA:HBC2	2.00	0.44
31:c:608:CLA:H152	31:c:608:CLA:H112	1.77	0.44
19:s:221:LEU:HD12	31:s:311:CLA:H12	2.00	0.44
1:1:94:HIS:CE1	31:1:603:CLA:C4D	3.00	0.44
1:1:246:LEU:H	1:1:246:LEU:HD22	1.83	0.44
2:2:139:ASN:OD1	2:2:148:HIS:HA	2.18	0.44
3:3:245:PHE:HB3	31:3:314:CLA:C2	2.48	0.44
31:3:304:CLA:H93	31:3:304:CLA:H111	1.64	0.44
2:4:146:LEU:HD13	30:4:605:CHL:O1D	2.18	0.44
3:5:91:HIS:HE1	31:5:603:CLA:C4D	2.30	0.44
3:5:121:TRP:CE2	3:5:122:PHE:HD1	2.36	0.44
3:5:161:LEU:HB3	3:5:165:TYR:CE2	2.52	0.44
32:5:617:LUT:H31	32:5:617:LUT:H391	1.87	0.44
32:5:617:LUT:H35	32:5:617:LUT:H401	1.91	0.44
4:6:45:ASP:OD1	4:6:45:ASP:N	2.47	0.44
7:C:132:PHE:HD1	33:C:623:LHG:HC11	1.82	0.44
31:N:310:CLA:H52	32:N:316:LUT:C30	2.48	0.44
31:0:611:CLA:C3C	33:0:619:LHG:HC62	2.48	0.44
1:7:251:LEU:HD23	30:7:321:CHL:O1A	2.17	0.44
30:7:306:CHL:CMA	18:r:270:ALA:HB2	2.47	0.44
2:9:90:ILE:HG23	30:9:311:CHL:OBD	2.17	0.44
2:9:241:HIS:CB	31:9:315:CLA:HAA2	2.48	0.44
2:q:200:ASP:OD1	2:q:201:THR:N	2.51	0.44
2:q:220:MET:HE2	32:q:318:LUT:H12	2.00	0.44
31:q:304:CLA:H92	31:q:305:CLA:HMA1	1.99	0.44
31:b:612:CLA:H151	31:b:614:CLA:C3D	2.48	0.44
43:b:618:BCR:H332	34:b:622:LMG:H111	1.99	0.44
7:c:267:ILE:HD11	31:c:603:CLA:H142	2.00	0.44
30:n:308:CHL:HMA2	31:y:615:CLA:CHC	2.48	0.44
32:n:318:LUT:H35	32:n:318:LUT:H401	1.87	0.44
18:r:174:TYR:HD1	31:r:306:CLA:HBA1	1.83	0.44
23:x:88:GLY:O	23:x:91:THR:HG22	2.18	0.44
26:u:157:ALA:HB2	26:u:197:LYS:HZ1	1.83	0.44
1:1:176:ALA:HB2	18:R:38:ARG:HH21	1.82	0.43
34:1:618:LMG:H151	31:R:313:CLA:NC	2.33	0.43
2:2:260:LEU:O	34:2:620:LMG:HC61	2.18	0.43
3:3:127:GLN:HE22	31:3:306:CLA:HED2	1.82	0.43
31:3:305:CLA:HBC2	30:3:310:CHL:HHD	1.99	0.43
2:4:147:ILE:HG23	30:4:605:CHL:CHD	2.48	0.43
34:4:620:LMG:HC91	34:4:621:LMG:C15	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:197:PHE:CE2	45:C:617:DGD:HBV2	2.53	0.43
5:A:299:GLY:O	7:C:391:SER:HB2	2.18	0.43
31:B:607:CLA:H141	31:B:607:CLA:H162	1.73	0.43
3:N:47:GLN:HG3	3:N:53:SER:CB	2.44	0.43
30:N:302:CHL:HED1	33:N:319:LHG:H292	2.00	0.43
30:N:307:CHL:HMB1	30:N:309:CHL:HAC1	2.00	0.43
2:9:230:THR:HG21	2:9:237:ASN:ND2	2.33	0.43
3:p:38:VAL:HA	3:p:41:TYR:O	2.18	0.43
2:q:138:LEU:O	2:q:138:LEU:HD23	2.18	0.43
2:q:254:ALA:O	37:q:321:XAT:H42	2.18	0.43
31:q:315:CLA:C2B	35:q:317:RRX:H53	2.47	0.43
31:q:315:CLA:H2	31:q:315:CLA:H61	1.61	0.43
33:a:415:LHG:HC92	7:c:24:TRP:CZ3	2.53	0.43
6:b:202:HIS:HE1	31:b:604:CLA:NA	2.13	0.43
7:c:117:GLY:O	7:c:121:SER:OG	2.28	0.43
7:c:120:HIS:HE1	31:c:613:CLA:C1A	2.30	0.43
7:c:219:GLU:HG3	26:u:173:ARG:NH1	2.33	0.43
7:c:392:LEU:HD22	7:c:392:LEU:HA	1.86	0.43
31:c:610:CLA:H152	31:c:610:CLA:H112	1.84	0.43
9:e:8:ARG:CD	9:e:13:ILE:HG12	2.48	0.43
2:g:72:TRP:CZ3	32:g:316:LUT:H383	2.53	0.43
2:g:107:THR:HB	2:g:108:PRO:HD3	2.00	0.43
38:g:301:SQD:H111	37:g:321:XAT:H222	1.99	0.43
31:n:303:CLA:HBA1	32:n:318:LUT:H382	1.99	0.43
36:r:301:NEX:H35	36:r:301:NEX:H401	1.84	0.43
34:w:202:LMG:H252	31:y:612:CLA:C16	2.47	0.43
31:y:603:CLA:HED2	31:y:603:CLA:H2A	2.00	0.43
1:1:246:LEU:HD23	1:1:247:TYR:CD2	2.52	0.43
2:2:62:LEU:HD13	2:2:71:GLY:HA2	2.00	0.43
2:2:139:ASN:CG	2:2:144:PRO:HA	2.43	0.43
3:3:169:GLY:HA2	30:3:309:CHL:HAC1	2.00	0.43
2:4:99:MET:HG3	2:4:213:GLY:HA2	2.00	0.43
3:5:206:LYS:HG2	33:5:619:LHG:H252	1.99	0.43
31:5:610:CLA:H2	32:5:616:LUT:C28	2.44	0.43
5:A:77:ILE:HD13	15:L:30:VAL:HG13	1.98	0.43
5:A:333:GLU:HB3	5:A:336:ALA:HB3	2.00	0.43
31:A:409:CLA:H122	34:A:412:LMG:H162	2.00	0.43
43:A:410:BCR:H24C	43:A:410:BCR:H371	1.89	0.43
6:B:75:TRP:CE2	38:a:412:SQD:H441	2.53	0.43
43:B:617:BCR:C2	34:B:621:LMG:H292	2.45	0.43
7:C:151:ILE:HG21	31:C:612:CLA:C3B	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:155:SER:HA	8:D:159:ILE:HB	1.98	0.43
8:D:201:VAL:HG22	31:D:403:CLA:C2B	2.48	0.43
18:R:44:TYR:HB2	36:R:301:NEX:O3	2.18	0.43
18:R:163:ALA:O	18:R:167:LEU:HG	2.17	0.43
31:S:303:CLA:CAB	32:S:318:LUT:H32	2.49	0.43
1:7:92:VAL:HG11	1:7:177:VAL:CG1	2.49	0.43
1:7:188:LEU:HB2	31:7:311:CLA:O1A	2.18	0.43
3:8:106:GLU:O	3:8:110:ARG:HG2	2.17	0.43
2:9:96:ARG:HA	2:9:99:MET:HE3	1.98	0.43
3:p:233:LEU:HA	31:p:613:CLA:HMA2	1.98	0.43
5:a:32:TRP:O	5:a:35:VAL:HG22	2.19	0.43
7:c:112:VAL:HG21	43:c:614:BCR:C17	2.48	0.43
45:c:619:DGD:O4E	33:y:619:LHG:HC12	2.18	0.43
38:g:318:SQD:H462	38:g:318:SQD:H2	2.00	0.43
31:r:306:CLA:HMA3	30:r:308:CHL:C3C	2.48	0.43
2:2:253:SER:HB2	2:2:256:LYS:HG2	2.00	0.43
2:4:96:ARG:HD2	30:4:608:CHL:OBD	2.17	0.43
4:6:110:LEU:HD21	34:6:322:LMG:C33	2.40	0.43
7:C:274:ALA:HB2	31:C:602:CLA:HMD1	1.99	0.43
34:D:410:LMG:H202	34:D:410:LMG:H172	1.82	0.43
31:R:316:CLA:HBA2	31:R:316:CLA:H3A	1.24	0.43
24:Y:145:LEU:HD11	34:Y:319:LMG:H301	1.99	0.43
30:Y:301:CHL:H51	30:Y:301:CHL:NC	2.34	0.43
26:U:93:ASN:O	26:U:96:VAL:HG22	2.18	0.43
4:0:255:LEU:O	4:0:256:ALA:C	2.61	0.43
1:7:100:LEU:HB3	31:7:305:CLA:HAB	1.99	0.43
31:8:612:CLA:H193	31:8:612:CLA:H152	1.99	0.43
2:9:205:LEU:HD22	31:9:312:CLA:H43	2.00	0.43
34:9:301:LMG:H161	34:9:301:LMG:H132	1.75	0.43
3:p:247:VAL:HG22	2:q:133:PHE:HD2	1.82	0.43
3:p:247:VAL:HG22	2:q:133:PHE:CE2	2.54	0.43
31:p:602:CLA:H62	31:p:603:CLA:H3A	1.99	0.43
31:p:613:CLA:C1	31:p:614:CLA:HMD2	2.48	0.43
2:q:190:PHE:HZ	30:q:310:CHL:NB	2.16	0.43
31:b:612:CLA:C4B	31:b:614:CLA:HMA2	2.48	0.43
31:b:614:CLA:H92	31:b:614:CLA:H61	1.60	0.43
31:c:608:CLA:HBC3	31:c:610:CLA:H71	2.01	0.43
2:g:162:ILE:HD12	30:g:307:CHL:HED2	2.00	0.43
3:n:252:LYS:HB2	3:n:258:TYR:HD2	1.83	0.43
31:n:314:CLA:H151	31:n:315:CLA:CMD	2.48	0.43
17:o:122:THR:HG22	17:o:164:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:49:TRP:H	2:2:49:TRP:CD1	2.36	0.43
2:2:112:GLN:HA	2:2:117:ALA:HA	2.00	0.43
3:3:91:HIS:HE1	31:3:305:CLA:ND	2.13	0.43
3:3:218:PHE:HD1	3:3:229:PRO:HB3	1.83	0.43
3:3:223:LEU:HD22	3:3:223:LEU:HA	1.87	0.43
3:3:233:LEU:C	3:3:233:LEU:HD13	2.43	0.43
3:3:246:TRP:HA	3:3:250:ALA:HB3	2.00	0.43
31:3:304:CLA:H93	31:3:305:CLA:HMB1	2.00	0.43
2:4:168:ALA:HB1	3:5:52:PHE:CG	2.52	0.43
31:4:611:CLA:CHD	33:4:618:LHG:HC62	2.49	0.43
3:5:96:MET:HG3	3:5:208:GLY:HA2	2.00	0.43
5:A:27:ARG:NH2	8:D:258:GLY:O	2.46	0.43
5:A:133:LEU:HD11	8:D:255:GLN:HB2	2.01	0.43
33:A:417:LHG:H292	33:A:417:LHG:H322	1.77	0.43
6:B:30:VAL:HG12	31:B:605:CLA:HHD	2.00	0.43
6:B:204:ALA:HA	34:B:625:LMG:H322	1.99	0.43
33:C:623:LHG:H331	33:C:623:LHG:H362	1.68	0.43
8:D:241:GLU:CD	8:D:241:GLU:H	2.26	0.43
31:G:612:CLA:HMA1	35:G:614:RRX:C4	2.48	0.43
16:M:4:ASN:C	16:M:6:LEU:N	2.76	0.43
31:N:305:CLA:H152	31:S:306:CLA:C4A	2.48	0.43
18:R:56:ASN:ND2	18:R:56:ASN:O	2.52	0.43
31:R:312:CLA:H3A	31:R:312:CLA:HBA2	1.25	0.43
24:Y:187:PRO:HD2	31:Y:310:CLA:OBD	2.18	0.43
1:7:96:ARG:HA	1:7:99:MET:HE3	2.00	0.43
1:7:183:PHE:HZ	30:7:309:CHL:C1C	2.32	0.43
34:9:301:LMG:H321	34:9:301:LMG:H352	1.83	0.43
3:p:245:PHE:HB2	31:p:613:CLA:OBD	2.19	0.43
31:b:611:CLA:C2	31:b:611:CLA:H72	2.48	0.43
7:c:203:ARG:HG3	7:c:211:TRP:HA	1.98	0.43
8:d:12:ARG:NH1	8:d:16:ASP:HB3	2.33	0.43
31:s:311:CLA:H11	32:s:317:LUT:H373	2.00	0.43
33:y:619:LHG:H331	33:y:619:LHG:H362	1.85	0.43
25:z:15:VAL:HG11	25:z:50:LEU:HD12	2.00	0.43
29:f1:216:LYS:NZ	29:f1:217:ARG:HH12	2.16	0.43
1:1:150:LEU:CD1	37:2:619:XAT:H202	2.49	0.43
31:3:314:CLA:H2	31:3:314:CLA:C4D	2.48	0.43
2:4:171:TYR:CD2	3:5:49:LEU:HD12	2.54	0.43
37:4:619:XAT:H31	37:4:619:XAT:H391	1.77	0.43
34:4:620:LMG:H111	34:4:620:LMG:H142	1.72	0.43
3:5:141:SER:O	30:5:605:CHL:H2A	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:184:ALA:O	3:5:187:PRO:HD3	2.18	0.43
4:6:104:CYS:SG	4:6:217:MET:HE1	2.59	0.43
8:D:117:HIS:CE1	31:D:404:CLA:C4D	3.00	0.43
8:D:261:PHE:CE2	33:D:408:LHG:HC81	2.53	0.43
8:D:279:LEU:HD11	42:D:401:PHO:CMC	2.48	0.43
14:K:21:ILE:HD11	33:K:102:LHG:H271	2.00	0.43
32:N:316:LUT:H15	32:N:316:LUT:H201	1.82	0.43
22:W:87:ILE:O	22:W:91:ILE:HG13	2.18	0.43
1:7:99:MET:SD	31:7:311:CLA:HAB	2.59	0.43
1:7:244:TYR:CD1	31:7:315:CLA:HED3	2.53	0.43
31:8:602:CLA:H141	31:8:602:CLA:H162	1.82	0.43
31:8:604:CLA:HBB1	31:8:604:CLA:CMB	2.48	0.43
2:9:99:MET:HB3	35:9:317:RRX:C18	2.48	0.43
2:9:146:LEU:O	2:9:148:HIS:N	2.51	0.43
2:9:230:THR:HG23	2:9:232:LYS:N	2.27	0.43
2:q:96:ARG:HA	2:q:99:MET:HE3	1.99	0.43
2:q:124:VAL:HG13	2:q:126:PHE:CE1	2.54	0.43
2:q:127:LYS:HA	30:q:309:CHL:HED2	2.00	0.43
31:b:612:CLA:H93	31:b:612:CLA:H62	1.86	0.43
31:c:613:CLA:HMB1	31:c:613:CLA:HBB1	2.00	0.43
45:c:616:DGD:HBW2	45:c:616:DGD:HB92	1.63	0.43
31:g:313:CLA:HBB1	31:g:313:CLA:CMB	2.49	0.43
3:n:191:ALA:HB2	31:n:311:CLA:HAA2	1.99	0.43
19:s:59:LEU:HD13	19:s:71:ILE:HD11	1.99	0.43
31:s:305:CLA:H93	36:s:319:NEX:C37	2.48	0.43
23:x:82:VAL:O	23:x:86:ILE:HG13	2.18	0.43
24:y:194:LEU:HD12	32:y:616:LUT:H222	2.01	0.43
2:2:139:ASN:HB3	2:2:143:ASN:C	2.44	0.43
31:2:602:CLA:H72	32:2:615:LUT:H31	2.00	0.43
3:3:252:LYS:HA	3:3:256:ILE:CG2	2.37	0.43
2:4:89:GLU:O	2:4:93:ILE:HG12	2.19	0.43
2:4:110:LEU:O	2:4:114:ASN:N	2.52	0.43
2:4:122:ALA:HB1	31:4:604:CLA:HED3	2.00	0.43
31:4:612:CLA:HHC	31:4:612:CLA:CBB	2.48	0.43
3:5:181:PRO:HB3	30:5:608:CHL:HBC2	2.00	0.43
30:6:309:CHL:CMA	36:6:319:NEX:H30	2.46	0.43
31:C:605:CLA:H202	31:C:605:CLA:H162	1.77	0.43
2:G:133:PHE:CE1	30:N:301:CHL:HMD3	2.53	0.43
31:G:612:CLA:HMA1	35:G:614:RRX:H57	2.00	0.43
32:G:615:LUT:H361	32:G:615:LUT:C28	2.48	0.43
34:G:621:LMG:C41	30:N:309:CHL:H161	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:U:151:LYS:O	26:U:155:GLN:HG2	2.18	0.43
3:8:200:LEU:HB3	31:8:609:CLA:CMA	2.48	0.43
3:8:220:VAL:O	3:8:224:ILE:HG12	2.19	0.43
3:8:245:PHE:CD1	3:8:249:TYR:HB2	2.53	0.43
32:8:616:LUT:H31	32:8:616:LUT:H391	1.95	0.43
31:9:306:CLA:HMB1	31:9:306:CLA:HBB1	1.99	0.43
30:p:609:CHL:HBD	30:p:609:CHL:HAA1	2.00	0.43
2:q:54:SER:O	2:q:58:VAL:HG23	2.18	0.43
35:q:317:RRX:H26	35:q:317:RRX:H22	1.79	0.43
2:g:97:TRP:CE2	30:g:308:CHL:HED3	2.53	0.43
31:s:312:CLA:H3A	31:s:312:CLA:HBA2	1.50	0.43
24:y:59:PRO:HG2	24:y:73:ASP:HB3	2.00	0.43
31:y:610:CLA:H61	31:y:610:CLA:H92	1.61	0.43
34:Q1:101:LMG:HC8	34:Q1:101:LMG:H111	1.32	0.43
29:F1:181:VAL:HG13	29:F1:195:GLN:HB2	2.00	0.43
1:1:48:LYS:HD3	1:1:58:VAL:HG22	2.00	0.43
1:1:223:THR:HA	1:1:247:TYR:CZ	2.54	0.43
30:1:605:CHL:HED3	18:R:266:LEU:HD21	2.00	0.43
2:2:193:LEU:HB2	2:2:195:LEU:HG	2.00	0.43
2:2:258:LEU:HD23	2:2:259:PRO:N	2.34	0.43
31:2:609:CLA:HBA1	35:2:614:RRX:C40	2.48	0.43
31:2:613:CLA:HBB1	31:2:613:CLA:CMB	2.49	0.43
3:3:93:ARG:HA	3:3:96:MET:HE3	1.99	0.43
3:3:206:LYS:HE3	33:3:320:LHG:O10	2.18	0.43
3:3:258:TYR:CE2	31:3:316:CLA:CHD	3.00	0.43
2:4:93:ILE:HD12	2:4:170:ARG:HH21	1.84	0.43
2:4:164:GLY:HA2	30:4:609:CHL:HAB	2.01	0.43
2:4:207:VAL:HA	2:4:210:ILE:HG22	2.00	0.43
3:5:40:TRP:HE3	3:5:46:PRO:HG3	1.82	0.43
7:C:158:LEU:HD22	34:C:621:LMG:H371	2.01	0.43
7:C:187:ILE:HG21	7:C:222:ILE:HG12	2.01	0.43
7:C:348:ASP:OD1	7:C:348:ASP:N	2.40	0.43
31:G:612:CLA:HMA1	35:G:614:RRX:H4	2.00	0.43
17:O:153:ASP:CG	17:O:154:GLY:H	2.26	0.43
22:W:93:TRP:HZ2	34:W:201:LMG:C11	2.31	0.43
24:Y:175:PRO:HB2	36:Y:317:NEX:H183	2.01	0.43
24:Y:206:LEU:HB3	31:Y:310:CLA:CMA	2.48	0.43
43:Z:101:BCR:H24C	43:Z:101:BCR:H371	1.81	0.43
1:7:72:TRP:O	32:7:318:LUT:H24	2.18	0.43
34:7:320:LMG:HC1	31:r:313:CLA:CMA	2.47	0.43
2:9:99:MET:O	35:9:317:RRX:H28	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:219:SER:O	2:9:223:PHE:HD1	2.01	0.43
31:p:611:CLA:H92	31:p:612:CLA:CED	2.48	0.43
2:q:170:ARG:HA	30:q:310:CHL:C4C	2.49	0.43
32:q:318:LUT:H31	32:q:318:LUT:H391	1.91	0.43
5:a:51:ALA:HA	5:a:55:ALA:HB2	2.01	0.43
7:c:135:PHE:HA	31:c:612:CLA:HMC1	2.00	0.43
7:c:261:SER:HB2	7:c:433:ALA:HB2	2.01	0.43
43:c:615:BCR:H15C	34:w:201:LMG:H402	2.00	0.43
8:d:257:PHE:O	33:d:408:LHG:H341	2.18	0.43
3:n:100:LEU:HD13	31:n:313:CLA:HBB2	2.00	0.43
31:n:303:CLA:H141	31:n:303:CLA:H162	1.81	0.43
18:r:141:ARG:HA	18:r:144:MET:HE3	2.00	0.43
18:r:220:LEU:HD12	32:r:317:LUT:H222	2.01	0.43
19:s:236:ILE:HD12	19:s:237:LYS:N	2.33	0.43
26:u:130:ARG:C	26:u:132:VAL:H	2.25	0.43
2:2:138:LEU:HD13	30:2:606:CHL:HHD	2.01	0.43
2:4:126:PHE:CB	31:5:615:CLA:HMB3	2.49	0.43
31:4:604:CLA:NC	36:4:617:NEX:H222	2.33	0.43
3:5:162:ILE:HD11	36:5:618:NEX:C35	2.49	0.43
31:6:305:CLA:H42	36:6:319:NEX:H23	1.99	0.43
7:C:155:VAL:HG12	34:C:621:LMG:C36	2.42	0.43
31:D:403:CLA:H62	31:D:403:CLA:H41	1.61	0.43
2:G:160:LEU:HA	30:G:608:CHL:HBB2	2.01	0.43
38:G:624:SQD:H252	31:7:312:CLA:H43	2.00	0.43
22:W:117:LEU:HD23	22:W:117:LEU:HA	1.86	0.43
31:Y:310:CLA:C2	32:Y:315:LUT:H28	2.48	0.43
1:7:94:HIS:CE1	31:7:304:CLA:C4D	3.02	0.43
1:7:178:TYR:HA	31:7:311:CLA:O1D	2.19	0.43
3:8:85:ARG:HG3	31:8:602:CLA:HMA3	2.01	0.43
31:p:610:CLA:HBB1	31:p:610:CLA:CMB	2.49	0.43
2:q:153:VAL:O	2:q:157:LEU:HD13	2.19	0.43
2:q:163:MET:HE1	30:q:308:CHL:HMA3	2.00	0.43
31:q:312:CLA:NA	35:q:317:RRX:H7	2.33	0.43
5:a:286:THR:OG1	31:a:406:CLA:O1D	2.32	0.43
7:c:132:PHE:CE1	31:c:613:CLA:HAA1	2.53	0.43
8:d:148:ALA:HB1	8:d:279:LEU:HB2	2.01	0.43
10:f:44:ARG:NH1	29:f1:60:ILE:HG21	2.33	0.43
32:g:316:LUT:H11	32:g:316:LUT:H191	1.82	0.43
32:g:316:LUT:H8	32:g:316:LUT:H181	2.01	0.43
18:r:139:HIS:CE1	31:r:305:CLA:C4D	3.02	0.43
37:r:318:XAT:H35	37:r:318:XAT:H401	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:124:VAL:HG13	2:2:127:LYS:HB2	2.00	0.43
2:2:153:VAL:O	2:2:156:LEU:HB2	2.19	0.43
3:3:41:TYR:OH	3:3:198:ALA:O	2.33	0.43
3:3:145:ALA:HA	30:3:307:CHL:CHC	2.48	0.43
3:3:160:GLY:HA2	30:3:310:CHL:CBB	2.48	0.43
3:3:166:ARG:HG3	3:3:167:VAL:HG13	2.01	0.43
2:4:116:ALA:HA	34:Q1:101:LMG:H112	2.01	0.43
2:4:132:ILE:CG1	2:4:152:ILE:HG13	2.48	0.43
30:4:606:CHL:HMC	32:4:616:LUT:H163	2.00	0.43
4:6:248:TYR:CD1	31:6:315:CLA:HED2	2.54	0.43
31:C:609:CLA:H141	31:C:609:CLA:H161	1.75	0.43
32:G:615:LUT:H402	32:G:615:LUT:H31	1.18	0.43
30:N:306:CHL:H122	32:S:317:LUT:H171	2.01	0.43
38:R:322:SQD:H161	38:R:322:SQD:H131	1.92	0.43
26:U:130:ARG:O	26:U:131:GLN:HB3	2.18	0.43
30:0:605:CHL:HAA1	31:r:315:CLA:CMD	2.49	0.43
30:0:607:CHL:CAA	37:q:321:XAT:C4	2.97	0.43
31:7:311:CLA:H62	31:7:313:CLA:CMA	2.49	0.43
31:p:615:CLA:C4C	34:q:302:LMG:H301	2.48	0.43
38:a:411:SQD:H312	31:c:608:CLA:H62	2.00	0.43
6:b:74:SER:OG	6:b:94:GLU:OE2	2.23	0.43
6:b:112:ILE:HG22	43:b:620:BCR:H402	2.01	0.43
6:b:124:ARG:O	11:h:31:LYS:NZ	2.48	0.43
33:b:628:LHG:H252	30:r:309:CHL:CHD	2.49	0.43
34:c:624:LMG:C31	33:y:619:LHG:HC92	2.48	0.43
3:n:245:PHE:CD1	3:n:249:TYR:HB2	2.53	0.43
48:r:302:LMU:H12	48:r:302:LMU:H41	1.37	0.43
30:r:310:CHL:HBB2	38:r:322:SQD:H81	2.01	0.43
31:2:603:CLA:H11	3:3:74:LEU:HD11	2.01	0.43
31:2:611:CLA:HBB1	31:2:611:CLA:HMB3	2.00	0.43
3:3:46:PRO:HB2	30:3:303:CHL:CBC	2.49	0.43
3:3:75:SER:HB3	3:3:81:PHE:CD1	2.54	0.43
31:3:314:CLA:CGA	31:3:314:CLA:C1A	2.97	0.43
2:4:54:SER:O	2:4:58:VAL:HG23	2.18	0.43
31:4:604:CLA:C1B	36:4:617:NEX:H383	2.49	0.43
32:4:616:LUT:H15	32:4:616:LUT:H201	1.85	0.43
31:5:610:CLA:H52	32:5:616:LUT:C28	2.48	0.43
36:5:618:NEX:H35	36:5:618:NEX:H401	1.90	0.43
4:6:49:PHE:CD2	30:6:302:CHL:HAA1	2.54	0.43
31:6:315:CLA:H42	31:6:315:CLA:C2D	2.49	0.43
31:6:315:CLA:H62	31:6:315:CLA:H2	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:338:ILE:HG21	7:C:347:TRP:HB2	2.00	0.43
7:C:361:ASN:O	7:C:361:ASN:ND2	2.51	0.43
8:D:117:HIS:HE1	31:D:404:CLA:ND	2.14	0.43
43:H:101:BCR:H11C	43:H:101:BCR:H341	1.82	0.43
34:I:101:LMG:O9	34:I:101:LMG:HC71	2.18	0.43
14:K:46:ARG:NH2	21:V:33:LEU:O	2.51	0.43
30:N:301:CHL:HBD	30:N:301:CHL:HAA1	2.00	0.43
31:N:303:CLA:HED2	31:N:303:CLA:H2A	2.01	0.43
30:7:302:CHL:HHC	30:7:302:CHL:CBB	2.47	0.43
31:7:312:CLA:HHC	31:7:312:CLA:CBB	2.49	0.43
30:7:321:CHL:H42	30:7:321:CHL:C1D	2.49	0.43
2:9:95:ALA:HB1	2:9:213:GLY:HA3	2.01	0.43
32:9:318:LUT:H31	32:9:318:LUT:H391	1.72	0.43
31:p:604:CLA:HMA3	30:p:606:CHL:C2C	2.49	0.43
44:a:414:PL9:H303	33:e:101:LHG:H382	2.01	0.43
6:b:121:GLU:HG3	11:h:22:ILE:O	2.19	0.43
31:b:615:CLA:HBB1	31:b:615:CLA:CMB	2.49	0.43
7:c:426:PHE:CE1	31:c:605:CLA:HAB	2.54	0.43
33:j:102:LHG:C3	29:f1:58:GLY:HA2	2.49	0.43
31:n:305:CLA:HBB1	31:n:305:CLA:CMB	2.47	0.43
22:w:111:ASN:C	22:w:111:ASN:HD22	2.26	0.43
27:q1:31:LEU:HA	27:q1:34:MET:HG2	2.01	0.43
28:p1:25:MET:HB3	28:p1:27:LYS:HE2	2.00	0.43
31:1:603:CLA:CMC	30:1:607:CHL:H122	2.49	0.42
31:1:614:CLA:C8	31:1:614:CLA:H2	2.48	0.42
2:2:238:LEU:HD11	34:2:618:LMG:H162	2.00	0.42
3:3:95:ALA:HA	32:3:318:LUT:C11	2.46	0.42
3:3:157:VAL:O	3:3:161:LEU:HG	2.19	0.42
33:3:320:LHG:H281	33:3:320:LHG:C7	2.49	0.42
2:4:223:PHE:CE1	35:4:615:RRX:H51	2.53	0.42
31:4:602:CLA:HED2	31:4:602:CLA:H2A	2.00	0.42
31:4:603:CLA:HED2	31:4:603:CLA:H2A	2.00	0.42
3:5:143:ILE:O	3:5:144:HIS:C	2.62	0.42
31:B:604:CLA:H143	31:B:615:CLA:HMA3	2.01	0.42
31:B:613:CLA:H141	31:B:613:CLA:H162	1.86	0.42
7:C:299:GLN:OE1	7:C:343:THR:OG1	2.37	0.42
7:C:336:GLU:H	7:C:336:GLU:HG2	1.57	0.42
31:C:603:CLA:HMB1	31:C:603:CLA:HBB1	2.01	0.42
44:D:406:PL9:H101	33:D:408:LHG:H101	2.01	0.42
2:G:254:ALA:O	37:G:620:XAT:H42	2.18	0.42
30:N:306:CHL:H101	30:N:306:CHL:H61	1.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:168:TYR:CZ	24:Y:175:PRO:HD3	2.53	0.42
30:Y:301:CHL:C12	30:Y:302:CHL:H61	2.49	0.42
1:7:198:LEU:CB	31:7:311:CLA:HMA2	2.49	0.42
30:8:605:CHL:H101	30:8:605:CHL:H61	1.67	0.42
31:q:314:CLA:H2A	31:q:314:CLA:O1D	2.19	0.42
6:b:357:ARG:HD2	6:b:366:PHE:CE2	2.54	0.42
7:c:264:LEU:HD21	31:c:608:CLA:CAB	2.49	0.42
34:c:620:LMG:H331	34:c:620:LMG:H362	1.90	0.42
33:g:319:LHG:HC61	37:g:321:XAT:H382	2.01	0.42
30:n:308:CHL:H42	30:n:308:CHL:C1D	2.49	0.42
36:n:319:NEX:H201	36:n:319:NEX:H15	1.78	0.42
18:r:78:LEU:HD13	31:r:304:CLA:H42	2.01	0.42
36:r:301:NEX:H15	36:r:301:NEX:H201	1.90	0.42
19:s:236:ILE:H	19:s:236:ILE:HG13	1.64	0.42
24:y:90:ILE:HD13	31:y:603:CLA:HBA1	2.01	0.42
25:z:33:TRP:CE2	25:z:37:LYS:HE2	2.54	0.42
29:F1:99:ASP:HB3	29:F1:102:ASP:O	2.19	0.42
1:1:157:MET:HE1	36:R:301:NEX:H30	2.01	0.42
1:1:170:ALA:O	1:1:182:ASN:ND2	2.52	0.42
3:3:245:PHE:CG	3:3:246:TRP:N	2.86	0.42
30:3:309:CHL:HAA1	30:3:309:CHL:CBD	2.48	0.42
30:5:605:CHL:HHC	30:5:605:CHL:CBB	2.45	0.42
4:6:71:TRP:CZ2	30:6:302:CHL:HAA2	2.55	0.42
4:6:165:GLU:HG3	30:6:310:CHL:C4B	2.49	0.42
4:6:182:TYR:CE2	4:6:203:LYS:HE3	2.54	0.42
31:6:303:CLA:H52	32:6:318:LUT:H28	2.01	0.42
31:6:313:CLA:HHC	31:6:313:CLA:CBB	2.49	0.42
5:A:93:PHE:HZ	31:A:409:CLA:HAA1	1.83	0.42
30:G:601:CHL:H171	30:G:623:CHL:C4B	2.50	0.42
31:G:604:CLA:HBB1	31:G:604:CLA:CMB	2.49	0.42
38:G:617:SQD:O6	38:G:617:SQD:C6	2.67	0.42
34:I:101:LMG:HC8	34:I:101:LMG:HC1	1.79	0.42
16:M:30:ALA:HB3	38:M:102:SQD:H462	2.01	0.42
3:N:203:LYS:HD3	31:N:312:CLA:HAA2	2.00	0.42
32:N:317:LUT:H11	32:N:317:LUT:H191	1.81	0.42
17:O:65:VAL:HG13	17:O:70:ILE:HG13	2.00	0.42
17:O:75:PRO:HD2	17:O:98:CYS:SG	2.59	0.42
18:R:50:ASP:CG	18:R:59:ARG:HH21	2.26	0.42
43:T:101:BCR:C33	43:b:619:BCR:H14C	2.49	0.42
31:Y:304:CLA:HHC	31:Y:304:CLA:CBB	2.49	0.42
32:Y:315:LUT:H35	32:Y:315:LUT:H401	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:0:49:PHE:CG	4:0:71:TRP:HB2	2.54	0.42
31:0:615:CLA:HBB2	3:p:121:TRP:CH2	2.54	0.42
34:7:301:LMG:HC8	34:7:301:LMG:HC1	1.77	0.42
30:7:307:CHL:HMB2	30:7:310:CHL:OMC	2.19	0.42
3:8:222:GLY:O	3:8:226:ARG:HA	2.19	0.42
2:9:92:VAL:HB	2:9:184:LEU:HD21	1.99	0.42
35:q:317:RRX:H8	35:q:317:RRX:H21	2.00	0.42
5:a:141:PRO:HG3	7:c:434:GLY:C	2.45	0.42
6:b:469:HIS:HE1	31:b:612:CLA:NA	2.16	0.42
31:b:606:CLA:H142	31:b:611:CLA:C2	2.49	0.42
7:c:177:TRP:HZ3	7:c:355:GLU:HG3	1.83	0.42
10:f:14:ILE:HD13	27:q1:23:ILE:HD11	2.02	0.42
2:g:167:GLU:HG2	30:g:309:CHL:CHB	2.49	0.42
31:g:303:CLA:H13	31:g:303:CLA:H102	1.88	0.42
31:y:604:CLA:HBB1	31:y:604:CLA:CMB	2.48	0.42
27:Q1:3:ASN:HB2	34:Q1:101:LMG:O6	2.19	0.42
29:f1:170:ASP:OD1	29:f1:171:LYS:N	2.47	0.42
1:1:59:PRO:HB3	1:1:61:TYR:CZ	2.55	0.42
2:2:246:SER:O	2:2:249:ASN:ND2	2.52	0.42
2:4:169:TYR:CB	2:4:174:GLU:HG3	2.49	0.42
2:4:254:ALA:HA	37:4:619:XAT:H172	2.02	0.42
31:4:604:CLA:H11	30:4:606:CHL:C4D	2.49	0.42
3:5:98:GLY:HA2	32:5:617:LUT:C18	2.49	0.42
34:5:620:LMG:H331	34:5:620:LMG:H362	1.71	0.42
31:B:604:CLA:H12	31:B:605:CLA:C4D	2.49	0.42
11:H:78:THR:OG1	11:H:83:SER:HB3	2.19	0.42
3:N:51:PRO:O	3:N:53:SER:N	2.52	0.42
3:N:223:LEU:HD21	31:N:321:CLA:C4	2.48	0.42
17:O:173:LEU:HD12	17:O:197:TYR:HA	1.99	0.42
19:S:161:ASN:HD21	19:S:163:LEU:HD23	1.84	0.42
34:X:202:LMG:H322	34:X:202:LMG:H351	1.79	0.42
4:0:175:GLY:HA2	18:r:56:ASN:HB2	2.01	0.42
30:0:607:CHL:HAA2	37:q:321:XAT:H42	2.01	0.42
31:p:602:CLA:H42	32:p:617:LUT:C37	2.49	0.42
30:p:605:CHL:HHC	30:p:605:CHL:CBB	2.44	0.42
2:q:140:TYR:O	2:q:141:LEU:C	2.62	0.42
30:q:307:CHL:HHC	30:q:307:CHL:CBB	2.45	0.42
5:a:307:VAL:HG11	29:f1:81:LYS:HE3	2.01	0.42
6:b:115:TRP:CD2	43:b:618:BCR:H291	2.54	0.42
31:b:610:CLA:OBD	11:h:46:THR:OG1	2.36	0.42
7:c:113:LEU:HD12	7:c:113:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:449:ARG:NH2	8:d:241:GLU:HB3	2.35	0.42
31:s:305:CLA:HMA3	30:s:307:CHL:C3C	2.49	0.42
31:s:306:CLA:H3A	31:s:306:CLA:HBA1	1.72	0.42
33:s:322:LHG:H132	33:s:322:LHG:O10	2.19	0.42
30:y:609:CHL:HHC	30:y:609:CHL:CBB	2.48	0.42
27:q1:16:ILE:O	27:q1:20:LEU:HD13	2.19	0.42
29:F1:208:LEU:HD23	29:F1:208:LEU:C	2.44	0.42
29:f1:102:ASP:HB2	29:f1:217:ARG:HE	1.85	0.42
2:2:150:GLN:HB2	30:2:605:CHL:CBB	2.49	0.42
2:2:174:GLU:HA	2:2:179:THR:HG21	2.01	0.42
2:2:177:VAL:HB	2:2:189:PHE:CG	2.54	0.42
31:2:603:CLA:H93	31:2:603:CLA:H62	1.79	0.42
30:3:302:CHL:H61	30:3:302:CHL:H101	1.75	0.42
31:3:314:CLA:HHC	31:3:314:CLA:CBB	2.49	0.42
30:5:601:CHL:HHC	30:5:601:CHL:CBB	2.47	0.42
4:6:168:ARG:NH2	30:6:310:CHL:O1D	2.50	0.42
5:A:102:LEU:H	34:A:414:LMG:HC61	1.85	0.42
31:A:406:CLA:H92	31:A:406:CLA:H62	1.76	0.42
6:B:230:ARG:NH2	38:B:623:SQD:O4	2.52	0.42
31:C:604:CLA:O2A	45:C:617:DGD:HB31	2.19	0.42
31:C:605:CLA:H142	31:C:605:CLA:H111	1.84	0.42
33:G:618:LHG:HC62	37:G:620:XAT:C38	2.49	0.42
34:G:621:LMG:H111	34:G:621:LMG:H142	1.75	0.42
3:N:215:MET:HE2	32:N:317:LUT:H10	2.02	0.42
31:N:310:CLA:H92	31:N:310:CLA:H61	1.62	0.42
18:R:164:ALA:CB	31:R:306:CLA:HED1	2.45	0.42
43:T:101:BCR:H332	6:b:33:TRP:HD1	1.84	0.42
30:0:601:CHL:HED1	33:0:619:LHG:H281	2.01	0.42
30:0:607:CHL:H122	30:0:607:CHL:H93	2.01	0.42
31:8:613:CLA:H2A	31:8:613:CLA:HED3	2.02	0.42
5:a:191:ASN:HB2	7:c:399:ALA:HB1	2.01	0.42
7:c:104:VAL:HG22	43:z:101:BCR:HC41	2.01	0.42
7:c:134:PHE:HD1	34:c:620:LMG:HC4	1.84	0.42
7:c:205:PRO:O	45:c:616:DGD:HG12	2.19	0.42
7:c:310:GLN:HG3	7:c:316:VAL:CG1	2.49	0.42
8:d:191:TRP:CE3	8:d:289:LEU:HD11	2.54	0.42
8:d:197:HIS:HE1	31:d:404:CLA:C1C	2.32	0.42
33:d:408:LHG:H292	20:t:17:ILE:HG23	2.00	0.42
2:g:40:GLU:O	2:g:41:PHE:HB2	2.18	0.42
2:g:238:LEU:HD21	34:g:320:LMG:H162	2.00	0.42
14:k:15:TYR:CZ	25:z:5:PHE:HZ	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:s:318:LUT:H15	32:s:318:LUT:H201	1.93	0.42
24:y:95:ALA:HB1	24:y:214:GLY:HA3	2.01	0.42
24:y:139:TYR:HH	36:y:618:NEX:H1	1.55	0.42
33:z:102:LHG:HC82	33:z:102:LHG:HC5	1.90	0.42
31:1:604:CLA:CMA	30:1:606:CHL:HBC3	2.45	0.42
31:1:612:CLA:H3A	31:1:612:CLA:HBA1	1.63	0.42
34:2:621:LMG:HC2	31:3:316:CLA:CGA	2.50	0.42
3:3:87:LEU:HD13	31:3:305:CLA:CBA	2.48	0.42
30:3:307:CHL:HBB1	34:3:321:LMG:H351	2.02	0.42
2:4:94:HIS:CE1	31:4:603:CLA:C4D	3.02	0.42
31:4:611:CLA:C4D	31:4:612:CLA:HMD3	2.49	0.42
3:5:54:ASN:O	3:5:55:PRO:C	2.62	0.42
4:6:219:GLY:O	4:6:223:GLN:HG3	2.20	0.42
6:B:382:PRO:HG3	6:B:391:SER:HB3	2.01	0.42
45:C:618:DGD:HB51	45:C:618:DGD:HB21	1.89	0.42
31:D:404:CLA:H91	31:D:404:CLA:H112	1.74	0.42
9:E:64:PRO:HB3	9:E:79:LEU:HD13	2.01	0.42
30:G:601:CHL:H11	30:Y:309:CHL:C1B	2.49	0.42
31:G:602:CLA:H102	31:G:602:CLA:H13	1.78	0.42
30:R:309:CHL:HBD	30:R:309:CHL:HAA1	2.02	0.42
38:R:322:SQD:H311	38:R:322:SQD:H342	1.79	0.42
4:0:120:GLU:HB2	4:0:129:GLN:HG3	2.00	0.42
4:0:202:LEU:CB	31:0:610:CLA:HMA2	2.42	0.42
30:0:605:CHL:HBA1	30:0:605:CHL:CBD	2.45	0.42
30:0:608:CHL:HMB2	36:0:618:NEX:C35	2.49	0.42
31:8:614:CLA:H12	2:9:257:PHE:HE1	1.84	0.42
2:9:205:LEU:CD2	31:9:312:CLA:H43	2.50	0.42
3:p:118:GLU:HB2	3:p:123:LYS:O	2.19	0.42
3:p:217:GLY:O	3:p:221:GLN:HG2	2.20	0.42
3:p:218:PHE:HA	3:p:221:GLN:NE2	2.35	0.42
31:p:610:CLA:H2	32:p:616:LUT:C38	2.49	0.42
2:q:146:LEU:HD12	30:q:307:CHL:HED3	2.01	0.42
6:b:115:TRP:CG	43:b:618:BCR:H291	2.55	0.42
6:b:270:PRO:HG3	6:b:312:TYR:HD1	1.84	0.42
8:d:266:TRP:CZ3	33:l:101:LHG:HC42	2.54	0.42
33:e:101:LHG:HC62	34:k:102:LMG:H342	2.02	0.42
31:n:303:CLA:H161	31:n:303:CLA:H202	1.87	0.42
31:n:316:CLA:H61	31:n:316:CLA:H92	1.68	0.42
36:r:319:NEX:H15	36:r:319:NEX:H201	1.88	0.42
31:s:305:CLA:HMA3	30:s:307:CHL:C4C	2.49	0.42
34:Q1:101:LMG:H342	34:Q1:101:LMG:H311	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f1:110:LEU:HD12	29:f1:110:LEU:N	2.34	0.42
2:2:83:THR:HG22	2:2:87:TYR:CE2	2.54	0.42
31:2:611:CLA:HMC3	35:2:614:RRX:H44	2.01	0.42
3:3:252:LYS:HB3	3:3:256:ILE:HG23	2.01	0.42
2:4:111:LEU:HB3	2:4:117:ALA:HB3	2.01	0.42
2:4:173:GLY:HA2	30:4:608:CHL:HMC	2.02	0.42
3:5:107:LEU:O	3:5:110:ARG:HG2	2.20	0.42
3:5:166:ARG:HG3	30:5:608:CHL:C1D	2.48	0.42
3:5:190:LEU:HB2	31:5:610:CLA:O1A	2.20	0.42
3:5:209:ARG:HA	3:5:212:MET:HE3	2.01	0.42
3:5:225:THR:HG21	3:5:232:ASN:CG	2.45	0.42
31:A:405:CLA:H62	31:A:405:CLA:H2	1.79	0.42
31:C:601:CLA:H143	31:C:601:CLA:H112	1.79	0.42
34:C:624:LMG:H121	34:C:624:LMG:H152	1.78	0.42
8:D:56:THR:HG21	9:E:50:PRO:HD3	2.02	0.42
8:D:87:HIS:CD2	8:D:166:GLY:HA2	2.54	0.42
11:H:76:ASP:OD1	11:H:76:ASP:N	2.51	0.42
34:J:101:LMG:H151	33:F1:301:LHG:H281	2.02	0.42
3:N:249:TYR:C	3:N:251:PRO:HD2	2.44	0.42
18:R:123:TYR:OH	18:R:134:GLU:OE1	2.30	0.42
23:X:96:PHE:CE2	27:Q1:34:MET:HE2	2.55	0.42
2:9:223:PHE:CE1	35:9:317:RRX:H48	2.54	0.42
31:9:304:CLA:CHA	31:9:304:CLA:HBA1	2.40	0.42
30:p:608:CHL:HAA1	30:p:608:CHL:CBD	2.49	0.42
32:p:616:LUT:H35	32:p:616:LUT:H401	1.33	0.42
2:q:180:SER:O	2:q:181:GLY:C	2.62	0.42
2:q:256:LYS:HD3	2:q:257:PHE:CE1	2.55	0.42
31:a:409:CLA:CMA	45:c:616:DGD:HBW1	2.49	0.42
6:b:52:LEU:HD12	6:b:52:LEU:HA	1.81	0.42
7:c:61:ALA:HB2	14:k:11:LEU:HD13	2.01	0.42
7:c:104:VAL:HG11	43:c:614:BCR:HC42	2.01	0.42
7:c:361:ASN:O	7:c:361:ASN:ND2	2.50	0.42
45:c:617:DGD:HBV1	34:d:409:LMG:H152	2.01	0.42
2:g:92:VAL:HB	2:g:184:LEU:HD21	2.01	0.42
37:g:321:XAT:H202	24:y:155:LEU:HD21	2.01	0.42
3:n:243:THR:HA	3:n:248:ASP:OD2	2.19	0.42
19:s:154:VAL:HG11	31:s:306:CLA:CED	2.50	0.42
19:s:264:TRP:HE1	31:s:315:CLA:HMC2	1.85	0.42
1:1:89:GLU:O	1:1:93:ILE:HG12	2.20	0.42
1:1:251:LEU:O	1:1:252:ALA:HB2	2.19	0.42
3:3:180:TYR:CE2	3:3:201:LYS:HE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:197:PHE:CZ	31:5:610:CLA:HED3	2.55	0.42
31:B:610:CLA:H122	31:B:615:CLA:HAA1	2.00	0.42
31:C:604:CLA:H92	31:C:604:CLA:H62	1.76	0.42
33:D:407:LHG:H341	33:D:407:LHG:H101	2.02	0.42
9:E:25:ILE:C	9:E:28:PRO:HD2	2.45	0.42
34:I:101:LMG:H112	34:I:101:LMG:H141	1.80	0.42
17:O:150:LYS:HE3	17:O:150:LYS:HB3	1.90	0.42
31:S:312:CLA:H3A	31:S:312:CLA:HBA2	1.51	0.42
31:S:313:CLA:HED1	31:S:313:CLA:H2	2.01	0.42
31:Y:313:CLA:H2	31:Y:313:CLA:H61	1.77	0.42
3:8:252:LYS:HB2	3:8:258:TYR:HD2	1.83	0.42
2:9:205:LEU:HB3	31:9:312:CLA:CMA	2.50	0.42
2:9:205:LEU:HB3	31:9:312:CLA:HMA2	2.01	0.42
32:9:318:LUT:H15	32:9:318:LUT:H201	1.75	0.42
3:p:96:MET:HG3	3:p:208:GLY:HA2	2.00	0.42
3:p:190:LEU:HD22	32:p:616:LUT:H371	2.02	0.42
2:q:104:GLY:HA3	32:q:318:LUT:C18	2.50	0.42
5:a:266:ASN:HD21	34:a:416:LMG:HC62	1.84	0.42
31:a:409:CLA:H11	12:i:9:TYR:CZ	2.55	0.42
31:b:604:CLA:HBB1	31:b:604:CLA:HMB1	2.02	0.42
7:c:239:HIS:HE1	31:c:606:CLA:NA	2.14	0.42
31:c:601:CLA:H41	31:c:601:CLA:H61	1.84	0.42
45:c:619:DGD:HE62	24:y:40:VAL:HG11	2.02	0.42
32:g:316:LUT:H361	32:g:316:LUT:C28	2.50	0.42
19:s:108:ALA:HB1	19:s:239:GLY:HA3	2.02	0.42
43:t:101:BCR:H341	43:t:101:BCR:H11C	1.26	0.42
22:w:111:ASN:HA	22:w:115:PHE:CG	2.54	0.42
30:y:606:CHL:OMC	30:y:606:CHL:HAC2	2.18	0.42
36:y:618:NEX:H15	36:y:618:NEX:H201	1.90	0.42
1:1:61:TYR:OH	1:1:76:GLY:HA2	2.20	0.42
30:1:607:CHL:HAA2	37:2:619:XAT:H42	2.02	0.42
31:1:610:CLA:H61	31:1:610:CLA:H41	1.66	0.42
3:3:190:LEU:HB2	31:3:311:CLA:CGA	2.49	0.42
2:4:90:ILE:HD13	31:4:603:CLA:HBA1	2.01	0.42
30:4:606:CHL:OMC	30:4:606:CHL:HAC2	2.20	0.42
34:4:620:LMG:H351	3:5:223:LEU:HD21	2.01	0.42
3:5:106:GLU:HB3	3:5:230:ILE:HD12	1.99	0.42
4:6:146:HIS:O	4:6:148:GLN:NE2	2.50	0.42
31:6:311:CLA:H2	32:6:317:LUT:H28	2.02	0.42
36:6:319:NEX:H173	18:R:53:TRP:HH2	1.83	0.42
5:A:317:TRP:HZ3	8:D:180:ARG:HD2	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:226:TYR:CD2	6:B:231:MET:HB2	2.55	0.42
6:B:477:ASP:HB2	18:R:100:LYS:NZ	2.35	0.42
7:C:418:HIS:CD2	31:C:602:CLA:ND	2.88	0.42
31:N:304:CLA:NC	30:N:309:CHL:H102	2.34	0.42
31:N:310:CLA:H62	31:N:310:CLA:H41	1.90	0.42
24:Y:145:LEU:O	24:Y:147:HIS:N	2.52	0.42
31:Y:305:CLA:HBB1	31:Y:305:CLA:CMB	2.49	0.42
43:Z:101:BCR:H15C	43:Z:101:BCR:H351	1.89	0.42
31:0:602:CLA:H61	31:0:602:CLA:H41	1.58	0.42
3:8:67:TYR:HE2	30:8:601:CHL:HBC2	1.85	0.42
30:8:606:CHL:H12	30:8:606:CHL:H51	1.72	0.42
31:9:306:CLA:NA	36:9:319:NEX:H242	2.34	0.42
31:p:611:CLA:H12	31:p:612:CLA:OBD	2.19	0.42
34:p:620:LMG:C28	34:p:620:LMG:HC72	2.49	0.42
31:b:608:CLA:C4A	31:b:608:CLA:HBA2	2.49	0.42
7:c:56:ASN:ND2	7:c:99:TYR:O	2.52	0.42
45:c:616:DGD:HBT1	45:c:616:DGD:HBN2	2.02	0.42
43:d:406:BCR:H15C	43:d:406:BCR:H351	1.25	0.42
31:n:305:CLA:H152	31:s:306:CLA:C1B	2.50	0.42
17:o:79:SER:O	17:o:250:LYS:HD3	2.19	0.42
18:r:127:PHE:HA	18:r:132:PHE:CZ	2.54	0.42
19:s:211:TYR:HB3	31:s:311:CLA:HED3	2.01	0.42
32:s:318:LUT:H31	32:s:318:LUT:H391	1.96	0.42
2:2:254:ALA:HA	37:2:619:XAT:H22	2.01	0.42
32:3:318:LUT:H31	32:3:318:LUT:H391	1.94	0.42
3:5:160:GLY:HA2	30:5:609:CHL:CAB	2.49	0.42
31:5:611:CLA:C2B	33:5:619:LHG:HC11	2.49	0.42
4:6:72:ASP:OD2	4:6:77:SER:OG	2.31	0.42
30:6:309:CHL:HHC	30:6:309:CHL:CBB	2.46	0.42
32:6:317:LUT:H15	32:6:317:LUT:H201	1.97	0.42
5:A:155:THR:HG22	5:A:160:ILE:HD13	2.02	0.42
31:B:609:CLA:HBA2	43:H:101:BCR:HC32	2.01	0.42
7:C:132:PHE:CD1	33:C:623:LHG:HC11	2.54	0.42
7:C:142:LYS:HE3	7:C:254:TRP:CG	2.55	0.42
17:O:272:LEU:HD12	17:O:272:LEU:HA	1.88	0.42
31:S:304:CLA:HBB1	31:S:304:CLA:HMB3	2.00	0.42
31:S:305:CLA:H203	31:S:316:CLA:H3A	2.02	0.42
22:W:62:ASP:N	22:W:62:ASP:OD1	2.53	0.42
26:U:128:LEU:HD12	26:U:128:LEU:HA	1.89	0.42
4:0:217:MET:HE2	32:0:617:LUT:H10	2.02	0.42
1:7:90:ILE:CD1	31:7:304:CLA:HBA1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:243:THR:HA	3:8:248:ASP:OD2	2.19	0.42
2:9:101:GLY:HA2	32:9:318:LUT:C18	2.50	0.42
31:9:306:CLA:H61	30:9:308:CHL:HAA1	2.01	0.42
3:p:48:PHE:HA	30:p:601:CHL:C1D	2.49	0.42
3:p:91:HIS:HE1	31:p:603:CLA:C4D	2.32	0.42
31:a:406:CLA:H72	31:a:406:CLA:H111	1.83	0.42
6:b:312:TYR:O	6:b:313:ASP:CB	2.67	0.42
34:c:624:LMG:H371	30:y:601:CHL:HMB3	2.00	0.42
38:g:301:SQD:C10	37:g:321:XAT:H222	2.49	0.42
34:j:101:LMG:H332	33:j:102:LHG:H322	2.01	0.42
31:r:306:CLA:C1C	36:r:319:NEX:H222	2.50	0.42
43:t:101:BCR:H351	43:t:101:BCR:H15C	1.28	0.42
29:F1:95:LEU:HD11	29:F1:97:TYR:HE1	1.85	0.42
1:1:52:PRO:HD2	30:1:601:CHL:CBB	2.48	0.42
2:2:168:ALA:HB1	3:3:52:PHE:CD2	2.55	0.42
37:2:619:XAT:H28	37:2:619:XAT:C36	2.30	0.42
3:3:139:ASN:OD1	3:3:141:SER:OG	2.28	0.42
30:3:307:CHL:HHC	30:3:307:CHL:CBB	2.45	0.42
2:4:119:PHE:HB3	2:4:122:ALA:HB3	2.02	0.42
2:4:138:LEU:HD13	30:4:606:CHL:HMD2	2.02	0.42
2:4:253:SER:HB2	2:4:256:LYS:CD	2.48	0.42
3:5:165:TYR:HA	3:5:169:GLY:O	2.19	0.42
3:5:177:ASP:HB3	3:5:180:TYR:C	2.45	0.42
3:5:250:ALA:N	3:5:251:PRO:CD	2.81	0.42
31:A:405:CLA:H92	31:A:405:CLA:H61	1.71	0.42
6:B:383:PHE:CZ	17:O:213:GLY:HA2	2.55	0.42
33:C:623:LHG:H312	33:S:320:LHG:HC81	2.02	0.42
8:D:15:PHE:HE1	34:D:410:LMG:H172	1.84	0.42
8:D:156:VAL:HG12	8:D:171:PRO:HG3	2.02	0.42
43:D:405:BCR:H372	34:D:409:LMG:H301	2.01	0.42
31:G:602:CLA:HMC2	32:G:615:LUT:H31	2.01	0.42
33:G:618:LHG:H261	37:G:620:XAT:C39	2.50	0.42
3:N:45:ARG:HD3	3:N:61:GLY:HA3	2.01	0.42
3:N:193:ASP:OD2	3:N:196:THR:HG23	2.20	0.42
3:N:233:LEU:O	3:N:237:LEU:HG	2.19	0.42
31:N:305:CLA:HMB3	31:N:305:CLA:HBB1	2.02	0.42
19:S:155:PRO:HG2	31:S:306:CLA:C4B	2.50	0.42
25:Z:26:VAL:HG21	25:Z:40:VAL:HG21	2.02	0.42
34:0:622:LMG:H351	34:0:622:LMG:H322	1.72	0.42
1:7:175:ASP:HB3	1:7:178:TYR:O	2.20	0.42
31:7:312:CLA:HHC	31:7:312:CLA:HBB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:66:ASP:HA	31:8:602:CLA:O1D	2.20	0.42
3:p:52:PHE:HE2	2:q:169:TYR:CE1	2.38	0.42
3:p:107:LEU:HA	3:p:110:ARG:HH21	1.85	0.42
2:q:96:ARG:HD3	31:q:312:CLA:CHD	2.49	0.42
2:q:146:LEU:HA	30:q:307:CHL:HED3	2.02	0.42
2:q:150:GLN:HB3	30:q:307:CHL:CBB	2.49	0.42
2:q:183:SER:HA	30:q:310:CHL:HBC1	2.02	0.42
5:a:227:THR:HG21	5:a:235:GLU:HB2	2.02	0.42
44:a:414:PL9:HC2	44:a:414:PL9:C10	2.46	0.42
31:b:603:CLA:H192	31:b:603:CLA:H161	1.79	0.42
3:n:67:TYR:HE2	30:n:302:CHL:HBC2	1.85	0.42
31:n:314:CLA:HHB	31:n:315:CLA:HBC3	2.01	0.42
17:o:65:VAL:HG13	17:o:70:ILE:HB	2.02	0.42
1:1:201:LYS:HD3	31:1:612:CLA:HAA2	2.01	0.41
2:2:178:GLU:OE2	2:2:180:SER:N	2.48	0.41
2:2:187:GLY:CA	31:2:609:CLA:HED2	2.48	0.41
2:2:256:LYS:HE2	2:2:256:LYS:HB2	1.55	0.41
3:3:206:LYS:NZ	33:3:320:LHG:O4	2.52	0.41
31:3:306:CLA:NB	36:3:319:NEX:H242	2.35	0.41
32:3:317:LUT:H15	32:3:317:LUT:H201	1.92	0.41
3:5:127:GLN:HG2	3:5:130:GLN:NE2	2.35	0.41
31:5:603:CLA:HMB3	31:5:603:CLA:HBB1	2.02	0.41
5:A:96:ILE:HG13	5:A:97:TRP:N	2.35	0.41
5:A:257:ARG:HG2	6:B:498:LEU:HD11	2.02	0.41
34:A:412:LMG:H331	7:C:205:PRO:HD3	2.02	0.41
31:B:604:CLA:H12	31:B:605:CLA:ND	2.35	0.41
2:G:226:GLN:HE22	35:G:614:RRX:H2	1.85	0.41
34:G:622:LMG:HC92	31:N:315:CLA:O2A	2.19	0.41
19:S:264:TRP:HE1	31:S:315:CLA:HMC2	1.85	0.41
24:Y:197:ALA:HB1	24:Y:203:LEU:HG	2.02	0.41
30:Y:301:CHL:H62	30:Y:302:CHL:H13	2.01	0.41
31:Y:304:CLA:HHC	31:Y:304:CLA:HBB1	2.01	0.41
4:0:197:ASP:N	4:0:197:ASP:OD1	2.51	0.41
30:0:608:CHL:HMA3	36:0:618:NEX:H30	2.01	0.41
31:0:610:CLA:H52	31:0:610:CLA:H8	1.65	0.41
2:9:163:MET:HE2	30:9:308:CHL:HMA1	2.02	0.41
2:9:195:LEU:HB2	31:9:312:CLA:CGA	2.49	0.41
37:9:322:XAT:H381	37:9:322:XAT:H27	1.83	0.41
2:q:146:LEU:O	2:q:147:ILE:C	2.63	0.41
2:q:232:LYS:HE2	2:q:232:LYS:HB2	1.73	0.41
30:q:309:CHL:H2A	30:q:309:CHL:O1D	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:409:CLA:H2	12:i:12:VAL:HG11	2.02	0.41
31:b:603:CLA:H91	31:b:610:CLA:H191	2.02	0.41
31:b:608:CLA:H92	31:b:608:CLA:H61	1.84	0.41
7:c:430:LEU:HD11	31:c:605:CLA:HMB2	2.01	0.41
31:c:606:CLA:H143	43:c:615:BCR:C18	2.50	0.41
8:d:274:VAL:N	8:d:275:PRO:HD2	2.34	0.41
14:k:12:PRO:HG3	19:s:288:VAL:HG11	2.02	0.41
3:n:66:ASP:HA	31:n:303:CLA:O1D	2.19	0.41
17:o:247:SER:O	17:o:260:GLY:HA3	2.20	0.41
18:r:154:GLU:HG2	18:r:159:ASP:O	2.20	0.41
19:s:191:GLY:HA3	31:s:316:CLA:C2D	2.49	0.41
32:s:317:LUT:H31	32:s:317:LUT:H391	1.92	0.41
43:z:101:BCR:H15C	43:z:101:BCR:H351	1.86	0.41
29:f1:171:LYS:HD3	29:f1:172:LYS:HZ3	1.85	0.41
30:1:606:CHL:HBB2	30:1:607:CHL:CAB	2.50	0.41
3:3:69:TRP:CZ2	30:3:303:CHL:HAA2	2.55	0.41
2:4:46:ARG:HD2	2:4:69:ASP:O	2.20	0.41
2:4:162:ILE:HG23	36:4:617:NEX:C15	2.51	0.41
2:4:170:ARG:NH2	30:4:608:CHL:O1D	2.53	0.41
2:4:198:ASP:HB3	2:4:201:THR:OG1	2.19	0.41
2:4:207:VAL:O	2:4:209:GLU:N	2.53	0.41
31:4:604:CLA:CGA	31:4:604:CLA:C3A	2.96	0.41
30:4:608:CHL:HBA1	31:4:610:CLA:HBC2	2.01	0.41
32:4:616:LUT:H31	32:4:616:LUT:H391	1.84	0.41
3:5:39:GLU:O	3:5:46:PRO:HD3	2.19	0.41
4:6:71:TRP:O	4:6:71:TRP:CD1	2.73	0.41
30:6:306:CHL:HHC	30:6:306:CHL:CBB	2.44	0.41
5:A:324:ALA:O	5:A:328:MET:HG3	2.19	0.41
43:B:619:BCR:H15C	43:B:619:BCR:H351	1.71	0.41
7:C:384:MET:HE2	7:C:384:MET:HB3	1.86	0.41
7:C:440:ALA:HB1	22:W:117:LEU:HD22	2.02	0.41
43:H:101:BCR:H15C	43:H:101:BCR:H351	1.88	0.41
36:R:319:NEX:H161	38:R:322:SQD:H112	2.01	0.41
24:Y:94:HIS:CE1	31:Y:304:CLA:C4D	3.01	0.41
31:Y:312:CLA:H92	31:Y:312:CLA:H62	1.75	0.41
31:0:602:CLA:H72	32:0:617:LUT:H30	2.01	0.41
31:0:603:CLA:H93	31:p:603:CLA:H93	2.01	0.41
34:0:620:LMG:H352	34:7:301:LMG:H172	2.03	0.41
1:7:103:LEU:HD13	31:7:305:CLA:HMC1	2.01	0.41
30:9:309:CHL:H43	30:9:309:CHL:CHC	2.51	0.41
30:9:309:CHL:C7	30:9:309:CHL:H41	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:p:197:PHE:O	3:p:201:LYS:HG3	2.20	0.41
2:q:148:HIS:HB3	30:q:307:CHL:C1B	2.51	0.41
6:b:159:THR:O	33:b:628:LHG:HC12	2.19	0.41
6:b:224:ARG:HG2	11:h:44:TRP:CZ2	2.55	0.41
6:b:440:ASP:OD1	6:b:440:ASP:N	2.52	0.41
31:b:606:CLA:H61	31:b:606:CLA:H41	1.74	0.41
33:b:628:LHG:H151	33:b:628:LHG:H192	2.01	0.41
7:c:388:PRO:HA	7:c:409:SER:HB2	2.02	0.41
9:e:12:ASP:OD1	13:j:9:ARG:NH1	2.49	0.41
9:e:25:ILE:C	9:e:28:PRO:HD2	2.45	0.41
31:g:314:CLA:HHC	31:g:314:CLA:CBB	2.49	0.41
33:l:101:LHG:H141	33:l:101:LHG:H111	1.79	0.41
30:n:308:CHL:H102	30:y:601:CHL:H102	2.00	0.41
18:r:198:GLU:HG3	31:r:311:CLA:C4B	2.51	0.41
19:s:153:ALA:CB	31:s:306:CLA:HBC3	2.51	0.41
22:w:94:GLY:O	22:w:98:VAL:HG23	2.19	0.41
24:y:107:PHE:HB3	24:y:108:PRO:HD3	2.02	0.41
24:y:111:LEU:HD21	34:y:620:LMG:H302	2.02	0.41
1:1:242:ASN:OD1	1:1:245:ALA:N	2.51	0.41
30:2:607:CHL:HHC	30:2:607:CHL:CBB	2.47	0.41
31:2:613:CLA:H2	31:2:613:CLA:H61	1.53	0.41
30:3:307:CHL:CHC	34:3:321:LMG:H371	2.51	0.41
33:4:618:LHG:HC92	37:4:619:XAT:C27	2.50	0.41
3:5:70:ASP:CB	31:5:602:CLA:HBA2	2.48	0.41
30:6:302:CHL:HHC	30:6:302:CHL:CBB	2.48	0.41
32:6:318:LUT:H35	32:6:318:LUT:H401	1.85	0.41
5:A:28:LEU:HD12	34:b:624:LMG:H311	2.03	0.41
5:A:160:ILE:HG12	7:C:419:PHE:CE2	2.56	0.41
6:B:297:SER:HB3	6:B:300:GLN:HG2	2.02	0.41
6:B:307:GLU:OE2	6:B:340:TRP:N	2.45	0.41
31:B:610:CLA:H72	31:B:610:CLA:H111	1.80	0.41
7:C:261:SER:HB2	7:C:433:ALA:HB2	2.01	0.41
31:C:613:CLA:H93	31:C:613:CLA:H61	1.88	0.41
33:G:618:LHG:H112	33:G:618:LHG:HC82	1.21	0.41
16:M:29:THR:O	16:M:32:GLN:HG2	2.19	0.41
31:N:304:CLA:HBC2	30:N:309:CHL:HHD	2.01	0.41
19:S:252:GLN:NE2	19:S:263:ASN:HD22	2.17	0.41
25:Z:5:PHE:HD1	25:Z:57:LEU:HB3	1.84	0.41
30:0:609:CHL:CMB	30:q:303:CHL:HHB	2.51	0.41
32:7:318:LUT:H31	32:7:318:LUT:H391	1.93	0.41
31:8:603:CLA:H2	31:8:603:CLA:H62	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:109:GLU:CD	2:9:235:LEU:HB2	2.45	0.41
34:9:321:LMG:HC1	34:9:321:LMG:HC8	1.71	0.41
3:p:239:ALA:O	3:p:243:THR:HG22	2.20	0.41
31:p:615:CLA:CAB	30:q:309:CHL:HMA2	2.49	0.41
2:q:140:TYR:C	2:q:142:GLY:N	2.75	0.41
2:q:218:PHE:CG	33:q:320:LHG:H281	2.56	0.41
36:q:319:NEX:H15	36:q:319:NEX:H201	1.87	0.41
5:a:18:CYS:SG	12:i:30:ARG:NH2	2.93	0.41
5:a:133:LEU:HD11	8:d:255:GLN:HB2	2.02	0.41
31:b:617:CLA:H11	31:b:617:CLA:H52	1.81	0.41
7:c:338:ILE:HG21	7:c:347:TRP:HB2	2.02	0.41
45:c:617:DGD:O1A	34:k:101:LMG:H302	2.20	0.41
3:n:93:ARG:HA	3:n:96:MET:HE3	2.02	0.41
31:n:314:CLA:H172	31:n:315:CLA:ND	2.35	0.41
34:r:321:LMG:HO2	34:r:321:LMG:C10	2.33	0.41
19:s:241:LEU:O	19:s:244:VAL:HG22	2.21	0.41
31:s:313:CLA:H12	34:s:321:LMG:O2	2.20	0.41
27:Q1:10:LEU:HG	34:Q1:101:LMG:O3	2.20	0.41
1:1:59:PRO:CG	1:1:62:LEU:HD12	2.49	0.41
2:2:224:PHE:CD1	31:3:316:CLA:HBB2	2.56	0.41
31:3:305:CLA:HMB3	31:3:305:CLA:HBB1	2.01	0.41
2:4:107:THR:N	2:4:108:PRO:HD2	2.34	0.41
3:5:106:GLU:HA	3:5:119:ALA:HB1	2.02	0.41
3:5:249:TYR:CB	3:5:258:TYR:CD2	3.02	0.41
31:5:603:CLA:H12	31:5:603:CLA:HBA2	1.85	0.41
31:6:305:CLA:H72	31:R:315:CLA:H92	2.01	0.41
31:6:314:CLA:H62	31:6:314:CLA:CHC	2.50	0.41
38:A:413:SQD:H5	6:b:75:TRP:HB3	2.02	0.41
6:B:148:LEU:HG	33:B:624:LHG:H361	2.02	0.41
6:B:161:LEU:HD12	33:B:624:LHG:H241	2.02	0.41
31:B:616:CLA:HMA3	43:B:619:BCR:C17	2.50	0.41
7:C:120:HIS:HE1	31:C:613:CLA:C1A	2.33	0.41
7:C:203:ARG:HG3	22:W:71:GLY:HA2	2.03	0.41
7:C:416:THR:HG22	45:C:617:DGD:HBF2	2.01	0.41
33:D:408:LHG:O2	15:L:14:ASN:ND2	2.54	0.41
47:E:101:HEM:HBC2	47:E:101:HEM:CHD	2.30	0.41
15:L:37:PHE:HD1	16:M:3:VAL:HG13	1.85	0.41
31:N:315:CLA:H61	31:N:315:CLA:H41	1.64	0.41
19:S:68:ARG:HA	19:S:71:ILE:HD13	2.02	0.41
22:W:76:ILE:HG23	22:W:81:LEU:HB2	2.01	0.41
30:Y:307:CHL:OMC	30:Y:307:CHL:HAC2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:0:93:HIS:HE1	31:0:603:CLA:ND	2.04	0.41
4:0:149:SER:CB	34:0:622:LMG:HC92	2.47	0.41
2:9:46:ARG:HG2	2:9:48:LYS:HE3	2.01	0.41
2:9:147:ILE:H	30:9:307:CHL:CGD	2.32	0.41
36:9:319:NEX:H15	36:9:319:NEX:H201	1.96	0.41
3:p:180:TYR:CE2	3:p:201:LYS:HE3	2.55	0.41
6:b:307:GLU:OE2	6:b:340:TRP:N	2.54	0.41
31:b:613:CLA:H161	31:b:613:CLA:H122	1.76	0.41
34:f:101:LMG:HC8	34:f:101:LMG:HC1	1.88	0.41
2:g:198:ASP:HB3	2:g:201:THR:HB	2.02	0.41
31:g:303:CLA:H93	31:g:304:CLA:HMA1	2.02	0.41
31:g:313:CLA:CGA	31:g:313:CLA:C1A	2.98	0.41
37:g:321:XAT:H201	37:g:321:XAT:H15	1.85	0.41
3:n:67:TYR:CE2	30:n:302:CHL:HBC2	2.55	0.41
31:r:303:CLA:CBD	33:r:320:LHG:HC82	2.50	0.41
31:r:315:CLA:HBB1	32:r:317:LUT:H192	2.01	0.41
31:s:311:CLA:H51	31:s:311:CLA:H11	1.85	0.41
31:y:604:CLA:H43	30:y:606:CHL:HBD	2.02	0.41
31:y:613:CLA:H61	31:y:613:CLA:H2	1.52	0.41
1:1:57:PHE:CE2	1:1:74:THR:HG22	2.56	0.41
31:1:610:CLA:H8	31:1:610:CLA:H52	1.33	0.41
2:2:186:PRO:O	2:2:190:PHE:HD1	2.04	0.41
31:3:315:CLA:HHC	31:3:315:CLA:HBB1	2.02	0.41
32:3:317:LUT:H31	32:3:317:LUT:H391	1.91	0.41
2:4:87:TYR:HB3	31:4:602:CLA:HMA1	2.02	0.41
2:4:215:LEU:HG	35:4:615:RRX:H36	2.02	0.41
3:5:38:VAL:HG23	3:5:40:TRP:N	2.36	0.41
36:6:319:NEX:H11	36:6:319:NEX:H191	1.90	0.41
5:A:228:THR:OG1	5:A:230:ASN:OD1	2.22	0.41
6:B:13:LEU:HD23	31:B:612:CLA:HBC1	2.02	0.41
6:B:94:GLU:H	6:B:94:GLU:HG2	1.49	0.41
31:B:607:CLA:H111	31:B:607:CLA:H143	1.73	0.41
31:C:610:CLA:HBA2	31:C:610:CLA:HBD	2.01	0.41
43:C:614:BCR:H15C	43:C:614:BCR:H351	1.79	0.41
45:C:620:DGD:O1A	34:W:201:LMG:O9	2.38	0.41
45:C:620:DGD:HB42	45:C:620:DGD:HA92	2.01	0.41
10:F:19:TRP:CE2	10:F:23:HIS:CE1	3.09	0.41
2:G:223:PHE:CE1	35:G:614:RRX:H52	2.54	0.41
16:M:-10:UNK:HA	6:b:46:ASP:OD2	2.21	0.41
3:N:143:ILE:HA	30:N:306:CHL:C4D	2.50	0.41
36:R:319:NEX:H11	36:R:319:NEX:H191	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:S:305:CLA:H203	31:S:316:CLA:HBA1	2.03	0.41
31:0:611:CLA:C2C	33:0:619:LHG:HC62	2.50	0.41
1:7:177:VAL:C	1:7:179:PRO:HD3	2.46	0.41
31:7:311:CLA:H111	31:7:311:CLA:H93	1.61	0.41
31:7:311:CLA:O2A	32:7:317:LUT:H26	2.20	0.41
2:9:89:GLU:O	2:9:93:ILE:HG12	2.20	0.41
31:p:603:CLA:HBC2	30:p:609:CHL:HHD	2.03	0.41
44:a:414:PL9:H171	44:a:414:PL9:H151	1.82	0.41
31:b:602:CLA:HAC1	43:h:101:BCR:H383	2.01	0.41
34:b:629:LMG:H371	34:b:629:LMG:H341	1.87	0.41
31:c:605:CLA:H62	31:c:605:CLA:H2	1.81	0.41
45:c:619:DGD:HB41	45:c:619:DGD:HA51	2.03	0.41
8:d:92:LEU:HD13	34:d:410:LMG:H141	2.02	0.41
2:g:49:TRP:N	2:g:70:TYR:HB3	2.35	0.41
34:n:322:LMG:H151	31:y:615:CLA:H11	2.02	0.41
18:r:190:ASN:ND2	30:r:308:CHL:O1D	2.53	0.41
36:r:301:NEX:O3	36:r:301:NEX:H162	2.21	0.41
31:r:312:CLA:H3A	31:r:312:CLA:HBA2	1.23	0.41
31:r:313:CLA:NB	33:r:320:LHG:O4	2.54	0.41
19:s:115:ALA:HB1	32:s:317:LUT:H12	2.01	0.41
32:s:317:LUT:H35	32:s:317:LUT:H401	1.84	0.41
34:w:202:LMG:H453	34:w:202:LMG:H411	2.03	0.41
24:y:206:LEU:CB	31:y:610:CLA:HMA2	2.50	0.41
24:y:227:GLN:O	24:y:231:THR:OG1	2.34	0.41
30:y:608:CHL:H2	32:y:616:LUT:C38	2.50	0.41
25:z:33:TRP:O	25:z:37:LYS:HB2	2.20	0.41
43:z:101:BCR:HC8	43:z:101:BCR:H331	2.02	0.41
1:1:139:GLY:HA2	1:1:142:ASN:ND2	2.35	0.41
1:1:167:GLY:HA3	18:R:39:SER:O	2.20	0.41
2:2:179:THR:C	2:2:181:GLY:N	2.76	0.41
3:3:147:SER:O	3:3:151:ILE:HG13	2.20	0.41
3:3:225:THR:O	3:3:226:ARG:HB2	2.21	0.41
31:3:301:CLA:HHC	31:3:301:CLA:CBB	2.51	0.41
2:4:50:LEU:HD12	2:4:50:LEU:HA	1.80	0.41
32:5:616:LUT:H35	32:5:616:LUT:H401	1.82	0.41
4:6:72:ASP:HA	32:6:318:LUT:H24	2.02	0.41
4:6:139:LEU:HD13	4:6:139:LEU:HA	1.91	0.41
34:6:321:LMG:HC71	18:R:273:PHE:CD1	2.56	0.41
6:B:307:GLU:HG3	6:B:340:TRP:HB2	2.01	0.41
43:C:615:BCR:H351	43:C:615:BCR:H15C	1.17	0.41
8:D:53:THR:HG22	10:F:39:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:148:ALA:HB3	8:D:149:PRO:HD3	2.03	0.41
42:D:401:PHO:HMB1	42:D:401:PHO:HBB1	2.03	0.41
43:D:405:BCR:H311	43:D:405:BCR:C8	2.49	0.41
2:G:75:ALA:HB3	2:G:77:LEU:HG	2.03	0.41
2:G:259:PRO:HA	34:G:621:LMG:C4	2.50	0.41
31:G:604:CLA:H41	31:G:604:CLA:H61	1.79	0.41
30:G:606:CHL:OMC	30:G:606:CHL:HAC2	2.20	0.41
3:N:162:ILE:HD11	36:N:318:NEX:C35	2.51	0.41
31:N:313:CLA:H102	31:N:314:CLA:HMD3	2.02	0.41
18:R:222:LEU:HB2	31:R:312:CLA:HBA1	2.03	0.41
48:R:302:LMU:H3'	48:R:302:LMU:H1B	1.75	0.41
31:S:312:CLA:H141	31:S:312:CLA:H161	1.82	0.41
22:W:89:PHE:CZ	34:W:201:LMG:H371	2.56	0.41
43:Z:101:BCR:H11C	43:Z:101:BCR:H341	1.76	0.41
4:0:85:ARG:HH22	2:q:59:PRO:HA	1.86	0.41
4:0:199:LEU:HD11	4:0:203:LYS:NZ	2.34	0.41
1:7:218:ILE:HD12	31:7:314:CLA:CAC	2.50	0.41
3:8:67:TYR:CE2	30:8:601:CHL:HBC2	2.55	0.41
3:8:93:ARG:HA	3:8:96:MET:HE3	2.02	0.41
2:q:127:LYS:C	2:q:129:GLY:H	2.28	0.41
31:q:312:CLA:HED2	31:q:312:CLA:HBD	1.91	0.41
43:a:410:BCR:H15C	43:a:410:BCR:H351	1.94	0.41
31:b:608:CLA:OBD	34:b:622:LMG:O2	2.37	0.41
31:b:613:CLA:H62	31:b:613:CLA:H102	1.86	0.41
31:b:617:CLA:H152	31:b:617:CLA:H112	1.53	0.41
7:c:156:LEU:HD12	7:c:156:LEU:HA	1.89	0.41
43:c:615:BCR:H15C	43:c:615:BCR:H351	1.67	0.41
2:g:78:SER:HB3	2:g:84:PHE:CD1	2.56	0.41
2:g:147:ILE:N	30:g:306:CHL:O1D	2.49	0.41
30:g:308:CHL:HHC	30:g:308:CHL:CBB	2.47	0.41
31:g:311:CLA:C4D	31:g:312:CLA:HMD3	2.50	0.41
31:g:314:CLA:HHC	31:g:314:CLA:HBB1	2.03	0.41
3:n:102:CYS:SG	32:n:318:LUT:H41	2.61	0.41
19:s:133:GLY:O	19:s:139:THR:HG22	2.21	0.41
24:y:121:GLU:N	24:y:130:GLN:OE1	2.51	0.41
24:y:227:GLN:HE21	24:y:238:ASN:HD22	1.69	0.41
29:F1:60:ILE:N	29:F1:60:ILE:HD12	2.36	0.41
30:2:606:CHL:HAC2	30:2:606:CHL:OMC	2.20	0.41
2:4:132:ILE:HG21	2:4:152:ILE:HG23	2.01	0.41
2:4:175:GLY:O	2:4:176:PRO:C	2.63	0.41
31:4:604:CLA:CHC	36:4:617:NEX:H362	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:91:HIS:HD2	32:5:617:LUT:H15	1.85	0.41
3:5:134:LEU:HD21	31:5:604:CLA:HAA1	2.03	0.41
3:5:169:GLY:HA2	30:5:608:CHL:HMC	2.02	0.41
3:5:200:LEU:CA	3:5:203:LYS:HD2	2.40	0.41
3:5:251:PRO:HG2	3:5:252:LYS:CD	2.47	0.41
34:5:620:LMG:H361	34:5:620:LMG:HC8	2.03	0.41
4:6:50:LEU:HD12	4:6:50:LEU:HA	1.83	0.41
4:6:218:PHE:CE2	31:6:314:CLA:HAC1	2.56	0.41
31:B:609:CLA:H142	31:B:609:CLA:H112	1.86	0.41
7:C:211:TRP:CG	7:C:212:ILE:H	2.37	0.41
45:C:620:DGD:HG11	45:C:620:DGD:C2B	2.47	0.41
8:D:274:VAL:N	8:D:275:PRO:HD2	2.36	0.41
9:E:23:HIS:HA	9:E:26:THR:OG1	2.20	0.41
31:G:602:CLA:HBA1	32:G:615:LUT:H382	2.02	0.41
31:G:603:CLA:NC	30:G:608:CHL:H111	2.36	0.41
31:G:611:CLA:HED2	31:G:611:CLA:H2A	2.02	0.41
37:G:620:XAT:H41	30:G:623:CHL:HAA1	2.02	0.41
17:O:127:ARG:NH2	22:W:68:GLU:OE1	2.27	0.41
17:O:138:GLN:NE2	17:O:140:LYS:HD2	2.35	0.41
18:R:153:GLN:O	18:R:157:THR:OG1	2.37	0.41
19:S:57:ARG:HH12	19:S:84:GLY:N	2.18	0.41
19:S:108:ALA:HB1	19:S:239:GLY:HA3	2.01	0.41
24:Y:47:PRO:HB2	30:Y:302:CHL:CBC	2.51	0.41
31:Y:303:CLA:H93	31:Y:303:CLA:H111	1.78	0.41
4:0:111:GLN:HG2	4:0:118:PHE:HD1	1.85	0.41
1:7:185:PRO:HD2	32:7:317:LUT:C23	2.49	0.41
30:7:302:CHL:C2D	33:7:319:LHG:HC81	2.51	0.41
34:7:320:LMG:HC1	31:r:313:CLA:HMA3	2.03	0.41
3:8:224:ILE:HD12	3:8:258:TYR:OH	2.20	0.41
3:p:240:PRO:HG3	31:p:614:CLA:CMB	2.50	0.41
2:q:104:GLY:HA3	32:q:318:LUT:H183	2.03	0.41
2:q:186:PRO:HB2	2:q:190:PHE:CD2	2.56	0.41
5:a:307:VAL:HG23	10:f:44:ARG:CD	2.50	0.41
7:c:97:TYR:OH	25:z:58:ASN:ND2	2.54	0.41
7:c:105:LEU:HD12	7:c:105:LEU:HA	1.76	0.41
31:c:613:CLA:OBD	19:s:62:PRO:HB2	2.21	0.41
43:c:614:BCR:H10C	43:c:614:BCR:HC7	1.83	0.41
33:c:622:LHG:H242	31:s:312:CLA:CAB	2.47	0.41
33:c:622:LHG:H331	33:c:622:LHG:H301	1.96	0.41
8:d:279:LEU:HD11	42:d:402:PHO:HMC3	2.02	0.41
11:h:37:TYR:CE2	18:r:89:LEU:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:h:101:BCR:H21C	34:x:202:LMG:H311	2.03	0.41
34:k:101:LMG:H111	34:k:101:LMG:H142	1.85	0.41
31:r:305:CLA:H41	31:r:305:CLA:H62	1.85	0.41
19:s:110:TRP:CD2	31:s:310:CLA:HAC2	2.56	0.41
33:s:322:LHG:H271	33:s:322:LHG:H241	1.97	0.41
21:v:15:ILE:O	43:v:101:BCR:H14C	2.21	0.41
24:y:139:TYR:OH	36:y:618:NEX:O23	2.32	0.41
29:F1:105:ASN:ND2	29:F1:214:GLY:H	2.18	0.41
31:1:614:CLA:H2	31:1:614:CLA:H61	1.77	0.41
31:2:613:CLA:NC	31:2:613:CLA:H51	2.36	0.41
3:3:44:ASN:OD1	3:3:44:ASN:N	2.54	0.41
3:3:245:PHE:CD1	3:3:249:TYR:HB2	2.56	0.41
30:3:303:CHL:HHC	30:3:303:CHL:CBB	2.46	0.41
31:3:306:CLA:C1B	36:3:319:NEX:H383	2.51	0.41
2:4:175:GLY:N	2:4:176:PRO:CD	2.83	0.41
2:4:179:THR:H	2:4:188:GLY:CA	2.24	0.41
2:4:205:LEU:HD12	31:4:610:CLA:H12	2.03	0.41
2:4:207:VAL:O	2:4:208:LYS:C	2.63	0.41
30:4:607:CHL:HHB	31:5:615:CLA:HAB	2.03	0.41
30:4:609:CHL:HHC	30:4:609:CHL:CBB	2.46	0.41
3:5:69:TRP:CE2	30:5:601:CHL:HBA2	2.56	0.41
3:5:187:PRO:HD2	32:5:616:LUT:C23	2.50	0.41
3:5:197:PHE:CD1	31:5:610:CLA:HMA3	2.56	0.41
3:5:220:VAL:CG2	31:5:613:CLA:HAC2	2.48	0.41
3:5:252:LYS:CB	3:5:258:TYR:HA	2.51	0.41
31:5:611:CLA:H8	31:5:612:CLA:ND	2.35	0.41
5:A:250:ALA:HA	6:B:490:VAL:HG11	2.02	0.41
31:A:405:CLA:H192	31:A:405:CLA:H162	1.95	0.41
6:B:243:ALA:HA	6:B:246:PHE:CD2	2.55	0.41
7:C:385:THR:HG21	26:U:75:ARG:HB3	2.03	0.41
31:C:611:CLA:H91	31:C:611:CLA:H111	1.95	0.41
45:C:620:DGD:HBH2	31:Y:311:CLA:C5	2.50	0.41
8:D:134:ARG:HD2	8:D:134:ARG:HA	1.87	0.41
8:D:297:ASP:HB2	8:D:315:TYR:OH	2.21	0.41
2:G:140:TYR:O	2:G:146:LEU:HD12	2.20	0.41
2:G:169:TYR:CE1	3:N:52:PHE:HE2	2.38	0.41
2:G:259:PRO:HG3	30:G:623:CHL:H42	2.03	0.41
34:G:622:LMG:H151	31:N:321:CLA:H12	2.02	0.41
14:K:21:ILE:HG13	33:K:102:LHG:H292	2.03	0.41
31:N:313:CLA:H43	31:N:314:CLA:OBD	2.21	0.41
31:R:316:CLA:H143	31:R:316:CLA:H162	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:175:PRO:HD2	30:Y:308:CHL:CBB	2.50	0.41
4:0:161:MET:HE2	4:0:161:MET:HA	2.03	0.41
4:0:219:GLY:O	4:0:223:GLN:HG3	2.20	0.41
34:0:620:LMG:H311	34:0:620:LMG:H342	1.89	0.41
31:7:303:CLA:H61	31:7:303:CLA:H101	1.85	0.41
3:8:253:SER:HB2	30:9:309:CHL:HAA1	2.01	0.41
34:9:321:LMG:HC2	34:9:321:LMG:HC71	1.79	0.41
31:p:610:CLA:H2	32:p:616:LUT:C26	2.50	0.41
2:q:48:LYS:HB2	2:q:54:SER:OG	2.20	0.41
5:a:120:PHE:CD2	45:c:616:DGD:HBT2	2.56	0.41
6:b:39:PHE:CD1	34:b:601:LMG:HC92	2.55	0.41
31:b:610:CLA:H91	31:b:610:CLA:H111	1.82	0.41
7:c:35:GLY:HA3	7:c:125:PRO:O	2.20	0.41
7:c:95:ASP:OD1	7:c:96:THR:N	2.54	0.41
7:c:306:LEU:HD23	7:c:306:LEU:C	2.45	0.41
31:d:404:CLA:H162	31:d:404:CLA:H193	1.79	0.41
37:g:321:XAT:H31	37:g:321:XAT:H391	1.77	0.41
3:n:75:SER:HB2	3:n:81:PHE:CD1	2.56	0.41
3:n:206:LYS:HD3	31:n:312:CLA:O1D	2.21	0.41
30:n:308:CHL:HAA1	30:n:308:CHL:CBD	2.51	0.41
17:o:208:ARG:HB2	17:o:235:LYS:HE2	2.01	0.41
19:s:189:PRO:O	19:s:204:TYR:OH	2.32	0.41
30:s:307:CHL:HBB1	32:s:318:LUT:H161	2.02	0.41
24:y:94:HIS:CE1	31:y:603:CLA:C4D	3.00	0.41
29:f1:106:ASN:OD1	29:f1:212:GLN:HB3	2.21	0.41
1:1:90:ILE:HD11	2:2:75:ALA:HA	2.03	0.41
31:1:602:CLA:H92	31:1:602:CLA:H61	1.81	0.41
31:1:604:CLA:HMA2	30:1:606:CHL:C3C	2.50	0.41
30:1:607:CHL:HAA2	37:2:619:XAT:C4	2.51	0.41
31:2:604:CLA:C4A	36:2:616:NEX:H242	2.50	0.41
37:2:619:XAT:H381	37:2:619:XAT:H27	1.83	0.41
3:3:104:THR:O	3:3:108:LEU:HD13	2.20	0.41
3:3:215:MET:HA	3:3:218:PHE:HD2	1.85	0.41
30:4:607:CHL:H102	30:4:607:CHL:NB	2.35	0.41
3:5:58:TYR:OH	3:5:73:GLY:HA2	2.19	0.41
3:5:107:LEU:HA	3:5:110:ARG:HG2	2.03	0.41
3:5:203:LYS:HD3	31:5:612:CLA:HBA2	2.02	0.41
30:5:606:CHL:HAC2	30:5:606:CHL:OMC	2.21	0.41
32:5:616:LUT:H11	32:5:616:LUT:H191	1.98	0.41
4:6:136:LEU:HD21	31:6:305:CLA:HAA2	2.03	0.41
4:6:147:ALA:HA	30:6:306:CHL:C1C	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:6:303:CLA:HMB1	31:6:303:CLA:HBB1	2.03	0.41
31:6:311:CLA:HBB1	31:6:311:CLA:CMB	2.51	0.41
5:A:96:ILE:HG22	5:A:105:TRP:CE2	2.56	0.41
6:B:24:LEU:HD21	31:B:616:CLA:CAB	2.51	0.41
31:B:601:CLA:C4B	34:X:202:LMG:H321	2.51	0.41
31:B:612:CLA:C17	31:B:613:CLA:HBB2	2.50	0.41
31:B:613:CLA:H62	31:B:613:CLA:H41	1.65	0.41
31:B:616:CLA:H11	31:B:616:CLA:H52	1.80	0.41
34:B:621:LMG:H151	34:B:621:LMG:H182	1.90	0.41
7:C:199:GLY:O	7:C:203:ARG:HB2	2.21	0.41
7:C:250:ARG:HH22	34:W:201:LMG:HC1	1.85	0.41
31:C:612:CLA:HBB1	31:C:612:CLA:HMB3	2.02	0.41
42:D:401:PHO:H2	42:D:401:PHO:H61	1.75	0.41
31:D:404:CLA:H143	31:D:404:CLA:H162	1.88	0.41
2:G:89:GLU:HA	2:G:184:LEU:HD11	2.02	0.41
14:K:23:ASP:OD2	21:V:8:GLN:NE2	2.54	0.41
3:N:86:GLU:HA	3:N:179:LEU:HD21	2.02	0.41
32:N:317:LUT:H35	32:N:317:LUT:H401	1.90	0.41
18:R:54:LEU:HD12	18:R:54:LEU:HA	1.89	0.41
18:R:180:PRO:HG2	18:R:181:PHE:CE1	2.56	0.41
19:S:70:GLU:HB3	33:S:322:LHG:HC12	2.03	0.41
38:S:301:SQD:H301	38:S:301:SQD:H332	1.93	0.41
23:X:82:VAL:O	23:X:86:ILE:HG13	2.20	0.41
38:X:201:SQD:H242	38:X:201:SQD:H462	1.86	0.41
31:Y:310:CLA:HMB3	31:Y:310:CLA:CBB	2.47	0.41
31:Y:310:CLA:H152	31:Y:310:CLA:H18	1.87	0.41
31:Y:312:CLA:H121	31:Y:312:CLA:H161	1.46	0.41
25:Z:5:PHE:HA	25:Z:57:LEU:HD23	2.03	0.41
4:0:71:TRP:O	32:0:617:LUT:H24	2.21	0.41
4:0:94:ALA:HB1	4:0:210:GLY:HA3	2.03	0.41
38:0:621:SQD:H1	31:9:313:CLA:O2A	2.21	0.41
3:8:75:SER:HB2	3:8:81:PHE:CD1	2.56	0.41
2:9:63:LYS:HB2	2:9:63:LYS:HZ3	1.85	0.41
2:9:101:GLY:HA2	32:9:318:LUT:H182	2.02	0.41
2:9:205:LEU:HD22	31:9:312:CLA:H12	2.03	0.41
30:9:303:CHL:HMD2	33:9:320:LHG:H251	2.03	0.41
31:9:315:CLA:H61	31:9:315:CLA:H2	1.70	0.41
3:p:96:MET:SD	31:p:610:CLA:HAB	2.61	0.41
3:p:173:GLY:O	30:p:608:CHL:HBC3	2.21	0.41
3:p:191:ALA:HB1	3:p:197:PHE:HB2	2.02	0.41
30:p:608:CHL:HHC	30:p:608:CHL:CBB	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:p:608:CHL:H11	31:p:610:CLA:HMD2	2.02	0.41
2:q:112:GLN:HB2	2:q:119:PHE:HD1	1.85	0.41
2:q:130:ALA:O	2:q:131:SER:C	2.64	0.41
2:q:132:ILE:HG13	2:q:149:ALA:C	2.46	0.41
2:q:144:PRO:C	2:q:146:LEU:H	2.29	0.41
31:a:409:CLA:H41	31:a:409:CLA:H62	1.55	0.41
6:b:55:MET:HE3	6:b:55:MET:HB2	1.84	0.41
6:b:238:LEU:N	31:b:613:CLA:HMD2	2.36	0.41
34:b:601:LMG:H332	34:b:601:LMG:H361	1.74	0.41
31:b:602:CLA:O1A	34:r:321:LMG:H112	2.21	0.41
31:b:606:CLA:H142	31:b:611:CLA:H2	2.02	0.41
31:b:611:CLA:H202	31:b:611:CLA:H161	1.81	0.41
31:b:614:CLA:HBB1	31:b:614:CLA:CMB	2.51	0.41
34:b:629:LMG:HC71	34:b:629:LMG:HC2	1.93	0.41
7:c:122:LEU:HD11	31:c:611:CLA:H92	2.03	0.41
7:c:153:LEU:HD13	31:c:607:CLA:HED1	2.03	0.41
7:c:265:GLY:C	31:c:605:CLA:HBC2	2.45	0.41
31:c:606:CLA:H91	43:c:615:BCR:H14C	2.02	0.41
45:c:619:DGD:HAN1	33:y:619:LHG:H341	2.03	0.41
33:g:319:LHG:H291	33:g:319:LHG:H261	1.48	0.41
14:k:12:PRO:HB2	14:k:15:TYR:HD1	1.86	0.41
15:l:23:LEU:HG	33:l:101:LHG:H181	2.02	0.41
3:n:51:PRO:HG2	3:n:52:PHE:CE1	2.56	0.41
3:n:85:ARG:HG3	31:n:303:CLA:HMA3	2.03	0.41
3:n:222:GLY:O	3:n:226:ARG:HA	2.19	0.41
30:n:306:CHL:H61	30:n:306:CHL:H101	1.67	0.41
31:n:311:CLA:HBA2	31:n:311:CLA:H3A	1.49	0.41
17:o:84:VAL:HA	17:o:251:VAL:HG11	2.03	0.41
18:r:75:PRO:HG2	37:r:318:XAT:H222	2.03	0.41
18:r:137:LEU:HD23	18:r:137:LEU:HA	1.92	0.41
18:r:182:ASP:OD1	18:r:182:ASP:N	2.54	0.41
34:r:321:LMG:O9	34:r:321:LMG:O2	2.37	0.41
19:s:153:ALA:HB1	31:s:306:CLA:HBC3	2.03	0.41
19:s:251:VAL:HG12	31:s:314:CLA:HMD3	2.03	0.41
34:s:321:LMG:H151	34:s:321:LMG:H182	1.85	0.41
25:z:23:VAL:O	25:z:27:LEU:HG	2.21	0.41
28:p1:50:TYR:CZ	28:p1:52:PHE:HB2	2.56	0.41
1:1:161:GLU:HG3	30:1:609:CHL:C4B	2.50	0.41
2:2:109:GLU:HA	2:2:123:ALA:HB1	2.03	0.41
3:3:197:PHE:CZ	3:3:201:LYS:HD2	2.55	0.41
2:4:124:VAL:HB	2:4:127:LYS:CB	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:38:VAL:HG23	3:5:40:TRP:H	1.85	0.41
3:5:75:SER:HB3	3:5:81:PHE:HD1	1.81	0.41
3:5:141:SER:HA	30:5:605:CHL:HMA1	2.03	0.41
3:5:233:LEU:HD23	31:5:613:CLA:CMA	2.50	0.41
30:5:601:CHL:HED1	33:5:619:LHG:H292	2.03	0.41
31:5:610:CLA:H52	32:5:616:LUT:C30	2.48	0.41
4:6:113:ASN:HD22	34:6:322:LMG:H292	1.86	0.41
30:6:309:CHL:HMB2	36:6:319:NEX:C35	2.50	0.41
5:A:38:ILE:HB	5:A:39:PRO:HD3	2.02	0.41
6:B:65:PHE:CE1	31:B:604:CLA:HED2	2.56	0.41
31:B:611:CLA:HBB1	31:B:611:CLA:CMB	2.44	0.41
31:B:613:CLA:H61	31:B:613:CLA:H92	1.64	0.41
34:B:625:LMG:H371	34:B:625:LMG:H341	1.87	0.41
7:C:426:PHE:CE1	31:C:605:CLA:HAB	2.56	0.41
8:D:118:GLY:O	8:D:121:SER:OG	2.37	0.41
8:D:201:VAL:HG13	31:D:403:CLA:HMB1	2.03	0.41
31:G:610:CLA:O1A	38:G:617:SQD:H111	2.21	0.41
14:K:35:LEU:HA	14:K:38:VAL:HG12	2.02	0.41
33:L:101:LHG:H202	33:L:101:LHG:H171	1.88	0.41
3:N:94:TRP:CD1	30:N:309:CHL:HMD3	2.56	0.41
31:N:305:CLA:H152	31:N:305:CLA:H18	1.90	0.41
30:N:307:CHL:H62	31:S:313:CLA:H72	2.03	0.41
32:R:317:LUT:H191	32:R:317:LUT:H11	1.79	0.41
36:S:319:NEX:H15	36:S:319:NEX:H201	1.91	0.41
31:Y:303:CLA:H142	32:Y:316:LUT:H31	2.03	0.41
26:U:71:ILE:HG22	26:U:75:ARG:CZ	2.51	0.41
34:0:620:LMG:H332	34:0:620:LMG:H301	1.91	0.41
3:8:215:MET:HG3	32:8:616:LUT:H12	2.02	0.41
30:8:606:CHL:HBA1	36:8:617:NEX:C32	2.51	0.41
2:9:229:VAL:HA	2:9:257:PHE:HZ	1.86	0.41
31:9:306:CLA:NC	36:9:319:NEX:H222	2.35	0.41
3:p:160:GLY:HA2	30:p:609:CHL:HAB	2.03	0.41
3:p:245:PHE:HD1	3:p:249:TYR:HB2	1.82	0.41
2:q:139:ASN:HA	2:q:148:HIS:H	1.86	0.41
37:q:321:XAT:H15	37:q:321:XAT:H201	1.85	0.41
5:a:47:VAL:HG21	5:a:114:LEU:HD22	2.02	0.41
5:a:312:ARG:NH2	9:e:61:GLN:O	2.53	0.41
8:d:148:ALA:HB3	8:d:149:PRO:HD3	2.03	0.41
47:e:102:HEM:CAC	10:f:26:ALA:HB1	2.51	0.41
37:g:321:XAT:H11	37:g:321:XAT:H191	1.99	0.41
31:r:314:CLA:HBA1	31:r:314:CLA:H3A	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:241:LEU:HD21	31:s:313:CLA:CBC	2.46	0.41
31:s:312:CLA:H192	31:s:313:CLA:HBB2	2.02	0.41
24:y:187:PRO:HD2	31:y:610:CLA:OBD	2.21	0.41
31:y:610:CLA:H18	31:y:610:CLA:H152	1.88	0.41
26:u:190:LYS:O	26:u:194:VAL:HG23	2.21	0.41
29:f1:196:LEU:HD22	29:f1:196:LEU:N	2.36	0.41
2:2:204:GLU:HG2	2:2:208:LYS:HE2	2.03	0.40
3:3:136:TYR:O	3:3:142:LEU:HD12	2.21	0.40
3:3:245:PHE:CE1	3:3:249:TYR:HB2	2.56	0.40
2:4:151:SER:HB3	30:4:605:CHL:OMC	2.20	0.40
34:4:621:LMG:H301	31:5:615:CLA:CHD	2.51	0.40
31:5:602:CLA:H92	31:5:602:CLA:C4	2.51	0.40
31:5:610:CLA:C2	32:5:616:LUT:H26	2.47	0.40
5:A:136:ARG:NH2	12:I:27:ASP:OD1	2.52	0.40
5:A:174:LEU:HD22	42:A:408:PHO:H143	2.02	0.40
31:B:613:CLA:HED2	31:B:614:CLA:HMC2	2.02	0.40
38:B:623:SQD:H212	8:D:36:LEU:HB2	2.03	0.40
31:C:610:CLA:HBB1	31:C:610:CLA:HMB1	2.02	0.40
44:D:406:PL9:H422	44:D:406:PL9:H461	1.90	0.40
31:N:310:CLA:H192	31:S:306:CLA:HBB2	2.03	0.40
31:N:313:CLA:H122	31:N:314:CLA:CMD	2.51	0.40
18:R:180:PRO:HG2	18:R:181:PHE:CZ	2.55	0.40
31:R:306:CLA:HMA3	30:R:308:CHL:C3C	2.52	0.40
31:R:315:CLA:HBA1	31:R:315:CLA:H3A	1.73	0.40
19:S:112:MET:HG3	19:S:239:GLY:HA2	2.04	0.40
30:Y:309:CHL:HBD	30:Y:309:CHL:HAA1	2.03	0.40
26:U:147:PRO:O	26:U:151:LYS:N	2.47	0.40
34:9:301:LMG:HC2	34:9:301:LMG:HC71	1.71	0.40
2:q:241:HIS:HB2	31:q:315:CLA:HAA2	2.02	0.40
31:q:304:CLA:CHA	31:q:304:CLA:HBA1	2.48	0.40
6:b:451:PHE:CZ	31:b:605:CLA:HED2	2.56	0.40
24:y:155:LEU:HD13	30:y:607:CHL:HBC3	2.02	0.40
43:z:101:BCR:HC7	43:z:101:BCR:H321	1.91	0.40
30:1:606:CHL:HMB2	30:1:609:CHL:OMC	2.21	0.40
3:3:91:HIS:CE1	31:3:305:CLA:C4D	3.04	0.40
2:4:109:GLU:HA	2:4:123:ALA:HB1	2.01	0.40
2:4:159:GLN:HE21	2:4:159:GLN:HB2	1.66	0.40
3:5:160:GLY:HA2	30:5:609:CHL:HAB	2.03	0.40
31:5:610:CLA:HBA2	32:5:616:LUT:C24	2.52	0.40
4:6:144:LEU:HD23	4:6:144:LEU:HA	1.91	0.40
32:6:318:LUT:H31	32:6:318:LUT:H391	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:257:TRP:CZ2	6:B:272:ARG:HG2	2.56	0.40
31:B:607:CLA:H61	31:B:607:CLA:H92	1.76	0.40
31:B:610:CLA:H92	31:B:610:CLA:H61	1.86	0.40
34:B:621:LMG:H332	34:B:621:LMG:H361	1.54	0.40
7:C:201:LEU:HD21	43:C:615:BCR:C22	2.51	0.40
31:C:608:CLA:H111	31:C:608:CLA:H152	1.90	0.40
2:G:47:ALA:HB1	30:G:601:CHL:CBC	2.52	0.40
2:G:241:HIS:CD2	31:G:613:CLA:NC	2.88	0.40
31:N:311:CLA:C4D	31:N:312:CLA:HMD3	2.51	0.40
18:R:198:GLU:HG3	31:R:311:CLA:C4B	2.51	0.40
36:R:301:NEX:H35	36:R:301:NEX:H401	1.76	0.40
19:S:60:TYR:HB2	30:S:302:CHL:C4D	2.50	0.40
19:S:251:VAL:HG21	31:S:314:CLA:HAC2	2.03	0.40
33:S:322:LHG:H121	33:S:322:LHG:HC91	1.82	0.40
24:Y:62:LEU:HD23	24:Y:62:LEU:HA	1.92	0.40
3:8:206:LYS:HD3	31:8:610:CLA:O1D	2.21	0.40
2:q:88:ARG:O	2:q:92:VAL:HG23	2.21	0.40
2:q:163:MET:HE1	36:q:319:NEX:H30	2.03	0.40
2:q:251:PHE:CG	37:q:321:XAT:H192	2.56	0.40
5:a:324:ALA:O	5:a:328:MET:HG3	2.21	0.40
31:b:611:CLA:H142	31:b:613:CLA:H2	2.02	0.40
7:c:152:HIS:HE1	31:c:612:CLA:C1D	2.35	0.40
7:c:331:ARG:NH2	17:o:71:ALA:O	2.54	0.40
31:c:602:CLA:H62	31:c:603:CLA:C1B	2.52	0.40
31:g:305:CLA:NB	36:g:317:NEX:H242	2.36	0.40
19:s:284:ASP:OD1	19:s:284:ASP:N	2.47	0.40
31:s:305:CLA:H161	31:s:316:CLA:C2B	2.51	0.40
25:z:47:TRP:O	25:z:51:VAL:HG23	2.21	0.40
28:p1:86:LEU:HD12	28:p1:86:LEU:HA	1.89	0.40
29:F1:149:GLU:HG3	29:F1:157:VAL:HG12	2.03	0.40
31:1:602:CLA:H2	32:1:616:LUT:H26	2.02	0.40
2:2:202:LEU:CG	2:2:206:LYS:HE3	2.49	0.40
3:3:38:VAL:CA	3:3:42:GLY:H	2.33	0.40
3:3:236:HIS:O	3:3:240:PRO:N	2.55	0.40
30:3:302:CHL:HHC	30:3:302:CHL:CBB	2.48	0.40
2:4:99:MET:HG2	35:4:615:RRX:C16	2.51	0.40
2:4:152:ILE:HG22	2:4:156:LEU:HD21	2.02	0.40
2:4:221:PHE:CD2	31:4:613:CLA:HAC1	2.57	0.40
31:4:613:CLA:H2	31:4:614:CLA:HMD2	2.03	0.40
3:5:182:GLY:HA2	3:5:186:ASP:HB2	2.03	0.40
31:5:611:CLA:H62	31:5:611:CLA:H92	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:145:VAL:HG13	30:6:306:CHL:C1D	2.51	0.40
4:6:191:GLY:HA3	18:R:45:ARG:HB2	2.03	0.40
30:6:307:CHL:OMC	30:6:307:CHL:HAC2	2.21	0.40
34:A:418:LMG:H292	34:A:418:LMG:HC91	1.95	0.40
6:B:224:ARG:HG2	11:H:44:TRP:CZ2	2.56	0.40
31:B:610:CLA:H193	31:B:612:CLA:HMD2	2.04	0.40
7:C:201:LEU:HD13	7:C:201:LEU:HA	1.83	0.40
31:C:606:CLA:HBB2	31:C:607:CLA:H61	2.03	0.40
2:G:129:GLY:HA3	30:N:301:CHL:C3D	2.52	0.40
31:G:612:CLA:H101	31:G:612:CLA:H62	1.63	0.40
3:N:177:ASP:HB3	3:N:180:TYR:O	2.21	0.40
3:N:191:ALA:HB1	3:N:197:PHE:CD1	2.57	0.40
30:N:309:CHL:H101	30:N:309:CHL:H62	1.87	0.40
18:R:248:PHE:CZ	37:R:318:XAT:H8	2.57	0.40
31:R:306:CLA:C1B	36:R:319:NEX:H383	2.51	0.40
30:R:309:CHL:HAC2	30:R:309:CHL:OMC	2.22	0.40
19:S:110:TRP:CD2	31:S:310:CLA:HAC2	2.56	0.40
30:Y:309:CHL:HHC	30:Y:309:CHL:CBB	2.47	0.40
31:Y:312:CLA:H161	31:Y:312:CLA:H202	1.84	0.40
4:0:120:GLU:OE1	4:0:132:GLN:NE2	2.55	0.40
4:0:194:ASP:N	18:r:45:ARG:HH22	2.19	0.40
4:0:256:ALA:O	30:p:607:CHL:HMA2	2.22	0.40
30:0:606:CHL:HBA2	30:0:606:CHL:HBD	2.03	0.40
31:0:615:CLA:O2A	34:q:301:LMG:H292	2.21	0.40
3:8:71:THR:HG21	30:9:311:CHL:HAA2	2.03	0.40
31:8:602:CLA:HBA1	32:8:616:LUT:H382	2.02	0.40
32:8:616:LUT:H35	32:8:616:LUT:H401	1.87	0.40
34:9:302:LMG:H302	34:9:302:LMG:C9	2.52	0.40
3:p:96:MET:HB3	32:p:616:LUT:C34	2.51	0.40
31:p:615:CLA:C3B	30:q:309:CHL:HMA2	2.52	0.40
2:q:205:LEU:HD12	31:q:312:CLA:HHB	2.02	0.40
31:q:304:CLA:HBA1	32:q:318:LUT:H382	2.03	0.40
5:a:263:ALA:HA	33:e:101:LHG:H131	2.02	0.40
31:a:407:CLA:H52	44:d:407:PL9:H151	2.02	0.40
6:b:391:SER:O	6:b:395:VAL:HG23	2.21	0.40
31:b:605:CLA:H41	31:b:605:CLA:H61	1.76	0.40
31:b:608:CLA:H193	15:l:29:ALA:HA	2.02	0.40
7:c:418:HIS:CD2	31:c:602:CLA:ND	2.89	0.40
45:c:619:DGD:HBS1	31:y:614:CLA:HBC1	2.03	0.40
8:d:146:PHE:C	8:d:149:PRO:HD2	2.47	0.40
8:d:160:TYR:O	8:d:164:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:d:320:LEU:HD12	8:d:320:LEU:HA	1.90	0.40
9:e:37:PHE:CZ	9:e:47:PHE:HE2	2.39	0.40
10:f:35:ALA:O	10:f:39:MET:HG3	2.22	0.40
2:g:126:PHE:CD1	2:g:127:LYS:HG3	2.56	0.40
31:g:313:CLA:H61	31:g:313:CLA:H92	1.76	0.40
3:n:200:LEU:HB3	31:n:311:CLA:CMA	2.50	0.40
32:n:317:LUT:H35	32:n:317:LUT:H401	1.86	0.40
18:r:145:LEU:HD11	38:r:322:SQD:H372	2.03	0.40
19:s:191:GLY:HA3	31:s:316:CLA:C3D	2.51	0.40
32:y:617:LUT:H15	32:y:617:LUT:H201	1.89	0.40
32:y:617:LUT:H35	32:y:617:LUT:H401	1.88	0.40
30:2:607:CHL:HBA2	31:2:609:CLA:CMD	2.50	0.40
3:3:118:GLU:OE2	3:3:130:GLN:NE2	2.54	0.40
3:3:188:LEU:HB2	3:3:190:LEU:HG	2.03	0.40
2:4:152:ILE:O	2:4:153:VAL:C	2.64	0.40
30:4:606:CHL:HMB1	30:4:606:CHL:CBB	2.49	0.40
31:4:612:CLA:HHC	31:4:612:CLA:HBB1	2.03	0.40
34:4:620:LMG:HC72	34:4:620:LMG:O9	2.22	0.40
31:5:603:CLA:HBB1	31:5:603:CLA:CMB	2.52	0.40
4:6:139:LEU:HD11	34:6:321:LMG:O9	2.22	0.40
34:6:321:LMG:H132	34:6:321:LMG:H161	1.89	0.40
43:B:619:BCR:H371	43:B:619:BCR:H24C	1.90	0.40
7:C:14:ARG:HE	7:C:14:ARG:HA	1.86	0.40
2:G:89:GLU:O	2:G:93:ILE:HG12	2.22	0.40
2:G:121:GLU:HB2	2:G:127:LYS:HE2	2.04	0.40
2:G:146:LEU:O	2:G:147:ILE:C	2.65	0.40
2:G:167:GLU:HG3	30:G:608:CHL:C4B	2.50	0.40
14:K:15:TYR:CZ	25:Z:5:PHE:HZ	2.40	0.40
3:N:252:LYS:HA	3:N:256:ILE:CG2	2.48	0.40
17:O:100:GLU:HA	17:O:131:THR:HG22	2.03	0.40
17:O:116:ASP:O	17:O:118:GLU:HG3	2.22	0.40
31:R:304:CLA:H93	31:R:304:CLA:H62	1.90	0.40
19:S:114:ALA:O	19:S:118:ALA:N	2.53	0.40
19:S:155:PRO:HD3	31:S:306:CLA:ND	2.35	0.40
31:S:305:CLA:NC	36:S:319:NEX:H222	2.36	0.40
31:S:312:CLA:CHD	33:S:320:LHG:HC62	2.51	0.40
20:T:18:PHE:HA	43:T:101:BCR:H403	2.04	0.40
4:0:191:GLY:HA3	18:r:45:ARG:HB2	2.04	0.40
4:0:253:LYS:HE2	4:0:253:LYS:HB2	1.90	0.40
31:7:316:CLA:HBB1	3:8:222:GLY:HA3	2.03	0.40
3:8:51:PRO:HG2	3:8:52:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:8:602:CLA:C9	31:9:305:CLA:H52	2.52	0.40
31:8:614:CLA:C3D	34:9:302:LMG:H292	2.51	0.40
2:q:116:ALA:HA	34:q1:101:LMG:HC8	2.03	0.40
2:q:195:LEU:HB2	31:q:312:CLA:O1A	2.21	0.40
5:a:198:HIS:HE1	31:a:406:CLA:C4B	2.35	0.40
6:b:149:LEU:HD22	31:b:605:CLA:H162	2.04	0.40
31:c:606:CLA:H111	31:c:606:CLA:H93	1.84	0.40
45:c:619:DGD:HA61	45:c:619:DGD:HA92	1.91	0.40
30:n:306:CHL:H93	30:n:306:CHL:H111	1.85	0.40
48:r:302:LMU:H22	31:r:307:CLA:CBB	2.51	0.40
31:r:312:CLA:HBA2	31:r:312:CLA:H12	1.94	0.40
1:1:134:TYR:CE1	31:1:604:CLA:H2	2.57	0.40
1:1:246:LEU:HD23	1:1:247:TYR:CE2	2.57	0.40
30:1:606:CHL:HAC1	30:1:606:CHL:OMC	2.22	0.40
31:1:611:CLA:CHD	33:1:617:LHG:HC62	2.52	0.40
30:2:608:CHL:HHC	30:2:608:CHL:CBB	2.47	0.40
3:3:241:ASP:N	3:3:241:ASP:OD1	2.55	0.40
31:3:305:CLA:HBB1	31:3:305:CLA:CMB	2.51	0.40
31:3:311:CLA:H2	32:3:317:LUT:H28	2.03	0.40
31:3:312:CLA:H92	31:3:312:CLA:H62	1.82	0.40
2:4:77:LEU:HD23	31:4:602:CLA:H11	2.04	0.40
2:4:152:ILE:H	2:4:152:ILE:CD1	2.21	0.40
2:4:158:THR:O	2:4:162:ILE:HD13	2.21	0.40
3:5:91:HIS:CD2	32:5:617:LUT:H15	2.57	0.40
31:5:610:CLA:H51	31:5:610:CLA:C2B	2.51	0.40
34:5:620:LMG:H122	34:5:620:LMG:H152	1.79	0.40
4:6:235:LEU:C	4:6:235:LEU:HD13	2.47	0.40
30:6:307:CHL:H3A	36:6:319:NEX:H31	2.02	0.40
34:6:323:LMG:C28	34:6:323:LMG:HC72	2.51	0.40
34:6:323:LMG:C28	34:X:202:LMG:H121	2.52	0.40
6:B:225:LEU:HD12	6:B:225:LEU:HA	1.90	0.40
31:B:610:CLA:H202	31:B:610:CLA:H161	1.87	0.40
31:B:616:CLA:H161	31:B:616:CLA:H141	1.81	0.40
31:C:602:CLA:H141	31:C:602:CLA:H161	1.90	0.40
45:C:620:DGD:HB42	45:C:620:DGD:HB71	1.72	0.40
14:K:19:ASP:N	14:K:20:PRO:HD2	2.36	0.40
19:S:163:LEU:HD13	19:S:163:LEU:HA	1.94	0.40
31:S:315:CLA:HBA2	31:S:315:CLA:H3A	1.53	0.40
20:T:26:PRO:HA	20:T:27:PRO:HD3	1.93	0.40
31:Y:312:CLA:H143	31:Y:312:CLA:H111	1.65	0.40
4:0:61:LEU:HD23	4:0:70:GLY:HA2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:0:602:CLA:H52	32:0:617:LUT:H28	2.02	0.40
3:8:87:LEU:CD1	31:8:603:CLA:HBA1	2.43	0.40
31:p:610:CLA:HBA2	32:p:616:LUT:H24	2.03	0.40
2:q:138:LEU:HD23	2:q:138:LEU:C	2.47	0.40
6:b:280:PHE:O	6:b:284:ILE:HG13	2.22	0.40
31:b:614:CLA:H112	31:b:614:CLA:H152	1.86	0.40
9:e:40:THR:HB	27:q1:4:ARG:HD2	2.03	0.40
2:g:185:TYR:CE2	2:g:206:LYS:HE3	2.56	0.40
31:g:304:CLA:H52	31:g:304:CLA:H8	1.50	0.40
31:g:313:CLA:H102	33:g:319:LHG:H281	2.02	0.40
3:n:226:ARG:NH1	31:y:615:CLA:HMA2	2.37	0.40
18:r:266:LEU:HD12	18:r:266:LEU:HA	1.92	0.40
31:s:315:CLA:H3A	31:s:315:CLA:HBA2	1.49	0.40
24:y:46:ARG:NH2	24:y:62:LEU:O	2.54	0.40
24:y:46:ARG:HD2	24:y:69:ASP:O	2.21	0.40
24:y:178:PHE:HD1	38:y:621:SQD:H2	1.86	0.40
24:y:251:PHE:HB2	31:y:613:CLA:CAD	2.52	0.40
31:y:610:CLA:C2	32:y:616:LUT:H28	2.48	0.40
27:q1:3:ASN:HB2	34:q1:101:LMG:C5	2.51	0.40
27:q1:23:ILE:HD12	27:q1:23:ILE:HA	2.00	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	212/214 (99%)	202 (95%)	10 (5%)	0	100 100
1	7	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	24 40
2	2	220/222 (99%)	203 (92%)	15 (7%)	2 (1%)	14 26
2	4	220/222 (99%)	200 (91%)	15 (7%)	5 (2%)	5 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	9	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
2	G	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
2	g	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
2	q	220/222 (99%)	196 (89%)	22 (10%)	2 (1%)	14	26
3	3	219/221 (99%)	198 (90%)	21 (10%)	0	100	100
3	5	219/221 (99%)	202 (92%)	15 (7%)	2 (1%)	14	26
3	8	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
3	N	219/221 (99%)	211 (96%)	7 (3%)	1 (0%)	24	40
3	n	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
3	p	219/221 (99%)	200 (91%)	16 (7%)	3 (1%)	9	15
4	0	215/217 (99%)	202 (94%)	12 (6%)	1 (0%)	24	40
4	6	215/217 (99%)	205 (95%)	9 (4%)	1 (0%)	24	40
5	A	334/336 (99%)	329 (98%)	5 (2%)	0	100	100
5	a	334/336 (99%)	329 (98%)	5 (2%)	0	100	100
6	B	502/504 (100%)	493 (98%)	9 (2%)	0	100	100
6	b	502/504 (100%)	491 (98%)	11 (2%)	0	100	100
7	C	446/448 (100%)	437 (98%)	9 (2%)	0	100	100
7	c	446/448 (100%)	438 (98%)	8 (2%)	0	100	100
8	D	340/342 (99%)	330 (97%)	10 (3%)	0	100	100
8	d	340/342 (99%)	329 (97%)	10 (3%)	1 (0%)	36	54
9	E	79/81 (98%)	79 (100%)	0	0	100	100
9	e	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
10	F	35/37 (95%)	35 (100%)	0	0	100	100
10	f	35/37 (95%)	35 (100%)	0	0	100	100
11	H	65/67 (97%)	65 (100%)	0	0	100	100
11	h	65/67 (97%)	65 (100%)	0	0	100	100
12	I	32/34 (94%)	32 (100%)	0	0	100	100
12	i	32/34 (94%)	32 (100%)	0	0	100	100
13	J	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
13	j	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
14	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
15	L	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
15	l	35/37 (95%)	35 (100%)	0	0	100	100
16	M	31/57 (54%)	30 (97%)	0	1 (3%)	3	5
16	m	31/57 (54%)	31 (100%)	0	0	100	100
17	O	238/240 (99%)	227 (95%)	11 (5%)	0	100	100
17	o	238/240 (99%)	227 (95%)	11 (5%)	0	100	100
18	R	233/236 (99%)	227 (97%)	6 (3%)	0	100	100
18	r	233/236 (99%)	230 (99%)	3 (1%)	0	100	100
19	S	255/257 (99%)	249 (98%)	6 (2%)	0	100	100
19	s	255/257 (99%)	249 (98%)	6 (2%)	0	100	100
20	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
20	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
21	V	30/32 (94%)	30 (100%)	0	0	100	100
21	v	30/32 (94%)	30 (100%)	0	0	100	100
22	W	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
22	w	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
23	X	35/37 (95%)	35 (100%)	0	0	100	100
23	x	35/37 (95%)	35 (100%)	0	0	100	100
24	Y	219/221 (99%)	215 (98%)	4 (2%)	0	100	100
24	y	219/221 (99%)	215 (98%)	4 (2%)	0	100	100
25	Z	60/62 (97%)	60 (100%)	0	0	100	100
25	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
26	U	142/144 (99%)	139 (98%)	2 (1%)	1 (1%)	18	32
26	u	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
27	Q1	32/34 (94%)	32 (100%)	0	0	100	100
27	q1	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
28	P1	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
28	p1	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
29	F1	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
29	f1	186/188 (99%)	180 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	10672/10854 (98%)	10317 (97%)	334 (3%)	21 (0%)	44 62

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	4	181	GLY
2	4	188	GLY
2	4	191	ASP
3	N	52	PHE
4	0	252	ALA
2	q	191	ASP
2	4	186	PRO
26	U	110	ALA
2	q	188	GLY
2	2	125	TRP
2	2	257	PHE
3	5	248	ASP
4	6	251	TYR
1	7	140	LEU
3	p	39	GLU
3	p	246	TRP
2	4	146	LEU
16	M	5	ILE
3	5	256	ILE
3	p	51	PRO
8	d	140	PRO

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	165/165 (100%)	156 (94%)	9 (6%)	19 35
1	7	165/165 (100%)	158 (96%)	7 (4%)	26 47
2	2	171/171 (100%)	164 (96%)	7 (4%)	27 48
2	4	171/171 (100%)	161 (94%)	10 (6%)	18 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	9	171/171 (100%)	165 (96%)	6 (4%)	32 54
2	G	171/171 (100%)	164 (96%)	7 (4%)	27 48
2	g	171/171 (100%)	161 (94%)	10 (6%)	18 33
2	q	171/171 (100%)	164 (96%)	7 (4%)	27 48
3	3	168/168 (100%)	156 (93%)	12 (7%)	13 24
3	5	168/168 (100%)	156 (93%)	12 (7%)	13 24
3	8	168/168 (100%)	159 (95%)	9 (5%)	20 36
3	N	168/168 (100%)	158 (94%)	10 (6%)	17 31
3	n	168/168 (100%)	159 (95%)	9 (5%)	20 36
3	p	168/168 (100%)	161 (96%)	7 (4%)	26 47
4	0	169/169 (100%)	159 (94%)	10 (6%)	18 32
4	6	169/169 (100%)	161 (95%)	8 (5%)	23 43
5	A	274/274 (100%)	261 (95%)	13 (5%)	23 43
5	a	274/274 (100%)	265 (97%)	9 (3%)	33 55
6	B	402/402 (100%)	375 (93%)	27 (7%)	15 27
6	b	402/402 (100%)	377 (94%)	25 (6%)	16 30
7	C	350/350 (100%)	324 (93%)	26 (7%)	13 23
7	c	350/350 (100%)	332 (95%)	18 (5%)	21 39
8	D	277/277 (100%)	268 (97%)	9 (3%)	34 56
8	d	277/277 (100%)	260 (94%)	17 (6%)	17 30
9	E	72/72 (100%)	69 (96%)	3 (4%)	26 47
9	e	72/72 (100%)	69 (96%)	3 (4%)	26 47
10	F	31/31 (100%)	31 (100%)	0	100 100
10	f	31/31 (100%)	31 (100%)	0	100 100
11	H	57/57 (100%)	56 (98%)	1 (2%)	51 69
11	h	57/57 (100%)	55 (96%)	2 (4%)	32 54
12	I	31/31 (100%)	30 (97%)	1 (3%)	34 56
12	i	31/31 (100%)	30 (97%)	1 (3%)	34 56
13	J	27/27 (100%)	24 (89%)	3 (11%)	6 11
13	j	27/27 (100%)	25 (93%)	2 (7%)	13 23
14	K	33/33 (100%)	29 (88%)	4 (12%)	5 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	k	33/33 (100%)	28 (85%)	5 (15%)	3 3
15	L	34/34 (100%)	32 (94%)	2 (6%)	18 32
15	l	34/34 (100%)	32 (94%)	2 (6%)	18 32
16	M	28/28 (100%)	27 (96%)	1 (4%)	31 53
16	m	28/28 (100%)	27 (96%)	1 (4%)	31 53
17	O	189/189 (100%)	176 (93%)	13 (7%)	14 26
17	o	189/189 (100%)	181 (96%)	8 (4%)	26 47
18	R	184/184 (100%)	178 (97%)	6 (3%)	33 55
18	r	184/184 (100%)	177 (96%)	7 (4%)	29 51
19	S	192/192 (100%)	185 (96%)	7 (4%)	31 53
19	s	192/192 (100%)	186 (97%)	6 (3%)	35 57
20	T	26/26 (100%)	26 (100%)	0	100 100
20	t	26/26 (100%)	23 (88%)	3 (12%)	5 10
21	V	26/26 (100%)	24 (92%)	2 (8%)	12 21
21	v	26/26 (100%)	25 (96%)	1 (4%)	29 51
22	W	50/50 (100%)	49 (98%)	1 (2%)	48 67
22	w	50/50 (100%)	50 (100%)	0	100 100
23	X	25/25 (100%)	23 (92%)	2 (8%)	11 20
23	x	25/25 (100%)	25 (100%)	0	100 100
24	Y	170/170 (100%)	161 (95%)	9 (5%)	20 37
24	y	170/170 (100%)	160 (94%)	10 (6%)	18 32
25	Z	52/52 (100%)	50 (96%)	2 (4%)	29 51
25	z	52/52 (100%)	49 (94%)	3 (6%)	18 33
26	U	108/108 (100%)	106 (98%)	2 (2%)	50 68
26	u	108/108 (100%)	100 (93%)	8 (7%)	13 23
27	Q1	28/28 (100%)	28 (100%)	0	100 100
27	q1	28/28 (100%)	28 (100%)	0	100 100
28	P1	88/88 (100%)	88 (100%)	0	100 100
28	p1	88/88 (100%)	84 (96%)	4 (4%)	24 44
29	F1	147/147 (100%)	139 (95%)	8 (5%)	20 36
29	f1	147/147 (100%)	146 (99%)	1 (1%)	76 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	8504/8504 (100%)	8086 (95%)	418 (5%)	24 41

All (418) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	40	GLN
1	1	48	LYS
1	1	77	LEU
1	1	103	LEU
1	1	146	ILE
1	1	150	LEU
1	1	231	LEU
1	1	246	LEU
1	1	249	LYS
2	2	77	LEU
2	2	124	VAL
2	2	127	LYS
2	2	152	ILE
2	2	184	LEU
2	2	189	PHE
2	2	256	LYS
3	3	86	GLU
3	3	118	GLU
3	3	153	LEU
3	3	166	ARG
3	3	168	ASN
3	3	200	LEU
3	3	202	VAL
3	3	223	LEU
3	3	241	ASP
3	3	252	LYS
3	3	256	ILE
3	3	258	TYR
2	4	50	LEU
2	4	77	LEU
2	4	113	ASN
2	4	146	LEU
2	4	152	ILE
2	4	155	VAL
2	4	159	GLN
2	4	170	ARG
2	4	202	LEU

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Mol	Chain	Res	Type
2	4	205	LEU
3	5	74	LEU
3	5	86	GLU
3	5	107	LEU
3	5	113	VAL
3	5	115	ASN
3	5	152	LEU
3	5	158	LEU
3	5	230	ILE
3	5	233	LEU
3	5	241	ASP
3	5	249	TYR
3	5	256	ILE
4	6	76	LEU
4	6	106	THR
4	6	139	LEU
4	6	148	GLN
4	6	177	VAL
4	6	178	VAL
4	6	251	TYR
4	6	253	LYS
5	A	35	VAL
5	A	36	LEU
5	A	96	ILE
5	A	121	LEU
5	A	133	LEU
5	A	194	MET
5	A	214	MET
5	A	218	LEU
5	A	275	LEU
5	A	313	VAL
5	A	326	LEU
5	A	334	ARG
5	A	343	LEU
6	B	10	THR
6	B	22	VAL
6	B	37	MET
6	B	51	VAL
6	B	52	LEU
6	B	57	ARG
6	B	94	GLU
6	B	159	THR

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Mol	Chain	Res	Type
6	B	161	LEU
6	B	181	VAL
6	B	214	LEU
6	B	236	THR
6	B	245	VAL
6	B	252	VAL
6	B	272	ARG
6	B	292	LEU
6	B	345	VAL
6	B	362	PHE
6	B	368	VAL
6	B	369	VAL
6	B	373	LYS
6	B	393	GLU
6	B	422	ARG
6	B	437	LEU
6	B	440	ASP
6	B	473	THR
6	B	486	LEU
7	C	56	ASN
7	C	101	VAL
7	C	105	LEU
7	C	112	VAL
7	C	113	LEU
7	C	123	VAL
7	C	155	VAL
7	C	156	LEU
7	C	158	LEU
7	C	164	VAL
7	C	173	ILE
7	C	201	LEU
7	C	222	ILE
7	C	228	ILE
7	C	243	LYS
7	C	302	THR
7	C	304	THR
7	C	308	ARG
7	C	309	ASP
7	C	336	GLU
7	C	357	LEU
7	C	361	ASN
7	C	369	LYS

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Mol	Chain	Res	Type
7	C	392	LEU
7	C	398	VAL
7	C	416	THR
8	D	28	VAL
8	D	35	LEU
8	D	74	LEU
8	D	90	LEU
8	D	92	LEU
8	D	107	LEU
8	D	131	GLU
8	D	178	ILE
8	D	264	LYS
9	E	7	GLU
9	E	62	GLU
9	E	67	THR
2	G	50	LEU
2	G	100	LEU
2	G	132	ILE
2	G	198	ASP
2	G	202	LEU
2	G	244	GLU
2	G	258	LEU
11	H	77	VAL
12	I	4	LEU
13	J	6	THR
13	J	12	LEU
13	J	42	LEU
14	K	25	LEU
14	K	33	LEU
14	K	35	LEU
14	K	37	LEU
15	L	12	GLU
15	L	16	THR
16	M	3	VAL
3	N	59	LEU
3	N	62	GLU
3	N	131	GLU
3	N	146	GLN
3	N	152	LEU
3	N	156	LEU
3	N	158	LEU
3	N	226	ARG

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Mol	Chain	Res	Type
3	N	241	ASP
3	N	256	ILE
17	O	60	LEU
17	O	86	ASP
17	O	87	LEU
17	O	148	GLU
17	O	151	GLU
17	O	170	VAL
17	O	173	LEU
17	O	179	LEU
17	O	184	ASN
17	O	250	LYS
17	O	251	VAL
17	O	255	THR
17	O	272	LEU
18	R	54	LEU
18	R	56	ASN
18	R	137	LEU
18	R	162	VAL
18	R	243	LEU
18	R	249	LEU
19	S	36	SER
19	S	51	LYS
19	S	92	LYS
19	S	149	LEU
19	S	196	VAL
19	S	201	GLU
19	S	209	ASN
21	V	2	ASN
21	V	7	LEU
22	W	119	LEU
23	X	72	LEU
23	X	100	ARG
24	Y	57	LEU
24	Y	77	LEU
24	Y	155	LEU
24	Y	167	ILE
24	Y	185	LEU
24	Y	203	LEU
24	Y	219	LEU
24	Y	222	LEU
24	Y	236	LEU

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Mol	Chain	Res	Type
25	Z	9	LEU
25	Z	53	LEU
26	U	89	GLN
26	U	92	GLU
4	0	76	LEU
4	0	106	THR
4	0	111	GLN
4	0	133	GLU
4	0	148	GLN
4	0	177	VAL
4	0	197	ASP
4	0	227	THR
4	0	235	LEU
4	0	250	LEU
1	7	50	LEU
1	7	61	TYR
1	7	103	LEU
1	7	140	LEU
1	7	150	LEU
1	7	221	ILE
1	7	251	LEU
3	8	38	VAL
3	8	52	PHE
3	8	59	LEU
3	8	62	GLU
3	8	131	GLU
3	8	146	GLN
3	8	152	LEU
3	8	158	LEU
3	8	256	ILE
2	9	63	LYS
2	9	119	PHE
2	9	124	VAL
2	9	184	LEU
2	9	238	LEU
2	9	258	LEU
3	p	74	LEU
3	p	100	LEU
3	p	128	ILE
3	p	179	LEU
3	p	232	ASN
3	p	233	LEU

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Mol	Chain	Res	Type
3	p	258	TYR
2	q	50	LEU
2	q	77	LEU
2	q	152	ILE
2	q	170	ARG
2	q	192	PRO
2	q	202	LEU
2	q	205	LEU
5	a	133	LEU
5	a	165	GLN
5	a	194	MET
5	a	257	ARG
5	a	266	ASN
5	a	275	LEU
5	a	313	VAL
5	a	334	ARG
5	a	343	LEU
6	b	10	THR
6	b	13	LEU
6	b	22	VAL
6	b	51	VAL
6	b	52	LEU
6	b	94	GLU
6	b	159	THR
6	b	181	VAL
6	b	214	LEU
6	b	224	ARG
6	b	225	LEU
6	b	236	THR
6	b	246	PHE
6	b	252	VAL
6	b	272	ARG
6	b	289	GLN
6	b	292	LEU
6	b	362	PHE
6	b	368	VAL
6	b	369	VAL
6	b	374	ASP
6	b	399	VAL
6	b	445	THR
6	b	489	GLN
6	b	498	LEU

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Mol	Chain	Res	Type
7	c	55	MET
7	c	56	ASN
7	c	101	VAL
7	c	105	LEU
7	c	155	VAL
7	c	156	LEU
7	c	164	VAL
7	c	166	LYS
7	c	173	ILE
7	c	267	ILE
7	c	275	CYS
7	c	302	THR
7	c	323	THR
7	c	361	ASN
7	c	392	LEU
7	c	398	VAL
7	c	430	LEU
7	c	458	ARG
8	d	28	VAL
8	d	45	LEU
8	d	74	LEU
8	d	90	LEU
8	d	92	LEU
8	d	102	THR
8	d	107	LEU
8	d	158	LEU
8	d	178	ILE
8	d	192	THR
8	d	213	ILE
8	d	279	LEU
8	d	320	LEU
8	d	323	GLU
8	d	340	VAL
8	d	345	VAL
8	d	352	LEU
9	e	49	SER
9	e	65	LEU
9	e	66	ILE
2	g	50	LEU
2	g	74	THR
2	g	100	LEU
2	g	152	ILE

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Mol	Chain	Res	Type
2	g	156	LEU
2	g	158	THR
2	g	167	GLU
2	g	184	LEU
2	g	202	LEU
2	g	204	GLU
11	h	74	LEU
11	h	77	VAL
12	i	4	LEU
13	j	12	LEU
13	j	42	LEU
14	k	11	LEU
14	k	25	LEU
14	k	33	LEU
14	k	35	LEU
14	k	37	LEU
15	l	3	LYS
15	l	16	THR
16	m	9	ILE
3	n	38	VAL
3	n	52	PHE
3	n	59	LEU
3	n	62	GLU
3	n	131	GLU
3	n	146	GLN
3	n	152	LEU
3	n	158	LEU
3	n	256	ILE
17	o	77	LEU
17	o	88	LYS
17	o	170	VAL
17	o	173	LEU
17	o	179	LEU
17	o	186	ASP
17	o	250	LYS
17	o	251	VAL
18	r	54	LEU
18	r	145	LEU
18	r	151	LEU
18	r	162	VAL
18	r	179	LEU
18	r	243	LEU

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Mol	Chain	Res	Type
18	r	249	LEU
19	s	45	GLN
19	s	90	LEU
19	s	92	LYS
19	s	149	LEU
19	s	196	VAL
19	s	236	ILE
20	t	1	MET
20	t	2	GLU
20	t	30	VAL
21	v	5	ILE
24	y	57	LEU
24	y	77	LEU
24	y	121	GLU
24	y	167	ILE
24	y	185	LEU
24	y	203	LEU
24	y	219	LEU
24	y	222	LEU
24	y	236	LEU
24	y	257	ASN
25	z	3	LEU
25	z	9	LEU
25	z	49	LEU
26	u	55	LEU
26	u	62	LYS
26	u	98	LYS
26	u	106	LYS
26	u	113	ASP
26	u	122	THR
26	u	152	LYS
26	u	153	GLU
28	p1	7	ILE
28	p1	28	SER
28	p1	60	VAL
28	p1	79	TYR
29	F1	63	LYS
29	F1	89	ASP
29	F1	120	ASP
29	F1	175	LYS
29	F1	181	VAL
29	F1	187	ASP

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Mol	Chain	Res	Type
29	F1	216	LYS
29	F1	235	VAL
29	f1	181	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	182	ASN
3	3	115	ASN
3	3	221	GLN
2	4	113	ASN
2	4	114	ASN
3	5	47	GLN
3	5	115	ASN
3	5	130	GLN
3	5	146	GLN
3	5	155	GLN
5	A	181	ASN
5	A	247	ASN
5	A	322	ASN
6	B	394	GLN
7	C	62	HIS
7	C	143	ASN
2	G	150	GLN
2	G	237	ASN
12	I	26	ASN
14	K	40	GLN
3	N	54	ASN
3	N	115	ASN
17	O	58	GLN
18	R	46	GLN
18	R	130	GLN
18	R	267	ASN
19	S	103	ASN
19	S	160	ASN
22	W	111	ASN
24	Y	238	ASN
26	U	131	GLN
26	U	171	GLN
4	0	148	GLN
4	0	170	ASN
4	0	234	ASN

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Mol	Chain	Res	Type
2	9	143	ASN
3	p	127	GLN
3	p	146	GLN
3	p	221	GLN
3	p	232	ASN
3	p	244	ASN
5	a	108	ASN
5	a	165	GLN
5	a	241	GLN
5	a	266	ASN
5	a	267	ASN
5	a	337	HIS
6	b	331	ASN
7	c	315	ASN
7	c	376	GLN
8	d	142	ASN
8	d	332	GLN
2	g	148	HIS
2	g	237	ASN
16	m	4	ASN
17	o	56	GLN
17	o	243	GLN
19	s	45	GLN
19	s	158	ASN
26	u	171	GLN
28	P1	17	ASN
28	P1	54	ASN
29	F1	59	ASN
29	F1	105	ASN
29	F1	203	ASN
29	f1	59	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	CSU	r	211	18	7,9,10	3.21	4 (57%)	4,12,14	2.29	2 (50%)
18	CSU	R	211	18	7,9,10	3.21	4 (57%)	4,12,14	2.30	2 (50%)

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
18	CSU	r	211	18	-	4/4/8/10	-
18	CSU	R	211	18	-	4/4/8/10	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	r	211	CSU	OD1-S	6.06	1.63	1.45
18	R	211	CSU	OD3-S	6.04	1.63	1.45
18	R	211	CSU	O-C	4.22	1.36	1.20
18	r	211	CSU	O-C	4.20	1.35	1.20
18	R	211	CSU	OD1-S	-2.73	1.37	1.45
18	r	211	CSU	OD3-S	-2.66	1.37	1.45
18	r	211	CSU	OD2-S	-2.38	1.37	1.49
18	R	211	CSU	OD2-S	-2.38	1.37	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	r	211	CSU	OD2-S-OD3	3.85	125.57	112.74
18	R	211	CSU	OD2-S-OD1	3.44	124.19	112.74
18	R	211	CSU	OD2-S-OD3	-2.93	102.99	112.74
18	r	211	CSU	OD2-S-OD1	-2.28	105.16	112.74

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	R	211	CSU	N-CA-CB-SG
18	R	211	CSU	OD2-S-SG-CB
18	r	211	CSU	OD2-S-SG-CB
18	R	211	CSU	OD1-S-SG-CB
18	R	211	CSU	OD3-S-SG-CB
18	r	211	CSU	OD1-S-SG-CB
18	r	211	CSU	OD3-S-SG-CB
18	r	211	CSU	N-CA-CB-SG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	r	211	CSU	1	0
18	R	211	CSU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 672 ligands modelled in this entry, 6 are monoatomic - leaving 666 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	$\#\|Z\| > 2$
34	LMG	b	601	-	45,45,55	1.00	3 (6%)	53,53,63	1.09	3 (5%)
31	CLA	s	306	-	54,58,73	1.52	7 (12%)	64,95,113	2.17	19 (29%)
31	CLA	S	303	19	69,73,73	1.35	7 (10%)	82,113,113	1.93	20 (24%)
33	LHG	Y	318	31	41,41,48	0.46	0	44,47,54	1.08	3 (6%)
32	LUT	1	615	-	42,43,43	6.32	25 (59%)	51,60,60	2.17	21 (41%)
34	LMG	5	620	-	38,38,55	0.68	1 (2%)	46,46,63	1.10	2 (4%)
30	CHL	5	605	3	40,54,74	1.54	8 (20%)	34,90,114	2.09	11 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	q	312	2	56,61,73	1.40	7 (12%)	69,98,113	2.18	20 (28%)
31	CLA	9	312	2	58,62,73	1.48	6 (10%)	68,99,113	2.13	22 (32%)
31	CLA	4	604	30	55,59,73	1.50	6 (10%)	64,96,113	2.17	18 (28%)
43	BCR	b	619	-	41,41,41	4.92	26 (63%)	56,56,56	2.33	18 (32%)
30	CHL	9	309	-	47,61,74	1.81	8 (17%)	41,98,114	1.93	12 (29%)
33	LHG	8	618	31	48,48,48	0.38	0	51,54,54	1.04	2 (3%)
31	CLA	3	311	-	58,62,73	1.49	7 (12%)	68,99,113	2.08	19 (27%)
31	CLA	7	315	-	58,62,73	1.46	5 (8%)	68,99,113	2.01	19 (27%)
31	CLA	B	609	-	69,73,73	1.36	6 (8%)	82,113,113	1.92	19 (23%)
30	CHL	S	309	49	43,57,74	1.66	9 (20%)	37,93,114	2.05	10 (27%)
34	LMG	D	412	-	48,48,55	1.12	5 (10%)	56,56,63	1.12	2 (3%)
30	CHL	q	311	2	50,64,74	1.40	8 (16%)	46,102,114	1.77	9 (19%)
31	CLA	N	303	3	69,73,73	1.35	6 (8%)	82,113,113	1.90	21 (25%)
31	CLA	7	303	1	64,68,73	1.40	6 (9%)	76,107,113	1.93	21 (27%)
31	CLA	r	312	18	61,65,73	1.46	6 (9%)	72,103,113	2.03	20 (27%)
33	LHG	b	628	-	48,48,48	0.40	0	51,54,54	1.12	3 (5%)
42	PHO	D	401	-	58,69,69	2.04	9 (15%)	55,99,99	1.46	8 (14%)
31	CLA	n	311	3	69,73,73	1.34	7 (10%)	82,113,113	1.89	20 (24%)
34	LMG	Y	319	-	38,38,55	0.69	1 (2%)	46,46,63	1.14	3 (6%)
31	CLA	R	314	-	53,57,73	1.55	6 (11%)	61,93,113	2.10	17 (27%)
31	CLA	r	316	18	69,73,73	1.37	6 (8%)	82,113,113	1.92	19 (23%)
31	CLA	y	613	24	69,73,73	1.44	6 (8%)	82,113,113	1.95	18 (21%)
34	LMG	G	622	-	40,40,55	0.76	2 (5%)	48,48,63	1.11	4 (8%)
36	NEX	2	616	31	40,46,46	2.72	11 (27%)	50,70,70	1.60	6 (12%)
38	SQD	g	301	-	36,38,54	0.89	0	46,49,65	0.93	2 (4%)
30	CHL	g	307	49	44,58,74	1.72	8 (18%)	37,94,114	1.96	11 (29%)
31	CLA	p	604	36	54,58,73	1.52	8 (14%)	64,95,113	2.09	19 (29%)
33	LHG	b	625	-	43,43,48	0.42	0	46,49,54	1.08	3 (6%)
31	CLA	8	603	-	59,63,73	1.46	6 (10%)	70,101,113	2.05	17 (24%)
31	CLA	B	601	49	53,57,73	1.56	6 (11%)	61,93,113	2.14	17 (27%)
31	CLA	g	303	2	69,73,73	1.33	6 (8%)	82,113,113	1.88	17 (20%)
31	CLA	6	304	-	60,64,73	1.46	7 (11%)	71,102,113	2.04	21 (29%)
38	SQD	S	301	-	49,51,54	0.79	0	59,62,65	0.88	2 (3%)
30	CHL	n	310	3	60,74,74	1.58	7 (11%)	58,114,114	1.68	11 (18%)
34	LMG	a	416	-	38,38,55	0.67	1 (2%)	46,46,63	1.07	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	A	405	-	69,73,73	1.36	6 (8%)	82,113,113	1.95	20 (24%)
34	LMG	f	101	-	38,38,55	0.63	1 (2%)	46,46,63	1.14	2 (4%)
30	CHL	1	609	1	60,74,74	1.55	10 (16%)	58,114,114	1.65	12 (20%)
31	CLA	B	608	-	69,73,73	1.38	6 (8%)	82,113,113	1.86	15 (18%)
33	LHG	r	320	31	37,37,48	0.46	0	40,43,54	1.16	3 (7%)
34	LMG	b	622	-	51,51,55	1.23	7 (13%)	59,59,63	1.35	7 (11%)
30	CHL	7	308	49	60,74,74	1.22	7 (11%)	58,114,114	1.64	11 (18%)
31	CLA	G	613	-	53,57,73	1.56	6 (11%)	61,93,113	2.10	18 (29%)
31	CLA	a	407	49	69,73,73	1.37	7 (10%)	82,113,113	1.92	18 (21%)
31	CLA	6	316	4	59,63,73	1.46	6 (10%)	70,101,113	2.03	18 (25%)
31	CLA	C	613	-	69,73,73	1.36	7 (10%)	82,113,113	2.02	20 (24%)
31	CLA	c	613	-	69,73,73	1.36	7 (10%)	82,113,113	1.96	21 (25%)
31	CLA	9	305	-	59,63,73	1.46	6 (10%)	70,101,113	2.05	21 (30%)
31	CLA	1	613	1	69,73,73	1.36	7 (10%)	82,113,113	1.86	16 (19%)
32	LUT	0	616	-	42,43,43	6.33	25 (59%)	51,60,60	2.14	17 (33%)
30	CHL	Y	302	24	60,74,74	1.28	7 (11%)	58,114,114	1.69	12 (20%)
33	LHG	C	623	-	39,39,48	0.43	0	42,45,54	1.23	4 (9%)
31	CLA	9	316	-	50,54,73	1.58	6 (12%)	59,90,113	2.03	17 (28%)
36	NEX	0	618	-	40,46,46	2.73	11 (27%)	50,70,70	1.57	9 (18%)
31	CLA	C	606	-	61,65,73	1.45	6 (9%)	72,103,113	2.00	17 (23%)
30	CHL	G	606	49	44,58,74	1.62	8 (18%)	37,94,114	1.98	12 (32%)
31	CLA	c	606	-	69,73,73	1.39	6 (8%)	82,113,113	1.88	14 (17%)
32	LUT	9	318	-	42,43,43	6.41	27 (64%)	51,60,60	2.30	16 (31%)
34	LMG	0	622	-	38,38,55	0.70	1 (2%)	46,46,63	1.14	3 (6%)
34	LMG	J	102	-	38,38,55	0.65	1 (2%)	46,46,63	1.11	2 (4%)
30	CHL	6	306	4	40,54,74	1.43	8 (20%)	34,90,114	1.98	9 (26%)
30	CHL	n	306	3	60,74,74	1.35	9 (15%)	58,114,114	1.65	13 (22%)
32	LUT	7	317	-	42,43,43	6.31	25 (59%)	51,60,60	2.25	17 (33%)
30	CHL	p	606	-	45,59,74	1.49	8 (17%)	40,96,114	1.94	13 (32%)
30	CHL	3	307	3	40,54,74	1.64	9 (22%)	34,90,114	2.03	10 (29%)
48	LMU	c	623	-	29,29,36	0.44	0	40,40,47	1.13	3 (7%)
31	CLA	D	403	-	69,73,73	1.39	6 (8%)	82,113,113	1.85	16 (19%)
30	CHL	4	609	2	51,65,74	1.53	9 (17%)	47,103,114	1.81	12 (25%)
30	CHL	q	307	2	40,54,74	1.57	7 (17%)	34,90,114	2.02	10 (29%)
32	LUT	2	615	-	42,43,43	6.23	27 (64%)	51,60,60	3.08	18 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	LHG	1	617	31	34,34,48	0.45	0	37,40,54	1.19	3 (8%)
30	CHL	2	601	2	60,74,74	1.36	9 (15%)	58,114,114	1.67	13 (22%)
31	CLA	R	315	18	59,63,73	1.48	7 (11%)	70,101,113	2.05	17 (24%)
34	LMG	k	101	-	48,48,55	1.12	5 (10%)	56,56,63	1.15	4 (7%)
32	LUT	R	317	-	42,43,43	6.35	25 (59%)	51,60,60	3.16	17 (33%)
31	CLA	C	608	-	69,73,73	1.38	6 (8%)	82,113,113	1.81	19 (23%)
31	CLA	c	604	49	60,64,73	1.44	6 (10%)	71,102,113	2.03	20 (28%)
31	CLA	c	608	-	69,73,73	1.38	6 (8%)	82,113,113	1.79	19 (23%)
46	BCT	D	402	40	3,3,3	3.12	1 (33%)	2,3,3	2.76	2 (100%)
31	CLA	b	613	-	69,73,73	1.35	7 (10%)	82,113,113	1.95	21 (25%)
31	CLA	C	605	-	69,73,73	1.46	7 (10%)	82,113,113	1.90	17 (20%)
30	CHL	G	605	2	42,56,74	1.61	9 (21%)	36,92,114	2.01	11 (30%)
32	LUT	S	318	-	42,43,43	6.42	26 (61%)	51,60,60	2.14	13 (25%)
31	CLA	1	611	33	69,73,73	1.34	7 (10%)	82,113,113	1.86	20 (24%)
34	LMG	3	321	-	38,38,55	0.68	1 (2%)	46,46,63	0.97	2 (4%)
31	CLA	3	301	1	58,62,73	1.51	6 (10%)	68,99,113	2.12	20 (29%)
30	CHL	n	302	3	50,64,74	1.46	8 (16%)	46,102,114	1.85	12 (26%)
31	CLA	b	606	-	69,73,73	1.37	6 (8%)	82,113,113	1.91	18 (21%)
30	CHL	y	606	49	53,67,74	1.44	8 (15%)	49,105,114	1.78	12 (24%)
42	PHO	d	402	-	58,69,69	0.80	4 (6%)	55,99,99	0.92	3 (5%)
33	LHG	S	322	-	43,43,48	0.41	0	46,49,54	1.10	3 (6%)
30	CHL	0	608	49	44,58,74	1.71	8 (18%)	37,94,114	1.98	10 (27%)
32	LUT	3	317	-	42,43,43	6.40	26 (61%)	51,60,60	2.00	15 (29%)
31	CLA	r	305	-	64,68,73	1.39	6 (9%)	76,107,113	1.96	19 (25%)
31	CLA	r	303	18	53,57,73	1.60	6 (11%)	61,93,113	2.31	18 (29%)
33	LHG	z	102	-	35,35,48	0.43	0	38,41,54	1.22	3 (7%)
31	CLA	Y	311	33	69,73,73	1.37	6 (8%)	82,113,113	1.85	15 (18%)
38	SQD	6	301	-	40,42,54	0.86	1 (2%)	50,53,65	0.92	2 (4%)
34	LMG	A	414	-	38,38,55	0.69	1 (2%)	46,46,63	1.16	4 (8%)
30	CHL	1	601	1	60,74,74	1.93	8 (13%)	58,114,114	1.62	10 (17%)
38	SQD	a	412	-	43,45,54	0.90	1 (2%)	53,56,65	0.95	3 (5%)
48	LMU	K	101	-	36,36,36	0.42	0	47,47,47	1.11	4 (8%)
31	CLA	b	608	49	69,73,73	1.37	7 (10%)	82,113,113	1.95	15 (18%)
36	NEX	g	317	31	40,46,46	2.72	12 (30%)	50,70,70	1.51	7 (14%)
31	CLA	c	603	-	69,73,73	1.38	7 (10%)	82,113,113	1.96	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	BCR	D	405	-	41,41,41	4.98	27 (65%)	56,56,56	2.70	22 (39%)
31	CLA	0	604	49	59,63,73	1.46	6 (10%)	70,101,113	2.05	15 (21%)
33	LHG	s	322	-	43,43,48	0.40	0	46,49,54	1.16	3 (6%)
38	SQD	G	617	-	40,42,54	0.85	1 (2%)	50,53,65	0.90	2 (4%)
34	LMG	D	409	-	46,46,55	1.06	4 (8%)	54,54,63	1.15	4 (7%)
31	CLA	S	315	-	52,56,73	1.57	6 (11%)	61,92,113	2.04	16 (26%)
31	CLA	s	303	19	69,73,73	1.35	7 (10%)	82,113,113	1.92	21 (25%)
31	CLA	N	304	-	59,63,73	1.45	6 (10%)	70,101,113	2.04	19 (27%)
36	NEX	S	319	-	40,46,46	2.76	12 (30%)	50,70,70	1.52	8 (16%)
31	CLA	7	314	1	69,73,73	1.37	7 (10%)	82,113,113	1.86	18 (21%)
34	LMG	p	620	-	38,38,55	0.67	1 (2%)	46,46,63	1.11	3 (6%)
31	CLA	3	313	3	54,58,73	1.53	5 (9%)	64,95,113	2.10	20 (31%)
31	CLA	4	613	2	65,69,73	1.39	7 (10%)	77,108,113	1.92	20 (25%)
45	DGD	c	617	-	63,63,67	1.25	7 (11%)	77,77,81	1.28	8 (10%)
32	LUT	8	615	-	42,43,43	6.40	25 (59%)	51,60,60	1.97	17 (33%)
33	LHG	G	618	31	43,43,48	0.40	0	46,49,54	1.11	3 (6%)
31	CLA	S	312	33	69,73,73	1.35	6 (8%)	82,113,113	1.89	16 (19%)
37	XAT	R	318	-	41,47,47	0.63	0	54,74,74	1.94	11 (20%)
34	LMG	w	203	-	38,38,55	0.66	1 (2%)	46,46,63	1.48	8 (17%)
46	BCT	d	403	40	3,3,3	1.30	0	2,3,3	4.34	2 (100%)
30	CHL	3	303	3	44,58,74	1.62	8 (18%)	37,94,114	1.97	11 (29%)
31	CLA	S	313	19	60,64,73	1.49	6 (10%)	71,102,113	2.07	20 (28%)
31	CLA	6	312	33	64,68,73	1.42	7 (10%)	76,107,113	1.94	16 (21%)
30	CHL	5	608	-	44,58,74	1.55	7 (15%)	37,94,114	1.95	11 (29%)
34	LMG	B	625	-	38,38,55	0.67	1 (2%)	46,46,63	1.10	4 (8%)
31	CLA	b	611	49	69,73,73	1.35	6 (8%)	82,113,113	1.88	18 (21%)
43	BCR	A	410	-	41,41,41	4.86	25 (60%)	56,56,56	2.59	21 (37%)
31	CLA	R	306	49	52,56,73	1.58	7 (13%)	61,92,113	2.31	17 (27%)
31	CLA	B	613	-	69,73,73	1.35	6 (8%)	82,113,113	1.82	18 (21%)
31	CLA	B	605	-	69,73,73	1.37	6 (8%)	82,113,113	1.91	15 (18%)
31	CLA	B	611	-	69,73,73	1.37	6 (8%)	82,113,113	1.88	18 (21%)
34	LMG	q1	101	-	38,38,55	0.69	1 (2%)	46,46,63	1.11	2 (4%)
31	CLA	9	304	2	69,73,73	1.35	6 (8%)	82,113,113	1.94	21 (25%)
34	LMG	S	321	-	41,41,55	0.92	2 (4%)	49,49,63	1.24	4 (8%)
30	CHL	3	310	3	55,69,74	1.56	7 (12%)	52,108,114	1.77	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CHL	g	309	2	57,71,74	1.57	8 (14%)	54,110,114	1.72	12 (22%)
38	SQD	X	201	-	36,38,54	0.90	0	46,49,65	0.94	2 (4%)
38	SQD	y	621	-	40,42,54	0.86	0	50,53,65	0.92	2 (4%)
33	LHG	l	101	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
34	LMG	2	621	-	40,40,55	0.74	2 (5%)	48,48,63	1.17	4 (8%)
34	LMG	0	620	-	42,42,55	0.89	3 (7%)	50,50,63	1.18	4 (8%)
32	LUT	N	316	-	42,43,43	6.40	26 (61%)	51,60,60	2.11	13 (25%)
43	BCR	t	101	-	41,41,41	4.85	27 (65%)	56,56,56	4.03	27 (48%)
34	LMG	9	301	-	51,51,55	1.23	6 (11%)	59,59,63	1.69	10 (16%)
30	CHL	R	309	18	50,64,74	1.39	8 (16%)	46,102,114	1.85	10 (21%)
31	CLA	Y	314	-	58,62,73	1.47	6 (10%)	68,99,113	2.05	20 (29%)
32	LUT	7	318	-	42,43,43	6.39	25 (59%)	51,60,60	2.00	16 (31%)
30	CHL	0	606	49	45,59,74	1.57	9 (20%)	40,96,114	2.05	13 (32%)
34	LMG	c	620	-	38,38,55	0.67	1 (2%)	46,46,63	1.19	5 (10%)
45	DGD	C	618	-	67,67,67	1.28	7 (10%)	81,81,81	0.94	3 (3%)
45	DGD	c	618	-	67,67,67	1.29	7 (10%)	81,81,81	1.03	3 (3%)
31	CLA	p	612	3	50,54,73	1.59	6 (12%)	59,90,113	2.06	18 (30%)
31	CLA	7	313	1	69,73,73	1.36	6 (8%)	82,113,113	1.87	20 (24%)
38	SQD	s	301	-	49,51,54	0.78	1 (2%)	59,62,65	0.87	2 (3%)
30	CHL	6	308	49	60,74,74	1.25	8 (13%)	58,114,114	1.60	9 (15%)
35	RRX	2	614	-	42,42,42	5.11	24 (57%)	56,58,58	2.54	17 (30%)
30	CHL	2	605	2	40,54,74	1.53	8 (20%)	34,90,114	2.04	10 (29%)
38	SQD	b	621	-	52,54,54	0.77	0	62,65,65	0.85	2 (3%)
33	LHG	q	320	31	45,45,48	0.44	1 (2%)	48,51,54	1.10	2 (4%)
30	CHL	0	605	4	46,60,74	2.30	9 (19%)	40,97,114	1.99	11 (27%)
38	SQD	0	621	-	40,42,54	0.85	1 (2%)	50,53,65	0.90	2 (4%)
31	CLA	c	609	-	69,73,73	1.38	7 (10%)	82,113,113	1.89	19 (23%)
31	CLA	0	602	4	69,73,73	1.35	6 (8%)	82,113,113	1.89	19 (23%)
30	CHL	1	606	49	60,74,74	1.46	9 (15%)	58,114,114	1.59	12 (20%)
31	CLA	2	603	-	59,63,73	1.45	5 (8%)	70,101,113	2.01	20 (28%)
31	CLA	3	306	49	59,63,73	1.46	6 (10%)	70,101,113	2.04	18 (25%)
36	NEX	8	617	31	40,46,46	2.72	12 (30%)	50,70,70	1.64	10 (20%)
34	LMG	A	418	-	38,38,55	0.67	1 (2%)	46,46,63	1.10	3 (6%)
31	CLA	S	306	-	54,58,73	1.52	6 (11%)	64,95,113	2.14	18 (28%)
31	CLA	Y	310	24	69,73,73	1.35	6 (8%)	82,113,113	1.87	19 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	A	407	49	53,57,73	1.56	6 (11%)	61,93,113	2.15	18 (29%)
30	CHL	G	608	2	57,71,74	1.68	9 (15%)	54,110,114	1.74	13 (24%)
35	RRX	G	614	-	42,42,42	5.12	24 (57%)	56,58,58	2.50	17 (30%)
30	CHL	p	609	3	50,64,74	1.63	10 (20%)	46,102,114	1.81	12 (26%)
30	CHL	9	308	-	46,60,74	1.65	9 (19%)	40,97,114	1.92	11 (27%)
31	CLA	1	602	1	64,68,73	1.42	6 (9%)	76,107,113	1.93	18 (23%)
30	CHL	0	609	4	55,69,74	1.60	10 (18%)	52,108,114	1.73	12 (23%)
33	LHG	n	320	31	48,48,48	0.38	0	51,54,54	1.04	2 (3%)
31	CLA	p	615	3	50,54,73	1.58	7 (14%)	59,90,113	2.04	15 (25%)
30	CHL	8	607	49	44,58,74	1.59	8 (18%)	37,94,114	2.00	11 (29%)
31	CLA	A	406	49	69,73,73	1.36	7 (10%)	82,113,113	1.95	18 (21%)
34	LMG	C	624	-	44,44,55	0.98	3 (6%)	52,52,63	1.07	2 (3%)
34	LMG	c	624	-	44,44,55	0.97	3 (6%)	52,52,63	1.06	3 (5%)
33	LHG	7	319	31	34,34,48	0.45	0	37,40,54	1.13	3 (8%)
45	DGD	C	616	-	51,51,67	0.85	2 (3%)	65,65,81	1.01	2 (3%)
30	CHL	g	306	2	42,56,74	1.69	8 (19%)	36,92,114	1.98	11 (30%)
31	CLA	0	615	-	59,63,73	1.46	6 (10%)	70,101,113	2.03	18 (25%)
31	CLA	n	314	3	69,73,73	1.35	6 (8%)	82,113,113	1.86	20 (24%)
30	CHL	0	601	4	50,64,74	1.50	9 (18%)	46,102,114	1.84	12 (26%)
34	LMG	4	620	-	51,51,55	1.20	6 (11%)	59,59,63	1.08	3 (5%)
30	CHL	p	601	3	45,59,74	1.49	10 (22%)	40,96,114	2.03	11 (27%)
30	CHL	3	309	-	44,58,74	1.68	9 (20%)	37,94,114	2.10	10 (27%)
34	LMG	7	322	-	38,38,55	0.69	1 (2%)	46,46,63	1.08	4 (8%)
34	LMG	q	301	-	51,51,55	1.20	6 (11%)	59,59,63	1.17	6 (10%)
48	LMU	r	302	-	36,36,36	0.38	0	47,47,47	0.80	1 (2%)
31	CLA	n	305	49	69,73,73	1.34	5 (7%)	82,113,113	1.90	19 (23%)
34	LMG	A	412	-	41,41,55	0.83	2 (4%)	49,49,63	1.07	2 (4%)
31	CLA	N	305	49	69,73,73	1.34	5 (7%)	82,113,113	1.92	18 (21%)
36	NEX	R	319	-	40,46,46	2.73	12 (30%)	50,70,70	1.60	8 (16%)
43	BCR	B	617	-	41,41,41	4.83	24 (58%)	56,56,56	2.58	21 (37%)
31	CLA	7	316	1	55,59,73	1.52	6 (10%)	64,96,113	2.11	19 (29%)
33	LHG	6	320	31	36,36,48	0.45	0	39,42,54	1.21	4 (10%)
31	CLA	Y	312	24	69,73,73	1.38	6 (8%)	82,113,113	1.89	18 (21%)
33	LHG	p	619	31	34,34,48	0.45	0	37,40,54	1.20	3 (8%)
34	LMG	g	320	-	38,38,55	0.67	1 (2%)	46,46,63	1.14	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	DGD	c	619	-	67,67,67	1.28	7 (10%)	81,81,81	1.02	3 (3%)
31	CLA	N	313	3	69,73,73	1.35	6 (8%)	82,113,113	1.87	19 (23%)
31	CLA	S	304	-	46,50,73	1.70	6 (13%)	53,85,113	1.99	17 (32%)
33	LHG	N	319	31	48,48,48	0.38	0	51,54,54	1.03	2 (3%)
32	LUT	5	616	-	42,43,43	6.42	27 (64%)	51,60,60	2.00	13 (25%)
30	CHL	4	605	2	40,54,74	1.58	7 (17%)	34,90,114	2.02	10 (29%)
34	LMG	6	321	-	42,42,55	0.86	2 (4%)	50,50,63	1.26	5 (10%)
30	CHL	9	307	2	40,54,74	1.73	8 (20%)	34,90,114	2.05	9 (26%)
31	CLA	s	304	-	46,50,73	1.63	5 (10%)	53,85,113	2.16	17 (32%)
32	LUT	y	616	-	42,43,43	6.30	25 (59%)	51,60,60	2.20	21 (41%)
43	BCR	v	101	-	41,41,41	4.89	25 (60%)	56,56,56	2.28	19 (33%)
31	CLA	5	612	3	54,58,73	1.54	7 (12%)	64,95,113	2.10	20 (31%)
31	CLA	n	315	-	53,57,73	1.54	6 (11%)	61,93,113	2.16	18 (29%)
33	LHG	B	624	-	48,48,48	0.37	0	51,54,54	0.99	2 (3%)
33	LHG	K	102	-	35,35,48	0.46	0	38,41,54	1.22	3 (7%)
30	CHL	q	308	-	45,59,74	1.71	7 (15%)	40,96,114	1.99	11 (27%)
31	CLA	b	615	-	69,73,73	1.35	7 (10%)	82,113,113	1.92	18 (21%)
33	LHG	0	619	31	35,35,48	0.45	0	38,41,54	1.21	4 (10%)
31	CLA	g	313	2	69,73,73	1.35	6 (8%)	82,113,113	1.86	19 (23%)
44	PL9	A	416	-	55,55,55	1.16	7 (12%)	68,69,69	1.57	13 (19%)
36	NEX	4	617	-	40,46,46	2.73	12 (30%)	50,70,70	1.54	7 (14%)
31	CLA	b	603	-	69,73,73	1.36	7 (10%)	82,113,113	1.99	17 (20%)
31	CLA	n	312	33	53,57,73	1.53	7 (13%)	61,93,113	2.13	18 (29%)
32	LUT	6	317	-	42,43,43	6.36	25 (59%)	51,60,60	2.09	16 (31%)
31	CLA	6	313	4	64,68,73	1.40	7 (10%)	76,107,113	1.94	21 (27%)
36	NEX	r	301	-	40,46,46	2.71	10 (25%)	50,70,70	1.57	10 (20%)
31	CLA	6	315	-	58,62,73	1.46	5 (8%)	68,99,113	2.07	20 (29%)
44	PL9	a	414	-	55,55,55	1.20	5 (9%)	68,69,69	1.49	14 (20%)
30	CHL	5	609	3	50,64,74	1.70	9 (18%)	46,102,114	1.85	12 (26%)
38	SQD	B	623	-	50,52,54	0.80	0	60,63,65	0.88	2 (3%)
30	CHL	n	301	49	44,58,74	1.69	8 (18%)	37,94,114	1.97	11 (29%)
32	LUT	Y	315	-	42,43,43	6.30	25 (59%)	51,60,60	2.15	17 (33%)
33	LHG	D	408	-	48,48,48	0.39	0	51,54,54	1.09	4 (7%)
43	BCR	b	620	-	41,41,41	4.89	26 (63%)	56,56,56	2.37	21 (37%)
34	LMG	j	101	-	43,43,55	0.91	2 (4%)	51,51,63	1.05	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	LMU	R	302	-	36,36,36	0.44	0	47,47,47	0.96	2 (4%)
33	LHG	4	618	31	46,46,48	0.40	0	49,52,54	1.07	4 (8%)
43	BCR	a	410	-	41,41,41	4.87	25 (60%)	56,56,56	2.58	20 (35%)
31	CLA	N	311	33	53,57,73	1.53	6 (11%)	61,93,113	2.17	18 (29%)
34	LMG	7	320	-	38,38,55	0.67	1 (2%)	46,46,63	1.17	3 (6%)
31	CLA	b	609	-	69,73,73	1.38	6 (8%)	82,113,113	1.87	15 (18%)
30	CHL	N	301	-	44,58,74	1.67	8 (18%)	37,94,114	1.96	10 (27%)
30	CHL	7	310	1	60,74,74	1.38	10 (16%)	58,114,114	1.62	12 (20%)
35	RRX	q	317	-	42,42,42	5.06	24 (57%)	56,58,58	2.61	18 (32%)
31	CLA	q	313	33	46,51,73	1.54	5 (10%)	57,86,113	2.21	16 (28%)
34	LMG	a	413	-	38,38,55	0.69	1 (2%)	46,46,63	1.50	6 (13%)
39	OEX	A	401	7,5	0,15,15	-	-	-		
39	OEX	a	402	7,5	0,15,15	-	-	-		
30	CHL	n	309	49	44,58,74	1.61	8 (18%)	37,94,114	2.00	11 (29%)
43	BCR	h	101	-	41,41,41	4.86	25 (60%)	56,56,56	2.44	20 (35%)
31	CLA	r	313	33	53,57,73	1.56	7 (13%)	61,93,113	2.13	16 (26%)
31	CLA	d	404	-	69,73,73	1.37	6 (8%)	82,113,113	1.84	16 (19%)
30	CHL	n	308	49	57,71,74	1.40	8 (14%)	54,110,114	1.73	12 (22%)
38	SQD	r	322	-	49,51,54	0.79	1 (2%)	59,62,65	0.86	2 (3%)
42	PHO	a	408	-	58,69,69	0.79	2 (3%)	55,99,99	0.90	2 (3%)
30	CHL	S	307	19	38,52,74	1.74	9 (23%)	31,87,114	2.06	10 (32%)
33	LHG	s	320	31	40,40,48	0.44	0	43,46,54	1.13	4 (9%)
34	LMG	X	203	-	38,38,55	0.66	1 (2%)	46,46,63	1.13	3 (6%)
34	LMG	m	102	-	45,45,55	1.02	3 (6%)	53,53,63	1.26	5 (9%)
30	CHL	2	608	2	51,65,74	1.69	10 (19%)	47,103,114	1.83	12 (25%)
30	CHL	s	307	19	38,52,74	1.72	9 (23%)	31,87,114	2.08	10 (32%)
34	LMG	R	321	-	38,38,55	0.68	1 (2%)	46,46,63	1.13	2 (4%)
31	CLA	r	304	18	64,68,73	1.40	6 (9%)	76,107,113	1.95	21 (27%)
44	PL9	d	407	-	55,55,55	0.75	1 (1%)	68,69,69	0.59	2 (2%)
31	CLA	8	610	33	53,57,73	1.53	6 (11%)	61,93,113	2.13	18 (29%)
32	LUT	S	317	-	42,43,43	6.39	25 (59%)	51,60,60	2.07	16 (31%)
31	CLA	7	305	49	69,73,73	1.35	6 (8%)	82,113,113	1.95	18 (21%)
30	CHL	y	608	49	44,58,74	1.65	8 (18%)	37,94,114	1.97	11 (29%)
36	NEX	Y	317	-	40,46,46	2.72	12 (30%)	50,70,70	1.69	11 (22%)
31	CLA	c	607	49	69,73,73	1.39	6 (8%)	82,113,113	1.89	19 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	BCR	B	619	-	41,41,41	4.88	26 (63%)	56,56,56	2.49	19 (33%)
31	CLA	p	613	-	58,62,73	1.47	6 (10%)	68,99,113	2.04	14 (20%)
31	CLA	p	611	33	64,68,73	1.41	7 (10%)	76,107,113	1.93	17 (22%)
30	CHL	n	307	49	52,66,74	1.49	8 (15%)	48,104,114	1.83	13 (27%)
31	CLA	5	613	3	58,62,73	1.47	6 (10%)	68,99,113	2.02	19 (27%)
34	LMG	g	322	-	49,49,55	1.16	5 (10%)	57,57,63	1.23	3 (5%)
31	CLA	r	306	49	52,56,73	1.57	7 (13%)	61,92,113	2.13	17 (27%)
31	CLA	S	305	49	69,73,73	1.34	5 (7%)	82,113,113	1.89	18 (21%)
33	LHG	c	622	-	46,46,48	0.40	0	49,52,54	1.03	2 (4%)
34	LMG	B	621	-	51,51,55	1.22	6 (11%)	59,59,63	1.30	4 (6%)
31	CLA	7	304	-	59,63,73	1.46	6 (10%)	70,101,113	2.04	20 (28%)
37	XAT	9	322	-	41,47,47	0.63	0	54,74,74	1.92	12 (22%)
31	CLA	n	303	3	69,73,73	1.34	7 (10%)	82,113,113	1.89	21 (25%)
30	CHL	7	302	1	60,74,74	1.38	9 (15%)	58,114,114	1.64	12 (20%)
43	BCR	H	101	-	41,41,41	4.88	27 (65%)	56,56,56	2.41	20 (35%)
33	LHG	j	102	-	48,48,48	0.39	0	51,54,54	1.10	3 (5%)
31	CLA	3	315	-	58,62,73	1.47	7 (12%)	68,99,113	2.05	20 (29%)
31	CLA	2	610	33	64,68,73	1.39	5 (7%)	76,107,113	1.97	17 (22%)
31	CLA	Y	304	-	59,63,73	1.46	6 (10%)	70,101,113	2.02	20 (28%)
31	CLA	R	313	33	53,57,73	1.56	7 (13%)	61,93,113	2.11	18 (29%)
31	CLA	y	603	-	59,63,73	1.46	6 (10%)	70,101,113	2.02	19 (27%)
31	CLA	R	311	18	62,66,73	1.45	6 (9%)	73,104,113	1.95	17 (23%)
31	CLA	3	314	3	59,63,73	1.46	6 (10%)	70,101,113	2.02	20 (28%)
31	CLA	9	313	33	51,55,73	1.58	7 (13%)	60,91,113	2.07	16 (26%)
36	NEX	r	319	-	40,46,46	2.74	12 (30%)	50,70,70	1.60	7 (14%)
31	CLA	C	604	49	60,64,73	1.47	6 (10%)	71,102,113	2.02	16 (22%)
30	CHL	r	309	18	50,64,74	1.30	8 (16%)	46,102,114	1.88	10 (21%)
47	HEM	e	102	10,9	50,50,50	1.58	8 (16%)	67,82,82	1.62	9 (13%)
32	LUT	N	317	-	42,43,43	6.39	26 (61%)	51,60,60	2.17	15 (29%)
30	CHL	S	308	49	37,51,74	1.86	9 (24%)	30,86,114	2.30	11 (36%)
31	CLA	B	615	-	69,73,73	1.36	7 (10%)	82,113,113	1.96	17 (20%)
34	LMG	w	202	-	55,55,55	1.28	6 (10%)	63,63,63	1.15	4 (6%)
43	BCR	T	101	-	41,41,41	4.91	27 (65%)	56,56,56	2.35	20 (35%)
30	CHL	6	309	49	44,58,74	1.75	8 (18%)	37,94,114	1.96	11 (29%)
31	CLA	B	610	49	69,73,73	1.35	6 (8%)	82,113,113	1.92	21 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CHL	6	310	4	55,69,74	1.46	9 (16%)	52,108,114	1.73	13 (25%)
31	CLA	0	611	33	64,68,73	1.41	7 (10%)	76,107,113	1.89	15 (19%)
31	CLA	N	321	24	58,62,73	1.47	7 (12%)	68,99,113	2.04	18 (26%)
34	LMG	C	621	-	38,38,55	0.67	1 (2%)	46,46,63	1.13	3 (6%)
34	LMG	c	621	-	38,38,55	0.68	1 (2%)	46,46,63	1.13	5 (10%)
30	CHL	p	605	3	40,54,74	1.57	7 (17%)	34,90,114	2.06	9 (26%)
30	CHL	6	302	4	50,64,74	1.45	8 (16%)	46,102,114	1.88	12 (26%)
31	CLA	2	604	36,49	58,62,73	1.48	6 (10%)	68,99,113	2.09	20 (29%)
30	CHL	2	606	-	45,59,74	1.43	7 (15%)	40,96,114	1.94	11 (27%)
31	CLA	s	305	49	69,73,73	1.35	6 (8%)	82,113,113	1.93	18 (21%)
31	CLA	R	304	18	64,68,73	1.42	6 (9%)	76,107,113	1.91	16 (21%)
31	CLA	8	612	3	69,73,73	1.35	6 (8%)	82,113,113	1.86	20 (24%)
34	LMG	w	201	-	48,48,55	1.13	5 (10%)	56,56,63	1.09	3 (5%)
45	DGD	C	620	-	67,67,67	1.30	7 (10%)	81,81,81	1.02	4 (4%)
31	CLA	b	605	-	69,73,73	1.40	7 (10%)	82,113,113	1.93	16 (19%)
31	CLA	g	305	36,49	59,63,73	1.46	6 (10%)	70,101,113	2.04	17 (24%)
30	CHL	R	308	18	50,64,74	1.58	8 (16%)	46,102,114	1.81	12 (26%)
31	CLA	D	404	-	69,73,73	1.36	7 (10%)	82,113,113	1.98	22 (26%)
31	CLA	R	316	18	69,73,73	1.36	7 (10%)	82,113,113	1.95	19 (23%)
31	CLA	8	604	36,49	69,73,73	1.34	5 (7%)	82,113,113	1.92	19 (23%)
30	CHL	y	607	49	60,74,74	1.34	8 (13%)	58,114,114	1.68	12 (20%)
30	CHL	8	606	49	52,66,74	1.49	8 (15%)	48,104,114	1.84	13 (27%)
38	SQD	x	201	-	40,42,54	0.87	1 (2%)	50,53,65	0.92	3 (6%)
44	PL9	D	406	-	55,55,55	0.69	1 (1%)	68,69,69	0.62	1 (1%)
30	CHL	6	307	49	45,59,74	1.34	7 (15%)	40,96,114	1.93	10 (25%)
32	LUT	y	617	-	42,43,43	6.32	25 (59%)	51,60,60	2.16	18 (35%)
38	SQD	A	413	-	43,45,54	0.83	1 (2%)	53,56,65	0.90	2 (3%)
43	BCR	B	618	-	41,41,41	4.91	25 (60%)	56,56,56	2.23	19 (33%)
31	CLA	1	610	1	69,73,73	1.35	6 (8%)	82,113,113	1.90	19 (23%)
31	CLA	d	405	-	69,73,73	1.36	7 (10%)	82,113,113	1.99	21 (25%)
31	CLA	8	602	3	69,73,73	1.35	6 (8%)	82,113,113	1.88	21 (25%)
31	CLA	y	604	49	59,63,73	1.47	6 (10%)	70,101,113	2.07	19 (27%)
31	CLA	y	612	24	69,73,73	1.37	6 (8%)	82,113,113	1.90	17 (20%)
31	CLA	B	607	49	69,73,73	1.43	7 (10%)	82,113,113	2.06	20 (24%)
30	CHL	Y	307	49	53,67,74	1.64	8 (15%)	49,105,114	1.74	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CHL	8	608	3	60,74,74	1.40	8 (13%)	58,114,114	1.68	11 (18%)
31	CLA	5	610	3	64,68,73	1.39	6 (9%)	76,107,113	1.99	19 (25%)
30	CHL	4	601	2	60,74,74	1.38	9 (15%)	58,114,114	1.68	13 (22%)
31	CLA	B	616	-	69,73,73	1.38	6 (8%)	82,113,113	1.91	14 (17%)
32	LUT	p	617	-	42,43,43	6.38	26 (61%)	51,60,60	2.93	17 (33%)
31	CLA	B	612	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	19 (23%)
30	CHL	3	308	-	41,55,74	1.60	10 (24%)	35,91,114	2.07	10 (28%)
34	LMG	6	322	-	39,39,55	0.65	1 (2%)	47,47,63	1.19	4 (8%)
32	LUT	6	318	-	42,43,43	6.38	26 (61%)	51,60,60	2.06	14 (27%)
30	CHL	N	308	49	44,58,74	1.76	8 (18%)	37,94,114	1.99	12 (32%)
34	LMG	w	205	-	38,38,55	0.67	1 (2%)	46,46,63	1.14	2 (4%)
31	CLA	B	602	-	69,73,73	1.37	7 (10%)	82,113,113	1.98	20 (24%)
35	RRX	4	615	-	42,42,42	5.13	24 (57%)	56,58,58	2.50	17 (30%)
34	LMG	a	401	-	38,38,55	0.67	1 (2%)	46,46,63	1.05	3 (6%)
43	BCR	C	614	-	41,41,41	4.84	26 (63%)	56,56,56	2.65	21 (37%)
43	BCR	c	614	-	41,41,41	4.90	26 (63%)	56,56,56	3.00	26 (46%)
31	CLA	y	615	24	58,62,73	1.47	7 (12%)	68,99,113	2.14	20 (29%)
31	CLA	Y	305	49	59,63,73	1.46	6 (10%)	70,101,113	2.03	18 (25%)
34	LMG	9	321	-	38,38,55	0.70	1 (2%)	46,46,63	1.16	4 (8%)
30	CHL	q	303	2	60,74,74	1.27	8 (13%)	58,114,114	1.66	11 (18%)
36	NEX	N	318	-	40,46,46	2.71	12 (30%)	50,70,70	1.73	13 (26%)
30	CHL	g	308	49	45,59,74	1.53	8 (17%)	40,96,114	1.97	12 (30%)
34	LMG	7	301	-	39,39,55	0.67	1 (2%)	47,47,63	1.01	2 (4%)
34	LMG	I	101	-	38,38,55	0.66	1 (2%)	46,46,63	1.11	2 (4%)
34	LMG	b	626	-	46,46,55	1.03	3 (6%)	54,54,63	1.12	4 (7%)
31	CLA	2	612	2	69,73,73	1.34	7 (10%)	82,113,113	1.88	19 (23%)
30	CHL	s	302	19	40,54,74	1.60	9 (22%)	34,90,114	2.13	10 (29%)
31	CLA	0	612	4	50,54,73	1.61	6 (12%)	59,90,113	2.02	16 (27%)
30	CHL	R	310	49	49,63,74	1.77	9 (18%)	44,100,114	1.94	10 (22%)
31	CLA	Y	303	24	64,68,73	1.40	6 (9%)	76,107,113	2.00	20 (26%)
30	CHL	1	607	-	60,74,74	1.26	7 (11%)	58,114,114	1.65	12 (20%)
31	CLA	8	614	3	58,62,73	1.47	6 (10%)	68,99,113	2.00	19 (27%)
30	CHL	p	607	-	45,59,74	1.83	8 (17%)	40,96,114	1.84	10 (25%)
42	PHO	A	408	-	58,69,69	2.03	10 (17%)	55,99,99	1.44	6 (10%)
31	CLA	g	314	-	53,57,73	1.54	6 (11%)	61,93,113	2.17	19 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	s	314	19	69,73,73	1.38	7 (10%)	82,113,113	1.90	18 (21%)
31	CLA	B	603	-	69,73,73	1.39	6 (8%)	82,113,113	1.84	16 (19%)
32	LUT	s	317	-	42,43,43	6.38	25 (59%)	51,60,60	2.04	19 (37%)
37	XAT	G	620	-	41,47,47	0.63	1 (2%)	54,74,74	1.92	12 (22%)
31	CLA	N	315	3	58,62,73	1.47	6 (10%)	68,99,113	2.05	19 (27%)
31	CLA	9	306	36,49	69,73,73	1.35	6 (8%)	82,113,113	1.95	18 (21%)
33	LHG	A	417	-	38,38,48	0.45	0	41,44,54	1.11	3 (7%)
43	BCR	d	406	-	41,41,41	4.84	25 (60%)	56,56,56	3.63	25 (44%)
31	CLA	S	316	19	50,54,73	1.58	6 (12%)	59,90,113	2.06	15 (25%)
30	CHL	y	609	24	60,74,74	1.38	9 (15%)	58,114,114	1.61	10 (17%)
32	LUT	n	317	-	42,43,43	6.40	25 (59%)	51,60,60	1.97	17 (33%)
30	CHL	9	303	2	60,74,74	1.25	10 (16%)	58,114,114	1.69	12 (20%)
34	LMG	X	202	-	38,38,55	0.67	1 (2%)	46,46,63	1.07	2 (4%)
36	NEX	3	319	-	40,46,46	2.75	11 (27%)	50,70,70	1.64	10 (20%)
43	BCR	V	101	-	41,41,41	4.85	25 (60%)	56,56,56	2.43	21 (37%)
31	CLA	3	312	33	69,73,73	1.35	7 (10%)	82,113,113	1.85	17 (20%)
31	CLA	y	614	-	58,62,73	1.46	6 (10%)	68,99,113	2.04	20 (29%)
31	CLA	b	616	-	69,73,73	1.35	7 (10%)	82,113,113	1.92	16 (19%)
34	LMG	d	411	-	48,48,55	1.12	5 (10%)	56,56,63	1.17	3 (5%)
31	CLA	q	314	2	50,54,73	1.60	6 (12%)	59,90,113	2.08	14 (23%)
33	LHG	F1	301	-	34,34,48	0.44	0	37,40,54	1.10	3 (8%)
30	CHL	N	309	3	60,74,74	1.48	7 (11%)	58,114,114	1.66	12 (20%)
31	CLA	4	612	2	50,54,73	1.59	6 (12%)	59,90,113	2.17	16 (27%)
31	CLA	g	304	-	59,63,73	1.45	6 (10%)	70,101,113	2.04	19 (27%)
30	CHL	2	607	49	44,58,74	1.59	9 (20%)	37,94,114	2.02	11 (29%)
30	CHL	0	607	49	60,74,74	1.23	8 (13%)	58,114,114	1.67	11 (18%)
34	LMG	d	410	-	51,51,55	1.22	6 (11%)	59,59,63	1.09	3 (5%)
31	CLA	g	310	2	69,73,73	1.37	7 (10%)	82,113,113	1.87	21 (25%)
31	CLA	s	312	33	69,73,73	1.35	7 (10%)	82,113,113	1.89	14 (17%)
31	CLA	9	315	2	59,63,73	1.46	6 (10%)	70,101,113	1.98	18 (25%)
30	CHL	4	606	31	45,59,74	1.48	7 (15%)	40,96,114	2.00	13 (32%)
31	CLA	5	604	-	54,58,73	1.52	6 (11%)	64,95,113	2.09	19 (29%)
31	CLA	0	610	4	69,73,73	1.41	6 (8%)	82,113,113	1.90	21 (25%)
36	NEX	n	319	-	40,46,46	2.67	11 (27%)	50,70,70	1.74	14 (28%)
31	CLA	G	610	33	64,68,73	1.42	7 (10%)	76,107,113	1.90	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	LMG	d	409	-	41,41,55	0.79	2 (4%)	49,49,63	1.10	3 (6%)
31	CLA	4	602	2	69,73,73	1.35	7 (10%)	82,113,113	1.93	21 (25%)
31	CLA	C	612	-	59,63,73	1.48	7 (11%)	70,101,113	2.09	16 (22%)
31	CLA	s	315	-	52,56,73	1.56	6 (11%)	61,92,113	2.04	14 (22%)
31	CLA	r	315	18	59,63,73	1.46	7 (11%)	70,101,113	2.09	20 (28%)
31	CLA	N	310	3	69,73,73	1.35	7 (10%)	82,113,113	1.91	20 (24%)
31	CLA	p	610	3	60,64,73	1.45	7 (11%)	71,102,113	1.99	20 (28%)
34	LMG	G	621	-	51,51,55	1.21	6 (11%)	59,59,63	1.09	3 (5%)
34	LMG	x	202	-	38,38,55	0.66	1 (2%)	46,46,63	1.15	4 (8%)
31	CLA	r	311	18	62,66,73	1.43	6 (9%)	73,104,113	1.99	17 (23%)
31	CLA	5	615	3	50,54,73	1.59	6 (12%)	59,90,113	2.18	16 (27%)
33	LHG	L	101	-	48,48,48	0.40	0	51,54,54	1.03	3 (5%)
31	CLA	q	305	-	59,63,73	1.44	6 (10%)	70,101,113	2.04	19 (27%)
34	LMG	2	618	-	38,38,55	0.67	1 (2%)	46,46,63	1.12	4 (8%)
31	CLA	q	316	-	54,58,73	1.54	7 (12%)	64,95,113	2.10	17 (26%)
30	CHL	s	308	49	37,51,74	1.53	8 (21%)	30,86,114	2.18	9 (30%)
32	LUT	q	318	-	42,43,43	6.39	26 (61%)	51,60,60	2.20	13 (25%)
31	CLA	q	315	2	69,73,73	1.38	6 (8%)	82,113,113	1.90	18 (21%)
33	LHG	y	619	31	45,45,48	0.44	0	48,51,54	1.06	3 (6%)
31	CLA	C	607	49	69,73,73	1.37	7 (10%)	82,113,113	1.96	21 (25%)
31	CLA	s	310	19	64,68,73	1.41	7 (10%)	76,107,113	1.97	16 (21%)
36	NEX	q	319	-	40,46,46	2.75	12 (30%)	50,70,70	1.52	9 (18%)
32	LUT	8	616	-	42,43,43	6.39	25 (59%)	51,60,60	2.05	16 (31%)
31	CLA	0	613	4	60,64,73	1.46	7 (11%)	71,102,113	1.99	19 (26%)
36	NEX	9	319	31	40,46,46	2.77	12 (30%)	50,70,70	1.60	8 (16%)
31	CLA	n	313	3	49,53,73	1.59	6 (12%)	58,89,113	2.06	14 (24%)
38	SQD	B	620	-	52,54,54	0.76	0	62,65,65	0.84	2 (3%)
32	LUT	3	318	-	42,43,43	6.39	27 (64%)	51,60,60	2.10	14 (27%)
34	LMG	b	623	-	38,38,55	0.67	1 (2%)	46,46,63	1.10	2 (4%)
33	LHG	2	617	31	48,48,48	0.39	0	51,54,54	1.10	3 (5%)
31	CLA	s	316	19	50,54,73	1.58	7 (14%)	59,90,113	2.07	17 (28%)
38	SQD	m	101	-	48,50,54	0.81	1 (2%)	58,61,65	0.90	2 (3%)
38	SQD	a	411	-	46,48,54	0.81	0	56,59,65	0.90	2 (3%)
31	CLA	8	611	3	49,53,73	1.59	6 (12%)	58,89,113	2.06	14 (24%)
33	LHG	g	319	31	43,43,48	0.40	0	46,49,54	1.15	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	LUT	1	616	-	42,43,43	6.34	25 (59%)	51,60,60	2.07	18 (35%)
30	CHL	S	302	19	40,54,74	1.64	9 (22%)	34,90,114	2.09	10 (29%)
33	LHG	a	415	-	38,38,48	0.46	0	41,44,54	1.26	3 (7%)
33	LHG	e	101	-	43,43,48	0.41	0	46,49,54	1.20	4 (8%)
37	XAT	g	321	-	41,47,47	0.63	0	54,74,74	1.93	12 (22%)
31	CLA	q	306	49	59,63,73	1.49	6 (10%)	70,101,113	1.99	19 (27%)
33	LHG	9	320	31	32,32,48	0.47	0	35,38,54	1.27	4 (11%)
31	CLA	R	303	18	53,57,73	1.56	7 (13%)	61,93,113	2.30	18 (29%)
31	CLA	n	316	3	58,62,73	1.47	6 (10%)	68,99,113	2.03	21 (30%)
31	CLA	6	311	4	69,73,73	1.34	6 (8%)	82,113,113	1.89	20 (24%)
34	LMG	G	619	-	38,38,55	0.68	1 (2%)	46,46,63	1.12	4 (8%)
30	CHL	5	607	-	45,59,74	1.90	9 (20%)	40,96,114	1.87	10 (25%)
31	CLA	C	610	-	69,73,73	1.38	7 (10%)	82,113,113	1.93	17 (20%)
31	CLA	c	610	-	69,73,73	1.37	7 (10%)	82,113,113	1.97	18 (21%)
31	CLA	r	307	49	52,56,73	1.59	7 (13%)	61,92,113	2.05	16 (26%)
31	CLA	S	311	19	69,73,73	1.37	7 (10%)	82,113,113	1.88	21 (25%)
31	CLA	G	602	2	69,73,73	1.35	7 (10%)	82,113,113	1.87	21 (25%)
36	NEX	5	618	-	40,46,46	2.71	11 (27%)	50,70,70	1.56	6 (12%)
30	CHL	8	601	3	50,64,74	1.46	8 (16%)	46,102,114	1.85	12 (26%)
31	CLA	5	614	-	55,59,73	1.51	6 (10%)	64,96,113	2.17	19 (29%)
36	NEX	6	319	-	40,46,46	2.73	12 (30%)	50,70,70	1.57	9 (18%)
36	NEX	p	618	31	40,46,46	2.72	12 (30%)	50,70,70	1.53	9 (18%)
30	CHL	N	307	49	52,66,74	1.65	8 (15%)	48,104,114	1.80	14 (29%)
33	LHG	t	102	-	40,40,48	0.43	0	43,46,54	1.20	4 (9%)
34	LMG	b	629	-	38,38,55	0.68	1 (2%)	46,46,63	1.13	3 (6%)
32	LUT	n	318	-	42,43,43	6.38	25 (59%)	51,60,60	2.06	16 (31%)
30	CHL	y	605	24	40,54,74	1.75	9 (22%)	34,90,114	2.08	9 (26%)
31	CLA	3	305	-	59,63,73	1.47	6 (10%)	70,101,113	2.00	18 (25%)
31	CLA	p	602	3	64,68,73	1.41	7 (10%)	76,107,113	1.92	19 (25%)
30	CHL	N	302	3	50,64,74	1.47	8 (16%)	46,102,114	1.84	12 (26%)
31	CLA	B	614	-	69,73,73	1.36	7 (10%)	82,113,113	1.86	18 (21%)
34	LMG	1	618	-	38,38,55	0.67	1 (2%)	46,46,63	1.05	3 (6%)
30	CHL	q	310	-	44,58,74	1.97	9 (20%)	37,94,114	2.05	13 (35%)
38	SQD	M	102	-	48,50,54	0.79	0	58,61,65	0.88	2 (3%)
30	CHL	9	310	49	44,58,74	1.45	8 (18%)	37,94,114	2.05	11 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CHL	q	309	-	51,65,74	2.21	8 (15%)	47,103,114	1.96	14 (29%)
36	NEX	s	319	-	40,46,46	2.78	11 (27%)	50,70,70	1.55	8 (16%)
34	LMG	q	302	-	40,40,55	0.76	2 (5%)	48,48,63	1.14	2 (4%)
30	CHL	s	309	49	43,57,74	1.73	9 (20%)	37,93,114	2.07	11 (29%)
31	CLA	0	603	-	60,64,73	1.47	7 (11%)	71,102,113	1.95	17 (23%)
32	LUT	4	616	-	42,43,43	6.38	25 (59%)	51,60,60	2.27	13 (25%)
31	CLA	b	617	-	69,73,73	1.39	6 (8%)	82,113,113	1.88	18 (21%)
30	CHL	5	601	3	45,59,74	1.44	8 (17%)	40,96,114	1.96	10 (25%)
38	SQD	G	624	-	36,38,54	0.93	1 (2%)	46,49,65	0.96	2 (4%)
31	CLA	y	602	24	64,68,73	1.40	7 (10%)	76,107,113	1.96	20 (26%)
32	LUT	s	318	-	42,43,43	6.36	25 (59%)	51,60,60	2.07	18 (35%)
30	CHL	r	308	18	50,64,74	1.68	8 (16%)	46,102,114	1.81	13 (28%)
34	LMG	4	621	-	40,40,55	0.75	2 (5%)	48,48,63	1.06	2 (4%)
38	SQD	b	627	-	50,52,54	0.86	1 (2%)	60,63,65	0.94	2 (3%)
31	CLA	2	613	-	58,62,73	1.48	6 (10%)	68,99,113	2.08	19 (27%)
30	CHL	Y	301	49	57,71,74	1.50	8 (14%)	54,110,114	1.74	12 (22%)
30	CHL	r	310	49	49,63,74	1.67	9 (18%)	44,100,114	1.87	11 (25%)
31	CLA	G	611	2	47,51,73	1.67	6 (12%)	55,86,113	2.08	14 (25%)
31	CLA	c	605	-	69,73,73	1.38	6 (8%)	82,113,113	1.84	15 (18%)
33	LHG	5	619	31	34,34,48	0.47	0	37,40,54	1.16	3 (8%)
34	LMG	n	322	-	40,40,55	0.78	3 (7%)	48,48,63	1.41	5 (10%)
34	LMG	D	411	-	51,51,55	1.22	6 (11%)	59,59,63	1.09	3 (5%)
31	CLA	p	603	-	59,63,73	1.47	7 (11%)	70,101,113	2.09	18 (25%)
43	BCR	z	101	-	41,41,41	4.91	26 (63%)	56,56,56	2.39	21 (37%)
32	LUT	5	617	-	42,43,43	6.41	27 (64%)	51,60,60	1.95	13 (25%)
30	CHL	G	623	49	60,74,74	1.37	8 (13%)	58,114,114	1.71	12 (20%)
35	RRX	9	317	-	42,42,42	5.12	24 (57%)	56,58,58	2.50	17 (30%)
31	CLA	G	612	2	69,73,73	1.37	7 (10%)	82,113,113	1.90	16 (19%)
33	LHG	M	101	-	40,40,48	0.42	0	43,46,54	1.12	3 (6%)
34	LMG	W	202	-	38,38,55	0.69	1 (2%)	46,46,63	1.27	7 (15%)
36	NEX	R	301	-	40,46,46	2.75	12 (30%)	50,70,70	1.50	9 (18%)
34	LMG	C	619	-	51,51,55	1.21	6 (11%)	59,59,63	1.19	5 (8%)
34	LMG	k	102	-	38,38,55	0.66	1 (2%)	46,46,63	1.11	3 (6%)
31	CLA	c	611	7	69,73,73	1.37	7 (10%)	82,113,113	1.95	19 (23%)
31	CLA	8	613	-	53,57,73	1.54	6 (11%)	61,93,113	2.15	18 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CHL	Y	308	49	44,58,74	1.71	10 (22%)	37,94,114	1.98	12 (32%)
31	CLA	b	610	-	69,73,73	1.36	7 (10%)	82,113,113	1.94	18 (21%)
31	CLA	5	611	33	62,66,73	1.42	6 (9%)	73,104,113	1.99	18 (24%)
31	CLA	q	304	2	69,73,73	1.35	8 (11%)	82,113,113	1.91	18 (21%)
34	LMG	W	201	-	55,55,55	1.32	7 (12%)	63,63,63	1.21	4 (6%)
30	CHL	1	619	-	55,69,74	2.41	8 (14%)	52,108,114	1.91	14 (26%)
31	CLA	C	602	-	69,73,73	1.37	6 (8%)	82,113,113	1.91	18 (21%)
31	CLA	c	602	-	69,73,73	1.38	6 (8%)	82,113,113	1.89	16 (19%)
33	LHG	A	415	-	43,43,48	0.41	0	46,49,54	1.17	5 (10%)
31	CLA	y	611	33	69,73,73	1.36	6 (8%)	82,113,113	1.81	16 (19%)
34	LMG	B	622	-	38,38,55	0.69	1 (2%)	46,46,63	1.23	4 (8%)
37	XAT	r	318	-	41,47,47	0.64	0	54,74,74	1.95	12 (22%)
34	LMG	2	620	-	51,51,55	1.20	6 (11%)	59,59,63	1.08	3 (5%)
38	SQD	A	411	-	49,51,54	0.79	1 (2%)	59,62,65	0.90	2 (3%)
30	CHL	7	306	1	60,74,74	1.61	9 (15%)	58,114,114	1.70	13 (22%)
31	CLA	A	409	-	64,68,73	1.42	7 (10%)	76,107,113	2.05	18 (23%)
33	LHG	S	320	31	40,40,48	0.44	0	43,46,54	1.18	4 (9%)
30	CHL	1	608	49	44,58,74	1.74	9 (20%)	37,94,114	1.99	11 (29%)
31	CLA	6	303	4	69,73,73	1.34	6 (8%)	82,113,113	1.90	20 (24%)
31	CLA	G	603	-	59,63,73	1.45	6 (10%)	70,101,113	2.03	18 (25%)
31	CLA	S	314	19	69,73,73	1.37	7 (10%)	82,113,113	1.88	20 (24%)
30	CHL	p	608	-	44,58,74	1.45	8 (18%)	37,94,114	2.02	10 (27%)
30	CHL	G	601	2	60,74,74	1.42	8 (13%)	58,114,114	1.65	12 (20%)
31	CLA	1	603	-	59,63,73	1.48	7 (11%)	70,101,113	1.98	16 (22%)
30	CHL	3	302	49	51,65,74	1.82	10 (19%)	47,103,114	1.92	13 (27%)
31	CLA	2	602	2	69,73,73	1.35	6 (8%)	82,113,113	1.90	19 (23%)
31	CLA	R	312	18	61,65,73	1.46	6 (9%)	72,103,113	2.02	18 (25%)
38	SQD	R	322	-	49,51,54	0.79	0	59,62,65	0.85	2 (3%)
30	CHL	G	607	49	45,59,74	1.62	8 (17%)	40,96,114	1.99	13 (32%)
31	CLA	7	311	1	69,73,73	1.35	7 (10%)	82,113,113	1.86	18 (21%)
31	CLA	B	606	-	69,73,73	1.38	6 (8%)	82,113,113	1.91	18 (21%)
31	CLA	b	602	49	53,57,73	1.54	6 (11%)	61,93,113	2.15	14 (22%)
33	LHG	D	407	-	43,43,48	0.41	0	46,49,54	1.11	3 (6%)
30	CHL	g	302	2	60,74,74	1.32	9 (15%)	58,114,114	1.71	12 (20%)
34	LMG	b	624	-	38,38,55	0.71	1 (2%)	46,46,63	1.35	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	5	603	-	56,60,73	1.49	5 (8%)	65,97,113	2.10	19 (29%)
31	CLA	6	305	49	59,63,73	1.45	6 (10%)	70,101,113	2.07	19 (27%)
31	CLA	y	610	24	69,73,73	1.35	6 (8%)	82,113,113	1.87	18 (21%)
31	CLA	C	611	7	69,73,73	1.38	7 (10%)	82,113,113	1.95	21 (25%)
32	LUT	0	617	-	42,43,43	6.33	25 (59%)	51,60,60	2.08	17 (33%)
34	LMG	C	622	-	32,32,55	0.49	0	40,40,63	1.09	2 (5%)
30	CHL	8	605	3	60,74,74	1.35	9 (15%)	58,114,114	1.65	13 (22%)
34	LMG	w	204	-	38,38,55	0.70	1 (2%)	46,46,63	1.13	4 (8%)
31	CLA	R	307	49	52,56,73	1.58	7 (13%)	61,92,113	2.07	15 (24%)
31	CLA	b	607	-	69,73,73	1.37	6 (8%)	82,113,113	1.93	17 (20%)
31	CLA	1	604	49	69,73,73	1.36	6 (8%)	82,113,113	1.94	17 (20%)
34	LMG	s	321	-	41,41,55	0.94	2 (4%)	49,49,63	1.28	5 (10%)
43	BCR	b	618	-	41,41,41	4.83	25 (60%)	56,56,56	2.58	25 (44%)
34	LMG	W	203	-	38,38,55	0.68	1 (2%)	46,46,63	1.14	2 (4%)
45	DGD	C	617	-	67,67,67	1.29	7 (10%)	81,81,81	0.92	3 (3%)
30	CHL	5	606	49	45,59,74	1.64	7 (15%)	40,96,114	1.94	11 (27%)
30	CHL	N	306	3	60,74,74	1.42	8 (13%)	58,114,114	1.68	12 (20%)
31	CLA	p	614	-	55,59,73	1.51	6 (10%)	64,96,113	2.14	19 (29%)
31	CLA	3	304	3	64,68,73	1.40	6 (9%)	76,107,113	1.97	21 (27%)
34	LMG	9	302	-	40,40,55	0.75	2 (5%)	48,48,63	1.10	4 (8%)
31	CLA	b	612	-	69,73,73	1.35	6 (8%)	82,113,113	1.89	19 (23%)
30	CHL	Y	306	24	40,54,74	1.77	9 (22%)	34,90,114	2.07	11 (32%)
31	CLA	4	610	2	64,68,73	1.44	6 (9%)	76,107,113	1.99	20 (26%)
31	CLA	5	602	3	64,68,73	1.40	7 (10%)	76,107,113	1.95	19 (25%)
32	LUT	Y	316	-	42,43,43	6.32	25 (59%)	51,60,60	2.18	17 (33%)
31	CLA	4	611	33	46,51,73	1.54	5 (10%)	57,86,113	2.12	16 (28%)
30	CHL	7	309	49	44,58,74	1.63	8 (18%)	37,94,114	2.00	11 (29%)
31	CLA	3	316	3	61,65,73	1.47	6 (9%)	72,103,113	2.04	21 (29%)
31	CLA	7	312	33	69,73,73	1.35	6 (8%)	82,113,113	1.91	18 (21%)
34	LMG	J	101	-	51,51,55	1.22	6 (11%)	59,59,63	1.09	3 (5%)
31	CLA	2	609	2	64,68,73	1.40	7 (10%)	76,107,113	1.98	20 (26%)
31	CLA	C	603	-	69,73,73	1.38	7 (10%)	82,113,113	1.95	15 (18%)
31	CLA	2	611	2	59,63,73	1.46	6 (10%)	70,101,113	1.98	18 (25%)
31	CLA	b	614	-	69,73,73	1.34	6 (8%)	82,113,113	1.87	19 (23%)
47	HEM	E	101	10,9	50,50,50	1.59	8 (16%)	67,82,82	1.64	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	LUT	g	316	-	42,43,43	6.42	27 (64%)	51,60,60	2.31	14 (27%)
30	CHL	7	321	49	57,71,74	1.40	8 (14%)	54,110,114	1.73	12 (22%)
43	BCR	C	615	-	41,41,41	4.84	25 (60%)	56,56,56	4.05	31 (55%)
34	LMG	n	321	-	38,38,55	0.71	1 (2%)	46,46,63	1.21	4 (8%)
43	BCR	c	615	-	41,41,41	4.93	25 (60%)	56,56,56	2.78	22 (39%)
31	CLA	G	604	49	59,63,73	1.45	6 (10%)	70,101,113	2.01	18 (25%)
34	LMG	6	323	-	38,38,55	0.68	1 (2%)	46,46,63	1.17	4 (8%)
34	LMG	y	620	-	38,38,55	0.65	1 (2%)	46,46,63	1.15	3 (6%)
31	CLA	C	609	-	69,73,73	1.37	7 (10%)	82,113,113	1.88	15 (18%)
31	CLA	N	314	-	53,57,73	1.54	6 (11%)	61,93,113	2.14	17 (27%)
32	LUT	p	616	-	42,43,43	6.42	26 (61%)	51,60,60	2.89	19 (37%)
38	SQD	Y	320	-	40,42,54	0.86	0	50,53,65	0.92	2 (4%)
31	CLA	0	614	-	58,62,73	1.46	6 (10%)	68,99,113	2.06	20 (29%)
35	RRX	g	315	-	42,42,42	5.14	24 (57%)	56,58,58	2.60	20 (35%)
31	CLA	a	406	-	69,73,73	1.37	6 (8%)	82,113,113	1.92	17 (20%)
36	NEX	G	616	-	40,46,46	2.72	11 (27%)	50,70,70	1.63	10 (20%)
33	LHG	3	320	31	32,32,48	0.46	0	35,38,54	1.31	4 (11%)
36	NEX	y	618	-	40,46,46	2.75	12 (30%)	50,70,70	1.55	11 (22%)
31	CLA	G	609	2	69,73,73	1.37	6 (8%)	82,113,113	1.85	18 (21%)
30	CHL	7	307	49	60,74,74	1.48	8 (13%)	58,114,114	1.68	12 (20%)
31	CLA	1	612	1	69,73,73	1.37	6 (8%)	82,113,113	1.83	18 (21%)
31	CLA	4	603	-	59,63,73	1.46	6 (10%)	70,101,113	2.00	20 (28%)
33	LHG	R	320	31	37,37,48	0.47	0	40,43,54	1.23	3 (7%)
30	CHL	1	605	1	60,74,74	1.44	9 (15%)	58,114,114	1.58	11 (18%)
34	LMG	D	410	-	46,46,55	1.04	3 (6%)	54,54,63	1.08	4 (7%)
37	XAT	q	321	-	41,47,47	0.63	1 (2%)	54,74,74	1.92	12 (22%)
31	CLA	R	305	-	64,68,73	1.42	7 (10%)	76,107,113	1.99	16 (21%)
34	LMG	Q1	101	-	38,38,55	0.69	1 (2%)	46,46,63	1.22	4 (8%)
31	CLA	b	604	-	69,73,73	1.39	6 (8%)	82,113,113	1.85	16 (19%)
38	SQD	g	318	-	40,42,54	0.87	1 (2%)	50,53,65	0.89	2 (4%)
33	LHG	d	408	-	48,48,48	0.39	0	51,54,54	1.10	3 (5%)
30	CHL	4	607	-	51,65,74	1.72	8 (15%)	47,103,114	1.68	8 (17%)
30	CHL	Y	309	24	60,74,74	1.33	9 (15%)	58,114,114	1.62	11 (18%)
34	LMG	r	321	-	38,38,55	0.74	2 (5%)	46,46,63	1.28	4 (8%)
37	XAT	4	619	-	41,47,47	0.63	1 (2%)	54,74,74	1.92	12 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	s	311	19	69,73,73	1.37	7 (10%)	82,113,113	1.89	22 (26%)
30	CHL	y	601	24	60,74,74	1.29	7 (11%)	58,114,114	1.69	11 (18%)
31	CLA	4	614	-	58,62,73	1.48	7 (12%)	68,99,113	2.08	21 (30%)
31	CLA	6	314	4	69,73,73	1.35	6 (8%)	82,113,113	1.91	19 (23%)
31	CLA	9	314	2	54,58,73	1.55	6 (11%)	64,95,113	2.08	17 (26%)
31	CLA	g	311	33	64,68,73	1.43	7 (10%)	76,107,113	1.93	17 (22%)
31	CLA	d	401	49	53,57,73	1.55	6 (11%)	61,93,113	2.18	18 (29%)
31	CLA	N	312	3	49,53,73	1.59	7 (14%)	58,89,113	2.04	17 (29%)
31	CLA	8	609	3	69,73,73	1.35	6 (8%)	82,113,113	1.90	19 (23%)
31	CLA	c	612	-	59,63,73	1.48	7 (11%)	70,101,113	2.09	18 (25%)
31	CLA	S	310	19	64,68,73	1.41	7 (10%)	76,107,113	1.94	17 (22%)
31	CLA	Y	313	24	69,73,73	1.38	7 (10%)	82,113,113	1.89	16 (19%)
31	CLA	s	313	19	60,64,73	1.47	6 (10%)	71,102,113	2.06	19 (26%)
37	XAT	2	619	-	41,47,47	0.63	0	54,74,74	1.92	12 (22%)
31	CLA	a	409	-	64,68,73	1.41	7 (10%)	76,107,113	2.05	17 (22%)
43	BCR	Z	101	-	41,41,41	4.92	26 (63%)	56,56,56	2.40	18 (32%)
34	LMG	N	320	-	38,38,55	0.68	1 (2%)	46,46,63	1.02	2 (4%)
31	CLA	g	312	2	47,51,73	1.63	6 (12%)	55,86,113	2.11	16 (29%)
30	CHL	4	608	-	44,58,74	1.51	8 (18%)	37,94,114	1.97	9 (24%)
45	DGD	c	616	-	67,67,67	1.28	7 (10%)	81,81,81	1.07	2 (2%)
31	CLA	n	304	-	59,63,73	1.45	6 (10%)	70,101,113	2.05	18 (25%)
30	CHL	9	311	2	55,69,74	1.45	9 (16%)	52,108,114	1.72	13 (25%)
31	CLA	r	314	-	53,57,73	1.56	6 (11%)	61,93,113	2.10	17 (27%)
31	CLA	B	604	-	69,73,73	1.40	7 (10%)	82,113,113	2.01	16 (19%)
32	LUT	r	317	-	42,43,43	6.31	25 (59%)	51,60,60	2.24	21 (41%)
32	LUT	G	615	-	42,43,43	6.44	26 (61%)	51,60,60	6.58	18 (35%)
31	CLA	1	614	-	58,62,73	1.46	6 (10%)	68,99,113	2.03	19 (27%)
31	CLA	C	601	-	69,73,73	1.37	7 (10%)	82,113,113	1.89	18 (21%)
31	CLA	c	601	-	69,73,73	1.36	6 (8%)	82,113,113	1.87	20 (24%)

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
34	LMG	b	601	-	-	10/40/60/70	0/1/1/1
31	CLA	s	306	-	1/1/12/20	5/21/97/115	-
31	CLA	S	303	19	1/1/15/20	15/39/115/115	-
33	LHG	Y	318	31	-	28/46/46/53	-
32	LUT	1	615	-	-	0/29/67/67	0/2/2/2
34	LMG	5	620	-	-	14/33/53/70	0/1/1/1
30	CHL	5	605	3	3/3/16/26	5/15/113/137	-
31	CLA	q	312	2	1/1/13/20	9/25/101/115	-
31	CLA	9	312	2	1/1/12/20	11/26/102/115	-
31	CLA	4	604	30	1/1/12/20	10/23/99/115	-
43	BCR	b	619	-	-	15/29/63/63	0/2/2/2
30	CHL	9	309	-	3/3/17/26	9/24/122/137	-
33	LHG	8	618	31	-	33/53/53/53	-
31	CLA	3	311	-	1/1/12/20	6/26/102/115	-
31	CLA	7	315	-	1/1/12/20	14/26/102/115	-
31	CLA	B	609	-	1/1/15/20	19/39/115/115	-
30	CHL	S	309	49	3/3/16/26	1/19/117/137	-
34	LMG	D	412	-	-	7/43/63/70	0/1/1/1
30	CHL	q	311	2	3/3/18/26	5/27/125/137	-
31	CLA	N	303	3	1/1/15/20	18/39/115/115	-
31	CLA	7	303	1	1/1/14/20	10/33/109/115	-
31	CLA	r	312	18	1/1/13/20	11/30/106/115	-
33	LHG	b	628	-	-	30/53/53/53	-
42	PHO	D	401	-	-	10/37/103/103	0/5/6/6
31	CLA	n	311	3	1/1/15/20	10/39/115/115	-
34	LMG	Y	319	-	-	8/33/53/70	0/1/1/1
31	CLA	R	314	-	1/1/11/20	6/20/96/115	-
31	CLA	r	316	18	1/1/15/20	18/39/115/115	-
31	CLA	y	613	24	1/1/15/20	15/39/115/115	-
34	LMG	G	622	-	-	8/35/55/70	0/1/1/1
36	NEX	2	616	31	-	14/27/83/83	0/3/3/3
38	SQD	g	301	-	-	6/33/53/69	0/1/1/1
30	CHL	g	307	49	3/3/16/26	3/20/118/137	-
31	CLA	p	604	36	1/1/12/20	8/21/97/115	-
33	LHG	b	625	-	-	29/48/48/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	8	603	-	1/1/13/20	12/27/103/115	-
31	CLA	B	601	49	1/1/11/20	8/20/96/115	-
31	CLA	g	303	2	1/1/15/20	10/39/115/115	-
31	CLA	6	304	-	1/1/13/20	18/29/105/115	-
38	SQD	S	301	-	-	13/46/66/69	0/1/1/1
30	CHL	n	310	3	3/3/20/26	8/39/137/137	-
34	LMG	a	416	-	-	11/33/53/70	0/1/1/1
31	CLA	A	405	-	1/1/15/20	7/39/115/115	-
34	LMG	f	101	-	-	11/33/53/70	0/1/1/1
30	CHL	1	609	1	3/3/20/26	8/39/137/137	-
31	CLA	B	608	-	1/1/15/20	10/39/115/115	-
33	LHG	r	320	31	-	22/42/42/53	-
34	LMG	b	622	-	-	15/46/66/70	0/1/1/1
30	CHL	7	308	49	3/3/20/26	10/39/137/137	-
31	CLA	G	613	-	1/1/11/20	10/20/96/115	-
31	CLA	a	407	49	1/1/15/20	11/39/115/115	-
31	CLA	6	316	4	1/1/13/20	15/27/103/115	-
31	CLA	C	613	-	1/1/15/20	13/39/115/115	-
31	CLA	c	613	-	1/1/15/20	10/39/115/115	-
31	CLA	9	305	-	1/1/13/20	12/27/103/115	-
31	CLA	1	613	1	1/1/15/20	14/39/115/115	-
32	LUT	0	616	-	-	2/29/67/67	0/2/2/2
30	CHL	Y	302	24	3/3/20/26	9/39/137/137	-
33	LHG	C	623	-	-	27/44/44/53	-
31	CLA	9	316	-	1/1/11/20	6/17/93/115	-
36	NEX	0	618	-	-	9/27/83/83	0/3/3/3
31	CLA	C	606	-	1/1/13/20	13/30/106/115	-
30	CHL	G	606	49	3/3/16/26	4/20/118/137	-
31	CLA	c	606	-	1/1/15/20	18/39/115/115	-
32	LUT	9	318	-	-	4/29/67/67	0/2/2/2
34	LMG	0	622	-	-	15/33/53/70	0/1/1/1
34	LMG	J	102	-	-	5/33/53/70	0/1/1/1
30	CHL	6	306	4	3/3/16/26	5/15/113/137	-
30	CHL	n	306	3	3/3/20/26	15/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LUT	7	317	-	-	6/29/67/67	0/2/2/2
30	CHL	p	606	-	3/3/17/26	3/21/119/137	-
30	CHL	3	307	3	3/3/16/26	5/15/113/137	-
48	LMU	c	623	-	-	5/14/54/61	0/2/2/2
31	CLA	D	403	-	1/1/15/20	14/39/115/115	-
30	CHL	4	609	2	3/3/18/26	11/29/127/137	-
30	CHL	q	307	2	3/3/16/26	2/15/113/137	-
32	LUT	2	615	-	-	5/29/67/67	0/2/2/2
33	LHG	1	617	31	-	29/39/39/53	-
30	CHL	2	601	2	3/3/20/26	9/39/137/137	-
31	CLA	R	315	18	1/1/13/20	7/27/103/115	-
34	LMG	k	101	-	-	9/43/63/70	0/1/1/1
32	LUT	R	317	-	-	8/29/67/67	0/2/2/2
31	CLA	C	608	-	1/1/15/20	11/39/115/115	-
31	CLA	c	604	49	1/1/13/20	10/29/105/115	-
31	CLA	c	608	-	1/1/15/20	7/39/115/115	-
31	CLA	b	613	-	1/1/15/20	17/39/115/115	-
31	CLA	C	605	-	1/1/15/20	17/39/115/115	-
30	CHL	G	605	2	3/3/16/26	4/18/116/137	-
32	LUT	S	318	-	-	9/29/67/67	0/2/2/2
31	CLA	1	611	33	1/1/15/20	9/39/115/115	-
34	LMG	3	321	-	-	10/33/53/70	0/1/1/1
31	CLA	3	301	1	1/1/12/20	11/26/102/115	-
30	CHL	n	302	3	3/3/18/26	7/27/125/137	-
31	CLA	b	606	-	1/1/15/20	14/39/115/115	-
30	CHL	y	606	49	3/3/18/26	7/31/129/137	-
42	PHO	d	402	-	-	6/37/103/103	0/5/6/6
33	LHG	S	322	-	-	29/48/48/53	-
30	CHL	0	608	49	3/3/16/26	5/20/118/137	-
32	LUT	3	317	-	-	2/29/67/67	0/2/2/2
31	CLA	r	305	-	1/1/14/20	13/33/109/115	-
31	CLA	r	303	18	1/1/11/20	9/20/96/115	-
33	LHG	z	102	-	-	21/40/40/53	-
31	CLA	Y	311	33	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	SQD	6	301	-	-	18/37/57/69	0/1/1/1
34	LMG	A	414	-	-	10/33/53/70	0/1/1/1
30	CHL	1	601	1	3/3/20/26	8/39/137/137	-
38	SQD	a	412	-	-	18/40/60/69	0/1/1/1
48	LMU	K	101	-	-	7/21/61/61	0/2/2/2
31	CLA	b	608	49	1/1/15/20	22/39/115/115	-
36	NEX	g	317	31	-	12/27/83/83	0/3/3/3
31	CLA	c	603	-	1/1/15/20	19/39/115/115	-
43	BCR	D	405	-	-	13/29/63/63	0/2/2/2
31	CLA	0	604	49	1/1/13/20	12/27/103/115	-
33	LHG	s	322	-	-	28/48/48/53	-
38	SQD	G	617	-	-	11/37/57/69	0/1/1/1
34	LMG	D	409	-	-	12/41/61/70	0/1/1/1
31	CLA	S	315	-	1/1/11/20	5/19/95/115	-
31	CLA	s	303	19	1/1/15/20	13/39/115/115	-
31	CLA	N	304	-	1/1/13/20	12/27/103/115	-
36	NEX	S	319	-	-	2/27/83/83	0/3/3/3
31	CLA	7	314	1	1/1/15/20	14/39/115/115	-
34	LMG	p	620	-	-	7/33/53/70	0/1/1/1
31	CLA	3	313	3	1/1/12/20	11/21/97/115	-
31	CLA	4	613	2	1/1/14/20	13/35/111/115	-
45	DGD	c	617	-	-	23/51/91/95	0/2/2/2
32	LUT	8	615	-	-	6/29/67/67	0/2/2/2
33	LHG	G	618	31	-	28/48/48/53	-
31	CLA	S	312	33	1/1/15/20	17/39/115/115	-
37	XAT	R	318	-	-	6/31/93/93	0/4/4/4
34	LMG	w	203	-	-	6/33/53/70	0/1/1/1
30	CHL	3	303	3	3/3/16/26	5/20/118/137	-
31	CLA	S	313	19	1/1/13/20	7/29/105/115	-
31	CLA	6	312	33	1/1/14/20	17/33/109/115	-
30	CHL	5	608	-	3/3/16/26	5/20/118/137	-
34	LMG	B	625	-	-	13/33/53/70	0/1/1/1
31	CLA	b	611	49	1/1/15/20	12/39/115/115	-
43	BCR	A	410	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	R	306	49	1/1/11/20	7/19/95/115	-
31	CLA	B	613	-	1/1/15/20	10/39/115/115	-
31	CLA	B	605	-	1/1/15/20	18/39/115/115	-
31	CLA	B	611	-	1/1/15/20	13/39/115/115	-
34	LMG	q1	101	-	-	7/33/53/70	0/1/1/1
31	CLA	9	304	2	1/1/15/20	20/39/115/115	-
34	LMG	S	321	-	-	9/36/56/70	0/1/1/1
30	CHL	3	310	3	3/3/19/26	10/33/131/137	-
30	CHL	g	309	2	3/3/19/26	10/36/134/137	-
38	SQD	X	201	-	-	10/33/53/69	0/1/1/1
38	SQD	y	621	-	-	9/37/57/69	0/1/1/1
33	LHG	l	101	-	-	29/53/53/53	-
34	LMG	2	621	-	-	9/35/55/70	0/1/1/1
34	LMG	0	620	-	-	13/37/57/70	0/1/1/1
32	LUT	N	316	-	-	6/29/67/67	0/2/2/2
43	BCR	t	101	-	-	6/29/63/63	0/2/2/2
34	LMG	9	301	-	-	11/46/66/70	0/1/1/1
30	CHL	R	309	18	3/3/18/26	7/27/125/137	-
31	CLA	Y	314	-	1/1/12/20	7/26/102/115	-
32	LUT	7	318	-	-	6/29/67/67	0/2/2/2
30	CHL	0	606	49	3/3/17/26	2/21/119/137	-
34	LMG	c	620	-	-	14/33/53/70	0/1/1/1
45	DGD	C	618	-	-	16/55/95/95	0/2/2/2
45	DGD	c	618	-	-	19/55/95/95	0/2/2/2
31	CLA	p	612	3	1/1/11/20	7/17/93/115	-
31	CLA	7	313	1	1/1/15/20	15/39/115/115	-
38	SQD	s	301	-	-	16/46/66/69	0/1/1/1
30	CHL	6	308	49	3/3/20/26	12/39/137/137	-
35	RRX	2	614	-	-	15/29/65/65	0/2/2/2
30	CHL	2	605	2	3/3/16/26	2/15/113/137	-
38	SQD	b	621	-	-	13/49/69/69	0/1/1/1
33	LHG	q	320	31	-	31/50/50/53	-
30	CHL	0	605	4	3/3/17/26	8/23/121/137	-
38	SQD	0	621	-	-	9/37/57/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	c	609	-	1/1/15/20	11/39/115/115	-
31	CLA	0	602	4	1/1/15/20	16/39/115/115	-
30	CHL	1	606	49	3/3/20/26	14/39/137/137	-
31	CLA	2	603	-	1/1/13/20	13/27/103/115	-
31	CLA	3	306	49	1/1/13/20	16/27/103/115	-
36	NEX	8	617	31	-	11/27/83/83	0/3/3/3
34	LMG	A	418	-	-	11/33/53/70	0/1/1/1
31	CLA	S	306	-	1/1/12/20	5/21/97/115	-
31	CLA	Y	310	24	1/1/15/20	8/39/115/115	-
31	CLA	A	407	49	1/1/11/20	4/20/96/115	-
30	CHL	G	608	2	3/3/19/26	7/36/134/137	-
35	RRX	G	614	-	-	15/29/65/65	0/2/2/2
30	CHL	p	609	3	3/3/18/26	6/27/125/137	-
30	CHL	9	308	-	3/3/17/26	5/23/121/137	-
31	CLA	1	602	1	1/1/14/20	14/33/109/115	-
30	CHL	0	609	4	3/3/19/26	3/33/131/137	-
33	LHG	n	320	31	-	33/53/53/53	-
31	CLA	p	615	3	1/1/11/20	6/17/93/115	-
30	CHL	8	607	49	3/3/16/26	6/20/118/137	-
31	CLA	A	406	49	1/1/15/20	10/39/115/115	-
34	LMG	C	624	-	-	14/39/59/70	0/1/1/1
34	LMG	c	624	-	-	10/39/59/70	0/1/1/1
33	LHG	7	319	31	-	25/39/39/53	-
45	DGD	C	616	-	-	10/39/79/95	0/2/2/2
30	CHL	g	306	2	3/3/16/26	4/18/116/137	-
31	CLA	0	615	-	1/1/13/20	14/27/103/115	-
31	CLA	n	314	3	1/1/15/20	13/39/115/115	-
30	CHL	0	601	4	3/3/18/26	7/27/125/137	-
34	LMG	4	620	-	-	15/46/66/70	0/1/1/1
30	CHL	p	601	3	3/3/17/26	7/21/119/137	-
30	CHL	3	309	-	3/3/16/26	7/20/118/137	-
34	LMG	7	322	-	-	13/33/53/70	0/1/1/1
34	LMG	q	301	-	-	14/46/66/70	0/1/1/1
48	LMU	r	302	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	n	305	49	1/1/15/20	17/39/115/115	-
34	LMG	A	412	-	-	11/36/56/70	0/1/1/1
31	CLA	N	305	49	1/1/15/20	17/39/115/115	-
36	NEX	R	319	-	-	7/27/83/83	0/3/3/3
43	BCR	B	617	-	-	14/29/63/63	0/2/2/2
31	CLA	7	316	1	1/1/12/20	7/23/99/115	-
33	LHG	6	320	31	-	22/41/41/53	-
31	CLA	Y	312	24	1/1/15/20	16/39/115/115	-
33	LHG	p	619	31	-	27/39/39/53	-
34	LMG	g	320	-	-	11/33/53/70	0/1/1/1
45	DGD	c	619	-	-	17/55/95/95	0/2/2/2
31	CLA	N	313	3	1/1/15/20	12/39/115/115	-
31	CLA	S	304	-	1/1/10/20	6/12/88/115	-
33	LHG	N	319	31	-	31/53/53/53	-
32	LUT	5	616	-	-	6/29/67/67	0/2/2/2
30	CHL	4	605	2	3/3/16/26	1/15/113/137	-
34	LMG	6	321	-	-	13/37/57/70	0/1/1/1
30	CHL	9	307	2	3/3/16/26	5/15/113/137	-
31	CLA	s	304	-	1/1/10/20	6/12/88/115	-
32	LUT	y	616	-	-	2/29/67/67	0/2/2/2
43	BCR	v	101	-	-	15/29/63/63	0/2/2/2
31	CLA	5	612	3	1/1/12/20	8/21/97/115	-
31	CLA	n	315	-	1/1/11/20	8/20/96/115	-
33	LHG	B	624	-	-	33/53/53/53	-
33	LHG	K	102	-	-	23/40/40/53	-
30	CHL	q	308	-	3/3/17/26	6/21/119/137	-
31	CLA	b	615	-	1/1/15/20	15/39/115/115	-
33	LHG	0	619	31	-	28/40/40/53	-
31	CLA	g	313	2	1/1/15/20	10/39/115/115	-
44	PL9	A	416	-	-	14/53/73/73	0/1/1/1
36	NEX	4	617	-	-	6/27/83/83	0/3/3/3
31	CLA	b	603	-	1/1/15/20	16/39/115/115	-
31	CLA	n	312	33	1/1/11/20	5/20/96/115	-
32	LUT	6	317	-	-	6/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	6	313	4	1/1/14/20	12/33/109/115	-
36	NEX	r	301	-	-	2/27/83/83	0/3/3/3
31	CLA	6	315	-	1/1/12/20	14/26/102/115	-
44	PL9	a	414	-	-	15/53/73/73	0/1/1/1
30	CHL	5	609	3	3/3/18/26	3/27/125/137	-
38	SQD	B	623	-	-	20/47/67/69	0/1/1/1
30	CHL	n	301	49	3/3/16/26	5/20/118/137	-
32	LUT	Y	315	-	-	0/29/67/67	0/2/2/2
33	LHG	D	408	-	-	28/53/53/53	-
43	BCR	b	620	-	-	9/29/63/63	0/2/2/2
34	LMG	j	101	-	-	12/38/58/70	0/1/1/1
48	LMU	R	302	-	-	12/21/61/61	0/2/2/2
33	LHG	4	618	31	-	27/51/51/53	-
43	BCR	a	410	-	-	11/29/63/63	0/2/2/2
31	CLA	N	311	33	1/1/11/20	8/20/96/115	-
34	LMG	7	320	-	-	7/33/53/70	0/1/1/1
31	CLA	b	609	-	1/1/15/20	12/39/115/115	-
30	CHL	N	301	-	3/3/16/26	5/20/118/137	-
30	CHL	7	310	1	3/3/20/26	10/39/137/137	-
35	RRX	q	317	-	-	9/29/65/65	0/2/2/2
31	CLA	q	313	33	1/1/11/20	5/13/89/115	-
34	LMG	a	413	-	-	9/33/53/70	0/1/1/1
30	CHL	n	309	49	3/3/16/26	6/20/118/137	-
43	BCR	h	101	-	-	8/29/63/63	0/2/2/2
31	CLA	r	313	33	1/1/11/20	8/20/96/115	-
31	CLA	d	404	-	1/1/15/20	13/39/115/115	-
30	CHL	n	308	49	3/3/19/26	12/36/134/137	-
38	SQD	r	322	-	-	15/46/66/69	0/1/1/1
42	PHO	a	408	-	-	9/37/103/103	0/5/6/6
30	CHL	S	307	19	3/3/15/26	2/13/111/137	-
33	LHG	s	320	31	-	24/45/45/53	-
34	LMG	X	203	-	-	10/33/53/70	0/1/1/1
34	LMG	m	102	-	-	10/40/60/70	0/1/1/1
30	CHL	2	608	2	3/3/18/26	9/29/127/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	s	307	19	3/3/15/26	2/13/111/137	-
34	LMG	R	321	-	-	9/33/53/70	0/1/1/1
31	CLA	r	304	18	1/1/14/20	9/33/109/115	-
44	PL9	d	407	-	-	7/53/73/73	0/1/1/1
31	CLA	8	610	33	1/1/11/20	5/20/96/115	-
32	LUT	S	317	-	-	6/29/67/67	0/2/2/2
31	CLA	7	305	49	1/1/15/20	15/39/115/115	-
30	CHL	y	608	49	3/3/16/26	5/20/118/137	-
36	NEX	Y	317	-	-	2/27/83/83	0/3/3/3
31	CLA	c	607	49	1/1/15/20	11/39/115/115	-
43	BCR	B	619	-	-	8/29/63/63	0/2/2/2
31	CLA	p	613	-	1/1/12/20	8/26/102/115	-
31	CLA	p	611	33	1/1/14/20	16/33/109/115	-
30	CHL	n	307	49	3/3/18/26	2/30/128/137	-
31	CLA	5	613	3	1/1/12/20	9/26/102/115	-
34	LMG	g	322	-	-	15/44/64/70	0/1/1/1
31	CLA	r	306	49	1/1/11/20	7/19/95/115	-
31	CLA	S	305	49	1/1/15/20	9/39/115/115	-
33	LHG	c	622	-	-	32/51/51/53	-
34	LMG	B	621	-	-	15/46/66/70	0/1/1/1
31	CLA	7	304	-	1/1/13/20	12/27/103/115	-
37	XAT	9	322	-	-	9/31/93/93	0/4/4/4
31	CLA	n	303	3	1/1/15/20	13/39/115/115	-
30	CHL	7	302	1	3/3/20/26	14/39/137/137	-
43	BCR	H	101	-	-	5/29/63/63	0/2/2/2
33	LHG	j	102	-	-	36/53/53/53	-
31	CLA	3	315	-	1/1/12/20	12/26/102/115	-
31	CLA	2	610	33	1/1/14/20	12/33/109/115	-
31	CLA	Y	304	-	1/1/13/20	13/27/103/115	-
31	CLA	R	313	33	1/1/11/20	8/20/96/115	-
31	CLA	y	603	-	1/1/13/20	12/27/103/115	-
31	CLA	R	311	18	1/1/13/20	16/31/107/115	-
31	CLA	3	314	3	1/1/13/20	6/27/103/115	-
31	CLA	9	313	33	1/1/11/20	8/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	NEX	r	319	-	-	4/27/83/83	0/3/3/3
31	CLA	C	604	49	1/1/13/20	9/29/105/115	-
30	CHL	r	309	18	3/3/18/26	5/27/125/137	-
47	HEM	e	102	10,9	-	5/14/54/54	-
32	LUT	N	317	-	-	6/29/67/67	0/2/2/2
30	CHL	S	308	49	3/3/15/26	0/12/110/137	-
31	CLA	B	615	-	1/1/15/20	11/39/115/115	-
34	LMG	w	202	-	-	12/50/70/70	0/1/1/1
43	BCR	T	101	-	-	13/29/63/63	0/2/2/2
30	CHL	6	309	49	3/3/16/26	4/20/118/137	-
31	CLA	B	610	49	1/1/15/20	15/39/115/115	-
30	CHL	6	310	4	3/3/19/26	10/33/131/137	-
31	CLA	0	611	33	1/1/14/20	10/33/109/115	-
31	CLA	N	321	24	1/1/12/20	9/26/102/115	-
34	LMG	C	621	-	-	9/33/53/70	0/1/1/1
34	LMG	c	621	-	-	7/33/53/70	0/1/1/1
30	CHL	p	605	3	3/3/16/26	1/15/113/137	-
30	CHL	6	302	4	3/3/18/26	4/27/125/137	-
31	CLA	2	604	36,49	1/1/12/20	11/26/102/115	-
30	CHL	2	606	-	3/3/17/26	6/21/119/137	-
31	CLA	s	305	49	1/1/15/20	16/39/115/115	-
31	CLA	R	304	18	1/1/14/20	12/33/109/115	-
31	CLA	8	612	3	1/1/15/20	13/39/115/115	-
34	LMG	w	201	-	-	13/43/63/70	0/1/1/1
45	DGD	C	620	-	-	18/55/95/95	0/2/2/2
31	CLA	b	605	-	1/1/15/20	24/39/115/115	-
31	CLA	g	305	36,49	1/1/13/20	11/27/103/115	-
30	CHL	R	308	18	3/3/18/26	6/27/125/137	-
31	CLA	D	404	-	1/1/15/20	17/39/115/115	-
31	CLA	R	316	18	1/1/15/20	18/39/115/115	-
31	CLA	8	604	36,49	1/1/15/20	17/39/115/115	-
30	CHL	y	607	49	3/3/20/26	13/39/137/137	-
30	CHL	8	606	49	3/3/18/26	2/30/128/137	-
38	SQD	x	201	-	-	14/37/57/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	PL9	D	406	-	-	9/53/73/73	0/1/1/1
30	CHL	6	307	49	3/3/17/26	7/21/119/137	-
32	LUT	y	617	-	-	2/29/67/67	0/2/2/2
38	SQD	A	413	-	-	13/40/60/69	0/1/1/1
43	BCR	B	618	-	-	9/29/63/63	0/2/2/2
31	CLA	1	610	1	1/1/15/20	17/39/115/115	-
31	CLA	d	405	-	1/1/15/20	13/39/115/115	-
31	CLA	8	602	3	1/1/15/20	13/39/115/115	-
31	CLA	y	604	49	1/1/13/20	13/27/103/115	-
31	CLA	y	612	24	1/1/15/20	20/39/115/115	-
31	CLA	B	607	49	1/1/15/20	18/39/115/115	-
30	CHL	Y	307	49	3/3/18/26	9/31/129/137	-
30	CHL	8	608	3	3/3/20/26	10/39/137/137	-
31	CLA	5	610	3	1/1/14/20	11/33/109/115	-
30	CHL	4	601	2	3/3/20/26	11/39/137/137	-
31	CLA	B	616	-	1/1/15/20	17/39/115/115	-
32	LUT	p	617	-	-	9/29/67/67	0/2/2/2
31	CLA	B	612	-	1/1/15/20	10/39/115/115	-
30	CHL	3	308	-	3/3/16/26	1/17/115/137	-
34	LMG	6	322	-	-	12/34/54/70	0/1/1/1
32	LUT	6	318	-	-	6/29/67/67	0/2/2/2
30	CHL	N	308	49	3/3/16/26	9/20/118/137	-
34	LMG	w	205	-	-	13/33/53/70	0/1/1/1
31	CLA	B	602	-	1/1/15/20	14/39/115/115	-
35	RRX	4	615	-	-	15/29/65/65	0/2/2/2
34	LMG	a	401	-	-	5/33/53/70	0/1/1/1
43	BCR	C	614	-	-	12/29/63/63	0/2/2/2
43	BCR	c	614	-	-	16/29/63/63	0/2/2/2
31	CLA	y	615	24	1/1/12/20	11/26/102/115	-
31	CLA	Y	305	49	1/1/13/20	11/27/103/115	-
34	LMG	9	321	-	-	10/33/53/70	0/1/1/1
30	CHL	q	303	2	3/3/20/26	8/39/137/137	-
36	NEX	N	318	-	-	15/27/83/83	0/3/3/3
30	CHL	g	308	49	3/3/17/26	5/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	7	301	-	-	11/34/54/70	0/1/1/1
34	LMG	I	101	-	-	15/33/53/70	0/1/1/1
34	LMG	b	626	-	-	14/41/61/70	0/1/1/1
31	CLA	2	612	2	1/1/15/20	14/39/115/115	-
30	CHL	s	302	19	3/3/16/26	4/15/113/137	-
31	CLA	0	612	4	1/1/11/20	8/17/93/115	-
30	CHL	R	310	49	3/3/17/26	6/26/124/137	-
31	CLA	Y	303	24	1/1/14/20	9/33/109/115	-
30	CHL	1	607	-	3/3/20/26	11/39/137/137	-
31	CLA	8	614	3	1/1/12/20	8/26/102/115	-
30	CHL	p	607	-	3/3/17/26	5/21/119/137	-
42	PHO	A	408	-	-	12/37/103/103	0/5/6/6
31	CLA	g	314	-	1/1/11/20	7/20/96/115	-
31	CLA	s	314	19	1/1/15/20	15/39/115/115	-
31	CLA	B	603	-	1/1/15/20	18/39/115/115	-
32	LUT	s	317	-	-	6/29/67/67	0/2/2/2
37	XAT	G	620	-	-	9/31/93/93	0/4/4/4
31	CLA	N	315	3	1/1/12/20	9/26/102/115	-
31	CLA	9	306	36,49	1/1/15/20	15/39/115/115	-
33	LHG	A	417	-	-	22/43/43/53	-
43	BCR	d	406	-	-	11/29/63/63	0/2/2/2
31	CLA	S	316	19	1/1/11/20	7/17/93/115	-
30	CHL	y	609	24	3/3/20/26	7/39/137/137	-
32	LUT	n	317	-	-	6/29/67/67	0/2/2/2
30	CHL	9	303	2	3/3/20/26	9/39/137/137	-
34	LMG	X	202	-	-	5/33/53/70	0/1/1/1
36	NEX	3	319	-	-	9/27/83/83	0/3/3/3
43	BCR	V	101	-	-	15/29/63/63	0/2/2/2
31	CLA	3	312	33	1/1/15/20	13/39/115/115	-
31	CLA	y	614	-	1/1/12/20	8/26/102/115	-
31	CLA	b	616	-	1/1/15/20	15/39/115/115	-
34	LMG	d	411	-	-	9/43/63/70	0/1/1/1
31	CLA	q	314	2	1/1/11/20	6/17/93/115	-
33	LHG	F1	301	-	-	26/39/39/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	N	309	3	3/3/20/26	8/39/137/137	-
31	CLA	4	612	2	1/1/11/20	6/17/93/115	-
31	CLA	g	304	-	1/1/13/20	12/27/103/115	-
30	CHL	2	607	49	3/3/16/26	5/20/118/137	-
30	CHL	0	607	49	3/3/20/26	18/39/137/137	-
34	LMG	d	410	-	-	14/46/66/70	0/1/1/1
31	CLA	g	310	2	1/1/15/20	12/39/115/115	-
31	CLA	s	312	33	1/1/15/20	22/39/115/115	-
31	CLA	9	315	2	1/1/13/20	5/27/103/115	-
30	CHL	4	606	31	3/3/17/26	6/21/119/137	-
31	CLA	5	604	-	1/1/12/20	6/21/97/115	-
31	CLA	0	610	4	1/1/15/20	15/39/115/115	-
36	NEX	n	319	-	-	10/27/83/83	0/3/3/3
31	CLA	G	610	33	1/1/14/20	14/33/109/115	-
34	LMG	d	409	-	-	10/36/56/70	0/1/1/1
31	CLA	4	602	2	1/1/15/20	16/39/115/115	-
31	CLA	C	612	-	1/1/13/20	13/27/103/115	-
31	CLA	s	315	-	1/1/11/20	6/19/95/115	-
31	CLA	r	315	18	1/1/13/20	12/27/103/115	-
31	CLA	N	310	3	1/1/15/20	10/39/115/115	-
31	CLA	p	610	3	1/1/13/20	13/29/105/115	-
34	LMG	G	621	-	-	13/46/66/70	0/1/1/1
34	LMG	x	202	-	-	18/33/53/70	0/1/1/1
31	CLA	r	311	18	1/1/13/20	14/31/107/115	-
31	CLA	5	615	3	1/1/11/20	11/17/93/115	-
33	LHG	L	101	-	-	31/53/53/53	-
31	CLA	q	305	-	1/1/13/20	12/27/103/115	-
34	LMG	2	618	-	-	13/33/53/70	0/1/1/1
31	CLA	q	316	-	1/1/12/20	10/21/97/115	-
30	CHL	s	308	49	3/3/15/26	2/12/110/137	-
32	LUT	q	318	-	-	6/29/67/67	0/2/2/2
31	CLA	q	315	2	1/1/15/20	12/39/115/115	-
33	LHG	y	619	31	-	30/50/50/53	-
31	CLA	C	607	49	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	s	310	19	1/1/14/20	15/33/109/115	-
36	NEX	q	319	-	-	11/27/83/83	0/3/3/3
32	LUT	8	616	-	-	6/29/67/67	0/2/2/2
31	CLA	0	613	4	1/1/13/20	10/29/105/115	-
36	NEX	9	319	31	-	6/27/83/83	0/3/3/3
31	CLA	n	313	3	1/1/11/20	4/15/91/115	-
38	SQD	B	620	-	-	18/49/69/69	0/1/1/1
32	LUT	3	318	-	-	7/29/67/67	0/2/2/2
34	LMG	b	623	-	-	7/33/53/70	0/1/1/1
33	LHG	2	617	31	-	32/53/53/53	-
31	CLA	s	316	19	1/1/11/20	6/17/93/115	-
38	SQD	m	101	-	-	13/45/65/69	0/1/1/1
38	SQD	a	411	-	-	16/43/63/69	0/1/1/1
31	CLA	8	611	3	1/1/11/20	4/15/91/115	-
33	LHG	g	319	31	-	25/48/48/53	-
32	LUT	1	616	-	-	3/29/67/67	0/2/2/2
30	CHL	S	302	19	3/3/16/26	0/15/113/137	-
33	LHG	a	415	-	-	23/43/43/53	-
33	LHG	e	101	-	-	32/48/48/53	-
37	XAT	g	321	-	-	9/31/93/93	0/4/4/4
31	CLA	q	306	49	1/1/13/20	10/27/103/115	-
33	LHG	9	320	31	-	22/37/37/53	-
31	CLA	R	303	18	1/1/11/20	11/20/96/115	-
31	CLA	n	316	3	1/1/12/20	8/26/102/115	-
31	CLA	6	311	4	1/1/15/20	14/39/115/115	-
34	LMG	G	619	-	-	11/33/53/70	0/1/1/1
30	CHL	5	607	-	3/3/17/26	7/21/119/137	-
31	CLA	C	610	-	1/1/15/20	14/39/115/115	-
31	CLA	c	610	-	1/1/15/20	14/39/115/115	-
31	CLA	r	307	49	1/1/11/20	10/19/95/115	-
31	CLA	S	311	19	1/1/15/20	13/39/115/115	-
31	CLA	G	602	2	1/1/15/20	16/39/115/115	-
36	NEX	5	618	-	-	9/27/83/83	0/3/3/3
30	CHL	8	601	3	3/3/18/26	7/27/125/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	5	614	-	1/1/12/20	8/23/99/115	-
36	NEX	6	319	-	-	9/27/83/83	0/3/3/3
36	NEX	p	618	31	-	9/27/83/83	0/3/3/3
30	CHL	N	307	49	3/3/18/26	5/30/128/137	-
33	LHG	t	102	-	-	30/45/45/53	-
34	LMG	b	629	-	-	12/33/53/70	0/1/1/1
32	LUT	n	318	-	-	6/29/67/67	0/2/2/2
30	CHL	y	605	24	3/3/16/26	3/15/113/137	-
31	CLA	3	305	-	1/1/13/20	11/27/103/115	-
31	CLA	p	602	3	1/1/14/20	13/33/109/115	-
30	CHL	N	302	3	3/3/18/26	3/27/125/137	-
31	CLA	B	614	-	1/1/15/20	18/39/115/115	-
34	LMG	1	618	-	-	8/33/53/70	0/1/1/1
30	CHL	q	310	-	3/3/16/26	4/20/118/137	-
38	SQD	M	102	-	-	16/45/65/69	0/1/1/1
30	CHL	9	310	49	3/3/16/26	9/20/118/137	-
30	CHL	q	309	-	3/3/18/26	17/29/127/137	-
36	NEX	s	319	-	-	3/27/83/83	0/3/3/3
34	LMG	q	302	-	-	9/35/55/70	0/1/1/1
30	CHL	s	309	49	3/3/16/26	2/19/117/137	-
31	CLA	0	603	-	1/1/13/20	16/29/105/115	-
32	LUT	4	616	-	-	6/29/67/67	0/2/2/2
31	CLA	b	617	-	1/1/15/20	14/39/115/115	-
30	CHL	5	601	3	3/3/17/26	7/21/119/137	-
38	SQD	G	624	-	-	11/33/53/69	0/1/1/1
31	CLA	y	602	24	1/1/14/20	10/33/109/115	-
32	LUT	s	318	-	-	5/29/67/67	0/2/2/2
30	CHL	r	308	18	3/3/18/26	7/27/125/137	-
34	LMG	4	621	-	-	11/35/55/70	0/1/1/1
38	SQD	b	627	-	-	13/47/67/69	0/1/1/1
31	CLA	2	613	-	1/1/12/20	13/26/102/115	-
30	CHL	Y	301	49	3/3/19/26	10/36/134/137	-
30	CHL	r	310	49	3/3/17/26	5/26/124/137	-
31	CLA	G	611	2	1/1/10/20	4/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	c	605	-	1/1/15/20	16/39/115/115	-
33	LHG	5	619	31	-	28/39/39/53	-
34	LMG	n	322	-	-	12/35/55/70	0/1/1/1
34	LMG	D	411	-	-	14/46/66/70	0/1/1/1
31	CLA	p	603	-	1/1/13/20	13/27/103/115	-
43	BCR	z	101	-	-	4/29/63/63	0/2/2/2
32	LUT	5	617	-	-	7/29/67/67	0/2/2/2
30	CHL	G	623	49	3/3/20/26	10/39/137/137	-
35	RRX	9	317	-	-	15/29/65/65	0/2/2/2
31	CLA	G	612	2	1/1/15/20	16/39/115/115	-
33	LHG	M	101	-	-	24/45/45/53	-
34	LMG	W	202	-	-	11/33/53/70	0/1/1/1
36	NEX	R	301	-	-	3/27/83/83	0/3/3/3
34	LMG	C	619	-	-	9/46/66/70	0/1/1/1
34	LMG	k	102	-	-	10/33/53/70	0/1/1/1
31	CLA	c	611	7	1/1/15/20	13/39/115/115	-
31	CLA	8	613	-	1/1/11/20	8/20/96/115	-
30	CHL	Y	308	49	3/3/16/26	9/20/118/137	-
31	CLA	b	610	-	1/1/15/20	18/39/115/115	-
31	CLA	5	611	33	1/1/13/20	12/31/107/115	-
31	CLA	q	304	2	1/1/15/20	12/39/115/115	-
34	LMG	W	201	-	-	19/50/70/70	0/1/1/1
30	CHL	1	619	-	3/3/19/26	13/33/131/137	-
31	CLA	C	602	-	1/1/15/20	11/39/115/115	-
31	CLA	c	602	-	1/1/15/20	9/39/115/115	-
33	LHG	A	415	-	-	30/48/48/53	-
31	CLA	y	611	33	1/1/15/20	13/39/115/115	-
34	LMG	B	622	-	-	8/33/53/70	0/1/1/1
37	XAT	r	318	-	-	2/31/93/93	0/4/4/4
34	LMG	2	620	-	-	19/46/66/70	0/1/1/1
38	SQD	A	411	-	-	14/46/66/69	0/1/1/1
30	CHL	7	306	1	3/3/20/26	15/39/137/137	-
31	CLA	A	409	-	1/1/14/20	16/33/109/115	-
33	LHG	S	320	31	-	29/45/45/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	1	608	49	3/3/16/26	7/20/118/137	-
31	CLA	6	303	4	1/1/15/20	15/39/115/115	-
31	CLA	G	603	-	1/1/13/20	11/27/103/115	-
31	CLA	S	314	19	1/1/15/20	13/39/115/115	-
30	CHL	p	608	-	3/3/16/26	8/20/118/137	-
30	CHL	G	601	2	3/3/20/26	8/39/137/137	-
31	CLA	1	603	-	1/1/13/20	9/27/103/115	-
30	CHL	3	302	49	3/3/18/26	11/29/127/137	-
31	CLA	2	602	2	1/1/15/20	22/39/115/115	-
31	CLA	R	312	18	1/1/13/20	11/30/106/115	-
38	SQD	R	322	-	-	16/46/66/69	0/1/1/1
30	CHL	G	607	49	3/3/17/26	3/21/119/137	-
31	CLA	7	311	1	1/1/15/20	15/39/115/115	-
31	CLA	B	606	-	1/1/15/20	14/39/115/115	-
31	CLA	b	602	49	1/1/11/20	12/20/96/115	-
33	LHG	D	407	-	-	31/48/48/53	-
30	CHL	g	302	2	3/3/20/26	12/39/137/137	-
34	LMG	b	624	-	-	13/33/53/70	0/1/1/1
31	CLA	5	603	-	1/1/12/20	10/24/100/115	-
31	CLA	6	305	49	1/1/13/20	14/27/103/115	-
31	CLA	y	610	24	1/1/15/20	9/39/115/115	-
31	CLA	C	611	7	1/1/15/20	13/39/115/115	-
32	LUT	0	617	-	-	0/29/67/67	0/2/2/2
34	LMG	C	622	-	-	6/27/47/70	0/1/1/1
30	CHL	8	605	3	3/3/20/26	17/39/137/137	-
34	LMG	w	204	-	-	11/33/53/70	0/1/1/1
31	CLA	R	307	49	1/1/11/20	10/19/95/115	-
31	CLA	b	607	-	1/1/15/20	13/39/115/115	-
31	CLA	1	604	49	1/1/15/20	14/39/115/115	-
34	LMG	s	321	-	-	11/36/56/70	0/1/1/1
43	BCR	b	618	-	-	14/29/63/63	0/2/2/2
34	LMG	W	203	-	-	12/33/53/70	0/1/1/1
45	DGD	C	617	-	-	16/55/95/95	0/2/2/2
30	CHL	5	606	49	3/3/17/26	2/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	N	306	3	3/3/20/26	9/39/137/137	-
31	CLA	p	614	-	1/1/12/20	9/23/99/115	-
31	CLA	3	304	3	1/1/14/20	12/33/109/115	-
34	LMG	9	302	-	-	14/35/55/70	0/1/1/1
31	CLA	b	612	-	1/1/15/20	12/39/115/115	-
30	CHL	Y	306	24	3/3/16/26	2/15/113/137	-
31	CLA	4	610	2	1/1/14/20	18/33/109/115	-
31	CLA	5	602	3	1/1/14/20	14/33/109/115	-
32	LUT	Y	316	-	-	3/29/67/67	0/2/2/2
31	CLA	4	611	33	1/1/11/20	5/13/89/115	-
30	CHL	7	309	49	3/3/16/26	8/20/118/137	-
31	CLA	3	316	3	1/1/13/20	12/30/106/115	-
31	CLA	7	312	33	1/1/15/20	17/39/115/115	-
34	LMG	J	101	-	-	12/46/66/70	0/1/1/1
31	CLA	2	609	2	1/1/14/20	16/33/109/115	-
31	CLA	C	603	-	1/1/15/20	18/39/115/115	-
31	CLA	2	611	2	1/1/13/20	9/27/103/115	-
31	CLA	b	614	-	1/1/15/20	13/39/115/115	-
47	HEM	E	101	10,9	-	5/14/54/54	-
32	LUT	g	316	-	-	10/29/67/67	0/2/2/2
30	CHL	7	321	49	3/3/19/26	12/36/134/137	-
43	BCR	C	615	-	-	9/29/63/63	0/2/2/2
34	LMG	n	321	-	-	12/33/53/70	0/1/1/1
43	BCR	c	615	-	-	11/29/63/63	0/2/2/2
31	CLA	G	604	49	1/1/13/20	15/27/103/115	-
34	LMG	6	323	-	-	12/33/53/70	0/1/1/1
34	LMG	y	620	-	-	10/33/53/70	0/1/1/1
31	CLA	C	609	-	1/1/15/20	10/39/115/115	-
31	CLA	N	314	-	1/1/11/20	7/20/96/115	-
32	LUT	p	616	-	-	8/29/67/67	0/2/2/2
38	SQD	Y	320	-	-	8/37/57/69	0/1/1/1
31	CLA	0	614	-	1/1/12/20	10/26/102/115	-
35	RRX	g	315	-	-	7/29/65/65	0/2/2/2
31	CLA	a	406	-	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	NEX	G	616	-	-	2/27/83/83	0/3/3/3
33	LHG	3	320	31	-	25/37/37/53	-
36	NEX	y	618	-	-	2/27/83/83	0/3/3/3
31	CLA	G	609	2	1/1/15/20	7/39/115/115	-
30	CHL	7	307	49	3/3/20/26	8/39/137/137	-
31	CLA	1	612	1	1/1/15/20	18/39/115/115	-
31	CLA	4	603	-	1/1/13/20	10/27/103/115	-
33	LHG	R	320	31	-	24/42/42/53	-
30	CHL	1	605	1	3/3/20/26	11/39/137/137	-
34	LMG	D	410	-	-	13/41/61/70	0/1/1/1
37	XAT	q	321	-	-	9/31/93/93	0/4/4/4
31	CLA	R	305	-	1/1/14/20	7/33/109/115	-
34	LMG	Q1	101	-	-	10/33/53/70	0/1/1/1
31	CLA	b	604	-	1/1/15/20	15/39/115/115	-
38	SQD	g	318	-	-	3/37/57/69	0/1/1/1
33	LHG	d	408	-	-	27/53/53/53	-
30	CHL	4	607	-	3/3/18/26	16/29/127/137	-
30	CHL	Y	309	24	3/3/20/26	12/39/137/137	-
34	LMG	r	321	-	-	15/33/53/70	0/1/1/1
37	XAT	4	619	-	-	9/31/93/93	0/4/4/4
31	CLA	s	311	19	1/1/15/20	13/39/115/115	-
30	CHL	y	601	24	3/3/20/26	11/39/137/137	-
31	CLA	4	614	-	1/1/12/20	7/26/102/115	-
31	CLA	6	314	4	1/1/15/20	12/39/115/115	-
31	CLA	9	314	2	1/1/12/20	5/21/97/115	-
31	CLA	g	311	33	1/1/14/20	13/33/109/115	-
31	CLA	d	401	49	1/1/11/20	6/20/96/115	-
31	CLA	N	312	3	1/1/11/20	4/15/91/115	-
31	CLA	8	609	3	1/1/15/20	10/39/115/115	-
31	CLA	c	612	-	1/1/13/20	13/27/103/115	-
31	CLA	S	310	19	1/1/14/20	15/33/109/115	-
31	CLA	Y	313	24	1/1/15/20	10/39/115/115	-
31	CLA	s	313	19	1/1/13/20	7/29/105/115	-
37	XAT	2	619	-	-	9/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	a	409	-	1/1/14/20	16/33/109/115	-
43	BCR	Z	101	-	-	4/29/63/63	0/2/2/2
34	LMG	N	320	-	-	9/33/53/70	0/1/1/1
31	CLA	g	312	2	1/1/10/20	4/13/89/115	-
30	CHL	4	608	-	3/3/16/26	5/20/118/137	-
45	DGD	c	616	-	-	22/55/95/95	0/2/2/2
31	CLA	n	304	-	1/1/13/20	12/27/103/115	-
30	CHL	9	311	2	3/3/19/26	12/33/131/137	-
31	CLA	r	314	-	1/1/11/20	6/20/96/115	-
31	CLA	B	604	-	1/1/15/20	14/39/115/115	-
32	LUT	r	317	-	-	4/29/67/67	0/2/2/2
32	LUT	G	615	-	-	10/29/67/67	0/2/2/2
31	CLA	1	614	-	1/1/12/20	14/26/102/115	-
31	CLA	C	601	-	1/1/15/20	16/39/115/115	-
31	CLA	c	601	-	1/1/15/20	21/39/115/115	-

All (4939) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	N	316	LUT	C24-C25	24.45	1.62	1.33
32	5	616	LUT	C24-C25	24.40	1.62	1.33
32	G	615	LUT	C24-C25	24.40	1.62	1.33
32	3	317	LUT	C24-C25	24.39	1.62	1.33
32	9	318	LUT	C24-C25	24.38	1.62	1.33
32	8	615	LUT	C24-C25	24.37	1.62	1.33
32	n	317	LUT	C24-C25	24.36	1.62	1.33
32	p	616	LUT	C24-C25	24.35	1.62	1.33
32	S	318	LUT	C24-C25	24.33	1.62	1.33
32	q	318	LUT	C24-C25	24.32	1.62	1.33
32	g	316	LUT	C24-C25	24.31	1.62	1.33
32	8	616	LUT	C24-C25	24.30	1.62	1.33
32	N	317	LUT	C24-C25	24.29	1.62	1.33
32	n	318	LUT	C24-C25	24.28	1.62	1.33
32	6	318	LUT	C24-C25	24.24	1.61	1.33
32	6	317	LUT	C24-C25	24.24	1.61	1.33
32	p	617	LUT	C24-C25	24.23	1.61	1.33
32	7	318	LUT	C24-C25	24.22	1.61	1.33
32	3	318	LUT	C24-C25	24.22	1.61	1.33
32	S	317	LUT	C24-C25	24.19	1.61	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	s	317	LUT	C24-C25	24.18	1.61	1.33
32	s	318	LUT	C24-C25	24.16	1.61	1.33
32	4	616	LUT	C24-C25	24.14	1.61	1.33
32	1	616	LUT	C24-C25	24.13	1.61	1.33
32	5	617	LUT	C24-C25	24.13	1.61	1.33
32	0	616	LUT	C24-C25	24.10	1.61	1.33
32	R	317	LUT	C24-C25	24.08	1.61	1.33
32	1	615	LUT	C24-C25	24.06	1.61	1.33
32	r	317	LUT	C24-C25	23.99	1.61	1.33
32	Y	315	LUT	C24-C25	23.93	1.61	1.33
32	7	317	LUT	C24-C25	23.93	1.61	1.33
32	0	617	LUT	C24-C25	23.89	1.61	1.33
32	y	617	LUT	C24-C25	23.89	1.61	1.33
32	y	616	LUT	C24-C25	23.83	1.61	1.33
32	Y	316	LUT	C24-C25	23.76	1.61	1.33
32	2	615	LUT	C24-C25	22.75	1.60	1.33
43	B	618	BCR	C26-C25	16.22	1.61	1.34
43	b	619	BCR	C26-C25	16.16	1.61	1.34
43	Z	101	BCR	C26-C25	15.93	1.61	1.34
43	z	101	BCR	C26-C25	15.90	1.61	1.34
43	D	405	BCR	C26-C25	15.85	1.61	1.34
35	9	317	RRX	C26-C25	15.82	1.61	1.34
35	4	615	RRX	C26-C25	15.81	1.61	1.34
35	G	614	RRX	C26-C25	15.79	1.61	1.34
32	8	615	LUT	C5-C6	15.79	1.61	1.34
32	n	317	LUT	C5-C6	15.78	1.61	1.34
35	2	614	RRX	C26-C25	15.78	1.61	1.34
43	b	620	BCR	C26-C25	15.75	1.60	1.34
35	g	315	RRX	C26-C25	15.74	1.60	1.34
32	G	615	LUT	C5-C6	15.72	1.60	1.34
43	t	101	BCR	C26-C25	15.72	1.60	1.34
43	c	615	BCR	C26-C25	15.72	1.60	1.34
32	s	317	LUT	C5-C6	15.72	1.60	1.34
32	5	617	LUT	C5-C6	15.72	1.60	1.34
32	S	317	LUT	C5-C6	15.70	1.60	1.34
35	q	317	RRX	C26-C25	15.70	1.60	1.34
43	H	101	BCR	C26-C25	15.70	1.60	1.34
32	6	318	LUT	C5-C6	15.69	1.60	1.34
32	7	318	LUT	C5-C6	15.69	1.60	1.34
32	5	616	LUT	C5-C6	15.68	1.60	1.34
32	9	318	LUT	C5-C6	15.67	1.60	1.34
43	T	101	BCR	C26-C25	15.67	1.60	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	8	616	LUT	C5-C6	15.66	1.60	1.34
32	n	318	LUT	C5-C6	15.65	1.60	1.34
43	c	614	BCR	C26-C25	15.65	1.60	1.34
43	v	101	BCR	C26-C25	15.64	1.60	1.34
43	a	410	BCR	C26-C25	15.64	1.60	1.34
43	C	615	BCR	C26-C25	15.63	1.60	1.34
43	B	619	BCR	C26-C25	15.61	1.60	1.34
32	p	616	LUT	C5-C6	15.61	1.60	1.34
32	4	616	LUT	C5-C6	15.61	1.60	1.34
43	h	101	BCR	C26-C25	15.59	1.60	1.34
32	3	317	LUT	C5-C6	15.58	1.60	1.34
32	0	617	LUT	C5-C6	15.56	1.60	1.34
32	N	316	LUT	C5-C6	15.53	1.60	1.34
32	g	316	LUT	C5-C6	15.53	1.60	1.34
32	r	317	LUT	C5-C6	15.53	1.60	1.34
32	S	318	LUT	C5-C6	15.53	1.60	1.34
43	d	406	BCR	C26-C25	15.53	1.60	1.34
32	y	617	LUT	C5-C6	15.49	1.60	1.34
32	Y	315	LUT	C5-C6	15.48	1.60	1.34
32	p	617	LUT	C5-C6	15.47	1.60	1.34
32	s	318	LUT	C5-C6	15.47	1.60	1.34
32	N	317	LUT	C5-C6	15.46	1.60	1.34
32	Y	316	LUT	C5-C6	15.46	1.60	1.34
43	A	410	BCR	C26-C25	15.46	1.60	1.34
32	1	616	LUT	C5-C6	15.43	1.60	1.34
32	3	318	LUT	C5-C6	15.43	1.60	1.34
32	6	317	LUT	C5-C6	15.42	1.60	1.34
32	R	317	LUT	C5-C6	15.40	1.60	1.34
32	q	318	LUT	C5-C6	15.39	1.60	1.34
32	y	616	LUT	C5-C6	15.38	1.60	1.34
43	B	617	BCR	C26-C25	15.37	1.60	1.34
32	0	616	LUT	C5-C6	15.36	1.60	1.34
32	1	615	LUT	C5-C6	15.27	1.60	1.34
32	7	317	LUT	C5-C6	15.27	1.60	1.34
32	2	615	LUT	C5-C6	15.26	1.60	1.34
43	b	618	BCR	C26-C25	15.24	1.60	1.34
43	C	614	BCR	C26-C25	15.19	1.60	1.34
43	V	101	BCR	C26-C25	15.15	1.59	1.34
35	g	315	RRX	C5-C6	14.74	1.59	1.34
35	4	615	RRX	C5-C6	14.68	1.59	1.34
43	D	405	BCR	C5-C6	14.67	1.59	1.34
35	9	317	RRX	C5-C6	14.66	1.59	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	1	619	CHL	C3A-C2A	-14.63	1.42	1.54
35	G	614	RRX	C5-C6	14.63	1.59	1.34
35	2	614	RRX	C5-C6	14.61	1.59	1.34
43	z	101	BCR	C5-C6	14.58	1.59	1.34
43	Z	101	BCR	C5-C6	14.48	1.58	1.34
43	B	618	BCR	C5-C6	14.41	1.58	1.34
35	q	317	RRX	C5-C6	14.37	1.58	1.34
43	T	101	BCR	C5-C6	14.33	1.58	1.34
43	a	410	BCR	C5-C6	14.32	1.58	1.34
43	b	619	BCR	C5-C6	14.31	1.58	1.34
43	c	614	BCR	C5-C6	14.28	1.58	1.34
43	H	101	BCR	C5-C6	14.26	1.58	1.34
43	v	101	BCR	C5-C6	14.24	1.58	1.34
43	A	410	BCR	C5-C6	14.23	1.58	1.34
43	b	620	BCR	C5-C6	14.23	1.58	1.34
43	B	619	BCR	C5-C6	14.20	1.58	1.34
43	V	101	BCR	C5-C6	14.16	1.58	1.34
43	C	614	BCR	C5-C6	14.14	1.58	1.34
43	h	101	BCR	C5-C6	14.14	1.58	1.34
43	b	618	BCR	C5-C6	14.10	1.58	1.34
43	c	615	BCR	C5-C6	14.03	1.58	1.34
43	B	617	BCR	C5-C6	13.98	1.57	1.34
43	d	406	BCR	C5-C6	13.97	1.57	1.34
43	t	101	BCR	C5-C6	13.79	1.57	1.34
32	R	317	LUT	C22-C21	-13.68	1.38	1.54
32	y	617	LUT	C22-C21	-13.67	1.38	1.54
32	Y	315	LUT	C22-C21	-13.65	1.38	1.54
32	r	317	LUT	C22-C21	-13.64	1.38	1.54
32	y	616	LUT	C22-C21	-13.61	1.38	1.54
32	1	616	LUT	C22-C21	-13.59	1.38	1.54
32	Y	316	LUT	C22-C21	-13.53	1.38	1.54
32	1	615	LUT	C22-C21	-13.51	1.38	1.54
32	7	317	LUT	C22-C21	-13.49	1.38	1.54
32	0	616	LUT	C22-C21	-13.42	1.38	1.54
32	9	318	LUT	C22-C21	-13.41	1.38	1.54
32	S	317	LUT	C22-C21	-13.40	1.38	1.54
32	n	317	LUT	C22-C21	-13.37	1.38	1.54
43	C	615	BCR	C5-C6	13.37	1.56	1.34
32	6	317	LUT	C22-C21	-13.36	1.38	1.54
32	8	615	LUT	C22-C21	-13.34	1.38	1.54
32	N	316	LUT	C22-C21	-13.31	1.38	1.54
32	8	616	LUT	C22-C21	-13.31	1.38	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	5	616	LUT	C22-C21	-13.30	1.38	1.54
32	S	318	LUT	C22-C21	-13.30	1.38	1.54
32	G	615	LUT	C22-C21	-13.29	1.38	1.54
32	s	317	LUT	C22-C21	-13.28	1.38	1.54
32	3	317	LUT	C22-C21	-13.27	1.38	1.54
32	n	318	LUT	C22-C21	-13.23	1.38	1.54
32	q	318	LUT	C22-C21	-13.22	1.38	1.54
32	N	317	LUT	C22-C21	-13.21	1.38	1.54
32	7	318	LUT	C22-C21	-13.19	1.38	1.54
32	g	316	LUT	C22-C21	-13.19	1.38	1.54
32	3	318	LUT	C22-C21	-13.18	1.38	1.54
32	4	616	LUT	C22-C21	-13.17	1.38	1.54
32	s	318	LUT	C22-C21	-13.16	1.38	1.54
32	6	318	LUT	C22-C21	-13.12	1.38	1.54
32	0	617	LUT	C22-C21	-13.06	1.38	1.54
32	p	616	LUT	C22-C21	-13.04	1.38	1.54
32	5	617	LUT	C22-C21	-12.92	1.38	1.54
32	p	617	LUT	C22-C21	-12.82	1.39	1.54
32	S	318	LUT	C22-C23	12.61	1.67	1.52
32	2	615	LUT	C22-C21	-12.50	1.39	1.54
32	5	617	LUT	C22-C23	12.42	1.67	1.52
32	g	316	LUT	C22-C23	12.28	1.66	1.52
32	7	318	LUT	C22-C23	12.21	1.66	1.52
32	s	318	LUT	C22-C23	12.21	1.66	1.52
32	p	617	LUT	C22-C23	12.12	1.66	1.52
30	q	309	CHL	C3A-C2A	-12.11	1.44	1.54
32	p	616	LUT	C22-C23	12.10	1.66	1.52
32	2	615	LUT	C22-C23	12.09	1.66	1.52
32	5	616	LUT	C22-C23	12.07	1.66	1.52
32	4	616	LUT	C22-C23	12.07	1.66	1.52
32	G	615	LUT	C22-C23	12.05	1.66	1.52
32	q	318	LUT	C22-C23	12.01	1.66	1.52
30	0	605	CHL	C3A-C2A	-11.98	1.44	1.54
32	6	318	LUT	C22-C23	11.98	1.66	1.52
32	3	318	LUT	C22-C23	11.98	1.66	1.52
32	0	617	LUT	C22-C23	11.90	1.66	1.52
32	N	317	LUT	C22-C23	11.88	1.66	1.52
32	s	317	LUT	C22-C23	11.88	1.66	1.52
32	8	616	LUT	C22-C23	11.88	1.66	1.52
32	n	318	LUT	C22-C23	11.87	1.66	1.52
32	S	317	LUT	C22-C23	11.83	1.66	1.52
32	1	615	LUT	C22-C23	11.82	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	6	317	LUT	C22-C23	11.81	1.66	1.52
32	0	616	LUT	C22-C23	11.76	1.66	1.52
32	y	616	LUT	C2-C3	-11.76	1.35	1.52
32	3	317	LUT	C22-C23	11.76	1.66	1.52
32	1	616	LUT	C22-C23	11.74	1.66	1.52
32	9	318	LUT	C22-C23	11.73	1.66	1.52
32	n	317	LUT	C22-C23	11.69	1.66	1.52
32	Y	316	LUT	C22-C23	11.68	1.66	1.52
32	8	615	LUT	C22-C23	11.68	1.66	1.52
32	r	317	LUT	C2-C3	-11.65	1.35	1.52
32	N	316	LUT	C22-C23	11.65	1.66	1.52
32	y	616	LUT	C22-C23	11.63	1.66	1.52
32	y	617	LUT	C2-C3	-11.63	1.35	1.52
32	7	317	LUT	C22-C23	11.61	1.66	1.52
32	Y	315	LUT	C2-C3	-11.58	1.35	1.52
32	Y	316	LUT	C2-C3	-11.58	1.35	1.52
32	r	317	LUT	C22-C23	11.56	1.66	1.52
32	y	617	LUT	C22-C23	11.55	1.66	1.52
32	8	615	LUT	C2-C3	-11.52	1.36	1.52
32	Y	315	LUT	C22-C23	11.49	1.65	1.52
32	S	317	LUT	C2-C3	-11.48	1.36	1.52
32	n	317	LUT	C2-C3	-11.48	1.36	1.52
32	s	317	LUT	C2-C3	-11.46	1.36	1.52
32	R	317	LUT	C22-C23	11.45	1.65	1.52
32	1	615	LUT	C2-C3	-11.45	1.36	1.52
32	R	317	LUT	C2-C3	-11.44	1.36	1.52
32	7	317	LUT	C2-C3	-11.42	1.36	1.52
32	0	617	LUT	C2-C3	-11.42	1.36	1.52
32	1	616	LUT	C2-C3	-11.38	1.36	1.52
32	3	317	LUT	C2-C3	-11.33	1.36	1.52
32	5	616	LUT	C2-C3	-11.32	1.36	1.52
32	6	318	LUT	C2-C3	-11.30	1.36	1.52
32	N	316	LUT	C2-C3	-11.27	1.36	1.52
32	G	615	LUT	C2-C3	-11.25	1.36	1.52
32	0	616	LUT	C2-C3	-11.25	1.36	1.52
32	6	317	LUT	C2-C3	-11.25	1.36	1.52
32	4	616	LUT	C2-C3	-11.25	1.36	1.52
32	7	318	LUT	C2-C3	-11.24	1.36	1.52
32	n	318	LUT	C2-C3	-11.19	1.36	1.52
32	9	318	LUT	C2-C3	-11.18	1.36	1.52
32	S	318	LUT	C2-C3	-11.18	1.36	1.52
32	8	616	LUT	C2-C3	-11.16	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	5	617	LUT	C2-C3	-11.14	1.36	1.52
32	g	316	LUT	C2-C3	-11.12	1.36	1.52
32	N	317	LUT	C2-C3	-11.11	1.36	1.52
32	p	616	LUT	C2-C3	-11.09	1.36	1.52
32	s	318	LUT	C2-C3	-11.03	1.36	1.52
32	2	615	LUT	C2-C3	-11.02	1.36	1.52
32	3	318	LUT	C2-C3	-11.01	1.36	1.52
32	q	318	LUT	C2-C3	-10.99	1.36	1.52
32	p	617	LUT	C2-C3	-10.88	1.36	1.52
30	1	601	CHL	C3A-C2A	-10.86	1.45	1.54
35	q	317	RRX	C29-C28	-10.51	1.37	1.52
35	G	614	RRX	C29-C28	-10.49	1.37	1.52
35	2	614	RRX	C29-C28	-10.48	1.37	1.52
35	9	317	RRX	C29-C28	-10.47	1.37	1.52
35	4	615	RRX	C29-C28	-10.45	1.37	1.52
35	g	315	RRX	C29-C28	-10.43	1.37	1.52
30	q	310	CHL	C3A-C2A	-9.31	1.46	1.54
30	3	302	CHL	C3A-C2A	-9.15	1.46	1.54
42	A	408	PHO	C1B-C2B	8.94	1.49	1.39
30	G	608	CHL	C3A-C2A	-8.93	1.47	1.54
30	5	607	CHL	C3A-C2A	-8.82	1.47	1.54
42	D	401	PHO	C1B-C2B	8.79	1.49	1.39
30	n	310	CHL	C3A-C2A	-8.73	1.47	1.54
43	B	617	BCR	C30-C25	-8.58	1.42	1.53
30	7	306	CHL	C3A-C2A	-8.57	1.47	1.54
35	g	315	RRX	C27-C28	8.27	1.66	1.52
42	D	401	PHO	C3B-C4B	8.15	1.49	1.41
43	C	615	BCR	C30-C25	-8.14	1.43	1.53
43	b	618	BCR	C30-C25	-8.11	1.43	1.53
30	5	609	CHL	C3A-C2A	-8.10	1.47	1.54
32	3	318	LUT	C4-C3	8.07	1.66	1.52
35	4	615	RRX	C27-C28	8.06	1.66	1.52
43	V	101	BCR	C30-C25	-8.06	1.43	1.53
43	d	406	BCR	C30-C25	-8.06	1.43	1.53
35	9	317	RRX	C27-C28	8.05	1.66	1.52
30	2	608	CHL	C3A-C2A	-8.02	1.47	1.54
30	9	309	CHL	C3A-C2A	-8.02	1.47	1.54
32	p	617	LUT	C4-C3	8.01	1.66	1.52
35	G	614	RRX	C27-C28	8.00	1.66	1.52
32	N	317	LUT	C4-C3	7.99	1.66	1.52
30	p	607	CHL	C3A-C2A	-7.97	1.47	1.54
32	g	316	LUT	C4-C3	7.97	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	q	318	LUT	C4-C3	7.96	1.66	1.52
32	G	615	LUT	C32-C33	7.94	1.63	1.46
35	2	614	RRX	C27-C28	7.94	1.66	1.52
32	S	318	LUT	C4-C3	7.93	1.66	1.52
43	C	614	BCR	C30-C25	-7.93	1.43	1.53
32	5	617	LUT	C4-C3	7.92	1.66	1.52
32	2	615	LUT	C4-C3	7.92	1.66	1.52
42	A	408	PHO	C3B-C4B	7.91	1.49	1.41
30	R	310	CHL	C3A-C2A	-7.89	1.47	1.54
32	8	616	LUT	C4-C3	7.88	1.66	1.52
32	n	318	LUT	C4-C3	7.86	1.66	1.52
35	q	317	RRX	C27-C28	7.86	1.66	1.52
32	p	616	LUT	C4-C3	7.86	1.66	1.52
43	c	615	BCR	C30-C25	-7.85	1.43	1.53
32	3	317	LUT	C4-C3	7.84	1.66	1.52
32	N	316	LUT	C4-C3	7.81	1.65	1.52
32	9	318	LUT	C4-C3	7.79	1.65	1.52
32	s	318	LUT	C4-C3	7.78	1.65	1.52
32	6	317	LUT	C4-C3	7.78	1.65	1.52
32	S	317	LUT	C4-C3	7.78	1.65	1.52
32	G	615	LUT	C4-C3	7.77	1.65	1.52
32	4	616	LUT	C4-C3	7.77	1.65	1.52
30	N	308	CHL	C3A-C2A	-7.76	1.48	1.54
30	g	309	CHL	C3A-C2A	-7.76	1.48	1.54
32	7	318	LUT	C4-C3	7.76	1.65	1.52
30	1	609	CHL	C3A-C2A	-7.75	1.48	1.54
30	3	310	CHL	C3A-C2A	-7.75	1.48	1.54
32	0	616	LUT	C4-C3	7.73	1.65	1.52
32	s	317	LUT	C4-C3	7.73	1.65	1.52
30	0	609	CHL	C3A-C2A	-7.72	1.48	1.54
32	5	616	LUT	C4-C3	7.71	1.65	1.52
32	0	617	LUT	C4-C3	7.70	1.65	1.52
32	p	616	LUT	C32-C33	7.70	1.62	1.46
43	A	410	BCR	C30-C25	-7.69	1.43	1.53
32	6	318	LUT	C4-C3	7.69	1.65	1.52
43	h	101	BCR	C30-C25	-7.66	1.44	1.53
32	8	615	LUT	C4-C3	7.64	1.65	1.52
32	Y	316	LUT	C4-C3	7.64	1.65	1.52
43	t	101	BCR	C30-C25	-7.64	1.44	1.53
43	B	619	BCR	C30-C25	-7.62	1.44	1.53
32	n	317	LUT	C4-C3	7.62	1.65	1.52
32	2	615	LUT	C32-C33	7.61	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	309	CHL	C3A-C2A	-7.61	1.48	1.54
43	Z	101	BCR	C30-C25	-7.60	1.44	1.53
43	B	617	BCR	C1-C6	-7.58	1.44	1.53
32	g	316	LUT	C32-C33	7.58	1.62	1.46
32	1	615	LUT	C4-C3	7.58	1.65	1.52
43	H	101	BCR	C30-C25	-7.58	1.44	1.53
43	b	620	BCR	C30-C25	-7.58	1.44	1.53
43	v	101	BCR	C30-C25	-7.57	1.44	1.53
32	p	617	LUT	C32-C33	7.57	1.62	1.46
32	7	317	LUT	C4-C3	7.56	1.65	1.52
32	9	318	LUT	C32-C33	7.55	1.62	1.46
43	c	615	BCR	C1-C6	-7.54	1.44	1.53
32	y	617	LUT	C4-C3	7.54	1.65	1.52
32	5	617	LUT	C32-C33	7.54	1.62	1.46
32	R	317	LUT	C4-C3	7.53	1.65	1.52
43	c	614	BCR	C30-C25	-7.52	1.44	1.53
32	3	318	LUT	C32-C33	7.52	1.62	1.46
43	t	101	BCR	C2-C3	-7.50	1.34	1.52
43	z	101	BCR	C1-C6	-7.50	1.44	1.53
32	5	616	LUT	C32-C33	7.50	1.62	1.46
32	q	318	LUT	C32-C33	7.50	1.62	1.46
32	4	616	LUT	C32-C33	7.49	1.62	1.46
30	Y	301	CHL	C3A-C2A	-7.48	1.48	1.54
43	D	405	BCR	C30-C25	-7.47	1.44	1.53
43	z	101	BCR	C30-C25	-7.47	1.44	1.53
43	Z	101	BCR	C1-C6	-7.46	1.44	1.53
32	N	317	LUT	C32-C33	7.46	1.61	1.46
32	1	616	LUT	C4-C3	7.46	1.65	1.52
32	S	318	LUT	C32-C33	7.44	1.61	1.46
32	Y	315	LUT	C4-C3	7.43	1.65	1.52
32	3	317	LUT	C32-C33	7.43	1.61	1.46
32	6	318	LUT	C32-C33	7.42	1.61	1.46
32	r	317	LUT	C4-C3	7.41	1.65	1.52
32	N	316	LUT	C32-C33	7.41	1.61	1.46
43	B	618	BCR	C30-C25	-7.41	1.44	1.53
43	T	101	BCR	C30-C25	-7.38	1.44	1.53
32	y	616	LUT	C4-C3	7.38	1.65	1.52
30	Y	307	CHL	C3A-C2A	-7.37	1.48	1.54
32	8	616	LUT	C32-C33	7.37	1.61	1.46
43	C	614	BCR	C1-C6	-7.37	1.44	1.53
32	7	318	LUT	C32-C33	7.36	1.61	1.46
32	n	318	LUT	C32-C33	7.35	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	6	309	CHL	C3A-C2A	-7.35	1.48	1.54
43	C	615	BCR	C1-C6	-7.35	1.44	1.53
32	1	615	LUT	C1-C6	-7.34	1.44	1.53
43	B	619	BCR	C1-C6	-7.34	1.44	1.53
43	V	101	BCR	C1-C6	-7.32	1.44	1.53
32	Y	316	LUT	C1-C6	-7.31	1.44	1.53
43	T	101	BCR	C2-C3	-7.30	1.35	1.52
35	g	315	RRX	C30-C25	-7.30	1.44	1.53
32	n	317	LUT	C32-C33	7.30	1.61	1.46
43	b	619	BCR	C1-C6	-7.30	1.44	1.53
32	8	615	LUT	C32-C33	7.30	1.61	1.46
32	R	317	LUT	C1-C6	-7.29	1.44	1.53
32	s	317	LUT	C32-C33	7.29	1.61	1.46
43	b	619	BCR	C30-C25	-7.28	1.44	1.53
32	S	317	LUT	C32-C33	7.28	1.61	1.46
32	6	317	LUT	C32-C33	7.28	1.61	1.46
32	s	318	LUT	C32-C33	7.27	1.61	1.46
32	y	617	LUT	C1-C6	-7.27	1.44	1.53
43	b	620	BCR	C1-C6	-7.27	1.44	1.53
43	d	406	BCR	C2-C3	-7.26	1.35	1.52
43	C	615	BCR	C2-C3	-7.25	1.35	1.52
43	v	101	BCR	C1-C6	-7.24	1.44	1.53
43	a	410	BCR	C30-C25	-7.22	1.44	1.53
32	0	617	LUT	C32-C33	7.21	1.61	1.46
30	1	608	CHL	C3A-C2A	-7.21	1.48	1.54
32	R	317	LUT	C32-C33	7.21	1.61	1.46
32	0	617	LUT	C1-C6	-7.20	1.44	1.53
43	h	101	BCR	C1-C6	-7.17	1.44	1.53
43	Z	101	BCR	C2-C3	-7.17	1.35	1.52
32	7	317	LUT	C1-C6	-7.17	1.44	1.53
32	y	616	LUT	C1-C6	-7.17	1.44	1.53
43	a	410	BCR	C1-C6	-7.17	1.44	1.53
43	z	101	BCR	C2-C3	-7.12	1.35	1.52
43	c	614	BCR	C2-C3	-7.10	1.35	1.52
43	h	101	BCR	C2-C3	-7.10	1.35	1.52
32	2	615	LUT	C1-C6	-7.10	1.44	1.53
32	3	318	LUT	C1-C6	-7.09	1.44	1.53
43	B	617	BCR	C2-C3	-7.09	1.35	1.52
32	8	616	LUT	C1-C6	-7.09	1.44	1.53
43	H	101	BCR	C2-C3	-7.09	1.35	1.52
32	0	616	LUT	C1-C6	-7.09	1.44	1.53
32	Y	316	LUT	C32-C33	7.08	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1	616	LUT	C32-C33	7.08	1.61	1.46
32	r	317	LUT	C1-C6	-7.08	1.44	1.53
32	N	317	LUT	C1-C6	-7.08	1.44	1.53
32	Y	315	LUT	C1-C6	-7.08	1.44	1.53
32	0	616	LUT	C32-C33	7.07	1.61	1.46
43	b	620	BCR	C2-C3	-7.07	1.35	1.52
43	B	619	BCR	C2-C3	-7.06	1.35	1.52
43	a	410	BCR	C2-C3	-7.06	1.35	1.52
43	H	101	BCR	C1-C6	-7.05	1.44	1.53
32	7	317	LUT	C32-C33	7.04	1.61	1.46
43	v	101	BCR	C2-C3	-7.03	1.35	1.52
32	n	318	LUT	C1-C6	-7.03	1.44	1.53
30	r	308	CHL	C3A-C2A	-7.03	1.48	1.54
43	b	618	BCR	C2-C3	-7.02	1.35	1.52
43	C	615	BCR	C29-C28	-7.02	1.35	1.52
43	A	410	BCR	C2-C3	-7.02	1.35	1.52
43	V	101	BCR	C2-C3	-7.00	1.36	1.52
32	y	617	LUT	C32-C33	7.00	1.60	1.46
43	A	410	BCR	C1-C6	-6.99	1.44	1.53
30	N	307	CHL	C3A-C2A	-6.98	1.48	1.54
43	D	405	BCR	C2-C3	-6.98	1.36	1.52
43	C	614	BCR	C2-C3	-6.98	1.36	1.52
43	t	101	BCR	C1-C6	-6.96	1.44	1.53
32	1	616	LUT	C1-C6	-6.94	1.44	1.53
30	8	608	CHL	C3A-C2A	-6.94	1.48	1.54
32	g	316	LUT	C1-C6	-6.94	1.44	1.53
32	q	318	LUT	C1-C6	-6.94	1.44	1.53
32	1	615	LUT	C32-C33	6.93	1.60	1.46
30	p	609	CHL	C3A-C2A	-6.93	1.48	1.54
30	q	308	CHL	C3A-C2A	-6.93	1.48	1.54
43	b	618	BCR	C1-C6	-6.92	1.44	1.53
43	c	615	BCR	C2-C3	-6.92	1.36	1.52
43	B	618	BCR	C1-C6	-6.92	1.44	1.53
35	q	317	RRX	C2-C3	-6.91	1.36	1.52
32	p	617	LUT	C1-C6	-6.91	1.44	1.53
43	B	618	BCR	C2-C3	-6.91	1.36	1.52
43	T	101	BCR	C1-C6	-6.90	1.45	1.53
35	2	614	RRX	C30-C25	-6.88	1.45	1.53
30	4	607	CHL	C3A-C2A	-6.88	1.48	1.54
32	Y	315	LUT	C32-C33	6.87	1.60	1.46
32	6	317	LUT	C1-C6	-6.87	1.45	1.53
32	s	318	LUT	C1-C6	-6.86	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	N	316	LUT	C1-C6	-6.86	1.45	1.53
32	6	318	LUT	C1-C6	-6.85	1.45	1.53
43	B	617	BCR	C29-C28	-6.85	1.36	1.52
43	b	619	BCR	C2-C3	-6.85	1.36	1.52
43	d	406	BCR	C1-C6	-6.84	1.45	1.53
43	a	410	BCR	C29-C28	-6.84	1.36	1.52
32	S	317	LUT	C1-C6	-6.84	1.45	1.53
32	4	616	LUT	C1-C6	-6.84	1.45	1.53
43	d	406	BCR	C29-C28	-6.84	1.36	1.52
32	y	616	LUT	C32-C33	6.84	1.60	1.46
30	Y	306	CHL	C3A-C2A	-6.83	1.48	1.54
32	7	318	LUT	C1-C6	-6.83	1.45	1.53
32	S	318	LUT	C1-C6	-6.82	1.45	1.53
32	r	317	LUT	C32-C33	6.81	1.60	1.46
43	z	101	BCR	C29-C28	-6.80	1.36	1.52
32	5	617	LUT	C1-C6	-6.80	1.45	1.53
35	G	614	RRX	C30-C25	-6.80	1.45	1.53
43	Z	101	BCR	C29-C28	-6.80	1.36	1.52
35	2	614	RRX	C2-C3	-6.78	1.36	1.52
43	c	614	BCR	C29-C28	-6.78	1.36	1.52
35	4	615	RRX	C30-C25	-6.78	1.45	1.53
35	G	614	RRX	C2-C3	-6.78	1.36	1.52
35	q	317	RRX	C30-C25	-6.78	1.45	1.53
32	s	317	LUT	C1-C6	-6.77	1.45	1.53
32	p	616	LUT	C1-C6	-6.76	1.45	1.53
43	D	405	BCR	C1-C6	-6.76	1.45	1.53
32	9	318	LUT	C1-C6	-6.76	1.45	1.53
43	B	618	BCR	C29-C28	-6.75	1.36	1.52
35	9	317	RRX	C2-C3	-6.74	1.36	1.52
35	4	615	RRX	C2-C3	-6.74	1.36	1.52
32	G	615	LUT	C1-C6	-6.74	1.45	1.53
35	9	317	RRX	C30-C25	-6.74	1.45	1.53
43	c	614	BCR	C1-C6	-6.74	1.45	1.53
35	g	315	RRX	C2-C3	-6.74	1.36	1.52
43	b	619	BCR	C29-C28	-6.73	1.36	1.52
43	B	619	BCR	C29-C28	-6.72	1.36	1.52
30	r	310	CHL	C3A-C2A	-6.71	1.48	1.54
43	h	101	BCR	C29-C28	-6.70	1.36	1.52
36	3	319	NEX	C35-C15	-6.70	1.17	1.36
32	8	615	LUT	C1-C6	-6.69	1.45	1.53
30	0	608	CHL	C3A-C2A	-6.68	1.48	1.54
35	q	317	RRX	C1-C6	-6.67	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	H	101	BCR	C29-C28	-6.67	1.36	1.52
43	b	620	BCR	C29-C28	-6.66	1.36	1.52
32	n	317	LUT	C1-C6	-6.66	1.45	1.53
32	3	317	LUT	C1-C6	-6.65	1.45	1.53
43	T	101	BCR	C29-C28	-6.65	1.36	1.52
36	s	319	NEX	C35-C15	-6.65	1.18	1.36
35	2	614	RRX	C1-C6	-6.64	1.45	1.53
43	t	101	BCR	C29-C28	-6.64	1.36	1.52
36	9	319	NEX	C35-C15	-6.64	1.18	1.36
43	v	101	BCR	C29-C28	-6.64	1.36	1.52
36	R	301	NEX	C35-C15	-6.64	1.18	1.36
36	S	319	NEX	C35-C15	-6.62	1.18	1.36
36	R	319	NEX	C35-C15	-6.60	1.18	1.36
43	A	410	BCR	C29-C28	-6.60	1.37	1.52
36	r	319	NEX	C35-C15	-6.59	1.18	1.36
36	G	616	NEX	C35-C15	-6.59	1.18	1.36
43	c	615	BCR	C29-C28	-6.58	1.37	1.52
36	p	618	NEX	C35-C15	-6.57	1.18	1.36
30	9	308	CHL	C3A-C2A	-6.57	1.49	1.54
43	b	618	BCR	C29-C28	-6.57	1.37	1.52
35	4	615	RRX	C1-C6	-6.56	1.45	1.53
36	y	618	NEX	C35-C15	-6.56	1.18	1.36
35	9	317	RRX	C1-C6	-6.56	1.45	1.53
30	9	307	CHL	C3A-C2A	-6.56	1.49	1.54
36	6	319	NEX	C35-C15	-6.55	1.18	1.36
36	0	618	NEX	C35-C15	-6.55	1.18	1.36
30	9	311	CHL	C3A-C2A	-6.55	1.49	1.54
36	r	301	NEX	C35-C15	-6.55	1.18	1.36
35	G	614	RRX	C1-C6	-6.54	1.45	1.53
36	q	319	NEX	C35-C15	-6.54	1.18	1.36
36	8	617	NEX	C35-C15	-6.54	1.18	1.36
36	2	616	NEX	C35-C15	-6.53	1.18	1.36
43	D	405	BCR	C29-C28	-6.52	1.37	1.52
36	Y	317	NEX	C35-C15	-6.52	1.18	1.36
36	5	618	NEX	C35-C15	-6.52	1.18	1.36
43	C	614	BCR	C29-C28	-6.51	1.37	1.52
36	4	617	NEX	C35-C15	-6.51	1.18	1.36
30	4	609	CHL	C3A-C2A	-6.50	1.49	1.54
32	5	616	LUT	C1-C6	-6.48	1.45	1.53
31	B	604	CLA	MG-NA	6.48	2.21	2.06
36	g	317	NEX	C35-C15	-6.47	1.18	1.36
36	N	318	NEX	C35-C15	-6.47	1.18	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	605	CLA	MG-NA	6.46	2.21	2.06
31	5	615	CLA	MG-NA	6.46	2.21	2.06
35	g	315	RRX	C1-C6	-6.46	1.45	1.53
36	n	319	NEX	C35-C15	-6.45	1.18	1.36
30	g	307	CHL	C3A-C2A	-6.44	1.49	1.54
36	9	319	NEX	C11-C12	-6.43	1.17	1.34
36	s	319	NEX	C11-C12	-6.42	1.17	1.34
30	g	306	CHL	C3A-C2A	-6.42	1.49	1.54
30	Y	308	CHL	C3A-C2A	-6.41	1.49	1.54
30	N	306	CHL	C3A-C2A	-6.41	1.49	1.54
36	9	319	NEX	C31-C32	-6.41	1.18	1.34
43	V	101	BCR	C29-C28	-6.39	1.37	1.52
30	1	606	CHL	C3A-C2A	-6.38	1.49	1.54
31	G	610	CLA	MG-NA	6.38	2.21	2.06
36	3	319	NEX	C11-C12	-6.38	1.18	1.34
31	g	311	CLA	MG-NA	6.37	2.21	2.06
30	7	307	CHL	C3A-C2A	-6.37	1.49	1.54
31	2	604	CLA	MG-NA	6.37	2.21	2.06
36	S	319	NEX	C11-C12	-6.37	1.18	1.34
36	s	319	NEX	C31-C32	-6.37	1.18	1.34
36	G	616	NEX	C31-C32	-6.36	1.18	1.34
36	R	301	NEX	C11-C12	-6.35	1.18	1.34
36	y	618	NEX	C11-C12	-6.35	1.18	1.34
30	7	321	CHL	C3A-C2A	-6.35	1.49	1.54
31	6	304	CLA	MG-NA	6.35	2.21	2.06
36	p	618	NEX	C11-C12	-6.35	1.18	1.34
30	n	308	CHL	C3A-C2A	-6.34	1.49	1.54
36	4	617	NEX	C11-C12	-6.34	1.18	1.34
36	g	317	NEX	C11-C12	-6.33	1.18	1.34
30	G	601	CHL	C3A-C2A	-6.33	1.49	1.54
31	G	613	CLA	MG-NA	6.33	2.21	2.06
30	5	606	CHL	C3A-C2A	-6.33	1.49	1.54
36	S	319	NEX	C31-C32	-6.33	1.18	1.34
30	n	309	CHL	C3A-C2A	-6.32	1.49	1.54
31	q	304	CLA	MG-NA	6.32	2.21	2.06
36	2	616	NEX	C11-C12	-6.32	1.18	1.34
36	6	319	NEX	C11-C12	-6.32	1.18	1.34
36	R	319	NEX	C11-C12	-6.32	1.18	1.34
31	6	312	CLA	MG-NA	6.32	2.21	2.06
30	0	606	CHL	C3A-C2A	-6.31	1.49	1.54
36	R	319	NEX	C31-C32	-6.31	1.18	1.34
31	q	316	CLA	MG-NA	6.31	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	609	CLA	MG-NA	6.31	2.21	2.06
31	Y	313	CLA	MG-NA	6.31	2.21	2.06
36	y	618	NEX	C31-C32	-6.31	1.18	1.34
36	0	618	NEX	C11-C12	-6.31	1.18	1.34
31	S	314	CLA	MG-NA	6.31	2.21	2.06
36	G	616	NEX	C11-C12	-6.31	1.18	1.34
31	b	607	CLA	MG-NA	6.30	2.21	2.06
36	0	618	NEX	C31-C32	-6.30	1.18	1.34
31	4	603	CLA	MG-NA	6.30	2.21	2.06
31	7	314	CLA	MG-NA	6.30	2.21	2.06
31	p	612	CLA	MG-NA	6.30	2.21	2.06
36	3	319	NEX	C31-C32	-6.30	1.18	1.34
31	0	603	CLA	MG-NA	6.30	2.21	2.06
31	9	315	CLA	MG-NA	6.29	2.21	2.06
36	r	319	NEX	C31-C32	-6.29	1.18	1.34
31	5	612	CLA	MG-NA	6.29	2.21	2.06
31	B	606	CLA	MG-NA	6.29	2.21	2.06
31	n	314	CLA	MG-NA	6.29	2.21	2.06
36	6	319	NEX	C31-C32	-6.29	1.18	1.34
36	5	618	NEX	C11-C12	-6.29	1.18	1.34
31	N	311	CLA	MG-NA	6.29	2.21	2.06
31	7	304	CLA	MG-NA	6.29	2.21	2.06
31	3	305	CLA	MG-NA	6.29	2.21	2.06
31	9	305	CLA	MG-NA	6.28	2.21	2.06
36	Y	317	NEX	C11-C12	-6.28	1.18	1.34
31	7	313	CLA	MG-NA	6.28	2.21	2.06
36	p	618	NEX	C31-C32	-6.28	1.18	1.34
31	N	313	CLA	MG-NA	6.28	2.21	2.06
36	r	319	NEX	C11-C12	-6.27	1.18	1.34
31	8	612	CLA	MG-NA	6.27	2.21	2.06
31	3	315	CLA	MG-NA	6.27	2.21	2.06
31	5	603	CLA	MG-NA	6.27	2.21	2.06
31	9	313	CLA	MG-NA	6.27	2.21	2.06
31	4	604	CLA	MG-NA	6.27	2.21	2.06
31	Y	304	CLA	MG-NA	6.27	2.21	2.06
31	q	305	CLA	MG-NA	6.27	2.21	2.06
31	4	611	CLA	MG-NA	6.27	2.21	2.06
31	5	602	CLA	MG-NA	6.27	2.21	2.06
31	G	611	CLA	MG-NA	6.27	2.21	2.06
36	2	616	NEX	C31-C32	-6.26	1.18	1.34
31	0	613	CLA	MG-NA	6.26	2.21	2.06
36	Y	317	NEX	C31-C32	-6.26	1.18	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	611	CLA	MG-NA	6.26	2.21	2.06
31	R	307	CLA	MG-NA	6.26	2.21	2.06
31	n	315	CLA	MG-NA	6.26	2.21	2.06
31	s	304	CLA	MG-NA	6.26	2.21	2.06
31	0	612	CLA	MG-NA	6.26	2.21	2.06
31	p	611	CLA	MG-NA	6.26	2.21	2.06
36	8	617	NEX	C31-C32	-6.26	1.18	1.34
31	3	313	CLA	MG-NA	6.26	2.21	2.06
31	8	613	CLA	MG-NA	6.26	2.21	2.06
31	s	314	CLA	MG-NA	6.26	2.21	2.06
31	g	313	CLA	MG-NA	6.25	2.21	2.06
31	5	614	CLA	MG-NA	6.25	2.21	2.06
31	c	601	CLA	MG-NA	6.25	2.21	2.06
31	0	614	CLA	MG-NA	6.25	2.21	2.06
31	1	613	CLA	MG-NA	6.25	2.21	2.06
36	5	618	NEX	C31-C32	-6.25	1.18	1.34
31	p	602	CLA	MG-NA	6.25	2.21	2.06
31	1	612	CLA	MG-NA	6.25	2.21	2.06
31	6	314	CLA	MG-NA	6.25	2.21	2.06
31	G	602	CLA	MG-NA	6.24	2.21	2.06
36	8	617	NEX	C11-C12	-6.24	1.18	1.34
31	9	316	CLA	MG-NA	6.24	2.21	2.06
31	p	610	CLA	MG-NA	6.24	2.21	2.06
31	2	602	CLA	MG-NA	6.24	2.21	2.06
36	N	318	NEX	C31-C32	-6.24	1.18	1.34
31	3	312	CLA	MG-NA	6.24	2.21	2.06
31	S	316	CLA	MG-NA	6.24	2.21	2.06
31	0	611	CLA	MG-NA	6.24	2.21	2.06
31	3	304	CLA	MG-NA	6.23	2.21	2.06
31	y	603	CLA	MG-NA	6.23	2.21	2.06
36	r	301	NEX	C31-C32	-6.23	1.18	1.34
31	2	603	CLA	MG-NA	6.23	2.21	2.06
31	S	310	CLA	MG-NA	6.23	2.21	2.06
31	1	603	CLA	MG-NA	6.23	2.21	2.06
31	7	303	CLA	MG-NA	6.23	2.21	2.06
31	n	312	CLA	MG-NA	6.23	2.21	2.06
31	B	611	CLA	MG-NA	6.23	2.21	2.06
31	5	613	CLA	MG-NA	6.23	2.21	2.06
31	g	305	CLA	MG-NA	6.23	2.21	2.06
31	8	603	CLA	MG-NA	6.23	2.21	2.06
31	y	614	CLA	MG-NA	6.23	2.21	2.06
31	4	610	CLA	MG-NA	6.23	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	602	CLA	MG-NA	6.23	2.21	2.06
36	R	301	NEX	C31-C32	-6.23	1.18	1.34
31	4	602	CLA	MG-NA	6.23	2.21	2.06
31	s	312	CLA	MG-NA	6.23	2.21	2.06
31	3	314	CLA	MG-NA	6.23	2.21	2.06
31	G	612	CLA	MG-NA	6.22	2.21	2.06
31	r	307	CLA	MG-NA	6.22	2.21	2.06
31	Y	303	CLA	MG-NA	6.22	2.21	2.06
31	n	313	CLA	MG-NA	6.22	2.21	2.06
31	C	603	CLA	MG-NA	6.22	2.21	2.06
31	b	609	CLA	MG-NA	6.22	2.21	2.06
31	S	306	CLA	MG-NA	6.22	2.21	2.06
31	8	609	CLA	MG-NA	6.22	2.21	2.06
31	Y	310	CLA	MG-NA	6.22	2.21	2.06
30	s	309	CHL	C3A-C2A	-6.22	1.49	1.54
31	s	306	CLA	MG-NA	6.21	2.21	2.06
31	b	612	CLA	MG-NA	6.21	2.21	2.06
31	5	611	CLA	MG-NA	6.21	2.21	2.06
36	4	617	NEX	C31-C32	-6.21	1.18	1.34
31	N	314	CLA	MG-NA	6.21	2.21	2.06
31	Y	312	CLA	MG-NA	6.21	2.21	2.06
31	c	603	CLA	MG-NA	6.21	2.21	2.06
31	g	314	CLA	MG-NA	6.21	2.21	2.06
31	n	311	CLA	MG-NA	6.21	2.21	2.06
31	7	311	CLA	MG-NA	6.21	2.21	2.06
31	8	610	CLA	MG-NA	6.21	2.21	2.06
31	7	316	CLA	MG-NA	6.21	2.21	2.06
31	p	603	CLA	MG-NA	6.21	2.21	2.06
31	7	315	CLA	MG-NA	6.21	2.21	2.06
31	s	316	CLA	MG-NA	6.21	2.21	2.06
31	5	604	CLA	MG-NA	6.21	2.21	2.06
31	N	312	CLA	MG-NA	6.21	2.21	2.06
31	7	312	CLA	MG-NA	6.21	2.21	2.06
31	4	614	CLA	MG-NA	6.20	2.21	2.06
31	N	315	CLA	MG-NA	6.20	2.21	2.06
31	b	614	CLA	MG-NA	6.20	2.21	2.06
31	6	316	CLA	MG-NA	6.20	2.21	2.06
31	B	614	CLA	MG-NA	6.20	2.21	2.06
31	S	304	CLA	MG-NA	6.20	2.21	2.06
31	8	614	CLA	MG-NA	6.20	2.21	2.06
31	2	610	CLA	MG-NA	6.20	2.21	2.06
31	1	614	CLA	MG-NA	6.20	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	611	CLA	MG-NA	6.20	2.21	2.06
31	g	312	CLA	MG-NA	6.20	2.21	2.06
31	8	604	CLA	MG-NA	6.20	2.21	2.06
31	r	313	CLA	MG-NA	6.20	2.21	2.06
31	s	303	CLA	MG-NA	6.20	2.21	2.06
31	C	611	CLA	MG-NA	6.19	2.21	2.06
31	9	306	CLA	MG-NA	6.19	2.21	2.06
31	3	311	CLA	MG-NA	6.19	2.21	2.06
31	N	304	CLA	MG-NA	6.19	2.21	2.06
31	N	303	CLA	MG-NA	6.19	2.21	2.06
31	b	603	CLA	MG-NA	6.19	2.21	2.06
31	y	602	CLA	MG-NA	6.19	2.21	2.06
31	S	305	CLA	MG-NA	6.19	2.21	2.06
31	8	611	CLA	MG-NA	6.19	2.21	2.06
31	n	303	CLA	MG-NA	6.19	2.21	2.06
36	g	317	NEX	C31-C32	-6.19	1.18	1.34
36	r	301	NEX	C11-C12	-6.19	1.18	1.34
31	C	601	CLA	MG-NA	6.19	2.21	2.06
31	p	614	CLA	MG-NA	6.19	2.21	2.06
31	B	610	CLA	MG-NA	6.18	2.21	2.06
31	p	604	CLA	MG-NA	6.18	2.21	2.06
31	N	321	CLA	MG-NA	6.18	2.21	2.06
31	y	610	CLA	MG-NA	6.18	2.21	2.06
31	3	306	CLA	MG-NA	6.18	2.21	2.06
31	N	310	CLA	MG-NA	6.18	2.20	2.06
31	q	312	CLA	MG-NA	6.18	2.20	2.06
31	2	613	CLA	MG-NA	6.18	2.20	2.06
31	2	612	CLA	MG-NA	6.18	2.20	2.06
31	a	407	CLA	MG-NA	6.18	2.20	2.06
31	6	313	CLA	MG-NA	6.18	2.20	2.06
31	G	603	CLA	MG-NA	6.17	2.20	2.06
36	q	319	NEX	C31-C32	-6.17	1.18	1.34
31	R	303	CLA	MG-NA	6.17	2.20	2.06
31	y	604	CLA	MG-NA	6.17	2.20	2.06
31	B	613	CLA	MG-NA	6.17	2.20	2.06
31	b	613	CLA	MG-NA	6.17	2.20	2.06
31	6	311	CLA	MG-NA	6.17	2.20	2.06
31	b	604	CLA	MG-NA	6.17	2.20	2.06
31	R	306	CLA	MG-NA	6.17	2.20	2.06
31	R	313	CLA	MG-NA	6.17	2.20	2.06
31	b	615	CLA	MG-NA	6.17	2.20	2.06
31	r	314	CLA	MG-NA	6.17	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y	314	CLA	MG-NA	6.17	2.20	2.06
31	c	602	CLA	MG-NA	6.17	2.20	2.06
31	s	310	CLA	MG-NA	6.17	2.20	2.06
36	q	319	NEX	C11-C12	-6.17	1.18	1.34
31	6	303	CLA	MG-NA	6.17	2.20	2.06
31	S	313	CLA	MG-NA	6.17	2.20	2.06
31	n	305	CLA	MG-NA	6.17	2.20	2.06
31	4	613	CLA	MG-NA	6.16	2.20	2.06
31	g	304	CLA	MG-NA	6.16	2.20	2.06
31	s	305	CLA	MG-NA	6.16	2.20	2.06
31	S	303	CLA	MG-NA	6.16	2.20	2.06
31	0	615	CLA	MG-NA	6.16	2.20	2.06
31	1	602	CLA	MG-NA	6.16	2.20	2.06
31	n	316	CLA	MG-NA	6.15	2.20	2.06
30	G	607	CHL	C3A-C2A	-6.15	1.49	1.54
31	Y	311	CLA	MG-NA	6.15	2.20	2.06
30	S	308	CHL	C3A-C2A	-6.15	1.49	1.54
31	B	608	CLA	MG-NA	6.15	2.20	2.06
31	Y	305	CLA	MG-NA	6.14	2.20	2.06
31	5	610	CLA	MG-NA	6.14	2.20	2.06
36	n	319	NEX	C11-C12	-6.14	1.18	1.34
31	G	604	CLA	MG-NA	6.14	2.20	2.06
31	N	305	CLA	MG-NA	6.14	2.20	2.06
35	9	317	RRX	C19-C18	6.14	1.59	1.46
31	r	305	CLA	MG-NA	6.14	2.20	2.06
31	s	313	CLA	MG-NA	6.14	2.20	2.06
31	y	615	CLA	MG-NA	6.14	2.20	2.06
31	c	611	CLA	MG-NA	6.14	2.20	2.06
31	y	612	CLA	MG-NA	6.13	2.20	2.06
31	n	304	CLA	MG-NA	6.13	2.20	2.06
31	6	315	CLA	MG-NA	6.13	2.20	2.06
31	c	607	CLA	MG-NA	6.13	2.20	2.06
35	4	615	RRX	C19-C18	6.13	1.59	1.46
31	2	611	CLA	MG-NA	6.13	2.20	2.06
31	B	612	CLA	MG-NA	6.13	2.20	2.06
31	b	617	CLA	MG-NA	6.12	2.20	2.06
31	r	316	CLA	MG-NA	6.12	2.20	2.06
31	B	601	CLA	MG-NA	6.12	2.20	2.06
31	S	315	CLA	MG-NA	6.12	2.20	2.06
31	p	615	CLA	MG-NA	6.12	2.20	2.06
31	6	305	CLA	MG-NA	6.12	2.20	2.06
31	C	602	CLA	MG-NA	6.11	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	305	CLA	MG-NA	6.11	2.20	2.06
31	C	612	CLA	MG-NA	6.11	2.20	2.06
31	C	607	CLA	MG-NA	6.11	2.20	2.06
31	0	602	CLA	MG-NA	6.11	2.20	2.06
31	S	312	CLA	MG-NA	6.11	2.20	2.06
31	9	304	CLA	MG-NA	6.11	2.20	2.06
31	B	602	CLA	MG-NA	6.10	2.20	2.06
31	c	608	CLA	MG-NA	6.10	2.20	2.06
31	b	610	CLA	MG-NA	6.10	2.20	2.06
31	c	609	CLA	MG-NA	6.10	2.20	2.06
31	q	306	CLA	MG-NA	6.10	2.20	2.06
36	n	319	NEX	C31-C32	-6.10	1.18	1.34
31	r	304	CLA	MG-NA	6.10	2.20	2.06
31	r	306	CLA	MG-NA	6.10	2.20	2.06
31	p	613	CLA	MG-NA	6.09	2.20	2.06
31	d	405	CLA	MG-NA	6.09	2.20	2.06
31	C	606	CLA	MG-NA	6.09	2.20	2.06
31	C	613	CLA	MG-NA	6.09	2.20	2.06
31	b	616	CLA	MG-NA	6.09	2.20	2.06
31	B	603	CLA	MG-NA	6.09	2.20	2.06
31	R	314	CLA	MG-NA	6.09	2.20	2.06
31	s	315	CLA	MG-NA	6.08	2.20	2.06
35	G	614	RRX	C19-C18	6.08	1.59	1.46
31	B	616	CLA	MG-NA	6.08	2.20	2.06
31	1	610	CLA	MG-NA	6.08	2.20	2.06
31	B	615	CLA	MG-NA	6.08	2.20	2.06
31	S	311	CLA	MG-NA	6.08	2.20	2.06
31	R	305	CLA	MG-NA	6.07	2.20	2.06
31	y	611	CLA	MG-NA	6.07	2.20	2.06
31	s	311	CLA	MG-NA	6.07	2.20	2.06
31	C	610	CLA	MG-NA	6.07	2.20	2.06
31	c	613	CLA	MG-NA	6.07	2.20	2.06
31	c	612	CLA	MG-NA	6.07	2.20	2.06
30	n	301	CHL	C3A-C2A	-6.06	1.49	1.54
31	B	609	CLA	MG-NA	6.06	2.20	2.06
31	R	304	CLA	MG-NA	6.06	2.20	2.06
31	c	605	CLA	MG-NA	6.06	2.20	2.06
35	2	614	RRX	C19-C18	6.06	1.58	1.46
30	R	308	CHL	C3A-C2A	-6.05	1.49	1.54
31	q	314	CLA	MG-NA	6.05	2.20	2.06
31	C	609	CLA	MG-NA	6.05	2.20	2.06
31	B	605	CLA	MG-NA	6.05	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	604	CLA	MG-NA	6.05	2.20	2.06
36	N	318	NEX	C11-C12	-6.05	1.18	1.34
31	D	403	CLA	MG-NA	6.04	2.20	2.06
31	R	312	CLA	MG-NA	6.04	2.20	2.06
31	d	401	CLA	MG-NA	6.04	2.20	2.06
31	R	316	CLA	MG-NA	6.04	2.20	2.06
31	c	606	CLA	MG-NA	6.04	2.20	2.06
31	g	310	CLA	MG-NA	6.03	2.20	2.06
35	g	315	RRX	C19-C18	6.03	1.58	1.46
31	A	406	CLA	MG-NA	6.03	2.20	2.06
31	a	406	CLA	MG-NA	6.03	2.20	2.06
31	C	608	CLA	MG-NA	6.02	2.20	2.06
31	b	606	CLA	MG-NA	6.02	2.20	2.06
31	b	608	CLA	MG-NA	6.02	2.20	2.06
31	0	604	CLA	MG-NA	6.01	2.20	2.06
31	b	602	CLA	MG-NA	6.01	2.20	2.06
31	R	315	CLA	MG-NA	6.01	2.20	2.06
31	c	610	CLA	MG-NA	6.00	2.20	2.06
31	D	404	CLA	MG-NA	6.00	2.20	2.06
31	d	404	CLA	MG-NA	6.00	2.20	2.06
31	R	311	CLA	MG-NA	5.99	2.20	2.06
31	G	609	CLA	MG-NA	5.99	2.20	2.06
31	0	610	CLA	MG-NA	5.99	2.20	2.06
30	y	605	CHL	C3A-C2A	-5.99	1.49	1.54
31	A	405	CLA	MG-NA	5.98	2.20	2.06
30	3	309	CHL	C3A-C2A	-5.97	1.49	1.54
30	y	608	CHL	C3A-C2A	-5.97	1.49	1.54
31	A	407	CLA	MG-NA	5.96	2.20	2.06
31	r	312	CLA	MG-NA	5.96	2.20	2.06
31	1	604	CLA	MG-NA	5.96	2.20	2.06
31	y	613	CLA	MG-NA	5.95	2.20	2.06
31	c	604	CLA	MG-NA	5.95	2.20	2.06
30	6	310	CHL	C3A-C2A	-5.93	1.49	1.54
30	8	607	CHL	C3A-C2A	-5.93	1.49	1.54
31	r	315	CLA	MG-NA	5.93	2.20	2.06
30	N	301	CHL	C3A-C2A	-5.92	1.49	1.54
31	3	301	CLA	MG-NA	5.92	2.20	2.06
31	g	303	CLA	MG-NA	5.90	2.20	2.06
30	1	605	CHL	C3A-C2A	-5.89	1.49	1.54
31	A	409	CLA	MG-NA	5.88	2.20	2.06
31	9	314	CLA	MG-NA	5.88	2.20	2.06
31	3	316	CLA	MG-NA	5.88	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	r	311	CLA	MG-NA	5.88	2.20	2.06
31	q	313	CLA	MG-NA	5.88	2.20	2.06
31	a	409	CLA	MG-NA	5.86	2.20	2.06
31	4	612	CLA	MG-NA	5.86	2.20	2.06
30	S	302	CHL	C3A-C2A	-5.84	1.49	1.54
31	r	303	CLA	MG-NA	5.84	2.20	2.06
43	c	614	BCR	C12-C13	5.84	1.58	1.46
43	D	405	BCR	C12-C13	5.83	1.58	1.46
31	B	607	CLA	MG-NA	5.82	2.20	2.06
31	q	315	CLA	MG-NA	5.81	2.20	2.06
31	9	312	CLA	MG-NA	5.80	2.20	2.06
30	7	309	CHL	C3A-C2A	-5.76	1.49	1.54
43	T	101	BCR	C12-C13	5.76	1.58	1.46
36	p	618	NEX	C7-C8	5.75	1.41	1.31
36	N	318	NEX	C7-C8	5.72	1.41	1.31
30	G	605	CHL	C3A-C2A	-5.69	1.49	1.54
35	q	317	RRX	C19-C18	5.69	1.58	1.46
31	C	605	CLA	MG-NA	5.69	2.19	2.06
43	c	615	BCR	C12-C13	5.68	1.58	1.46
30	3	307	CHL	C3A-C2A	-5.68	1.49	1.54
30	S	309	CHL	C3A-C2A	-5.66	1.49	1.54
36	n	319	NEX	C7-C8	5.63	1.41	1.31
30	s	302	CHL	C3A-C2A	-5.60	1.49	1.54
36	y	618	NEX	C28-C29	-5.58	1.34	1.46
36	q	319	NEX	C7-C8	5.58	1.41	1.31
43	v	101	BCR	C12-C13	5.58	1.57	1.46
30	3	303	CHL	C3A-C2A	-5.57	1.49	1.54
36	0	618	NEX	C28-C29	-5.56	1.34	1.46
36	r	319	NEX	C28-C29	-5.56	1.34	1.46
43	A	410	BCR	C12-C13	5.56	1.57	1.46
36	6	319	NEX	C28-C29	-5.56	1.34	1.46
43	D	405	BCR	C8-C9	5.56	1.57	1.46
36	R	319	NEX	C28-C29	-5.56	1.34	1.46
30	5	608	CHL	C3A-C2A	-5.56	1.49	1.54
43	z	101	BCR	C12-C13	5.55	1.57	1.46
36	q	319	NEX	C28-C29	-5.55	1.34	1.46
36	s	319	NEX	C28-C29	-5.55	1.34	1.46
43	B	619	BCR	C12-C13	5.55	1.57	1.46
36	S	319	NEX	C28-C29	-5.54	1.34	1.46
43	C	614	BCR	C12-C13	5.54	1.57	1.46
43	H	101	BCR	C12-C13	5.52	1.57	1.46
36	9	319	NEX	C28-C29	-5.52	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	S	319	NEX	C7-C8	5.51	1.40	1.31
36	2	616	NEX	C28-C29	-5.50	1.34	1.46
43	b	618	BCR	C12-C13	5.50	1.57	1.46
36	r	301	NEX	C28-C29	-5.49	1.34	1.46
36	4	617	NEX	C28-C29	-5.49	1.34	1.46
43	V	101	BCR	C12-C13	5.49	1.57	1.46
36	r	301	NEX	C7-C8	5.49	1.40	1.31
36	Y	317	NEX	C7-C8	5.49	1.40	1.31
43	Z	101	BCR	C12-C13	5.49	1.57	1.46
36	3	319	NEX	C28-C29	-5.48	1.34	1.46
36	5	618	NEX	C28-C29	-5.48	1.34	1.46
36	s	319	NEX	C7-C8	5.48	1.40	1.31
36	G	616	NEX	C28-C29	-5.46	1.34	1.46
30	2	607	CHL	C3A-C2A	-5.46	1.50	1.54
36	8	617	NEX	C28-C29	-5.46	1.34	1.46
43	b	620	BCR	C12-C13	5.46	1.57	1.46
36	3	319	NEX	C7-C8	5.46	1.40	1.31
30	s	307	CHL	C3A-C2A	-5.44	1.50	1.54
36	R	301	NEX	C28-C29	-5.43	1.34	1.46
43	C	615	BCR	C12-C13	5.43	1.57	1.46
36	Y	317	NEX	C28-C29	-5.43	1.34	1.46
36	8	617	NEX	C7-C8	5.43	1.40	1.31
30	7	310	CHL	C3A-C2A	-5.43	1.50	1.54
30	4	607	CHL	C3B-C4B	5.42	1.46	1.41
36	r	319	NEX	C7-C8	5.42	1.40	1.31
43	h	101	BCR	C12-C13	5.42	1.57	1.46
36	0	618	NEX	C7-C8	5.41	1.40	1.31
36	6	319	NEX	C7-C8	5.41	1.40	1.31
36	p	618	NEX	C28-C29	-5.41	1.34	1.46
30	4	601	CHL	C3A-C2A	-5.41	1.50	1.54
30	8	605	CHL	C3A-C2A	-5.41	1.50	1.54
36	g	317	NEX	C28-C29	-5.40	1.34	1.46
43	t	101	BCR	C12-C13	5.40	1.57	1.46
36	N	318	NEX	C28-C29	-5.40	1.34	1.46
30	G	606	CHL	C3A-C2A	-5.39	1.50	1.54
43	b	619	BCR	C12-C13	5.39	1.57	1.46
30	2	601	CHL	C3A-C2A	-5.38	1.50	1.54
36	y	618	NEX	C7-C8	5.38	1.40	1.31
30	N	307	CHL	C3B-C4B	5.38	1.46	1.41
30	n	306	CHL	C3A-C2A	-5.37	1.50	1.54
36	5	618	NEX	C7-C8	5.37	1.40	1.31
43	B	618	BCR	C12-C13	5.36	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	c	614	BCR	C8-C9	5.35	1.57	1.46
43	c	615	BCR	C8-C9	5.35	1.57	1.46
43	t	101	BCR	C29-C30	5.35	1.66	1.54
30	G	623	CHL	C3A-C2A	-5.34	1.50	1.54
43	D	405	BCR	C23-C22	5.34	1.57	1.46
36	R	319	NEX	C7-C8	5.34	1.40	1.31
30	S	307	CHL	C3A-C2A	-5.33	1.50	1.54
43	a	410	BCR	C12-C13	5.33	1.57	1.46
30	7	302	CHL	C3A-C2A	-5.33	1.50	1.54
36	g	317	NEX	C7-C8	5.31	1.40	1.31
30	y	609	CHL	C3A-C2A	-5.31	1.50	1.54
43	v	101	BCR	C8-C9	5.30	1.57	1.46
36	n	319	NEX	C28-C29	-5.30	1.34	1.46
47	E	101	HEM	FE-NB	5.29	2.11	1.94
43	T	101	BCR	C8-C9	5.29	1.57	1.46
36	4	617	NEX	C7-C8	5.29	1.40	1.31
43	V	101	BCR	C29-C30	5.28	1.66	1.54
36	2	616	NEX	C7-C8	5.27	1.40	1.31
43	d	406	BCR	C12-C13	5.26	1.57	1.46
43	V	101	BCR	C8-C9	5.25	1.57	1.46
43	B	617	BCR	C12-C13	5.24	1.57	1.46
47	e	102	HEM	FE-NB	5.23	2.11	1.94
30	N	302	CHL	C3A-C2A	-5.22	1.50	1.54
43	D	405	BCR	C29-C30	5.21	1.66	1.54
43	T	101	BCR	C29-C30	5.21	1.66	1.54
43	b	619	BCR	C23-C22	5.21	1.57	1.46
43	b	618	BCR	C8-C9	5.20	1.57	1.46
43	b	619	BCR	C8-C9	5.19	1.57	1.46
43	A	410	BCR	C8-C9	5.19	1.57	1.46
30	8	606	CHL	C3B-C4B	5.18	1.46	1.41
43	B	618	BCR	C8-C9	5.16	1.57	1.46
43	B	619	BCR	C8-C9	5.16	1.57	1.46
36	9	319	NEX	C7-C8	5.15	1.40	1.31
43	b	620	BCR	C23-C22	5.14	1.57	1.46
36	R	301	NEX	C7-C8	5.14	1.40	1.31
43	H	101	BCR	C29-C30	5.14	1.65	1.54
43	h	101	BCR	C29-C30	5.14	1.65	1.54
30	n	302	CHL	C3A-C2A	-5.12	1.50	1.54
43	z	101	BCR	C8-C9	5.12	1.56	1.46
43	v	101	BCR	C29-C30	5.11	1.65	1.54
43	c	615	BCR	C23-C22	5.11	1.56	1.46
43	v	101	BCR	C23-C22	5.10	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	q	317	RRX	C8-C9	5.10	1.56	1.46
30	y	607	CHL	C3A-C2A	-5.10	1.50	1.54
36	G	616	NEX	C7-C8	5.10	1.40	1.31
32	p	616	LUT	C8-C9	5.10	1.56	1.46
30	n	307	CHL	C3B-C4B	5.09	1.46	1.41
30	8	601	CHL	C3A-C2A	-5.09	1.50	1.54
35	G	614	RRX	C8-C9	5.09	1.56	1.46
35	4	615	RRX	C8-C9	5.09	1.56	1.46
30	q	309	CHL	C3B-C4B	5.08	1.46	1.41
32	5	617	LUT	C8-C9	5.08	1.56	1.46
30	1	601	CHL	C1A-CHA	-5.08	1.34	1.40
43	C	614	BCR	C29-C30	5.08	1.65	1.54
35	9	317	RRX	C8-C9	5.08	1.56	1.46
46	D	402	BCT	O1-C	5.06	1.43	1.25
32	5	616	LUT	C8-C9	5.06	1.56	1.46
35	g	315	RRX	C8-C9	5.06	1.56	1.46
43	B	618	BCR	C29-C30	5.06	1.65	1.54
43	a	410	BCR	C8-C9	5.06	1.56	1.46
43	C	614	BCR	C8-C9	5.05	1.56	1.46
43	H	101	BCR	C8-C9	5.05	1.56	1.46
43	B	618	BCR	C23-C22	5.04	1.56	1.46
43	A	410	BCR	C29-C30	5.04	1.65	1.54
30	y	601	CHL	C3A-C2A	-5.04	1.50	1.54
43	c	615	BCR	C29-C30	5.04	1.65	1.54
32	9	318	LUT	C8-C9	5.03	1.56	1.46
30	y	606	CHL	C3A-C2A	-5.03	1.50	1.54
43	B	619	BCR	C23-C22	5.03	1.56	1.46
43	T	101	BCR	C23-C22	5.03	1.56	1.46
43	b	620	BCR	C8-C9	5.03	1.56	1.46
43	b	620	BCR	C29-C30	5.03	1.65	1.54
43	b	619	BCR	C29-C30	5.02	1.65	1.54
43	b	618	BCR	C29-C30	5.02	1.65	1.54
43	B	619	BCR	C29-C30	5.02	1.65	1.54
43	a	410	BCR	C29-C30	5.02	1.65	1.54
43	H	101	BCR	C23-C22	5.02	1.56	1.46
30	g	307	CHL	C3B-C4B	5.01	1.46	1.41
43	A	410	BCR	C23-C22	5.01	1.56	1.46
43	d	406	BCR	C8-C9	5.00	1.56	1.46
30	g	302	CHL	C3A-C2A	-5.00	1.50	1.54
32	3	318	LUT	C8-C9	5.00	1.56	1.46
32	G	615	LUT	C8-C9	4.99	1.56	1.46
35	2	614	RRX	C8-C9	4.99	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	601	CHL	C3A-C2A	-4.99	1.50	1.54
43	d	406	BCR	C29-C30	4.98	1.65	1.54
32	g	316	LUT	C8-C9	4.98	1.56	1.46
32	2	615	LUT	C8-C9	4.98	1.56	1.46
43	B	617	BCR	C8-C9	4.97	1.56	1.46
32	q	318	LUT	C8-C9	4.97	1.56	1.46
32	p	617	LUT	C8-C9	4.97	1.56	1.46
35	g	315	RRX	C2-C1	4.96	1.65	1.54
43	z	101	BCR	C29-C30	4.96	1.65	1.54
43	D	405	BCR	C15-C14	4.96	1.58	1.43
43	h	101	BCR	C8-C9	4.96	1.56	1.46
30	4	606	CHL	C3A-C2A	-4.96	1.50	1.54
43	t	101	BCR	C8-C9	4.95	1.56	1.46
43	a	410	BCR	C23-C22	4.95	1.56	1.46
32	3	317	LUT	C8-C9	4.95	1.56	1.46
44	d	407	PL9	C3-C4	-4.93	1.41	1.49
30	s	309	CHL	C3B-C4B	4.93	1.46	1.41
43	C	615	BCR	C15-C14	4.93	1.58	1.43
43	h	101	BCR	C23-C22	4.92	1.56	1.46
43	Z	101	BCR	C29-C30	4.91	1.65	1.54
35	4	615	RRX	C23-C22	4.91	1.56	1.46
43	c	615	BCR	C15-C14	4.90	1.58	1.43
32	y	616	LUT	C4-C5	-4.90	1.43	1.51
43	Z	101	BCR	C8-C9	4.90	1.56	1.46
35	9	317	RRX	C23-C22	4.89	1.56	1.46
32	S	318	LUT	C8-C9	4.89	1.56	1.46
35	2	614	RRX	C23-C22	4.89	1.56	1.46
43	C	615	BCR	C23-C22	4.88	1.56	1.46
43	c	614	BCR	C15-C14	4.88	1.58	1.43
32	Y	315	LUT	C4-C5	-4.88	1.43	1.51
30	6	302	CHL	C3A-C2A	-4.88	1.50	1.54
32	7	318	LUT	C8-C9	4.87	1.56	1.46
32	N	316	LUT	C8-C9	4.87	1.56	1.46
35	G	614	RRX	C23-C22	4.87	1.56	1.46
30	G	623	CHL	C3B-C4B	4.87	1.46	1.41
32	N	317	LUT	C8-C9	4.87	1.56	1.46
35	g	315	RRX	C23-C22	4.87	1.56	1.46
43	t	101	BCR	C23-C22	4.86	1.56	1.46
43	c	614	BCR	C29-C30	4.86	1.65	1.54
43	Z	101	BCR	C23-C22	4.85	1.56	1.46
30	7	307	CHL	C3B-C4B	4.85	1.46	1.41
30	r	308	CHL	C3B-C4B	4.85	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	p	606	CHL	C3A-C2A	-4.84	1.50	1.54
35	G	614	RRX	C2-C1	4.84	1.65	1.54
32	n	318	LUT	C8-C9	4.84	1.56	1.46
32	p	616	LUT	C12-C13	4.83	1.56	1.46
32	7	317	LUT	C4-C5	-4.83	1.43	1.51
32	4	616	LUT	C8-C9	4.83	1.56	1.46
32	n	317	LUT	C8-C9	4.83	1.56	1.46
43	T	101	BCR	C15-C14	4.83	1.58	1.43
32	6	317	LUT	C8-C9	4.82	1.56	1.46
30	s	308	CHL	C3B-C4B	4.82	1.46	1.41
35	4	615	RRX	C2-C1	4.82	1.65	1.54
32	8	616	LUT	C8-C9	4.82	1.56	1.46
43	V	101	BCR	C23-C22	4.82	1.56	1.46
30	n	307	CHL	C3A-C2A	-4.82	1.50	1.54
30	6	308	CHL	C3B-C4B	4.81	1.46	1.41
35	4	615	RRX	C12-C13	4.81	1.56	1.46
32	6	318	LUT	C8-C9	4.81	1.56	1.46
30	9	309	CHL	C3B-C4B	4.81	1.46	1.41
43	C	615	BCR	C29-C30	4.81	1.65	1.54
32	s	318	LUT	C8-C9	4.80	1.56	1.46
30	Y	302	CHL	C3A-C2A	-4.80	1.50	1.54
32	s	317	LUT	C8-C9	4.80	1.56	1.46
43	c	614	BCR	C23-C22	4.80	1.56	1.46
30	p	605	CHL	C3A-C2A	-4.80	1.50	1.54
43	C	614	BCR	C23-C22	4.80	1.56	1.46
32	8	615	LUT	C8-C9	4.80	1.56	1.46
43	a	410	BCR	C19-C18	4.79	1.56	1.46
32	S	317	LUT	C8-C9	4.79	1.56	1.46
35	9	317	RRX	C12-C13	4.79	1.56	1.46
35	9	317	RRX	C2-C1	4.79	1.65	1.54
35	2	614	RRX	C2-C1	4.78	1.65	1.54
35	G	614	RRX	C12-C13	4.78	1.56	1.46
35	4	615	RRX	C24-C25	4.78	1.61	1.45
30	g	308	CHL	C3A-C2A	-4.78	1.50	1.54
35	g	315	RRX	C12-C13	4.77	1.56	1.46
43	A	410	BCR	C15-C14	4.77	1.58	1.43
30	8	606	CHL	C3A-C2A	-4.77	1.50	1.54
35	g	315	RRX	C24-C25	4.76	1.61	1.45
32	Y	316	LUT	C4-C5	-4.76	1.43	1.51
35	9	317	RRX	C24-C25	4.76	1.61	1.45
43	z	101	BCR	C23-C22	4.75	1.56	1.46
35	G	614	RRX	C24-C25	4.75	1.61	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	r	317	LUT	C4-C5	-4.75	1.43	1.51
35	2	614	RRX	C24-C25	4.74	1.61	1.45
43	d	406	BCR	C23-C22	4.74	1.56	1.46
43	D	405	BCR	C19-C18	4.74	1.56	1.46
32	1	616	LUT	C4-C5	-4.74	1.43	1.51
30	r	310	CHL	C3B-C4B	4.74	1.46	1.41
30	1	619	CHL	C3B-C4B	4.72	1.46	1.41
30	4	605	CHL	C3A-C2A	-4.72	1.50	1.54
43	D	405	BCR	C2-C1	4.72	1.64	1.54
35	2	614	RRX	C12-C13	4.72	1.56	1.46
43	B	617	BCR	C29-C30	4.72	1.64	1.54
43	Z	101	BCR	C15-C14	4.71	1.57	1.43
43	b	618	BCR	C23-C22	4.71	1.56	1.46
30	G	606	CHL	C3B-C4B	4.71	1.46	1.41
35	q	317	RRX	C24-C25	4.70	1.61	1.45
43	C	615	BCR	C8-C9	4.70	1.56	1.46
30	Y	307	CHL	C3B-C4B	4.70	1.46	1.41
32	p	617	LUT	C12-C13	4.69	1.56	1.46
43	v	101	BCR	C15-C14	4.69	1.57	1.43
35	q	317	RRX	C12-C13	4.69	1.56	1.46
32	R	317	LUT	C4-C5	-4.68	1.43	1.51
43	c	615	BCR	C19-C18	4.68	1.56	1.46
30	1	606	CHL	C3B-C4B	4.68	1.45	1.41
30	N	301	CHL	C3B-C4B	4.68	1.45	1.41
32	y	617	LUT	C4-C5	-4.68	1.43	1.51
32	G	615	LUT	C12-C13	4.67	1.55	1.46
43	V	101	BCR	C15-C14	4.66	1.57	1.43
32	5	616	LUT	C12-C13	4.65	1.55	1.46
32	0	616	LUT	C8-C9	4.65	1.55	1.46
35	q	317	RRX	C23-C22	4.65	1.55	1.46
32	g	316	LUT	C12-C13	4.65	1.55	1.46
32	1	616	LUT	C8-C9	4.65	1.55	1.46
32	1	615	LUT	C4-C5	-4.64	1.43	1.51
43	d	406	BCR	C15-C14	4.64	1.57	1.43
43	t	101	BCR	C15-C14	4.63	1.57	1.43
32	0	617	LUT	C8-C9	4.63	1.55	1.46
30	n	301	CHL	C3B-C4B	4.63	1.45	1.41
43	B	618	BCR	C15-C14	4.62	1.57	1.43
43	H	101	BCR	C15-C14	4.62	1.57	1.43
32	5	617	LUT	C12-C13	4.62	1.55	1.46
43	C	614	BCR	C15-C14	4.62	1.57	1.43
43	b	620	BCR	C15-C14	4.61	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	R	310	CHL	C3B-C4B	4.61	1.45	1.41
30	y	606	CHL	C3B-C4B	4.61	1.45	1.41
32	s	318	LUT	C4-C5	-4.60	1.43	1.51
32	9	318	LUT	C12-C13	4.60	1.55	1.46
32	p	616	LUT	C15-C14	4.60	1.57	1.43
32	7	317	LUT	C8-C9	4.59	1.55	1.46
32	4	616	LUT	C12-C13	4.59	1.55	1.46
32	q	318	LUT	C12-C13	4.59	1.55	1.46
43	z	101	BCR	C15-C14	4.58	1.57	1.43
43	h	101	BCR	C15-C14	4.58	1.57	1.43
32	N	317	LUT	C12-C13	4.58	1.55	1.46
32	Y	316	LUT	C8-C9	4.57	1.55	1.46
32	S	318	LUT	C12-C13	4.57	1.55	1.46
36	9	319	NEX	C7-C6	-4.57	1.25	1.30
43	a	410	BCR	C15-C14	4.57	1.57	1.43
30	1	607	CHL	C3A-C2A	-4.57	1.50	1.54
32	3	318	LUT	C12-C13	4.56	1.55	1.46
30	y	607	CHL	C3B-C4B	4.56	1.45	1.41
32	3	317	LUT	C12-C13	4.56	1.55	1.46
32	N	316	LUT	C12-C13	4.56	1.55	1.46
43	b	619	BCR	C15-C14	4.56	1.57	1.43
32	R	317	LUT	C8-C9	4.55	1.55	1.46
36	S	319	NEX	C10-C9	-4.55	1.25	1.35
43	C	615	BCR	C19-C18	4.55	1.55	1.46
36	3	319	NEX	C14-C13	-4.54	1.25	1.35
36	3	319	NEX	C10-C9	-4.54	1.25	1.35
36	R	301	NEX	C34-C33	-4.54	1.25	1.35
43	b	618	BCR	C15-C14	4.54	1.57	1.43
36	9	319	NEX	C30-C29	-4.54	1.25	1.35
32	2	615	LUT	C15-C14	4.53	1.57	1.43
36	9	319	NEX	C34-C33	-4.53	1.25	1.35
30	Y	308	CHL	C3B-C4B	4.53	1.45	1.41
36	R	301	NEX	C14-C13	-4.53	1.25	1.35
32	p	616	LUT	C31-C30	4.53	1.57	1.43
36	s	319	NEX	C34-C33	-4.53	1.25	1.35
43	B	619	BCR	C15-C14	4.52	1.57	1.43
32	2	615	LUT	C35-C34	4.52	1.57	1.43
32	p	616	LUT	C35-C34	4.51	1.57	1.43
32	2	615	LUT	C31-C30	4.51	1.57	1.43
32	R	317	LUT	C12-C13	4.50	1.55	1.46
30	4	607	CHL	C1A-CHA	-4.50	1.34	1.40
32	2	615	LUT	C12-C13	4.50	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	G	614	RRX	C3-C4	4.50	1.66	1.52
32	p	617	LUT	C15-C14	4.50	1.57	1.43
32	7	318	LUT	C12-C13	4.50	1.55	1.46
35	q	317	RRX	C11-C10	4.49	1.57	1.43
35	4	615	RRX	C3-C4	4.49	1.66	1.52
35	2	614	RRX	C29-C30	4.49	1.68	1.54
30	R	308	CHL	C3B-C4B	4.49	1.45	1.41
32	0	617	LUT	C4-C5	-4.49	1.44	1.51
30	7	309	CHL	C3B-C4B	4.49	1.45	1.41
36	s	319	NEX	C30-C29	-4.49	1.25	1.35
30	p	607	CHL	C3B-C4B	4.49	1.45	1.41
32	G	615	LUT	C15-C14	4.48	1.57	1.43
31	S	304	CLA	CBB-CAB	4.48	1.51	1.30
35	2	614	RRX	C3-C4	4.48	1.66	1.52
36	s	319	NEX	C10-C9	-4.48	1.25	1.35
32	p	617	LUT	C31-C30	4.48	1.57	1.43
35	G	614	RRX	C29-C30	4.47	1.68	1.54
30	9	308	CHL	C3B-C4B	4.47	1.45	1.41
36	9	319	NEX	C10-C9	-4.47	1.25	1.35
35	9	317	RRX	C3-C4	4.47	1.66	1.52
30	5	605	CHL	C3A-C2A	-4.47	1.50	1.54
35	4	615	RRX	C29-C30	4.47	1.68	1.54
36	3	319	NEX	C34-C33	-4.47	1.25	1.35
36	G	616	NEX	C34-C33	-4.47	1.25	1.35
35	9	317	RRX	C29-C30	4.46	1.68	1.54
44	D	406	PL9	C3-C4	-4.46	1.42	1.49
35	q	317	RRX	C29-C30	4.46	1.68	1.54
35	g	315	RRX	C11-C10	4.46	1.57	1.43
43	b	619	BCR	C2-C1	4.46	1.64	1.54
36	G	616	NEX	C30-C29	-4.46	1.25	1.35
36	s	319	NEX	C14-C13	-4.46	1.25	1.35
43	B	619	BCR	C2-C1	4.46	1.64	1.54
43	D	405	BCR	C20-C21	4.46	1.57	1.43
43	B	618	BCR	C2-C1	4.46	1.64	1.54
30	S	307	CHL	C3B-C4B	4.46	1.45	1.41
43	B	617	BCR	C15-C14	4.45	1.57	1.43
32	r	317	LUT	C8-C9	4.45	1.55	1.46
32	3	318	LUT	C15-C14	4.45	1.57	1.43
36	G	616	NEX	C14-C13	-4.45	1.25	1.35
36	y	618	NEX	C34-C33	-4.45	1.25	1.35
32	n	317	LUT	C12-C13	4.45	1.55	1.46
32	9	318	LUT	C15-C14	4.45	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	q	317	RRX	C2-C1	4.45	1.64	1.54
30	0	607	CHL	C3B-C4B	4.44	1.45	1.41
43	T	101	BCR	C19-C18	4.44	1.55	1.46
32	5	617	LUT	C15-C14	4.44	1.57	1.43
43	c	615	BCR	C20-C21	4.44	1.57	1.43
32	n	317	LUT	C4-C5	-4.44	1.44	1.51
30	5	607	CHL	C3B-C4B	4.44	1.45	1.41
32	g	316	LUT	C31-C30	4.44	1.57	1.43
36	3	319	NEX	C30-C29	-4.44	1.25	1.35
35	4	615	RRX	C11-C10	4.44	1.56	1.43
31	p	604	CLA	CBB-CAB	4.44	1.51	1.30
31	C	605	CLA	MG-ND	-4.44	1.97	2.05
32	q	318	LUT	C31-C30	4.44	1.56	1.43
30	0	601	CHL	C3B-C4B	4.44	1.45	1.41
35	9	317	RRX	C11-C10	4.43	1.56	1.43
43	c	614	BCR	C2-C1	4.43	1.64	1.54
32	G	615	LUT	C31-C30	4.43	1.56	1.43
32	0	616	LUT	C4-C5	-4.43	1.44	1.51
43	a	410	BCR	C2-C1	4.43	1.64	1.54
43	d	406	BCR	C2-C1	4.43	1.64	1.54
30	p	609	CHL	C3B-C4B	4.43	1.45	1.41
36	S	319	NEX	C30-C29	-4.43	1.25	1.35
32	q	318	LUT	C15-C14	4.43	1.56	1.43
36	N	318	NEX	C14-C13	-4.43	1.25	1.35
32	5	617	LUT	C31-C30	4.42	1.56	1.43
32	5	616	LUT	C15-C14	4.42	1.56	1.43
32	g	316	LUT	C15-C14	4.42	1.56	1.43
32	8	615	LUT	C4-C5	-4.42	1.44	1.51
35	G	614	RRX	C11-C10	4.42	1.56	1.43
32	S	317	LUT	C4-C5	-4.42	1.44	1.51
32	S	318	LUT	C4-C5	-4.42	1.44	1.51
32	n	318	LUT	C12-C13	4.42	1.55	1.46
32	s	318	LUT	C12-C13	4.42	1.55	1.46
43	b	618	BCR	C2-C1	4.42	1.64	1.54
31	s	316	CLA	CBB-CAB	4.42	1.51	1.30
32	6	318	LUT	C4-C5	-4.42	1.44	1.51
43	A	410	BCR	C2-C1	4.42	1.64	1.54
43	H	101	BCR	C2-C1	4.42	1.64	1.54
30	p	601	CHL	C3B-C4B	4.41	1.45	1.41
31	4	614	CLA	CBB-CAB	4.41	1.51	1.30
36	2	616	NEX	C10-C9	-4.41	1.25	1.35
32	p	617	LUT	C35-C34	4.41	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	N	316	LUT	C4-C5	-4.41	1.44	1.51
32	5	616	LUT	C31-C30	4.41	1.56	1.43
32	9	318	LUT	C31-C30	4.41	1.56	1.43
36	4	617	NEX	C10-C9	-4.41	1.25	1.35
31	3	304	CLA	CBB-CAB	4.41	1.51	1.30
36	y	618	NEX	C10-C9	-4.41	1.25	1.35
43	c	615	BCR	C2-C1	4.41	1.64	1.54
32	6	318	LUT	C12-C13	4.41	1.55	1.46
32	8	615	LUT	C12-C13	4.41	1.55	1.46
31	8	602	CLA	CBB-CAB	4.41	1.51	1.30
32	7	318	LUT	C4-C5	-4.41	1.44	1.51
32	6	317	LUT	C12-C13	4.40	1.55	1.46
32	3	318	LUT	C31-C30	4.40	1.56	1.43
32	4	616	LUT	C15-C14	4.40	1.56	1.43
32	4	616	LUT	C4-C5	-4.40	1.44	1.51
31	3	312	CLA	CBB-CAB	4.40	1.51	1.30
31	3	314	CLA	CBB-CAB	4.40	1.51	1.30
30	6	302	CHL	C3B-C4B	4.40	1.45	1.41
31	9	306	CLA	CBB-CAB	4.40	1.51	1.30
32	S	318	LUT	C15-C14	4.40	1.56	1.43
32	8	616	LUT	C12-C13	4.40	1.55	1.46
32	1	615	LUT	C8-C9	4.40	1.55	1.46
43	c	614	BCR	C19-C18	4.40	1.55	1.46
31	3	315	CLA	CBB-CAB	4.40	1.51	1.30
36	R	301	NEX	C10-C9	-4.40	1.25	1.35
43	A	410	BCR	C19-C18	4.40	1.55	1.46
31	5	603	CLA	CBB-CAB	4.39	1.51	1.30
31	5	613	CLA	CBB-CAB	4.39	1.51	1.30
31	3	313	CLA	CBB-CAB	4.39	1.51	1.30
36	g	317	NEX	C10-C9	-4.39	1.25	1.35
31	5	612	CLA	CBB-CAB	4.39	1.51	1.30
31	6	315	CLA	CBB-CAB	4.39	1.51	1.30
31	5	610	CLA	CBB-CAB	4.39	1.51	1.30
31	0	611	CLA	CBB-CAB	4.39	1.51	1.30
31	p	612	CLA	CBB-CAB	4.39	1.51	1.30
31	7	303	CLA	CBB-CAB	4.39	1.51	1.30
31	b	615	CLA	CBB-CAB	4.39	1.51	1.30
32	y	616	LUT	C8-C9	4.39	1.55	1.46
31	9	304	CLA	CBB-CAB	4.39	1.51	1.30
31	q	304	CLA	CBB-CAB	4.39	1.51	1.30
32	6	317	LUT	C4-C5	-4.39	1.44	1.51
31	6	313	CLA	CBB-CAB	4.39	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	y	618	NEX	C30-C29	-4.39	1.25	1.35
35	2	614	RRX	C11-C10	4.39	1.56	1.43
31	8	614	CLA	CBB-CAB	4.39	1.51	1.30
36	8	617	NEX	C34-C33	-4.39	1.25	1.35
31	n	303	CLA	CBB-CAB	4.39	1.51	1.30
30	1	609	CHL	C3B-C4B	4.39	1.45	1.41
31	s	305	CLA	CBB-CAB	4.39	1.51	1.30
31	5	611	CLA	CBB-CAB	4.39	1.51	1.30
31	s	303	CLA	CBB-CAB	4.39	1.51	1.30
31	5	602	CLA	CBB-CAB	4.39	1.51	1.30
31	7	311	CLA	CBB-CAB	4.39	1.51	1.30
31	N	312	CLA	CBB-CAB	4.39	1.51	1.30
31	7	315	CLA	CBB-CAB	4.39	1.51	1.30
31	3	306	CLA	CBB-CAB	4.39	1.51	1.30
31	S	303	CLA	CBB-CAB	4.39	1.51	1.30
31	8	603	CLA	CBB-CAB	4.39	1.51	1.30
31	y	610	CLA	CBB-CAB	4.39	1.51	1.30
43	h	101	BCR	C2-C1	4.39	1.64	1.54
31	6	304	CLA	CBB-CAB	4.39	1.51	1.30
31	8	610	CLA	CBB-CAB	4.38	1.51	1.30
43	C	614	BCR	C2-C1	4.38	1.64	1.54
31	6	312	CLA	CBB-CAB	4.38	1.51	1.30
32	R	317	LUT	C15-C14	4.38	1.56	1.43
31	Y	310	CLA	CBB-CAB	4.38	1.51	1.30
36	S	319	NEX	C14-C13	-4.38	1.25	1.35
31	0	612	CLA	CBB-CAB	4.38	1.51	1.30
31	9	316	CLA	CBB-CAB	4.38	1.51	1.30
31	4	604	CLA	CBB-CAB	4.38	1.51	1.30
31	c	607	CLA	CBB-CAB	4.38	1.51	1.30
31	n	305	CLA	CBB-CAB	4.38	1.51	1.30
31	5	604	CLA	CBB-CAB	4.38	1.51	1.30
31	2	604	CLA	CBB-CAB	4.38	1.51	1.30
31	3	305	CLA	CBB-CAB	4.38	1.51	1.30
31	N	303	CLA	CBB-CAB	4.38	1.51	1.30
31	N	314	CLA	CBB-CAB	4.38	1.51	1.30
31	p	610	CLA	CBB-CAB	4.38	1.51	1.30
32	q	318	LUT	C4-C5	-4.38	1.44	1.51
31	7	312	CLA	CBB-CAB	4.38	1.51	1.30
31	n	313	CLA	CBB-CAB	4.38	1.51	1.30
32	N	317	LUT	C31-C30	4.38	1.56	1.43
31	6	303	CLA	CBB-CAB	4.38	1.51	1.30
31	S	305	CLA	CBB-CAB	4.38	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	615	LUT	C4-C5	-4.38	1.44	1.51
31	B	611	CLA	CBB-CAB	4.38	1.51	1.30
31	N	305	CLA	CBB-CAB	4.38	1.51	1.30
31	p	614	CLA	CBB-CAB	4.38	1.51	1.30
31	y	603	CLA	CBB-CAB	4.38	1.51	1.30
31	1	614	CLA	CBB-CAB	4.38	1.51	1.30
32	N	316	LUT	C15-C14	4.38	1.56	1.43
31	5	614	CLA	CBB-CAB	4.38	1.51	1.30
31	3	311	CLA	CBB-CAB	4.38	1.51	1.30
31	4	603	CLA	CBB-CAB	4.38	1.51	1.30
31	r	305	CLA	CBB-CAB	4.38	1.51	1.30
31	g	314	CLA	CBB-CAB	4.38	1.51	1.30
31	2	610	CLA	CBB-CAB	4.38	1.51	1.30
31	4	602	CLA	CBB-CAB	4.38	1.51	1.30
31	N	304	CLA	CBB-CAB	4.38	1.51	1.30
31	0	614	CLA	CBB-CAB	4.38	1.51	1.30
31	G	602	CLA	CBB-CAB	4.38	1.51	1.30
31	s	304	CLA	CBB-CAB	4.38	1.51	1.30
31	6	311	CLA	CBB-CAB	4.38	1.51	1.30
31	n	312	CLA	CBB-CAB	4.38	1.51	1.30
31	y	612	CLA	CBB-CAB	4.38	1.51	1.30
31	9	305	CLA	CBB-CAB	4.38	1.51	1.30
31	n	315	CLA	CBB-CAB	4.38	1.51	1.30
43	v	101	BCR	C19-C18	4.38	1.55	1.46
31	g	305	CLA	CBB-CAB	4.38	1.51	1.30
36	r	319	NEX	C30-C29	-4.38	1.25	1.35
31	9	315	CLA	CBB-CAB	4.38	1.51	1.30
31	B	614	CLA	CBB-CAB	4.38	1.51	1.30
32	g	316	LUT	C35-C34	4.38	1.56	1.43
36	6	319	NEX	C30-C29	-4.38	1.25	1.35
31	N	313	CLA	CBB-CAB	4.38	1.51	1.30
31	8	604	CLA	CBB-CAB	4.38	1.51	1.30
31	1	611	CLA	CBB-CAB	4.38	1.51	1.30
31	Y	303	CLA	CBB-CAB	4.37	1.51	1.30
30	1	605	CHL	C3B-C4B	4.37	1.45	1.41
31	8	609	CLA	CBB-CAB	4.37	1.51	1.30
32	s	317	LUT	C12-C13	4.37	1.55	1.46
31	9	312	CLA	CBB-CAB	4.37	1.51	1.30
36	y	618	NEX	C14-C13	-4.37	1.25	1.35
32	S	318	LUT	C31-C30	4.37	1.56	1.43
31	6	314	CLA	CBB-CAB	4.37	1.51	1.30
31	N	310	CLA	CBB-CAB	4.37	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	R	319	NEX	C14-C13	-4.37	1.25	1.35
31	s	306	CLA	CBB-CAB	4.37	1.51	1.30
31	R	313	CLA	CBB-CAB	4.37	1.51	1.30
32	G	615	LUT	C35-C34	4.37	1.56	1.43
43	b	620	BCR	C2-C1	4.37	1.64	1.54
31	Y	305	CLA	CBB-CAB	4.37	1.51	1.30
31	q	316	CLA	CBB-CAB	4.37	1.51	1.30
32	4	616	LUT	C31-C30	4.37	1.56	1.43
31	0	603	CLA	CBB-CAB	4.37	1.51	1.30
31	9	313	CLA	CBB-CAB	4.37	1.51	1.30
31	b	613	CLA	CBB-CAB	4.37	1.51	1.30
31	G	610	CLA	CBB-CAB	4.37	1.51	1.30
31	q	306	CLA	CBB-CAB	4.37	1.51	1.30
31	r	304	CLA	CBB-CAB	4.37	1.51	1.30
31	8	611	CLA	CBB-CAB	4.37	1.51	1.30
36	S	319	NEX	C34-C33	-4.37	1.25	1.35
43	b	619	BCR	C19-C18	4.37	1.55	1.46
32	N	317	LUT	C4-C5	-4.37	1.44	1.51
31	p	611	CLA	CBB-CAB	4.37	1.51	1.30
31	b	614	CLA	CBB-CAB	4.37	1.51	1.30
31	n	316	CLA	CBB-CAB	4.37	1.51	1.30
31	g	303	CLA	CBB-CAB	4.37	1.51	1.30
31	N	315	CLA	CBB-CAB	4.37	1.51	1.30
31	B	610	CLA	CBB-CAB	4.37	1.51	1.30
32	3	318	LUT	C35-C34	4.37	1.56	1.43
31	0	602	CLA	CBB-CAB	4.37	1.51	1.30
31	6	305	CLA	CBB-CAB	4.37	1.51	1.30
31	2	609	CLA	CBB-CAB	4.37	1.51	1.30
31	8	613	CLA	CBB-CAB	4.37	1.51	1.30
31	n	314	CLA	CBB-CAB	4.37	1.51	1.30
36	R	319	NEX	C30-C29	-4.37	1.25	1.35
30	2	606	CHL	C3A-C2A	-4.37	1.50	1.54
36	0	618	NEX	C30-C29	-4.37	1.25	1.35
31	S	306	CLA	CBB-CAB	4.37	1.51	1.30
31	q	305	CLA	CBB-CAB	4.37	1.51	1.30
36	R	319	NEX	C10-C9	-4.37	1.25	1.35
32	9	318	LUT	C4-C5	-4.37	1.44	1.51
31	b	612	CLA	CBB-CAB	4.37	1.51	1.30
30	7	306	CHL	C3B-C4B	4.36	1.45	1.41
31	g	311	CLA	CBB-CAB	4.36	1.51	1.30
31	p	602	CLA	CBB-CAB	4.36	1.51	1.30
31	R	316	CLA	CBB-CAB	4.36	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	n	304	CLA	CBB-CAB	4.36	1.51	1.30
31	7	305	CLA	CBB-CAB	4.36	1.51	1.30
35	g	315	RRX	C3-C4	4.36	1.66	1.52
31	p	603	CLA	CBB-CAB	4.36	1.51	1.30
31	y	602	CLA	CBB-CAB	4.36	1.51	1.30
31	8	612	CLA	CBB-CAB	4.36	1.51	1.30
31	0	613	CLA	CBB-CAB	4.36	1.51	1.30
32	S	317	LUT	C12-C13	4.36	1.55	1.46
31	y	604	CLA	CBB-CAB	4.36	1.51	1.30
31	G	604	CLA	CBB-CAB	4.36	1.51	1.30
31	7	316	CLA	CBB-CAB	4.36	1.51	1.30
31	s	315	CLA	CBB-CAB	4.36	1.51	1.30
31	2	613	CLA	CBB-CAB	4.36	1.51	1.30
31	r	313	CLA	CBB-CAB	4.36	1.51	1.30
31	1	610	CLA	CBB-CAB	4.36	1.51	1.30
31	G	613	CLA	CBB-CAB	4.36	1.51	1.30
31	7	304	CLA	CBB-CAB	4.36	1.51	1.30
36	Y	317	NEX	C14-C13	-4.36	1.25	1.35
30	1	608	CHL	C3B-C4B	4.36	1.45	1.41
31	y	615	CLA	CBB-CAB	4.36	1.51	1.30
31	b	611	CLA	CBB-CAB	4.36	1.51	1.30
36	5	618	NEX	C14-C13	-4.36	1.25	1.35
31	g	304	CLA	CBB-CAB	4.36	1.51	1.30
31	N	311	CLA	CBB-CAB	4.36	1.51	1.30
31	s	311	CLA	CBB-CAB	4.36	1.51	1.30
31	N	321	CLA	CBB-CAB	4.36	1.51	1.30
36	r	301	NEX	C30-C29	-4.36	1.25	1.35
32	3	317	LUT	C15-C14	4.36	1.56	1.43
32	3	317	LUT	C31-C30	4.36	1.56	1.43
31	G	603	CLA	CBB-CAB	4.36	1.51	1.30
36	r	319	NEX	C34-C33	-4.36	1.25	1.35
31	g	313	CLA	CBB-CAB	4.36	1.51	1.30
31	2	611	CLA	CBB-CAB	4.35	1.51	1.30
31	Y	314	CLA	CBB-CAB	4.35	1.51	1.30
32	7	317	LUT	C12-C13	4.35	1.55	1.46
32	N	317	LUT	C15-C14	4.35	1.56	1.43
30	4	601	CHL	C3B-C4B	4.35	1.45	1.41
31	0	615	CLA	CBB-CAB	4.35	1.51	1.30
36	R	301	NEX	C7-C6	-4.35	1.25	1.30
31	g	312	CLA	CBB-CAB	4.35	1.51	1.30
32	3	317	LUT	C4-C5	-4.35	1.44	1.51
31	5	615	CLA	CBB-CAB	4.35	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	G	612	CLA	CBB-CAB	4.35	1.51	1.30
36	4	617	NEX	C14-C13	-4.35	1.25	1.35
31	b	609	CLA	CBB-CAB	4.35	1.51	1.30
31	B	608	CLA	CBB-CAB	4.35	1.51	1.30
36	p	618	NEX	C30-C29	-4.35	1.25	1.35
31	2	603	CLA	CBB-CAB	4.35	1.51	1.30
31	B	613	CLA	CBB-CAB	4.35	1.51	1.30
36	R	319	NEX	C34-C33	-4.35	1.25	1.35
36	q	319	NEX	C30-C29	-4.35	1.25	1.35
32	5	616	LUT	C35-C34	4.35	1.56	1.43
32	5	617	LUT	C35-C34	4.35	1.56	1.43
36	2	616	NEX	C34-C33	-4.35	1.25	1.35
31	S	316	CLA	CBB-CAB	4.35	1.51	1.30
31	R	314	CLA	CBB-CAB	4.35	1.51	1.30
31	B	612	CLA	CBB-CAB	4.35	1.51	1.30
36	9	319	NEX	C14-C13	-4.35	1.25	1.35
32	6	318	LUT	C31-C30	4.35	1.56	1.43
31	C	610	CLA	CBB-CAB	4.35	1.51	1.30
31	9	314	CLA	CBB-CAB	4.35	1.51	1.30
36	2	616	NEX	C14-C13	-4.35	1.25	1.35
35	q	317	RRX	C3-C4	4.35	1.66	1.52
36	q	319	NEX	C34-C33	-4.35	1.25	1.35
32	q	318	LUT	C35-C34	4.35	1.56	1.43
31	R	307	CLA	CBB-CAB	4.34	1.51	1.30
36	G	616	NEX	C10-C9	-4.34	1.25	1.35
31	D	404	CLA	CBB-CAB	4.34	1.51	1.30
31	R	303	CLA	CBB-CAB	4.34	1.51	1.30
31	Y	304	CLA	CBB-CAB	4.34	1.51	1.30
32	0	617	LUT	C12-C13	4.34	1.55	1.46
31	7	314	CLA	CBB-CAB	4.34	1.51	1.30
32	s	317	LUT	C4-C5	-4.34	1.44	1.51
36	Y	317	NEX	C34-C33	-4.34	1.25	1.35
31	n	311	CLA	CBB-CAB	4.34	1.51	1.30
31	2	612	CLA	CBB-CAB	4.34	1.51	1.30
30	Y	309	CHL	C3A-C2A	-4.34	1.51	1.54
31	7	313	CLA	CBB-CAB	4.34	1.51	1.30
31	1	612	CLA	CBB-CAB	4.34	1.51	1.30
31	p	615	CLA	CBB-CAB	4.34	1.51	1.30
31	1	613	CLA	CBB-CAB	4.34	1.51	1.30
31	4	612	CLA	CBB-CAB	4.34	1.51	1.30
31	s	310	CLA	CBB-CAB	4.34	1.51	1.30
31	S	310	CLA	CBB-CAB	4.34	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	602	CLA	CBB-CAB	4.34	1.51	1.30
31	s	312	CLA	CBB-CAB	4.34	1.51	1.30
31	S	312	CLA	CBB-CAB	4.34	1.51	1.30
31	S	315	CLA	CBB-CAB	4.34	1.51	1.30
43	C	615	BCR	C20-C21	4.34	1.56	1.43
30	9	310	CHL	C3B-C4B	4.33	1.45	1.41
32	N	316	LUT	C31-C30	4.33	1.56	1.43
31	4	610	CLA	CBB-CAB	4.33	1.51	1.30
31	p	613	CLA	CBB-CAB	4.33	1.51	1.30
31	R	311	CLA	CBB-CAB	4.33	1.51	1.30
31	6	316	CLA	CBB-CAB	4.33	1.51	1.30
30	q	307	CHL	C3A-C2A	-4.33	1.51	1.54
31	r	311	CLA	CBB-CAB	4.33	1.51	1.30
31	s	313	CLA	CBB-CAB	4.33	1.51	1.30
36	4	617	NEX	C30-C29	-4.33	1.25	1.35
31	S	313	CLA	CBB-CAB	4.33	1.51	1.30
31	B	615	CLA	CBB-CAB	4.33	1.51	1.30
31	2	602	CLA	CBB-CAB	4.33	1.51	1.30
36	8	617	NEX	C14-C13	-4.33	1.25	1.35
31	b	606	CLA	CBB-CAB	4.33	1.51	1.30
31	c	604	CLA	CBB-CAB	4.33	1.51	1.30
31	3	301	CLA	CBB-CAB	4.33	1.51	1.30
31	r	303	CLA	CBB-CAB	4.33	1.51	1.30
32	n	318	LUT	C4-C5	-4.33	1.44	1.51
31	1	603	CLA	CBB-CAB	4.33	1.51	1.30
31	Y	313	CLA	CBB-CAB	4.33	1.51	1.30
30	7	310	CHL	C3B-C4B	4.33	1.45	1.41
31	r	314	CLA	CBB-CAB	4.33	1.51	1.30
36	5	618	NEX	C30-C29	-4.33	1.25	1.35
31	0	604	CLA	CBB-CAB	4.33	1.51	1.30
36	q	319	NEX	C14-C13	-4.33	1.25	1.35
31	B	609	CLA	CBB-CAB	4.33	1.51	1.30
32	G	615	LUT	C4-C5	-4.32	1.44	1.51
31	B	604	CLA	CBB-CAB	4.32	1.51	1.30
36	r	301	NEX	C10-C9	-4.32	1.25	1.35
31	B	602	CLA	CBB-CAB	4.32	1.51	1.30
31	r	307	CLA	CBB-CAB	4.32	1.51	1.30
31	r	316	CLA	CBB-CAB	4.32	1.51	1.30
36	p	618	NEX	C34-C33	-4.32	1.25	1.35
31	R	306	CLA	CBB-CAB	4.32	1.51	1.30
36	r	319	NEX	C14-C13	-4.32	1.25	1.35
43	V	101	BCR	C2-C1	4.32	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	b	619	BCR	C20-C21	4.32	1.56	1.43
31	b	608	CLA	CBB-CAB	4.32	1.51	1.30
32	7	318	LUT	C15-C14	4.32	1.56	1.43
31	C	601	CLA	CBB-CAB	4.32	1.51	1.30
31	S	314	CLA	CBB-CAB	4.32	1.51	1.30
36	r	301	NEX	C14-C13	-4.32	1.25	1.35
31	S	311	CLA	CBB-CAB	4.32	1.51	1.30
31	c	606	CLA	CBB-CAB	4.32	1.51	1.30
31	G	609	CLA	CBB-CAB	4.32	1.51	1.30
36	r	301	NEX	C34-C33	-4.32	1.25	1.35
31	b	604	CLA	CBB-CAB	4.32	1.51	1.30
31	y	614	CLA	CBB-CAB	4.32	1.51	1.30
31	G	611	CLA	CBB-CAB	4.32	1.51	1.30
36	Y	317	NEX	C10-C9	-4.32	1.25	1.35
43	t	101	BCR	C4-C5	-4.32	1.43	1.51
30	G	601	CHL	C3B-C4B	4.32	1.45	1.41
31	R	305	CLA	CBB-CAB	4.32	1.51	1.30
32	2	615	LUT	C23-C24	-4.32	1.44	1.50
31	r	315	CLA	CBB-CAB	4.32	1.51	1.30
31	A	406	CLA	CBB-CAB	4.32	1.51	1.30
36	8	617	NEX	C30-C29	-4.32	1.25	1.35
36	4	617	NEX	C34-C33	-4.32	1.25	1.35
31	R	315	CLA	CBB-CAB	4.32	1.51	1.30
31	q	315	CLA	CBB-CAB	4.32	1.51	1.30
31	c	610	CLA	CBB-CAB	4.32	1.51	1.30
31	C	608	CLA	CBB-CAB	4.32	1.51	1.30
35	g	315	RRX	C29-C30	4.31	1.67	1.54
36	5	618	NEX	C34-C33	-4.31	1.25	1.35
31	q	314	CLA	CBB-CAB	4.31	1.51	1.30
31	b	605	CLA	CBB-CAB	4.31	1.51	1.30
36	R	301	NEX	C30-C29	-4.31	1.25	1.35
31	Y	312	CLA	CBB-CAB	4.31	1.51	1.30
31	c	601	CLA	CBB-CAB	4.31	1.51	1.30
36	p	618	NEX	C14-C13	-4.31	1.25	1.35
31	b	603	CLA	CBB-CAB	4.31	1.51	1.30
31	b	610	CLA	CBB-CAB	4.31	1.51	1.30
31	s	314	CLA	CBB-CAB	4.31	1.51	1.30
31	R	312	CLA	CBB-CAB	4.31	1.51	1.30
31	c	603	CLA	CBB-CAB	4.31	1.51	1.30
31	c	602	CLA	CBB-CAB	4.31	1.51	1.30
30	g	302	CHL	C3B-C4B	4.31	1.45	1.41
31	c	605	CLA	CBB-CAB	4.31	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	g	317	NEX	C34-C33	-4.31	1.25	1.35
36	r	319	NEX	C10-C9	-4.31	1.25	1.35
32	7	318	LUT	C31-C30	4.30	1.56	1.43
31	b	607	CLA	CBB-CAB	4.30	1.51	1.30
31	g	310	CLA	CBB-CAB	4.30	1.51	1.30
31	y	611	CLA	CBB-CAB	4.30	1.51	1.30
32	g	316	LUT	C4-C5	-4.30	1.44	1.51
32	6	318	LUT	C15-C14	4.30	1.56	1.43
30	4	608	CHL	C3B-C4B	4.30	1.45	1.41
43	Z	101	BCR	C2-C1	4.30	1.63	1.54
31	R	304	CLA	CBB-CAB	4.30	1.51	1.30
31	C	607	CLA	CBB-CAB	4.30	1.51	1.30
32	8	616	LUT	C4-C5	-4.30	1.44	1.51
31	C	612	CLA	CBB-CAB	4.30	1.51	1.30
36	2	616	NEX	C30-C29	-4.30	1.25	1.35
32	R	317	LUT	C35-C34	4.30	1.56	1.43
36	5	618	NEX	C10-C9	-4.30	1.25	1.35
31	C	603	CLA	CBB-CAB	4.30	1.51	1.30
31	c	611	CLA	CBB-CAB	4.30	1.51	1.30
36	8	617	NEX	C10-C9	-4.30	1.25	1.35
31	r	312	CLA	CBB-CAB	4.30	1.51	1.30
32	N	316	LUT	C35-C34	4.30	1.56	1.43
32	s	317	LUT	C31-C30	4.30	1.56	1.43
31	r	306	CLA	CBB-CAB	4.30	1.51	1.30
31	C	613	CLA	CBB-CAB	4.30	1.51	1.30
43	T	101	BCR	C2-C1	4.30	1.63	1.54
31	B	606	CLA	CBB-CAB	4.30	1.51	1.30
36	0	618	NEX	C34-C33	-4.29	1.25	1.35
32	Y	315	LUT	C8-C9	4.29	1.55	1.46
32	n	318	LUT	C15-C14	4.29	1.56	1.43
31	b	617	CLA	CBB-CAB	4.29	1.51	1.30
32	p	617	LUT	C4-C5	-4.29	1.44	1.51
30	S	309	CHL	C3B-C4B	4.29	1.45	1.41
36	6	319	NEX	C34-C33	-4.29	1.25	1.35
31	4	613	CLA	CBB-CAB	4.29	1.51	1.30
30	G	608	CHL	C3B-C4B	4.29	1.45	1.41
32	S	317	LUT	C31-C30	4.29	1.56	1.43
31	1	604	CLA	CBB-CAB	4.29	1.51	1.30
31	a	406	CLA	CBB-CAB	4.29	1.51	1.30
31	b	616	CLA	CBB-CAB	4.29	1.51	1.30
30	0	608	CHL	C3B-C4B	4.29	1.45	1.41
36	6	319	NEX	C14-C13	-4.29	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	0	618	NEX	C14-C13	-4.29	1.25	1.35
31	A	405	CLA	CBB-CAB	4.29	1.51	1.30
43	V	101	BCR	C28-C27	4.29	1.65	1.52
31	C	611	CLA	CBB-CAB	4.29	1.51	1.30
36	Y	317	NEX	C30-C29	-4.28	1.25	1.35
31	d	401	CLA	CBB-CAB	4.28	1.51	1.30
31	a	409	CLA	CBB-CAB	4.28	1.51	1.30
36	g	317	NEX	C14-C13	-4.28	1.25	1.35
32	5	616	LUT	C4-C5	-4.28	1.44	1.51
32	p	616	LUT	C4-C5	-4.28	1.44	1.51
30	3	303	CHL	C3B-C4B	4.28	1.45	1.41
31	A	407	CLA	CBB-CAB	4.28	1.51	1.30
31	a	407	CLA	CBB-CAB	4.28	1.51	1.30
43	T	101	BCR	C20-C21	4.28	1.56	1.43
31	d	404	CLA	CBB-CAB	4.28	1.51	1.30
43	B	617	BCR	C2-C1	4.28	1.63	1.54
30	y	608	CHL	C3B-C4B	4.28	1.45	1.41
31	c	608	CLA	CBB-CAB	4.28	1.51	1.30
32	8	616	LUT	C15-C14	4.28	1.56	1.43
32	8	616	LUT	C31-C30	4.28	1.56	1.43
47	E	101	HEM	FE-NC	4.28	2.09	1.95
32	S	318	LUT	C35-C34	4.28	1.56	1.43
31	B	603	CLA	CBB-CAB	4.28	1.50	1.30
31	B	605	CLA	CBB-CAB	4.28	1.50	1.30
43	B	617	BCR	C23-C22	4.28	1.55	1.46
31	d	405	CLA	CBB-CAB	4.28	1.50	1.30
36	q	319	NEX	C10-C9	-4.28	1.25	1.35
30	R	309	CHL	C3A-C2A	-4.28	1.51	1.54
32	6	318	LUT	C35-C34	4.28	1.56	1.43
43	v	101	BCR	C2-C1	4.28	1.63	1.54
32	n	318	LUT	C31-C30	4.28	1.56	1.43
43	V	101	BCR	C19-C18	4.28	1.55	1.46
32	4	616	LUT	C35-C34	4.28	1.56	1.43
32	s	317	LUT	C15-C14	4.28	1.56	1.43
32	s	318	LUT	C15-C14	4.28	1.56	1.43
31	A	409	CLA	CBB-CAB	4.28	1.50	1.30
31	B	616	CLA	CBB-CAB	4.28	1.50	1.30
31	C	604	CLA	CBB-CAB	4.27	1.50	1.30
36	s	319	NEX	C7-C6	-4.27	1.25	1.30
30	y	605	CHL	C3B-C4B	4.27	1.45	1.41
31	C	602	CLA	CBB-CAB	4.27	1.50	1.30
31	3	316	CLA	CBB-CAB	4.27	1.50	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	p	616	LUT	C7-C6	4.27	1.59	1.45
36	g	317	NEX	C30-C29	-4.27	1.25	1.35
32	3	317	LUT	C35-C34	4.27	1.56	1.43
43	z	101	BCR	C2-C1	4.27	1.63	1.54
43	b	620	BCR	C19-C18	4.27	1.55	1.46
32	9	318	LUT	C35-C34	4.27	1.56	1.43
31	c	613	CLA	CBB-CAB	4.27	1.50	1.30
43	Z	101	BCR	C19-C18	4.27	1.55	1.46
32	6	317	LUT	C31-C30	4.27	1.56	1.43
30	6	309	CHL	C3B-C4B	4.26	1.45	1.41
32	N	317	LUT	C35-C34	4.26	1.56	1.43
32	s	318	LUT	C31-C30	4.26	1.56	1.43
32	0	617	LUT	C31-C30	4.26	1.56	1.43
31	D	403	CLA	CBB-CAB	4.26	1.50	1.30
32	1	616	LUT	C12-C13	4.26	1.55	1.46
31	S	304	CLA	MG-ND	-4.26	1.97	2.05
43	D	405	BCR	C28-C27	4.26	1.65	1.52
32	5	617	LUT	C4-C5	-4.26	1.44	1.51
32	8	615	LUT	C15-C14	4.26	1.56	1.43
36	N	318	NEX	C30-C29	-4.26	1.26	1.35
36	N	318	NEX	C34-C33	-4.26	1.26	1.35
32	n	317	LUT	C15-C14	4.25	1.56	1.43
32	Y	316	LUT	C12-C13	4.25	1.55	1.46
31	C	609	CLA	CBB-CAB	4.25	1.50	1.30
36	q	319	NEX	C7-C6	-4.25	1.25	1.30
43	H	101	BCR	C19-C18	4.25	1.55	1.46
43	h	101	BCR	C19-C18	4.25	1.55	1.46
31	c	607	CLA	MG-ND	-4.25	1.97	2.05
31	c	612	CLA	CBB-CAB	4.25	1.50	1.30
32	5	616	LUT	C7-C6	4.25	1.59	1.45
32	y	617	LUT	C8-C9	4.25	1.55	1.46
30	q	311	CHL	C3A-C2A	-4.25	1.51	1.54
31	b	617	CLA	MG-ND	-4.25	1.97	2.05
32	6	317	LUT	C15-C14	4.25	1.56	1.43
36	p	618	NEX	C10-C9	-4.25	1.26	1.35
31	0	610	CLA	CBB-CAB	4.25	1.50	1.30
31	c	609	CLA	CBB-CAB	4.24	1.50	1.30
32	S	317	LUT	C15-C14	4.24	1.56	1.43
36	N	318	NEX	C10-C9	-4.24	1.26	1.35
30	4	608	CHL	C3A-C2A	-4.24	1.51	1.54
32	7	317	LUT	C15-C14	4.24	1.56	1.43
32	R	317	LUT	C31-C30	4.24	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	g	317	NEX	C7-C6	-4.23	1.25	1.30
43	B	618	BCR	C19-C18	4.23	1.55	1.46
30	7	302	CHL	C3B-C4B	4.23	1.45	1.41
47	e	102	HEM	FE-NC	4.23	2.09	1.95
36	n	319	NEX	C14-C13	-4.23	1.26	1.35
32	3	318	LUT	C4-C5	-4.23	1.44	1.51
32	n	317	LUT	C31-C30	4.23	1.56	1.43
31	B	607	CLA	CBB-CAB	4.23	1.50	1.30
31	Y	311	CLA	CBB-CAB	4.23	1.50	1.30
43	b	620	BCR	C20-C21	4.23	1.56	1.43
31	B	601	CLA	CBB-CAB	4.23	1.50	1.30
31	C	603	CLA	MG-ND	-4.23	1.97	2.05
32	8	615	LUT	C31-C30	4.23	1.56	1.43
36	6	319	NEX	C10-C9	-4.23	1.26	1.35
43	v	101	BCR	C20-C21	4.22	1.56	1.43
32	0	617	LUT	C15-C14	4.22	1.56	1.43
30	4	605	CHL	C3B-C4B	4.22	1.45	1.41
30	9	303	CHL	C3B-C4B	4.22	1.45	1.41
30	g	309	CHL	C3B-C4B	4.22	1.45	1.41
35	q	317	RRX	C27-C26	-4.22	1.44	1.51
43	v	101	BCR	C28-C27	4.22	1.65	1.52
43	C	614	BCR	C19-C18	4.21	1.55	1.46
36	0	618	NEX	C10-C9	-4.21	1.26	1.35
32	9	318	LUT	C7-C6	4.21	1.59	1.45
43	c	615	BCR	C28-C27	4.20	1.65	1.52
32	7	318	LUT	C35-C34	4.20	1.56	1.43
32	5	617	LUT	C7-C6	4.20	1.59	1.45
30	6	310	CHL	C3B-C4B	4.20	1.45	1.41
31	b	602	CLA	CBB-CAB	4.20	1.50	1.30
32	g	316	LUT	C7-C6	4.20	1.59	1.45
45	C	620	DGD	O1G-C1A	4.20	1.45	1.33
31	G	611	CLA	MG-ND	-4.20	1.97	2.05
36	4	617	NEX	C7-C6	-4.20	1.25	1.30
32	0	617	LUT	C35-C34	4.20	1.56	1.43
31	C	606	CLA	CBB-CAB	4.20	1.50	1.30
32	8	616	LUT	C35-C34	4.20	1.56	1.43
32	G	615	LUT	C7-C6	4.20	1.59	1.45
31	c	603	CLA	MG-ND	-4.20	1.97	2.05
30	Y	309	CHL	C3B-C4B	4.20	1.45	1.41
31	C	605	CLA	CBB-CAB	4.19	1.50	1.30
32	n	318	LUT	C35-C34	4.19	1.56	1.43
30	y	609	CHL	C3B-C4B	4.19	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	8	601	CHL	C3B-C4B	4.19	1.45	1.41
32	8	615	LUT	C35-C34	4.19	1.56	1.43
32	n	317	LUT	C35-C34	4.19	1.56	1.43
30	n	302	CHL	C3B-C4B	4.19	1.45	1.41
32	0	616	LUT	C15-C14	4.18	1.56	1.43
32	Y	316	LUT	C15-C14	4.18	1.56	1.43
43	A	410	BCR	C20-C21	4.18	1.56	1.43
36	2	616	NEX	C7-C6	-4.18	1.25	1.30
43	C	614	BCR	C28-C27	4.18	1.65	1.52
32	0	616	LUT	C12-C13	4.18	1.54	1.46
36	n	319	NEX	C10-C9	-4.18	1.26	1.35
32	p	617	LUT	C7-C6	4.17	1.59	1.45
30	3	308	CHL	C3B-C4B	4.17	1.45	1.41
32	q	318	LUT	C7-C6	4.17	1.59	1.45
30	s	307	CHL	C3B-C4B	4.17	1.45	1.41
30	5	601	CHL	C3B-C4B	4.17	1.45	1.41
31	B	603	CLA	MG-ND	-4.17	1.97	2.05
32	S	317	LUT	C35-C34	4.17	1.56	1.43
43	Z	101	BCR	C20-C21	4.17	1.56	1.43
36	R	319	NEX	C7-C6	-4.17	1.25	1.30
31	c	609	CLA	MG-ND	-4.17	1.97	2.05
43	B	619	BCR	C19-C18	4.17	1.54	1.46
43	T	101	BCR	C28-C27	4.17	1.65	1.52
32	s	318	LUT	C35-C34	4.17	1.56	1.43
36	n	319	NEX	C34-C33	-4.16	1.26	1.35
30	p	608	CHL	C3B-C4B	4.16	1.45	1.41
32	6	317	LUT	C35-C34	4.16	1.56	1.43
30	5	606	CHL	C3B-C4B	4.16	1.45	1.41
43	H	101	BCR	C20-C21	4.16	1.56	1.43
32	Y	316	LUT	C31-C30	4.16	1.56	1.43
31	B	616	CLA	MG-ND	-4.16	1.97	2.05
30	q	308	CHL	C1A-CHA	-4.16	1.35	1.40
45	c	619	DGD	O1G-C1A	4.16	1.45	1.33
43	B	618	BCR	C20-C21	4.16	1.56	1.43
43	c	614	BCR	C20-C21	4.16	1.56	1.43
43	b	618	BCR	C28-C27	4.16	1.65	1.52
31	C	610	CLA	MG-ND	-4.15	1.97	2.05
32	s	317	LUT	C35-C34	4.15	1.56	1.43
32	3	318	LUT	C7-C6	4.15	1.59	1.45
32	Y	316	LUT	C35-C34	4.15	1.56	1.43
30	3	308	CHL	C3A-C2A	-4.15	1.51	1.54
32	1	616	LUT	C31-C30	4.15	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	615	LUT	C21-C26	4.15	1.67	1.56
30	N	302	CHL	C3B-C4B	4.15	1.45	1.41
35	4	615	RRX	C15-C14	4.15	1.56	1.43
31	C	607	CLA	MG-ND	-4.15	1.97	2.05
30	q	303	CHL	C3B-C4B	4.15	1.45	1.41
32	2	615	LUT	C7-C6	4.15	1.59	1.45
35	g	315	RRX	C15-C14	4.15	1.56	1.43
45	C	618	DGD	O1G-C1A	4.14	1.45	1.33
31	y	613	CLA	CBB-CAB	4.14	1.50	1.30
32	7	318	LUT	C7-C6	4.14	1.59	1.45
32	N	317	LUT	C7-C6	4.14	1.59	1.45
31	b	605	CLA	MG-ND	-4.14	1.97	2.05
32	1	616	LUT	C15-C14	4.14	1.56	1.43
32	5	616	LUT	C28-C29	4.14	1.54	1.46
32	4	616	LUT	C7-C6	4.14	1.59	1.45
30	q	307	CHL	C3B-C4B	4.14	1.45	1.41
43	B	619	BCR	C20-C21	4.14	1.56	1.43
36	y	618	NEX	C7-C6	-4.14	1.25	1.30
43	A	410	BCR	C28-C27	4.13	1.65	1.52
43	V	101	BCR	C20-C21	4.13	1.56	1.43
30	q	311	CHL	C3B-C4B	4.13	1.45	1.41
43	d	406	BCR	C28-C27	4.13	1.65	1.52
31	c	612	CLA	MG-ND	-4.13	1.97	2.05
43	Z	101	BCR	C28-C27	4.13	1.65	1.52
35	9	317	RRX	C15-C14	4.13	1.56	1.43
43	a	410	BCR	C28-C27	4.13	1.65	1.52
32	1	615	LUT	C12-C13	4.13	1.54	1.46
43	h	101	BCR	C20-C21	4.13	1.56	1.43
32	1	615	LUT	C31-C30	4.12	1.56	1.43
43	H	101	BCR	C28-C27	4.12	1.65	1.52
35	G	614	RRX	C15-C14	4.12	1.56	1.43
43	B	617	BCR	C4-C5	-4.12	1.43	1.51
43	b	620	BCR	C28-C27	4.12	1.65	1.52
43	t	101	BCR	C2-C1	4.12	1.63	1.54
32	3	317	LUT	C7-C6	4.12	1.59	1.45
36	n	319	NEX	C30-C29	-4.12	1.26	1.35
36	G	616	NEX	C7-C6	-4.12	1.25	1.30
32	y	617	LUT	C12-C13	4.12	1.54	1.46
31	y	613	CLA	C4B-NB	-4.11	1.32	1.37
31	C	612	CLA	MG-ND	-4.11	1.97	2.05
35	2	614	RRX	C15-C14	4.11	1.55	1.43
30	2	608	CHL	C3B-C4B	4.11	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	b	619	BCR	C28-C27	4.11	1.65	1.52
32	g	316	LUT	C28-C29	4.11	1.54	1.46
43	t	101	BCR	C28-C27	4.11	1.65	1.52
31	C	609	CLA	MG-ND	-4.11	1.97	2.05
31	D	403	CLA	MG-ND	-4.11	1.97	2.05
31	c	606	CLA	MG-ND	-4.11	1.97	2.05
43	z	101	BCR	C19-C18	4.10	1.54	1.46
32	s	317	LUT	C7-C6	4.10	1.59	1.45
31	r	303	CLA	MG-ND	-4.10	1.97	2.05
32	6	318	LUT	C7-C6	4.10	1.59	1.45
31	B	604	CLA	MG-ND	-4.10	1.97	2.05
32	N	316	LUT	C7-C6	4.10	1.59	1.45
43	t	101	BCR	C19-C18	4.10	1.54	1.46
32	S	318	LUT	C7-C6	4.10	1.59	1.45
43	B	618	BCR	C28-C27	4.10	1.65	1.52
31	b	604	CLA	MG-ND	-4.10	1.97	2.05
32	n	318	LUT	C7-C6	4.10	1.59	1.45
30	9	307	CHL	C3B-C4B	4.10	1.45	1.41
43	C	615	BCR	C27-C26	-4.10	1.43	1.51
32	5	617	LUT	C28-C29	4.10	1.54	1.46
32	n	317	LUT	C7-C6	4.09	1.59	1.45
43	B	619	BCR	C28-C27	4.09	1.65	1.52
43	C	614	BCR	C20-C21	4.09	1.55	1.43
36	5	618	NEX	C7-C6	-4.09	1.25	1.30
30	g	308	CHL	C3B-C4B	4.09	1.45	1.41
32	8	615	LUT	C7-C6	4.09	1.59	1.45
32	8	616	LUT	C7-C6	4.09	1.59	1.45
32	1	616	LUT	C35-C34	4.08	1.55	1.43
35	q	317	RRX	C15-C14	4.08	1.55	1.43
32	y	617	LUT	C15-C14	4.08	1.55	1.43
31	S	313	CLA	MG-ND	-4.08	1.97	2.05
32	1	615	LUT	C15-C14	4.08	1.55	1.43
43	h	101	BCR	C28-C27	4.08	1.65	1.52
43	c	614	BCR	C28-C27	4.08	1.65	1.52
32	0	616	LUT	C31-C30	4.08	1.55	1.43
45	C	617	DGD	O1G-C1A	4.07	1.45	1.33
32	p	617	LUT	C21-C26	4.07	1.67	1.56
45	C	616	DGD	O1G-C1A	4.07	1.45	1.33
32	7	317	LUT	C31-C30	4.07	1.55	1.43
31	r	307	CLA	MG-ND	-4.07	1.97	2.05
31	q	315	CLA	MG-ND	-4.07	1.97	2.05
32	S	317	LUT	C7-C6	4.07	1.59	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	607	CHL	C3B-C4B	4.07	1.45	1.41
43	c	614	BCR	C11-C10	4.07	1.55	1.43
32	7	317	LUT	C35-C34	4.07	1.55	1.43
31	y	613	CLA	MG-ND	-4.07	1.97	2.05
35	2	614	RRX	C27-C26	-4.07	1.44	1.51
30	n	306	CHL	C3B-C4B	4.07	1.45	1.41
31	1	604	CLA	MG-ND	-4.06	1.97	2.05
45	c	616	DGD	O1G-C1A	4.06	1.45	1.33
32	3	318	LUT	C28-C29	4.06	1.54	1.46
32	N	317	LUT	C28-C29	4.06	1.54	1.46
30	8	605	CHL	C3B-C4B	4.06	1.45	1.41
30	p	606	CHL	C3B-C4B	4.06	1.45	1.41
32	q	318	LUT	C28-C29	4.06	1.54	1.46
30	g	306	CHL	C3B-C4B	4.06	1.45	1.41
36	Y	317	NEX	C7-C6	-4.06	1.25	1.30
45	c	618	DGD	O1G-C1A	4.06	1.45	1.33
31	r	314	CLA	MG-ND	-4.06	1.97	2.05
45	c	617	DGD	O1G-C1A	4.05	1.45	1.33
43	d	406	BCR	C20-C21	4.05	1.55	1.43
32	s	318	LUT	C7-C6	4.05	1.58	1.45
32	R	317	LUT	C7-C6	4.05	1.58	1.45
31	R	305	CLA	MG-ND	-4.05	1.97	2.05
31	c	602	CLA	MG-ND	-4.05	1.97	2.05
32	6	317	LUT	C7-C6	4.05	1.58	1.45
32	3	317	LUT	C28-C29	4.05	1.54	1.46
31	0	610	CLA	MG-ND	-4.05	1.97	2.05
43	z	101	BCR	C20-C21	4.05	1.55	1.43
32	N	316	LUT	C28-C29	4.05	1.54	1.46
30	2	605	CHL	C3B-C4B	4.04	1.45	1.41
36	r	319	NEX	C7-C6	-4.04	1.25	1.30
31	1	603	CLA	MG-ND	-4.04	1.97	2.05
32	y	616	LUT	C15-C14	4.04	1.55	1.43
43	t	101	BCR	C20-C21	4.04	1.55	1.43
31	R	307	CLA	MG-ND	-4.04	1.97	2.05
32	0	616	LUT	C35-C34	4.03	1.55	1.43
43	b	618	BCR	C19-C18	4.03	1.54	1.46
31	c	613	CLA	MG-ND	-4.03	1.97	2.05
43	a	410	BCR	C20-C21	4.03	1.55	1.43
32	Y	316	LUT	C7-C6	4.03	1.58	1.45
31	Y	312	CLA	MG-ND	-4.02	1.97	2.05
32	0	616	LUT	C7-C6	4.02	1.58	1.45
31	0	603	CLA	MG-ND	-4.02	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	p	603	CLA	MG-ND	-4.02	1.97	2.05
31	c	610	CLA	MG-ND	-4.02	1.97	2.05
30	8	607	CHL	C3B-C4B	4.02	1.45	1.41
43	z	101	BCR	C28-C27	4.02	1.65	1.52
35	4	615	RRX	C27-C26	-4.02	1.44	1.51
31	R	306	CLA	MG-ND	-4.02	1.97	2.05
32	1	615	LUT	C35-C34	4.02	1.55	1.43
31	7	314	CLA	MG-ND	-4.02	1.97	2.05
31	0	612	CLA	MG-ND	-4.02	1.97	2.05
30	2	601	CHL	C3B-C4B	4.02	1.45	1.41
31	c	608	CLA	MG-ND	-4.02	1.97	2.05
31	1	613	CLA	MG-ND	-4.01	1.97	2.05
35	G	614	RRX	C27-C26	-4.01	1.44	1.51
31	S	314	CLA	MG-ND	-4.01	1.97	2.05
30	N	308	CHL	C3B-C4B	4.01	1.45	1.41
30	5	609	CHL	C3B-C4B	4.01	1.45	1.41
35	9	317	RRX	C27-C26	-4.01	1.44	1.51
32	y	617	LUT	C31-C30	4.01	1.55	1.43
31	g	311	CLA	MG-ND	-4.01	1.97	2.05
32	Y	315	LUT	C15-C14	4.00	1.55	1.43
30	2	605	CHL	C3A-C2A	-4.00	1.51	1.54
31	r	316	CLA	MG-ND	-4.00	1.97	2.05
30	N	306	CHL	C3B-C4B	4.00	1.45	1.41
31	R	313	CLA	MG-ND	-4.00	1.97	2.05
31	G	610	CLA	MG-ND	-4.00	1.97	2.05
32	0	617	LUT	C7-C6	4.00	1.58	1.45
31	b	608	CLA	MG-ND	-4.00	1.97	2.05
31	Y	311	CLA	MG-ND	-4.00	1.97	2.05
32	y	616	LUT	C12-C13	4.00	1.54	1.46
31	s	314	CLA	MG-ND	-3.99	1.97	2.05
32	y	617	LUT	C35-C34	3.99	1.55	1.43
32	S	318	LUT	C28-C29	3.99	1.54	1.46
32	9	318	LUT	C28-C29	3.99	1.54	1.46
32	6	318	LUT	C28-C29	3.99	1.54	1.46
31	Y	313	CLA	MG-ND	-3.99	1.97	2.05
32	6	317	LUT	C28-C29	3.99	1.54	1.46
32	5	617	LUT	C11-C10	3.99	1.55	1.43
31	C	602	CLA	MG-ND	-3.99	1.97	2.05
31	B	608	CLA	MG-ND	-3.99	1.97	2.05
32	r	317	LUT	C31-C30	3.99	1.55	1.43
31	R	314	CLA	MG-ND	-3.98	1.97	2.05
32	G	615	LUT	C28-C29	3.98	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	C	615	BCR	C2-C1	3.98	1.63	1.54
31	b	609	CLA	MG-ND	-3.98	1.97	2.05
32	4	616	LUT	C28-C29	3.98	1.54	1.46
32	y	616	LUT	C31-C30	3.98	1.55	1.43
31	d	404	CLA	MG-ND	-3.98	1.97	2.05
36	r	301	NEX	C7-C6	-3.98	1.25	1.30
32	0	617	LUT	C21-C26	3.98	1.67	1.56
32	p	616	LUT	C11-C10	3.98	1.55	1.43
32	1	616	LUT	C7-C6	3.98	1.58	1.45
31	s	313	CLA	MG-ND	-3.98	1.97	2.05
31	1	612	CLA	MG-ND	-3.97	1.97	2.05
31	y	612	CLA	MG-ND	-3.97	1.97	2.05
32	7	317	LUT	C7-C6	3.97	1.58	1.45
30	G	607	CHL	C3B-C4B	3.97	1.45	1.41
30	0	609	CHL	C3B-C4B	3.97	1.45	1.41
32	Y	315	LUT	C35-C34	3.97	1.55	1.43
31	C	605	CLA	C4B-NB	-3.97	1.32	1.37
36	3	319	NEX	C7-C6	-3.97	1.26	1.30
43	D	405	BCR	C16-C17	3.96	1.55	1.43
43	B	617	BCR	C28-C27	3.96	1.64	1.52
31	C	604	CLA	MG-ND	-3.96	1.97	2.05
31	a	406	CLA	MG-ND	-3.96	1.97	2.05
31	c	605	CLA	MG-ND	-3.96	1.97	2.05
32	n	317	LUT	C28-C29	3.95	1.54	1.46
30	3	307	CHL	C3B-C4B	3.95	1.45	1.41
31	4	612	CLA	MG-ND	-3.95	1.98	2.05
31	R	303	CLA	MG-ND	-3.95	1.98	2.05
32	r	317	LUT	C12-C13	3.95	1.54	1.46
32	Y	315	LUT	C31-C30	3.95	1.55	1.43
31	C	606	CLA	MG-ND	-3.95	1.98	2.05
35	2	614	RRX	C16-C17	3.95	1.55	1.43
31	C	608	CLA	MG-ND	-3.95	1.98	2.05
35	G	614	RRX	C16-C17	3.95	1.55	1.43
32	8	615	LUT	C28-C29	3.95	1.54	1.46
31	R	316	CLA	MG-ND	-3.95	1.98	2.05
32	Y	315	LUT	C12-C13	3.95	1.54	1.46
31	3	301	CLA	MG-ND	-3.95	1.98	2.05
31	q	306	CLA	MG-ND	-3.95	1.98	2.05
32	s	317	LUT	C28-C29	3.95	1.54	1.46
31	3	316	CLA	MG-ND	-3.94	1.98	2.05
43	d	406	BCR	C19-C18	3.94	1.54	1.46
31	B	615	CLA	MG-ND	-3.94	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	606	CLA	MG-ND	-3.94	1.98	2.05
36	S	319	NEX	C7-C6	-3.94	1.26	1.30
31	S	315	CLA	MG-ND	-3.94	1.98	2.05
35	9	317	RRX	C16-C17	3.94	1.55	1.43
31	B	605	CLA	MG-ND	-3.94	1.98	2.05
31	r	312	CLA	MG-ND	-3.94	1.98	2.05
43	b	618	BCR	C20-C21	3.94	1.55	1.43
31	c	611	CLA	MG-ND	-3.94	1.98	2.05
32	p	617	LUT	C28-C29	3.94	1.54	1.46
31	r	313	CLA	MG-ND	-3.94	1.98	2.05
31	y	611	CLA	MG-ND	-3.94	1.98	2.05
31	G	612	CLA	MG-ND	-3.94	1.98	2.05
32	3	317	LUT	C21-C26	3.93	1.67	1.56
43	C	614	BCR	C27-C26	-3.93	1.43	1.51
32	7	318	LUT	C28-C29	3.93	1.54	1.46
31	r	311	CLA	MG-ND	-3.93	1.98	2.05
35	4	615	RRX	C16-C17	3.93	1.55	1.43
31	R	315	CLA	MG-ND	-3.93	1.98	2.05
30	Y	306	CHL	C3B-C4B	3.93	1.45	1.41
31	B	601	CLA	MG-ND	-3.93	1.98	2.05
32	y	616	LUT	C35-C34	3.93	1.55	1.43
31	6	312	CLA	MG-ND	-3.93	1.98	2.05
31	R	312	CLA	MG-ND	-3.93	1.98	2.05
36	0	618	NEX	C7-C6	-3.93	1.26	1.30
32	r	317	LUT	C15-C14	3.93	1.55	1.43
31	C	611	CLA	MG-ND	-3.93	1.98	2.05
31	C	613	CLA	MG-ND	-3.93	1.98	2.05
32	p	616	LUT	C21-C26	3.92	1.67	1.56
31	p	602	CLA	MG-ND	-3.92	1.98	2.05
43	b	618	BCR	C27-C26	-3.92	1.43	1.51
32	n	318	LUT	C28-C29	3.92	1.54	1.46
36	8	617	NEX	C7-C6	-3.92	1.26	1.30
32	3	318	LUT	C11-C10	3.92	1.55	1.43
32	G	615	LUT	C21-C26	3.92	1.67	1.56
32	1	615	LUT	C7-C6	3.92	1.58	1.45
43	C	615	BCR	C28-C27	3.92	1.64	1.52
32	8	616	LUT	C28-C29	3.92	1.54	1.46
31	3	311	CLA	MG-ND	-3.92	1.98	2.05
30	p	605	CHL	C3B-C4B	3.92	1.45	1.41
32	y	616	LUT	C7-C6	3.92	1.58	1.45
30	6	306	CHL	C3B-C4B	3.92	1.45	1.41
31	B	606	CLA	MG-ND	-3.91	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	G	614	RRX	C20-C21	3.91	1.55	1.43
43	b	619	BCR	C3-C4	3.91	1.64	1.52
32	p	616	LUT	C28-C29	3.91	1.54	1.46
32	S	317	LUT	C28-C29	3.91	1.54	1.46
30	S	308	CHL	C1A-CHA	-3.91	1.35	1.40
31	0	613	CLA	MG-ND	-3.91	1.98	2.05
43	d	406	BCR	C4-C5	-3.91	1.43	1.51
35	g	315	RRX	C16-C17	3.91	1.55	1.43
36	6	319	NEX	C7-C6	-3.90	1.26	1.30
30	y	601	CHL	C3B-C4B	3.90	1.45	1.41
32	y	617	LUT	C7-C6	3.90	1.58	1.45
31	g	310	CLA	MG-ND	-3.90	1.98	2.05
31	A	405	CLA	MG-ND	-3.90	1.98	2.05
43	V	101	BCR	C3-C4	3.90	1.64	1.52
31	R	311	CLA	MG-ND	-3.90	1.98	2.05
30	5	605	CHL	C3B-C4B	3.90	1.45	1.41
32	r	317	LUT	C7-C6	3.90	1.58	1.45
31	4	610	CLA	MG-ND	-3.90	1.98	2.05
30	1	607	CHL	C3B-C4B	3.89	1.45	1.41
43	c	615	BCR	C3-C4	3.89	1.64	1.52
31	B	607	CLA	C1C-NC	-3.89	1.31	1.37
35	q	317	RRX	C16-C17	3.89	1.55	1.43
30	5	608	CHL	C3B-C4B	3.89	1.45	1.41
35	g	315	RRX	C20-C21	3.89	1.55	1.43
35	4	615	RRX	C20-C21	3.89	1.55	1.43
32	2	615	LUT	C28-C29	3.89	1.54	1.46
31	S	312	CLA	MG-ND	-3.89	1.98	2.05
30	7	308	CHL	C3B-C4B	3.89	1.45	1.41
31	9	314	CLA	MG-ND	-3.89	1.98	2.05
31	4	613	CLA	MG-ND	-3.89	1.98	2.05
32	R	317	LUT	C21-C26	3.89	1.67	1.56
31	0	611	CLA	MG-ND	-3.89	1.98	2.05
31	3	312	CLA	MG-ND	-3.89	1.98	2.05
43	C	615	BCR	C3-C4	3.88	1.64	1.52
32	s	318	LUT	C28-C29	3.88	1.54	1.46
32	5	617	LUT	C21-C26	3.88	1.67	1.56
31	s	312	CLA	MG-ND	-3.88	1.98	2.05
30	n	309	CHL	C3B-C4B	3.88	1.45	1.41
31	a	407	CLA	MG-ND	-3.88	1.98	2.05
35	9	317	RRX	C20-C21	3.88	1.55	1.43
32	p	617	LUT	C11-C10	3.88	1.55	1.43
43	B	617	BCR	C27-C26	-3.88	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	304	CLA	MG-ND	-3.87	1.98	2.05
31	0	604	CLA	MG-ND	-3.87	1.98	2.05
43	B	618	BCR	C3-C4	3.87	1.64	1.52
32	g	316	LUT	C21-C26	3.87	1.67	1.56
31	9	313	CLA	MG-ND	-3.87	1.98	2.05
31	A	406	CLA	MG-ND	-3.87	1.98	2.05
31	b	602	CLA	MG-ND	-3.87	1.98	2.05
31	b	607	CLA	MG-ND	-3.87	1.98	2.05
43	H	101	BCR	C4-C5	-3.87	1.43	1.51
32	9	318	LUT	C21-C26	3.87	1.67	1.56
31	1	602	CLA	MG-ND	-3.87	1.98	2.05
31	C	605	CLA	C1C-NC	-3.86	1.31	1.37
30	4	606	CHL	C3B-C4B	3.86	1.45	1.41
31	A	407	CLA	MG-ND	-3.86	1.98	2.05
30	q	303	CHL	C3A-C2A	-3.86	1.51	1.54
31	d	401	CLA	MG-ND	-3.86	1.98	2.05
31	r	306	CLA	MG-ND	-3.86	1.98	2.05
31	S	311	CLA	MG-ND	-3.86	1.98	2.05
31	S	316	CLA	MG-ND	-3.85	1.98	2.05
32	q	318	LUT	C21-C26	3.85	1.67	1.56
31	0	602	CLA	MG-ND	-3.85	1.98	2.05
30	G	605	CHL	C3B-C4B	3.85	1.45	1.41
31	q	316	CLA	MG-ND	-3.85	1.98	2.05
32	S	318	LUT	C21-C26	3.85	1.67	1.56
32	G	615	LUT	C11-C10	3.85	1.55	1.43
31	b	610	CLA	MG-ND	-3.85	1.98	2.05
31	s	310	CLA	MG-ND	-3.85	1.98	2.05
32	4	616	LUT	C21-C26	3.85	1.67	1.56
32	g	316	LUT	C11-C10	3.85	1.55	1.43
31	G	609	CLA	MG-ND	-3.85	1.98	2.05
35	2	614	RRX	C20-C21	3.85	1.55	1.43
32	s	317	LUT	C21-C26	3.85	1.67	1.56
32	N	317	LUT	C21-C26	3.85	1.67	1.56
32	0	617	LUT	C28-C29	3.85	1.54	1.46
31	s	311	CLA	MG-ND	-3.84	1.98	2.05
43	v	101	BCR	C3-C4	3.84	1.64	1.52
32	6	318	LUT	C21-C26	3.84	1.67	1.56
32	N	316	LUT	C21-C26	3.84	1.67	1.56
30	7	308	CHL	C3A-C2A	-3.84	1.51	1.54
30	R	309	CHL	C3B-C4B	3.84	1.45	1.41
31	B	602	CLA	MG-ND	-3.84	1.98	2.05
32	S	317	LUT	C21-C26	3.84	1.67	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	D	405	BCR	C11-C10	3.84	1.55	1.43
43	T	101	BCR	C4-C5	-3.84	1.43	1.51
31	G	613	CLA	MG-ND	-3.84	1.98	2.05
32	r	317	LUT	C35-C34	3.84	1.55	1.43
31	s	315	CLA	MG-ND	-3.83	1.98	2.05
31	c	604	CLA	MG-ND	-3.83	1.98	2.05
45	c	616	DGD	CAB-C9B	-3.83	1.32	1.51
31	b	616	CLA	MG-ND	-3.83	1.98	2.05
32	5	616	LUT	C11-C10	3.83	1.55	1.43
43	t	101	BCR	C27-C26	-3.83	1.43	1.51
30	0	605	CHL	C1A-CHA	-3.82	1.35	1.40
32	3	318	LUT	C21-C26	3.82	1.67	1.56
30	p	608	CHL	C3A-C2A	-3.82	1.51	1.54
32	5	616	LUT	C21-C26	3.82	1.67	1.56
32	8	615	LUT	C21-C26	3.82	1.67	1.56
32	Y	315	LUT	C7-C6	3.82	1.58	1.45
43	C	614	BCR	C4-C5	-3.82	1.43	1.51
31	r	315	CLA	MG-ND	-3.82	1.98	2.05
35	g	315	RRX	C27-C26	-3.82	1.45	1.51
31	q	314	CLA	MG-ND	-3.82	1.98	2.05
31	S	310	CLA	MG-ND	-3.82	1.98	2.05
31	q	315	CLA	C1C-NC	-3.82	1.31	1.37
34	B	621	LMG	C37-C36	-3.81	1.32	1.51
31	C	601	CLA	MG-ND	-3.81	1.98	2.05
31	B	609	CLA	MG-ND	-3.81	1.98	2.05
32	n	317	LUT	C21-C26	3.81	1.67	1.56
31	y	613	CLA	C1C-NC	-3.81	1.31	1.37
43	c	614	BCR	C16-C17	3.81	1.55	1.43
32	8	616	LUT	C21-C26	3.81	1.67	1.56
34	g	322	LMG	C37-C36	-3.81	1.32	1.51
43	z	101	BCR	C3-C4	3.81	1.64	1.52
43	A	410	BCR	C27-C26	-3.80	1.43	1.51
43	B	617	BCR	C19-C18	3.80	1.54	1.46
43	h	101	BCR	C4-C5	-3.80	1.43	1.51
31	B	607	CLA	MG-ND	-3.80	1.98	2.05
34	9	301	LMG	C19-C18	-3.80	1.32	1.51
31	0	615	CLA	MG-ND	-3.80	1.98	2.05
31	4	614	CLA	MG-ND	-3.80	1.98	2.05
43	T	101	BCR	C16-C17	3.80	1.55	1.43
45	c	617	DGD	CGB-CFB	-3.80	1.32	1.51
32	7	318	LUT	C21-C26	3.80	1.67	1.56
43	a	410	BCR	C27-C26	-3.80	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	6	317	LUT	C21-C26	3.79	1.67	1.56
31	b	603	CLA	MG-ND	-3.79	1.98	2.05
32	Y	316	LUT	C28-C29	3.79	1.54	1.46
34	m	102	LMG	C37-C36	-3.79	1.32	1.51
30	Y	302	CHL	C3B-C4B	3.79	1.45	1.41
43	c	614	BCR	C4-C5	-3.79	1.43	1.51
32	q	318	LUT	C11-C10	3.79	1.54	1.43
30	N	309	CHL	C3B-C4B	3.79	1.45	1.41
43	C	615	BCR	C4-C5	-3.79	1.43	1.51
32	2	615	LUT	C11-C10	3.79	1.54	1.43
31	d	405	CLA	MG-ND	-3.79	1.98	2.05
43	B	619	BCR	C4-C5	-3.79	1.43	1.51
43	C	614	BCR	C3-C4	3.78	1.64	1.52
30	3	309	CHL	C1A-CHA	-3.78	1.35	1.40
32	n	318	LUT	C21-C26	3.78	1.66	1.56
45	c	618	DGD	CAA-C9A	-3.78	1.33	1.51
31	s	316	CLA	MG-ND	-3.78	1.98	2.05
32	9	318	LUT	C11-C10	3.78	1.54	1.43
32	7	317	LUT	C28-C29	3.78	1.54	1.46
34	d	410	LMG	C40-C39	-3.78	1.33	1.51
31	a	409	CLA	MG-ND	-3.78	1.98	2.05
31	7	313	CLA	MG-ND	-3.77	1.98	2.05
43	B	619	BCR	C3-C4	3.77	1.64	1.52
34	D	411	LMG	C40-C39	-3.77	1.33	1.51
43	c	614	BCR	C27-C26	-3.77	1.44	1.51
32	4	616	LUT	C11-C10	3.77	1.54	1.43
34	b	601	LMG	C37-C36	-3.77	1.33	1.51
45	c	616	DGD	CGA-CFA	-3.77	1.33	1.51
32	Y	316	LUT	C23-C24	-3.77	1.45	1.50
43	b	620	BCR	C3-C4	3.76	1.64	1.52
45	c	617	DGD	CAB-C9B	-3.76	1.33	1.51
34	D	409	LMG	C19-C18	-3.76	1.33	1.51
31	c	601	CLA	MG-ND	-3.76	1.98	2.05
43	c	615	BCR	C27-C26	-3.76	1.44	1.51
32	N	317	LUT	C11-C10	3.76	1.54	1.43
34	D	410	LMG	C37-C36	-3.76	1.33	1.51
45	c	617	DGD	CAA-C9A	-3.76	1.33	1.51
31	b	617	CLA	C1C-NC	-3.76	1.31	1.37
32	S	318	LUT	C11-C10	3.76	1.54	1.43
31	5	615	CLA	MG-ND	-3.76	1.98	2.05
32	3	317	LUT	C11-C10	3.76	1.54	1.43
34	m	102	LMG	C40-C39	-3.76	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C	617	DGD	CGB-CFB	-3.76	1.33	1.51
43	c	614	BCR	C3-C4	3.76	1.64	1.52
32	5	617	LUT	C19-C9	3.76	1.58	1.50
30	r	309	CHL	C3B-C4B	3.76	1.45	1.41
45	C	617	DGD	CAB-C9B	-3.76	1.33	1.51
31	A	409	CLA	MG-ND	-3.76	1.98	2.05
34	s	321	LMG	C19-C18	-3.76	1.33	1.51
32	1	616	LUT	C28-C29	3.76	1.54	1.46
30	4	609	CHL	C3B-C4B	3.76	1.45	1.41
34	W	201	LMG	C19-C18	-3.76	1.33	1.51
32	s	318	LUT	C21-C26	3.76	1.66	1.56
34	b	601	LMG	C40-C39	-3.76	1.33	1.51
34	w	201	LMG	C19-C18	-3.75	1.33	1.51
32	N	316	LUT	C11-C10	3.75	1.54	1.43
34	b	622	LMG	C37-C36	-3.75	1.33	1.51
32	0	616	LUT	C28-C29	3.75	1.54	1.46
45	C	617	DGD	CDB-CCB	-3.75	1.33	1.51
43	d	406	BCR	C27-C26	-3.75	1.44	1.51
43	z	101	BCR	C27-C26	-3.75	1.44	1.51
43	b	618	BCR	C3-C4	3.75	1.64	1.52
34	W	201	LMG	C37-C36	-3.75	1.33	1.51
45	c	618	DGD	CAB-C9B	-3.75	1.33	1.51
45	c	619	DGD	CDA-CCA	-3.75	1.33	1.51
32	R	317	LUT	C11-C10	3.75	1.54	1.43
34	W	201	LMG	C25-C24	-3.74	1.33	1.51
43	A	410	BCR	C3-C4	3.74	1.64	1.52
45	c	616	DGD	CGB-CFB	-3.74	1.33	1.51
34	W	201	LMG	C22-C21	-3.74	1.33	1.51
31	B	616	CLA	C1C-NC	-3.74	1.32	1.37
43	a	410	BCR	C3-C4	3.74	1.64	1.52
30	2	606	CHL	C3B-C4B	3.74	1.45	1.41
34	w	201	LMG	C40-C39	-3.74	1.33	1.51
45	c	619	DGD	CAB-C9B	-3.74	1.33	1.51
34	J	101	LMG	C37-C36	-3.74	1.33	1.51
31	p	604	CLA	MG-ND	-3.74	1.98	2.05
43	D	405	BCR	C3-C4	3.74	1.64	1.52
34	D	411	LMG	C37-C36	-3.74	1.33	1.51
43	v	101	BCR	C16-C17	3.74	1.54	1.43
34	b	622	LMG	C22-C21	-3.73	1.33	1.51
31	n	315	CLA	MG-ND	-3.73	1.98	2.05
34	B	621	LMG	C22-C21	-3.73	1.33	1.51
43	h	101	BCR	C27-C26	-3.73	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	D	409	LMG	C22-C21	-3.73	1.33	1.51
45	C	617	DGD	CAA-C9A	-3.73	1.33	1.51
34	J	101	LMG	C19-C18	-3.73	1.33	1.51
43	b	619	BCR	C16-C17	3.73	1.54	1.43
34	2	620	LMG	C40-C39	-3.73	1.33	1.51
43	t	101	BCR	C11-C10	3.73	1.54	1.43
34	d	410	LMG	C37-C36	-3.73	1.33	1.51
43	Z	101	BCR	C3-C4	3.73	1.64	1.52
34	C	619	LMG	C40-C39	-3.73	1.33	1.51
34	J	101	LMG	C40-C39	-3.73	1.33	1.51
43	T	101	BCR	C11-C10	3.73	1.54	1.43
34	B	621	LMG	C19-C18	-3.73	1.33	1.51
34	D	412	LMG	C37-C36	-3.73	1.33	1.51
35	g	315	RRX	C7-C6	3.73	1.57	1.45
45	c	616	DGD	CDA-CCA	-3.73	1.33	1.51
32	7	318	LUT	C11-C10	3.73	1.54	1.43
34	9	301	LMG	C37-C36	-3.73	1.33	1.51
32	y	617	LUT	C23-C24	-3.73	1.45	1.50
34	C	624	LMG	C19-C18	-3.73	1.33	1.51
43	h	101	BCR	C3-C4	3.72	1.64	1.52
34	b	626	LMG	C37-C36	-3.72	1.33	1.51
32	S	317	LUT	C38-C25	3.72	1.57	1.50
34	C	619	LMG	C19-C18	-3.72	1.33	1.51
31	8	613	CLA	MG-ND	-3.72	1.98	2.05
35	q	317	RRX	C20-C21	3.72	1.54	1.43
43	c	615	BCR	C11-C10	3.72	1.54	1.43
34	c	624	LMG	C40-C39	-3.72	1.33	1.51
32	8	615	LUT	C11-C10	3.72	1.54	1.43
32	n	317	LUT	C11-C10	3.72	1.54	1.43
45	C	620	DGD	CAA-C9A	-3.72	1.33	1.51
45	c	616	DGD	CDB-CCB	-3.72	1.33	1.51
34	0	620	LMG	C19-C18	-3.72	1.33	1.51
34	A	412	LMG	C19-C18	-3.72	1.33	1.51
34	w	202	LMG	C37-C36	-3.72	1.33	1.51
34	j	101	LMG	C19-C18	-3.72	1.33	1.51
34	g	322	LMG	C19-C18	-3.72	1.33	1.51
32	s	317	LUT	C38-C25	3.72	1.57	1.50
45	c	618	DGD	CDA-CCA	-3.72	1.33	1.51
34	C	624	LMG	C22-C21	-3.72	1.33	1.51
45	C	618	DGD	CAA-C9A	-3.72	1.33	1.51
32	0	616	LUT	C21-C26	3.72	1.66	1.56
31	N	314	CLA	MG-ND	-3.72	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	J	101	LMG	C22-C21	-3.72	1.33	1.51
34	w	202	LMG	C25-C24	-3.72	1.33	1.51
43	B	619	BCR	C27-C26	-3.71	1.44	1.51
43	B	617	BCR	C3-C4	3.71	1.64	1.52
32	y	617	LUT	C21-C26	3.71	1.66	1.56
30	Y	301	CHL	C3B-C4B	3.71	1.45	1.41
45	C	620	DGD	CGA-CFA	-3.71	1.33	1.51
31	p	612	CLA	MG-ND	-3.71	1.98	2.05
45	C	620	DGD	CDB-CCB	-3.71	1.33	1.51
34	b	622	LMG	C19-C18	-3.71	1.33	1.51
34	s	321	LMG	C22-C21	-3.71	1.33	1.51
34	G	621	LMG	C22-C21	-3.71	1.33	1.51
43	H	101	BCR	C3-C4	3.71	1.64	1.52
45	c	617	DGD	CDB-CCB	-3.71	1.33	1.51
43	b	620	BCR	C27-C26	-3.71	1.44	1.51
32	q	318	LUT	C19-C9	3.70	1.58	1.50
34	D	412	LMG	C19-C18	-3.70	1.33	1.51
34	w	202	LMG	C22-C21	-3.70	1.33	1.51
32	8	616	LUT	C11-C10	3.70	1.54	1.43
31	D	404	CLA	MG-ND	-3.70	1.98	2.05
34	D	412	LMG	C40-C39	-3.70	1.33	1.51
34	4	620	LMG	C40-C39	-3.70	1.33	1.51
34	d	410	LMG	C22-C21	-3.70	1.33	1.51
34	d	411	LMG	C19-C18	-3.70	1.33	1.51
34	w	202	LMG	C19-C18	-3.70	1.33	1.51
45	C	617	DGD	CGA-CFA	-3.70	1.33	1.51
34	j	101	LMG	C37-C36	-3.70	1.33	1.51
34	c	624	LMG	C37-C36	-3.70	1.33	1.51
32	Y	315	LUT	C21-C26	3.70	1.66	1.56
34	C	619	LMG	C22-C21	-3.70	1.33	1.51
34	W	201	LMG	C43-C42	-3.70	1.33	1.51
32	9	318	LUT	C19-C9	3.70	1.58	1.50
45	C	617	DGD	CDA-CCA	-3.70	1.33	1.51
32	8	616	LUT	C19-C9	3.70	1.58	1.50
43	b	620	BCR	C4-C5	-3.70	1.44	1.51
34	k	101	LMG	C19-C18	-3.70	1.33	1.51
32	n	318	LUT	C11-C10	3.70	1.54	1.43
34	D	410	LMG	C19-C18	-3.70	1.33	1.51
32	s	318	LUT	C11-C10	3.70	1.54	1.43
34	9	301	LMG	C22-C21	-3.70	1.33	1.51
43	B	617	BCR	C20-C21	3.70	1.54	1.43
31	7	316	CLA	MG-ND	-3.70	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C	620	DGD	CDA-CCA	-3.70	1.33	1.51
43	c	615	BCR	C16-C17	3.69	1.54	1.43
32	6	317	LUT	C38-C25	3.69	1.57	1.50
32	7	317	LUT	C21-C26	3.69	1.66	1.56
34	D	411	LMG	C22-C21	-3.69	1.33	1.51
31	6	316	CLA	MG-ND	-3.69	1.98	2.05
31	5	612	CLA	MG-ND	-3.69	1.98	2.05
45	c	618	DGD	CDB-CCB	-3.69	1.33	1.51
31	2	611	CLA	MG-ND	-3.69	1.98	2.05
32	1	616	LUT	C21-C26	3.69	1.66	1.56
34	C	619	LMG	C37-C36	-3.69	1.33	1.51
32	1	615	LUT	C21-C26	3.69	1.66	1.56
34	2	620	LMG	C22-C21	-3.69	1.33	1.51
34	k	101	LMG	C40-C39	-3.69	1.33	1.51
45	C	620	DGD	CAB-C9B	-3.69	1.33	1.51
34	4	620	LMG	C37-C36	-3.69	1.33	1.51
31	C	608	CLA	C1C-NC	-3.69	1.32	1.37
32	6	317	LUT	C11-C10	3.69	1.54	1.43
34	G	621	LMG	C19-C18	-3.69	1.33	1.51
45	c	619	DGD	CGA-CFA	-3.69	1.33	1.51
34	4	620	LMG	C22-C21	-3.69	1.33	1.51
34	w	202	LMG	C40-C39	-3.69	1.33	1.51
31	B	607	CLA	C4B-NB	-3.69	1.33	1.37
31	5	611	CLA	MG-ND	-3.69	1.98	2.05
45	C	618	DGD	CDA-CCA	-3.69	1.33	1.51
45	c	618	DGD	CGB-CFB	-3.69	1.33	1.51
45	c	619	DGD	CAA-C9A	-3.69	1.33	1.51
43	V	101	BCR	C16-C17	3.69	1.54	1.43
32	3	318	LUT	C19-C9	3.69	1.58	1.50
32	4	616	LUT	C38-C25	3.69	1.57	1.50
34	d	411	LMG	C37-C36	-3.69	1.33	1.51
32	p	617	LUT	C38-C25	3.69	1.57	1.50
32	s	317	LUT	C11-C10	3.68	1.54	1.43
43	C	615	BCR	C11-C10	3.68	1.54	1.43
34	k	101	LMG	C37-C36	-3.68	1.33	1.51
32	n	318	LUT	C19-C9	3.68	1.58	1.50
34	S	321	LMG	C22-C21	-3.68	1.33	1.51
34	q	301	LMG	C22-C21	-3.68	1.33	1.51
43	A	410	BCR	C4-C5	-3.68	1.44	1.51
34	B	621	LMG	C40-C39	-3.68	1.33	1.51
43	D	405	BCR	C24-C25	3.68	1.57	1.45
34	b	622	LMG	C40-C39	-3.68	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	B	618	BCR	C24-C25	3.68	1.57	1.45
32	3	317	LUT	C19-C9	3.68	1.58	1.50
34	d	410	LMG	C19-C18	-3.68	1.33	1.51
35	9	317	RRX	C7-C6	3.68	1.57	1.45
34	2	620	LMG	C37-C36	-3.68	1.33	1.51
31	9	312	CLA	MG-ND	-3.68	1.98	2.05
45	C	618	DGD	CAB-C9B	-3.68	1.33	1.51
31	2	612	CLA	MG-ND	-3.68	1.98	2.05
32	g	316	LUT	C38-C25	3.68	1.57	1.50
32	6	317	LUT	C19-C9	3.68	1.58	1.50
32	N	316	LUT	C19-C9	3.68	1.58	1.50
34	D	411	LMG	C19-C18	-3.68	1.33	1.51
45	C	618	DGD	CGB-CFB	-3.68	1.33	1.51
31	C	602	CLA	C1C-NC	-3.68	1.32	1.37
30	1	619	CHL	C3B-C2B	-3.67	1.35	1.40
31	p	613	CLA	MG-ND	-3.67	1.98	2.05
35	G	614	RRX	C7-C6	3.67	1.57	1.45
32	6	318	LUT	C11-C10	3.67	1.54	1.43
32	S	317	LUT	C19-C9	3.67	1.58	1.50
32	s	317	LUT	C19-C9	3.67	1.58	1.50
34	G	621	LMG	C37-C36	-3.67	1.33	1.51
43	Z	101	BCR	C27-C26	-3.67	1.44	1.51
31	N	313	CLA	MG-ND	-3.67	1.98	2.05
32	R	317	LUT	C23-C24	-3.67	1.45	1.50
34	6	321	LMG	C19-C18	-3.67	1.33	1.51
43	a	410	BCR	C4-C5	-3.67	1.44	1.51
43	b	618	BCR	C4-C5	-3.67	1.44	1.51
34	d	411	LMG	C40-C39	-3.67	1.33	1.51
43	B	618	BCR	C16-C17	3.67	1.54	1.43
31	r	303	CLA	C1C-NC	-3.67	1.32	1.37
34	q	301	LMG	C37-C36	-3.67	1.33	1.51
34	S	321	LMG	C19-C18	-3.67	1.33	1.51
32	S	317	LUT	C11-C10	3.67	1.54	1.43
43	d	406	BCR	C3-C4	3.66	1.63	1.52
45	c	618	DGD	CGA-CFA	-3.66	1.33	1.51
32	R	317	LUT	C28-C29	3.66	1.53	1.46
31	B	614	CLA	MG-ND	-3.66	1.98	2.05
43	b	619	BCR	C24-C25	3.66	1.57	1.45
45	C	618	DGD	CGA-CFA	-3.66	1.33	1.51
31	8	610	CLA	MG-ND	-3.66	1.98	2.05
32	8	615	LUT	C38-C25	3.66	1.57	1.50
45	c	619	DGD	CDB-CCB	-3.66	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	w	202	LMG	C43-C42	-3.66	1.33	1.51
32	5	616	LUT	C19-C9	3.66	1.58	1.50
32	G	615	LUT	C19-C9	3.66	1.58	1.50
32	n	317	LUT	C19-C9	3.66	1.58	1.50
43	T	101	BCR	C27-C26	-3.66	1.44	1.51
32	g	316	LUT	C19-C9	3.66	1.58	1.50
34	4	620	LMG	C19-C18	-3.66	1.33	1.51
43	Z	101	BCR	C16-C17	3.66	1.54	1.43
35	4	615	RRX	C7-C6	3.66	1.57	1.45
31	A	407	CLA	C1C-NC	-3.66	1.32	1.37
31	3	314	CLA	MG-ND	-3.66	1.98	2.05
32	1	615	LUT	C28-C29	3.65	1.53	1.46
32	5	617	LUT	C38-C25	3.65	1.57	1.50
34	2	620	LMG	C19-C18	-3.65	1.33	1.51
31	b	608	CLA	C1C-NC	-3.65	1.32	1.37
34	q	301	LMG	C19-C18	-3.65	1.33	1.51
45	C	618	DGD	CDB-CCB	-3.65	1.33	1.51
32	7	318	LUT	C19-C9	3.65	1.58	1.50
32	3	317	LUT	C38-C25	3.65	1.57	1.50
31	s	305	CLA	MG-ND	-3.65	1.98	2.05
32	y	616	LUT	C21-C26	3.65	1.66	1.56
43	A	410	BCR	C11-C10	3.65	1.54	1.43
31	g	313	CLA	MG-ND	-3.65	1.98	2.05
34	G	621	LMG	C40-C39	-3.65	1.33	1.51
31	N	321	CLA	MG-ND	-3.65	1.98	2.05
32	0	616	LUT	C38-C25	3.65	1.57	1.50
31	p	611	CLA	MG-ND	-3.65	1.98	2.05
31	q	313	CLA	MG-ND	-3.65	1.98	2.05
32	s	318	LUT	C19-C9	3.65	1.58	1.50
31	N	305	CLA	MG-ND	-3.65	1.98	2.05
32	S	318	LUT	C19-C9	3.65	1.58	1.50
32	7	318	LUT	C38-C25	3.65	1.57	1.50
32	n	317	LUT	C38-C25	3.65	1.57	1.50
34	g	322	LMG	C40-C39	-3.64	1.33	1.51
34	W	201	LMG	C40-C39	-3.64	1.33	1.51
45	c	619	DGD	CGB-CFB	-3.64	1.33	1.51
43	B	619	BCR	C11-C10	3.64	1.54	1.43
43	b	618	BCR	C11-C10	3.64	1.54	1.43
31	y	604	CLA	MG-ND	-3.64	1.98	2.05
31	B	612	CLA	MG-ND	-3.64	1.98	2.05
34	9	301	LMG	C40-C39	-3.64	1.33	1.51
32	8	615	LUT	C19-C9	3.64	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	g	312	CLA	MG-ND	-3.64	1.98	2.05
32	Y	315	LUT	C28-C29	3.64	1.53	1.46
32	Y	316	LUT	C21-C26	3.64	1.66	1.56
31	5	614	CLA	MG-ND	-3.64	1.98	2.05
43	D	405	BCR	C4-C5	-3.64	1.44	1.51
43	c	615	BCR	C4-C5	-3.64	1.44	1.51
31	5	604	CLA	MG-ND	-3.64	1.98	2.05
43	v	101	BCR	C11-C10	3.63	1.54	1.43
43	V	101	BCR	C11-C10	3.63	1.54	1.43
43	v	101	BCR	C24-C25	3.63	1.57	1.45
31	2	604	CLA	MG-ND	-3.63	1.98	2.05
32	p	617	LUT	C19-C9	3.63	1.58	1.50
34	w	201	LMG	C37-C36	-3.63	1.33	1.51
31	8	614	CLA	MG-ND	-3.63	1.98	2.05
36	n	319	NEX	C7-C6	-3.63	1.26	1.30
31	B	611	CLA	MG-ND	-3.63	1.98	2.05
32	4	616	LUT	C19-C9	3.63	1.58	1.50
32	s	318	LUT	C38-C25	3.63	1.57	1.50
31	n	312	CLA	MG-ND	-3.63	1.98	2.05
32	6	318	LUT	C38-C25	3.63	1.57	1.50
31	6	313	CLA	MG-ND	-3.63	1.98	2.05
43	C	614	BCR	C11-C10	3.63	1.54	1.43
36	N	318	NEX	C7-C6	-3.63	1.26	1.30
32	N	317	LUT	C19-C9	3.63	1.58	1.50
35	q	317	RRX	C7-C6	3.62	1.57	1.45
34	q	301	LMG	C40-C39	-3.62	1.33	1.51
31	3	313	CLA	MG-ND	-3.62	1.98	2.05
32	2	615	LUT	C19-C9	3.62	1.58	1.50
32	6	318	LUT	C19-C9	3.62	1.58	1.50
31	r	304	CLA	MG-ND	-3.62	1.98	2.05
32	7	317	LUT	C11-C10	3.62	1.54	1.43
43	T	101	BCR	C3-C4	3.62	1.63	1.52
32	y	617	LUT	C28-C29	3.62	1.53	1.46
32	Y	316	LUT	C11-C10	3.62	1.54	1.43
32	9	318	LUT	C38-C25	3.62	1.57	1.50
43	z	101	BCR	C11-C10	3.62	1.54	1.43
31	p	614	CLA	MG-ND	-3.62	1.98	2.05
31	7	312	CLA	MG-ND	-3.62	1.98	2.05
30	q	309	CHL	C1A-CHA	-3.62	1.35	1.40
31	Y	314	CLA	MG-ND	-3.62	1.98	2.05
31	4	611	CLA	MG-ND	-3.62	1.98	2.05
31	G	602	CLA	MG-ND	-3.62	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	626	LMG	C19-C18	-3.62	1.33	1.51
31	2	613	CLA	MG-ND	-3.61	1.98	2.05
31	g	314	CLA	MG-ND	-3.61	1.98	2.05
43	A	410	BCR	C16-C17	3.61	1.54	1.43
43	H	101	BCR	C27-C26	-3.61	1.44	1.51
31	B	610	CLA	MG-ND	-3.61	1.98	2.05
31	p	610	CLA	MG-ND	-3.61	1.98	2.05
30	p	601	CHL	C3A-C2A	-3.61	1.51	1.54
31	c	602	CLA	C1C-NC	-3.61	1.32	1.37
31	c	606	CLA	C1C-NC	-3.61	1.32	1.37
43	T	101	BCR	C24-C25	3.61	1.57	1.45
31	a	406	CLA	C1C-NC	-3.61	1.32	1.37
31	y	615	CLA	MG-ND	-3.61	1.98	2.05
31	9	316	CLA	MG-ND	-3.60	1.98	2.05
43	h	101	BCR	C16-C17	3.60	1.54	1.43
31	n	316	CLA	MG-ND	-3.60	1.98	2.05
43	h	101	BCR	C11-C10	3.60	1.54	1.43
31	G	604	CLA	MG-ND	-3.60	1.98	2.05
31	8	611	CLA	MG-ND	-3.60	1.98	2.05
31	p	615	CLA	MG-ND	-3.60	1.98	2.05
32	0	617	LUT	C11-C10	3.60	1.54	1.43
35	2	614	RRX	C7-C6	3.60	1.57	1.45
43	B	618	BCR	C27-C26	-3.60	1.44	1.51
43	V	101	BCR	C27-C26	-3.60	1.44	1.51
43	Z	101	BCR	C11-C10	3.60	1.54	1.43
32	p	616	LUT	C19-C9	3.60	1.58	1.50
31	3	301	CLA	C1C-NC	-3.60	1.32	1.37
31	N	315	CLA	MG-ND	-3.60	1.98	2.05
43	c	615	BCR	C24-C25	3.60	1.57	1.45
43	Z	101	BCR	C4-C5	-3.60	1.44	1.51
31	3	315	CLA	MG-ND	-3.60	1.98	2.05
31	8	603	CLA	MG-ND	-3.60	1.98	2.05
30	3	310	CHL	C3B-C4B	3.60	1.44	1.41
31	N	312	CLA	MG-ND	-3.60	1.98	2.05
31	S	305	CLA	MG-ND	-3.60	1.98	2.05
31	7	315	CLA	MG-ND	-3.60	1.98	2.05
31	8	602	CLA	MG-ND	-3.60	1.98	2.05
31	7	305	CLA	MG-ND	-3.60	1.98	2.05
31	8	612	CLA	MG-ND	-3.60	1.98	2.05
31	n	314	CLA	MG-ND	-3.59	1.98	2.05
30	n	310	CHL	C3B-C4B	3.59	1.44	1.41
32	p	616	LUT	C2-C1	3.59	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C	620	DGD	CGB-CFB	-3.59	1.33	1.51
31	n	313	CLA	MG-ND	-3.59	1.98	2.05
43	a	410	BCR	C16-C17	3.59	1.54	1.43
31	6	314	CLA	MG-ND	-3.59	1.98	2.05
31	5	613	CLA	MG-ND	-3.59	1.98	2.05
43	b	620	BCR	C11-C10	3.59	1.54	1.43
31	R	311	CLA	C1C-NC	-3.59	1.32	1.37
31	n	304	CLA	MG-ND	-3.59	1.98	2.05
32	G	615	LUT	C38-C25	3.59	1.57	1.50
34	b	626	LMG	C22-C21	-3.59	1.33	1.51
32	0	616	LUT	C11-C10	3.59	1.54	1.43
42	D	401	PHO	C1D-C2D	3.59	1.43	1.39
43	b	620	BCR	C16-C17	3.59	1.54	1.43
31	r	312	CLA	C1C-NC	-3.59	1.32	1.37
32	n	318	LUT	C38-C25	3.59	1.57	1.50
31	B	613	CLA	MG-ND	-3.58	1.98	2.05
43	b	619	BCR	C11-C10	3.58	1.54	1.43
34	D	410	LMG	C22-C21	-3.58	1.34	1.51
32	1	616	LUT	C19-C9	3.58	1.58	1.50
31	N	304	CLA	MG-ND	-3.58	1.98	2.05
31	y	614	CLA	MG-ND	-3.58	1.98	2.05
31	g	305	CLA	MG-ND	-3.58	1.98	2.05
32	0	616	LUT	C19-C9	3.58	1.58	1.50
31	1	614	CLA	MG-ND	-3.58	1.98	2.05
31	7	303	CLA	MG-ND	-3.58	1.98	2.05
43	H	101	BCR	C24-C25	3.58	1.57	1.45
43	t	101	BCR	C24-C25	3.58	1.57	1.45
32	1	616	LUT	C11-C10	3.58	1.54	1.43
31	0	614	CLA	MG-ND	-3.58	1.98	2.05
30	6	307	CHL	C3B-C4B	3.58	1.44	1.41
32	q	318	LUT	C38-C25	3.58	1.57	1.50
43	b	620	BCR	C24-C25	3.58	1.57	1.45
31	6	303	CLA	MG-ND	-3.58	1.98	2.05
31	8	604	CLA	MG-ND	-3.58	1.98	2.05
31	c	609	CLA	C1C-NC	-3.57	1.32	1.37
43	C	614	BCR	C16-C17	3.57	1.54	1.43
31	y	602	CLA	MG-ND	-3.57	1.98	2.05
43	a	410	BCR	C24-C25	3.57	1.57	1.45
31	g	304	CLA	MG-ND	-3.57	1.98	2.05
30	q	310	CHL	C3B-C4B	3.57	1.44	1.41
31	5	602	CLA	MG-ND	-3.57	1.98	2.05
31	2	603	CLA	MG-ND	-3.57	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	7	317	LUT	C38-C25	3.57	1.57	1.50
32	8	616	LUT	C38-C25	3.57	1.57	1.50
31	d	401	CLA	C1C-NC	-3.57	1.32	1.37
43	H	101	BCR	C16-C17	3.57	1.54	1.43
31	b	611	CLA	MG-ND	-3.57	1.98	2.05
43	H	101	BCR	C11-C10	3.57	1.54	1.43
31	4	602	CLA	MG-ND	-3.57	1.98	2.05
31	Y	310	CLA	MG-ND	-3.57	1.98	2.05
31	n	305	CLA	MG-ND	-3.57	1.98	2.05
32	3	318	LUT	C38-C25	3.57	1.57	1.50
32	p	617	LUT	C2-C1	3.57	1.65	1.54
43	v	101	BCR	C27-C26	-3.57	1.44	1.51
32	r	317	LUT	C21-C26	3.56	1.66	1.56
31	9	315	CLA	MG-ND	-3.56	1.98	2.05
31	0	610	CLA	C1C-NC	-3.56	1.32	1.37
30	p	608	CHL	CBB-CAB	3.56	1.51	1.29
31	6	304	CLA	MG-ND	-3.56	1.98	2.05
31	r	311	CLA	C1C-NC	-3.56	1.32	1.37
32	1	616	LUT	C38-C25	3.56	1.57	1.50
32	5	616	LUT	C38-C25	3.56	1.57	1.50
30	3	309	CHL	C3B-C4B	3.56	1.44	1.41
30	9	307	CHL	CBB-CAB	3.56	1.51	1.29
45	c	616	DGD	CAA-C9A	-3.56	1.34	1.51
32	N	316	LUT	C38-C25	3.56	1.57	1.50
32	q	318	LUT	C2-C1	3.56	1.65	1.54
32	S	318	LUT	C38-C25	3.56	1.57	1.50
31	3	306	CLA	MG-ND	-3.56	1.98	2.05
31	6	305	CLA	MG-ND	-3.56	1.98	2.05
30	7	321	CHL	C3B-C4B	3.56	1.44	1.41
31	Y	303	CLA	MG-ND	-3.56	1.98	2.05
31	A	405	CLA	C1C-NC	-3.56	1.32	1.37
31	N	311	CLA	MG-ND	-3.56	1.98	2.05
32	9	318	LUT	C2-C1	3.56	1.65	1.54
30	4	609	CHL	CBB-CAB	3.55	1.51	1.29
43	z	101	BCR	C16-C17	3.55	1.54	1.43
31	c	608	CLA	C1C-NC	-3.55	1.32	1.37
30	5	605	CHL	CBB-CAB	3.55	1.51	1.29
31	9	306	CLA	MG-ND	-3.55	1.98	2.05
30	3	307	CHL	CBB-CAB	3.55	1.51	1.29
30	8	608	CHL	C3B-C4B	3.55	1.44	1.41
31	1	611	CLA	MG-ND	-3.55	1.98	2.05
31	Y	305	CLA	MG-ND	-3.55	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	311	CLA	MG-ND	-3.55	1.98	2.05
43	h	101	BCR	C24-C25	3.55	1.57	1.45
30	0	605	CHL	C3B-C4B	3.55	1.44	1.41
30	p	605	CHL	CBB-CAB	3.55	1.51	1.29
43	v	101	BCR	C4-C5	-3.55	1.44	1.51
31	2	610	CLA	MG-ND	-3.55	1.98	2.05
32	N	316	LUT	C2-C1	3.55	1.65	1.54
43	B	619	BCR	C16-C17	3.55	1.54	1.43
31	c	603	CLA	C1C-NC	-3.55	1.32	1.37
43	V	101	BCR	C4-C5	-3.55	1.44	1.51
32	1	615	LUT	C38-C25	3.55	1.57	1.50
30	g	306	CHL	CBB-CAB	3.54	1.51	1.29
31	S	303	CLA	MG-ND	-3.54	1.98	2.05
31	q	312	CLA	MG-ND	-3.54	1.98	2.05
31	b	613	CLA	MG-ND	-3.54	1.98	2.05
31	n	303	CLA	MG-ND	-3.54	1.98	2.05
30	p	601	CHL	CBB-CAB	3.54	1.51	1.29
31	C	607	CLA	C1C-NC	-3.54	1.32	1.37
31	N	310	CLA	MG-ND	-3.54	1.98	2.05
31	B	605	CLA	C1C-NC	-3.54	1.32	1.37
31	c	604	CLA	C1C-NC	-3.54	1.32	1.37
32	N	317	LUT	C38-C25	3.54	1.57	1.50
30	G	605	CHL	CBB-CAB	3.54	1.51	1.29
35	q	317	RRX	C4-C5	-3.54	1.44	1.51
31	B	604	CLA	C1C-NC	-3.54	1.32	1.37
31	g	310	CLA	C1C-NC	-3.54	1.32	1.37
31	9	305	CLA	MG-ND	-3.54	1.98	2.05
30	n	308	CHL	C3B-C4B	3.54	1.44	1.41
43	B	618	BCR	C11-C10	3.54	1.54	1.43
31	9	304	CLA	MG-ND	-3.54	1.98	2.05
31	G	609	CLA	C1C-NC	-3.54	1.32	1.37
31	b	615	CLA	MG-ND	-3.54	1.98	2.05
31	c	607	CLA	C1C-NC	-3.54	1.32	1.37
30	2	605	CHL	CBB-CAB	3.54	1.51	1.29
30	G	607	CHL	CBB-CAB	3.54	1.51	1.29
43	b	619	BCR	C27-C26	-3.53	1.44	1.51
31	C	604	CLA	C1C-NC	-3.53	1.32	1.37
31	G	603	CLA	MG-ND	-3.53	1.98	2.05
31	7	311	CLA	MG-ND	-3.53	1.98	2.05
32	r	317	LUT	C38-C25	3.53	1.57	1.50
31	0	610	CLA	C4B-NB	-3.53	1.33	1.37
30	2	608	CHL	CBB-CAB	3.53	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	316	CLA	C1C-NC	-3.53	1.32	1.37
32	r	317	LUT	C28-C29	3.53	1.53	1.46
43	c	614	BCR	C24-C25	3.53	1.57	1.45
30	9	311	CHL	CBB-CAB	3.53	1.51	1.29
43	z	101	BCR	C4-C5	-3.53	1.44	1.51
30	2	607	CHL	CBB-CAB	3.53	1.51	1.29
32	0	617	LUT	C19-C9	3.53	1.58	1.50
30	p	609	CHL	CBB-CAB	3.53	1.51	1.29
30	Y	302	CHL	CBB-CAB	3.53	1.51	1.29
30	4	605	CHL	CBB-CAB	3.53	1.51	1.29
31	2	602	CLA	MG-ND	-3.53	1.98	2.05
31	N	303	CLA	MG-ND	-3.53	1.98	2.05
30	6	306	CHL	CBB-CAB	3.53	1.51	1.29
30	q	307	CHL	CBB-CAB	3.53	1.51	1.29
31	b	606	CLA	C1C-NC	-3.52	1.32	1.37
31	1	610	CLA	MG-ND	-3.52	1.98	2.05
43	C	615	BCR	C24-C25	3.52	1.57	1.45
32	5	616	LUT	C2-C1	3.52	1.65	1.54
30	g	309	CHL	CBB-CAB	3.52	1.51	1.29
30	8	607	CHL	CBB-CAB	3.52	1.51	1.29
32	6	317	LUT	C2-C1	3.52	1.65	1.54
31	3	304	CLA	MG-ND	-3.52	1.98	2.05
36	p	618	NEX	C7-C6	-3.52	1.26	1.30
30	1	605	CHL	CBB-CAB	3.52	1.51	1.29
31	n	311	CLA	MG-ND	-3.52	1.98	2.05
32	5	617	LUT	C2-C1	3.52	1.65	1.54
30	G	608	CHL	CBB-CAB	3.52	1.51	1.29
32	s	318	LUT	C2-C1	3.52	1.65	1.54
32	0	617	LUT	C23-C24	-3.52	1.45	1.50
30	3	303	CHL	CBB-CAB	3.52	1.51	1.29
31	2	609	CLA	MG-ND	-3.52	1.98	2.05
31	4	604	CLA	MG-ND	-3.52	1.98	2.05
30	8	601	CHL	CBB-CAB	3.52	1.51	1.29
43	a	410	BCR	C11-C10	3.52	1.54	1.43
30	n	302	CHL	CBB-CAB	3.52	1.51	1.29
31	b	605	CLA	C1C-NC	-3.52	1.32	1.37
43	V	101	BCR	C24-C25	3.52	1.57	1.45
31	q	304	CLA	MG-ND	-3.52	1.98	2.05
30	7	309	CHL	CBB-CAB	3.52	1.51	1.29
31	R	315	CLA	C1C-NC	-3.52	1.32	1.37
30	7	306	CHL	CBB-CAB	3.52	1.51	1.29
43	b	618	BCR	C16-C17	3.52	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	q	311	CHL	CBB-CAB	3.52	1.51	1.29
43	Z	101	BCR	C24-C25	3.52	1.57	1.45
31	s	303	CLA	MG-ND	-3.52	1.98	2.05
43	A	410	BCR	C24-C25	3.52	1.57	1.45
31	3	305	CLA	MG-ND	-3.51	1.98	2.05
30	g	308	CHL	CBB-CAB	3.51	1.51	1.29
43	t	101	BCR	C16-C17	3.51	1.54	1.43
30	0	609	CHL	CBB-CAB	3.51	1.51	1.29
31	b	612	CLA	MG-ND	-3.51	1.98	2.05
30	5	609	CHL	CBB-CAB	3.51	1.51	1.29
30	N	302	CHL	CBB-CAB	3.51	1.51	1.29
30	Y	309	CHL	CBB-CAB	3.51	1.51	1.29
32	6	318	LUT	C2-C1	3.51	1.65	1.54
32	y	617	LUT	C19-C9	3.51	1.57	1.50
30	r	309	CHL	CBB-CAB	3.51	1.51	1.29
31	C	611	CLA	C1C-NC	-3.51	1.32	1.37
30	9	310	CHL	CBB-CAB	3.51	1.51	1.29
32	y	616	LUT	C28-C29	3.51	1.53	1.46
31	5	610	CLA	MG-ND	-3.51	1.98	2.05
30	3	310	CHL	CBB-CAB	3.51	1.51	1.29
43	z	101	BCR	C24-C25	3.51	1.57	1.45
30	n	309	CHL	CBB-CAB	3.51	1.51	1.29
30	1	608	CHL	CBB-CAB	3.51	1.51	1.29
32	y	616	LUT	C19-C9	3.51	1.57	1.50
30	y	601	CHL	CBB-CAB	3.51	1.51	1.29
32	4	616	LUT	C2-C1	3.51	1.65	1.54
30	7	310	CHL	CBB-CAB	3.51	1.51	1.29
31	1	604	CLA	C1C-NC	-3.51	1.32	1.37
30	g	302	CHL	CBB-CAB	3.51	1.51	1.29
30	y	609	CHL	CBB-CAB	3.51	1.51	1.29
32	7	318	LUT	C2-C1	3.50	1.65	1.54
43	d	406	BCR	C24-C25	3.50	1.57	1.45
32	2	615	LUT	C2-C1	3.50	1.65	1.54
32	0	617	LUT	C38-C25	3.50	1.57	1.50
31	A	409	CLA	C1C-NC	-3.50	1.32	1.37
31	9	312	CLA	C1C-NC	-3.50	1.32	1.37
32	Y	315	LUT	C38-C25	3.50	1.57	1.50
30	N	308	CHL	CBB-CAB	3.50	1.51	1.29
30	9	303	CHL	CBB-CAB	3.50	1.51	1.29
30	n	310	CHL	CBB-CAB	3.50	1.51	1.29
30	s	308	CHL	CBB-CAB	3.50	1.51	1.29
30	R	309	CHL	CBB-CAB	3.50	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1	615	LUT	C19-C9	3.50	1.57	1.50
43	d	406	BCR	C16-C17	3.50	1.54	1.43
30	4	606	CHL	CBB-CAB	3.50	1.51	1.29
32	G	615	LUT	C2-C1	3.50	1.65	1.54
30	5	608	CHL	CBB-CAB	3.50	1.51	1.29
32	3	317	LUT	C2-C1	3.50	1.65	1.54
30	5	601	CHL	CBB-CAB	3.50	1.51	1.29
31	C	612	CLA	C1C-NC	-3.50	1.32	1.37
30	8	608	CHL	CBB-CAB	3.49	1.51	1.29
30	N	309	CHL	CBB-CAB	3.49	1.51	1.29
30	9	309	CHL	CBB-CAB	3.49	1.51	1.29
31	D	403	CLA	C1C-NC	-3.49	1.32	1.37
31	B	603	CLA	C1C-NC	-3.49	1.32	1.37
30	7	308	CHL	CBB-CAB	3.49	1.51	1.29
32	1	616	LUT	C2-C1	3.49	1.65	1.54
30	y	608	CHL	CBB-CAB	3.49	1.51	1.29
30	S	302	CHL	CBB-CAB	3.49	1.51	1.29
43	B	617	BCR	C11-C10	3.49	1.54	1.43
31	b	614	CLA	MG-ND	-3.49	1.98	2.05
30	q	303	CHL	CBB-CAB	3.49	1.51	1.29
30	3	302	CHL	C3B-C4B	3.49	1.44	1.41
43	B	619	BCR	C24-C25	3.49	1.57	1.45
31	8	609	CLA	MG-ND	-3.49	1.98	2.05
31	a	409	CLA	C1C-NC	-3.49	1.32	1.37
30	6	302	CHL	CBB-CAB	3.49	1.51	1.29
31	6	315	CLA	MG-ND	-3.49	1.98	2.05
30	2	601	CHL	CBB-CAB	3.49	1.51	1.29
30	0	601	CHL	CBB-CAB	3.49	1.51	1.29
32	7	317	LUT	C19-C9	3.49	1.57	1.50
30	3	309	CHL	CBB-CAB	3.49	1.51	1.29
30	G	601	CHL	CBB-CAB	3.49	1.51	1.29
31	R	304	CLA	C1C-NC	-3.49	1.32	1.37
32	8	615	LUT	C2-C1	3.49	1.65	1.54
43	B	618	BCR	C4-C5	-3.49	1.44	1.51
30	Y	301	CHL	CBB-CAB	3.48	1.51	1.29
32	y	616	LUT	C38-C25	3.48	1.57	1.50
30	1	607	CHL	CBB-CAB	3.48	1.51	1.29
30	7	302	CHL	CBB-CAB	3.48	1.51	1.29
32	n	317	LUT	C2-C1	3.48	1.65	1.54
32	g	316	LUT	C2-C1	3.48	1.65	1.54
30	s	302	CHL	CBB-CAB	3.48	1.51	1.29
31	A	406	CLA	C1C-NC	-3.48	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	n	306	CHL	CBB-CAB	3.48	1.51	1.29
30	4	608	CHL	CBB-CAB	3.48	1.51	1.29
30	Y	308	CHL	CBB-CAB	3.48	1.51	1.29
32	r	317	LUT	C19-C9	3.48	1.57	1.50
32	p	616	LUT	C38-C25	3.48	1.57	1.50
30	4	601	CHL	CBB-CAB	3.48	1.51	1.29
30	9	311	CHL	C3B-C4B	3.48	1.44	1.41
30	1	609	CHL	CBB-CAB	3.48	1.51	1.29
30	n	301	CHL	CBB-CAB	3.48	1.51	1.29
30	5	606	CHL	CBB-CAB	3.48	1.51	1.29
30	0	608	CHL	CBB-CAB	3.48	1.51	1.29
31	C	603	CLA	C1C-NC	-3.48	1.32	1.37
30	p	607	CHL	CBB-CAB	3.48	1.51	1.29
32	0	616	LUT	C23-C24	-3.47	1.45	1.50
30	Y	306	CHL	CBB-CAB	3.47	1.51	1.29
30	0	607	CHL	CBB-CAB	3.47	1.51	1.29
31	y	610	CLA	MG-ND	-3.47	1.98	2.05
31	q	313	CLA	C1C-NC	-3.47	1.32	1.37
30	S	308	CHL	C3B-C2B	-3.47	1.35	1.40
31	s	304	CLA	MG-ND	-3.47	1.98	2.05
35	g	315	RRX	C4-C5	-3.47	1.44	1.51
30	S	309	CHL	CBB-CAB	3.47	1.51	1.29
32	S	318	LUT	C2-C1	3.47	1.65	1.54
30	6	310	CHL	CBB-CAB	3.47	1.51	1.29
31	Y	304	CLA	MG-ND	-3.47	1.98	2.05
30	1	605	CHL	C1A-CHA	-3.47	1.36	1.40
31	y	603	CLA	MG-ND	-3.47	1.98	2.05
30	s	309	CHL	CBB-CAB	3.47	1.51	1.29
30	p	606	CHL	CBB-CAB	3.47	1.51	1.29
30	8	605	CHL	CBB-CAB	3.47	1.51	1.29
30	5	607	CHL	CBB-CAB	3.47	1.51	1.29
31	Y	311	CLA	C1C-NC	-3.47	1.32	1.37
30	N	306	CHL	CBB-CAB	3.47	1.51	1.29
32	0	616	LUT	C2-C1	3.47	1.65	1.54
31	c	613	CLA	C1C-NC	-3.47	1.32	1.37
30	9	308	CHL	CBB-CAB	3.47	1.51	1.29
31	S	313	CLA	C1C-NC	-3.47	1.32	1.37
32	7	317	LUT	C23-C24	-3.47	1.45	1.50
32	7	317	LUT	C2-C1	3.46	1.65	1.54
31	S	311	CLA	C1C-NC	-3.46	1.32	1.37
30	N	301	CHL	CBB-CAB	3.46	1.51	1.29
30	n	308	CHL	CBB-CAB	3.46	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	7	321	CHL	CBB-CAB	3.46	1.51	1.29
30	6	308	CHL	CBB-CAB	3.46	1.51	1.29
43	b	619	BCR	C4-C5	-3.46	1.44	1.51
31	r	307	CLA	C1C-NC	-3.46	1.32	1.37
32	5	616	LUT	C40-C33	3.46	1.57	1.50
30	G	623	CHL	CBB-CAB	3.46	1.51	1.29
30	1	606	CHL	CBB-CAB	3.46	1.51	1.29
31	r	305	CLA	MG-ND	-3.46	1.98	2.05
31	R	312	CLA	C1C-NC	-3.46	1.32	1.37
32	Y	315	LUT	C19-C9	3.46	1.57	1.50
30	7	307	CHL	CBB-CAB	3.46	1.51	1.29
31	R	314	CLA	C1C-NC	-3.46	1.32	1.37
32	N	317	LUT	C2-C1	3.46	1.65	1.54
30	8	606	CHL	C1A-CHA	-3.46	1.36	1.40
31	Y	313	CLA	C1C-NC	-3.46	1.32	1.37
32	8	615	LUT	C40-C33	3.46	1.57	1.50
30	y	605	CHL	CBB-CAB	3.46	1.51	1.29
32	q	318	LUT	C40-C33	3.45	1.57	1.50
32	1	615	LUT	C11-C10	3.45	1.53	1.43
31	5	603	CLA	MG-ND	-3.45	1.98	2.05
32	Y	316	LUT	C19-C9	3.45	1.57	1.50
30	6	307	CHL	CBB-CAB	3.45	1.50	1.29
30	Y	307	CHL	CBB-CAB	3.45	1.50	1.29
31	B	609	CLA	C1C-NC	-3.44	1.32	1.37
31	7	313	CLA	C1C-NC	-3.44	1.32	1.37
31	c	605	CLA	C1C-NC	-3.44	1.32	1.37
32	Y	315	LUT	C23-C24	-3.44	1.45	1.50
32	n	318	LUT	C2-C1	3.44	1.65	1.54
32	4	616	LUT	C40-C33	3.44	1.57	1.50
31	a	407	CLA	C1C-NC	-3.44	1.32	1.37
32	6	317	LUT	C40-C33	3.44	1.57	1.50
30	y	607	CHL	CBB-CAB	3.44	1.50	1.29
30	2	606	CHL	CBB-CAB	3.44	1.50	1.29
32	S	317	LUT	C40-C33	3.44	1.57	1.50
32	3	318	LUT	C2-C1	3.44	1.65	1.54
30	6	309	CHL	CBB-CAB	3.44	1.50	1.29
31	s	306	CLA	MG-ND	-3.44	1.99	2.05
32	6	318	LUT	C40-C33	3.44	1.57	1.50
32	R	317	LUT	C38-C25	3.44	1.56	1.50
43	C	614	BCR	C24-C25	3.44	1.56	1.45
31	c	611	CLA	C1C-NC	-3.44	1.32	1.37
30	y	606	CHL	CBB-CAB	3.44	1.50	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	p	617	LUT	C23-C24	-3.43	1.45	1.50
32	5	617	LUT	C40-C33	3.43	1.57	1.50
31	R	316	CLA	C1C-NC	-3.43	1.32	1.37
32	S	318	LUT	C40-C33	3.43	1.57	1.50
31	r	316	CLA	C1C-NC	-3.43	1.32	1.37
31	g	303	CLA	MG-ND	-3.43	1.99	2.05
30	5	601	CHL	C3A-C2A	-3.43	1.51	1.54
43	C	615	BCR	C16-C17	3.43	1.53	1.43
30	g	307	CHL	CBB-CAB	3.43	1.50	1.29
32	8	616	LUT	C2-C1	3.43	1.65	1.54
32	y	616	LUT	C2-C1	3.43	1.65	1.54
43	d	406	BCR	C11-C10	3.43	1.53	1.43
32	y	617	LUT	C11-C10	3.43	1.53	1.43
30	p	607	CHL	C1A-CHA	-3.43	1.36	1.40
30	8	606	CHL	CBB-CAB	3.43	1.50	1.29
30	s	307	CHL	CBB-CAB	3.43	1.50	1.29
30	q	310	CHL	CBB-CAB	3.43	1.50	1.29
32	y	616	LUT	C23-C24	-3.43	1.45	1.50
30	G	606	CHL	CBB-CAB	3.42	1.50	1.29
43	D	405	BCR	C27-C26	-3.42	1.44	1.51
32	G	615	LUT	C40-C33	3.42	1.57	1.50
32	Y	315	LUT	C11-C10	3.42	1.53	1.43
32	8	615	LUT	C23-C24	-3.42	1.45	1.50
31	B	606	CLA	C1C-NC	-3.42	1.32	1.37
32	p	616	LUT	C40-C33	3.42	1.57	1.50
32	8	616	LUT	C23-C24	-3.42	1.45	1.50
30	9	303	CHL	C3A-C2A	-3.42	1.51	1.54
32	n	317	LUT	C40-C33	3.42	1.57	1.50
31	7	304	CLA	MG-ND	-3.42	1.99	2.05
31	B	602	CLA	C1C-NC	-3.42	1.32	1.37
43	t	101	BCR	C3-C4	3.42	1.63	1.52
30	n	307	CHL	CBB-CAB	3.42	1.50	1.29
31	1	603	CLA	C1C-NC	-3.42	1.32	1.37
30	n	307	CHL	C1A-CHA	-3.42	1.36	1.40
30	S	307	CHL	CBB-CAB	3.41	1.50	1.29
31	B	615	CLA	C1C-NC	-3.41	1.32	1.37
30	9	310	CHL	C3A-C2A	-3.41	1.51	1.54
32	N	316	LUT	C40-C33	3.41	1.57	1.50
30	q	308	CHL	CBB-CAB	3.41	1.50	1.29
32	9	318	LUT	C23-C24	-3.41	1.45	1.50
30	S	302	CHL	C3B-C4B	3.41	1.44	1.41
31	C	601	CLA	C1C-NC	-3.41	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	7	318	LUT	C40-C33	3.41	1.57	1.50
32	R	317	LUT	C2-C1	3.41	1.65	1.54
32	N	317	LUT	C40-C33	3.41	1.57	1.50
32	S	317	LUT	C2-C1	3.41	1.65	1.54
43	b	618	BCR	C24-C25	3.41	1.56	1.45
32	s	318	LUT	C40-C33	3.41	1.57	1.50
31	9	312	CLA	C4B-NB	-3.41	1.33	1.37
31	9	314	CLA	C1C-NC	-3.40	1.32	1.37
31	4	603	CLA	MG-ND	-3.40	1.99	2.05
31	C	606	CLA	C1C-NC	-3.40	1.32	1.37
32	n	317	LUT	C23-C24	-3.40	1.45	1.50
31	s	310	CLA	C1C-NC	-3.40	1.32	1.37
32	r	317	LUT	C11-C10	3.40	1.53	1.43
32	s	317	LUT	C2-C1	3.40	1.65	1.54
32	9	318	LUT	C40-C33	3.40	1.57	1.50
30	R	308	CHL	CBB-CAB	3.40	1.50	1.29
31	R	306	CLA	C1C-NC	-3.40	1.32	1.37
30	0	605	CHL	C3B-C2B	-3.40	1.35	1.40
30	7	309	CHL	C1A-CHA	-3.40	1.36	1.40
31	r	306	CLA	C1C-NC	-3.40	1.32	1.37
31	R	307	CLA	C1C-NC	-3.40	1.32	1.37
32	n	318	LUT	C23-C24	-3.40	1.45	1.50
30	N	307	CHL	CBB-CAB	3.40	1.50	1.29
32	s	317	LUT	C40-C33	3.39	1.57	1.50
47	E	101	HEM	C1B-NB	-3.39	1.34	1.40
31	G	612	CLA	C1C-NC	-3.39	1.32	1.37
32	n	318	LUT	C40-C33	3.39	1.57	1.50
32	3	318	LUT	C40-C33	3.39	1.57	1.50
31	1	602	CLA	C1C-NC	-3.39	1.32	1.37
31	B	601	CLA	C1C-NC	-3.39	1.32	1.37
31	d	405	CLA	C1C-NC	-3.39	1.32	1.37
32	3	317	LUT	C40-C33	3.39	1.57	1.50
32	8	616	LUT	C40-C33	3.38	1.57	1.50
30	9	309	CHL	C1A-CHA	-3.38	1.36	1.40
31	b	602	CLA	C1C-NC	-3.38	1.32	1.37
31	c	612	CLA	C1C-NC	-3.38	1.32	1.37
32	r	317	LUT	C2-C1	3.38	1.64	1.54
31	C	613	CLA	C1C-NC	-3.38	1.32	1.37
31	s	316	CLA	C1C-NC	-3.38	1.32	1.37
31	q	315	CLA	C4B-NB	-3.38	1.33	1.37
31	B	608	CLA	C1C-NC	-3.38	1.32	1.37
30	4	607	CHL	CBB-CAB	3.38	1.50	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	606	CHL	CBB-CAB	3.38	1.50	1.29
31	y	611	CLA	C1C-NC	-3.37	1.32	1.37
32	y	616	LUT	C11-C10	3.37	1.53	1.43
30	N	301	CHL	C1A-CHA	-3.37	1.36	1.40
44	a	414	PL9	C3-C4	-3.37	1.44	1.49
32	g	316	LUT	C40-C33	3.37	1.57	1.50
32	1	615	LUT	C2-C1	3.37	1.64	1.54
31	S	314	CLA	C1C-NC	-3.37	1.32	1.37
30	r	310	CHL	CBB-CAB	3.37	1.50	1.29
31	R	313	CLA	C1C-NC	-3.37	1.32	1.37
30	1	619	CHL	CHB-C4A	-3.37	1.34	1.38
30	r	308	CHL	CBB-CAB	3.37	1.50	1.29
31	Y	312	CLA	C1C-NC	-3.37	1.32	1.37
31	s	311	CLA	C1C-NC	-3.37	1.32	1.37
32	N	316	LUT	C23-C24	-3.37	1.45	1.50
31	4	612	CLA	C1C-NC	-3.37	1.32	1.37
31	r	315	CLA	C1C-NC	-3.37	1.32	1.37
31	q	306	CLA	C4B-NB	-3.37	1.33	1.37
47	E	101	HEM	C4D-ND	-3.37	1.34	1.40
31	g	303	CLA	C1C-NC	-3.36	1.32	1.37
30	3	302	CHL	CBB-CAB	3.36	1.50	1.29
31	3	301	CLA	C4B-NB	-3.36	1.33	1.37
31	3	316	CLA	C4B-NB	-3.36	1.33	1.37
31	R	303	CLA	C1C-NC	-3.36	1.32	1.37
31	r	314	CLA	C1C-NC	-3.36	1.32	1.37
31	S	313	CLA	C4B-NB	-3.36	1.33	1.37
32	y	617	LUT	C38-C25	3.36	1.56	1.50
31	C	609	CLA	C1C-NC	-3.36	1.32	1.37
31	0	602	CLA	C1C-NC	-3.36	1.32	1.37
31	r	303	CLA	C4B-NB	-3.36	1.33	1.37
31	s	314	CLA	C1C-NC	-3.36	1.32	1.37
31	q	305	CLA	MG-ND	-3.35	1.99	2.05
31	A	407	CLA	C4B-NB	-3.35	1.33	1.37
31	b	604	CLA	C1C-NC	-3.35	1.32	1.37
31	D	404	CLA	C1C-NC	-3.35	1.32	1.37
32	Y	315	LUT	C2-C1	3.35	1.64	1.54
32	Y	316	LUT	C2-C1	3.35	1.64	1.54
32	p	617	LUT	C40-C33	3.35	1.57	1.50
31	S	306	CLA	MG-ND	-3.35	1.99	2.05
32	0	616	LUT	C40-C33	3.35	1.57	1.50
30	0	605	CHL	CBB-CAB	3.35	1.50	1.29
31	s	313	CLA	C1C-NC	-3.35	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	3	308	CHL	CBB-CAB	3.35	1.50	1.29
32	1	615	LUT	C23-C24	-3.35	1.45	1.50
32	r	317	LUT	C23-C24	-3.35	1.45	1.50
31	y	612	CLA	C1C-NC	-3.34	1.32	1.37
31	0	604	CLA	C1C-NC	-3.34	1.32	1.37
31	b	610	CLA	C1C-NC	-3.34	1.32	1.37
31	4	613	CLA	C1C-NC	-3.34	1.32	1.37
47	e	102	HEM	C1B-NB	-3.34	1.34	1.40
30	S	308	CHL	CBB-CAB	3.34	1.50	1.29
32	0	617	LUT	C40-C33	3.34	1.57	1.50
32	0	617	LUT	C2-C1	3.34	1.64	1.54
32	y	617	LUT	C2-C1	3.33	1.64	1.54
31	3	311	CLA	C1C-NC	-3.33	1.32	1.37
32	4	616	LUT	C23-C24	-3.33	1.45	1.50
30	1	601	CHL	CBB-CAB	3.33	1.50	1.29
31	R	305	CLA	C1C-NC	-3.33	1.32	1.37
32	q	318	LUT	C23-C24	-3.33	1.45	1.50
31	S	315	CLA	C1C-NC	-3.33	1.32	1.37
32	R	317	LUT	C19-C9	3.32	1.57	1.50
43	B	617	BCR	C16-C17	3.32	1.53	1.43
31	b	607	CLA	C1C-NC	-3.32	1.32	1.37
30	N	307	CHL	C1A-CHA	-3.32	1.36	1.40
30	y	605	CHL	C1A-CHA	-3.32	1.36	1.40
32	6	317	LUT	C23-C24	-3.32	1.45	1.50
30	4	608	CHL	C1A-CHA	-3.32	1.36	1.40
31	1	613	CLA	C1C-NC	-3.32	1.32	1.37
30	R	310	CHL	CBB-CAB	3.31	1.50	1.29
32	N	317	LUT	C23-C24	-3.31	1.45	1.50
31	s	315	CLA	C1C-NC	-3.31	1.32	1.37
30	R	308	CHL	C1A-CHA	-3.31	1.36	1.40
47	e	102	HEM	C4D-ND	-3.31	1.34	1.40
31	G	613	CLA	C1C-NC	-3.30	1.32	1.37
31	C	604	CLA	C4B-NB	-3.30	1.33	1.37
31	q	314	CLA	C1C-NC	-3.30	1.32	1.37
32	7	317	LUT	C40-C33	3.30	1.57	1.50
31	C	610	CLA	C1C-NC	-3.29	1.32	1.37
31	1	612	CLA	C1C-NC	-3.29	1.32	1.37
31	B	603	CLA	C4B-NB	-3.29	1.33	1.37
31	b	616	CLA	C1C-NC	-3.29	1.32	1.37
44	a	414	PL9	C7-C3	-3.29	1.46	1.51
31	c	610	CLA	C1C-NC	-3.29	1.32	1.37
30	r	308	CHL	C1A-CHA	-3.28	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1	616	LUT	C40-C33	3.28	1.57	1.50
31	d	404	CLA	C1C-NC	-3.28	1.32	1.37
32	S	317	LUT	C23-C24	-3.28	1.45	1.50
31	A	409	CLA	C4B-NB	-3.28	1.33	1.37
31	c	607	CLA	C4B-NB	-3.28	1.33	1.37
31	q	306	CLA	C1C-NC	-3.27	1.32	1.37
31	S	312	CLA	C1C-NC	-3.27	1.32	1.37
31	9	313	CLA	C1C-NC	-3.27	1.32	1.37
31	6	312	CLA	C1C-NC	-3.27	1.32	1.37
31	c	601	CLA	C1C-NC	-3.27	1.32	1.37
30	g	308	CHL	C1A-CHA	-3.27	1.36	1.40
31	0	615	CLA	C4B-NB	-3.27	1.33	1.37
31	0	613	CLA	C1C-NC	-3.27	1.32	1.37
31	D	403	CLA	C4B-NB	-3.26	1.33	1.37
31	S	310	CLA	C1C-NC	-3.26	1.32	1.37
31	4	614	CLA	C1C-NC	-3.26	1.32	1.37
31	b	609	CLA	C1C-NC	-3.26	1.32	1.37
31	r	313	CLA	C1C-NC	-3.26	1.32	1.37
35	2	614	RRX	C4-C5	-3.26	1.44	1.51
31	c	612	CLA	C4B-NB	-3.26	1.33	1.37
30	q	309	CHL	CBB-CAB	3.26	1.49	1.29
32	3	317	LUT	C23-C24	-3.26	1.45	1.50
30	7	307	CHL	C1A-CHA	-3.25	1.36	1.40
35	4	615	RRX	C4-C5	-3.25	1.44	1.51
30	1	601	CHL	C3B-C2B	-3.25	1.36	1.40
31	g	311	CLA	C1C-NC	-3.25	1.32	1.37
30	8	601	CHL	C1A-CHA	-3.25	1.36	1.40
31	0	612	CLA	C1C-NC	-3.25	1.32	1.37
31	c	602	CLA	C4B-NB	-3.25	1.33	1.37
35	G	614	RRX	C4-C5	-3.25	1.45	1.51
30	q	309	CHL	C3B-C2B	-3.25	1.36	1.40
31	b	603	CLA	C1C-NC	-3.25	1.32	1.37
31	B	616	CLA	C4B-NB	-3.25	1.33	1.37
30	q	307	CHL	C1A-CHA	-3.25	1.36	1.40
32	Y	315	LUT	C40-C33	3.24	1.57	1.50
32	1	616	LUT	C23-C24	-3.24	1.45	1.50
30	3	308	CHL	C3B-C2B	-3.24	1.36	1.40
31	G	611	CLA	C1C-NC	-3.24	1.32	1.37
31	7	314	CLA	C1C-NC	-3.24	1.32	1.37
32	1	615	LUT	C40-C33	3.24	1.57	1.50
31	C	613	CLA	C4B-NB	-3.24	1.33	1.37
31	0	603	CLA	C1C-NC	-3.23	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	s	312	CLA	C1C-NC	-3.23	1.32	1.37
31	p	602	CLA	C1C-NC	-3.23	1.32	1.37
32	r	317	LUT	C40-C33	3.23	1.57	1.50
31	B	610	CLA	C1C-NC	-3.23	1.32	1.37
31	A	406	CLA	C4B-NB	-3.23	1.33	1.37
30	1	619	CHL	CBB-CAB	3.22	1.49	1.29
31	a	409	CLA	C4B-NB	-3.22	1.33	1.37
31	R	304	CLA	C4B-NB	-3.22	1.33	1.37
31	c	609	CLA	C4B-NB	-3.22	1.33	1.37
31	p	615	CLA	C1C-NC	-3.22	1.32	1.37
30	n	302	CHL	C1A-CHA	-3.22	1.36	1.40
31	C	607	CLA	C4B-NB	-3.22	1.33	1.37
31	0	615	CLA	C1C-NC	-3.22	1.32	1.37
31	2	611	CLA	C1C-NC	-3.22	1.32	1.37
31	4	610	CLA	C4B-NB	-3.22	1.33	1.37
32	s	317	LUT	C23-C24	-3.22	1.45	1.50
35	9	317	RRX	C4-C5	-3.22	1.45	1.51
43	B	617	BCR	C24-C25	3.22	1.56	1.45
42	A	408	PHO	C1D-C2D	3.21	1.43	1.39
30	n	301	CHL	C1A-CHA	-3.21	1.36	1.40
42	D	401	PHO	C4D-CHA	3.21	1.44	1.39
31	4	610	CLA	C1C-NC	-3.21	1.32	1.37
31	R	315	CLA	C4B-NB	-3.21	1.33	1.37
31	r	311	CLA	C4B-NB	-3.21	1.33	1.37
32	6	318	LUT	C23-C24	-3.21	1.45	1.50
31	B	604	CLA	C4B-NB	-3.21	1.33	1.37
30	N	302	CHL	C1A-CHA	-3.21	1.36	1.40
30	q	310	CHL	C1A-CHA	-3.21	1.36	1.40
32	3	318	LUT	C23-C24	-3.21	1.45	1.50
30	0	608	CHL	C1A-CHA	-3.20	1.36	1.40
31	c	613	CLA	C4B-NB	-3.20	1.33	1.37
32	Y	316	LUT	C38-C25	3.20	1.56	1.50
31	C	602	CLA	C4B-NB	-3.20	1.33	1.37
32	2	615	LUT	C40-C33	3.20	1.57	1.50
31	c	605	CLA	C4B-NB	-3.20	1.33	1.37
32	R	317	LUT	C40-C33	3.20	1.57	1.50
32	y	616	LUT	C40-C33	3.20	1.57	1.50
31	B	611	CLA	C1C-NC	-3.20	1.32	1.37
31	a	407	CLA	C4B-NB	-3.19	1.33	1.37
30	0	607	CHL	C1A-CHA	-3.19	1.36	1.40
30	R	310	CHL	C3B-C2B	-3.19	1.36	1.40
32	Y	316	LUT	C40-C33	3.19	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	615	CLA	C4B-NB	-3.19	1.33	1.37
31	3	313	CLA	C1C-NC	-3.19	1.32	1.37
31	B	605	CLA	C4B-NB	-3.19	1.33	1.37
32	y	617	LUT	C40-C33	3.18	1.57	1.50
31	b	617	CLA	C4B-NB	-3.18	1.33	1.37
31	q	316	CLA	C1C-NC	-3.18	1.32	1.37
30	Y	309	CHL	C1A-CHA	-3.18	1.36	1.40
30	0	607	CHL	C3A-C2A	-3.18	1.52	1.54
30	s	307	CHL	C1A-CHA	-3.18	1.36	1.40
31	q	312	CLA	C1C-NC	-3.18	1.32	1.37
30	2	601	CHL	C1A-CHA	-3.17	1.36	1.40
31	G	609	CLA	C4B-NB	-3.17	1.33	1.37
31	Y	314	CLA	C1C-NC	-3.17	1.32	1.37
31	p	614	CLA	C1C-NC	-3.17	1.32	1.37
30	y	608	CHL	C1A-CHA	-3.17	1.36	1.40
31	C	611	CLA	C4B-NB	-3.17	1.33	1.37
31	B	602	CLA	C4B-NB	-3.17	1.33	1.37
31	q	312	CLA	C3B-C4B	3.17	1.46	1.39
30	9	310	CHL	C1A-CHA	-3.17	1.36	1.40
31	n	316	CLA	C1C-NC	-3.17	1.32	1.37
31	r	305	CLA	C1C-NC	-3.17	1.32	1.37
31	5	615	CLA	C1C-NC	-3.16	1.32	1.37
31	2	613	CLA	C1C-NC	-3.16	1.32	1.37
30	6	306	CHL	C1A-CHA	-3.16	1.36	1.40
31	6	314	CLA	C1C-NC	-3.16	1.32	1.37
31	p	603	CLA	C1C-NC	-3.16	1.32	1.37
31	S	316	CLA	C1C-NC	-3.16	1.32	1.37
31	Y	305	CLA	C1C-NC	-3.16	1.32	1.37
31	4	611	CLA	C3B-C4B	3.16	1.46	1.39
31	6	305	CLA	C1C-NC	-3.16	1.32	1.37
30	0	601	CHL	C1A-CHA	-3.16	1.36	1.40
32	5	617	LUT	C23-C24	-3.15	1.45	1.50
31	r	304	CLA	C1C-NC	-3.15	1.32	1.37
30	7	302	CHL	C1A-CHA	-3.15	1.36	1.40
31	1	610	CLA	C1C-NC	-3.15	1.32	1.37
31	g	310	CLA	C4B-NB	-3.15	1.33	1.37
31	N	310	CLA	C1C-NC	-3.15	1.32	1.37
31	R	311	CLA	C4B-NB	-3.15	1.33	1.37
32	7	318	LUT	C23-C24	-3.15	1.46	1.50
31	7	316	CLA	C1C-NC	-3.14	1.32	1.37
32	p	616	LUT	C23-C24	-3.14	1.46	1.50
31	A	405	CLA	C4B-NB	-3.14	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y	604	CLA	C1C-NC	-3.14	1.32	1.37
30	s	302	CHL	C3B-C4B	3.14	1.44	1.41
31	r	312	CLA	C4B-NB	-3.14	1.33	1.37
31	s	304	CLA	C1C-NC	-3.14	1.32	1.37
31	N	312	CLA	C1C-NC	-3.14	1.32	1.37
31	G	612	CLA	C4B-NB	-3.14	1.33	1.37
31	0	611	CLA	C1C-NC	-3.14	1.32	1.37
31	n	304	CLA	C1C-NC	-3.14	1.32	1.37
30	Y	302	CHL	C1A-CHA	-3.14	1.36	1.40
31	s	305	CLA	C1C-NC	-3.14	1.32	1.37
31	d	401	CLA	C4B-NB	-3.14	1.33	1.37
31	B	614	CLA	C1C-NC	-3.13	1.33	1.37
31	q	305	CLA	C1C-NC	-3.13	1.33	1.37
31	b	612	CLA	C1C-NC	-3.13	1.33	1.37
31	c	606	CLA	C4B-NB	-3.13	1.33	1.37
31	3	314	CLA	C1C-NC	-3.13	1.33	1.37
31	r	306	CLA	C4B-NB	-3.13	1.33	1.37
31	q	314	CLA	C4B-NB	-3.13	1.33	1.37
31	N	314	CLA	C1C-NC	-3.13	1.33	1.37
31	7	304	CLA	C1C-NC	-3.13	1.33	1.37
31	b	605	CLA	C4B-NB	-3.13	1.33	1.37
31	N	321	CLA	C1C-NC	-3.13	1.33	1.37
31	p	612	CLA	C1C-NC	-3.13	1.33	1.37
31	8	612	CLA	C1C-NC	-3.13	1.33	1.37
31	S	311	CLA	C4B-NB	-3.13	1.33	1.37
31	b	608	CLA	C4B-NB	-3.13	1.33	1.37
31	2	603	CLA	C1C-NC	-3.13	1.33	1.37
30	2	607	CHL	C1A-CHA	-3.13	1.36	1.40
42	A	408	PHO	C4D-CHA	3.12	1.44	1.39
31	3	305	CLA	C1C-NC	-3.12	1.33	1.37
31	g	304	CLA	C1C-NC	-3.12	1.33	1.37
42	a	408	PHO	C4D-CHA	3.12	1.44	1.39
31	C	612	CLA	C4B-NB	-3.12	1.33	1.37
31	a	406	CLA	C4B-NB	-3.12	1.33	1.37
31	G	610	CLA	C1C-NC	-3.12	1.33	1.37
31	N	303	CLA	C1C-NC	-3.12	1.33	1.37
31	7	305	CLA	C1C-NC	-3.12	1.33	1.37
31	Y	313	CLA	C4B-NB	-3.12	1.33	1.37
31	b	611	CLA	C1C-NC	-3.12	1.33	1.37
31	C	609	CLA	C4B-NB	-3.11	1.33	1.37
31	g	313	CLA	C1C-NC	-3.11	1.33	1.37
31	4	603	CLA	C1C-NC	-3.11	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	g	312	CLA	C1C-NC	-3.11	1.33	1.37
31	s	306	CLA	C1C-NC	-3.11	1.33	1.37
31	G	604	CLA	C1C-NC	-3.11	1.33	1.37
31	y	603	CLA	C1C-NC	-3.11	1.33	1.37
30	4	601	CHL	C1A-CHA	-3.11	1.36	1.40
31	2	610	CLA	C1C-NC	-3.11	1.33	1.37
31	6	304	CLA	C1C-NC	-3.11	1.33	1.37
32	s	318	LUT	C23-C24	-3.11	1.46	1.50
30	5	606	CHL	C1A-CHA	-3.11	1.36	1.40
30	0	605	CHL	CHB-C4A	-3.11	1.34	1.38
31	3	315	CLA	C1C-NC	-3.10	1.33	1.37
31	5	612	CLA	C1C-NC	-3.10	1.33	1.37
31	g	314	CLA	C1C-NC	-3.10	1.33	1.37
31	b	610	CLA	C4B-NB	-3.10	1.33	1.37
31	Y	304	CLA	C1C-NC	-3.10	1.33	1.37
31	9	304	CLA	C1C-NC	-3.10	1.33	1.37
31	6	303	CLA	C1C-NC	-3.10	1.33	1.37
31	5	613	CLA	C1C-NC	-3.10	1.33	1.37
31	S	305	CLA	C1C-NC	-3.10	1.33	1.37
31	y	602	CLA	C1C-NC	-3.10	1.33	1.37
31	n	311	CLA	C1C-NC	-3.10	1.33	1.37
31	8	610	CLA	C1C-NC	-3.10	1.33	1.37
30	7	308	CHL	C1A-CHA	-3.09	1.36	1.40
31	9	305	CLA	C1C-NC	-3.09	1.33	1.37
31	y	614	CLA	C1C-NC	-3.09	1.33	1.37
31	5	611	CLA	C1C-NC	-3.09	1.33	1.37
30	8	605	CHL	C1A-CHA	-3.09	1.36	1.40
31	G	602	CLA	C1C-NC	-3.09	1.33	1.37
31	7	312	CLA	C1C-NC	-3.09	1.33	1.37
31	n	315	CLA	C1C-NC	-3.09	1.33	1.37
30	1	606	CHL	C1A-CHA	-3.09	1.36	1.40
31	N	305	CLA	C1C-NC	-3.09	1.33	1.37
31	n	305	CLA	C1C-NC	-3.09	1.33	1.37
30	1	601	CHL	CHB-C4A	-3.09	1.34	1.38
31	r	315	CLA	C4B-NB	-3.09	1.33	1.37
31	N	304	CLA	C1C-NC	-3.09	1.33	1.37
31	7	311	CLA	C1C-NC	-3.09	1.33	1.37
31	n	312	CLA	C1C-NC	-3.09	1.33	1.37
31	p	611	CLA	C1C-NC	-3.09	1.33	1.37
31	n	314	CLA	C1C-NC	-3.09	1.33	1.37
31	5	604	CLA	C1C-NC	-3.08	1.33	1.37
31	y	610	CLA	C1C-NC	-3.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y	303	CLA	C1C-NC	-3.08	1.33	1.37
31	y	615	CLA	C1C-NC	-3.08	1.33	1.37
31	6	313	CLA	C1C-NC	-3.08	1.33	1.37
31	Y	311	CLA	C4B-NB	-3.08	1.33	1.37
31	1	604	CLA	C4B-NB	-3.08	1.33	1.37
31	D	404	CLA	C4B-NB	-3.08	1.33	1.37
34	y	620	LMG	C37-C36	-3.08	1.32	1.51
31	b	604	CLA	C4B-NB	-3.08	1.33	1.37
31	p	604	CLA	C1C-NC	-3.08	1.33	1.37
31	C	608	CLA	C4B-NB	-3.08	1.33	1.37
31	S	304	CLA	C4B-NB	-3.08	1.33	1.37
31	8	614	CLA	C1C-NC	-3.08	1.33	1.37
31	Y	310	CLA	C1C-NC	-3.08	1.33	1.37
31	1	611	CLA	C1C-NC	-3.08	1.33	1.37
31	S	306	CLA	C1C-NC	-3.08	1.33	1.37
31	s	303	CLA	C1C-NC	-3.08	1.33	1.37
31	2	612	CLA	C1C-NC	-3.08	1.33	1.37
34	0	622	LMG	C37-C36	-3.07	1.32	1.51
31	d	404	CLA	C4B-NB	-3.07	1.33	1.37
31	2	609	CLA	C1C-NC	-3.07	1.33	1.37
32	5	616	LUT	C23-C24	-3.07	1.46	1.50
31	1	614	CLA	C1C-NC	-3.07	1.33	1.37
31	8	604	CLA	C1C-NC	-3.07	1.33	1.37
30	G	606	CHL	C1A-CHA	-3.07	1.36	1.40
31	p	613	CLA	C1C-NC	-3.07	1.33	1.37
31	3	306	CLA	C1C-NC	-3.07	1.33	1.37
31	1	602	CLA	C4B-NB	-3.07	1.33	1.37
30	1	607	CHL	C1A-CHA	-3.07	1.36	1.40
31	s	311	CLA	C4B-NB	-3.07	1.33	1.37
31	S	303	CLA	C1C-NC	-3.07	1.33	1.37
31	R	306	CLA	C4B-NB	-3.06	1.33	1.37
31	2	613	CLA	C4B-NB	-3.06	1.33	1.37
31	d	405	CLA	C4B-NB	-3.06	1.33	1.37
31	9	306	CLA	C1C-NC	-3.06	1.33	1.37
30	n	306	CHL	C1A-CHA	-3.06	1.36	1.40
31	B	608	CLA	C4B-NB	-3.06	1.33	1.37
30	g	307	CHL	C1A-CHA	-3.06	1.36	1.40
31	5	603	CLA	C1C-NC	-3.06	1.33	1.37
31	3	304	CLA	C1C-NC	-3.06	1.33	1.37
31	9	316	CLA	C1C-NC	-3.06	1.33	1.37
31	b	614	CLA	C1C-NC	-3.06	1.33	1.37
31	4	602	CLA	C1C-NC	-3.05	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	G	615	LUT	C23-C24	-3.05	1.46	1.50
31	n	303	CLA	C1C-NC	-3.05	1.33	1.37
31	n	313	CLA	C1C-NC	-3.05	1.33	1.37
31	3	312	CLA	C1C-NC	-3.05	1.33	1.37
31	9	315	CLA	C1C-NC	-3.05	1.33	1.37
31	g	305	CLA	C1C-NC	-3.05	1.33	1.37
31	8	609	CLA	C1C-NC	-3.05	1.33	1.37
31	N	315	CLA	C1C-NC	-3.05	1.33	1.37
31	2	602	CLA	C1C-NC	-3.05	1.33	1.37
31	2	604	CLA	C1C-NC	-3.05	1.33	1.37
31	B	606	CLA	C4B-NB	-3.05	1.33	1.37
30	3	303	CHL	C1A-CHA	-3.05	1.36	1.40
31	5	614	CLA	C1C-NC	-3.05	1.33	1.37
31	8	611	CLA	C1C-NC	-3.05	1.33	1.37
31	b	613	CLA	C1C-NC	-3.04	1.33	1.37
31	B	613	CLA	C1C-NC	-3.04	1.33	1.37
31	b	615	CLA	C1C-NC	-3.04	1.33	1.37
30	N	306	CHL	C1A-CHA	-3.04	1.36	1.40
31	7	315	CLA	C1C-NC	-3.04	1.33	1.37
31	6	316	CLA	C4B-NB	-3.04	1.33	1.37
31	N	311	CLA	C1C-NC	-3.04	1.33	1.37
31	b	603	CLA	C4B-NB	-3.04	1.33	1.37
30	y	601	CHL	C1A-CHA	-3.04	1.36	1.40
30	y	609	CHL	C1A-CHA	-3.04	1.36	1.40
31	r	307	CLA	C4B-NB	-3.04	1.33	1.37
31	5	610	CLA	C1C-NC	-3.04	1.33	1.37
30	Y	307	CHL	C1A-CHA	-3.04	1.36	1.40
31	6	315	CLA	C1C-NC	-3.04	1.33	1.37
31	6	316	CLA	C1C-NC	-3.04	1.33	1.37
31	G	603	CLA	C1C-NC	-3.04	1.33	1.37
31	8	603	CLA	C1C-NC	-3.04	1.33	1.37
30	8	607	CHL	C1A-CHA	-3.03	1.36	1.40
31	5	602	CLA	C1C-NC	-3.03	1.33	1.37
31	R	312	CLA	C4B-NB	-3.03	1.33	1.37
31	6	311	CLA	C1C-NC	-3.03	1.33	1.37
31	N	313	CLA	C1C-NC	-3.03	1.33	1.37
31	y	604	CLA	C4B-NB	-3.03	1.33	1.37
31	q	313	CLA	C3B-C4B	3.03	1.46	1.39
31	S	306	CLA	C4B-NB	-3.02	1.33	1.37
31	S	315	CLA	C4B-NB	-3.02	1.33	1.37
31	8	613	CLA	C1C-NC	-3.02	1.33	1.37
30	r	310	CHL	C1A-CHA	-3.02	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	611	CLA	C4B-NB	-3.02	1.33	1.37
31	7	303	CLA	C1C-NC	-3.02	1.33	1.37
31	c	608	CLA	C4B-NB	-3.02	1.33	1.37
31	r	316	CLA	C4B-NB	-3.02	1.33	1.37
31	0	614	CLA	C1C-NC	-3.02	1.33	1.37
31	S	304	CLA	C1C-NC	-3.02	1.33	1.37
31	b	606	CLA	C4B-NB	-3.02	1.33	1.37
30	q	308	CHL	C3B-C4B	3.02	1.44	1.41
34	w	205	LMG	C37-C36	-3.02	1.33	1.51
31	B	609	CLA	C4B-NB	-3.02	1.33	1.37
31	Y	314	CLA	C4B-NB	-3.01	1.33	1.37
31	b	616	CLA	C4B-NB	-3.01	1.33	1.37
31	y	602	CLA	C4B-NB	-3.01	1.33	1.37
31	8	602	CLA	C1C-NC	-3.01	1.33	1.37
31	p	613	CLA	C4B-NB	-3.01	1.33	1.37
31	R	305	CLA	C4B-NB	-3.01	1.33	1.37
30	6	308	CHL	C3A-C2A	-3.01	1.52	1.54
31	c	610	CLA	C4B-NB	-3.01	1.33	1.37
34	b	624	LMG	C37-C36	-3.01	1.33	1.51
30	q	309	CHL	CHB-C4A	-3.01	1.35	1.38
34	r	321	LMG	C37-C36	-3.01	1.33	1.51
31	B	612	CLA	C1C-NC	-3.01	1.33	1.37
31	c	611	CLA	C4B-NB	-3.00	1.33	1.37
31	Y	305	CLA	C4B-NB	-3.00	1.33	1.37
31	p	610	CLA	C1C-NC	-3.00	1.33	1.37
31	s	314	CLA	C4B-NB	-3.00	1.33	1.37
31	s	303	CLA	C4B-NB	-3.00	1.33	1.37
31	2	611	CLA	C4B-NB	-3.00	1.33	1.37
30	5	601	CHL	C1A-CHA	-3.00	1.36	1.40
30	y	606	CHL	C1A-CHA	-3.00	1.36	1.40
31	b	607	CLA	C4B-NB	-3.00	1.33	1.37
34	n	321	LMG	C37-C36	-2.99	1.33	1.51
31	9	304	CLA	C4B-NB	-2.99	1.33	1.37
30	r	310	CHL	C3B-C2B	-2.99	1.36	1.40
34	R	321	LMG	C37-C36	-2.99	1.33	1.51
31	s	310	CLA	C4B-NB	-2.99	1.33	1.37
31	9	316	CLA	C4B-NB	-2.99	1.33	1.37
30	0	606	CHL	C3B-C4B	2.99	1.44	1.41
34	6	321	LMG	C37-C36	-2.99	1.33	1.51
31	4	604	CLA	C1C-NC	-2.99	1.33	1.37
30	S	308	CHL	C3B-C4B	2.99	1.44	1.41
45	c	617	DGD	CDA-CCA	-2.99	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	621	LMG	C37-C36	-2.99	1.33	1.51
31	G	611	CLA	C4B-NB	-2.99	1.33	1.37
45	C	616	DGD	CAB-C9B	-2.98	1.33	1.51
31	4	611	CLA	C1C-NC	-2.98	1.33	1.37
34	Q1	101	LMG	C37-C36	-2.98	1.33	1.51
31	R	316	CLA	C4B-NB	-2.98	1.33	1.37
31	7	305	CLA	C4B-NB	-2.98	1.33	1.37
34	b	623	LMG	C37-C36	-2.98	1.33	1.51
31	0	602	CLA	C4B-NB	-2.98	1.33	1.37
31	b	613	CLA	C4B-NB	-2.98	1.33	1.37
30	N	309	CHL	C1A-CHA	-2.98	1.36	1.40
31	3	304	CLA	C4B-NB	-2.98	1.33	1.37
31	4	612	CLA	C4B-NB	-2.98	1.33	1.37
31	3	311	CLA	C4B-NB	-2.98	1.34	1.37
30	S	309	CHL	C1A-CHA	-2.98	1.36	1.40
31	c	603	CLA	C4B-NB	-2.98	1.34	1.37
31	b	612	CLA	C4B-NB	-2.97	1.34	1.37
34	w	203	LMG	C37-C36	-2.97	1.33	1.51
31	4	614	CLA	C4B-NB	-2.97	1.34	1.37
34	A	418	LMG	C37-C36	-2.97	1.33	1.51
34	B	625	LMG	C37-C36	-2.97	1.33	1.51
31	N	310	CLA	C4B-NB	-2.97	1.34	1.37
31	7	315	CLA	C4B-NB	-2.97	1.34	1.37
31	r	304	CLA	C4B-NB	-2.97	1.34	1.37
30	Y	308	CHL	C1A-CHA	-2.97	1.36	1.40
34	A	414	LMG	C37-C36	-2.97	1.33	1.51
34	Y	319	LMG	C37-C36	-2.97	1.33	1.51
31	q	304	CLA	C1C-NC	-2.97	1.33	1.37
34	d	409	LMG	C19-C18	-2.97	1.33	1.51
34	4	621	LMG	C19-C18	-2.97	1.33	1.51
34	G	619	LMG	C37-C36	-2.97	1.33	1.51
31	G	604	CLA	C4B-NB	-2.97	1.34	1.37
31	b	609	CLA	C4B-NB	-2.97	1.34	1.37
31	S	303	CLA	C4B-NB	-2.97	1.34	1.37
31	s	313	CLA	C4B-NB	-2.97	1.34	1.37
34	7	322	LMG	C37-C36	-2.96	1.33	1.51
31	s	305	CLA	C4B-NB	-2.96	1.34	1.37
34	f	101	LMG	C37-C36	-2.96	1.33	1.51
34	m	102	LMG	C19-C18	-2.96	1.33	1.51
34	3	321	LMG	C37-C36	-2.96	1.33	1.51
31	0	613	CLA	C4B-NB	-2.96	1.34	1.37
34	6	322	LMG	C19-C18	-2.96	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	610	CLA	C4B-NB	-2.96	1.34	1.37
30	R	310	CHL	CHB-C4A	-2.96	1.35	1.38
34	X	203	LMG	C37-C36	-2.96	1.33	1.51
34	d	409	LMG	C37-C36	-2.96	1.33	1.51
34	N	320	LMG	C37-C36	-2.96	1.33	1.51
34	9	321	LMG	C37-C36	-2.96	1.33	1.51
31	B	601	CLA	C4B-NB	-2.96	1.34	1.37
31	7	316	CLA	C4B-NB	-2.95	1.34	1.37
32	y	617	LUT	O23-C23	-2.95	1.38	1.43
34	7	320	LMG	C37-C36	-2.95	1.33	1.51
31	6	305	CLA	C4B-NB	-2.95	1.34	1.37
30	N	308	CHL	C1A-CHA	-2.95	1.36	1.40
34	2	618	LMG	C37-C36	-2.95	1.33	1.51
31	1	613	CLA	C4B-NB	-2.95	1.34	1.37
31	n	311	CLA	C4B-NB	-2.95	1.34	1.37
30	6	309	CHL	C1A-CHA	-2.95	1.36	1.40
31	3	306	CLA	C4B-NB	-2.95	1.34	1.37
34	5	620	LMG	C37-C36	-2.95	1.33	1.51
34	9	302	LMG	C19-C18	-2.95	1.33	1.51
31	y	603	CLA	C4B-NB	-2.95	1.34	1.37
34	g	320	LMG	C37-C36	-2.95	1.33	1.51
31	b	602	CLA	C4B-NB	-2.95	1.34	1.37
34	p	620	LMG	C37-C36	-2.95	1.33	1.51
34	X	202	LMG	C37-C36	-2.95	1.33	1.51
34	1	618	LMG	C37-C36	-2.95	1.33	1.51
34	b	629	LMG	C37-C36	-2.95	1.33	1.51
31	B	612	CLA	C4B-NB	-2.95	1.34	1.37
31	C	610	CLA	C4B-NB	-2.95	1.34	1.37
34	q1	101	LMG	C37-C36	-2.95	1.33	1.51
34	k	102	LMG	C37-C36	-2.95	1.33	1.51
34	2	621	LMG	C19-C18	-2.95	1.33	1.51
34	W	203	LMG	C37-C36	-2.95	1.33	1.51
31	n	304	CLA	C4B-NB	-2.95	1.34	1.37
34	c	621	LMG	C37-C36	-2.95	1.33	1.51
31	p	603	CLA	C4B-NB	-2.95	1.34	1.37
34	B	622	LMG	C37-C36	-2.94	1.33	1.51
31	B	614	CLA	C4B-NB	-2.94	1.34	1.37
31	C	603	CLA	C4B-NB	-2.94	1.34	1.37
31	r	305	CLA	C4B-NB	-2.94	1.34	1.37
31	N	314	CLA	C4B-NB	-2.94	1.34	1.37
34	I	101	LMG	C37-C36	-2.94	1.33	1.51
32	g	316	LUT	C23-C24	-2.94	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	q	302	LMG	C19-C18	-2.94	1.33	1.51
31	C	601	CLA	C4B-NB	-2.94	1.34	1.37
34	6	323	LMG	C37-C36	-2.94	1.33	1.51
31	N	303	CLA	C4B-NB	-2.94	1.34	1.37
30	p	605	CHL	C1A-CHA	-2.94	1.36	1.40
34	b	601	LMG	C19-C18	-2.94	1.33	1.51
34	g	322	LMG	C22-C21	-2.94	1.33	1.51
30	q	310	CHL	C3B-C2B	-2.94	1.36	1.40
34	0	620	LMG	C37-C36	-2.94	1.33	1.51
31	s	315	CLA	C4B-NB	-2.94	1.34	1.37
34	7	301	LMG	C19-C18	-2.94	1.33	1.51
34	n	322	LMG	C19-C18	-2.94	1.33	1.51
31	N	313	CLA	C4B-NB	-2.94	1.34	1.37
31	4	602	CLA	C4B-NB	-2.94	1.34	1.37
31	Y	310	CLA	C4B-NB	-2.94	1.34	1.37
34	a	401	LMG	C37-C36	-2.94	1.33	1.51
31	8	609	CLA	C4B-NB	-2.93	1.34	1.37
34	J	102	LMG	C37-C36	-2.93	1.33	1.51
30	Y	301	CHL	C1A-CHA	-2.93	1.36	1.40
34	c	620	LMG	C37-C36	-2.93	1.33	1.51
31	Y	303	CLA	C4B-NB	-2.93	1.34	1.37
34	D	409	LMG	C37-C36	-2.93	1.33	1.51
31	7	314	CLA	C4B-NB	-2.93	1.34	1.37
34	W	202	LMG	C37-C36	-2.93	1.33	1.51
31	8	611	CLA	C4B-NB	-2.93	1.34	1.37
31	n	303	CLA	C4B-NB	-2.93	1.34	1.37
34	a	416	LMG	C37-C36	-2.93	1.33	1.51
31	S	310	CLA	C4B-NB	-2.93	1.34	1.37
30	3	302	CHL	CHB-C4A	-2.93	1.35	1.38
31	9	314	CLA	C4B-NB	-2.93	1.34	1.37
30	s	309	CHL	C1A-CHA	-2.93	1.36	1.40
31	G	602	CLA	C4B-NB	-2.93	1.34	1.37
31	8	603	CLA	C4B-NB	-2.93	1.34	1.37
34	G	622	LMG	C19-C18	-2.93	1.33	1.51
31	7	311	CLA	C4B-NB	-2.92	1.34	1.37
31	n	315	CLA	C4B-NB	-2.92	1.34	1.37
31	5	602	CLA	C4B-NB	-2.92	1.34	1.37
30	4	607	CHL	C1D-C2D	2.92	1.42	1.39
34	w	204	LMG	C37-C36	-2.92	1.33	1.51
31	6	303	CLA	C4B-NB	-2.92	1.34	1.37
43	D	405	BCR	C7-C6	2.92	1.55	1.45
31	N	315	CLA	C4B-NB	-2.92	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	609	CLA	C4B-NB	-2.92	1.34	1.37
30	4	606	CHL	C1A-CHA	-2.92	1.36	1.40
31	3	305	CLA	C4B-NB	-2.92	1.34	1.37
31	R	307	CLA	C4B-NB	-2.92	1.34	1.37
31	g	305	CLA	C4B-NB	-2.92	1.34	1.37
34	a	413	LMG	C37-C36	-2.92	1.33	1.51
30	2	605	CHL	C1A-CHA	-2.91	1.36	1.40
31	N	305	CLA	C4B-NB	-2.91	1.34	1.37
31	0	604	CLA	C4B-NB	-2.91	1.34	1.37
31	6	314	CLA	C4B-NB	-2.91	1.34	1.37
31	s	306	CLA	C4B-NB	-2.91	1.34	1.37
34	x	202	LMG	C37-C36	-2.91	1.33	1.51
31	5	612	CLA	C4B-NB	-2.91	1.34	1.37
31	n	305	CLA	C4B-NB	-2.91	1.34	1.37
31	g	313	CLA	C4B-NB	-2.90	1.34	1.37
31	8	612	CLA	C4B-NB	-2.90	1.34	1.37
31	n	313	CLA	C4B-NB	-2.90	1.34	1.37
31	6	315	CLA	C4B-NB	-2.90	1.34	1.37
31	8	613	CLA	C4B-NB	-2.90	1.34	1.37
31	p	615	CLA	C4B-NB	-2.90	1.34	1.37
31	g	312	CLA	C4B-NB	-2.90	1.34	1.37
30	7	306	CHL	C1A-CHA	-2.90	1.36	1.40
30	r	308	CHL	CHB-C4A	-2.89	1.35	1.38
30	S	307	CHL	C1A-CHA	-2.89	1.36	1.40
31	n	314	CLA	C4B-NB	-2.89	1.34	1.37
31	n	316	CLA	C4B-NB	-2.89	1.34	1.37
31	b	615	CLA	C4B-NB	-2.89	1.34	1.37
31	8	614	CLA	C4B-NB	-2.89	1.34	1.37
43	D	405	BCR	C34-C9	2.89	1.56	1.50
30	9	307	CHL	C1A-CHA	-2.89	1.36	1.40
31	N	304	CLA	C4B-NB	-2.89	1.34	1.37
31	6	311	CLA	C4B-NB	-2.89	1.34	1.37
31	S	314	CLA	C4B-NB	-2.88	1.34	1.37
31	b	614	CLA	C4B-NB	-2.88	1.34	1.37
30	3	302	CHL	C3B-C2B	-2.88	1.36	1.40
31	p	602	CLA	C4B-NB	-2.88	1.34	1.37
31	S	305	CLA	C4B-NB	-2.88	1.34	1.37
31	y	610	CLA	C4B-NB	-2.88	1.34	1.37
30	1	609	CHL	C1A-CHA	-2.88	1.36	1.40
31	2	602	CLA	C4B-NB	-2.88	1.34	1.37
31	0	614	CLA	C4B-NB	-2.88	1.34	1.37
43	c	614	BCR	C7-C6	2.88	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	N	321	CLA	C4B-NB	-2.88	1.34	1.37
30	G	601	CHL	C1A-CHA	-2.88	1.36	1.40
30	G	607	CHL	C1A-CHA	-2.88	1.36	1.40
32	r	317	LUT	O23-C23	-2.88	1.38	1.43
31	8	602	CLA	C4B-NB	-2.88	1.34	1.37
31	9	315	CLA	C4B-NB	-2.88	1.34	1.37
31	B	610	CLA	C4B-NB	-2.87	1.34	1.37
30	4	607	CHL	CHB-C4A	-2.87	1.35	1.38
32	R	317	LUT	O23-C23	-2.87	1.38	1.43
30	n	310	CHL	C1A-CHA	-2.87	1.36	1.40
31	1	614	CLA	C4B-NB	-2.87	1.34	1.37
31	7	303	CLA	C4B-NB	-2.87	1.34	1.37
31	B	613	CLA	C4B-NB	-2.87	1.34	1.37
31	r	313	CLA	C4B-NB	-2.87	1.34	1.37
31	y	615	CLA	C4B-NB	-2.86	1.34	1.37
31	5	615	CLA	C4B-NB	-2.86	1.34	1.37
31	5	603	CLA	C4B-NB	-2.86	1.34	1.37
31	8	604	CLA	C4B-NB	-2.86	1.34	1.37
30	1	601	CHL	C3B-C4B	2.86	1.44	1.41
30	S	302	CHL	CHB-C4A	-2.86	1.35	1.38
31	5	610	CLA	C4B-NB	-2.86	1.34	1.37
31	s	312	CLA	C4B-NB	-2.86	1.34	1.37
42	D	401	PHO	CMC-C2C	-2.85	1.46	1.50
31	S	316	CLA	C4B-NB	-2.85	1.34	1.37
30	0	609	CHL	C1A-CHA	-2.85	1.36	1.40
30	1	608	CHL	C1A-CHA	-2.85	1.36	1.40
32	2	615	LUT	O23-C23	-2.85	1.38	1.43
30	6	308	CHL	C1A-CHA	-2.85	1.36	1.40
32	2	615	LUT	C38-C25	2.85	1.55	1.50
31	2	604	CLA	C4B-NB	-2.85	1.34	1.37
30	p	606	CHL	C1D-C2D	2.84	1.42	1.39
31	R	303	CLA	C4B-NB	-2.84	1.34	1.37
30	g	306	CHL	C1A-CHA	-2.84	1.36	1.40
32	Y	315	LUT	O23-C23	-2.84	1.38	1.43
31	9	306	CLA	C4B-NB	-2.84	1.34	1.37
31	g	304	CLA	C4B-NB	-2.84	1.34	1.37
30	y	607	CHL	C1A-CHA	-2.84	1.36	1.40
42	A	408	PHO	CMC-C2C	-2.84	1.46	1.50
31	5	604	CLA	C4B-NB	-2.84	1.34	1.37
31	p	610	CLA	C4B-NB	-2.83	1.34	1.37
31	c	604	CLA	C4B-NB	-2.83	1.34	1.37
30	y	605	CHL	CHB-C4A	-2.83	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	604	CLA	C4B-NB	-2.83	1.34	1.37
30	5	608	CHL	C1A-CHA	-2.83	1.36	1.40
43	V	101	BCR	C34-C9	2.83	1.56	1.50
31	3	315	CLA	C4B-NB	-2.83	1.34	1.37
31	3	313	CLA	C4B-NB	-2.82	1.34	1.37
30	Y	307	CHL	CHB-C4A	-2.82	1.35	1.38
30	r	309	CHL	C1A-CHA	-2.82	1.36	1.40
32	0	616	LUT	O23-C23	-2.82	1.38	1.43
31	5	611	CLA	C4B-NB	-2.82	1.34	1.37
31	g	311	CLA	C4B-NB	-2.82	1.34	1.37
30	p	607	CHL	C1D-C2D	2.82	1.42	1.39
31	p	614	CLA	C4B-NB	-2.82	1.34	1.37
32	s	317	LUT	O23-C23	-2.82	1.38	1.43
30	Y	306	CHL	C3B-C2B	-2.82	1.36	1.40
30	7	307	CHL	CHB-C4A	-2.81	1.35	1.38
30	n	308	CHL	C1A-CHA	-2.81	1.36	1.40
31	g	303	CLA	C4B-NB	-2.81	1.34	1.37
30	5	605	CHL	C1A-CHA	-2.81	1.36	1.40
31	6	312	CLA	C4B-NB	-2.81	1.34	1.37
30	G	623	CHL	C1A-CHA	-2.81	1.36	1.40
30	6	307	CHL	C1A-CHA	-2.81	1.36	1.40
30	g	307	CHL	CHB-C4A	-2.81	1.35	1.38
30	3	309	CHL	CHB-C4A	-2.81	1.35	1.38
30	R	309	CHL	C1A-CHA	-2.81	1.36	1.40
30	r	310	CHL	CHB-C4A	-2.81	1.35	1.38
30	y	609	CHL	CHB-C4A	-2.81	1.35	1.38
31	2	612	CLA	C4B-NB	-2.81	1.34	1.37
31	r	314	CLA	C4B-NB	-2.81	1.34	1.37
30	Y	306	CHL	CHB-C4A	-2.80	1.35	1.38
30	5	605	CHL	C1B-C2B	2.80	1.42	1.39
31	y	614	CLA	C4B-NB	-2.80	1.34	1.37
43	v	101	BCR	C7-C6	2.80	1.54	1.45
30	3	303	CHL	CHB-C4A	-2.80	1.35	1.38
32	N	317	LUT	O23-C23	-2.80	1.38	1.43
30	7	321	CHL	C1A-CHA	-2.80	1.36	1.40
31	2	610	CLA	C4B-NB	-2.80	1.34	1.37
30	3	310	CHL	C1D-C2D	2.80	1.42	1.39
30	5	608	CHL	C1D-C2D	2.80	1.42	1.39
31	R	313	CLA	C4B-NB	-2.80	1.34	1.37
31	7	312	CLA	C4B-NB	-2.80	1.34	1.37
32	Y	316	LUT	O23-C23	-2.80	1.38	1.43
31	Y	304	CLA	C4B-NB	-2.80	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	608	CHL	C1D-C2D	2.79	1.42	1.39
30	y	607	CHL	CHB-C4A	-2.79	1.35	1.38
43	B	617	BCR	C39-C30	-2.79	1.48	1.53
30	1	606	CHL	C1D-C2D	2.79	1.42	1.39
30	0	609	CHL	C1D-C2D	2.79	1.42	1.39
30	p	608	CHL	C1D-C2D	2.79	1.42	1.39
30	s	308	CHL	C1A-CHA	-2.79	1.36	1.40
43	v	101	BCR	C34-C9	2.79	1.56	1.50
30	G	605	CHL	C1A-CHA	-2.79	1.36	1.40
30	Y	309	CHL	CHB-C4A	-2.79	1.35	1.38
30	2	601	CHL	C1D-C2D	2.79	1.42	1.39
30	n	310	CHL	C1D-C2D	2.79	1.42	1.39
30	N	307	CHL	CHB-C4A	-2.79	1.35	1.38
30	2	606	CHL	C1D-C2D	2.79	1.42	1.39
30	9	303	CHL	C1A-CHA	-2.79	1.36	1.40
30	6	302	CHL	CHB-C4A	-2.79	1.35	1.38
31	y	611	CLA	C4B-NB	-2.78	1.34	1.37
31	q	304	CLA	C4B-NB	-2.78	1.34	1.37
30	Y	309	CHL	C1D-C2D	2.78	1.42	1.39
30	5	609	CHL	CHB-C4A	-2.78	1.35	1.38
43	b	619	BCR	C34-C9	2.78	1.56	1.50
30	7	321	CHL	C1D-C2D	2.78	1.42	1.39
43	A	410	BCR	C34-C9	2.78	1.56	1.50
43	b	618	BCR	C34-C9	2.78	1.56	1.50
30	G	623	CHL	CHB-C4A	-2.78	1.35	1.38
30	p	609	CHL	C1A-CHA	-2.78	1.36	1.40
30	n	309	CHL	C1A-CHA	-2.78	1.36	1.40
30	7	307	CHL	C1D-C2D	2.78	1.42	1.39
30	9	308	CHL	C1D-C2D	2.78	1.42	1.39
30	1	606	CHL	CHB-C4A	-2.78	1.35	1.38
32	S	317	LUT	O23-C23	-2.78	1.38	1.43
30	4	609	CHL	C1D-C2D	2.78	1.42	1.39
31	3	314	CLA	C4B-NB	-2.77	1.34	1.37
43	B	618	BCR	C7-C6	2.77	1.54	1.45
31	n	312	CLA	C4B-NB	-2.77	1.34	1.37
30	S	307	CHL	CHB-C4A	-2.77	1.35	1.38
30	g	302	CHL	C1A-CHA	-2.77	1.36	1.40
30	y	605	CHL	C3B-C2B	-2.77	1.36	1.40
30	Y	302	CHL	CHB-C4A	-2.77	1.35	1.38
43	b	620	BCR	C34-C9	2.77	1.56	1.50
30	n	307	CHL	CHB-C4A	-2.77	1.35	1.38
30	2	605	CHL	C1B-C2B	2.77	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	r	308	CHL	C3B-C2B	-2.77	1.36	1.40
30	6	309	CHL	C1D-C2D	2.77	1.42	1.39
30	7	308	CHL	C1D-C2D	2.77	1.42	1.39
32	8	616	LUT	O23-C23	-2.77	1.38	1.43
30	5	607	CHL	C1A-CHA	-2.77	1.36	1.40
30	6	310	CHL	C1D-C2D	2.77	1.42	1.39
30	y	608	CHL	C1D-C2D	2.77	1.42	1.39
32	0	617	LUT	O23-C23	-2.77	1.38	1.43
30	2	608	CHL	CHB-C4A	-2.76	1.35	1.38
30	y	608	CHL	CHB-C4A	-2.76	1.35	1.38
32	y	616	LUT	O23-C23	-2.76	1.38	1.43
32	S	317	LUT	C18-C5	2.76	1.55	1.50
30	n	309	CHL	C1D-C2D	2.76	1.42	1.39
31	C	606	CLA	C4B-NB	-2.76	1.34	1.37
30	y	606	CHL	CHB-C4A	-2.76	1.35	1.38
30	y	606	CHL	C1D-C2D	2.76	1.42	1.39
43	c	615	BCR	C7-C6	2.76	1.54	1.45
30	G	605	CHL	C1B-C2B	2.76	1.42	1.39
31	5	613	CLA	C4B-NB	-2.76	1.34	1.37
31	q	316	CLA	C4B-NB	-2.76	1.34	1.37
30	2	606	CHL	C1A-CHA	-2.76	1.36	1.40
30	s	309	CHL	CHB-C4A	-2.76	1.35	1.38
30	0	608	CHL	C1D-C2D	2.76	1.42	1.39
30	4	608	CHL	C1B-C2B	2.76	1.42	1.39
30	R	308	CHL	CHB-C4A	-2.76	1.35	1.38
30	p	608	CHL	C1A-CHA	-2.75	1.36	1.40
30	8	607	CHL	C1D-C2D	2.75	1.42	1.39
30	q	307	CHL	C1B-C2B	2.75	1.42	1.39
31	N	311	CLA	C4B-NB	-2.75	1.34	1.37
43	c	614	BCR	C34-C9	2.75	1.56	1.50
31	g	314	CLA	C4B-NB	-2.75	1.34	1.37
30	y	609	CHL	C1D-C2D	2.75	1.42	1.39
30	7	302	CHL	CHB-C4A	-2.75	1.35	1.38
30	7	310	CHL	CHB-C4A	-2.75	1.35	1.38
30	2	608	CHL	C1D-C2D	2.75	1.42	1.39
30	p	601	CHL	C1D-C2D	2.75	1.42	1.39
30	n	306	CHL	C1D-C2D	2.75	1.42	1.39
31	9	313	CLA	C4B-NB	-2.75	1.34	1.37
30	0	608	CHL	C1B-C2B	2.75	1.42	1.39
30	n	308	CHL	C1D-C2D	2.75	1.42	1.39
30	9	309	CHL	CHB-C4A	-2.75	1.35	1.38
30	g	309	CHL	C1A-CHA	-2.75	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	5	616	LUT	C18-C5	2.75	1.55	1.50
30	8	607	CHL	C1B-C2B	2.75	1.42	1.39
30	g	309	CHL	C1D-C2D	2.75	1.42	1.39
32	6	318	LUT	O23-C23	-2.75	1.38	1.43
30	N	307	CHL	C1D-C2D	2.75	1.42	1.39
31	p	611	CLA	C4B-NB	-2.75	1.34	1.37
42	A	408	PHO	CMB-C2B	-2.75	1.46	1.51
31	6	313	CLA	C4B-NB	-2.75	1.34	1.37
32	6	318	LUT	C18-C5	2.75	1.55	1.50
32	n	317	LUT	O23-C23	-2.75	1.38	1.43
32	n	318	LUT	O23-C23	-2.75	1.38	1.43
30	n	301	CHL	C1D-C2D	2.75	1.42	1.39
30	n	302	CHL	C1D-C2D	2.74	1.42	1.39
30	n	308	CHL	C1B-C2B	2.74	1.42	1.39
30	2	607	CHL	C1D-C2D	2.74	1.42	1.39
30	9	310	CHL	C1D-C2D	2.74	1.42	1.39
31	5	614	CLA	C4B-NB	-2.74	1.34	1.37
30	5	607	CHL	C1D-C2D	2.74	1.42	1.39
30	7	321	CHL	C1B-C2B	2.74	1.42	1.39
30	g	309	CHL	CHB-C4A	-2.74	1.35	1.38
30	n	302	CHL	CHB-C4A	-2.74	1.35	1.38
30	N	308	CHL	C1D-C2D	2.74	1.42	1.39
31	b	611	CLA	C4B-NB	-2.74	1.34	1.37
30	y	607	CHL	C1D-C2D	2.74	1.42	1.39
30	S	308	CHL	CHB-C4A	-2.74	1.35	1.38
30	p	607	CHL	CHB-C4A	-2.74	1.35	1.38
32	n	317	LUT	C18-C5	2.74	1.55	1.50
30	N	309	CHL	C1D-C2D	2.74	1.42	1.39
30	S	307	CHL	C1D-C2D	2.74	1.42	1.39
30	7	310	CHL	C1D-C2D	2.74	1.42	1.39
31	8	610	CLA	C4B-NB	-2.74	1.34	1.37
43	V	101	BCR	C7-C6	2.74	1.54	1.45
42	d	402	PHO	C1B-C2B	2.74	1.42	1.39
32	3	317	LUT	C18-C5	2.74	1.55	1.50
30	p	606	CHL	C1A-CHA	-2.74	1.36	1.40
30	G	606	CHL	C1D-C2D	2.74	1.42	1.39
30	n	301	CHL	CHB-C4A	-2.73	1.35	1.38
30	1	605	CHL	C1B-C2B	2.73	1.42	1.39
30	S	309	CHL	CHB-C4A	-2.73	1.35	1.38
30	8	608	CHL	C1A-CHA	-2.73	1.36	1.40
30	6	307	CHL	C1D-C2D	2.73	1.42	1.39
30	1	609	CHL	CHB-C4A	-2.73	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	8	601	CHL	CHB-C4A	-2.73	1.35	1.38
30	9	311	CHL	CHB-C4A	-2.73	1.35	1.38
31	6	304	CLA	C4B-NB	-2.73	1.34	1.37
30	q	303	CHL	C1A-CHA	-2.73	1.36	1.40
30	p	605	CHL	C1D-C2D	2.73	1.42	1.39
30	0	601	CHL	CHB-C4A	-2.73	1.35	1.38
32	9	318	LUT	O23-C23	-2.73	1.38	1.43
30	G	607	CHL	C1B-C2B	2.73	1.42	1.39
32	1	616	LUT	O23-C23	-2.73	1.38	1.43
30	5	608	CHL	C1B-C2B	2.73	1.42	1.39
31	1	603	CLA	C4B-NB	-2.73	1.34	1.37
30	7	309	CHL	C1D-C2D	2.73	1.42	1.39
30	p	609	CHL	C1D-C2D	2.73	1.42	1.39
30	Y	308	CHL	CHB-C4A	-2.73	1.35	1.38
32	s	317	LUT	C18-C5	2.73	1.55	1.50
32	1	615	LUT	O23-C23	-2.73	1.38	1.43
32	6	317	LUT	O23-C23	-2.73	1.38	1.43
30	p	605	CHL	C1B-C2B	2.73	1.42	1.39
30	3	308	CHL	CHB-C4A	-2.72	1.35	1.38
30	9	309	CHL	C1D-C2D	2.72	1.42	1.39
30	q	303	CHL	C1B-C2B	2.72	1.42	1.39
32	6	317	LUT	C18-C5	2.72	1.55	1.50
30	6	308	CHL	CHB-C4A	-2.72	1.35	1.38
30	4	605	CHL	C1A-CHA	-2.72	1.36	1.40
30	G	623	CHL	C1D-C2D	2.72	1.42	1.39
30	8	606	CHL	CHB-C4A	-2.72	1.35	1.38
30	s	307	CHL	CHB-C4A	-2.72	1.35	1.38
30	8	605	CHL	C1D-C2D	2.72	1.42	1.39
32	8	615	LUT	O23-C23	-2.72	1.39	1.43
30	4	605	CHL	C1B-C2B	2.72	1.42	1.39
30	N	306	CHL	C1D-C2D	2.72	1.42	1.39
30	q	303	CHL	C1D-C2D	2.72	1.42	1.39
30	g	302	CHL	C1D-C2D	2.72	1.42	1.39
30	2	606	CHL	CHB-C4A	-2.72	1.35	1.38
32	3	317	LUT	O23-C23	-2.72	1.39	1.43
32	8	615	LUT	C18-C5	2.72	1.55	1.50
43	b	619	BCR	C7-C6	2.72	1.54	1.45
30	1	607	CHL	C1B-C2B	2.72	1.42	1.39
30	q	307	CHL	C1D-C2D	2.72	1.42	1.39
30	5	606	CHL	CHB-C4A	-2.72	1.35	1.38
42	D	401	PHO	CMD-C2D	-2.72	1.46	1.51
36	q	319	NEX	O24-C25	-2.72	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S	312	CLA	C4B-NB	-2.72	1.34	1.37
30	Y	307	CHL	C1D-C2D	2.72	1.42	1.39
30	9	311	CHL	C1D-C2D	2.72	1.42	1.39
31	G	613	CLA	C4B-NB	-2.72	1.34	1.37
43	c	615	BCR	C34-C9	2.72	1.56	1.50
30	p	601	CHL	CHB-C4A	-2.72	1.35	1.38
31	s	304	CLA	C4B-NB	-2.72	1.34	1.37
30	4	609	CHL	C1B-C2B	2.72	1.42	1.39
30	5	606	CHL	C1D-C2D	2.72	1.42	1.39
30	8	608	CHL	C1D-C2D	2.72	1.42	1.39
30	R	309	CHL	CHB-C4A	-2.72	1.35	1.38
30	s	308	CHL	CHB-C4A	-2.72	1.35	1.38
31	1	611	CLA	C4B-NB	-2.72	1.34	1.37
30	G	608	CHL	C1D-C2D	2.72	1.42	1.39
30	7	310	CHL	C1B-C2B	2.71	1.42	1.39
30	g	308	CHL	C1B-C2B	2.71	1.42	1.39
30	G	608	CHL	CHB-C4A	-2.71	1.35	1.38
30	G	605	CHL	C1D-C2D	2.71	1.42	1.39
30	1	607	CHL	C1D-C2D	2.71	1.42	1.39
30	6	308	CHL	C1D-C2D	2.71	1.42	1.39
30	g	306	CHL	C1B-C2B	2.71	1.42	1.39
30	n	310	CHL	C1B-C2B	2.71	1.42	1.39
30	0	609	CHL	CHB-C4A	-2.71	1.35	1.38
30	2	607	CHL	C1B-C2B	2.71	1.42	1.39
30	8	601	CHL	C1D-C2D	2.71	1.42	1.39
43	B	618	BCR	C34-C9	2.71	1.56	1.50
43	a	410	BCR	C34-C9	2.71	1.56	1.50
30	6	302	CHL	C1A-CHA	-2.71	1.36	1.40
30	6	310	CHL	C1A-CHA	-2.71	1.36	1.40
30	2	605	CHL	C1D-C2D	2.71	1.42	1.39
30	5	605	CHL	C1D-C2D	2.71	1.42	1.39
30	G	601	CHL	C1D-C2D	2.71	1.42	1.39
30	Y	302	CHL	C1D-C2D	2.71	1.42	1.39
30	g	302	CHL	CHB-C4A	-2.71	1.35	1.38
42	A	408	PHO	CMD-C2D	-2.71	1.46	1.51
30	R	309	CHL	C1D-C2D	2.71	1.42	1.39
30	5	608	CHL	CHB-C4A	-2.71	1.35	1.38
30	r	309	CHL	C3A-C2A	-2.71	1.52	1.54
31	c	601	CLA	C4B-NB	-2.71	1.34	1.37
31	C	605	CLA	C3D-C4D	-2.71	1.38	1.44
30	8	606	CHL	C1D-C2D	2.71	1.42	1.39
30	g	307	CHL	C1D-C2D	2.71	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	T	101	BCR	C7-C6	2.71	1.54	1.45
30	0	601	CHL	C1B-C2B	2.71	1.42	1.39
30	8	605	CHL	CHB-C4A	-2.71	1.35	1.38
30	N	302	CHL	CHB-C4A	-2.71	1.35	1.38
30	3	307	CHL	C1B-C2B	2.70	1.42	1.39
30	g	309	CHL	C1B-C2B	2.70	1.42	1.39
30	Y	301	CHL	CHB-C4A	-2.70	1.35	1.38
30	p	606	CHL	CHB-C4A	-2.70	1.35	1.38
30	n	310	CHL	CHB-C4A	-2.70	1.35	1.38
30	G	608	CHL	C1A-CHA	-2.70	1.36	1.40
30	N	308	CHL	CHB-C4A	-2.70	1.35	1.38
30	p	609	CHL	CHB-C4A	-2.70	1.35	1.38
30	q	311	CHL	CHB-C4A	-2.70	1.35	1.38
30	n	301	CHL	C1B-C2B	2.70	1.42	1.39
30	s	308	CHL	C1B-C2B	2.70	1.42	1.39
43	C	615	BCR	C39-C30	-2.70	1.48	1.53
32	S	318	LUT	C23-C24	-2.70	1.46	1.50
30	G	606	CHL	CHB-C4A	-2.70	1.35	1.38
30	7	309	CHL	CHB-C4A	-2.70	1.35	1.38
30	9	308	CHL	CHB-C4A	-2.70	1.35	1.38
30	N	301	CHL	C1D-C2D	2.70	1.42	1.39
30	9	311	CHL	C1B-C2B	2.70	1.42	1.39
30	5	607	CHL	CHB-C4A	-2.70	1.35	1.38
30	N	306	CHL	CHB-C4A	-2.70	1.35	1.38
30	N	309	CHL	CHB-C4A	-2.70	1.35	1.38
30	n	309	CHL	CHB-C4A	-2.70	1.35	1.38
30	1	608	CHL	C1D-C2D	2.70	1.42	1.39
31	0	611	CLA	C4B-NB	-2.70	1.34	1.37
30	6	308	CHL	C1B-C2B	2.70	1.42	1.39
30	4	606	CHL	C1D-C2D	2.70	1.42	1.39
32	q	318	LUT	O23-C23	-2.70	1.39	1.43
30	n	306	CHL	CHB-C4A	-2.70	1.35	1.38
30	y	601	CHL	CHB-C4A	-2.70	1.35	1.38
30	n	307	CHL	C1D-C2D	2.70	1.42	1.39
30	6	307	CHL	CHB-C4A	-2.70	1.35	1.38
30	6	310	CHL	CHB-C4A	-2.70	1.35	1.38
32	N	316	LUT	C18-C5	2.69	1.55	1.50
30	6	306	CHL	C1D-C2D	2.69	1.42	1.39
30	4	601	CHL	C1D-C2D	2.69	1.42	1.39
30	p	601	CHL	C1B-C2B	2.69	1.42	1.39
30	n	302	CHL	C1B-C2B	2.69	1.42	1.39
30	7	308	CHL	C1B-C2B	2.69	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	3	303	CHL	C1D-C2D	2.69	1.42	1.39
30	5	609	CHL	C1D-C2D	2.69	1.42	1.39
30	n	309	CHL	C1B-C2B	2.69	1.42	1.39
31	p	612	CLA	C4B-NB	-2.69	1.34	1.37
30	3	307	CHL	C1A-CHA	-2.69	1.36	1.40
30	2	601	CHL	CHB-C4A	-2.69	1.35	1.38
32	G	615	LUT	O23-C23	-2.69	1.39	1.43
30	7	302	CHL	C1B-C2B	2.69	1.42	1.39
31	G	603	CLA	C4B-NB	-2.69	1.34	1.37
30	G	608	CHL	C1B-C2B	2.69	1.42	1.39
30	q	311	CHL	C1D-C2D	2.69	1.42	1.39
30	5	601	CHL	C1D-C2D	2.69	1.42	1.39
30	8	608	CHL	C1B-C2B	2.69	1.42	1.39
30	9	303	CHL	C1D-C2D	2.69	1.42	1.39
30	9	303	CHL	CHB-C4A	-2.69	1.35	1.38
32	7	317	LUT	O23-C23	-2.69	1.39	1.43
30	q	308	CHL	C1B-C2B	2.69	1.42	1.39
30	G	601	CHL	CHB-C4A	-2.69	1.35	1.38
30	g	306	CHL	CHB-C4A	-2.68	1.35	1.38
32	5	617	LUT	O23-C23	-2.68	1.39	1.43
31	R	314	CLA	C4B-NB	-2.68	1.34	1.37
32	7	318	LUT	C18-C5	2.68	1.55	1.50
30	6	307	CHL	C3A-C2A	-2.68	1.52	1.54
30	3	307	CHL	CHB-C4A	-2.68	1.35	1.38
30	3	310	CHL	CHB-C4A	-2.68	1.35	1.38
30	q	311	CHL	C1B-C2B	2.68	1.42	1.39
30	y	601	CHL	C1D-C2D	2.68	1.42	1.39
30	3	307	CHL	C1D-C2D	2.68	1.42	1.39
30	7	309	CHL	C1B-C2B	2.68	1.42	1.39
32	N	316	LUT	O23-C23	-2.68	1.39	1.43
30	5	606	CHL	C1B-C2B	2.68	1.42	1.39
30	0	601	CHL	C1D-C2D	2.68	1.42	1.39
30	s	308	CHL	C1D-C2D	2.68	1.42	1.39
30	7	310	CHL	C1A-CHA	-2.68	1.37	1.40
30	6	302	CHL	C1B-C2B	2.68	1.42	1.39
30	N	302	CHL	C1D-C2D	2.68	1.42	1.39
30	7	306	CHL	C1D-C2D	2.68	1.42	1.39
30	1	605	CHL	C1D-C2D	2.68	1.42	1.39
32	5	617	LUT	C18-C5	2.68	1.55	1.50
43	T	101	BCR	C34-C9	2.68	1.56	1.50
30	R	308	CHL	C1D-C2D	2.68	1.42	1.39
30	g	308	CHL	C1D-C2D	2.67	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	r	308	CHL	C1D-C2D	2.67	1.42	1.39
32	p	616	LUT	C18-C5	2.67	1.55	1.50
30	n	308	CHL	CHB-C4A	-2.67	1.35	1.38
30	Y	306	CHL	C1D-C2D	2.67	1.42	1.39
30	4	601	CHL	CHB-C4A	-2.67	1.35	1.38
30	g	308	CHL	CHB-C4A	-2.67	1.35	1.38
31	y	612	CLA	C4B-NB	-2.67	1.34	1.37
30	8	607	CHL	CHB-C4A	-2.67	1.35	1.38
30	6	302	CHL	C1D-C2D	2.67	1.42	1.39
30	0	607	CHL	C1B-C2B	2.67	1.42	1.39
30	9	307	CHL	C1B-C2B	2.67	1.42	1.39
32	3	318	LUT	O23-C23	-2.67	1.39	1.43
44	a	414	PL9	C6-C1	-2.67	1.44	1.48
30	Y	302	CHL	C1B-C2B	2.67	1.42	1.39
30	9	303	CHL	C1B-C2B	2.67	1.42	1.39
30	r	309	CHL	C1D-C2D	2.67	1.42	1.39
32	4	616	LUT	O23-C23	-2.67	1.39	1.43
30	3	310	CHL	C1B-C2B	2.67	1.42	1.39
30	S	309	CHL	C1D-C2D	2.67	1.42	1.39
43	B	619	BCR	C7-C6	2.67	1.54	1.45
30	1	608	CHL	C1B-C2B	2.67	1.42	1.39
30	g	306	CHL	C1D-C2D	2.67	1.42	1.39
30	6	309	CHL	CHB-C4A	-2.67	1.35	1.38
30	2	608	CHL	C1B-C2B	2.67	1.42	1.39
30	5	607	CHL	C1B-C2B	2.67	1.42	1.39
30	1	609	CHL	C1D-C2D	2.67	1.42	1.39
30	0	609	CHL	C1B-C2B	2.67	1.42	1.39
30	Y	301	CHL	C1B-C2B	2.67	1.42	1.39
30	Y	301	CHL	C1D-C2D	2.67	1.42	1.39
30	Y	308	CHL	C1B-C2B	2.67	1.42	1.39
31	7	304	CLA	C4B-NB	-2.67	1.34	1.37
30	r	310	CHL	C1D-C2D	2.67	1.42	1.39
30	S	307	CHL	C1B-C2B	2.66	1.42	1.39
30	p	606	CHL	C1B-C2B	2.66	1.42	1.39
31	Y	312	CLA	C4B-NB	-2.66	1.34	1.37
30	G	601	CHL	C1B-C2B	2.66	1.42	1.39
30	1	605	CHL	CHB-C4A	-2.66	1.35	1.38
30	2	606	CHL	C1B-C2B	2.66	1.42	1.39
30	p	608	CHL	C1B-C2B	2.66	1.42	1.39
30	3	308	CHL	C1D-C2D	2.66	1.42	1.39
30	5	609	CHL	C1B-C2B	2.66	1.42	1.39
30	5	601	CHL	C1B-C2B	2.66	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	7	321	CHL	CHB-C4A	-2.66	1.35	1.38
42	a	408	PHO	C1B-C2B	2.66	1.42	1.39
31	7	313	CLA	C4B-NB	-2.66	1.34	1.37
30	Y	309	CHL	C1B-C2B	2.66	1.42	1.39
30	q	307	CHL	CHB-C4A	-2.66	1.35	1.38
30	4	601	CHL	C1B-C2B	2.66	1.42	1.39
30	y	601	CHL	C1B-C2B	2.66	1.42	1.39
47	E	101	HEM	C1C-C2C	-2.66	1.40	1.45
30	7	302	CHL	C1D-C2D	2.66	1.42	1.39
30	8	601	CHL	C1B-C2B	2.66	1.42	1.39
31	4	603	CLA	C4B-NB	-2.66	1.34	1.37
32	g	316	LUT	C18-C5	2.66	1.55	1.50
32	S	318	LUT	C18-C5	2.66	1.55	1.50
30	N	309	CHL	C1B-C2B	2.65	1.42	1.39
30	0	607	CHL	C1D-C2D	2.65	1.42	1.39
30	3	309	CHL	C3B-C2B	-2.65	1.36	1.40
30	4	606	CHL	C1B-C2B	2.65	1.42	1.39
30	Y	308	CHL	C1D-C2D	2.65	1.42	1.39
31	9	305	CLA	C4B-NB	-2.65	1.34	1.37
30	R	309	CHL	C1B-C2B	2.65	1.42	1.39
30	9	308	CHL	C1B-C2B	2.65	1.42	1.39
43	A	410	BCR	C7-C6	2.65	1.54	1.45
30	q	310	CHL	CHB-C4A	-2.65	1.35	1.38
30	N	302	CHL	C1B-C2B	2.65	1.42	1.39
43	z	101	BCR	C34-C9	2.65	1.56	1.50
30	4	609	CHL	CHB-C4A	-2.65	1.35	1.38
30	7	308	CHL	CHB-C4A	-2.65	1.35	1.38
43	h	101	BCR	C34-C9	2.65	1.56	1.50
30	2	601	CHL	C1B-C2B	2.65	1.42	1.39
30	N	301	CHL	CHB-C4A	-2.65	1.35	1.38
30	p	607	CHL	C1B-C2B	2.65	1.42	1.39
32	N	317	LUT	C18-C5	2.65	1.55	1.50
31	0	603	CLA	C4B-NB	-2.65	1.34	1.37
30	p	609	CHL	C1B-C2B	2.65	1.42	1.39
30	s	302	CHL	C1D-C2D	2.65	1.42	1.39
31	N	312	CLA	C4B-NB	-2.65	1.34	1.37
30	n	307	CHL	C1B-C2B	2.65	1.42	1.39
30	G	607	CHL	CHB-C4A	-2.64	1.35	1.38
30	3	303	CHL	C1B-C2B	2.64	1.42	1.39
30	y	609	CHL	C1B-C2B	2.64	1.42	1.39
31	2	603	CLA	C4B-NB	-2.64	1.34	1.37
31	G	610	CLA	C4B-NB	-2.64	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	307	CHL	C1D-C2D	2.64	1.42	1.39
30	r	309	CHL	C1B-C2B	2.64	1.42	1.39
30	s	302	CHL	CHB-C4A	-2.64	1.35	1.38
30	3	310	CHL	C1A-CHA	-2.64	1.37	1.40
32	7	317	LUT	C18-C5	2.64	1.55	1.50
32	0	617	LUT	C18-C5	2.64	1.55	1.50
32	9	318	LUT	C18-C5	2.63	1.55	1.50
30	9	309	CHL	C1B-C2B	2.63	1.42	1.39
43	C	614	BCR	C7-C6	2.63	1.54	1.45
43	b	618	BCR	C7-C6	2.63	1.54	1.45
32	G	615	LUT	C18-C5	2.63	1.55	1.50
30	4	605	CHL	CHB-C4A	-2.63	1.35	1.38
30	6	307	CHL	C1B-C2B	2.63	1.42	1.39
30	6	309	CHL	C1B-C2B	2.63	1.42	1.39
30	0	606	CHL	CHB-C4A	-2.63	1.35	1.38
32	Y	315	LUT	C18-C5	2.63	1.55	1.50
30	N	308	CHL	C1B-C2B	2.63	1.42	1.39
30	6	310	CHL	C1B-C2B	2.63	1.42	1.39
30	8	606	CHL	C1B-C2B	2.63	1.42	1.39
47	e	102	HEM	C1C-C2C	-2.63	1.40	1.45
30	N	301	CHL	C1B-C2B	2.63	1.42	1.39
32	g	316	LUT	O23-C23	-2.63	1.39	1.43
30	p	605	CHL	CHB-C4A	-2.63	1.35	1.38
30	s	307	CHL	C1D-C2D	2.63	1.42	1.39
31	B	607	CLA	C3D-C4D	-2.63	1.38	1.44
30	9	307	CHL	CHB-C4A	-2.62	1.35	1.38
30	s	302	CHL	C1B-C2B	2.62	1.42	1.39
43	B	619	BCR	C34-C9	2.62	1.56	1.50
32	0	616	LUT	C18-C5	2.62	1.55	1.50
30	5	609	CHL	C1A-CHA	-2.62	1.37	1.40
30	N	306	CHL	C1B-C2B	2.62	1.42	1.39
43	C	614	BCR	C34-C9	2.62	1.56	1.50
30	2	608	CHL	C1A-CHA	-2.62	1.37	1.40
32	7	318	LUT	O23-C23	-2.62	1.39	1.43
30	4	605	CHL	C1D-C2D	2.61	1.42	1.39
30	G	605	CHL	CHB-C4A	-2.61	1.35	1.38
32	p	617	LUT	C18-C5	2.61	1.55	1.50
30	y	607	CHL	C1B-C2B	2.61	1.42	1.39
30	4	607	CHL	C1B-C2B	2.61	1.42	1.39
30	Y	307	CHL	C1B-C2B	2.61	1.42	1.39
30	7	306	CHL	C1B-C2B	2.61	1.42	1.39
30	y	608	CHL	C1B-C2B	2.61	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	605	CHL	CHB-C4A	-2.61	1.35	1.38
30	G	623	CHL	C1B-C2B	2.61	1.42	1.39
30	q	311	CHL	C1A-CHA	-2.61	1.37	1.40
30	1	606	CHL	C1B-C2B	2.61	1.42	1.39
30	1	607	CHL	CHB-C4A	-2.61	1.35	1.38
30	7	306	CHL	CHB-C4A	-2.61	1.35	1.38
30	4	606	CHL	CHB-C4A	-2.61	1.35	1.38
30	0	608	CHL	CHB-C4A	-2.61	1.35	1.38
32	r	317	LUT	C18-C5	2.61	1.55	1.50
30	8	605	CHL	C1B-C2B	2.61	1.42	1.39
30	s	307	CHL	C1B-C2B	2.61	1.42	1.39
30	g	307	CHL	C1B-C2B	2.61	1.42	1.39
30	G	607	CHL	C1D-C2D	2.61	1.42	1.39
30	6	306	CHL	CHB-C4A	-2.60	1.35	1.38
30	2	607	CHL	CHB-C4A	-2.60	1.35	1.38
43	H	101	BCR	C34-C9	2.60	1.56	1.50
32	s	318	LUT	C18-C5	2.60	1.55	1.50
30	R	308	CHL	C1B-C2B	2.60	1.42	1.39
31	s	316	CLA	C4B-NB	-2.60	1.34	1.37
30	0	607	CHL	CHB-C4A	-2.60	1.35	1.38
30	p	608	CHL	CHB-C4A	-2.60	1.35	1.38
30	5	601	CHL	CHB-C4A	-2.60	1.35	1.38
32	q	318	LUT	C18-C5	2.60	1.55	1.50
32	8	616	LUT	C18-C5	2.60	1.55	1.50
31	0	612	CLA	C4B-NB	-2.60	1.34	1.37
32	4	616	LUT	C18-C5	2.59	1.55	1.50
30	q	308	CHL	CHB-C4A	-2.59	1.35	1.38
30	3	309	CHL	C1D-C2D	2.59	1.42	1.39
30	1	608	CHL	CHB-C4A	-2.59	1.35	1.38
30	q	303	CHL	CHB-C4A	-2.59	1.35	1.38
30	0	606	CHL	C1D-C2D	2.59	1.42	1.39
42	d	402	PHO	C4D-CHA	2.59	1.43	1.39
30	9	310	CHL	C1B-C2B	2.59	1.42	1.39
30	y	605	CHL	C1B-C2B	2.59	1.42	1.39
32	5	616	LUT	O23-C23	-2.59	1.39	1.43
31	1	612	CLA	C4B-NB	-2.59	1.34	1.37
32	n	318	LUT	C18-C5	2.59	1.55	1.50
30	S	309	CHL	C1B-C2B	2.59	1.42	1.39
32	s	318	LUT	O23-C23	-2.59	1.39	1.43
30	0	605	CHL	C1D-C2D	2.59	1.42	1.39
30	R	310	CHL	C1D-C2D	2.59	1.42	1.39
30	8	608	CHL	CHB-C4A	-2.58	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	n	306	CHL	C1B-C2B	2.58	1.42	1.39
30	6	306	CHL	C1B-C2B	2.58	1.42	1.39
30	9	310	CHL	CHB-C4A	-2.58	1.35	1.38
30	1	609	CHL	C1B-C2B	2.58	1.42	1.39
30	r	308	CHL	C1B-C2B	2.58	1.42	1.39
32	3	318	LUT	C18-C5	2.58	1.55	1.50
30	r	309	CHL	CHB-C4A	-2.58	1.35	1.38
30	S	302	CHL	C1B-C2B	2.58	1.42	1.39
31	4	613	CLA	C4B-NB	-2.58	1.34	1.37
30	y	606	CHL	C1B-C2B	2.57	1.42	1.39
30	g	307	CHL	C3B-C2B	-2.57	1.36	1.40
32	p	617	LUT	O23-C23	-2.57	1.39	1.43
30	1	601	CHL	C1D-C2D	2.57	1.42	1.39
30	g	302	CHL	C1B-C2B	2.57	1.42	1.39
43	b	620	BCR	C7-C6	2.57	1.53	1.45
30	7	307	CHL	C1B-C2B	2.56	1.42	1.39
30	y	605	CHL	C1D-C2D	2.56	1.42	1.39
43	d	406	BCR	C7-C6	2.56	1.53	1.45
30	1	619	CHL	C1A-CHA	-2.56	1.37	1.40
31	q	305	CLA	C4B-NB	-2.56	1.34	1.37
30	N	307	CHL	C1B-C2B	2.56	1.42	1.39
30	S	302	CHL	C1D-C2D	2.56	1.42	1.39
30	q	310	CHL	C1B-C2B	2.56	1.42	1.39
30	3	308	CHL	C1A-CHA	-2.56	1.37	1.40
43	Z	101	BCR	C34-C9	2.56	1.56	1.50
43	a	410	BCR	C7-C6	2.56	1.53	1.45
30	s	309	CHL	C1D-C2D	2.56	1.42	1.39
32	y	616	LUT	C18-C5	2.56	1.55	1.50
43	d	406	BCR	C34-C9	2.56	1.56	1.50
30	4	608	CHL	CHB-C4A	-2.55	1.35	1.38
32	1	616	LUT	C18-C5	2.55	1.55	1.50
30	N	307	CHL	C3B-C2B	-2.55	1.36	1.40
30	Y	306	CHL	C1B-C2B	2.55	1.42	1.39
30	R	308	CHL	C3B-C2B	-2.55	1.36	1.40
30	5	605	CHL	CHB-C4A	-2.55	1.35	1.38
30	S	308	CHL	C1D-C2D	2.55	1.42	1.39
43	z	101	BCR	C7-C6	2.55	1.53	1.45
43	C	615	BCR	C7-C6	2.55	1.53	1.45
30	0	606	CHL	C1B-C2B	2.55	1.42	1.39
30	R	310	CHL	C1A-CHA	-2.55	1.37	1.40
31	p	604	CLA	C4B-NB	-2.55	1.34	1.37
32	1	615	LUT	C18-C5	2.54	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	B	617	BCR	C34-C9	2.54	1.56	1.50
32	p	616	LUT	O23-C23	-2.54	1.39	1.43
30	3	308	CHL	C1B-C2B	2.54	1.42	1.39
32	S	318	LUT	O23-C23	-2.54	1.39	1.43
43	b	618	BCR	C39-C30	-2.54	1.49	1.53
42	D	401	PHO	CMB-C2B	-2.54	1.46	1.51
30	r	310	CHL	C1B-C2B	2.53	1.42	1.39
30	3	302	CHL	C1B-C2B	2.53	1.42	1.39
30	G	606	CHL	C1B-C2B	2.53	1.42	1.39
43	H	101	BCR	C7-C6	2.53	1.53	1.45
31	y	613	CLA	C3D-C4D	-2.53	1.38	1.44
44	A	416	PL9	C3-C4	-2.52	1.45	1.49
30	p	601	CHL	C2C-C3C	2.52	1.38	1.36
30	s	309	CHL	C1B-C2B	2.52	1.42	1.39
32	Y	316	LUT	C18-C5	2.51	1.54	1.50
30	1	619	CHL	C1D-C2D	2.51	1.42	1.39
32	2	615	LUT	C18-C5	2.51	1.54	1.50
31	3	312	CLA	C4B-NB	-2.51	1.34	1.37
35	9	317	RRX	C34-C9	2.51	1.55	1.50
30	R	310	CHL	C1B-C2B	2.51	1.42	1.39
44	a	414	PL9	C53-C6	-2.50	1.45	1.50
30	q	309	CHL	C1B-C2B	2.49	1.42	1.39
35	4	615	RRX	C34-C9	2.49	1.55	1.50
30	p	601	CHL	C1A-CHA	-2.49	1.37	1.40
30	6	309	CHL	C3B-C2B	-2.49	1.37	1.40
42	A	408	PHO	CAC-C3C	-2.49	1.47	1.51
30	0	608	CHL	C3B-C2B	-2.49	1.37	1.40
36	r	319	NEX	O24-C25	-2.49	1.43	1.46
31	0	610	CLA	C3D-C4D	-2.48	1.38	1.44
30	q	308	CHL	C1D-C2D	2.48	1.42	1.39
30	3	309	CHL	C1B-C2B	2.48	1.42	1.39
42	D	401	PHO	CAC-C3C	-2.48	1.47	1.51
30	3	302	CHL	C1D-C2D	2.48	1.42	1.39
43	H	101	BCR	C39-C30	-2.48	1.49	1.53
32	y	617	LUT	C18-C5	2.47	1.54	1.50
30	q	309	CHL	C1D-C2D	2.47	1.42	1.39
43	h	101	BCR	C7-C6	2.47	1.53	1.45
43	T	101	BCR	C36-C18	2.47	1.55	1.50
30	S	307	CHL	C3B-C2B	-2.47	1.37	1.40
30	8	606	CHL	C3B-C2B	-2.47	1.37	1.40
35	G	614	RRX	C34-C9	2.47	1.55	1.50
32	g	316	LUT	C26-C27	2.47	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	c	615	BCR	C39-C30	-2.47	1.49	1.53
31	r	303	CLA	C3D-C4D	-2.46	1.38	1.44
43	C	615	BCR	C34-C9	2.46	1.55	1.50
43	Z	101	BCR	C7-C6	2.46	1.53	1.45
47	e	102	HEM	FE-ND	-2.46	1.87	1.94
43	t	101	BCR	C34-C9	2.46	1.55	1.50
43	h	101	BCR	C39-C30	-2.45	1.49	1.53
30	n	307	CHL	C3B-C2B	-2.45	1.37	1.40
43	d	406	BCR	C39-C30	-2.45	1.49	1.53
30	q	310	CHL	C1D-C2D	2.45	1.42	1.39
42	D	401	PHO	C4D-ND	-2.45	1.34	1.38
43	b	620	BCR	C39-C30	-2.45	1.49	1.53
44	A	416	PL9	C6-C1	-2.45	1.44	1.48
44	A	416	PL9	C7-C3	-2.44	1.48	1.51
43	C	614	BCR	C39-C30	-2.44	1.49	1.53
36	8	617	NEX	O24-C25	-2.44	1.43	1.46
43	A	410	BCR	C39-C30	-2.44	1.49	1.53
43	c	614	BCR	C39-C30	-2.44	1.49	1.53
36	4	617	NEX	O24-C25	-2.44	1.43	1.46
43	V	101	BCR	C39-C30	-2.44	1.49	1.53
35	g	315	RRX	C34-C9	2.44	1.55	1.50
36	g	317	NEX	O24-C25	-2.43	1.43	1.46
43	a	410	BCR	C36-C18	2.43	1.55	1.50
30	2	601	CHL	C3B-C2B	-2.43	1.37	1.40
30	y	607	CHL	C3B-C2B	-2.42	1.37	1.40
34	g	322	LMG	C43-C42	-2.42	1.33	1.50
30	1	601	CHL	C1B-C2B	2.42	1.42	1.39
30	Y	308	CHL	C3B-C2B	-2.42	1.37	1.40
47	E	101	HEM	FE-ND	-2.42	1.87	1.94
30	S	309	CHL	C3B-C2B	-2.42	1.37	1.40
43	a	410	BCR	C39-C30	-2.42	1.49	1.53
30	0	605	CHL	C1B-C2B	2.41	1.42	1.39
31	3	301	CLA	C3D-C4D	-2.41	1.38	1.44
34	C	624	LMG	C25-C24	-2.41	1.33	1.50
30	S	308	CHL	C1B-C2B	2.41	1.42	1.39
32	R	317	LUT	C18-C5	2.41	1.54	1.50
34	n	322	LMG	C37-C36	-2.41	1.33	1.50
31	A	409	CLA	C3D-C4D	-2.41	1.38	1.44
43	z	101	BCR	C39-C30	-2.41	1.49	1.53
30	Y	307	CHL	C3B-C2B	-2.41	1.37	1.40
43	Z	101	BCR	C39-C30	-2.41	1.49	1.53
43	t	101	BCR	C7-C6	2.40	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	d	410	LMG	C25-C24	-2.40	1.33	1.50
34	w	201	LMG	C22-C21	-2.40	1.33	1.50
34	J	101	LMG	C25-C24	-2.40	1.33	1.50
34	d	411	LMG	C22-C21	-2.40	1.33	1.50
36	0	618	NEX	O24-C25	-2.40	1.43	1.46
34	k	101	LMG	C43-C42	-2.40	1.33	1.50
34	D	411	LMG	C43-C42	-2.40	1.33	1.50
30	s	309	CHL	C3B-C2B	-2.40	1.37	1.40
34	D	411	LMG	C25-C24	-2.40	1.33	1.50
45	c	617	DGD	O5D-C1E	2.40	1.44	1.40
31	c	608	CLA	C3D-C4D	-2.40	1.38	1.44
34	d	410	LMG	C43-C42	-2.40	1.33	1.50
34	B	621	LMG	C25-C24	-2.40	1.33	1.50
34	A	412	LMG	C22-C21	-2.40	1.33	1.50
35	2	614	RRX	C34-C9	2.39	1.55	1.50
30	G	623	CHL	C3B-C2B	-2.39	1.37	1.40
34	w	201	LMG	C43-C42	-2.39	1.33	1.50
42	A	408	PHO	C4D-ND	-2.39	1.35	1.38
30	s	307	CHL	C3B-C2B	-2.39	1.37	1.40
34	D	412	LMG	C22-C21	-2.39	1.33	1.50
30	G	606	CHL	C3B-C2B	-2.39	1.37	1.40
34	C	619	LMG	C43-C42	-2.39	1.33	1.50
34	c	624	LMG	C43-C42	-2.39	1.33	1.50
31	a	409	CLA	C3D-C4D	-2.39	1.38	1.44
30	0	601	CHL	C2C-C3C	2.39	1.38	1.36
34	D	409	LMG	C25-C24	-2.39	1.33	1.50
34	9	301	LMG	C43-C42	-2.39	1.33	1.50
34	D	412	LMG	C43-C42	-2.39	1.33	1.50
43	b	619	BCR	C39-C30	-2.39	1.49	1.53
34	q	302	LMG	C37-C36	-2.38	1.33	1.50
34	b	622	LMG	C25-C24	-2.38	1.33	1.50
34	9	302	LMG	C37-C36	-2.38	1.33	1.50
34	9	301	LMG	C25-C24	-2.38	1.33	1.50
34	2	621	LMG	C37-C36	-2.38	1.33	1.50
34	J	101	LMG	C43-C42	-2.38	1.33	1.50
43	B	619	BCR	C39-C30	-2.38	1.49	1.53
34	b	622	LMG	C43-C42	-2.38	1.33	1.50
36	R	319	NEX	O24-C25	-2.38	1.43	1.46
34	4	620	LMG	C43-C42	-2.38	1.33	1.50
34	4	621	LMG	C37-C36	-2.38	1.33	1.50
34	d	411	LMG	C43-C42	-2.37	1.33	1.50
34	C	619	LMG	C25-C24	-2.37	1.33	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	606	CHL	C1A-CHA	-2.37	1.37	1.40
34	2	620	LMG	C25-C24	-2.37	1.33	1.50
34	k	101	LMG	C22-C21	-2.37	1.33	1.50
34	B	621	LMG	C43-C42	-2.37	1.33	1.50
34	q	301	LMG	C43-C42	-2.37	1.33	1.50
34	G	621	LMG	C43-C42	-2.37	1.33	1.50
43	v	101	BCR	C39-C30	-2.37	1.49	1.53
31	4	610	CLA	C3D-C4D	-2.37	1.38	1.44
34	G	621	LMG	C25-C24	-2.37	1.33	1.50
43	D	405	BCR	C36-C18	2.37	1.55	1.50
31	c	605	CLA	C3D-C4D	-2.37	1.38	1.44
34	G	622	LMG	C37-C36	-2.37	1.33	1.50
31	B	603	CLA	C3D-C4D	-2.37	1.38	1.44
31	b	604	CLA	C3D-C4D	-2.36	1.38	1.44
34	4	620	LMG	C25-C24	-2.36	1.33	1.50
30	7	310	CHL	C3B-C2B	-2.36	1.37	1.40
30	Y	309	CHL	C2C-C3C	2.36	1.38	1.36
36	6	319	NEX	O24-C25	-2.36	1.43	1.46
34	q	301	LMG	C25-C24	-2.36	1.33	1.50
30	y	608	CHL	C3B-C2B	-2.36	1.37	1.40
43	B	617	BCR	C7-C6	2.36	1.53	1.45
43	B	618	BCR	C39-C30	-2.36	1.49	1.53
43	t	101	BCR	C39-C30	-2.36	1.49	1.53
30	q	303	CHL	C3B-C2B	-2.35	1.37	1.40
30	s	308	CHL	C3B-C2B	-2.35	1.37	1.40
34	2	620	LMG	C43-C42	-2.35	1.33	1.50
31	Y	312	CLA	C3D-C4D	-2.35	1.38	1.44
36	S	319	NEX	C1-C6	-2.35	1.50	1.54
30	G	608	CHL	C3B-C2B	-2.35	1.37	1.40
36	R	301	NEX	C1-C6	-2.35	1.50	1.54
32	G	615	LUT	C26-C27	2.35	1.53	1.50
31	b	607	CLA	C3D-C4D	-2.35	1.38	1.44
38	a	412	SQD	O47-C45	-2.35	1.41	1.46
31	C	608	CLA	C3D-C4D	-2.34	1.38	1.44
31	b	609	CLA	C3D-C4D	-2.34	1.38	1.44
30	3	302	CHL	C1A-CHA	-2.34	1.37	1.40
43	b	620	BCR	C36-C18	2.34	1.55	1.50
31	R	305	CLA	C3D-C4D	-2.34	1.38	1.44
30	6	310	CHL	C3B-C2B	-2.33	1.37	1.40
43	c	614	BCR	C36-C18	2.33	1.55	1.50
30	1	619	CHL	C1B-C2B	2.33	1.42	1.39
30	4	609	CHL	C1A-CHA	-2.33	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	306	CHL	C3B-C2B	-2.33	1.37	1.40
30	7	307	CHL	C3B-C2B	-2.32	1.37	1.40
30	y	609	CHL	C3B-C2B	-2.32	1.37	1.40
43	H	101	BCR	C36-C18	2.32	1.55	1.50
31	B	605	CLA	C3D-C4D	-2.32	1.39	1.44
43	v	101	BCR	C36-C18	2.31	1.55	1.50
31	B	615	CLA	C3D-C4D	-2.31	1.39	1.44
36	Y	317	NEX	O24-C25	-2.31	1.43	1.46
30	1	606	CHL	C3B-C2B	-2.31	1.37	1.40
31	4	612	CLA	C3D-C4D	-2.31	1.39	1.44
31	y	612	CLA	C3D-C4D	-2.31	1.39	1.44
30	6	308	CHL	C3B-C2B	-2.31	1.37	1.40
31	9	312	CLA	C3D-C4D	-2.30	1.39	1.44
30	s	302	CHL	C1A-CHA	-2.30	1.37	1.40
31	D	403	CLA	C3D-C4D	-2.30	1.39	1.44
31	A	407	CLA	C3D-C4D	-2.30	1.39	1.44
31	d	404	CLA	C3D-C4D	-2.30	1.39	1.44
30	6	306	CHL	C3A-C2A	-2.30	1.52	1.54
30	1	609	CHL	C3B-C2B	-2.30	1.37	1.40
31	B	608	CLA	C3D-C4D	-2.30	1.39	1.44
35	q	317	RRX	C34-C9	2.30	1.55	1.50
30	n	301	CHL	C3B-C2B	-2.30	1.37	1.40
43	V	101	BCR	C36-C18	2.29	1.55	1.50
31	a	406	CLA	C3D-C4D	-2.29	1.39	1.44
31	C	606	CLA	C3D-C4D	-2.29	1.39	1.44
31	q	315	CLA	C3D-C4D	-2.29	1.39	1.44
31	9	314	CLA	C3D-C4D	-2.29	1.39	1.44
30	y	606	CHL	C3B-C2B	-2.29	1.37	1.40
31	s	313	CLA	C3D-C4D	-2.29	1.39	1.44
31	R	304	CLA	C3D-C4D	-2.29	1.39	1.44
30	N	301	CHL	C3B-C2B	-2.29	1.37	1.40
31	B	604	CLA	C3D-C4D	-2.28	1.39	1.44
30	Y	309	CHL	C3B-C2B	-2.28	1.37	1.40
31	G	611	CLA	C3D-C4D	-2.28	1.39	1.44
31	B	606	CLA	C3D-C4D	-2.28	1.39	1.44
31	b	616	CLA	C3D-C4D	-2.28	1.39	1.44
36	y	618	NEX	O24-C25	-2.28	1.43	1.46
43	B	619	BCR	C36-C18	2.28	1.55	1.50
35	4	615	RRX	C33-C5	2.28	1.54	1.50
30	7	302	CHL	C3B-C2B	-2.28	1.37	1.40
35	G	614	RRX	C33-C5	2.28	1.54	1.50
43	Z	101	BCR	C36-C18	2.28	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	404	CLA	C3D-C4D	-2.28	1.39	1.44
31	b	606	CLA	C3D-C4D	-2.28	1.39	1.44
30	4	607	CHL	C3B-C2B	-2.27	1.37	1.40
30	g	309	CHL	C3B-C2B	-2.27	1.37	1.40
42	A	408	PHO	C3B-C2B	-2.27	1.37	1.40
43	T	101	BCR	C39-C30	-2.27	1.49	1.53
31	C	603	CLA	C3D-C4D	-2.27	1.39	1.44
31	d	401	CLA	C3D-C4D	-2.27	1.39	1.44
30	p	601	CHL	C3B-C2B	-2.27	1.37	1.40
31	R	312	CLA	C3D-C4D	-2.27	1.39	1.44
47	e	102	HEM	C1D-ND	-2.27	1.34	1.38
43	h	101	BCR	C36-C18	2.27	1.55	1.50
31	c	607	CLA	C3D-C4D	-2.27	1.39	1.44
30	9	308	CHL	C3B-C2B	-2.27	1.37	1.40
30	n	306	CHL	C3B-C2B	-2.27	1.37	1.40
31	C	605	CLA	C1D-ND	-2.27	1.34	1.37
30	0	609	CHL	C3B-C2B	-2.27	1.37	1.40
30	8	605	CHL	C3B-C2B	-2.27	1.37	1.40
31	B	609	CLA	C3D-C4D	-2.27	1.39	1.44
31	c	602	CLA	C3D-C4D	-2.27	1.39	1.44
30	y	609	CHL	C2C-C3C	2.27	1.38	1.36
30	4	601	CHL	C2C-C3C	2.26	1.38	1.36
31	A	405	CLA	C3D-C4D	-2.26	1.39	1.44
31	A	406	CLA	C3D-C4D	-2.26	1.39	1.44
35	9	317	RRX	C33-C5	2.26	1.54	1.50
36	N	318	NEX	O24-C25	-2.26	1.43	1.46
36	R	301	NEX	O24-C25	-2.26	1.43	1.46
30	S	308	CHL	CHA-CBD	2.25	1.54	1.51
36	2	616	NEX	C1-C6	-2.25	1.50	1.54
31	s	315	CLA	C3D-C4D	-2.25	1.39	1.44
31	c	606	CLA	C3D-C4D	-2.25	1.39	1.44
31	a	407	CLA	C3D-C4D	-2.25	1.39	1.44
31	R	314	CLA	C3D-C4D	-2.25	1.39	1.44
31	R	311	CLA	C3D-C4D	-2.25	1.39	1.44
31	b	617	CLA	C3D-C4D	-2.25	1.39	1.44
43	c	615	BCR	C36-C18	2.25	1.55	1.50
30	7	310	CHL	C2C-C3C	2.25	1.38	1.36
44	a	414	PL9	C52-C5	-2.25	1.46	1.50
31	C	604	CLA	C3D-C4D	-2.25	1.39	1.44
30	0	607	CHL	C3B-C2B	-2.25	1.37	1.40
31	q	314	CLA	C3D-C4D	-2.25	1.39	1.44
31	C	602	CLA	C3D-C4D	-2.25	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	C	614	BCR	C36-C18	2.24	1.55	1.50
31	c	609	CLA	C3D-C4D	-2.24	1.39	1.44
31	r	311	CLA	C3D-C4D	-2.24	1.39	1.44
32	S	318	LUT	C26-C27	2.24	1.53	1.50
36	s	319	NEX	O24-C25	-2.24	1.43	1.46
30	Y	308	CHL	C2C-C3C	2.24	1.38	1.36
31	S	304	CLA	C3D-C4D	-2.24	1.39	1.44
31	0	615	CLA	C3D-C4D	-2.24	1.39	1.44
32	p	616	LUT	C28-C27	2.24	1.37	1.32
31	b	605	CLA	C3D-C4D	-2.24	1.39	1.44
30	5	609	CHL	C3B-C2B	-2.23	1.37	1.40
31	0	612	CLA	C3D-C4D	-2.23	1.39	1.44
36	9	319	NEX	C1-C6	-2.23	1.50	1.54
31	R	307	CLA	C3D-C4D	-2.23	1.39	1.44
30	9	309	CHL	C3B-C2B	-2.23	1.37	1.40
38	G	624	SQD	O47-C45	-2.23	1.41	1.46
31	C	610	CLA	C3D-C4D	-2.23	1.39	1.44
43	D	405	BCR	C39-C30	-2.23	1.49	1.53
44	A	416	PL9	C36-C34	-2.23	1.46	1.51
31	R	315	CLA	C3D-C4D	-2.22	1.39	1.44
44	A	416	PL9	C53-C6	-2.22	1.46	1.50
30	9	303	CHL	C3B-C2B	-2.22	1.37	1.40
36	N	318	NEX	C1-C6	-2.22	1.50	1.54
30	9	311	CHL	C1A-CHA	-2.22	1.37	1.40
30	1	608	CHL	C3B-C2B	-2.22	1.37	1.40
31	C	609	CLA	C3D-C4D	-2.22	1.39	1.44
30	5	607	CHL	C3B-C2B	-2.22	1.37	1.40
31	B	602	CLA	C3D-C4D	-2.22	1.39	1.44
31	1	612	CLA	C3D-C4D	-2.22	1.39	1.44
31	b	610	CLA	C3D-C4D	-2.22	1.39	1.44
32	2	615	LUT	C28-C27	2.22	1.37	1.32
36	n	319	NEX	O24-C25	-2.22	1.43	1.46
36	r	319	NEX	C1-C6	-2.22	1.50	1.54
43	b	619	BCR	C36-C18	2.22	1.55	1.50
43	b	618	BCR	C36-C18	2.22	1.55	1.50
47	E	101	HEM	C1D-ND	-2.22	1.34	1.38
31	c	610	CLA	C3D-C4D	-2.22	1.39	1.44
35	2	614	RRX	C33-C5	2.21	1.54	1.50
44	A	416	PL9	C31-C29	-2.21	1.46	1.51
31	r	312	CLA	C3D-C4D	-2.21	1.39	1.44
31	b	602	CLA	C3D-C4D	-2.21	1.39	1.44
43	z	101	BCR	C36-C18	2.21	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	g	303	CLA	C3D-C4D	-2.21	1.39	1.44
31	1	603	CLA	C3D-C4D	-2.21	1.39	1.44
31	b	608	CLA	C3D-C4D	-2.21	1.39	1.44
43	A	410	BCR	C36-C18	2.21	1.55	1.50
31	3	316	CLA	C3D-C4D	-2.20	1.39	1.44
31	c	603	CLA	C3D-C4D	-2.20	1.39	1.44
30	6	302	CHL	C3B-C2B	-2.20	1.37	1.40
31	r	315	CLA	C3D-C4D	-2.20	1.39	1.44
30	1	605	CHL	C2C-C3C	2.20	1.38	1.36
31	Y	311	CLA	C3D-C4D	-2.20	1.39	1.44
36	S	319	NEX	O24-C25	-2.20	1.43	1.46
31	q	306	CLA	C3D-C4D	-2.20	1.39	1.44
31	0	603	CLA	C3D-C4D	-2.20	1.39	1.44
31	S	313	CLA	C3D-C4D	-2.19	1.39	1.44
30	s	308	CHL	CHA-CBD	2.19	1.54	1.51
31	G	613	CLA	C3D-C4D	-2.19	1.39	1.44
31	B	616	CLA	C3D-C4D	-2.19	1.39	1.44
31	y	611	CLA	C3D-C4D	-2.19	1.39	1.44
35	g	315	RRX	C33-C5	2.19	1.54	1.50
30	8	601	CHL	C3B-C2B	-2.19	1.37	1.40
31	S	315	CLA	C3D-C4D	-2.19	1.39	1.44
30	S	302	CHL	C1A-CHA	-2.19	1.37	1.40
30	3	302	CHL	C3D-C2D	-2.19	1.35	1.39
31	q	313	CLA	C3D-C4D	-2.19	1.39	1.44
31	r	314	CLA	C3D-C4D	-2.19	1.39	1.44
31	B	601	CLA	C3D-C4D	-2.19	1.39	1.44
31	C	607	CLA	C3D-C4D	-2.18	1.39	1.44
31	1	602	CLA	C3D-C4D	-2.18	1.39	1.44
47	e	102	HEM	C4B-NB	-2.18	1.34	1.38
31	7	313	CLA	C3D-C4D	-2.18	1.39	1.44
31	b	603	CLA	C3D-C4D	-2.18	1.39	1.44
31	r	316	CLA	C3D-C4D	-2.18	1.39	1.44
31	c	611	CLA	C3D-C4D	-2.18	1.39	1.44
30	7	302	CHL	C2C-C3C	2.18	1.38	1.36
31	s	314	CLA	C3D-C4D	-2.18	1.39	1.44
31	r	306	CLA	C3D-C4D	-2.18	1.39	1.44
32	5	617	LUT	C26-C27	2.17	1.53	1.50
31	C	612	CLA	C3D-C4D	-2.17	1.39	1.44
31	C	613	CLA	C3D-C4D	-2.17	1.39	1.44
31	c	612	CLA	C3D-C4D	-2.17	1.39	1.44
31	Y	313	CLA	C3D-C4D	-2.17	1.39	1.44
30	S	307	CHL	C2C-C3C	2.17	1.38	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	9	318	LUT	C26-C27	2.17	1.53	1.50
36	8	617	NEX	C1-C6	-2.17	1.50	1.54
36	G	616	NEX	O24-C25	-2.16	1.43	1.46
31	6	304	CLA	C3D-C4D	-2.16	1.39	1.44
30	0	601	CHL	C3B-C2B	-2.16	1.37	1.40
31	d	405	CLA	C3D-C4D	-2.16	1.39	1.44
43	t	101	BCR	C36-C18	2.16	1.55	1.50
31	R	306	CLA	C3D-C4D	-2.16	1.39	1.44
30	p	601	CHL	CHA-CBD	2.16	1.54	1.51
31	R	306	CLA	C1A-CHA	2.16	1.52	1.43
34	r	321	LMG	O7-C8	-2.16	1.41	1.46
31	C	601	CLA	C3D-C4D	-2.16	1.39	1.44
31	S	312	CLA	C3D-C4D	-2.16	1.39	1.44
31	R	316	CLA	C3D-C4D	-2.16	1.39	1.44
38	x	201	SQD	O47-C45	-2.16	1.41	1.46
30	S	309	CHL	CHA-CBD	2.15	1.54	1.51
31	0	604	CLA	C3D-C4D	-2.15	1.39	1.44
30	3	308	CHL	CHA-CBD	2.15	1.54	1.51
30	p	609	CHL	C2C-C3C	2.15	1.38	1.36
36	3	319	NEX	O24-C25	-2.15	1.43	1.46
31	B	612	CLA	C1C-C2C	2.15	1.48	1.44
31	s	312	CLA	C3D-C4D	-2.15	1.39	1.44
30	9	308	CHL	C1A-CHA	-2.15	1.37	1.40
31	C	611	CLA	C3D-C4D	-2.15	1.39	1.44
31	c	604	CLA	C3D-C4D	-2.15	1.39	1.44
43	z	101	BCR	C38-C26	2.15	1.54	1.50
31	8	603	CLA	C3D-C4D	-2.15	1.39	1.44
30	g	308	CHL	C3B-C2B	-2.15	1.37	1.40
30	2	608	CHL	C3B-C2B	-2.15	1.37	1.40
30	n	302	CHL	C3B-C2B	-2.15	1.37	1.40
31	3	305	CLA	C3D-C4D	-2.15	1.39	1.44
31	0	611	CLA	C3D-C4D	-2.15	1.39	1.44
30	3	303	CHL	C3B-C2B	-2.15	1.37	1.40
36	g	317	NEX	C1-C6	-2.15	1.51	1.54
30	s	302	CHL	CHA-CBD	2.15	1.54	1.51
31	1	604	CLA	C3D-C4D	-2.15	1.39	1.44
43	D	405	BCR	C38-C26	2.15	1.54	1.50
31	r	307	CLA	C3D-C4D	-2.14	1.39	1.44
31	r	313	CLA	C3D-C4D	-2.14	1.39	1.44
47	E	101	HEM	C4B-NB	-2.14	1.34	1.38
31	7	304	CLA	C3D-C4D	-2.14	1.39	1.44
43	Z	101	BCR	C38-C26	2.14	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	G	612	CLA	C3D-C4D	-2.14	1.39	1.44
30	4	609	CHL	C3B-C2B	-2.14	1.37	1.40
31	G	610	CLA	C1A-CHA	2.14	1.51	1.43
36	4	617	NEX	C1-C6	-2.14	1.51	1.54
30	7	309	CHL	C3B-C2B	-2.14	1.37	1.40
31	c	601	CLA	C3D-C4D	-2.14	1.39	1.44
31	p	603	CLA	C3D-C4D	-2.14	1.39	1.44
30	4	601	CHL	C3B-C2B	-2.14	1.37	1.40
31	p	615	CLA	C3D-C4D	-2.14	1.39	1.44
31	b	613	CLA	C1C-C2C	2.14	1.48	1.44
31	g	310	CLA	C3D-C4D	-2.14	1.39	1.44
31	b	605	CLA	C1A-CHA	2.14	1.51	1.43
30	S	302	CHL	CHA-CBD	2.13	1.54	1.51
43	D	405	BCR	C37-C22	2.13	1.55	1.50
31	7	314	CLA	C3D-C4D	-2.13	1.39	1.44
42	d	402	PHO	C1D-C2D	2.13	1.41	1.39
31	2	602	CLA	C1C-C2C	2.13	1.48	1.44
31	q	316	CLA	C3D-C4D	-2.13	1.39	1.44
31	0	613	CLA	C3D-C4D	-2.13	1.39	1.44
30	g	306	CHL	C3B-C2B	-2.13	1.37	1.40
31	0	602	CLA	C3D-C4D	-2.13	1.39	1.44
30	9	311	CHL	C2C-C3C	2.13	1.38	1.36
31	y	603	CLA	C3D-C4D	-2.13	1.39	1.44
36	q	319	NEX	C1-C6	-2.13	1.51	1.54
31	c	613	CLA	C3D-C4D	-2.13	1.39	1.44
36	p	618	NEX	C1-C6	-2.12	1.51	1.54
31	s	311	CLA	C3D-C4D	-2.12	1.39	1.44
31	1	603	CLA	C1A-CHA	2.12	1.51	1.43
30	0	606	CHL	CHA-CBD	2.12	1.54	1.51
31	p	610	CLA	C1C-C2C	2.12	1.48	1.44
30	N	302	CHL	C3B-C2B	-2.12	1.37	1.40
31	G	609	CLA	C3D-C4D	-2.12	1.39	1.44
31	S	310	CLA	C3D-C4D	-2.12	1.39	1.44
36	5	618	NEX	C1-C6	-2.12	1.51	1.54
32	3	317	LUT	C26-C27	2.12	1.53	1.50
30	2	607	CHL	C3B-C2B	-2.12	1.37	1.40
31	p	613	CLA	C3D-C4D	-2.12	1.39	1.44
32	p	617	LUT	C28-C27	2.12	1.37	1.32
43	C	615	BCR	C36-C18	2.12	1.55	1.50
31	r	305	CLA	C3D-C4D	-2.12	1.39	1.44
30	S	302	CHL	C2C-C3C	2.12	1.38	1.36
32	5	616	LUT	C26-C27	2.12	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	N	316	LUT	C26-C27	2.12	1.53	1.50
32	N	317	LUT	C26-C27	2.12	1.53	1.50
30	0	606	CHL	C2C-C3C	2.11	1.38	1.36
30	Y	306	CHL	CHA-CBD	2.11	1.54	1.51
42	d	402	PHO	C3A-C2A	-2.11	1.52	1.54
30	p	609	CHL	C3B-C2B	-2.11	1.37	1.40
30	4	608	CHL	C3B-C2B	-2.11	1.37	1.40
30	g	302	CHL	C3B-C2B	-2.11	1.37	1.40
43	T	101	BCR	C38-C26	2.11	1.54	1.50
31	B	612	CLA	C3D-C4D	-2.11	1.39	1.44
31	4	603	CLA	C3D-C4D	-2.11	1.39	1.44
31	g	311	CLA	C1A-CHA	2.11	1.51	1.43
31	S	314	CLA	C3D-C4D	-2.10	1.39	1.44
31	q	312	CLA	C3D-C4D	-2.10	1.39	1.44
30	3	307	CHL	C3B-C2B	-2.10	1.37	1.40
31	A	406	CLA	C1A-CHA	2.10	1.51	1.43
31	4	614	CLA	C3D-C4D	-2.10	1.39	1.44
31	9	313	CLA	C3D-C4D	-2.10	1.39	1.44
31	d	405	CLA	C1A-CHA	2.10	1.51	1.43
31	y	602	CLA	C3D-C4D	-2.10	1.39	1.44
43	T	101	BCR	C37-C22	2.10	1.55	1.50
30	q	310	CHL	CHA-CBD	2.10	1.54	1.51
30	q	311	CHL	C3B-C2B	-2.10	1.37	1.40
31	B	604	CLA	C1A-CHA	2.10	1.51	1.43
30	7	321	CHL	CHA-CBD	2.10	1.54	1.51
31	N	312	CLA	C3D-C4D	-2.10	1.39	1.44
31	S	316	CLA	C3D-C4D	-2.10	1.39	1.44
31	q	304	CLA	C1C-C2C	2.10	1.48	1.44
30	s	302	CHL	C2C-C3C	2.10	1.38	1.36
30	p	607	CHL	C3B-C2B	-2.10	1.37	1.40
30	3	309	CHL	CHA-CBD	2.10	1.54	1.51
36	Y	317	NEX	C1-C6	-2.10	1.51	1.54
31	C	613	CLA	C1A-CHA	2.10	1.51	1.43
31	D	404	CLA	C1A-CHA	2.10	1.51	1.43
31	g	312	CLA	C3D-C4D	-2.10	1.39	1.44
31	a	407	CLA	C1A-CHA	2.09	1.51	1.43
31	B	613	CLA	C3D-C4D	-2.09	1.39	1.44
30	9	308	CHL	CHA-CBD	2.09	1.54	1.51
31	C	610	CLA	C1A-CHA	2.09	1.51	1.43
43	b	619	BCR	C38-C26	2.09	1.54	1.50
31	6	312	CLA	C1A-CHA	2.09	1.51	1.43
31	1	613	CLA	C3D-C4D	-2.09	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	313	CLA	C3D-C4D	-2.09	1.39	1.44
31	S	311	CLA	C3D-C4D	-2.09	1.39	1.44
31	c	613	CLA	C1A-CHA	2.09	1.51	1.43
43	B	618	BCR	C36-C18	2.09	1.55	1.50
31	6	312	CLA	C3D-C4D	-2.09	1.39	1.44
43	H	101	BCR	C38-C26	2.09	1.54	1.50
43	d	406	BCR	C36-C18	2.09	1.55	1.50
31	B	602	CLA	C1A-CHA	2.09	1.51	1.43
30	R	309	CHL	C3B-C2B	-2.09	1.37	1.40
31	G	604	CLA	C3D-C4D	-2.09	1.39	1.44
31	p	602	CLA	C1A-CHA	2.09	1.51	1.43
38	m	101	SQD	O47-C45	-2.09	1.41	1.46
31	g	304	CLA	C3D-C4D	-2.09	1.39	1.44
31	s	310	CLA	C3D-C4D	-2.08	1.39	1.44
30	1	609	CHL	C2C-C3C	2.08	1.38	1.36
31	B	615	CLA	C1A-CHA	2.08	1.51	1.43
31	q	312	CLA	C1B-C2B	2.08	1.44	1.41
31	G	602	CLA	C3D-C4D	-2.08	1.39	1.44
31	g	311	CLA	C3D-C4D	-2.08	1.39	1.44
31	2	613	CLA	C3D-C4D	-2.08	1.39	1.44
31	G	603	CLA	C3D-C4D	-2.08	1.39	1.44
31	9	305	CLA	C3D-C4D	-2.08	1.39	1.44
31	s	316	CLA	C3D-C4D	-2.08	1.39	1.44
31	R	303	CLA	C1A-CHA	2.08	1.51	1.43
31	7	314	CLA	C1A-CHA	2.08	1.51	1.43
30	0	609	CHL	C2C-C3C	2.08	1.38	1.36
31	5	611	CLA	C3D-C4D	-2.08	1.39	1.44
31	3	306	CLA	C3D-C4D	-2.08	1.39	1.44
31	n	304	CLA	C3D-C4D	-2.08	1.39	1.44
31	S	303	CLA	C1C-C2C	2.08	1.48	1.44
31	1	610	CLA	C3D-C4D	-2.08	1.39	1.44
31	3	312	CLA	C3D-C4D	-2.08	1.39	1.44
31	p	614	CLA	C3D-C4D	-2.08	1.39	1.44
31	2	611	CLA	C3D-C4D	-2.08	1.39	1.44
31	q	305	CLA	C3D-C4D	-2.08	1.39	1.44
30	6	310	CHL	CHA-CBD	2.08	1.54	1.51
31	8	612	CLA	C3D-C4D	-2.08	1.39	1.44
34	n	322	LMG	O1-C1	2.07	1.43	1.40
31	N	304	CLA	C3D-C4D	-2.07	1.39	1.44
32	q	318	LUT	C26-C27	2.07	1.53	1.50
31	p	611	CLA	C1C-C2C	2.07	1.48	1.44
31	b	613	CLA	C3D-C4D	-2.07	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	614	CLA	C3D-C4D	-2.07	1.39	1.44
43	c	614	BCR	C37-C22	2.07	1.55	1.50
30	4	609	CHL	CHA-CBD	2.07	1.54	1.51
31	9	304	CLA	C1C-C2C	2.07	1.48	1.44
31	n	316	CLA	C3D-C4D	-2.07	1.39	1.44
31	5	612	CLA	C1C-C2C	2.07	1.48	1.44
32	2	615	LUT	C26-C27	2.07	1.53	1.50
31	B	614	CLA	C3D-C4D	-2.07	1.39	1.44
30	3	302	CHL	CHA-CBD	2.07	1.54	1.51
31	b	608	CLA	C1A-CHA	2.07	1.51	1.43
31	N	321	CLA	C3D-C4D	-2.07	1.39	1.44
31	p	610	CLA	C3D-C4D	-2.07	1.39	1.44
30	5	605	CHL	CHA-CBD	2.07	1.54	1.51
31	N	314	CLA	C1C-C2C	2.07	1.48	1.44
31	S	310	CLA	C1A-CHA	2.07	1.51	1.43
31	8	613	CLA	C1C-C2C	2.07	1.48	1.44
30	p	609	CHL	CHA-CBD	2.07	1.54	1.51
31	Y	313	CLA	C1A-CHA	2.07	1.51	1.43
30	1	605	CHL	C3B-C2B	-2.07	1.37	1.40
44	A	416	PL9	C52-C5	-2.07	1.46	1.50
30	G	601	CHL	C3B-C2B	-2.07	1.37	1.40
30	s	309	CHL	CHA-CBD	2.07	1.54	1.51
31	Y	304	CLA	C3D-C4D	-2.07	1.39	1.44
31	8	602	CLA	C1C-C2C	2.07	1.48	1.44
30	9	311	CHL	CHA-CBD	2.07	1.54	1.51
31	n	315	CLA	C1C-C2C	2.07	1.48	1.44
31	N	303	CLA	C3D-C4D	-2.06	1.39	1.44
31	2	609	CLA	C1C-C2C	2.06	1.48	1.44
31	q	312	CLA	C1C-C2C	2.06	1.48	1.44
31	R	313	CLA	C1A-CHA	2.06	1.51	1.43
30	n	308	CHL	CHA-CBD	2.06	1.54	1.51
31	R	313	CLA	C3D-C4D	-2.06	1.39	1.44
31	p	615	CLA	C1C-C2C	2.06	1.48	1.44
30	R	310	CHL	CHA-CBD	2.06	1.54	1.51
31	b	603	CLA	C1A-CHA	2.06	1.51	1.43
30	9	310	CHL	C3B-C2B	-2.06	1.37	1.40
31	3	314	CLA	C3D-C4D	-2.06	1.39	1.44
36	p	618	NEX	O24-C25	-2.06	1.43	1.46
31	s	306	CLA	C1C-C2C	2.06	1.48	1.44
30	7	306	CHL	C2C-C3C	2.06	1.38	1.36
31	r	306	CLA	C1A-CHA	2.06	1.51	1.43
31	1	613	CLA	C1A-CHA	2.06	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	603	CLA	C1A-CHA	2.06	1.51	1.43
31	7	316	CLA	C3D-C4D	-2.06	1.39	1.44
30	r	310	CHL	CHA-CBD	2.06	1.54	1.51
30	y	605	CHL	CHA-CBD	2.06	1.54	1.51
31	2	604	CLA	C3D-C4D	-2.06	1.39	1.44
31	y	615	CLA	C3D-C4D	-2.06	1.39	1.44
31	p	604	CLA	C3D-C4D	-2.06	1.39	1.44
31	3	311	CLA	C1A-CHA	2.06	1.51	1.43
30	9	303	CHL	C2C-C3C	2.06	1.38	1.36
31	4	602	CLA	C1C-C2C	2.06	1.48	1.44
36	9	319	NEX	O24-C25	-2.06	1.43	1.46
37	q	321	XAT	O24-C25	-2.06	1.43	1.46
31	b	616	CLA	C1A-CHA	2.06	1.51	1.43
31	4	613	CLA	C3D-C4D	-2.06	1.39	1.44
31	6	305	CLA	C3D-C4D	-2.06	1.39	1.44
31	S	314	CLA	C1A-CHA	2.05	1.51	1.43
30	s	307	CHL	C2C-C3C	2.05	1.38	1.36
38	0	621	SQD	O47-C45	-2.05	1.41	1.46
31	N	310	CLA	C3D-C4D	-2.05	1.39	1.44
31	R	303	CLA	C3D-C4D	-2.05	1.39	1.44
32	3	318	LUT	C26-C27	2.05	1.53	1.50
31	Y	310	CLA	C3D-C4D	-2.05	1.39	1.44
31	N	313	CLA	C3D-C4D	-2.05	1.39	1.44
31	7	311	CLA	C3D-C4D	-2.05	1.39	1.44
31	9	316	CLA	C3D-C4D	-2.05	1.39	1.44
31	0	603	CLA	C1A-CHA	2.05	1.51	1.43
34	W	201	LMG	O7-C8	-2.05	1.41	1.46
43	t	101	BCR	C37-C22	2.05	1.55	1.50
36	R	319	NEX	C1-C6	-2.05	1.51	1.54
30	5	607	CHL	CHA-CBD	2.05	1.54	1.51
31	G	612	CLA	C1A-CHA	2.05	1.51	1.43
31	s	314	CLA	C1A-CHA	2.05	1.51	1.43
31	p	603	CLA	C1A-CHA	2.05	1.51	1.43
31	Y	303	CLA	C3D-C4D	-2.05	1.39	1.44
31	n	314	CLA	C3D-C4D	-2.05	1.39	1.44
31	n	312	CLA	C3D-C4D	-2.05	1.39	1.44
31	y	610	CLA	C3D-C4D	-2.05	1.39	1.44
31	3	311	CLA	C3D-C4D	-2.05	1.39	1.44
31	C	612	CLA	C1A-CHA	2.05	1.51	1.43
31	p	612	CLA	C3D-C4D	-2.05	1.39	1.44
31	A	409	CLA	C1A-CHA	2.05	1.51	1.43
31	2	612	CLA	C3D-C4D	-2.05	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	614	CLA	C1A-CHA	2.05	1.51	1.43
43	C	614	BCR	C37-C22	2.05	1.55	1.50
38	r	322	SQD	O47-C45	-2.04	1.41	1.46
31	8	610	CLA	C3D-C4D	-2.04	1.39	1.44
31	N	311	CLA	C1C-C2C	2.04	1.48	1.44
31	9	315	CLA	C3D-C4D	-2.04	1.39	1.44
31	a	409	CLA	C1A-CHA	2.04	1.51	1.43
31	5	613	CLA	C3D-C4D	-2.04	1.39	1.44
31	p	602	CLA	C3D-C4D	-2.04	1.39	1.44
31	p	604	CLA	C1C-C2C	2.04	1.48	1.44
30	G	605	CHL	C3B-C2B	-2.04	1.37	1.40
31	4	611	CLA	C1B-C2B	2.04	1.44	1.41
33	q	320	LHG	O7-C5	-2.04	1.41	1.46
31	C	609	CLA	C1A-CHA	2.04	1.51	1.43
31	g	314	CLA	C1C-C2C	2.04	1.48	1.44
38	A	413	SQD	O47-C45	-2.04	1.41	1.46
38	G	617	SQD	O47-C45	-2.04	1.41	1.46
31	Y	305	CLA	C3D-C4D	-2.04	1.39	1.44
31	3	315	CLA	C1C-C2C	2.04	1.48	1.44
36	6	319	NEX	C1-C6	-2.04	1.51	1.54
32	5	617	LUT	C28-C27	2.04	1.37	1.32
30	1	609	CHL	CHA-CBD	2.04	1.54	1.51
31	9	313	CLA	C1A-CHA	2.04	1.51	1.43
31	2	612	CLA	C1A-CHA	2.04	1.51	1.43
31	b	611	CLA	C3D-C4D	-2.04	1.39	1.44
32	6	318	LUT	C26-C27	2.04	1.53	1.50
30	Y	301	CHL	CHA-CBD	2.04	1.54	1.51
31	6	303	CLA	C3D-C4D	-2.04	1.39	1.44
31	n	311	CLA	C3D-C4D	-2.03	1.39	1.44
31	R	316	CLA	C1A-CHA	2.03	1.51	1.43
30	p	608	CHL	CHA-CBD	2.03	1.54	1.51
31	g	310	CLA	C1A-CHA	2.03	1.51	1.43
30	G	605	CHL	CHA-CBD	2.03	1.54	1.51
30	0	605	CHL	CHA-CBD	2.03	1.54	1.51
30	8	607	CHL	CHA-CBD	2.03	1.54	1.51
31	S	306	CLA	C1C-C2C	2.03	1.48	1.44
31	8	609	CLA	C1C-C2C	2.03	1.48	1.44
31	b	615	CLA	C3D-C4D	-2.03	1.39	1.44
31	p	611	CLA	C3D-C4D	-2.03	1.39	1.44
31	c	612	CLA	C1A-CHA	2.03	1.51	1.43
31	s	310	CLA	C1A-CHA	2.03	1.51	1.43
31	B	610	CLA	C3D-C4D	-2.03	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	g	318	SQD	O47-C45	-2.03	1.41	1.46
31	3	312	CLA	C1C-C2C	2.03	1.48	1.44
30	5	601	CHL	C3B-C2B	-2.03	1.37	1.40
31	6	311	CLA	C3D-C4D	-2.03	1.39	1.44
38	6	301	SQD	O47-C45	-2.03	1.41	1.46
30	5	609	CHL	CHA-CBD	2.03	1.54	1.51
31	4	604	CLA	C1C-C2C	2.03	1.48	1.44
31	0	613	CLA	C1A-CHA	2.03	1.51	1.43
31	G	610	CLA	C3D-C4D	-2.03	1.39	1.44
31	q	304	CLA	C1A-CHA	2.03	1.51	1.43
31	B	611	CLA	C3D-C4D	-2.03	1.39	1.44
31	Y	314	CLA	C3D-C4D	-2.03	1.39	1.44
30	r	309	CHL	CHA-CBD	2.03	1.54	1.51
31	r	313	CLA	C1A-CHA	2.03	1.51	1.43
43	t	101	BCR	C38-C26	2.03	1.54	1.50
31	4	602	CLA	C3D-C4D	-2.03	1.39	1.44
31	C	607	CLA	C1A-CHA	2.03	1.51	1.43
31	y	602	CLA	C1C-C2C	2.03	1.48	1.44
31	C	603	CLA	C1A-CHA	2.03	1.51	1.43
30	2	608	CHL	CHA-CBD	2.03	1.54	1.51
30	8	608	CHL	CHA-CBD	2.03	1.54	1.51
31	s	316	CLA	C1A-CHA	2.03	1.51	1.43
31	5	604	CLA	C3D-C4D	-2.03	1.39	1.44
31	7	305	CLA	C3D-C4D	-2.03	1.39	1.44
30	n	309	CHL	CHA-CBD	2.03	1.54	1.51
31	s	303	CLA	C1C-C2C	2.03	1.48	1.44
37	G	620	XAT	O24-C25	-2.03	1.43	1.46
31	N	310	CLA	C1C-C2C	2.02	1.48	1.44
31	N	321	CLA	C1C-C2C	2.02	1.48	1.44
31	S	303	CLA	C3D-C4D	-2.02	1.39	1.44
31	g	313	CLA	C3D-C4D	-2.02	1.39	1.44
30	2	607	CHL	CHA-CBD	2.02	1.54	1.51
43	b	620	BCR	C38-C26	2.02	1.54	1.50
31	7	311	CLA	C1C-C2C	2.02	1.48	1.44
30	Y	306	CHL	C1A-CHA	-2.02	1.37	1.40
31	n	303	CLA	C3D-C4D	-2.02	1.39	1.44
31	R	307	CLA	C1A-CHA	2.02	1.51	1.43
32	5	616	LUT	C28-C27	2.02	1.37	1.32
31	7	303	CLA	C1C-C2C	2.02	1.48	1.44
31	n	311	CLA	C1C-C2C	2.02	1.48	1.44
31	b	610	CLA	C1A-CHA	2.02	1.51	1.43
34	0	620	LMG	O1-C1	2.02	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	q	317	RRX	C33-C5	2.02	1.54	1.50
31	1	611	CLA	C3D-C4D	-2.02	1.39	1.44
31	y	615	CLA	C1C-C2C	2.02	1.48	1.44
38	b	627	SQD	O47-C45	-2.02	1.41	1.46
31	p	604	CLA	C1A-CHA	2.02	1.51	1.43
31	2	609	CLA	C3D-C4D	-2.02	1.39	1.44
31	y	604	CLA	C3D-C4D	-2.02	1.39	1.44
31	c	611	CLA	C1A-CHA	2.02	1.51	1.43
31	g	305	CLA	C3D-C4D	-2.02	1.39	1.44
31	5	602	CLA	C1C-C2C	2.02	1.48	1.44
31	5	612	CLA	C3D-C4D	-2.02	1.39	1.44
31	n	312	CLA	C1C-C2C	2.02	1.48	1.44
31	B	607	CLA	CAA-C2A	-2.02	1.50	1.54
30	n	306	CHL	CHA-CBD	2.02	1.54	1.51
30	6	306	CHL	C3B-C2B	-2.02	1.37	1.40
31	N	312	CLA	C1C-C2C	2.02	1.48	1.44
31	4	614	CLA	C1A-CHA	2.02	1.51	1.43
30	3	307	CHL	CHA-CBD	2.02	1.54	1.51
30	Y	308	CHL	CHA-CBD	2.02	1.54	1.51
30	7	310	CHL	CHA-CBD	2.02	1.54	1.51
31	r	315	CLA	C1A-CHA	2.02	1.51	1.43
31	0	614	CLA	C3D-C4D	-2.02	1.39	1.44
31	C	611	CLA	C1A-CHA	2.02	1.51	1.43
36	y	618	NEX	C1-C6	-2.02	1.51	1.54
31	3	315	CLA	C3D-C4D	-2.02	1.39	1.44
31	5	615	CLA	C3D-C4D	-2.02	1.39	1.44
30	9	307	CHL	C3B-C2B	-2.02	1.37	1.40
38	s	301	SQD	O47-C45	-2.02	1.41	1.46
31	c	609	CLA	C1A-CHA	2.02	1.51	1.43
31	c	610	CLA	C1A-CHA	2.02	1.51	1.43
30	3	308	CHL	C2C-C3C	2.02	1.38	1.36
30	8	605	CHL	CHA-CBD	2.02	1.54	1.51
31	s	311	CLA	C1A-CHA	2.02	1.51	1.43
32	g	316	LUT	C28-C27	2.02	1.36	1.32
31	b	612	CLA	C1C-C2C	2.01	1.48	1.44
31	8	614	CLA	C3D-C4D	-2.01	1.39	1.44
31	s	303	CLA	C3D-C4D	-2.01	1.39	1.44
31	8	611	CLA	C3D-C4D	-2.01	1.39	1.44
31	s	312	CLA	C1A-CHA	2.01	1.51	1.43
30	2	608	CHL	C2C-C3C	2.01	1.38	1.36
38	A	411	SQD	O47-C45	-2.01	1.41	1.46
31	R	305	CLA	C1A-CHA	2.01	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	r	304	CLA	C3D-C4D	-2.01	1.39	1.44
31	s	305	CLA	C3D-C4D	-2.01	1.39	1.44
31	6	316	CLA	C3D-C4D	-2.01	1.39	1.44
30	2	605	CHL	C3B-C2B	-2.01	1.37	1.40
30	G	607	CHL	C3B-C2B	-2.01	1.37	1.40
31	q	316	CLA	C1A-CHA	2.01	1.51	1.43
31	b	615	CLA	C1C-C2C	2.01	1.48	1.44
31	5	610	CLA	C3D-C4D	-2.01	1.39	1.44
31	s	306	CLA	C3D-C4D	-2.01	1.39	1.44
32	9	318	LUT	C28-C27	2.01	1.36	1.32
31	N	315	CLA	C3D-C4D	-2.01	1.39	1.44
31	n	313	CLA	C3D-C4D	-2.01	1.39	1.44
31	y	614	CLA	C3D-C4D	-2.01	1.39	1.44
31	5	602	CLA	C3D-C4D	-2.01	1.39	1.44
30	G	608	CHL	CHA-CBD	2.01	1.54	1.51
31	1	614	CLA	C3D-C4D	-2.01	1.39	1.44
31	1	611	CLA	C1C-C2C	2.01	1.48	1.44
31	6	313	CLA	C1C-C2C	2.01	1.48	1.44
31	R	315	CLA	C1A-CHA	2.01	1.51	1.43
30	9	303	CHL	CHA-CBD	2.01	1.54	1.51
30	g	302	CHL	CHA-CBD	2.01	1.54	1.51
31	r	307	CLA	C1A-CHA	2.01	1.51	1.43
31	9	306	CLA	C3D-C4D	-2.01	1.39	1.44
31	0	611	CLA	C1A-CHA	2.01	1.51	1.43
31	7	312	CLA	C3D-C4D	-2.01	1.39	1.44
31	G	602	CLA	C1C-C2C	2.01	1.48	1.44
43	B	619	BCR	C38-C26	2.00	1.54	1.50
37	4	619	XAT	O24-C25	-2.00	1.43	1.46
30	1	606	CHL	CHA-CBD	2.00	1.54	1.51
32	3	318	LUT	C28-C27	2.00	1.36	1.32
31	3	304	CLA	C1C-C2C	2.00	1.48	1.44
30	0	609	CHL	CHA-CBD	2.00	1.54	1.51
31	B	614	CLA	C1C-C2C	2.00	1.48	1.44
43	H	101	BCR	C37-C22	2.00	1.54	1.50
31	4	613	CLA	C1A-CHA	2.00	1.51	1.43
31	S	311	CLA	C1A-CHA	2.00	1.51	1.43
31	6	314	CLA	C3D-C4D	-2.00	1.39	1.44
31	C	601	CLA	C1A-CHA	2.00	1.51	1.43
30	2	601	CHL	CHA-CBD	2.00	1.54	1.51
30	p	606	CHL	CHA-CBD	2.00	1.54	1.51
31	q	304	CLA	C3D-C4D	-2.00	1.39	1.44
34	b	622	LMG	O1-C1	2.00	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	7	306	CHL	C3B-C2B	-2.00	1.37	1.40
30	1	608	CHL	CHA-CBD	2.00	1.54	1.51
30	N	308	CHL	CHA-CBD	2.00	1.54	1.51
31	6	304	CLA	C1C-C2C	2.00	1.48	1.44
31	n	303	CLA	C1C-C2C	2.00	1.48	1.44

All (8361) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	G	615	LUT	C40-C33-C34	-28.87	76.04	122.82
32	G	615	LUT	C32-C33-C34	24.72	157.89	119.01
32	G	615	LUT	C40-C33-C32	-23.72	81.85	118.09
43	C	615	BCR	C15-C14-C13	-13.04	108.99	127.28
43	t	101	BCR	C11-C10-C9	-12.07	110.35	127.28
43	d	406	BCR	C15-C14-C13	-11.98	110.48	127.28
43	d	406	BCR	C7-C8-C9	-11.96	108.55	126.23
43	t	101	BCR	C15-C14-C13	-11.86	110.65	127.28
43	C	615	BCR	C7-C8-C9	-11.75	108.85	126.23
32	R	317	LUT	C35-C34-C33	-10.83	112.09	127.28
43	t	101	BCR	C7-C8-C9	-10.60	110.56	126.23
32	p	617	LUT	C35-C34-C33	-10.56	112.47	127.28
32	p	616	LUT	C35-C34-C33	-10.53	112.52	127.28
43	c	614	BCR	C20-C21-C22	-10.27	112.88	127.28
31	B	607	CLA	C4A-NA-C1A	10.14	111.31	106.68
31	b	608	CLA	C4A-NA-C1A	9.88	111.19	106.68
31	d	405	CLA	C4A-NA-C1A	9.86	111.18	106.68
31	B	615	CLA	C4A-NA-C1A	9.73	111.12	106.68
32	2	615	LUT	C35-C34-C33	-9.72	113.64	127.28
31	c	613	CLA	C4A-NA-C1A	9.70	111.11	106.68
31	R	306	CLA	C4A-NA-C1A	9.59	111.06	106.68
31	a	409	CLA	C4A-NA-C1A	9.56	111.04	106.68
31	A	409	CLA	C4A-NA-C1A	9.53	111.03	106.68
31	b	610	CLA	C4A-NA-C1A	9.52	111.02	106.68
31	g	305	CLA	C4A-NA-C1A	9.52	111.02	106.68
31	b	616	CLA	C4A-NA-C1A	9.49	111.01	106.68
31	D	404	CLA	C4A-NA-C1A	9.49	111.01	106.68
31	q	315	CLA	C4A-NA-C1A	9.47	111.00	106.68
31	C	612	CLA	C4A-NA-C1A	9.43	110.98	106.68
31	C	607	CLA	C4A-NA-C1A	9.41	110.97	106.68
31	c	606	CLA	C4A-NA-C1A	9.40	110.97	106.68
31	c	612	CLA	C4A-NA-C1A	9.37	110.95	106.68
31	R	316	CLA	C4A-NA-C1A	9.35	110.95	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	406	CLA	C4A-NA-C1A	9.34	110.94	106.68
31	b	609	CLA	C4A-NA-C1A	9.34	110.94	106.68
31	r	315	CLA	C4A-NA-C1A	9.33	110.93	106.68
31	A	405	CLA	C4A-NA-C1A	9.32	110.93	106.68
31	q	313	CLA	C4A-NA-C1A	9.32	110.93	106.68
31	C	609	CLA	C4A-NA-C1A	9.31	110.93	106.68
31	2	604	CLA	C4A-NA-C1A	9.30	110.92	106.68
31	9	312	CLA	C4A-NA-C1A	9.30	110.92	106.68
31	r	312	CLA	C4A-NA-C1A	9.29	110.92	106.68
31	4	612	CLA	C4A-NA-C1A	9.27	110.91	106.68
31	b	613	CLA	C4A-NA-C1A	9.26	110.90	106.68
31	s	310	CLA	C4A-NA-C1A	9.26	110.90	106.68
31	C	613	CLA	C4A-NA-C1A	9.25	110.90	106.68
31	B	609	CLA	C4A-NA-C1A	9.24	110.89	106.68
31	y	604	CLA	C4A-NA-C1A	9.22	110.88	106.68
31	c	610	CLA	C4A-NA-C1A	9.20	110.88	106.68
31	p	613	CLA	C4A-NA-C1A	9.20	110.88	106.68
31	7	305	CLA	C4A-NA-C1A	9.18	110.86	106.68
31	c	611	CLA	C4A-NA-C1A	9.12	110.84	106.68
31	y	613	CLA	C4A-NA-C1A	9.11	110.84	106.68
31	6	305	CLA	C4A-NA-C1A	9.10	110.83	106.68
43	D	405	BCR	C7-C8-C9	-9.10	112.78	126.23
31	a	406	CLA	C4A-NA-C1A	9.08	110.82	106.68
31	2	602	CLA	C4A-NA-C1A	9.07	110.82	106.68
31	4	604	CLA	C4A-NA-C1A	9.06	110.81	106.68
31	c	609	CLA	C4A-NA-C1A	9.06	110.81	106.68
31	G	604	CLA	C4A-NA-C1A	9.04	110.81	106.68
31	a	407	CLA	C4A-NA-C1A	9.04	110.80	106.68
31	0	604	CLA	C4A-NA-C1A	9.04	110.80	106.68
31	n	315	CLA	C4A-NA-C1A	9.04	110.80	106.68
31	R	312	CLA	C4A-NA-C1A	9.03	110.80	106.68
31	r	306	CLA	C4A-NA-C1A	9.03	110.80	106.68
31	4	610	CLA	C4A-NA-C1A	9.03	110.80	106.68
31	B	616	CLA	C4A-NA-C1A	9.02	110.79	106.68
31	S	306	CLA	C4A-NA-C1A	9.00	110.78	106.68
31	8	613	CLA	C4A-NA-C1A	8.99	110.78	106.68
31	9	306	CLA	C4A-NA-C1A	8.98	110.78	106.68
31	C	611	CLA	C4A-NA-C1A	8.98	110.78	106.68
31	1	613	CLA	C4A-NA-C1A	8.96	110.77	106.68
31	0	615	CLA	C4A-NA-C1A	8.96	110.77	106.68
31	0	610	CLA	C4A-NA-C1A	8.96	110.77	106.68
31	D	403	CLA	C4A-NA-C1A	8.96	110.77	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	N	314	CLA	C4A-NA-C1A	8.96	110.77	106.68
31	R	315	CLA	C4A-NA-C1A	8.95	110.76	106.68
31	S	310	CLA	C4A-NA-C1A	8.95	110.76	106.68
31	S	314	CLA	C4A-NA-C1A	8.94	110.76	106.68
31	s	312	CLA	C4A-NA-C1A	8.94	110.76	106.68
31	2	610	CLA	C4A-NA-C1A	8.93	110.75	106.68
31	q	304	CLA	C4A-NA-C1A	8.93	110.75	106.68
31	Y	305	CLA	C4A-NA-C1A	8.91	110.75	106.68
31	B	604	CLA	C4A-NA-C1A	8.91	110.75	106.68
31	y	615	CLA	C4A-NA-C1A	8.91	110.74	106.68
31	r	311	CLA	C4A-NA-C1A	8.91	110.74	106.68
31	q	312	CLA	C4A-NA-C1A	8.90	110.74	106.68
31	b	606	CLA	C4A-NA-C1A	8.89	110.74	106.68
31	R	303	CLA	C4A-NA-C1A	8.88	110.73	106.68
31	S	313	CLA	C4A-NA-C1A	8.88	110.73	106.68
31	Y	311	CLA	C4A-NA-C1A	8.88	110.73	106.68
31	N	304	CLA	C4A-NA-C1A	8.87	110.73	106.68
31	2	612	CLA	C4A-NA-C1A	8.86	110.72	106.68
31	9	314	CLA	C4A-NA-C1A	8.86	110.72	106.68
31	N	305	CLA	C4A-NA-C1A	8.85	110.72	106.68
31	N	311	CLA	C4A-NA-C1A	8.84	110.71	106.68
31	G	610	CLA	C4A-NA-C1A	8.83	110.71	106.68
31	c	605	CLA	C4A-NA-C1A	8.83	110.71	106.68
31	g	310	CLA	C4A-NA-C1A	8.83	110.71	106.68
31	1	603	CLA	C4A-NA-C1A	8.82	110.70	106.68
31	n	304	CLA	C4A-NA-C1A	8.82	110.70	106.68
31	b	614	CLA	C4A-NA-C1A	8.82	110.70	106.68
31	G	612	CLA	C4A-NA-C1A	8.81	110.70	106.68
31	b	605	CLA	C4A-NA-C1A	8.81	110.70	106.68
31	s	313	CLA	C4A-NA-C1A	8.81	110.70	106.68
31	2	611	CLA	C4A-NA-C1A	8.80	110.69	106.68
31	5	615	CLA	C4A-NA-C1A	8.80	110.69	106.68
31	6	314	CLA	C4A-NA-C1A	8.80	110.69	106.68
31	B	608	CLA	C4A-NA-C1A	8.79	110.69	106.68
31	5	603	CLA	C4A-NA-C1A	8.79	110.69	106.68
31	1	604	CLA	C4A-NA-C1A	8.78	110.69	106.68
31	1	614	CLA	C4A-NA-C1A	8.78	110.68	106.68
31	S	305	CLA	C4A-NA-C1A	8.78	110.68	106.68
31	0	602	CLA	C4A-NA-C1A	8.77	110.68	106.68
31	r	316	CLA	C4A-NA-C1A	8.77	110.68	106.68
31	8	604	CLA	C4A-NA-C1A	8.76	110.68	106.68
31	g	303	CLA	C4A-NA-C1A	8.76	110.68	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	305	CLA	C4A-NA-C1A	8.76	110.68	106.68
31	s	304	CLA	C4A-NA-C1A	8.76	110.67	106.68
31	G	611	CLA	C4A-NA-C1A	8.75	110.67	106.68
31	B	612	CLA	C4A-NA-C1A	8.75	110.67	106.68
31	n	305	CLA	C4A-NA-C1A	8.75	110.67	106.68
31	r	303	CLA	C4A-NA-C1A	8.74	110.67	106.68
31	3	306	CLA	C4A-NA-C1A	8.73	110.66	106.68
31	3	311	CLA	C4A-NA-C1A	8.73	110.66	106.68
31	b	602	CLA	C4A-NA-C1A	8.73	110.66	106.68
31	C	610	CLA	C4A-NA-C1A	8.72	110.66	106.68
31	Y	313	CLA	C4A-NA-C1A	8.72	110.66	106.68
31	c	604	CLA	C4A-NA-C1A	8.72	110.66	106.68
31	s	303	CLA	C4A-NA-C1A	8.71	110.66	106.68
31	S	303	CLA	C4A-NA-C1A	8.71	110.65	106.68
31	y	612	CLA	C4A-NA-C1A	8.70	110.65	106.68
31	R	305	CLA	C4A-NA-C1A	8.70	110.65	106.68
31	p	602	CLA	C4A-NA-C1A	8.70	110.65	106.68
31	c	607	CLA	C4A-NA-C1A	8.70	110.65	106.68
31	6	311	CLA	C4A-NA-C1A	8.69	110.64	106.68
31	0	614	CLA	C4A-NA-C1A	8.69	110.64	106.68
31	2	613	CLA	C4A-NA-C1A	8.68	110.64	106.68
31	3	313	CLA	C4A-NA-C1A	8.68	110.64	106.68
31	7	314	CLA	C4A-NA-C1A	8.68	110.64	106.68
31	5	604	CLA	C4A-NA-C1A	8.68	110.64	106.68
31	0	613	CLA	C4A-NA-C1A	8.68	110.64	106.68
31	s	316	CLA	C4A-NA-C1A	8.68	110.64	106.68
31	A	407	CLA	C4A-NA-C1A	8.67	110.64	106.68
31	d	401	CLA	C4A-NA-C1A	8.67	110.64	106.68
31	G	609	CLA	C4A-NA-C1A	8.67	110.64	106.68
31	R	313	CLA	C4A-NA-C1A	8.66	110.63	106.68
31	9	304	CLA	C4A-NA-C1A	8.66	110.63	106.68
31	n	314	CLA	C4A-NA-C1A	8.66	110.63	106.68
31	C	602	CLA	C4A-NA-C1A	8.65	110.63	106.68
31	5	602	CLA	C4A-NA-C1A	8.65	110.63	106.68
31	C	608	CLA	C4A-NA-C1A	8.65	110.63	106.68
31	2	609	CLA	C4A-NA-C1A	8.65	110.62	106.68
31	y	611	CLA	C4A-NA-C1A	8.65	110.62	106.68
31	g	312	CLA	C4A-NA-C1A	8.64	110.62	106.68
31	g	313	CLA	C4A-NA-C1A	8.64	110.62	106.68
31	r	313	CLA	C4A-NA-C1A	8.64	110.62	106.68
31	5	611	CLA	C4A-NA-C1A	8.62	110.61	106.68
31	8	603	CLA	C4A-NA-C1A	8.62	110.61	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	305	CLA	C4A-NA-C1A	8.62	110.61	106.68
31	n	312	CLA	C4A-NA-C1A	8.62	110.61	106.68
31	r	305	CLA	C4A-NA-C1A	8.62	110.61	106.68
31	q	316	CLA	C4A-NA-C1A	8.61	110.61	106.68
31	n	303	CLA	C4A-NA-C1A	8.61	110.61	106.68
31	s	306	CLA	C4A-NA-C1A	8.61	110.61	106.68
31	c	603	CLA	C4A-NA-C1A	8.61	110.61	106.68
31	q	314	CLA	C4A-NA-C1A	8.61	110.61	106.68
31	s	314	CLA	C4A-NA-C1A	8.61	110.61	106.68
31	6	313	CLA	C4A-NA-C1A	8.60	110.60	106.68
31	5	614	CLA	C4A-NA-C1A	8.60	110.60	106.68
31	3	312	CLA	C4A-NA-C1A	8.60	110.60	106.68
31	5	610	CLA	C4A-NA-C1A	8.60	110.60	106.68
31	B	610	CLA	C4A-NA-C1A	8.60	110.60	106.68
31	B	603	CLA	C4A-NA-C1A	8.60	110.60	106.68
31	6	315	CLA	C4A-NA-C1A	8.59	110.60	106.68
31	b	615	CLA	C4A-NA-C1A	8.59	110.60	106.68
31	4	614	CLA	C4A-NA-C1A	8.59	110.60	106.68
31	S	311	CLA	C4A-NA-C1A	8.59	110.60	106.68
31	Y	303	CLA	C4A-NA-C1A	8.59	110.60	106.68
31	8	612	CLA	C4A-NA-C1A	8.59	110.60	106.68
31	1	602	CLA	C4A-NA-C1A	8.58	110.59	106.68
31	7	315	CLA	C4A-NA-C1A	8.58	110.59	106.68
31	8	610	CLA	C4A-NA-C1A	8.58	110.59	106.68
31	c	602	CLA	C4A-NA-C1A	8.58	110.59	106.68
31	G	603	CLA	C4A-NA-C1A	8.56	110.58	106.68
31	N	313	CLA	C4A-NA-C1A	8.56	110.58	106.68
31	S	312	CLA	C4A-NA-C1A	8.56	110.58	106.68
31	8	609	CLA	C4A-NA-C1A	8.56	110.58	106.68
31	3	316	CLA	C4A-NA-C1A	8.55	110.58	106.68
31	B	605	CLA	C4A-NA-C1A	8.55	110.58	106.68
31	g	304	CLA	C4A-NA-C1A	8.55	110.58	106.68
31	N	303	CLA	C4A-NA-C1A	8.55	110.58	106.68
31	b	612	CLA	C4A-NA-C1A	8.55	110.58	106.68
31	r	304	CLA	C4A-NA-C1A	8.55	110.58	106.68
31	7	303	CLA	C4A-NA-C1A	8.54	110.58	106.68
31	9	315	CLA	C4A-NA-C1A	8.54	110.58	106.68
31	n	311	CLA	C4A-NA-C1A	8.54	110.57	106.68
31	b	607	CLA	C4A-NA-C1A	8.53	110.57	106.68
31	R	307	CLA	C4A-NA-C1A	8.52	110.57	106.68
31	6	316	CLA	C4A-NA-C1A	8.52	110.57	106.68
31	y	603	CLA	C4A-NA-C1A	8.52	110.57	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	617	CLA	C4A-NA-C1A	8.52	110.56	106.68
31	N	315	CLA	C4A-NA-C1A	8.51	110.56	106.68
31	Y	312	CLA	C4A-NA-C1A	8.51	110.56	106.68
31	7	312	CLA	C4A-NA-C1A	8.50	110.56	106.68
31	n	313	CLA	C4A-NA-C1A	8.50	110.56	106.68
31	S	316	CLA	C4A-NA-C1A	8.49	110.55	106.68
31	N	310	CLA	C4A-NA-C1A	8.48	110.55	106.68
31	p	611	CLA	C4A-NA-C1A	8.48	110.55	106.68
31	8	611	CLA	C4A-NA-C1A	8.47	110.54	106.68
31	Y	314	CLA	C4A-NA-C1A	8.47	110.54	106.68
31	d	404	CLA	C4A-NA-C1A	8.47	110.54	106.68
31	5	612	CLA	C4A-NA-C1A	8.46	110.54	106.68
31	3	314	CLA	C4A-NA-C1A	8.45	110.53	106.68
31	B	606	CLA	C4A-NA-C1A	8.45	110.53	106.68
31	C	601	CLA	C4A-NA-C1A	8.44	110.53	106.68
31	4	602	CLA	C4A-NA-C1A	8.44	110.53	106.68
31	6	303	CLA	C4A-NA-C1A	8.43	110.53	106.68
31	C	604	CLA	C4A-NA-C1A	8.42	110.52	106.68
31	p	603	CLA	C4A-NA-C1A	8.42	110.52	106.68
31	y	602	CLA	C4A-NA-C1A	8.42	110.52	106.68
31	4	611	CLA	C4A-NA-C1A	8.41	110.52	106.68
31	g	314	CLA	C4A-NA-C1A	8.41	110.52	106.68
31	Y	304	CLA	C4A-NA-C1A	8.41	110.52	106.68
31	1	612	CLA	C4A-NA-C1A	8.40	110.51	106.68
31	8	602	CLA	C4A-NA-C1A	8.40	110.51	106.68
31	3	301	CLA	C4A-NA-C1A	8.40	110.51	106.68
31	p	612	CLA	C4A-NA-C1A	8.39	110.51	106.68
31	7	304	CLA	C4A-NA-C1A	8.38	110.50	106.68
31	y	610	CLA	C4A-NA-C1A	8.38	110.50	106.68
31	3	305	CLA	C4A-NA-C1A	8.37	110.50	106.68
31	7	316	CLA	C4A-NA-C1A	8.37	110.50	106.68
31	q	305	CLA	C4A-NA-C1A	8.37	110.50	106.68
31	R	304	CLA	C4A-NA-C1A	8.36	110.50	106.68
31	6	304	CLA	C4A-NA-C1A	8.36	110.49	106.68
31	2	603	CLA	C4A-NA-C1A	8.36	110.49	106.68
31	3	304	CLA	C4A-NA-C1A	8.35	110.49	106.68
31	B	601	CLA	C4A-NA-C1A	8.35	110.49	106.68
31	7	311	CLA	C4A-NA-C1A	8.35	110.49	106.68
31	g	311	CLA	C4A-NA-C1A	8.34	110.48	106.68
31	6	312	CLA	C4A-NA-C1A	8.33	110.48	106.68
31	B	602	CLA	C4A-NA-C1A	8.32	110.48	106.68
31	4	613	CLA	C4A-NA-C1A	8.32	110.48	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	314	CLA	C4A-NA-C1A	8.32	110.48	106.68
31	3	315	CLA	C4A-NA-C1A	8.30	110.46	106.68
31	5	613	CLA	C4A-NA-C1A	8.29	110.46	106.68
31	R	311	CLA	C4A-NA-C1A	8.29	110.46	106.68
31	r	314	CLA	C4A-NA-C1A	8.29	110.46	106.68
31	B	611	CLA	C4A-NA-C1A	8.28	110.46	106.68
31	G	602	CLA	C4A-NA-C1A	8.28	110.46	106.68
31	n	316	CLA	C4A-NA-C1A	8.28	110.46	106.68
31	p	604	CLA	C4A-NA-C1A	8.27	110.45	106.68
31	C	605	CLA	C4A-NA-C1A	8.26	110.45	106.68
31	s	311	CLA	C4A-NA-C1A	8.26	110.45	106.68
31	N	321	CLA	C4A-NA-C1A	8.26	110.45	106.68
31	b	604	CLA	C4A-NA-C1A	8.25	110.44	106.68
31	Y	310	CLA	C4A-NA-C1A	8.25	110.44	106.68
31	C	606	CLA	C4A-NA-C1A	8.23	110.43	106.68
31	b	611	CLA	C4A-NA-C1A	8.22	110.43	106.68
31	9	313	CLA	C4A-NA-C1A	8.21	110.42	106.68
31	p	610	CLA	C4A-NA-C1A	8.21	110.42	106.68
31	9	316	CLA	C4A-NA-C1A	8.20	110.42	106.68
31	0	611	CLA	C4A-NA-C1A	8.20	110.42	106.68
31	4	603	CLA	C4A-NA-C1A	8.20	110.42	106.68
31	0	612	CLA	C4A-NA-C1A	8.19	110.42	106.68
31	r	307	CLA	C4A-NA-C1A	8.19	110.41	106.68
31	q	306	CLA	C4A-NA-C1A	8.18	110.41	106.68
31	1	611	CLA	C4A-NA-C1A	8.17	110.41	106.68
31	p	614	CLA	C4A-NA-C1A	8.17	110.41	106.68
31	c	608	CLA	C4A-NA-C1A	8.16	110.40	106.68
31	B	614	CLA	C4A-NA-C1A	8.16	110.40	106.68
43	D	405	BCR	C15-C14-C13	-8.15	115.85	127.28
31	c	601	CLA	C4A-NA-C1A	8.14	110.39	106.68
31	s	315	CLA	C4A-NA-C1A	8.14	110.39	106.68
31	0	603	CLA	C4A-NA-C1A	8.13	110.39	106.68
31	N	312	CLA	C4A-NA-C1A	8.11	110.38	106.68
31	b	603	CLA	C4A-NA-C1A	8.11	110.38	106.68
31	y	614	CLA	C4A-NA-C1A	8.11	110.38	106.68
31	1	610	CLA	C4A-NA-C1A	8.10	110.38	106.68
31	C	603	CLA	C4A-NA-C1A	8.07	110.36	106.68
43	C	615	BCR	C20-C21-C22	-8.07	115.96	127.28
31	8	614	CLA	C4A-NA-C1A	8.02	110.34	106.68
31	B	613	CLA	C4A-NA-C1A	8.01	110.33	106.68
31	S	315	CLA	C4A-NA-C1A	7.97	110.31	106.68
31	p	615	CLA	C4A-NA-C1A	7.89	110.28	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	313	CLA	C4A-NA-C1A	7.75	110.22	106.68
43	c	614	BCR	C24-C23-C22	-7.74	114.78	126.23
31	r	303	CLA	O2D-CGD-CBD	7.73	124.75	111.23
31	G	613	CLA	C4A-NA-C1A	7.62	110.16	106.68
30	3	309	CHL	C1B-CHB-C4A	7.51	126.15	121.32
43	c	615	BCR	C20-C21-C22	-7.50	116.76	127.28
43	t	101	BCR	C33-C5-C6	-7.40	116.40	124.48
43	A	410	BCR	C15-C14-C13	-7.35	116.97	127.28
32	R	317	LUT	C27-C28-C29	-7.34	110.55	126.32
31	R	303	CLA	O2D-CGD-CBD	7.31	124.01	111.23
32	G	615	LUT	C31-C30-C29	-7.26	117.09	127.28
43	z	101	BCR	C11-C10-C9	-7.26	117.10	127.28
43	t	101	BCR	C15-C16-C17	-7.25	108.68	123.52
43	C	615	BCR	C8-C9-C10	7.12	130.21	119.01
31	R	306	CLA	O2D-CGD-CBD	7.02	123.49	111.23
30	s	302	CHL	C1B-CHB-C4A	7.01	125.83	121.32
30	q	309	CHL	C1B-CHB-C4A	6.94	125.79	121.32
43	C	615	BCR	C10-C11-C12	-6.92	103.16	123.20
43	d	406	BCR	C10-C11-C12	-6.92	103.16	123.20
30	R	310	CHL	C1B-CHB-C4A	6.84	125.72	121.32
43	c	615	BCR	C15-C14-C13	-6.81	117.73	127.28
43	C	615	BCR	C12-C13-C14	6.77	129.66	119.01
35	g	315	RRX	C11-C10-C9	-6.67	117.92	127.28
30	p	601	CHL	C1B-CHB-C4A	6.66	125.61	121.32
32	g	316	LUT	C31-C30-C29	-6.66	117.94	127.28
43	H	101	BCR	C11-C10-C9	-6.65	117.95	127.28
43	c	614	BCR	C16-C17-C18	-6.64	117.97	127.28
43	B	619	BCR	C11-C10-C9	-6.62	118.00	127.28
35	g	315	RRX	C15-C14-C13	-6.60	118.02	127.28
32	Y	316	LUT	C11-C10-C9	-6.60	118.03	127.28
43	a	410	BCR	C24-C23-C22	-6.58	116.50	126.23
32	R	317	LUT	C30-C31-C32	-6.58	104.15	123.20
30	s	309	CHL	C1B-CHB-C4A	6.57	125.55	121.32
43	c	615	BCR	C1-C6-C5	-6.54	113.70	122.64
43	a	410	BCR	C20-C21-C22	-6.51	118.15	127.28
43	Z	101	BCR	C7-C8-C9	-6.48	116.65	126.23
30	S	302	CHL	C1B-CHB-C4A	6.45	125.47	121.32
30	y	605	CHL	C1B-CHB-C4A	6.41	125.45	121.32
30	9	310	CHL	C1B-CHB-C4A	6.40	125.44	121.32
43	d	406	BCR	C8-C9-C10	6.40	129.07	119.01
32	2	615	LUT	C30-C31-C32	-6.40	104.67	123.20
32	p	617	LUT	C21-C26-C27	-6.37	105.50	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	605	CHL	C1B-CHB-C4A	6.36	125.42	121.32
43	T	101	BCR	C33-C5-C6	-6.35	117.56	124.48
32	4	616	LUT	C11-C10-C9	-6.34	118.38	127.28
43	C	615	BCR	C11-C10-C9	6.34	136.17	127.28
43	t	101	BCR	C27-C26-C25	-6.34	114.14	122.70
43	t	101	BCR	C20-C21-C22	-6.34	118.39	127.28
31	3	316	CLA	CMD-C2D-C1D	6.33	135.88	124.73
35	q	317	RRX	C15-C14-C13	-6.33	118.40	127.28
32	p	617	LUT	C27-C28-C29	-6.32	112.73	126.32
32	3	318	LUT	C15-C14-C13	-6.31	118.43	127.28
31	B	604	CLA	O2D-CGD-CBD	6.31	122.26	111.23
30	3	308	CHL	C1B-CHB-C4A	6.31	125.38	121.32
43	Z	101	BCR	C11-C10-C9	-6.30	118.44	127.28
30	S	309	CHL	C1B-CHB-C4A	6.30	125.38	121.32
43	C	615	BCR	C1-C6-C5	-6.29	114.04	122.64
31	p	614	CLA	CMD-C2D-C1D	6.27	135.77	124.73
35	q	317	RRX	C1-C6-C5	-6.27	114.07	122.64
30	S	308	CHL	C1B-CHB-C4A	6.26	125.35	121.32
32	p	616	LUT	C27-C28-C29	-6.23	112.92	126.32
31	s	306	CLA	O2D-CGD-CBD	6.23	122.11	111.23
31	5	615	CLA	CMD-C2D-C1D	6.22	135.68	124.73
43	B	618	BCR	C15-C14-C13	-6.21	118.56	127.28
35	4	615	RRX	C20-C21-C22	-6.20	118.58	127.28
43	B	619	BCR	C15-C14-C13	-6.19	118.60	127.28
43	V	101	BCR	C16-C17-C18	-6.18	118.61	127.28
43	b	620	BCR	C7-C8-C9	-6.18	117.09	126.23
35	9	317	RRX	C20-C21-C22	-6.16	118.64	127.28
31	C	605	CLA	O2D-CGD-CBD	6.16	122.00	111.23
30	Y	306	CHL	C1B-CHB-C4A	6.16	125.29	121.32
35	G	614	RRX	C20-C21-C22	-6.16	118.64	127.28
30	g	302	CHL	C1B-CHB-C4A	6.16	125.28	121.32
43	b	618	BCR	C38-C26-C25	-6.14	117.78	124.48
32	2	615	LUT	C27-C28-C29	-6.13	113.14	126.32
43	C	614	BCR	C38-C26-C25	-6.12	117.81	124.48
37	r	318	XAT	C31-C30-C29	-6.11	118.71	127.28
31	5	614	CLA	O2D-CGD-CBD	6.09	121.87	111.23
35	2	614	RRX	C20-C21-C22	-6.09	118.74	127.28
31	B	606	CLA	O2D-CGD-CBD	6.09	121.87	111.23
30	0	606	CHL	C1B-CHB-C4A	6.08	125.24	121.32
31	1	604	CLA	O2D-CGD-CBD	6.08	121.86	111.23
30	q	303	CHL	C1B-CHB-C4A	6.07	125.23	121.32
31	S	313	CLA	O2D-CGD-CBD	6.07	121.84	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	A	410	BCR	C38-C26-C25	-6.07	117.87	124.48
43	B	617	BCR	C4-C5-C6	-6.06	114.51	122.70
31	c	612	CLA	O2D-CGD-CBD	6.06	121.83	111.23
31	R	312	CLA	CMD-C2D-C1D	6.00	135.29	124.73
30	r	309	CHL	C1B-CHB-C4A	5.96	125.16	121.32
32	R	317	LUT	C21-C26-C27	-5.96	105.98	112.83
43	b	618	BCR	C33-C5-C6	-5.95	117.99	124.48
43	C	614	BCR	C11-C10-C9	-5.95	118.94	127.28
43	d	406	BCR	C38-C26-C25	-5.94	118.00	124.48
43	b	618	BCR	C27-C26-C25	-5.93	114.69	122.70
43	v	101	BCR	C16-C17-C18	-5.92	118.98	127.28
31	q	312	CLA	CMD-C2D-C1D	5.92	135.15	124.73
31	S	304	CLA	C4A-NA-C1A	5.91	109.38	106.68
31	a	406	CLA	C1-C2-C3	-5.91	116.51	126.20
30	p	608	CHL	C1B-CHB-C4A	5.91	125.12	121.32
43	T	101	BCR	C7-C8-C9	-5.90	117.51	126.23
35	q	317	RRX	C20-C21-C22	-5.90	119.01	127.28
32	S	318	LUT	C35-C34-C33	-5.89	119.02	127.28
43	C	615	BCR	C33-C5-C6	-5.89	118.06	124.48
31	8	603	CLA	CMD-C2D-C1D	5.89	135.09	124.73
31	7	313	CLA	O2D-CGD-CBD	5.88	121.50	111.23
43	h	101	BCR	C11-C10-C9	-5.88	119.04	127.28
31	D	404	CLA	O2D-CGD-CBD	5.88	121.50	111.23
31	1	610	CLA	CMD-C2D-C1D	5.87	135.07	124.73
43	t	101	BCR	C11-C12-C13	-5.86	110.28	126.36
31	7	305	CLA	CMD-C2D-C1D	5.86	135.04	124.73
32	9	318	LUT	C31-C30-C29	-5.84	119.08	127.28
32	g	316	LUT	C11-C10-C9	-5.83	119.09	127.28
30	4	601	CHL	C1B-CHB-C4A	5.83	125.07	121.32
31	c	607	CLA	O2D-CGD-CBD	5.83	121.41	111.23
31	C	603	CLA	C1-C2-C3	-5.82	116.66	126.20
31	b	603	CLA	CAA-C2A-C3A	-5.82	97.27	113.00
30	R	309	CHL	C1B-CHB-C4A	5.82	125.07	121.32
43	d	406	BCR	C24-C23-C22	-5.81	117.64	126.23
30	2	601	CHL	C1B-CHB-C4A	5.80	125.06	121.32
32	2	615	LUT	C28-C29-C30	5.80	128.13	119.01
31	R	306	CLA	CMD-C2D-C1D	5.80	134.94	124.73
30	4	606	CHL	C1B-CHB-C4A	5.80	125.05	121.32
31	S	315	CLA	CMD-C2D-C1D	5.79	134.92	124.73
31	C	607	CLA	O2D-CGD-CBD	5.77	121.32	111.23
43	v	101	BCR	C38-C26-C25	-5.77	118.19	124.48
31	d	401	CLA	CMD-C2D-C1D	5.77	134.88	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	613	CLA	CMD-C2D-C1D	5.77	134.88	124.73
43	b	619	BCR	C20-C21-C22	-5.76	119.19	127.28
30	s	308	CHL	C1B-CHB-C4A	5.76	125.03	121.32
31	C	603	CLA	CMD-C2D-C1D	5.75	134.86	124.73
31	B	616	CLA	O2D-CGD-CBD	5.75	121.29	111.23
32	7	317	LUT	C7-C8-C9	-5.75	117.73	126.23
31	7	304	CLA	CMD-C2D-C1D	5.75	134.85	124.73
31	b	607	CLA	CMD-C2D-C1D	5.75	134.85	124.73
31	y	612	CLA	O2D-CGD-CBD	5.75	121.28	111.23
31	4	614	CLA	CMD-C2D-C1D	5.74	134.84	124.73
31	0	604	CLA	O2D-CGD-CBD	5.74	121.27	111.23
31	r	316	CLA	CMD-C2D-C1D	5.74	134.84	124.73
43	b	620	BCR	C11-C10-C9	-5.74	119.23	127.28
31	B	605	CLA	O2D-CGD-CBD	5.73	121.25	111.23
31	7	313	CLA	CMD-C2D-C1D	5.73	134.82	124.73
31	7	305	CLA	O2D-CGD-CBD	5.73	121.24	111.23
31	0	612	CLA	CMD-C2D-C1D	5.73	134.81	124.73
30	G	623	CHL	C1B-CHB-C4A	5.72	125.00	121.32
37	R	318	XAT	C31-C30-C29	-5.72	119.25	127.28
31	y	610	CLA	CMD-C2D-C1D	5.72	134.80	124.73
44	A	416	PL9	C7-C3-C4	5.72	121.62	116.91
31	B	601	CLA	O2D-CGD-CBD	5.72	121.22	111.23
31	p	604	CLA	CMD-C2D-C1D	5.72	134.79	124.73
31	C	612	CLA	O2D-CGD-CBD	5.72	121.22	111.23
43	V	101	BCR	C33-C5-C6	-5.71	118.25	124.48
31	N	310	CLA	CMD-C2D-C1D	5.71	134.78	124.73
35	4	615	RRX	C24-C23-C22	-5.70	117.80	126.23
31	R	314	CLA	CMD-C2D-C1D	5.70	134.76	124.73
31	1	602	CLA	O2D-CGD-CBD	5.70	121.19	111.23
31	q	316	CLA	CMD-C2D-C1D	5.70	134.76	124.73
31	B	615	CLA	O2D-CGD-CBD	5.70	121.19	111.23
30	G	607	CHL	C1B-CHB-C4A	5.70	124.99	121.32
32	9	318	LUT	C15-C14-C13	-5.70	119.29	127.28
35	9	317	RRX	C24-C23-C22	-5.69	117.81	126.23
30	1	619	CHL	C1B-CHB-C4A	5.69	124.98	121.32
31	b	605	CLA	O2D-CGD-CBD	5.69	121.18	111.23
31	s	315	CLA	CMD-C2D-C1D	5.68	134.74	124.73
35	G	614	RRX	C24-C23-C22	-5.68	117.84	126.23
31	b	607	CLA	O2D-CGD-CBD	5.68	121.15	111.23
31	B	605	CLA	CMD-C2D-C1D	5.67	134.71	124.73
31	5	610	CLA	CMD-C2D-C1D	5.67	134.71	124.73
31	p	610	CLA	CMD-C2D-C1D	5.67	134.71	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	q	312	CLA	O2D-CGD-CBD	5.67	121.13	111.23
31	g	304	CLA	CMD-C2D-C1D	5.66	134.70	124.73
31	g	303	CLA	CMD-C2D-C1D	5.66	134.70	124.73
31	C	610	CLA	O2D-CGD-CBD	5.66	121.13	111.23
31	s	303	CLA	CMD-C2D-C1D	5.66	134.70	124.73
31	G	602	CLA	CMD-C2D-C1D	5.66	134.70	124.73
30	7	308	CHL	C1B-CHB-C4A	5.66	124.96	121.32
30	n	307	CHL	C1B-CHB-C4A	5.66	124.96	121.32
31	r	313	CLA	O2A-C1-C2	5.66	122.45	108.99
31	G	603	CLA	CMD-C2D-C1D	5.65	134.68	124.73
31	C	611	CLA	O2D-CGD-CBD	5.65	121.11	111.23
30	8	606	CHL	C1B-CHB-C4A	5.65	124.96	121.32
31	R	305	CLA	O2D-CGD-CBD	5.65	121.11	111.23
31	y	615	CLA	O2D-CGD-CBD	5.65	121.10	111.23
31	B	602	CLA	O2D-CGD-CBD	5.65	121.10	111.23
35	2	614	RRX	C24-C23-C22	-5.65	117.88	126.23
30	Y	302	CHL	C1B-CHB-C4A	5.64	124.95	121.32
30	1	608	CHL	C1B-CHB-C4A	5.64	124.95	121.32
31	G	613	CLA	CMD-C2D-C1D	5.64	134.66	124.73
31	9	316	CLA	CMD-C2D-C1D	5.64	134.66	124.73
31	A	409	CLA	O2D-CGD-CBD	5.64	121.08	111.23
31	N	315	CLA	CMD-C2D-C1D	5.63	134.65	124.73
31	R	304	CLA	CMD-C2D-C1D	5.63	134.65	124.73
31	7	311	CLA	CMD-C2D-C1D	5.63	134.65	124.73
32	g	316	LUT	C35-C34-C33	-5.63	119.39	127.28
43	c	615	BCR	C11-C10-C9	-5.63	119.39	127.28
31	R	316	CLA	CMD-C2D-C1D	5.62	134.63	124.73
31	6	304	CLA	CMD-C2D-C1D	5.62	134.63	124.73
31	q	304	CLA	CMD-C2D-C1D	5.62	134.62	124.73
43	h	101	BCR	C15-C14-C13	-5.62	119.40	127.28
30	2	607	CHL	C1B-CHB-C4A	5.62	124.94	121.32
43	b	619	BCR	C16-C17-C18	-5.62	119.40	127.28
43	C	615	BCR	C4-C5-C6	-5.61	115.12	122.70
31	C	602	CLA	O2D-CGD-CBD	5.61	121.04	111.23
31	r	304	CLA	CMD-C2D-C1D	5.61	134.61	124.73
31	s	306	CLA	CMD-C2D-C1D	5.61	134.61	124.73
31	9	312	CLA	CMD-C2D-C1D	5.61	134.61	124.73
31	B	604	CLA	CMD-C2D-C1D	5.61	134.61	124.73
31	s	313	CLA	O2D-CGD-CBD	5.61	121.04	111.23
30	7	306	CHL	C1B-CHB-C4A	5.61	124.93	121.32
31	a	409	CLA	O2D-CGD-CBD	5.61	121.03	111.23
31	9	305	CLA	CMD-C2D-C1D	5.60	134.60	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	603	CLA	CMD-C2D-C1D	5.60	134.60	124.73
31	6	303	CLA	CMD-C2D-C1D	5.60	134.59	124.73
30	y	601	CHL	C1B-CHB-C4A	5.60	124.93	121.32
31	d	405	CLA	O2D-CGD-CBD	5.60	121.02	111.23
35	g	315	RRX	C20-C21-C22	-5.60	119.43	127.28
31	4	610	CLA	CMD-C2D-C1D	5.60	134.59	124.73
31	2	609	CLA	CMD-C2D-C1D	5.60	134.58	124.73
31	6	311	CLA	CMD-C2D-C1D	5.59	134.58	124.73
31	y	615	CLA	CMD-C2D-C1D	5.59	134.58	124.73
43	v	101	BCR	C33-C5-C6	-5.59	118.39	124.48
30	1	607	CHL	C1B-CHB-C4A	5.59	124.92	121.32
31	g	312	CLA	CMD-C2D-C1D	5.58	134.56	124.73
31	r	306	CLA	O2D-CGD-CBD	5.58	120.99	111.23
31	B	606	CLA	CMD-C2D-C1D	5.58	134.56	124.73
31	3	304	CLA	CMD-C2D-C1D	5.58	134.55	124.73
30	9	303	CHL	C1B-CHB-C4A	5.58	124.91	121.32
31	c	601	CLA	CMD-C2D-C1D	5.58	134.55	124.73
31	6	315	CLA	CMD-C2D-C1D	5.57	134.54	124.73
31	r	312	CLA	CMD-C2D-C1D	5.57	134.54	124.73
31	B	602	CLA	CAA-C2A-C3A	-5.57	97.96	113.00
31	p	603	CLA	CMD-C2D-C1D	5.56	134.53	124.73
31	n	316	CLA	CMD-C2D-C1D	5.56	134.53	124.73
43	C	614	BCR	C27-C26-C25	-5.56	115.19	122.70
31	4	602	CLA	CMD-C2D-C1D	5.56	134.52	124.73
31	q	314	CLA	CMD-C2D-C1D	5.56	134.52	124.73
31	1	614	CLA	CMD-C2D-C1D	5.56	134.52	124.73
31	p	615	CLA	CMD-C2D-C1D	5.56	134.52	124.73
31	c	603	CLA	C1-C2-C3	-5.56	117.09	126.20
30	6	310	CHL	C1B-CHB-C4A	5.56	124.90	121.32
31	2	602	CLA	CMD-C2D-C1D	5.55	134.51	124.73
31	b	602	CLA	CMD-C2D-C1D	5.55	134.51	124.73
31	R	315	CLA	CMD-C2D-C1D	5.55	134.51	124.73
31	6	305	CLA	CMD-C2D-C1D	5.55	134.50	124.73
31	N	303	CLA	CMD-C2D-C1D	5.55	134.50	124.73
31	b	603	CLA	O2D-CGD-CBD	5.55	120.93	111.23
43	H	101	BCR	C7-C8-C9	-5.55	118.03	126.23
32	R	317	LUT	C11-C10-C9	-5.54	119.50	127.28
30	6	302	CHL	C1B-CHB-C4A	5.54	124.89	121.32
31	G	604	CLA	CMD-C2D-C1D	5.54	134.49	124.73
32	S	318	LUT	C31-C30-C29	-5.54	119.50	127.28
31	p	603	CLA	O2D-CGD-CBD	5.54	120.92	111.23
31	b	602	CLA	O2D-CGD-CBD	5.54	120.92	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	g	314	CLA	CMD-C2D-C1D	5.54	134.49	124.73
31	8	614	CLA	CMD-C2D-C1D	5.54	134.48	124.73
31	A	406	CLA	CMD-C2D-C1D	5.54	134.48	124.73
31	c	609	CLA	O2D-CGD-CBD	5.54	120.91	111.23
31	3	313	CLA	CMD-C2D-C1D	5.54	134.48	124.73
31	S	303	CLA	CMD-C2D-C1D	5.54	134.48	124.73
31	S	306	CLA	CMD-C2D-C1D	5.53	134.47	124.73
31	b	608	CLA	CMD-C2D-C1D	5.53	134.47	124.73
32	y	616	LUT	C21-C26-C27	-5.53	106.46	112.83
30	p	605	CHL	C1B-CHB-C4A	5.53	124.88	121.32
31	p	612	CLA	CMD-C2D-C1D	5.53	134.47	124.73
31	p	613	CLA	O2D-CGD-CBD	5.53	120.90	111.23
31	6	314	CLA	CMD-C2D-C1D	5.53	134.47	124.73
31	5	603	CLA	CMD-C2D-C1D	5.53	134.47	124.73
31	q	305	CLA	CMD-C2D-C1D	5.53	134.46	124.73
31	n	303	CLA	CMD-C2D-C1D	5.53	134.46	124.73
31	b	615	CLA	CMD-C2D-C1D	5.53	134.46	124.73
31	c	603	CLA	CMD-C2D-C1D	5.53	134.46	124.73
32	7	317	LUT	C11-C10-C9	-5.53	119.53	127.28
30	r	310	CHL	C1B-CHB-C4A	5.52	124.88	121.32
31	Y	310	CLA	CMD-C2D-C1D	5.52	134.46	124.73
31	R	316	CLA	O2D-CGD-CBD	5.52	120.89	111.23
31	N	321	CLA	CMD-C2D-C1D	5.52	134.45	124.73
31	r	315	CLA	O2D-CGD-CBD	5.52	120.88	111.23
31	C	604	CLA	CMD-C2D-C1D	5.52	134.45	124.73
32	N	317	LUT	C11-C10-C9	-5.52	119.54	127.28
31	3	306	CLA	CMD-C2D-C1D	5.52	134.45	124.73
31	6	313	CLA	CMD-C2D-C1D	5.52	134.44	124.73
43	C	614	BCR	C7-C8-C9	-5.52	118.08	126.23
31	2	604	CLA	CMD-C2D-C1D	5.51	134.44	124.73
31	Y	304	CLA	CMD-C2D-C1D	5.51	134.44	124.73
31	9	306	CLA	CMD-C2D-C1D	5.51	134.44	124.73
31	B	612	CLA	O2D-CGD-CBD	5.51	120.86	111.23
37	R	318	XAT	C38-C25-C24	5.51	120.43	114.24
37	r	318	XAT	C38-C25-C24	5.51	120.43	114.24
31	8	609	CLA	CMD-C2D-C1D	5.51	134.43	124.73
31	G	611	CLA	O2D-CGD-CBD	5.51	120.86	111.23
32	N	316	LUT	C7-C8-C9	-5.51	118.09	126.23
31	Y	305	CLA	CMD-C2D-C1D	5.51	134.43	124.73
31	4	604	CLA	CMD-C2D-C1D	5.51	134.42	124.73
32	5	616	LUT	C18-C5-C6	-5.51	118.48	124.48
31	r	316	CLA	O2D-CGD-CBD	5.50	120.85	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	610	CLA	O2D-CGD-CBD	5.50	120.85	111.23
31	0	614	CLA	CMD-C2D-C1D	5.50	134.42	124.73
31	Y	303	CLA	CMD-C2D-C1D	5.50	134.42	124.73
31	y	614	CLA	CMD-C2D-C1D	5.50	134.42	124.73
31	7	303	CLA	CMD-C2D-C1D	5.50	134.42	124.73
32	Y	315	LUT	C26-C27-C28	-5.50	116.02	124.58
31	S	316	CLA	CMD-C2D-C1D	5.50	134.41	124.73
47	e	102	HEM	CHC-C4B-NB	5.50	130.34	124.42
31	y	603	CLA	CMD-C2D-C1D	5.50	134.41	124.73
31	7	316	CLA	O2D-CGD-CBD	5.50	120.84	111.23
31	5	602	CLA	CMD-C2D-C1D	5.50	134.41	124.73
31	8	602	CLA	CMD-C2D-C1D	5.50	134.41	124.73
31	R	307	CLA	O2D-CGD-CBD	5.49	120.84	111.23
35	q	317	RRX	C33-C5-C6	-5.49	118.49	124.48
31	s	304	CLA	CMD-C2D-C1D	5.49	134.40	124.73
31	N	313	CLA	CMD-C2D-C1D	5.49	134.40	124.73
31	1	604	CLA	CMD-C2D-C1D	5.49	134.40	124.73
31	1	612	CLA	CMD-C2D-C1D	5.49	134.39	124.73
31	b	617	CLA	O2D-CGD-CBD	5.49	120.83	111.23
31	c	604	CLA	CMD-C2D-C1D	5.49	134.39	124.73
31	n	304	CLA	CMD-C2D-C1D	5.49	134.39	124.73
31	r	315	CLA	CMD-C2D-C1D	5.49	134.39	124.73
31	N	304	CLA	CMD-C2D-C1D	5.49	134.39	124.73
43	d	406	BCR	C33-C5-C6	-5.49	118.50	124.48
31	Y	312	CLA	CMD-C2D-C1D	5.49	134.39	124.73
31	C	606	CLA	O2D-CGD-CBD	5.49	120.82	111.23
31	b	612	CLA	CMD-C2D-C1D	5.48	134.39	124.73
31	n	313	CLA	CMD-C2D-C1D	5.48	134.39	124.73
31	7	316	CLA	CMD-C2D-C1D	5.48	134.38	124.73
31	s	313	CLA	CMD-C2D-C1D	5.48	134.38	124.73
31	9	304	CLA	CMD-C2D-C1D	5.48	134.38	124.73
31	5	615	CLA	O2D-CGD-CBD	5.48	120.81	111.23
31	y	613	CLA	O2D-CGD-CBD	5.48	120.81	111.23
31	C	604	CLA	O2D-CGD-CBD	5.48	120.81	111.23
31	5	614	CLA	CMD-C2D-C1D	5.48	134.38	124.73
31	B	615	CLA	CMD-C2D-C1D	5.48	134.37	124.73
31	G	612	CLA	CMD-C2D-C1D	5.48	134.37	124.73
31	7	315	CLA	CMD-C2D-C1D	5.47	134.37	124.73
31	C	607	CLA	CMD-C2D-C1D	5.47	134.37	124.73
31	R	303	CLA	O2A-C1-C2	5.47	122.01	108.99
31	8	611	CLA	CMD-C2D-C1D	5.47	134.36	124.73
31	n	311	CLA	CMD-C2D-C1D	5.47	134.36	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	N	312	CLA	CMD-C2D-C1D	5.47	134.36	124.73
31	c	609	CLA	CMD-C2D-C1D	5.46	134.35	124.73
31	5	612	CLA	CMD-C2D-C1D	5.46	134.34	124.73
31	c	604	CLA	O2D-CGD-CBD	5.46	120.77	111.23
31	5	604	CLA	CMD-C2D-C1D	5.46	134.34	124.73
31	c	605	CLA	O2D-CGD-CBD	5.46	120.77	111.23
43	z	101	BCR	C24-C23-C22	-5.46	118.16	126.23
31	0	602	CLA	CMD-C2D-C1D	5.46	134.34	124.73
30	y	607	CHL	C1B-CHB-C4A	5.46	124.83	121.32
31	9	313	CLA	O2D-CGD-CBD	5.45	120.76	111.23
31	3	315	CLA	CMD-C2D-C1D	5.45	134.33	124.73
31	3	311	CLA	CMD-C2D-C1D	5.45	134.33	124.73
31	r	305	CLA	CMD-C2D-C1D	5.45	134.33	124.73
31	y	602	CLA	CMD-C2D-C1D	5.45	134.33	124.73
31	c	610	CLA	CMD-C2D-C1D	5.45	134.32	124.73
31	G	613	CLA	O2D-CGD-CBD	5.45	120.76	111.23
31	R	315	CLA	O2D-CGD-CBD	5.45	120.76	111.23
35	2	614	RRX	C11-C10-C9	-5.45	119.64	127.28
31	9	315	CLA	CMD-C2D-C1D	5.44	134.32	124.73
31	b	606	CLA	CMD-C2D-C1D	5.44	134.31	124.73
31	p	604	CLA	O2D-CGD-CBD	5.44	120.75	111.23
31	0	603	CLA	CMD-C2D-C1D	5.44	134.31	124.73
31	0	615	CLA	CMD-C2D-C1D	5.44	134.31	124.73
31	B	614	CLA	CMD-C2D-C1D	5.44	134.30	124.73
31	0	613	CLA	CMD-C2D-C1D	5.44	134.30	124.73
31	A	405	CLA	CMD-C2D-C1D	5.43	134.30	124.73
31	g	313	CLA	CMD-C2D-C1D	5.43	134.29	124.73
31	b	606	CLA	O2D-CGD-CBD	5.43	120.72	111.23
31	4	603	CLA	CMD-C2D-C1D	5.43	134.29	124.73
31	r	314	CLA	CMD-C2D-C1D	5.43	134.28	124.73
31	b	604	CLA	CMD-C2D-C1D	5.43	134.28	124.73
30	4	608	CHL	C1B-CHB-C4A	5.43	124.81	121.32
31	S	304	CLA	CMD-C2D-C1D	5.42	134.28	124.73
31	b	616	CLA	O2D-CGD-CBD	5.42	120.71	111.23
31	g	305	CLA	CMD-C2D-C1D	5.42	134.28	124.73
32	2	615	LUT	C38-C25-C24	-5.42	110.53	123.36
31	4	613	CLA	CMD-C2D-C1D	5.42	134.27	124.73
31	b	614	CLA	CMD-C2D-C1D	5.42	134.27	124.73
31	c	607	CLA	CMD-C2D-C1D	5.42	134.27	124.73
31	Y	314	CLA	CMD-C2D-C1D	5.42	134.27	124.73
31	s	310	CLA	CMD-C2D-C1D	5.42	134.27	124.73
31	R	313	CLA	O2A-C1-C2	5.41	121.88	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	305	CLA	CMD-C2D-C1D	5.41	134.26	124.73
43	B	617	BCR	C38-C26-C25	-5.41	118.58	124.48
31	r	305	CLA	O2D-CGD-CBD	5.41	120.69	111.23
31	4	612	CLA	O2D-CGD-CBD	5.41	120.69	111.23
31	S	310	CLA	CMD-C2D-C1D	5.41	134.25	124.73
31	N	305	CLA	CMD-C2D-C1D	5.41	134.25	124.73
31	0	610	CLA	CMD-C2D-C1D	5.41	134.25	124.73
31	c	603	CLA	O2D-CGD-CBD	5.41	120.68	111.23
35	q	317	RRX	C38-C26-C25	-5.41	118.58	124.48
31	c	602	CLA	O2D-CGD-CBD	5.41	120.68	111.23
31	B	601	CLA	CMD-C2D-C1D	5.40	134.24	124.73
31	b	611	CLA	CMD-C2D-C1D	5.40	134.24	124.73
31	y	604	CLA	CMD-C2D-C1D	5.40	134.23	124.73
31	8	604	CLA	CMD-C2D-C1D	5.40	134.23	124.73
31	3	314	CLA	CMD-C2D-C1D	5.40	134.23	124.73
31	r	314	CLA	O2A-C1-C2	5.40	121.83	108.99
31	n	305	CLA	CMD-C2D-C1D	5.39	134.23	124.73
31	S	313	CLA	CMD-C2D-C1D	5.39	134.22	124.73
31	s	316	CLA	CMD-C2D-C1D	5.39	134.22	124.73
35	g	315	RRX	C30-C25-C26	-5.39	115.27	122.64
31	A	409	CLA	CMD-C2D-C1D	5.39	134.22	124.73
31	a	409	CLA	CMD-C2D-C1D	5.39	134.22	124.73
30	5	601	CHL	C1B-CHB-C4A	5.39	124.79	121.32
31	g	314	CLA	O2D-CGD-CBD	5.39	120.65	111.23
31	C	610	CLA	CMD-C2D-C1D	5.39	134.22	124.73
31	Y	312	CLA	O2D-CGD-CBD	5.39	120.64	111.23
31	B	613	CLA	CMD-C2D-C1D	5.38	134.21	124.73
31	A	407	CLA	CMD-C2D-C1D	5.38	134.21	124.73
47	E	101	HEM	CHC-C4B-NB	5.38	130.22	124.42
31	a	406	CLA	CMD-C2D-C1D	5.38	134.21	124.73
30	G	606	CHL	C1B-CHB-C4A	5.38	124.78	121.32
31	s	311	CLA	CMD-C2D-C1D	5.38	134.20	124.73
31	s	311	CLA	O2D-CGD-CBD	5.38	120.63	111.23
36	2	616	NEX	C38-C25-C24	5.38	120.28	114.24
31	p	615	CLA	O2D-CGD-CBD	5.38	120.63	111.23
31	3	311	CLA	O2D-CGD-CBD	5.37	120.62	111.23
30	8	605	CHL	C1B-CHB-C4A	5.37	124.78	121.32
43	Z	101	BCR	C24-C23-C22	-5.37	118.29	126.23
31	B	610	CLA	CMD-C2D-C1D	5.37	134.19	124.73
32	2	615	LUT	C31-C30-C29	5.37	134.81	127.28
30	6	307	CHL	C1B-CHB-C4A	5.37	124.78	121.32
31	6	316	CLA	CMD-C2D-C1D	5.36	134.17	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	A	410	BCR	C16-C17-C18	-5.36	119.76	127.28
30	G	601	CHL	C1B-CHB-C4A	5.36	124.77	121.32
31	B	611	CLA	CMD-C2D-C1D	5.36	134.17	124.73
31	C	611	CLA	CMD-C2D-C1D	5.36	134.17	124.73
31	3	305	CLA	CMD-C2D-C1D	5.36	134.16	124.73
31	g	311	CLA	O2D-CGD-CBD	5.35	120.59	111.23
31	s	312	CLA	O2D-CGD-CBD	5.35	120.58	111.23
30	4	605	CHL	C1B-CHB-C4A	5.35	124.77	121.32
31	d	401	CLA	O2D-CGD-CBD	5.35	120.58	111.23
31	S	311	CLA	CMD-C2D-C1D	5.35	134.15	124.73
31	S	315	CLA	O2D-CGD-CBD	5.35	120.58	111.23
30	n	306	CHL	C1B-CHB-C4A	5.35	124.76	121.32
31	1	611	CLA	CMD-C2D-C1D	5.35	134.15	124.73
31	s	305	CLA	CMD-C2D-C1D	5.35	134.15	124.73
31	q	313	CLA	O2D-CGD-CBD	5.35	120.58	111.23
31	b	610	CLA	O2D-CGD-CBD	5.35	120.58	111.23
31	b	616	CLA	CMD-C2D-C1D	5.35	134.14	124.73
30	9	307	CHL	C1B-CHB-C4A	5.35	124.76	121.32
31	0	604	CLA	CMD-C2D-C1D	5.35	134.14	124.73
31	8	612	CLA	CMD-C2D-C1D	5.35	134.14	124.73
31	n	314	CLA	CMD-C2D-C1D	5.35	134.14	124.73
31	q	315	CLA	O2D-CGD-CBD	5.34	120.56	111.23
31	2	611	CLA	CMD-C2D-C1D	5.34	134.13	124.73
31	B	609	CLA	CMD-C2D-C1D	5.34	134.12	124.73
31	0	603	CLA	O2D-CGD-CBD	5.33	120.55	111.23
43	B	619	BCR	C16-C17-C18	-5.33	119.80	127.28
35	G	614	RRX	C15-C14-C13	-5.33	119.80	127.28
31	N	311	CLA	O2D-CGD-CBD	5.33	120.55	111.23
31	6	305	CLA	O2D-CGD-CBD	5.33	120.55	111.23
31	2	609	CLA	O2D-CGD-CBD	5.33	120.55	111.23
43	c	614	BCR	C15-C14-C13	-5.33	119.81	127.28
31	A	407	CLA	O2D-CGD-CBD	5.32	120.54	111.23
43	z	101	BCR	C7-C8-C9	-5.32	118.36	126.23
35	4	615	RRX	C15-C14-C13	-5.32	119.81	127.28
31	C	601	CLA	O2D-CGD-CBD	5.32	120.53	111.23
31	N	305	CLA	O2D-CGD-CBD	5.32	120.53	111.23
31	S	304	CLA	O2D-CGD-CBD	5.32	120.53	111.23
31	3	314	CLA	O2D-CGD-CBD	5.32	120.53	111.23
31	s	314	CLA	CMD-C2D-C1D	5.32	134.09	124.73
31	p	612	CLA	O2D-CGD-CBD	5.32	120.53	111.23
31	c	611	CLA	CMD-C2D-C1D	5.32	134.09	124.73
31	C	601	CLA	CMD-C2D-C1D	5.32	134.09	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	602	CLA	CMD-C2D-C1D	5.32	134.09	124.73
31	9	313	CLA	CMD-C2D-C1D	5.32	134.09	124.73
30	5	607	CHL	C1B-CHB-C4A	5.31	124.74	121.32
31	C	603	CLA	O2D-CGD-CBD	5.31	120.52	111.23
31	6	304	CLA	O2D-CGD-CBD	5.31	120.52	111.23
31	d	405	CLA	CMD-C2D-C1D	5.31	134.08	124.73
31	4	612	CLA	CMD-C2D-C1D	5.31	134.08	124.73
31	D	404	CLA	CMD-C2D-C1D	5.31	134.08	124.73
31	4	611	CLA	CMD-C2D-C1D	5.31	134.07	124.73
31	G	609	CLA	CMD-C2D-C1D	5.31	134.07	124.73
31	g	310	CLA	CMD-C2D-C1D	5.31	134.07	124.73
31	4	604	CLA	C1-C2-C3	-5.30	117.51	126.20
31	d	404	CLA	CMD-C2D-C1D	5.30	134.07	124.73
31	8	611	CLA	O2D-CGD-CBD	5.30	120.50	111.23
31	r	307	CLA	O2D-CGD-CBD	5.30	120.50	111.23
30	2	605	CHL	C1B-CHB-C4A	5.30	124.73	121.32
31	8	604	CLA	O2D-CGD-CBD	5.30	120.50	111.23
31	C	606	CLA	CMD-C2D-C1D	5.30	134.07	124.73
30	q	311	CHL	C1B-CHB-C4A	5.30	124.73	121.32
32	1	616	LUT	C26-C27-C28	-5.30	116.33	124.58
32	5	617	LUT	C15-C14-C13	-5.30	119.85	127.28
35	9	317	RRX	C15-C14-C13	-5.30	119.85	127.28
31	r	306	CLA	CMD-C2D-C1D	5.29	134.05	124.73
31	b	613	CLA	O2D-CGD-CBD	5.29	120.48	111.23
31	2	613	CLA	O2D-CGD-CBD	5.29	120.48	111.23
32	N	317	LUT	C7-C8-C9	-5.29	118.41	126.23
31	n	315	CLA	CMD-C2D-C1D	5.29	134.04	124.73
31	A	405	CLA	C1-C2-C3	-5.29	117.53	126.20
31	c	613	CLA	O2D-CGD-CBD	5.29	120.47	111.23
31	2	610	CLA	CMD-C2D-C1D	5.29	134.04	124.73
31	8	613	CLA	CMD-C2D-C1D	5.28	134.03	124.73
36	5	618	NEX	C38-C25-C24	5.28	120.18	114.24
31	A	407	CLA	O2A-C1-C2	5.28	121.56	108.99
31	B	607	CLA	O2D-CGD-CBD	5.28	120.47	111.23
31	0	613	CLA	O2D-CGD-CBD	5.28	120.47	111.23
31	0	612	CLA	O2D-CGD-CBD	5.28	120.46	111.23
31	b	603	CLA	CMD-C2D-C1D	5.28	134.03	124.73
31	6	312	CLA	O2D-CGD-CBD	5.28	120.46	111.23
31	s	315	CLA	O2D-CGD-CBD	5.28	120.46	111.23
31	2	612	CLA	CMD-C2D-C1D	5.28	134.02	124.73
31	B	609	CLA	O2D-CGD-CBD	5.28	120.45	111.23
31	n	313	CLA	O2D-CGD-CBD	5.28	120.45	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	613	CLA	CMD-C2D-C1D	5.27	134.02	124.73
31	Y	303	CLA	O2D-CGD-CBD	5.27	120.45	111.23
31	5	610	CLA	O2D-CGD-CBD	5.27	120.44	111.23
31	5	612	CLA	O2D-CGD-CBD	5.27	120.44	111.23
31	G	611	CLA	CMD-C2D-C1D	5.27	134.01	124.73
32	4	616	LUT	C15-C14-C13	-5.27	119.89	127.28
31	S	314	CLA	CMD-C2D-C1D	5.27	134.01	124.73
43	b	619	BCR	C15-C14-C13	-5.27	119.89	127.28
30	6	308	CHL	C1B-CHB-C4A	5.27	124.71	121.32
31	7	314	CLA	CMD-C2D-C1D	5.26	134.00	124.73
31	c	606	CLA	O2D-CGD-CBD	5.26	120.43	111.23
31	9	306	CLA	O2D-CGD-CBD	5.26	120.43	111.23
31	q	306	CLA	CMD-C2D-C1D	5.26	133.99	124.73
31	3	312	CLA	O2D-CGD-CBD	5.26	120.43	111.23
31	7	312	CLA	CMD-C2D-C1D	5.26	133.99	124.73
31	q	305	CLA	O2D-CGD-CBD	5.26	120.42	111.23
31	S	316	CLA	O2D-CGD-CBD	5.26	120.42	111.23
31	B	602	CLA	CMD-C2D-C1D	5.26	133.99	124.73
31	b	611	CLA	O2D-CGD-CBD	5.26	120.42	111.23
31	c	605	CLA	CMD-C2D-C1D	5.25	133.98	124.73
30	Y	301	CHL	C1B-CHB-C4A	5.25	124.70	121.32
31	B	608	CLA	O2D-CGD-CBD	5.25	120.41	111.23
31	C	609	CLA	O2D-CGD-CBD	5.25	120.41	111.23
43	C	614	BCR	C15-C14-C13	-5.25	119.92	127.28
31	r	311	CLA	CMD-C2D-C1D	5.25	133.97	124.73
31	Y	311	CLA	O2D-CGD-CBD	5.25	120.40	111.23
43	t	101	BCR	C38-C26-C25	-5.24	118.76	124.48
32	s	317	LUT	C35-C34-C33	-5.24	119.93	127.28
31	R	303	CLA	CMD-C2D-C1D	5.24	133.95	124.73
31	3	306	CLA	O2D-CGD-CBD	5.24	120.39	111.23
31	3	315	CLA	O2D-CGD-CBD	5.24	120.39	111.23
31	8	610	CLA	O2A-C1-C2	5.24	121.45	108.99
31	n	312	CLA	O2A-C1-C2	5.24	121.45	108.99
31	R	311	CLA	CMD-C2D-C1D	5.24	133.95	124.73
37	2	619	XAT	C15-C14-C13	-5.23	119.94	127.28
31	B	603	CLA	CMD-C2D-C1D	5.23	133.94	124.73
31	b	617	CLA	CMD-C2D-C1D	5.23	133.94	124.73
31	n	305	CLA	O2D-CGD-CBD	5.23	120.38	111.23
35	2	614	RRX	C15-C14-C13	-5.23	119.94	127.28
32	R	317	LUT	C28-C29-C30	5.23	127.23	119.01
32	y	616	LUT	C26-C27-C28	-5.23	116.44	124.58
31	n	312	CLA	O2D-CGD-CBD	5.23	120.37	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	1	612	CLA	O2D-CGD-CBD	5.23	120.37	111.23
46	d	403	BCT	O2-C-O1	5.23	133.04	119.68
31	s	313	CLA	C1-C2-C3	-5.23	117.64	126.20
31	c	610	CLA	O2D-CGD-CBD	5.22	120.36	111.23
32	G	615	LUT	C35-C15-C14	-5.22	112.83	123.52
31	D	403	CLA	CMD-C2D-C1D	5.22	133.93	124.73
37	4	619	XAT	C15-C14-C13	-5.22	119.95	127.28
31	N	311	CLA	CMD-C2D-C1D	5.22	133.92	124.73
31	8	610	CLA	O2D-CGD-CBD	5.22	120.36	111.23
37	G	620	XAT	C15-C14-C13	-5.22	119.96	127.28
31	y	603	CLA	O2D-CGD-CBD	5.22	120.35	111.23
31	Y	304	CLA	O2D-CGD-CBD	5.22	120.35	111.23
31	c	601	CLA	O2D-CGD-CBD	5.22	120.35	111.23
31	y	614	CLA	O2D-CGD-CBD	5.22	120.35	111.23
31	3	301	CLA	C1-C2-C3	-5.22	117.65	126.20
31	Y	313	CLA	O2D-CGD-CBD	5.21	120.35	111.23
31	9	314	CLA	CMD-C2D-C1D	5.21	133.91	124.73
31	y	604	CLA	O2D-CGD-CBD	5.21	120.34	111.23
32	6	317	LUT	C35-C34-C33	-5.21	119.97	127.28
31	G	609	CLA	O2D-CGD-CBD	5.21	120.34	111.23
37	g	321	XAT	C15-C14-C13	-5.21	119.97	127.28
36	q	319	NEX	C27-C28-C29	-5.21	117.44	125.53
43	c	614	BCR	C33-C5-C6	-5.21	118.80	124.48
37	q	321	XAT	C15-C14-C13	-5.21	119.97	127.28
31	B	603	CLA	O2D-CGD-CBD	5.21	120.33	111.23
31	0	611	CLA	O2D-CGD-CBD	5.21	120.33	111.23
31	b	612	CLA	O2D-CGD-CBD	5.21	120.33	111.23
31	5	611	CLA	O2D-CGD-CBD	5.20	120.33	111.23
31	S	312	CLA	O2D-CGD-CBD	5.20	120.33	111.23
35	G	614	RRX	C11-C10-C9	-5.20	119.98	127.28
30	0	607	CHL	C1B-CHB-C4A	5.20	124.67	121.32
36	R	319	NEX	C38-C25-C24	5.19	120.08	114.24
31	N	312	CLA	O2D-CGD-CBD	5.19	120.31	111.23
31	Y	313	CLA	CMD-C2D-C1D	5.19	133.87	124.73
31	6	311	CLA	O2D-CGD-CBD	5.19	120.30	111.23
31	1	602	CLA	CMD-C2D-C1D	5.19	133.87	124.73
31	Y	305	CLA	O2D-CGD-CBD	5.19	120.30	111.23
31	g	314	CLA	O2A-C1-C2	5.19	121.34	108.99
35	9	317	RRX	C11-C10-C9	-5.19	120.00	127.28
37	9	322	XAT	C15-C14-C13	-5.19	120.00	127.28
31	N	311	CLA	O2A-C1-C2	5.19	121.33	108.99
42	A	408	PHO	C4D-CHA-CBD	-5.18	105.97	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	h	101	BCR	C7-C8-C9	-5.18	118.57	126.23
30	N	307	CHL	C1B-CHB-C4A	5.18	124.66	121.32
43	z	101	BCR	C33-C5-C6	-5.18	118.83	124.48
31	b	613	CLA	CMD-C2D-C1D	5.18	133.85	124.73
43	C	615	BCR	C16-C17-C18	-5.18	120.02	127.28
31	7	314	CLA	O2D-CGD-CBD	5.18	120.28	111.23
31	r	307	CLA	CMD-C2D-C1D	5.18	133.85	124.73
31	4	604	CLA	O2D-CGD-CBD	5.18	120.28	111.23
32	p	616	LUT	C11-C10-C9	-5.18	120.02	127.28
32	9	318	LUT	C35-C34-C33	-5.17	120.02	127.28
31	s	303	CLA	O2D-CGD-CBD	5.17	120.27	111.23
31	4	614	CLA	O2D-CGD-CBD	5.17	120.27	111.23
31	1	603	CLA	O2D-CGD-CBD	5.17	120.27	111.23
31	G	602	CLA	O2D-CGD-CBD	5.17	120.27	111.23
31	5	611	CLA	CMD-C2D-C1D	5.17	133.82	124.73
31	0	602	CLA	O2D-CGD-CBD	5.17	120.26	111.23
31	d	401	CLA	O2A-C1-C2	5.17	121.28	108.99
31	4	603	CLA	O2D-CGD-CBD	5.16	120.26	111.23
31	y	611	CLA	O2D-CGD-CBD	5.16	120.26	111.23
35	4	615	RRX	C11-C10-C9	-5.16	120.04	127.28
31	y	602	CLA	O2D-CGD-CBD	5.16	120.25	111.23
32	p	616	LUT	C32-C33-C34	5.16	127.13	119.01
31	b	604	CLA	O2D-CGD-CBD	5.16	120.25	111.23
31	2	604	CLA	O2D-CGD-CBD	5.16	120.25	111.23
31	6	315	CLA	O2D-CGD-CBD	5.16	120.25	111.23
31	1	611	CLA	O2D-CGD-CBD	5.16	120.25	111.23
31	3	301	CLA	CMD-C2D-C1D	5.16	133.81	124.73
32	q	318	LUT	C7-C8-C9	-5.16	118.61	126.23
31	B	611	CLA	O2D-CGD-CBD	5.16	120.24	111.23
31	r	303	CLA	CMD-C2D-C1D	5.16	133.81	124.73
30	y	606	CHL	C1B-CHB-C4A	5.16	124.64	121.32
31	y	612	CLA	CMD-C2D-C1D	5.15	133.81	124.73
30	N	301	CHL	C1B-CHB-C4A	5.15	124.64	121.32
31	N	313	CLA	O2D-CGD-CBD	5.15	120.24	111.23
31	5	604	CLA	O2D-CGD-CBD	5.15	120.24	111.23
43	B	617	BCR	C33-C5-C6	-5.15	118.86	124.48
31	b	605	CLA	CMD-C2D-C1D	5.15	133.79	124.73
36	8	617	NEX	C38-C25-C24	5.15	120.02	114.24
32	0	617	LUT	C7-C8-C9	-5.15	118.62	126.23
31	B	604	CLA	C1-C2-C3	-5.15	117.77	126.20
32	R	317	LUT	C32-C33-C34	5.14	127.10	119.01
31	q	306	CLA	O2D-CGD-CBD	5.14	120.22	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	303	CLA	O2D-CGD-CBD	5.14	120.22	111.23
31	p	602	CLA	CMD-C2D-C1D	5.14	133.78	124.73
32	q	318	LUT	C11-C10-C9	-5.14	120.07	127.28
32	s	318	LUT	C26-C27-C28	-5.14	116.58	124.58
43	V	101	BCR	C27-C26-C25	-5.14	115.76	122.70
32	6	318	LUT	C7-C8-C9	-5.14	118.63	126.23
31	a	407	CLA	CMD-C2D-C1D	5.14	133.78	124.73
31	N	303	CLA	O2D-CGD-CBD	5.14	120.21	111.23
30	g	308	CHL	C1B-CHB-C4A	5.14	124.63	121.32
43	D	405	BCR	C8-C9-C10	5.14	127.09	119.01
31	1	613	CLA	O2D-CGD-CBD	5.14	120.21	111.23
31	q	313	CLA	CMD-C2D-C1D	5.13	133.77	124.73
31	S	305	CLA	O2D-CGD-CBD	5.13	120.20	111.23
31	r	304	CLA	O2D-CGD-CBD	5.13	120.20	111.23
31	p	602	CLA	O2D-CGD-CBD	5.13	120.20	111.23
31	N	315	CLA	O2D-CGD-CBD	5.13	120.20	111.23
31	5	613	CLA	O2D-CGD-CBD	5.13	120.20	111.23
31	R	304	CLA	O2D-CGD-CBD	5.13	120.19	111.23
31	S	311	CLA	O2D-CGD-CBD	5.13	120.19	111.23
31	c	611	CLA	O2D-CGD-CBD	5.13	120.19	111.23
43	c	615	BCR	C33-C5-C6	-5.13	118.89	124.48
42	D	401	PHO	C4D-CHA-CBD	-5.13	106.00	108.45
31	n	303	CLA	O2D-CGD-CBD	5.13	120.19	111.23
36	r	301	NEX	C38-C25-C24	5.13	120.00	114.24
31	3	301	CLA	O2D-CGD-CBD	5.12	120.19	111.23
31	8	612	CLA	O2D-CGD-CBD	5.12	120.19	111.23
31	c	608	CLA	CMD-C2D-C1D	5.12	133.75	124.73
43	c	615	BCR	C4-C5-C6	-5.12	115.78	122.70
31	c	613	CLA	CMD-C2D-C1D	5.12	133.75	124.73
31	B	614	CLA	O2D-CGD-CBD	5.12	120.18	111.23
31	1	603	CLA	CMD-C2D-C1D	5.11	133.73	124.73
31	s	316	CLA	O2D-CGD-CBD	5.11	120.17	111.23
31	n	314	CLA	O2D-CGD-CBD	5.11	120.17	111.23
36	r	319	NEX	C38-C25-C24	5.11	119.98	114.24
31	C	609	CLA	CMD-C2D-C1D	5.11	133.72	124.73
43	t	101	BCR	C20-C19-C18	-5.11	112.36	126.36
31	b	608	CLA	O2D-CGD-CBD	5.11	120.16	111.23
30	8	601	CHL	C1B-CHB-C4A	5.10	124.61	121.32
43	C	614	BCR	C33-C5-C6	-5.10	118.92	124.48
31	b	609	CLA	O2D-CGD-CBD	5.10	120.14	111.23
31	8	610	CLA	CMD-C2D-C1D	5.10	133.71	124.73
31	B	612	CLA	CMD-C2D-C1D	5.10	133.70	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	304	CLA	O2D-CGD-CBD	5.10	120.14	111.23
30	Y	308	CHL	C1B-CHB-C4A	5.10	124.60	121.32
31	R	311	CLA	O2D-CGD-CBD	5.09	120.14	111.23
43	A	410	BCR	C20-C21-C22	-5.09	120.13	127.28
30	G	605	CHL	C1B-CHB-C4A	5.09	124.60	121.32
31	6	303	CLA	O2D-CGD-CBD	5.09	120.13	111.23
31	4	610	CLA	O2D-CGD-CBD	5.09	120.13	111.23
31	s	305	CLA	O2D-CGD-CBD	5.09	120.13	111.23
31	1	610	CLA	O2D-CGD-CBD	5.09	120.13	111.23
31	p	611	CLA	O2D-CGD-CBD	5.09	120.13	111.23
31	9	316	CLA	O2D-CGD-CBD	5.09	120.12	111.23
31	p	611	CLA	CMD-C2D-C1D	5.09	133.69	124.73
43	h	101	BCR	C24-C23-C22	-5.09	118.71	126.23
31	C	613	CLA	CMD-C2D-C1D	5.09	133.69	124.73
31	S	312	CLA	CMD-C2D-C1D	5.09	133.69	124.73
31	g	304	CLA	O2D-CGD-CBD	5.09	120.12	111.23
43	Z	101	BCR	C33-C5-C6	-5.08	118.94	124.48
31	S	303	CLA	O2D-CGD-CBD	5.08	120.12	111.23
31	n	312	CLA	CMD-C2D-C1D	5.08	133.68	124.73
31	p	614	CLA	O2D-CGD-CBD	5.08	120.11	111.23
31	s	304	CLA	O2D-CGD-CBD	5.08	120.11	111.23
31	D	403	CLA	O2D-CGD-CBD	5.08	120.11	111.23
30	n	302	CHL	C1B-CHB-C4A	5.08	124.59	121.32
31	7	312	CLA	O2D-CGD-CBD	5.08	120.10	111.23
31	b	610	CLA	CMD-C2D-C1D	5.07	133.66	124.73
31	B	601	CLA	O2A-C1-C2	5.07	121.06	108.99
43	c	615	BCR	C38-C26-C25	-5.07	118.95	124.48
31	0	610	CLA	O2D-CGD-CBD	5.07	120.09	111.23
31	6	316	CLA	O2D-CGD-CBD	5.07	120.08	111.23
35	g	315	RRX	C38-C26-C25	-5.06	118.96	124.48
31	b	602	CLA	O2A-C1-C2	5.06	121.04	108.99
31	g	310	CLA	O2D-CGD-CBD	5.06	120.08	111.23
31	n	316	CLA	O2D-CGD-CBD	5.06	120.08	111.23
31	9	305	CLA	O2D-CGD-CBD	5.06	120.08	111.23
31	N	314	CLA	CMD-C2D-C1D	5.06	133.64	124.73
31	C	608	CLA	CMD-C2D-C1D	5.06	133.64	124.73
30	9	309	CHL	C1C-CHC-C4B	5.06	134.16	116.07
31	R	305	CLA	CMD-C2D-C1D	5.05	133.63	124.73
31	c	602	CLA	CMD-C2D-C1D	5.05	133.63	124.73
31	8	602	CLA	O2D-CGD-CBD	5.05	120.06	111.23
43	b	618	BCR	C16-C17-C18	-5.05	120.20	127.28
43	d	406	BCR	C12-C13-C14	5.05	126.95	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	p	610	CLA	O2D-CGD-CBD	5.04	120.05	111.23
32	S	317	LUT	C35-C34-C33	-5.04	120.21	127.28
37	9	322	XAT	C38-C25-C24	5.04	119.91	114.24
31	4	611	CLA	O2D-CGD-CBD	5.04	120.04	111.23
37	g	321	XAT	C38-C25-C24	5.04	119.90	114.24
32	4	616	LUT	C7-C8-C9	-5.04	118.78	126.23
31	G	604	CLA	O2D-CGD-CBD	5.04	120.04	111.23
31	G	610	CLA	O2D-CGD-CBD	5.04	120.04	111.23
31	C	608	CLA	O2D-CGD-CBD	5.04	120.04	111.23
31	s	312	CLA	CMD-C2D-C1D	5.04	133.60	124.73
43	c	615	BCR	C27-C26-C25	-5.03	115.90	122.70
31	n	304	CLA	O2D-CGD-CBD	5.03	120.03	111.23
31	r	303	CLA	O2A-C1-C2	5.03	120.97	108.99
31	0	611	CLA	CMD-C2D-C1D	5.03	133.59	124.73
31	C	606	CLA	C1-C2-C3	-5.03	117.95	126.20
31	G	612	CLA	O2D-CGD-CBD	5.03	120.02	111.23
31	N	304	CLA	O2D-CGD-CBD	5.03	120.02	111.23
37	2	619	XAT	C38-C25-C24	5.03	119.89	114.24
31	y	611	CLA	CMD-C2D-C1D	5.03	133.58	124.73
30	7	309	CHL	C1B-CHB-C4A	5.03	124.56	121.32
37	G	620	XAT	C38-C25-C24	5.03	119.89	114.24
43	a	410	BCR	C38-C26-C25	-5.02	119.01	124.48
31	p	613	CLA	CMD-C2D-C1D	5.02	133.57	124.73
32	q	318	LUT	C15-C14-C13	-5.02	120.24	127.28
35	q	317	RRX	C16-C17-C18	-5.02	120.24	127.28
30	1	601	CHL	C1C-CHC-C4B	5.02	134.02	116.07
37	4	619	XAT	C38-C25-C24	5.02	119.88	114.24
32	5	616	LUT	C35-C34-C33	-5.02	120.24	127.28
31	B	607	CLA	CMD-C2D-C1D	5.02	133.56	124.73
31	9	304	CLA	O2D-CGD-CBD	5.01	120.00	111.23
31	G	613	CLA	O2A-C1-C2	5.01	120.92	108.99
31	5	603	CLA	O2D-CGD-CBD	5.01	119.99	111.23
31	S	306	CLA	O2D-CGD-CBD	5.01	119.99	111.23
43	V	101	BCR	C38-C26-C25	-5.01	119.02	124.48
44	a	414	PL9	C7-C3-C4	5.01	121.03	116.91
32	p	616	LUT	C30-C31-C32	-5.01	108.69	123.20
31	N	310	CLA	O2D-CGD-CBD	5.01	119.98	111.23
32	r	317	LUT	C26-C27-C28	-5.01	116.79	124.58
31	r	312	CLA	O2D-CGD-CBD	5.01	119.98	111.23
32	g	316	LUT	C15-C14-C13	-5.00	120.26	127.28
31	C	613	CLA	O2D-CGD-CBD	5.00	119.98	111.23
32	0	616	LUT	C35-C34-C33	-5.00	120.26	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	q	321	XAT	C38-C25-C24	5.00	119.86	114.24
31	2	610	CLA	O2D-CGD-CBD	5.00	119.97	111.23
31	8	609	CLA	O2D-CGD-CBD	5.00	119.97	111.23
31	g	305	CLA	O2D-CGD-CBD	5.00	119.97	111.23
31	g	313	CLA	O2D-CGD-CBD	5.00	119.96	111.23
30	n	309	CHL	C1B-CHB-C4A	4.99	124.54	121.32
31	3	313	CLA	O2D-CGD-CBD	4.99	119.96	111.23
31	d	404	CLA	O2D-CGD-CBD	4.99	119.96	111.23
36	g	317	NEX	C38-C25-C24	4.99	119.85	114.24
31	g	312	CLA	O2D-CGD-CBD	4.99	119.96	111.23
31	9	315	CLA	O2D-CGD-CBD	4.99	119.95	111.23
31	0	615	CLA	O2D-CGD-CBD	4.99	119.95	111.23
31	3	304	CLA	O2D-CGD-CBD	4.99	119.95	111.23
31	4	613	CLA	O2D-CGD-CBD	4.98	119.94	111.23
43	B	619	BCR	C38-C26-C25	-4.98	119.05	124.48
31	q	316	CLA	O2D-CGD-CBD	4.98	119.94	111.23
30	3	307	CHL	C1B-CHB-C4A	4.98	124.53	121.32
31	b	615	CLA	O2D-CGD-CBD	4.98	119.93	111.23
31	6	312	CLA	CMD-C2D-C1D	4.98	133.49	124.73
31	s	310	CLA	O2D-CGD-CBD	4.98	119.93	111.23
32	3	317	LUT	C35-C34-C33	-4.98	120.30	127.28
31	n	315	CLA	O2A-C1-C2	4.97	120.82	108.99
31	a	407	CLA	O2D-CGD-CBD	4.97	119.92	111.23
32	y	617	LUT	C26-C27-C28	-4.97	116.85	124.58
30	N	308	CHL	C1B-CHB-C4A	4.97	124.52	121.32
30	q	310	CHL	C1C-CHC-C4B	4.96	133.82	116.07
31	R	312	CLA	O2D-CGD-CBD	4.96	119.90	111.23
43	A	410	BCR	C33-C5-C6	-4.96	119.07	124.48
32	s	318	LUT	C35-C34-C33	-4.96	120.33	127.28
30	3	310	CHL	C1B-CHB-C4A	4.96	124.51	121.32
30	Y	309	CHL	C1C-CHC-C4B	4.95	133.80	116.07
30	n	301	CHL	C1B-CHB-C4A	4.95	124.51	121.32
36	6	319	NEX	C38-C25-C24	4.95	119.81	114.24
31	8	614	CLA	O2D-CGD-CBD	4.95	119.89	111.23
31	0	614	CLA	O2D-CGD-CBD	4.95	119.89	111.23
36	4	617	NEX	C38-C25-C24	4.95	119.80	114.24
32	2	615	LUT	C32-C33-C34	4.95	126.80	119.01
30	N	306	CHL	C1B-CHB-C4A	4.95	124.51	121.32
31	r	313	CLA	CMD-C2D-C1D	4.95	133.44	124.73
31	R	314	CLA	O2D-CGD-CBD	4.95	119.88	111.23
31	8	613	CLA	O2A-C1-C2	4.95	120.76	108.99
31	6	314	CLA	O2D-CGD-CBD	4.94	119.87	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	1	613	CLA	CMD-C2D-C1D	4.94	133.43	124.73
30	1	606	CHL	C1B-CHB-C4A	4.94	124.50	121.32
31	B	607	CLA	C1-C2-C3	-4.94	118.10	126.20
31	r	313	CLA	O2D-CGD-CBD	4.94	119.87	111.23
31	N	314	CLA	O2A-C1-C2	4.94	120.75	108.99
31	3	305	CLA	O2D-CGD-CBD	4.94	119.87	111.23
31	7	315	CLA	O2D-CGD-CBD	4.94	119.86	111.23
32	p	616	LUT	C28-C29-C30	4.94	126.78	119.01
43	b	620	BCR	C15-C14-C13	-4.93	120.36	127.28
30	y	609	CHL	C1C-CHC-C4B	4.93	133.72	116.07
30	q	308	CHL	C1C-CHC-C4B	4.93	133.72	116.07
31	4	602	CLA	O2D-CGD-CBD	4.93	119.85	111.23
30	2	606	CHL	C1B-CHB-C4A	4.93	124.49	121.32
31	S	310	CLA	O2D-CGD-CBD	4.93	119.85	111.23
30	s	307	CHL	C1C-CHC-C4B	4.93	133.70	116.07
36	r	319	NEX	C27-C28-C29	-4.93	117.89	125.53
31	n	311	CLA	O2D-CGD-CBD	4.93	119.84	111.23
31	1	614	CLA	O2D-CGD-CBD	4.92	119.84	111.23
31	c	608	CLA	O2D-CGD-CBD	4.92	119.84	111.23
31	R	313	CLA	CMD-C2D-C1D	4.92	133.40	124.73
30	4	607	CHL	C1C-CHC-C4B	4.92	133.69	116.07
31	R	314	CLA	O2A-C1-C2	4.92	120.70	108.99
36	0	618	NEX	C38-C25-C24	4.92	119.77	114.24
30	S	307	CHL	C1C-CHC-C4B	4.92	133.67	116.07
30	1	605	CHL	C1C-CHC-C4B	4.92	133.67	116.07
30	q	307	CHL	C1B-CHB-C4A	4.92	124.49	121.32
30	N	302	CHL	C1C-CHC-C4B	4.92	133.66	116.07
31	8	603	CLA	O2D-CGD-CBD	4.92	119.82	111.23
30	8	607	CHL	C1B-CHB-C4A	4.91	124.48	121.32
31	B	616	CLA	CMD-C2D-C1D	4.91	133.38	124.73
31	G	610	CLA	CMD-C2D-C1D	4.91	133.37	124.73
31	g	311	CLA	CMD-C2D-C1D	4.91	133.37	124.73
30	3	302	CHL	C1-C2-C3	-4.90	118.16	126.20
31	q	304	CLA	O2D-CGD-CBD	4.90	119.80	111.23
43	a	410	BCR	C15-C14-C13	-4.90	120.40	127.28
32	4	616	LUT	C35-C34-C33	-4.90	120.40	127.28
30	7	302	CHL	C1C-CHC-C4B	4.90	133.60	116.07
32	6	318	LUT	C35-C34-C33	-4.90	120.41	127.28
30	R	308	CHL	C1C-CHC-C4B	4.90	133.59	116.07
32	N	317	LUT	C15-C14-C13	-4.89	120.41	127.28
31	A	406	CLA	O2D-CGD-CBD	4.89	119.79	111.23
31	9	314	CLA	O2D-CGD-CBD	4.89	119.78	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	307	CLA	CMD-C2D-C1D	4.89	133.34	124.73
30	q	307	CHL	C1C-CHC-C4B	4.89	133.57	116.07
37	g	321	XAT	C31-C30-C29	-4.89	120.42	127.28
31	q	314	CLA	O2D-CGD-CBD	4.88	119.77	111.23
37	G	620	XAT	C31-C30-C29	-4.88	120.43	127.28
31	3	312	CLA	CMD-C2D-C1D	4.88	133.33	124.73
30	3	302	CHL	C1C-CHC-C4B	4.88	133.54	116.07
30	7	310	CHL	C1C-CHC-C4B	4.88	133.54	116.07
30	5	606	CHL	C1C-CHC-C4B	4.88	133.54	116.07
30	n	308	CHL	C1C-CHC-C4B	4.88	133.54	116.07
31	Y	314	CLA	O2D-CGD-CBD	4.88	119.76	111.23
31	5	602	CLA	O2D-CGD-CBD	4.88	119.76	111.23
30	n	301	CHL	C1C-CHC-C4B	4.88	133.53	116.07
30	n	310	CHL	C1C-CHC-C4B	4.88	133.53	116.07
32	9	318	LUT	C11-C10-C9	-4.88	120.44	127.28
30	7	321	CHL	C1C-CHC-C4B	4.88	133.52	116.07
37	q	321	XAT	C31-C30-C29	-4.87	120.44	127.28
31	N	321	CLA	O2D-CGD-CBD	4.87	119.75	111.23
43	h	101	BCR	C33-C5-C6	-4.87	119.17	124.48
37	2	619	XAT	C31-C30-C29	-4.87	120.45	127.28
31	b	609	CLA	CMD-C2D-C1D	4.87	133.30	124.73
37	4	619	XAT	C31-C30-C29	-4.87	120.45	127.28
31	6	316	CLA	C1-C2-C3	-4.87	118.22	126.20
30	p	607	CHL	C1C-CHC-C4B	4.87	133.48	116.07
30	9	308	CHL	C1C-CHC-C4B	4.86	133.46	116.07
43	t	101	BCR	C4-C5-C6	-4.86	116.14	122.70
31	6	313	CLA	O2D-CGD-CBD	4.86	119.72	111.23
30	p	609	CHL	C1B-CHB-C4A	4.85	124.44	121.32
30	9	307	CHL	C1C-CHC-C4B	4.85	133.43	116.07
30	3	303	CHL	C1C-CHC-C4B	4.85	133.43	116.07
30	8	608	CHL	C1C-CHC-C4B	4.85	133.42	116.07
30	g	306	CHL	C1C-CHC-C4B	4.85	133.42	116.07
30	5	608	CHL	C1C-CHC-C4B	4.85	133.42	116.07
37	9	322	XAT	C31-C30-C29	-4.85	120.48	127.28
30	0	608	CHL	C1C-CHC-C4B	4.85	133.42	116.07
31	Y	310	CLA	O2D-CGD-CBD	4.85	119.70	111.23
30	1	609	CHL	C1C-CHC-C4B	4.85	133.41	116.07
31	2	603	CLA	O2D-CGD-CBD	4.85	119.70	111.23
30	g	309	CHL	C1C-CHC-C4B	4.85	133.41	116.07
30	r	310	CHL	C1C-CHC-C4B	4.84	133.40	116.07
31	s	314	CLA	O2D-CGD-CBD	4.84	119.70	111.23
31	y	613	CLA	CMD-C2D-C1D	4.84	133.26	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	g	307	CHL	C1B-CHB-C4A	4.84	124.44	121.32
32	1	615	LUT	C26-C27-C28	-4.84	117.04	124.58
43	C	614	BCR	C20-C21-C22	-4.84	120.49	127.28
30	4	605	CHL	C1C-CHC-C4B	4.84	133.37	116.07
30	Y	307	CHL	C1C-CHC-C4B	4.84	133.37	116.07
43	T	101	BCR	C38-C26-C25	-4.83	119.21	124.48
43	C	614	BCR	C4-C5-C6	-4.83	116.17	122.70
43	H	101	BCR	C24-C23-C22	-4.83	119.09	126.23
30	6	309	CHL	C1C-CHC-C4B	4.83	133.35	116.07
30	0	601	CHL	C1C-CHC-C4B	4.83	133.35	116.07
30	8	601	CHL	C1C-CHC-C4B	4.83	133.35	116.07
43	c	614	BCR	C38-C26-C25	-4.83	119.22	124.48
30	2	605	CHL	C1C-CHC-C4B	4.83	133.34	116.07
36	8	617	NEX	C27-C28-C29	-4.83	118.04	125.53
30	0	605	CHL	C1C-CHC-C4B	4.83	133.34	116.07
32	4	616	LUT	C18-C5-C6	-4.82	119.22	124.48
34	9	301	LMG	C1-O6-C5	-4.82	104.30	113.72
30	n	302	CHL	C1C-CHC-C4B	4.82	133.32	116.07
35	4	615	RRX	C1-C6-C5	-4.82	116.05	122.64
32	1	615	LUT	C18-C5-C6	-4.82	119.23	124.48
35	9	317	RRX	C1-C6-C5	-4.82	116.06	122.64
30	N	301	CHL	C1C-CHC-C4B	4.82	133.30	116.07
30	5	601	CHL	C1C-CHC-C4B	4.82	133.30	116.07
30	6	306	CHL	C1C-CHC-C4B	4.82	133.30	116.07
30	0	605	CHL	C1-O2A-CGA	4.81	128.30	116.65
30	7	307	CHL	C1C-CHC-C4B	4.81	133.29	116.07
35	G	614	RRX	C1-C6-C5	-4.81	116.06	122.64
31	A	405	CLA	O2D-CGD-CBD	4.81	119.64	111.23
31	Y	311	CLA	CMD-C2D-C1D	4.81	133.20	124.73
43	a	410	BCR	C33-C5-C6	-4.81	119.24	124.48
34	m	102	LMG	O7-C10-C11	4.81	121.88	111.48
30	0	609	CHL	C1C-CHC-C4B	4.80	133.26	116.07
30	G	605	CHL	C1C-CHC-C4B	4.80	133.26	116.07
43	H	101	BCR	C16-C17-C18	-4.80	120.54	127.28
30	N	309	CHL	C1C-CHC-C4B	4.80	133.25	116.07
32	N	316	LUT	C18-C5-C6	-4.80	119.25	124.48
43	B	617	BCR	C15-C14-C13	-4.80	120.55	127.28
36	9	319	NEX	C38-C25-C24	4.80	119.63	114.24
30	p	606	CHL	C1C-CHC-C4B	4.80	133.24	116.07
31	R	313	CLA	O2D-CGD-CBD	4.80	119.61	111.23
30	0	607	CHL	C1C-CHC-C4B	4.79	133.22	116.07
31	b	614	CLA	O2D-CGD-CBD	4.79	119.61	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	608	CLA	CMD-C2D-C1D	4.79	133.17	124.73
30	y	608	CHL	C1C-CHC-C4B	4.79	133.22	116.07
35	g	315	RRX	C24-C23-C22	-4.79	119.15	126.23
31	7	311	CLA	O2D-CGD-CBD	4.79	119.61	111.23
31	n	315	CLA	O2D-CGD-CBD	4.79	119.61	111.23
30	p	609	CHL	C1C-CHC-C4B	4.79	133.21	116.07
30	3	307	CHL	C1C-CHC-C4B	4.79	133.21	116.07
31	r	314	CLA	O2D-CGD-CBD	4.79	119.60	111.23
30	q	311	CHL	C1C-CHC-C4B	4.79	133.21	116.07
31	C	613	CLA	CAA-C2A-C3A	-4.79	100.06	113.00
43	a	410	BCR	C11-C10-C9	-4.79	120.57	127.28
30	4	609	CHL	C1C-CHC-C4B	4.78	133.19	116.07
30	s	308	CHL	C1C-CHC-C4B	4.78	133.18	116.07
30	g	308	CHL	C1C-CHC-C4B	4.78	133.17	116.07
30	G	608	CHL	C1C-CHC-C4B	4.78	133.17	116.07
31	q	315	CLA	CMD-C2D-C1D	4.78	133.14	124.73
30	N	306	CHL	C1C-CHC-C4B	4.78	133.16	116.07
30	S	309	CHL	C1C-CHC-C4B	4.78	133.16	116.07
30	p	605	CHL	C1C-CHC-C4B	4.77	133.15	116.07
30	Y	301	CHL	C1C-CHC-C4B	4.77	133.15	116.07
30	r	308	CHL	C1C-CHC-C4B	4.77	133.15	116.07
30	8	607	CHL	C1C-CHC-C4B	4.77	133.15	116.07
31	2	612	CLA	O2D-CGD-CBD	4.77	119.57	111.23
30	y	607	CHL	C1C-CHC-C4B	4.77	133.14	116.07
30	7	309	CHL	C1C-CHC-C4B	4.77	133.13	116.07
31	2	602	CLA	O2D-CGD-CBD	4.77	119.56	111.23
30	n	309	CHL	C1C-CHC-C4B	4.77	133.13	116.07
30	2	608	CHL	C1C-CHC-C4B	4.77	133.13	116.07
30	1	607	CHL	C1C-CHC-C4B	4.77	133.13	116.07
31	C	605	CLA	CMD-C2D-C1D	4.77	133.12	124.73
30	N	308	CHL	C1C-CHC-C4B	4.77	133.12	116.07
30	2	606	CHL	C1C-CHC-C4B	4.76	133.12	116.07
30	y	606	CHL	C1C-CHC-C4B	4.76	133.12	116.07
36	9	319	NEX	C27-C28-C29	-4.76	118.15	125.53
30	0	601	CHL	C1B-CHB-C4A	4.76	124.38	121.32
31	s	305	CLA	C1-C2-C3	-4.76	118.40	126.20
30	4	609	CHL	C1B-CHB-C4A	4.76	124.38	121.32
36	g	317	NEX	C27-C28-C29	-4.76	118.15	125.53
32	6	317	LUT	C26-C27-C28	-4.76	117.18	124.58
43	D	405	BCR	C33-C5-C6	-4.75	119.30	124.48
30	5	607	CHL	C1C-CHC-C4B	4.75	133.08	116.07
31	G	603	CLA	O2D-CGD-CBD	4.75	119.54	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	G	601	CHL	C1C-CHC-C4B	4.75	133.07	116.07
36	R	319	NEX	C27-C28-C29	-4.75	118.16	125.53
30	1	606	CHL	C1C-CHC-C4B	4.75	133.07	116.07
30	y	601	CHL	C1C-CHC-C4B	4.75	133.07	116.07
30	Y	308	CHL	C1C-CHC-C4B	4.75	133.06	116.07
30	5	609	CHL	C1B-CHB-C4A	4.75	124.38	121.32
30	6	308	CHL	C1C-CHC-C4B	4.75	133.06	116.07
30	5	609	CHL	C1C-CHC-C4B	4.75	133.06	116.07
30	Y	306	CHL	C1C-CHC-C4B	4.75	133.05	116.07
30	9	311	CHL	C1C-CHC-C4B	4.74	133.04	116.07
32	2	615	LUT	C1-C6-C5	-4.74	116.15	122.64
34	w	203	LMG	O7-C10-C11	4.74	121.74	111.48
30	7	308	CHL	C1C-CHC-C4B	4.74	133.01	116.07
30	4	608	CHL	C1C-CHC-C4B	4.73	133.01	116.07
31	9	312	CLA	O2D-CGD-CBD	4.73	119.51	111.23
30	2	607	CHL	C1C-CHC-C4B	4.73	133.01	116.07
30	6	302	CHL	C1C-CHC-C4B	4.73	133.00	116.07
30	9	303	CHL	C1C-CHC-C4B	4.73	133.00	116.07
35	2	614	RRX	C1-C6-C5	-4.73	116.17	122.64
30	g	307	CHL	C1C-CHC-C4B	4.73	133.00	116.07
32	n	317	LUT	C35-C34-C33	-4.73	120.65	127.28
30	6	307	CHL	C1C-CHC-C4B	4.73	132.99	116.07
43	b	619	BCR	C33-C5-C6	-4.73	119.33	124.48
30	3	308	CHL	C1C-CHC-C4B	4.72	132.98	116.07
32	0	616	LUT	C26-C27-C28	-4.72	117.23	124.58
30	G	623	CHL	C1C-CHC-C4B	4.72	132.96	116.07
37	r	318	XAT	C15-C14-C13	-4.72	120.66	127.28
30	3	310	CHL	C1C-CHC-C4B	4.72	132.95	116.07
30	3	303	CHL	C1B-CHB-C4A	4.72	124.36	121.32
30	8	605	CHL	C1C-CHC-C4B	4.72	132.94	116.07
43	A	410	BCR	C11-C10-C9	-4.71	120.67	127.28
30	G	606	CHL	C1C-CHC-C4B	4.71	132.94	116.07
31	B	613	CLA	O2D-CGD-CBD	4.71	119.47	111.23
43	d	406	BCR	C34-C9-C10	-4.71	115.18	122.82
32	8	615	LUT	C35-C34-C33	-4.71	120.67	127.28
30	p	608	CHL	C1C-CHC-C4B	4.71	132.93	116.07
30	n	306	CHL	C1C-CHC-C4B	4.71	132.93	116.07
31	a	406	CLA	O2D-CGD-CBD	4.71	119.46	111.23
32	3	318	LUT	C1-C6-C5	-4.71	116.20	122.64
35	q	317	RRX	C24-C23-C22	-4.71	119.27	126.23
37	R	318	XAT	C15-C14-C13	-4.70	120.68	127.28
32	6	317	LUT	C18-C5-C6	-4.70	119.36	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	S	302	CHL	C1C-CHC-C4B	4.70	132.89	116.07
30	r	309	CHL	C1C-CHC-C4B	4.70	132.89	116.07
30	r	308	CHL	C1B-CHB-C4A	4.70	124.35	121.32
43	B	618	BCR	C33-C5-C6	-4.70	119.36	124.48
43	B	618	BCR	C11-C10-C9	-4.70	120.69	127.28
31	C	612	CLA	CMD-C2D-C1D	4.70	133.00	124.73
31	2	611	CLA	O2D-CGD-CBD	4.70	119.44	111.23
30	Y	302	CHL	C1C-CHC-C4B	4.70	132.87	116.07
31	c	612	CLA	CMD-C2D-C1D	4.69	133.00	124.73
31	3	316	CLA	O2D-CGD-CBD	4.69	119.43	111.23
34	n	322	LMG	O7-C10-C11	4.69	121.63	111.48
30	n	307	CHL	C1C-CHC-C4B	4.69	132.85	116.07
30	4	601	CHL	C1C-CHC-C4B	4.69	132.85	116.07
30	1	608	CHL	C1C-CHC-C4B	4.69	132.85	116.07
32	8	616	LUT	C35-C34-C33	-4.69	120.70	127.28
31	8	613	CLA	O2D-CGD-CBD	4.69	119.42	111.23
30	6	310	CHL	C1C-CHC-C4B	4.69	132.84	116.07
30	G	607	CHL	C1C-CHC-C4B	4.69	132.84	116.07
30	8	606	CHL	C1C-CHC-C4B	4.68	132.83	116.07
31	y	610	CLA	O2D-CGD-CBD	4.68	119.42	111.23
32	7	317	LUT	C26-C27-C28	-4.68	117.29	124.58
43	T	101	BCR	C20-C21-C22	-4.68	120.72	127.28
30	s	302	CHL	C1C-CHC-C4B	4.68	132.81	116.07
30	p	606	CHL	C1B-CHB-C4A	4.68	124.33	121.32
32	Y	316	LUT	C7-C8-C9	-4.68	119.31	126.23
30	1	619	CHL	C1C-CHC-C4B	4.68	132.81	116.07
34	b	622	LMG	O7-C10-C11	4.68	121.60	111.48
31	R	305	CLA	C1-C2-C3	-4.68	118.54	126.20
30	q	303	CHL	C1C-CHC-C4B	4.67	132.79	116.07
32	p	617	LUT	C35-C15-C14	-4.67	113.96	123.52
32	N	316	LUT	C15-C14-C13	-4.67	120.72	127.28
32	R	317	LUT	C18-C5-C6	-4.67	119.39	124.48
35	2	614	RRX	C16-C17-C18	-4.67	120.73	127.28
31	S	313	CLA	C1-C2-C3	-4.67	118.55	126.20
32	n	318	LUT	C35-C34-C33	-4.67	120.73	127.28
32	p	617	LUT	C30-C31-C32	-4.67	109.67	123.20
30	7	306	CHL	C1C-CHC-C4B	4.67	132.77	116.07
30	2	601	CHL	C1C-CHC-C4B	4.67	132.77	116.07
30	0	606	CHL	C1C-CHC-C4B	4.67	132.76	116.07
30	R	309	CHL	C1C-CHC-C4B	4.66	132.76	116.07
30	N	307	CHL	C1C-CHC-C4B	4.66	132.76	116.07
36	n	319	NEX	C27-C28-C29	-4.66	118.30	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	g	315	RRX	C16-C17-C18	-4.66	120.74	127.28
35	g	315	RRX	C4-C5-C6	-4.66	116.41	122.70
34	w	205	LMG	O7-C10-C11	4.66	121.55	111.48
30	0	608	CHL	C1B-CHB-C4A	4.65	124.32	121.32
30	g	302	CHL	C1C-CHC-C4B	4.65	132.72	116.07
30	5	605	CHL	C1C-CHC-C4B	4.65	132.71	116.07
31	r	311	CLA	O2D-CGD-CBD	4.65	119.36	111.23
30	p	601	CHL	C1C-CHC-C4B	4.65	132.70	116.07
30	6	306	CHL	C1B-CHB-C4A	4.65	124.31	121.32
43	V	101	BCR	C24-C23-C22	-4.65	119.36	126.23
36	y	618	NEX	C38-C25-C24	4.64	119.45	114.24
36	r	301	NEX	C27-C28-C29	-4.64	118.33	125.53
30	s	309	CHL	C1C-CHC-C4B	4.64	132.68	116.07
30	g	306	CHL	C1B-CHB-C4A	4.64	124.31	121.32
32	7	318	LUT	C7-C8-C9	-4.64	119.37	126.23
37	r	318	XAT	C18-C5-C4	4.64	119.45	114.24
36	G	616	NEX	C38-C25-C24	4.63	119.44	114.24
30	9	311	CHL	C1B-CHB-C4A	4.63	124.30	121.32
30	9	310	CHL	C1C-CHC-C4B	4.63	132.64	116.07
32	0	617	LUT	C35-C34-C33	-4.63	120.79	127.28
43	D	405	BCR	C24-C23-C22	-4.63	119.39	126.23
36	2	616	NEX	C27-C28-C29	-4.62	118.35	125.53
32	n	317	LUT	C26-C27-C28	-4.62	117.38	124.58
32	8	615	LUT	C26-C27-C28	-4.62	117.38	124.58
30	7	310	CHL	C1B-CHB-C4A	4.62	124.30	121.32
32	0	616	LUT	C21-C26-C27	-4.62	107.51	112.83
33	z	102	LHG	O7-C7-C8	4.62	121.47	111.48
43	d	406	BCR	C11-C10-C9	4.62	133.76	127.28
32	p	616	LUT	C18-C5-C6	-4.62	119.45	124.48
43	b	618	BCR	C7-C8-C9	-4.61	119.41	126.23
31	S	314	CLA	O2D-CGD-CBD	4.61	119.30	111.23
34	W	201	LMG	O7-C10-C11	4.61	121.46	111.48
30	G	608	CHL	C1B-CHB-C4A	4.61	124.29	121.32
32	p	617	LUT	C1-C6-C5	-4.61	116.34	122.64
30	9	308	CHL	C1B-CHB-C4A	4.61	124.29	121.32
35	g	315	RRX	C1-C6-C5	-4.61	116.34	122.64
31	S	312	CLA	O2A-C1-C2	4.60	125.81	108.11
31	N	314	CLA	O2D-CGD-CBD	4.60	119.27	111.23
36	s	319	NEX	C38-C25-C24	4.60	119.41	114.24
43	B	617	BCR	C7-C8-C9	-4.60	119.44	126.23
43	A	410	BCR	C27-C26-C25	-4.59	116.50	122.70
43	c	614	BCR	C7-C8-C9	-4.59	119.44	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	3	302	CHL	C1B-CHB-C4A	4.59	124.28	121.32
32	7	317	LUT	C15-C14-C13	-4.59	120.84	127.28
35	G	614	RRX	C16-C17-C18	-4.59	120.84	127.28
35	2	614	RRX	C4-C5-C6	-4.59	116.50	122.70
30	2	608	CHL	C1B-CHB-C4A	4.59	124.27	121.32
37	g	321	XAT	C18-C5-C4	4.58	119.39	114.24
34	c	620	LMG	O7-C10-C11	4.58	121.40	111.48
32	3	317	LUT	C18-C5-C6	-4.58	119.48	124.48
30	4	606	CHL	C1C-CHC-C4B	4.58	132.47	116.07
32	p	617	LUT	C11-C10-C9	-4.58	120.86	127.28
30	y	605	CHL	C1C-CHC-C4B	4.58	132.45	116.07
36	Y	317	NEX	C2-C1-C6	4.58	113.66	109.21
31	Y	303	CLA	C1-C2-C3	-4.57	118.70	126.20
32	2	615	LUT	C39-C29-C30	-4.57	115.41	122.82
30	N	309	CHL	C1B-CHB-C4A	4.57	124.26	121.32
35	4	615	RRX	C16-C17-C18	-4.57	120.87	127.28
30	R	310	CHL	C1C-CHC-C4B	4.57	132.43	116.07
30	q	310	CHL	C1B-CHB-C4A	4.57	124.26	121.32
30	y	608	CHL	C1B-CHB-C4A	4.57	124.26	121.32
32	S	317	LUT	C18-C5-C6	-4.57	119.50	124.48
43	z	101	BCR	C20-C21-C22	-4.56	120.88	127.28
43	a	410	BCR	C36-C18-C19	4.56	125.06	118.09
37	G	620	XAT	C18-C5-C4	4.56	119.36	114.24
37	R	318	XAT	C18-C5-C4	4.56	119.36	114.24
30	q	308	CHL	CHA-C1A-C2A	-4.56	122.60	133.31
37	4	619	XAT	C18-C5-C4	4.56	119.36	114.24
36	R	301	NEX	C27-C28-C29	-4.56	118.46	125.53
33	C	623	LHG	O7-C7-C8	4.56	121.34	111.48
43	b	618	BCR	C15-C14-C13	-4.55	120.89	127.28
30	7	307	CHL	C1B-CHB-C4A	4.55	124.25	121.32
34	B	621	LMG	O7-C10-C11	4.55	121.32	111.48
37	q	321	XAT	C18-C5-C4	4.54	119.34	114.24
35	9	317	RRX	C16-C17-C18	-4.54	120.91	127.28
30	6	309	CHL	C1B-CHB-C4A	4.54	124.24	121.32
33	K	102	LHG	O7-C7-C8	4.54	121.30	111.48
32	N	316	LUT	C11-C10-C9	-4.54	120.91	127.28
35	q	317	RRX	C4-C5-C6	-4.54	116.57	122.70
32	9	318	LUT	C18-C5-C6	-4.54	119.53	124.48
36	3	319	NEX	C38-C25-C24	4.53	119.33	114.24
37	9	322	XAT	C18-C5-C4	4.53	119.33	114.24
30	S	308	CHL	C1C-CHC-C4B	4.53	132.27	116.07
32	q	318	LUT	C35-C34-C33	-4.53	120.93	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	C	614	BCR	C16-C17-C18	-4.53	120.93	127.28
31	7	312	CLA	C1-C2-C3	-4.53	118.78	126.20
33	a	415	LHG	O7-C7-C8	4.52	121.26	111.48
36	p	618	NEX	C38-C25-C24	4.52	119.31	114.24
30	n	308	CHL	C1B-CHB-C4A	4.51	124.23	121.32
30	7	321	CHL	C1B-CHB-C4A	4.51	124.23	121.32
37	2	619	XAT	C18-C5-C4	4.51	119.31	114.24
30	8	608	CHL	C1B-CHB-C4A	4.51	124.22	121.32
31	c	606	CLA	CMD-C2D-C1D	4.51	132.66	124.73
34	9	301	LMG	C8-O7-C10	-4.51	107.01	117.80
36	y	618	NEX	C27-C28-C29	-4.50	118.54	125.53
31	b	605	CLA	C1-C2-C3	-4.50	118.83	126.20
31	B	611	CLA	C1-C2-C3	-4.50	118.83	126.20
30	q	309	CHL	C1C-CHC-C4B	4.49	132.13	116.07
32	4	616	LUT	C31-C30-C29	-4.49	120.98	127.28
31	8	604	CLA	C1-C2-C3	-4.49	118.84	126.20
31	y	615	CLA	C1-C2-C3	-4.48	118.85	126.20
32	s	317	LUT	C26-C27-C28	-4.48	117.60	124.58
47	E	101	HEM	CHD-C1D-ND	4.48	129.25	124.42
32	y	617	LUT	C18-C5-C6	-4.48	119.59	124.48
32	Y	315	LUT	C21-C26-C27	-4.48	107.67	112.83
45	c	618	DGD	O2G-C1B-C2B	4.48	121.17	111.48
43	B	617	BCR	C11-C10-C9	-4.48	121.00	127.28
43	z	101	BCR	C15-C14-C13	-4.48	121.00	127.28
31	q	312	CLA	C1B-NB-C4B	4.48	109.45	106.31
43	C	615	BCR	C34-C9-C10	-4.48	115.56	122.82
31	b	615	CLA	C1-C2-C3	-4.47	118.87	126.20
32	9	318	LUT	C7-C8-C9	-4.47	119.62	126.23
32	7	318	LUT	C35-C34-C33	-4.47	121.01	127.28
34	6	321	LMG	O7-C10-C11	4.47	121.15	111.48
32	7	317	LUT	C21-C26-C27	-4.46	107.69	112.83
36	Y	317	NEX	C27-C28-C29	-4.46	118.60	125.53
35	2	614	RRX	C38-C26-C25	-4.46	119.61	124.48
32	q	318	LUT	C1-C6-C5	-4.46	116.54	122.64
43	B	619	BCR	C24-C23-C22	-4.46	119.63	126.23
31	g	303	CLA	O2D-CGD-CBD	4.46	119.03	111.23
32	1	616	LUT	C35-C34-C33	-4.46	121.02	127.28
34	g	320	LMG	O7-C10-C11	4.46	121.12	111.48
36	R	301	NEX	C38-C25-C24	4.46	119.25	114.24
36	n	319	NEX	C38-C25-C24	4.45	119.24	114.24
36	Y	317	NEX	C38-C25-C24	4.45	119.23	114.24
32	s	317	LUT	C18-C5-C6	-4.44	119.64	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	604	CLA	C1-C2-C3	-4.44	118.92	126.20
30	5	608	CHL	C1B-CHB-C4A	4.44	124.18	121.32
32	r	317	LUT	C21-C26-C27	-4.44	107.72	112.83
31	9	306	CLA	C1-C2-C3	-4.44	118.93	126.20
43	h	101	BCR	C20-C21-C22	-4.43	121.06	127.28
30	0	605	CHL	C1B-CHB-C4A	4.43	124.17	121.32
35	G	614	RRX	C38-C26-C25	-4.43	119.65	124.48
34	d	411	LMG	O7-C10-C11	4.43	121.06	111.48
33	t	102	LHG	O7-C7-C8	4.42	121.05	111.48
35	9	317	RRX	C38-C26-C25	-4.42	119.66	124.48
34	B	622	LMG	O7-C10-C11	4.42	121.05	111.48
36	S	319	NEX	C27-C28-C29	-4.42	118.67	125.53
30	3	309	CHL	C1C-CHC-C4B	4.42	131.89	116.07
32	p	617	LUT	C32-C33-C34	4.42	125.96	119.01
36	N	318	NEX	C38-C25-C24	4.42	119.20	114.24
35	4	615	RRX	C38-C26-C25	-4.42	119.67	124.48
32	n	318	LUT	C7-C8-C9	-4.41	119.70	126.23
47	e	102	HEM	CHD-C1D-ND	4.41	129.17	124.42
30	1	609	CHL	C1B-CHB-C4A	4.41	124.16	121.32
43	V	101	BCR	C20-C21-C22	-4.41	121.09	127.28
43	h	101	BCR	C16-C17-C18	-4.41	121.09	127.28
34	C	621	LMG	O7-C10-C11	4.41	121.01	111.48
34	G	622	LMG	O7-C10-C11	4.39	120.98	111.48
32	5	617	LUT	C18-C5-C6	-4.39	119.69	124.48
31	r	315	CLA	O2A-C1-C2	4.39	125.00	108.11
32	p	617	LUT	C28-C29-C30	4.39	125.91	119.01
43	b	620	BCR	C33-C5-C6	-4.39	119.70	124.48
35	2	614	RRX	C33-C5-C6	-4.39	119.70	124.48
30	7	302	CHL	C1B-CHB-C4A	4.38	124.14	121.32
43	b	620	BCR	C16-C17-C18	-4.38	121.13	127.28
43	B	617	BCR	C23-C24-C25	-4.38	115.30	127.00
32	2	615	LUT	C21-C26-C27	-4.38	107.79	112.83
31	4	602	CLA	C1-C2-C3	-4.38	119.03	126.20
32	8	616	LUT	C7-C8-C9	-4.38	119.76	126.23
43	d	406	BCR	C2-C1-C6	4.38	116.80	110.44
31	6	305	CLA	C1-C2-C3	-4.37	119.03	126.20
32	1	615	LUT	C21-C26-C27	-4.37	107.80	112.83
30	N	302	CHL	C1B-CHB-C4A	4.37	124.14	121.32
43	d	406	BCR	C27-C26-C25	-4.37	116.81	122.70
32	3	318	LUT	C18-C5-C6	-4.37	119.72	124.48
33	3	320	LHG	O7-C7-C8	4.37	120.92	111.48
31	y	604	CLA	C1-C2-C3	-4.36	119.05	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	609	CHL	C1B-CHB-C4A	4.36	124.13	121.32
32	G	615	LUT	C18-C5-C6	-4.36	119.73	124.48
32	y	617	LUT	C35-C34-C33	-4.35	121.17	127.28
43	V	101	BCR	C30-C25-C26	-4.35	116.69	122.64
43	t	101	BCR	C8-C9-C10	4.35	125.86	119.01
30	5	606	CHL	C1B-CHB-C4A	4.35	124.12	121.32
31	N	321	CLA	C1-C2-C3	-4.35	119.07	126.20
32	3	318	LUT	C7-C8-C9	-4.35	119.80	126.23
31	S	314	CLA	C1-C2-C3	-4.35	119.08	126.20
43	b	619	BCR	C4-C5-C6	-4.34	116.83	122.70
30	R	308	CHL	C1B-CHB-C4A	4.34	124.12	121.32
32	Y	316	LUT	C15-C14-C13	-4.34	121.19	127.28
31	C	612	CLA	C1-C2-C3	-4.34	119.09	126.20
43	Z	101	BCR	C20-C21-C22	-4.33	121.20	127.28
34	b	624	LMG	O7-C10-C11	4.32	120.83	111.48
30	q	308	CHL	C1A-CHA-C4D	4.32	126.19	118.98
32	8	616	LUT	C26-C27-C28	-4.32	117.86	124.58
30	S	308	CHL	C3D-C4D-CHA	4.32	115.11	108.54
36	N	318	NEX	C27-C28-C29	-4.32	118.83	125.53
30	y	609	CHL	C1B-CHB-C4A	4.31	124.10	121.32
32	R	317	LUT	C39-C29-C30	-4.31	115.83	122.82
30	n	310	CHL	C1B-CHB-C4A	4.30	124.09	121.32
36	s	319	NEX	C17-C1-C6	-4.30	106.62	110.47
32	n	318	LUT	C26-C27-C28	-4.30	117.88	124.58
30	1	605	CHL	CHA-C1A-C2A	-4.30	123.21	133.31
34	a	413	LMG	O7-C10-C11	4.30	120.77	111.48
34	W	203	LMG	O7-C10-C11	4.30	120.77	111.48
32	y	617	LUT	C21-C26-C27	-4.29	107.89	112.83
36	G	616	NEX	C27-C28-C29	-4.29	118.87	125.53
43	c	615	BCR	C16-C17-C18	-4.29	121.26	127.28
32	7	317	LUT	C35-C34-C33	-4.29	121.26	127.28
36	S	319	NEX	C38-C25-C24	4.29	119.06	114.24
32	1	616	LUT	C7-C8-C9	-4.29	119.89	126.23
31	y	602	CLA	C1-C2-C3	-4.29	119.17	126.20
31	3	304	CLA	C1-C2-C3	-4.28	119.18	126.20
34	q	302	LMG	O7-C10-C11	4.28	120.73	111.48
35	9	317	RRX	C4-C5-C6	-4.27	116.93	122.70
32	g	316	LUT	C7-C8-C9	-4.27	119.91	126.23
43	B	619	BCR	C4-C5-C6	-4.27	116.93	122.70
30	9	309	CHL	CHA-C1A-C2A	-4.27	123.28	133.31
32	S	317	LUT	C26-C27-C28	-4.27	117.93	124.58
32	8	615	LUT	C18-C5-C6	-4.27	119.83	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	c	619	DGD	O2G-C1B-C2B	4.27	120.71	111.48
32	S	317	LUT	C7-C8-C9	-4.27	119.92	126.23
43	C	615	BCR	C20-C19-C18	-4.26	114.67	126.36
43	b	618	BCR	C4-C5-C6	-4.26	116.94	122.70
32	n	317	LUT	C18-C5-C6	-4.26	119.83	124.48
33	9	320	LHG	O7-C7-C8	4.26	120.70	111.48
31	C	605	CLA	C1-C2-C3	-4.26	119.22	126.20
43	t	101	BCR	C30-C25-C26	-4.26	116.82	122.64
31	N	305	CLA	C1-C2-C3	-4.26	119.22	126.20
34	S	321	LMG	O7-C10-C11	4.25	120.68	111.48
32	p	616	LUT	C35-C15-C14	-4.25	114.82	123.52
30	6	306	CHL	CHA-C1A-C2A	-4.25	123.33	133.31
33	R	320	LHG	O7-C7-C8	4.25	120.67	111.48
34	w	202	LMG	O7-C10-C11	4.25	120.67	111.48
35	G	614	RRX	C4-C5-C6	-4.25	116.97	122.70
33	s	322	LHG	O7-C7-C8	4.24	120.66	111.48
32	Y	315	LUT	C18-C5-C6	-4.24	119.86	124.48
43	C	615	BCR	C16-C15-C14	4.24	132.20	123.52
43	H	101	BCR	C15-C14-C13	-4.24	121.33	127.28
34	b	601	LMG	O7-C10-C11	4.24	120.65	111.48
32	r	317	LUT	C18-C5-C6	-4.24	119.86	124.48
34	2	618	LMG	O7-C10-C11	4.24	120.65	111.48
35	4	615	RRX	C4-C5-C6	-4.24	116.98	122.70
34	9	301	LMG	O1-C7-C8	-4.24	100.51	110.82
44	A	416	PL9	C7-C3-C2	-4.23	118.41	123.39
43	A	410	BCR	C24-C23-C22	-4.23	119.98	126.23
31	c	612	CLA	C1-C2-C3	-4.22	119.28	126.20
32	N	316	LUT	C35-C34-C33	-4.22	121.36	127.28
43	B	619	BCR	C20-C21-C22	-4.22	121.36	127.28
36	s	319	NEX	C27-C28-C29	-4.22	118.99	125.53
43	c	614	BCR	C11-C12-C13	-4.22	114.80	126.36
34	f	101	LMG	O7-C10-C11	4.21	120.60	111.48
31	n	305	CLA	C1-C2-C3	-4.21	119.30	126.20
30	p	607	CHL	C1B-CHB-C4A	4.21	124.03	121.32
30	Y	307	CHL	C1B-CHB-C4A	4.21	124.03	121.32
34	I	101	LMG	O7-C10-C11	4.20	120.57	111.48
32	7	318	LUT	C26-C27-C28	-4.20	118.04	124.58
32	0	616	LUT	C18-C5-C6	-4.19	119.91	124.48
31	Y	305	CLA	C1-C2-C3	-4.19	119.33	126.20
30	1	601	CHL	CHA-C1A-C2A	-4.19	123.46	133.31
31	B	608	CLA	C1-C2-C3	-4.19	119.33	126.20
48	c	623	LMU	C1B-O1B-C4'	-4.19	108.05	117.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	r	317	LUT	C35-C34-C33	-4.19	121.40	127.28
36	3	319	NEX	C2-C1-C6	4.19	113.28	109.21
32	N	317	LUT	C35-C34-C33	-4.19	121.40	127.28
36	q	319	NEX	C38-C25-C24	4.19	118.94	114.24
43	b	620	BCR	C4-C5-C6	-4.19	117.05	122.70
31	q	313	CLA	C1B-NB-C4B	4.19	109.25	106.31
30	7	309	CHL	CHA-C1A-C2A	-4.18	123.48	133.31
30	1	619	CHL	C1-C2-C3	-4.18	119.35	126.20
31	4	611	CLA	C1B-NB-C4B	4.18	109.25	106.31
30	Y	309	CHL	CHA-C1A-C2A	-4.18	123.49	133.31
30	1	606	CHL	CHA-C1A-C2A	-4.18	123.50	133.31
30	s	307	CHL	CHA-C1A-C2A	-4.18	123.50	133.31
30	g	309	CHL	C1B-CHB-C4A	4.18	124.01	121.32
31	9	312	CLA	O2A-C1-C2	4.18	124.18	108.11
34	Y	319	LMG	O7-C10-C11	4.18	120.51	111.48
31	D	404	CLA	O2A-C1-C2	4.17	124.17	108.11
32	6	318	LUT	C15-C14-C13	-4.17	121.43	127.28
32	R	317	LUT	C35-C15-C14	-4.17	114.98	123.52
31	C	610	CLA	CAA-C2A-C3A	-4.17	101.73	113.00
43	H	101	BCR	C27-C26-C25	-4.17	117.07	122.70
43	H	101	BCR	C4-C5-C6	-4.17	117.07	122.70
43	B	618	BCR	C4-C5-C6	-4.17	117.07	122.70
43	a	410	BCR	C15-C16-C17	-4.16	115.00	123.52
45	C	620	DGD	O2G-C1B-C2B	4.16	120.49	111.48
30	0	607	CHL	CHA-C1A-C2A	-4.16	123.54	133.31
43	Z	101	BCR	C15-C14-C13	-4.16	121.44	127.28
30	S	307	CHL	C1B-CHB-C4A	4.16	124.00	121.32
31	Y	313	CLA	C1-C2-C3	-4.16	119.38	126.20
34	7	320	LMG	O7-C10-C11	4.16	120.48	111.48
32	2	615	LUT	C31-C32-C33	4.15	137.75	126.36
33	p	619	LHG	O7-C7-C8	4.15	120.46	111.48
30	8	607	CHL	CHA-C1A-C2A	-4.15	123.56	133.31
34	J	102	LMG	O7-C10-C11	4.15	120.46	111.48
34	6	322	LMG	O7-C10-C11	4.15	120.46	111.48
34	2	621	LMG	O7-C10-C11	4.15	120.46	111.48
33	A	415	LHG	O7-C7-C8	4.15	120.45	111.48
36	4	617	NEX	C27-C28-C29	-4.15	119.10	125.53
34	Q1	101	LMG	O7-C10-C11	4.14	120.44	111.48
43	b	620	BCR	C24-C23-C22	-4.14	120.11	126.23
33	D	407	LHG	O7-C7-C8	4.14	120.44	111.48
34	G	619	LMG	O7-C10-C11	4.14	120.44	111.48
31	y	612	CLA	C1-C2-C3	-4.14	119.42	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	c	614	BCR	C4-C5-C6	-4.14	117.11	122.70
32	n	318	LUT	C15-C14-C13	-4.14	121.47	127.28
32	N	317	LUT	C1-C6-C5	-4.14	116.98	122.64
32	g	316	LUT	C1-C6-C5	-4.14	116.98	122.64
32	8	616	LUT	C15-C14-C13	-4.14	121.48	127.28
31	s	314	CLA	C1-C2-C3	-4.13	119.43	126.20
43	b	619	BCR	C11-C10-C9	-4.13	121.49	127.28
31	0	614	CLA	C1-C2-C3	-4.13	119.43	126.20
43	B	617	BCR	C16-C17-C18	-4.13	121.49	127.28
30	N	302	CHL	CHA-C1A-C2A	-4.13	123.62	133.31
43	B	618	BCR	C20-C21-C22	-4.13	121.49	127.28
30	5	608	CHL	CHA-C1A-C2A	-4.12	123.63	133.31
31	S	306	CLA	C1-C2-C3	-4.12	120.09	126.76
30	s	308	CHL	C3D-C4D-CHA	4.12	114.80	108.54
31	c	606	CLA	C1-C2-C3	-4.12	119.45	126.20
34	b	629	LMG	O7-C10-C11	4.12	120.38	111.48
43	H	101	BCR	C33-C5-C6	-4.11	119.99	124.48
31	r	311	CLA	O2A-C1-C2	4.11	123.94	108.11
31	C	613	CLA	O2A-C1-C2	4.11	123.94	108.11
31	0	604	CLA	C1-C2-C3	-4.11	119.46	126.20
31	G	612	CLA	C1-C2-C3	-4.11	119.46	126.20
30	9	303	CHL	C1-C2-C3	-4.11	119.46	126.20
30	7	307	CHL	CHA-C1A-C2A	-4.11	123.66	133.31
32	y	617	LUT	C15-C14-C13	-4.11	121.52	127.28
34	7	322	LMG	O7-C10-C11	4.11	120.37	111.48
32	R	317	LUT	C31-C30-C29	4.11	133.04	127.28
34	b	623	LMG	O7-C10-C11	4.10	120.36	111.48
31	B	605	CLA	C1-C2-C3	-4.10	119.47	126.20
34	A	412	LMG	O7-C10-C11	4.10	120.36	111.48
43	v	101	BCR	C27-C26-C25	-4.10	117.16	122.70
34	D	412	LMG	O7-C10-C11	4.10	120.35	111.48
30	Y	309	CHL	C1B-CHB-C4A	4.10	123.96	121.32
31	0	602	CLA	C1-C2-C3	-4.10	119.48	126.20
31	q	316	CLA	C1-C2-C3	-4.10	120.13	126.76
30	n	308	CHL	CHA-C1A-C2A	-4.10	123.68	133.31
31	c	604	CLA	C1-C2-C3	-4.10	119.48	126.20
33	S	320	LHG	O7-C7-C8	4.10	120.34	111.48
31	a	407	CLA	C1-C2-C3	-4.09	119.49	126.20
30	R	308	CHL	CHA-C1A-C2A	-4.09	123.70	133.31
34	a	413	LMG	C1-O6-C5	-4.09	105.73	113.72
31	0	613	CLA	C1-C2-C3	-4.09	119.49	126.20
36	5	618	NEX	C27-C28-C29	-4.09	119.18	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2	615	LUT	C18-C5-C6	-4.09	120.02	124.48
43	b	619	BCR	C1-C6-C5	-4.09	117.05	122.64
43	h	101	BCR	C27-C26-C25	-4.09	117.18	122.70
30	y	608	CHL	CHA-C1A-C2A	-4.09	123.71	133.31
30	g	308	CHL	CHA-C1A-C2A	-4.09	123.71	133.31
30	7	321	CHL	CHA-C1A-C2A	-4.09	123.71	133.31
30	8	608	CHL	CHA-C1A-C2A	-4.08	123.72	133.31
30	5	606	CHL	CHA-C1A-C2A	-4.08	123.72	133.31
30	Y	307	CHL	CHA-C1A-C2A	-4.08	123.72	133.31
30	q	309	CHL	C1-O2A-CGA	4.08	126.53	116.65
34	w	204	LMG	O7-C10-C11	4.08	120.31	111.48
30	q	307	CHL	CHA-C1A-C2A	-4.08	123.73	133.31
30	8	601	CHL	CHA-C1A-C2A	-4.08	123.73	133.31
30	4	608	CHL	CHA-C1A-C2A	-4.08	123.73	133.31
32	6	318	LUT	C26-C27-C28	-4.08	118.23	124.58
31	1	610	CLA	C1-C2-C3	-4.08	119.52	126.20
30	1	605	CHL	C1B-CHB-C4A	4.08	123.94	121.32
30	0	601	CHL	CHA-C1A-C2A	-4.08	123.74	133.31
34	X	203	LMG	O7-C10-C11	4.07	120.29	111.48
30	n	302	CHL	CHA-C1A-C2A	-4.07	123.75	133.31
31	4	614	CLA	C1-C2-C3	-4.07	119.53	126.20
30	3	302	CHL	C1-O2A-CGA	4.07	126.50	116.65
30	s	307	CHL	C1B-CHB-C4A	4.07	123.94	121.32
31	y	614	CLA	C1-C2-C3	-4.07	119.53	126.20
31	Y	314	CLA	C1-C2-C3	-4.07	119.54	126.20
31	s	312	CLA	C1-C2-C3	-4.06	119.54	126.20
43	A	410	BCR	C7-C8-C9	-4.06	120.22	126.23
43	Z	101	BCR	C38-C26-C25	-4.06	120.05	124.48
30	0	608	CHL	CHA-C1A-C2A	-4.06	123.77	133.31
30	8	606	CHL	CHA-C1A-C2A	-4.06	123.77	133.31
34	J	101	LMG	O7-C10-C11	4.06	120.27	111.48
35	4	615	RRX	C33-C5-C6	-4.06	120.05	124.48
30	y	606	CHL	CHA-C1A-C2A	-4.06	123.77	133.31
35	q	317	RRX	C27-C26-C25	-4.06	112.41	120.76
45	c	617	DGD	O2G-C1B-C2B	4.06	120.27	111.48
30	2	607	CHL	CHA-C1A-C2A	-4.06	123.77	133.31
30	0	606	CHL	C3D-C4D-CHA	4.06	114.71	108.54
30	n	307	CHL	CHA-C1A-C2A	-4.06	123.77	133.31
31	b	609	CLA	C1-C2-C3	-4.06	119.55	126.20
34	k	102	LMG	O7-C10-C11	4.06	120.26	111.48
31	S	305	CLA	C1-C2-C3	-4.06	119.55	126.20
30	3	302	CHL	CHA-C1A-C2A	-4.06	123.78	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	y	620	LMG	O7-C10-C11	4.06	120.25	111.48
31	b	612	CLA	C1-C2-C3	-4.06	119.55	126.20
30	N	309	CHL	CHA-C1A-C2A	-4.05	123.79	133.31
33	b	625	LHG	O7-C7-C8	4.05	120.25	111.48
30	1	607	CHL	CHA-C1A-C2A	-4.05	123.80	133.31
36	3	319	NEX	C27-C28-C29	-4.04	119.25	125.53
31	9	304	CLA	O2A-C1-C2	4.04	123.67	108.11
30	g	307	CHL	CHA-C1A-C2A	-4.04	123.82	133.31
48	K	101	LMU	C1B-O1B-C4'	-4.04	108.40	117.98
30	n	310	CHL	CHA-C1A-C2A	-4.04	123.82	133.31
31	1	613	CLA	C1-C2-C3	-4.04	119.58	126.20
32	Y	315	LUT	C35-C34-C33	-4.04	121.61	127.28
43	B	618	BCR	C1-C6-C5	-4.04	117.12	122.64
35	2	614	RRX	C7-C8-C9	-4.04	120.26	126.23
30	N	307	CHL	CHA-C1A-C2A	-4.04	123.83	133.31
35	G	614	RRX	C33-C5-C6	-4.04	120.08	124.48
31	2	604	CLA	C1-C2-C3	-4.04	119.58	126.20
32	Y	316	LUT	C35-C34-C33	-4.04	121.62	127.28
34	s	321	LMG	O7-C10-C11	4.03	120.21	111.48
30	s	302	CHL	C3D-C4D-CHA	4.03	114.67	108.54
30	6	309	CHL	CHA-C1A-C2A	-4.03	123.84	133.31
30	p	606	CHL	CHA-C1A-C2A	-4.03	123.85	133.31
31	d	404	CLA	O2A-C1-C2	4.03	123.61	108.11
43	c	614	BCR	C15-C16-C17	-4.03	115.28	123.52
31	2	612	CLA	C1-C2-C3	-4.03	119.60	126.20
31	b	606	CLA	C1-C2-C3	-4.03	119.60	126.20
30	1	601	CHL	C1A-CHA-C4D	4.02	125.70	118.98
30	n	309	CHL	CHA-C1A-C2A	-4.02	123.86	133.31
33	c	622	LHG	O7-C7-C8	4.02	120.18	111.48
31	r	306	CLA	O2A-C1-C2	4.02	122.91	109.44
31	r	311	CLA	C1-C2-C3	-4.02	119.61	126.20
30	q	309	CHL	C3D-C4D-CHA	4.02	114.65	108.54
31	N	315	CLA	C1-C2-C3	-4.02	119.61	126.20
35	9	317	RRX	C33-C5-C6	-4.02	120.10	124.48
30	N	301	CHL	CHA-C1A-C2A	-4.02	123.87	133.31
30	r	308	CHL	CHA-C1A-C2A	-4.02	123.88	133.31
33	j	102	LHG	O7-C7-C8	4.02	120.17	111.48
30	Y	306	CHL	C3D-C4D-CHA	4.02	114.64	108.54
43	B	617	BCR	C1-C6-C5	-4.01	117.15	122.64
43	T	101	BCR	C27-C26-C25	-4.01	117.28	122.70
31	5	612	CLA	C1-C2-C3	-4.01	120.27	126.76
32	1	616	LUT	C15-C14-C13	-4.01	121.65	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	0	619	LHG	O7-C7-C8	4.01	120.16	111.48
34	c	621	LMG	O7-C10-C11	4.01	120.16	111.48
30	S	307	CHL	CHA-C1A-C2A	-4.01	123.89	133.31
34	W	202	LMG	O7-C10-C11	4.01	120.15	111.48
30	7	302	CHL	CHA-C1A-C2A	-4.01	123.90	133.31
30	3	303	CHL	CHA-C1A-C2A	-4.00	123.90	133.31
31	c	610	CLA	C1-C2-C3	-4.00	119.64	126.20
30	4	607	CHL	CHA-C1A-C2A	-4.00	123.91	133.31
30	7	302	CHL	C1A-CHA-C4D	4.00	125.66	118.98
31	C	613	CLA	C1-C2-C3	-4.00	119.64	126.20
30	R	310	CHL	C3D-C4D-CHA	4.00	114.62	108.54
43	B	619	BCR	C27-C26-C25	-4.00	117.30	122.70
30	1	605	CHL	C1A-CHA-C4D	4.00	125.65	118.98
30	r	309	CHL	C1-C2-C3	-4.00	119.65	126.20
30	y	605	CHL	C3D-C4D-CHA	4.00	114.61	108.54
32	5	617	LUT	C35-C34-C33	-4.00	121.67	127.28
33	L	101	LHG	O7-C7-C8	3.99	120.12	111.48
31	p	603	CLA	O2A-C1-C2	3.99	123.48	108.11
34	b	626	LMG	O7-C10-C11	3.99	120.12	111.48
30	p	601	CHL	C3D-C4D-CHA	3.99	114.61	108.54
31	9	314	CLA	C1-C2-C3	-3.99	120.31	126.76
33	1	617	LHG	O7-C7-C8	3.99	120.11	111.48
33	6	320	LHG	O7-C7-C8	3.99	120.11	111.48
31	R	306	CLA	O2A-C1-C2	3.99	122.79	109.44
31	7	314	CLA	C1-C2-C3	-3.99	119.67	126.20
31	6	312	CLA	O2A-C1-C2	3.99	123.45	108.11
43	h	101	BCR	C4-C5-C6	-3.99	117.32	122.70
30	2	605	CHL	CHA-C1A-C2A	-3.98	123.95	133.31
30	S	302	CHL	C3D-C4D-CHA	3.98	114.59	108.54
31	B	616	CLA	C1-C2-C3	-3.98	119.67	126.20
33	D	408	LHG	O7-C7-C8	3.98	120.09	111.48
32	Y	316	LUT	C26-C27-C28	-3.98	118.39	124.58
33	d	408	LHG	O7-C7-C8	3.98	120.09	111.48
30	g	309	CHL	CHA-C1A-C2A	-3.98	123.97	133.31
34	R	321	LMG	O7-C10-C11	3.98	120.08	111.48
34	B	625	LMG	O7-C10-C11	3.98	120.08	111.48
32	Y	316	LUT	C21-C26-C27	-3.98	108.25	112.83
32	r	317	LUT	C15-C14-C13	-3.98	121.70	127.28
43	Z	101	BCR	C16-C17-C18	-3.97	121.70	127.28
30	p	605	CHL	CHA-C1A-C2A	-3.97	123.97	133.31
30	p	608	CHL	CHA-C1A-C2A	-3.97	123.97	133.31
30	Y	308	CHL	CHA-C1A-C2A	-3.97	123.98	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	y	609	CHL	CHA-C1A-C2A	-3.97	123.98	133.31
30	r	309	CHL	CHA-C1A-C2A	-3.97	123.98	133.31
34	j	101	LMG	O7-C10-C11	3.97	120.07	111.48
31	8	609	CLA	C1-C2-C3	-3.97	119.69	126.20
31	5	604	CLA	C1-C2-C3	-3.97	120.34	126.76
34	d	409	LMG	O7-C10-C11	3.97	120.06	111.48
34	A	414	LMG	O7-C10-C11	3.97	120.06	111.48
31	C	601	CLA	C1-C2-C3	-3.97	119.70	126.20
43	t	101	BCR	C7-C6-C5	-3.97	112.42	121.56
31	9	304	CLA	C1-C2-C3	-3.97	119.70	126.20
43	d	406	BCR	C4-C5-C6	-3.97	117.35	122.70
43	d	406	BCR	C15-C16-C17	-3.96	115.41	123.52
34	9	302	LMG	O7-C10-C11	3.96	120.05	111.48
43	H	101	BCR	C38-C26-C25	-3.96	120.16	124.48
31	b	603	CLA	O2A-C1-C2	3.96	123.35	108.11
30	n	301	CHL	CHA-C1A-C2A	-3.96	124.00	133.31
31	b	603	CLA	C1-C2-C3	-3.96	119.71	126.20
34	q	301	LMG	O7-C10-C11	3.96	120.04	111.48
30	2	606	CHL	CHA-C1A-C2A	-3.96	124.01	133.31
30	G	606	CHL	CHA-C1A-C2A	-3.96	124.01	133.31
32	S	318	LUT	C1-C6-C5	-3.96	117.23	122.64
32	y	616	LUT	C18-C5-C6	-3.95	120.17	124.48
31	c	613	CLA	CAA-C2A-C3A	-3.95	102.32	113.00
31	C	613	CLA	C1-O2A-CGA	3.95	126.21	116.65
31	A	406	CLA	C1-C2-C3	-3.95	119.72	126.20
43	b	618	BCR	C11-C10-C9	-3.95	121.74	127.28
32	0	617	LUT	C15-C14-C13	-3.95	121.74	127.28
43	c	614	BCR	C30-C25-C26	-3.95	117.24	122.64
32	N	316	LUT	C26-C27-C28	-3.95	118.44	124.58
30	1	609	CHL	CHA-C1A-C2A	-3.95	124.04	133.31
30	s	307	CHL	C1A-CHA-C4D	3.95	125.57	118.98
31	5	602	CLA	C1-C2-C3	-3.95	119.73	126.20
30	g	306	CHL	CHA-C1A-C2A	-3.94	124.05	133.31
30	3	307	CHL	CHA-C1A-C2A	-3.94	124.05	133.31
30	4	606	CHL	CHA-C1A-C2A	-3.94	124.05	133.31
30	s	309	CHL	C3D-C4D-CHA	3.94	114.53	108.54
32	6	318	LUT	C11-C10-C9	-3.94	121.75	127.28
30	9	310	CHL	CHA-C1A-C2A	-3.94	124.06	133.31
32	3	318	LUT	C26-C27-C28	-3.94	118.45	124.58
30	9	309	CHL	C1A-CHA-C4D	3.93	125.55	118.98
31	B	613	CLA	C1-C2-C3	-3.93	119.75	126.20
34	C	619	LMG	O7-C10-C11	3.93	119.99	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	t	101	BCR	C24-C23-C22	-3.93	120.42	126.23
44	a	414	PL9	C7-C3-C2	-3.93	118.75	123.39
30	S	307	CHL	C1A-CHA-C4D	3.93	125.54	118.98
32	p	616	LUT	C1-C6-C5	-3.93	117.27	122.64
30	7	308	CHL	CHA-C1A-C2A	-3.93	124.08	133.31
30	N	306	CHL	CHA-C1A-C2A	-3.93	124.08	133.31
31	g	305	CLA	C1-C2-C3	-3.93	119.76	126.20
32	y	616	LUT	C35-C34-C33	-3.93	121.77	127.28
30	N	308	CHL	CHA-C1A-C2A	-3.92	124.09	133.31
32	6	317	LUT	C21-C26-C27	-3.92	108.32	112.83
33	M	101	LHG	O7-C7-C8	3.92	119.97	111.48
43	v	101	BCR	C1-C6-C5	-3.92	117.28	122.64
31	d	405	CLA	C1-C2-C3	-3.92	119.77	126.20
30	9	307	CHL	CHA-C1A-C2A	-3.92	124.10	133.31
43	C	615	BCR	C35-C13-C14	-3.92	116.47	122.82
33	e	101	LHG	O7-C7-C8	3.92	119.96	111.48
30	4	605	CHL	CHA-C1A-C2A	-3.92	124.11	133.31
30	6	308	CHL	CHA-C1A-C2A	-3.92	124.11	133.31
31	c	601	CLA	C1-C2-C3	-3.92	119.78	126.20
33	5	619	LHG	O7-C7-C8	3.91	119.95	111.48
31	n	316	CLA	C1-C2-C3	-3.91	119.79	126.20
43	D	405	BCR	C34-C9-C10	-3.91	116.48	122.82
34	r	321	LMG	O7-C10-C11	3.91	119.94	111.48
30	1	608	CHL	CHA-C1A-C2A	-3.91	124.13	133.31
31	D	404	CLA	C1-C2-C3	-3.91	119.80	126.20
30	5	601	CHL	CHA-C1A-C2A	-3.91	124.13	133.31
30	Y	301	CHL	CHA-C1A-C2A	-3.90	124.14	133.31
30	p	609	CHL	CHA-C1A-C2A	-3.90	124.14	133.31
31	g	303	CLA	C1D-ND-C4D	-3.90	103.57	106.31
30	5	605	CHL	CHA-C1A-C2A	-3.90	124.14	133.31
32	s	318	LUT	C15-C14-C13	-3.90	121.81	127.28
34	n	321	LMG	O7-C10-C11	3.90	119.92	111.48
43	Z	101	BCR	C27-C26-C25	-3.90	117.44	122.70
34	D	411	LMG	O7-C10-C11	3.89	119.91	111.48
30	r	310	CHL	C3D-C4D-CHA	3.89	114.46	108.54
30	9	303	CHL	CHA-C1A-C2A	-3.89	124.17	133.31
31	8	603	CLA	C1-C2-C3	-3.89	119.82	126.20
34	d	410	LMG	O7-C10-C11	3.89	119.89	111.48
31	3	313	CLA	C1-C2-C3	-3.89	120.47	126.76
31	q	306	CLA	C1-C2-C3	-3.89	119.83	126.20
31	R	311	CLA	O2A-C1-C2	3.89	123.07	108.11
30	0	609	CHL	CHA-C1A-C2A	-3.89	124.18	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	a	410	BCR	C4-C5-C6	-3.89	117.45	122.70
33	G	618	LHG	O7-C7-C8	3.89	119.89	111.48
32	y	617	LUT	C7-C8-C9	-3.88	120.50	126.23
31	N	310	CLA	C1-C2-C3	-3.88	119.84	126.20
32	q	318	LUT	C18-C5-C6	-3.88	120.25	124.48
33	r	320	LHG	O7-C7-C8	3.88	119.87	111.48
31	c	602	CLA	O2A-C1-C2	3.88	123.03	108.11
30	Y	309	CHL	C1A-CHA-C4D	3.87	125.44	118.98
32	7	318	LUT	C18-C5-C6	-3.87	120.26	124.48
33	2	617	LHG	O7-C7-C8	3.87	119.85	111.48
30	9	311	CHL	C3D-C4D-CHA	3.87	114.42	108.54
31	3	311	CLA	C1-C2-C3	-3.87	119.86	126.20
35	q	317	RRX	C20-C19-C18	-3.87	115.76	126.36
30	n	306	CHL	CHA-C1A-C2A	-3.87	124.22	133.31
34	X	202	LMG	O7-C10-C11	3.87	119.84	111.48
30	s	308	CHL	CHA-C1A-C2A	-3.87	124.23	133.31
30	8	605	CHL	CHA-C1A-C2A	-3.86	124.23	133.31
30	6	302	CHL	CHA-C1A-C2A	-3.86	124.23	133.31
30	9	308	CHL	CHA-C1A-C2A	-3.86	124.23	133.31
30	3	308	CHL	C3D-C4D-CHA	3.86	114.41	108.54
31	B	614	CLA	C1-C2-C3	-3.86	119.87	126.20
32	n	317	LUT	C15-C14-C13	-3.86	121.86	127.28
43	t	101	BCR	C19-C18-C17	3.86	125.08	119.01
30	R	308	CHL	C1A-CHA-C4D	3.86	125.42	118.98
34	C	622	LMG	O7-C10-C11	3.86	119.82	111.48
32	0	617	LUT	C21-C26-C27	-3.85	108.39	112.83
30	7	310	CHL	CHA-C1A-C2A	-3.85	124.26	133.31
34	n	322	LMG	C8-O7-C10	-3.85	108.58	117.80
30	3	310	CHL	C1-O2A-CGA	3.85	125.97	116.65
30	4	601	CHL	CHA-C1A-C2A	-3.85	124.27	133.31
32	s	318	LUT	C1-C6-C5	-3.85	117.38	122.64
34	6	323	LMG	O7-C10-C11	3.85	119.80	111.48
42	a	408	PHO	C4D-CHA-CBD	-3.84	106.61	108.45
30	y	601	CHL	CHA-C1A-C2A	-3.84	124.28	133.31
30	3	303	CHL	C1A-CHA-C4D	3.84	125.39	118.98
31	p	602	CLA	C1-C2-C3	-3.84	119.90	126.20
30	3	310	CHL	CHA-C1A-C2A	-3.84	124.29	133.31
45	C	616	DGD	O2G-C1B-C2B	3.84	119.79	111.48
32	p	617	LUT	C7-C8-C9	-3.84	120.56	126.23
33	S	322	LHG	O7-C7-C8	3.84	119.78	111.48
33	s	320	LHG	O7-C7-C8	3.84	119.78	111.48
32	7	318	LUT	C15-C14-C13	-3.84	121.90	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	y	609	CHL	C1A-CHA-C4D	3.84	125.38	118.98
43	v	101	BCR	C20-C21-C22	-3.84	121.90	127.28
31	6	314	CLA	C1-C2-C3	-3.84	119.91	126.20
34	5	620	LMG	O7-C10-C11	3.84	119.78	111.48
34	0	620	LMG	O7-C10-C11	3.84	119.78	111.48
30	p	607	CHL	C3D-C4D-CHA	3.84	114.37	108.54
43	V	101	BCR	C1-C6-C5	-3.84	117.39	122.64
30	6	310	CHL	CHA-C1A-C2A	-3.83	124.31	133.31
32	8	615	LUT	C15-C14-C13	-3.83	121.91	127.28
30	9	309	CHL	C1-O2A-CGA	3.83	125.92	116.65
30	R	309	CHL	CHA-C1A-C2A	-3.83	124.32	133.31
34	k	101	LMG	O7-C10-C11	3.83	119.76	111.48
31	a	406	CLA	O2A-C1-C2	3.83	122.84	108.11
30	Y	302	CHL	CHA-C1A-C2A	-3.83	124.32	133.31
34	7	301	LMG	O7-C10-C11	3.83	119.76	111.48
43	d	406	BCR	C35-C13-C14	-3.83	116.62	122.82
30	2	601	CHL	CHA-C1A-C2A	-3.82	124.33	133.31
33	g	319	LHG	O7-C7-C8	3.82	119.75	111.48
31	s	306	CLA	C1-C2-C3	-3.82	120.58	126.76
43	C	614	BCR	C30-C25-C26	-3.82	117.41	122.64
33	A	417	LHG	O7-C7-C8	3.82	119.75	111.48
34	4	621	LMG	O7-C10-C11	3.82	119.75	111.48
32	5	617	LUT	C7-C8-C9	-3.82	120.58	126.23
34	p	620	LMG	O7-C10-C11	3.82	119.74	111.48
30	3	307	CHL	C3D-C4D-CHA	3.82	114.34	108.54
31	b	607	CLA	O2A-C1-C2	3.82	122.79	108.11
43	B	617	BCR	C27-C26-C25	-3.81	117.55	122.70
30	G	623	CHL	C3D-C4D-CHA	3.81	114.34	108.54
30	y	607	CHL	CHA-C1A-C2A	-3.81	124.35	133.31
30	8	608	CHL	C1-O2A-CGA	3.81	125.88	116.65
34	G	621	LMG	O7-C10-C11	3.81	119.72	111.48
30	q	303	CHL	CHA-C1A-C2A	-3.81	124.36	133.31
30	Y	302	CHL	C3D-C4D-CHA	3.81	114.33	108.54
31	3	301	CLA	O2A-C1-C2	3.81	122.77	108.11
31	B	604	CLA	O2A-C1-C2	3.81	122.76	108.11
30	g	302	CHL	C3D-C4D-CHA	3.81	114.33	108.54
30	6	308	CHL	C3D-C4D-CHA	3.81	114.33	108.54
30	G	605	CHL	CHA-C1A-C2A	-3.80	124.37	133.31
31	S	310	CLA	O2A-C1-C2	3.80	122.75	108.11
30	S	309	CHL	C3D-C4D-CHA	3.80	114.32	108.54
34	D	409	LMG	O7-C10-C11	3.80	119.71	111.48
30	4	601	CHL	C1-C2-C3	-3.80	119.97	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	g	322	LMG	O7-C10-C11	3.80	119.71	111.48
30	q	311	CHL	C3D-C4D-CHA	3.80	114.32	108.54
30	3	310	CHL	C3D-C4D-CHA	3.80	114.32	108.54
30	G	607	CHL	CHA-C1A-C2A	-3.80	124.38	133.31
30	7	307	CHL	C1-C2-C3	-3.80	119.97	126.20
33	N	319	LHG	O7-C7-C8	3.80	119.70	111.48
31	b	617	CLA	C1-C2-C3	-3.80	119.97	126.20
30	0	607	CHL	C1A-CHA-C4D	3.80	125.32	118.98
30	9	303	CHL	C3D-C4D-CHA	3.80	114.31	108.54
30	7	307	CHL	C1A-CHA-C4D	3.80	125.32	118.98
30	2	608	CHL	CHA-C1A-C2A	-3.80	124.39	133.31
31	3	306	CLA	C1-C2-C3	-3.80	119.97	126.20
30	q	303	CHL	C3D-C4D-CHA	3.80	114.31	108.54
31	B	602	CLA	O2A-C1-C2	3.79	122.71	108.11
34	x	202	LMG	O7-C10-C11	3.79	119.69	111.48
34	9	321	LMG	O7-C10-C11	3.79	119.69	111.48
31	6	315	CLA	O2A-C1-C2	3.79	122.71	108.11
31	B	610	CLA	C1-C2-C3	-3.79	119.98	126.20
31	Y	312	CLA	C1-C2-C3	-3.79	119.98	126.20
30	5	609	CHL	CHA-C1A-C2A	-3.79	124.40	133.31
30	5	605	CHL	C3D-C4D-CHA	3.79	114.30	108.54
31	S	303	CLA	C1-C2-C3	-3.79	119.98	126.20
31	7	316	CLA	C1-C2-C3	-3.79	119.98	126.20
31	c	611	CLA	C1-C2-C3	-3.79	119.99	126.20
31	1	604	CLA	O2A-C1-C2	3.79	122.69	108.11
30	N	302	CHL	C1A-CHA-C4D	3.79	125.31	118.98
31	b	605	CLA	O2A-C1-C2	3.79	122.69	108.11
30	n	301	CHL	C1A-CHA-C4D	3.79	125.30	118.98
30	2	608	CHL	C3D-C4D-CHA	3.79	114.30	108.54
32	5	617	LUT	C26-C27-C28	-3.79	118.69	124.58
34	0	622	LMG	O7-C10-C11	3.79	119.67	111.48
30	G	601	CHL	CHA-C1A-C2A	-3.79	124.42	133.31
30	2	601	CHL	C3D-C4D-CHA	3.79	114.29	108.54
30	7	306	CHL	C3D-C4D-CHA	3.79	114.29	108.54
31	R	307	CLA	O2A-C1-C2	3.78	122.11	109.44
32	p	617	LUT	C18-C5-C6	-3.78	120.36	124.48
30	p	608	CHL	C3D-C4D-CHA	3.78	114.29	108.54
43	b	618	BCR	C30-C25-C26	-3.78	117.47	122.64
30	G	623	CHL	CHA-C1A-C2A	-3.78	124.42	133.31
30	4	609	CHL	C3D-C4D-CHA	3.78	114.29	108.54
35	g	315	RRX	C33-C5-C6	-3.78	120.36	124.48
36	p	618	NEX	C27-C28-C29	-3.78	119.66	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	c	616	DGD	O2G-C1B-C2B	3.78	119.66	111.48
30	7	306	CHL	CHA-C1A-C2A	-3.78	124.43	133.31
31	c	610	CLA	O2A-C1-C2	3.78	122.65	108.11
30	G	608	CHL	C3D-C4D-CHA	3.78	114.28	108.54
30	4	607	CHL	C1B-CHB-C4A	3.78	123.75	121.32
31	3	312	CLA	O2A-C1-C2	3.78	122.64	108.11
30	G	608	CHL	CHA-C1A-C2A	-3.78	124.44	133.31
30	6	310	CHL	C3D-C4D-CHA	3.77	114.28	108.54
30	7	321	CHL	C3D-C4D-CHA	3.77	114.28	108.54
31	s	310	CLA	O2A-C1-C2	3.77	122.62	108.11
30	y	607	CHL	C3D-C4D-CHA	3.77	114.27	108.54
31	b	610	CLA	C1-C2-C3	-3.77	120.02	126.20
30	7	310	CHL	C1A-CHA-C4D	3.77	125.27	118.98
33	F1	301	LHG	O7-C7-C8	3.77	119.63	111.48
31	A	409	CLA	C1-C2-C3	-3.77	120.02	126.20
30	5	607	CHL	C3D-C4D-CHA	3.77	114.27	108.54
31	B	607	CLA	O2A-C1-C2	3.77	122.60	108.11
30	4	606	CHL	C3D-C4D-CHA	3.77	114.26	108.54
30	R	309	CHL	C3D-C4D-CHA	3.77	114.26	108.54
43	z	101	BCR	C16-C17-C18	-3.76	122.00	127.28
43	T	101	BCR	C16-C15-C14	-3.76	115.82	123.52
30	n	308	CHL	C3D-C4D-CHA	3.76	114.26	108.54
32	r	317	LUT	C8-C7-C6	-3.76	116.95	127.00
32	5	616	LUT	C15-C14-C13	-3.76	122.00	127.28
32	N	317	LUT	C26-C27-C28	-3.76	118.72	124.58
34	w	201	LMG	O7-C10-C11	3.76	119.62	111.48
30	6	302	CHL	C3D-C4D-CHA	3.76	114.26	108.54
43	b	620	BCR	C27-C26-C25	-3.76	117.62	122.70
30	G	607	CHL	C3D-C4D-CHA	3.76	114.25	108.54
30	y	606	CHL	C3D-C4D-CHA	3.76	114.25	108.54
30	Y	301	CHL	C3D-C4D-CHA	3.76	114.25	108.54
30	4	601	CHL	C3D-C4D-CHA	3.76	114.25	108.54
30	q	307	CHL	C1A-CHA-C4D	3.76	125.25	118.98
31	9	313	CLA	O2A-C1-C2	3.76	121.87	108.40
32	q	318	LUT	C26-C27-C28	-3.75	118.74	124.58
30	5	609	CHL	C3D-C4D-CHA	3.75	114.25	108.54
31	4	614	CLA	O2A-C1-C2	3.75	122.56	108.11
31	q	305	CLA	C1-C2-C3	-3.75	120.05	126.20
30	r	309	CHL	C3D-C4D-CHA	3.75	114.25	108.54
32	4	616	LUT	C26-C27-C28	-3.75	118.74	124.58
30	6	307	CHL	CHA-C1A-C2A	-3.75	124.50	133.31
30	7	321	CHL	C1A-CHA-C4D	3.75	125.24	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	409	CLA	C1-C2-C3	-3.75	120.05	126.20
43	b	619	BCR	C38-C26-C25	-3.75	120.39	124.48
30	9	308	CHL	C1A-CHA-C4D	3.75	125.24	118.98
31	Y	312	CLA	O2A-C1-C2	3.75	122.53	108.11
33	l	101	LHG	O7-C7-C8	3.75	119.59	111.48
30	2	606	CHL	C3D-C4D-CHA	3.75	114.24	108.54
30	y	608	CHL	C1A-CHA-C4D	3.75	125.24	118.98
31	B	614	CLA	O2A-C1-C2	3.75	122.53	108.11
30	7	310	CHL	C3D-C4D-CHA	3.75	114.24	108.54
31	C	612	CLA	O2A-C1-C2	3.75	122.53	108.11
32	S	318	LUT	C22-C23-C24	3.75	116.75	111.18
31	2	613	CLA	C1-C2-C3	-3.75	120.06	126.20
43	b	620	BCR	C20-C21-C22	-3.75	122.02	127.28
30	0	609	CHL	C3D-C4D-CHA	3.75	114.23	108.54
32	2	615	LUT	C35-C15-C14	-3.75	115.86	123.52
30	0	601	CHL	C1A-CHA-C4D	3.74	125.23	118.98
31	9	312	CLA	C1-C2-C3	-3.74	120.06	126.20
31	s	313	CLA	O2A-C1-C2	3.74	122.52	108.11
34	2	620	LMG	O7-C10-C11	3.74	119.58	111.48
30	5	601	CHL	C1A-CHA-C4D	3.74	125.23	118.98
33	n	320	LHG	O7-C7-C8	3.74	119.58	111.48
30	4	607	CHL	C3D-C4D-CHA	3.74	114.23	108.54
43	C	615	BCR	C11-C12-C13	3.74	136.62	126.36
31	8	614	CLA	C1-C2-C3	-3.74	120.07	126.20
31	c	604	CLA	O2A-C1-C2	3.74	122.50	108.11
30	S	307	CHL	C3D-C4D-CHA	3.74	114.22	108.54
33	8	618	LHG	O7-C7-C8	3.74	119.57	111.48
30	9	309	CHL	C1B-CHB-C4A	3.74	123.73	121.32
30	p	605	CHL	C3D-C4D-CHA	3.74	114.22	108.54
30	g	306	CHL	C1A-CHA-C4D	3.73	125.21	118.98
30	p	609	CHL	C3D-C4D-CHA	3.73	114.22	108.54
30	6	306	CHL	C1A-CHA-C4D	3.73	125.21	118.98
30	n	310	CHL	C1A-CHA-C4D	3.73	125.21	118.98
30	6	307	CHL	C3D-C4D-CHA	3.73	114.21	108.54
30	g	307	CHL	C3D-C4D-CHA	3.73	114.21	108.54
32	y	616	LUT	C30-C31-C32	-3.73	112.39	123.20
30	5	606	CHL	C1A-CHA-C4D	3.73	125.21	118.98
43	T	101	BCR	C4-C5-C6	-3.73	117.66	122.70
30	N	308	CHL	C3D-C4D-CHA	3.73	114.21	108.54
30	n	301	CHL	C3D-C4D-CHA	3.73	114.21	108.54
32	S	317	LUT	C31-C30-C29	-3.73	122.05	127.28
36	n	319	NEX	C2-C1-C6	3.73	112.84	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	0	615	CLA	C1-C2-C3	-3.73	120.09	126.20
30	n	308	CHL	C1A-CHA-C4D	3.73	125.20	118.98
31	r	307	CLA	O2A-C1-C2	3.73	121.92	109.44
30	7	308	CHL	C3D-C4D-CHA	3.73	114.21	108.54
30	8	608	CHL	C1A-CHA-C4D	3.73	125.20	118.98
30	9	307	CHL	C3D-C4D-CHA	3.73	114.21	108.54
30	9	308	CHL	C3D-C4D-CHA	3.73	114.21	108.54
30	y	609	CHL	C3D-C4D-CHA	3.73	114.21	108.54
32	0	617	LUT	C18-C5-C6	-3.73	120.42	124.48
30	p	606	CHL	C3D-C4D-CHA	3.73	114.20	108.54
30	1	607	CHL	C3D-C4D-CHA	3.73	114.20	108.54
30	q	311	CHL	CHA-C1A-C2A	-3.73	124.56	133.31
30	G	606	CHL	C3D-C4D-CHA	3.73	114.20	108.54
31	6	303	CLA	C1-C2-C3	-3.72	120.09	126.20
32	5	617	LUT	C31-C30-C29	-3.72	122.05	127.28
31	R	305	CLA	O2A-C1-C2	3.72	122.44	108.11
32	p	616	LUT	C40-C33-C34	-3.72	116.78	122.82
30	g	309	CHL	C3D-C4D-CHA	3.72	114.20	108.54
30	7	321	CHL	C1-C2-C3	-3.72	120.09	126.20
31	g	311	CLA	O2A-C1-C2	3.72	122.44	108.11
31	y	613	CLA	C1-C2-C3	-3.72	120.10	126.20
30	Y	307	CHL	C1A-CHA-C4D	3.72	125.19	118.98
34	w	203	LMG	O8-C28-C29	3.72	123.18	111.83
30	Y	307	CHL	C3D-C4D-CHA	3.72	114.19	108.54
30	y	601	CHL	C3D-C4D-CHA	3.72	114.19	108.54
30	1	609	CHL	C3D-C4D-CHA	3.72	114.19	108.54
43	z	101	BCR	C27-C26-C25	-3.72	117.68	122.70
32	3	318	LUT	C35-C34-C33	-3.72	122.07	127.28
32	Y	315	LUT	C15-C14-C13	-3.72	122.07	127.28
33	q	320	LHG	O7-C7-C8	3.72	119.52	111.48
32	0	617	LUT	C26-C27-C28	-3.72	118.80	124.58
43	C	614	BCR	C23-C24-C25	-3.71	117.08	127.00
31	3	314	CLA	C1-C2-C3	-3.71	120.11	126.20
30	q	310	CHL	C3D-C4D-CHA	3.71	114.19	108.54
43	t	101	BCR	C2-C1-C6	3.71	115.83	110.44
34	c	624	LMG	O7-C10-C11	3.71	119.51	111.48
30	0	607	CHL	C3D-C4D-CHA	3.71	114.18	108.54
30	0	608	CHL	C1A-CHA-C4D	3.71	125.17	118.98
32	q	318	LUT	C31-C30-C29	-3.71	122.07	127.28
31	B	616	CLA	O2A-C1-C2	3.71	122.38	108.11
30	8	605	CHL	C3D-C4D-CHA	3.71	114.18	108.54
30	Y	308	CHL	C3D-C4D-CHA	3.71	114.18	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	619	CHL	C3D-C4D-CHA	3.71	114.18	108.54
32	2	615	LUT	C40-C33-C34	-3.71	116.81	122.82
34	a	401	LMG	O7-C10-C11	3.71	119.50	111.48
33	7	319	LHG	O7-C7-C8	3.71	119.50	111.48
30	r	308	CHL	C3D-C4D-CHA	3.71	114.17	108.54
30	3	309	CHL	CHA-C1A-C2A	-3.71	124.61	133.31
30	1	606	CHL	C3D-C4D-CHA	3.70	114.17	108.54
30	n	308	CHL	C1-C2-C3	-3.70	120.13	126.20
30	4	605	CHL	C3D-C4D-CHA	3.70	114.17	108.54
30	R	308	CHL	C1-C2-C3	-3.70	120.13	126.20
30	s	307	CHL	C3D-C4D-CHA	3.70	114.17	108.54
30	n	306	CHL	C3D-C4D-CHA	3.70	114.16	108.54
32	3	317	LUT	C21-C26-C27	-3.70	108.57	112.83
30	N	307	CHL	C3D-C4D-CHA	3.70	114.16	108.54
30	6	308	CHL	C1A-CHA-C4D	3.70	125.15	118.98
43	t	101	BCR	C12-C13-C14	3.70	124.83	119.01
30	5	608	CHL	C1A-CHA-C4D	3.70	125.15	118.98
33	y	619	LHG	O7-C7-C8	3.70	119.48	111.48
34	q1	101	LMG	O7-C10-C11	3.70	119.48	111.48
30	2	605	CHL	C1A-CHA-C4D	3.70	125.15	118.98
30	7	302	CHL	C3D-C4D-CHA	3.70	114.16	108.54
30	n	309	CHL	C3D-C4D-CHA	3.69	114.16	108.54
32	7	318	LUT	C31-C30-C29	-3.69	122.10	127.28
43	a	410	BCR	C30-C25-C26	-3.69	117.59	122.64
35	q	317	RRX	C30-C25-C26	-3.69	117.59	122.64
32	0	617	LUT	C11-C10-C9	-3.69	122.10	127.28
31	n	311	CLA	C1-C2-C3	-3.69	120.15	126.20
30	8	601	CHL	C3D-C4D-CHA	3.69	114.15	108.54
30	g	306	CHL	C3D-C4D-CHA	3.69	114.15	108.54
32	9	318	LUT	C1-C6-C5	-3.69	117.59	122.64
31	p	613	CLA	C1-O2A-CGA	3.69	125.58	116.65
31	2	603	CLA	C1-C2-C3	-3.69	120.15	126.20
30	2	605	CHL	C3D-C4D-CHA	3.69	114.14	108.54
30	N	306	CHL	C3D-C4D-CHA	3.69	114.14	108.54
31	B	611	CLA	O2A-C1-C2	3.69	122.29	108.11
43	a	410	BCR	C27-C26-C25	-3.69	117.72	122.70
30	N	301	CHL	C3D-C4D-CHA	3.68	114.14	108.54
30	7	309	CHL	C3D-C4D-CHA	3.68	114.14	108.54
30	8	608	CHL	C3D-C4D-CHA	3.68	114.14	108.54
30	g	302	CHL	CHA-C1A-C2A	-3.68	124.66	133.31
30	G	601	CHL	C3D-C4D-CHA	3.68	114.14	108.54
30	G	605	CHL	C3D-C4D-CHA	3.68	114.14	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	8	606	CHL	C3D-C4D-CHA	3.68	114.14	108.54
31	7	304	CLA	C1-C2-C3	-3.68	120.17	126.20
30	N	302	CHL	C3D-C4D-CHA	3.68	114.13	108.54
33	b	628	LHG	O7-C7-C8	3.68	119.44	111.48
30	0	601	CHL	C3D-C4D-CHA	3.68	114.13	108.54
32	3	317	LUT	C26-C27-C28	-3.68	118.86	124.58
30	n	302	CHL	C3D-C4D-CHA	3.68	114.13	108.54
30	n	307	CHL	C3D-C4D-CHA	3.68	114.13	108.54
30	p	605	CHL	C1A-CHA-C4D	3.68	125.11	118.98
30	6	309	CHL	C3D-C4D-CHA	3.68	114.13	108.54
31	d	405	CLA	O2A-C1-C2	3.67	122.25	108.11
31	B	609	CLA	C1-C2-C3	-3.67	120.18	126.20
30	4	605	CHL	C1A-CHA-C4D	3.67	125.11	118.98
30	q	308	CHL	C1B-CHB-C4A	3.67	123.69	121.32
31	R	316	CLA	C1-C2-C3	-3.67	120.18	126.20
31	C	602	CLA	O2A-C1-C2	3.67	122.23	108.11
30	2	606	CHL	C1A-CHA-C4D	3.67	125.11	118.98
30	q	310	CHL	C1A-CHA-C4D	3.67	125.11	118.98
30	r	310	CHL	CHA-C1A-C2A	-3.67	124.69	133.31
30	g	309	CHL	C1A-CHA-C4D	3.67	125.11	118.98
31	b	615	CLA	O2A-C1-C2	3.67	122.23	108.11
30	r	308	CHL	C1A-CHA-C4D	3.67	125.10	118.98
30	3	303	CHL	C3D-C4D-CHA	3.67	114.11	108.54
31	s	310	CLA	C1-C2-C3	-3.67	120.19	126.20
30	0	605	CHL	C3D-C4D-CHA	3.67	114.11	108.54
43	d	406	BCR	C16-C17-C18	-3.67	122.14	127.28
30	4	609	CHL	CHA-C1A-C2A	-3.67	124.70	133.31
31	4	613	CLA	C1-C2-C3	-3.66	120.19	126.20
31	q	316	CLA	O2A-C1-C2	3.66	122.20	108.11
43	B	617	BCR	C20-C21-C22	-3.66	122.14	127.28
30	9	309	CHL	C3D-C4D-CHA	3.66	114.11	108.54
43	c	614	BCR	C21-C20-C19	3.66	133.81	123.20
32	1	615	LUT	C35-C34-C33	-3.66	122.14	127.28
30	Y	309	CHL	C3D-C4D-CHA	3.66	114.11	108.54
30	8	607	CHL	C3D-C4D-CHA	3.66	114.11	108.54
30	p	606	CHL	C1A-CHA-C4D	3.66	125.09	118.98
30	5	601	CHL	C3D-C4D-CHA	3.66	114.10	108.54
30	1	608	CHL	C3D-C4D-CHA	3.66	114.10	108.54
31	Y	310	CLA	C1-C2-C3	-3.66	120.20	126.20
31	s	312	CLA	O2A-C1-C2	3.66	122.19	108.11
30	5	609	CHL	C1A-CHA-C4D	3.66	125.08	118.98
31	b	617	CLA	O2A-C1-C2	3.66	122.18	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	S	309	CHL	CHA-C1A-C2A	-3.66	124.72	133.31
30	N	309	CHL	C3D-C4D-CHA	3.66	114.10	108.54
32	1	615	LUT	C8-C7-C6	-3.65	117.24	127.00
32	3	317	LUT	C15-C14-C13	-3.65	122.16	127.28
31	s	311	CLA	O2A-C1-C2	3.65	122.16	108.11
31	C	604	CLA	O2A-C1-C2	3.65	122.16	108.11
30	7	307	CHL	C3D-C4D-CHA	3.65	114.09	108.54
30	4	609	CHL	C1A-CHA-C4D	3.65	125.07	118.98
30	9	310	CHL	C3D-C4D-CHA	3.65	114.09	108.54
31	5	610	CLA	C1-C2-C3	-3.65	120.22	126.20
43	A	410	BCR	C30-C25-C26	-3.65	117.65	122.64
30	S	308	CHL	CHA-C1A-C2A	-3.65	124.74	133.31
31	C	611	CLA	O2A-C1-C2	3.65	122.15	108.11
30	R	308	CHL	C3D-C4D-CHA	3.65	114.08	108.54
30	9	307	CHL	C1A-CHA-C4D	3.65	125.06	118.98
31	b	611	CLA	C1-C2-C3	-3.65	120.22	126.20
30	5	606	CHL	C3D-C4D-CHA	3.64	114.08	108.54
30	0	606	CHL	C1A-CHA-C4D	3.64	125.06	118.98
30	N	301	CHL	C1A-CHA-C4D	3.64	125.06	118.98
31	n	304	CLA	C1-C2-C3	-3.64	120.23	126.20
30	2	608	CHL	C1A-CHA-C4D	3.64	125.06	118.98
43	b	618	BCR	C24-C23-C22	-3.64	120.85	126.23
31	S	313	CLA	O2A-C1-C2	3.64	122.11	108.11
31	1	610	CLA	O2A-C1-C2	3.64	122.11	108.11
31	c	603	CLA	O2A-C1-C2	3.64	122.11	108.11
32	1	616	LUT	C21-C26-C27	-3.64	108.64	112.83
30	5	608	CHL	C3D-C4D-CHA	3.64	114.07	108.54
32	Y	315	LUT	C10-C11-C12	-3.64	112.66	123.20
32	S	317	LUT	C15-C14-C13	-3.64	122.18	127.28
32	1	616	LUT	C18-C5-C6	-3.64	120.52	124.48
30	1	609	CHL	C1A-CHA-C4D	3.64	125.05	118.98
30	G	605	CHL	C1A-CHA-C4D	3.64	125.05	118.98
31	0	604	CLA	O2A-C1-C2	3.64	122.10	108.11
31	c	611	CLA	O2A-C1-C2	3.64	122.10	108.11
32	p	616	LUT	C21-C26-C27	-3.64	108.65	112.83
43	B	617	BCR	C24-C23-C22	-3.63	120.86	126.23
30	1	619	CHL	CMA-C3A-C4A	3.63	122.44	114.61
34	4	620	LMG	O7-C10-C11	3.63	119.34	111.48
33	Y	318	LHG	O7-C7-C8	3.63	119.33	111.48
31	5	615	CLA	C2C-C1C-NC	3.63	113.79	109.98
30	3	309	CHL	C3D-C4D-CHA	3.63	114.05	108.54
30	0	609	CHL	C1A-CHA-C4D	3.62	125.03	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	p	609	CHL	C1A-CHA-C4D	3.62	125.03	118.98
30	3	307	CHL	C1A-CHA-C4D	3.62	125.03	118.98
30	7	309	CHL	C1A-CHA-C4D	3.62	125.03	118.98
31	g	304	CLA	C1-C2-C3	-3.62	120.26	126.20
34	D	410	LMG	O7-C10-C11	3.62	119.32	111.48
31	N	304	CLA	C1-C2-C3	-3.62	120.27	126.20
30	1	605	CHL	C3D-C4D-CHA	3.62	114.04	108.54
31	C	603	CLA	O2A-C1-C2	3.62	122.03	108.11
32	5	616	LUT	C26-C27-C28	-3.62	118.95	124.58
35	2	614	RRX	C30-C25-C26	-3.62	117.69	122.64
35	G	614	RRX	C7-C8-C9	-3.62	120.89	126.23
30	y	608	CHL	C3D-C4D-CHA	3.61	114.03	108.54
30	y	605	CHL	CHA-C1A-C2A	-3.61	124.83	133.31
30	3	302	CHL	C3D-C4D-CHA	3.61	114.03	108.54
30	g	308	CHL	C3D-C4D-CHA	3.61	114.03	108.54
43	V	101	BCR	C4-C5-C6	-3.61	117.83	122.70
43	b	618	BCR	C23-C24-C25	-3.61	117.36	127.00
30	q	307	CHL	C3D-C4D-CHA	3.61	114.02	108.54
31	Y	303	CLA	O2A-C1-C2	3.61	121.98	108.11
43	H	101	BCR	C2-C1-C6	3.61	115.68	110.44
30	n	310	CHL	C3D-C4D-CHA	3.60	114.02	108.54
31	y	612	CLA	O2A-C1-C2	3.60	121.98	108.11
31	R	315	CLA	C1-C2-C3	-3.60	120.30	126.20
30	9	311	CHL	CHA-C1A-C2A	-3.60	124.85	133.31
43	D	405	BCR	C10-C11-C12	-3.60	112.77	123.20
31	A	405	CLA	O2A-C1-C2	3.60	121.96	108.11
31	q	312	CLA	C1-C2-C3	-3.60	120.30	126.20
30	3	308	CHL	CHA-C1A-C2A	-3.60	124.86	133.31
34	a	413	LMG	O1-C7-C8	-3.59	102.08	110.82
32	Y	315	LUT	C7-C8-C9	-3.59	120.92	126.23
30	R	309	CHL	C1-C2-C3	-3.59	120.31	126.20
30	2	607	CHL	C3D-C4D-CHA	3.59	114.00	108.54
33	4	618	LHG	O7-C7-C8	3.59	119.25	111.48
31	S	311	CLA	O2A-C1-C2	3.59	121.93	108.11
31	b	614	CLA	C1-C2-C3	-3.59	120.31	126.20
30	0	608	CHL	C3D-C4D-CHA	3.59	114.00	108.54
43	D	405	BCR	C27-C26-C25	-3.59	117.86	122.70
30	g	307	CHL	C1A-CHA-C4D	3.59	124.97	118.98
31	3	304	CLA	O2A-C1-C2	3.59	121.92	108.11
31	1	604	CLA	C1-C2-C3	-3.59	120.32	126.20
30	6	306	CHL	C3D-C4D-CHA	3.59	113.99	108.54
32	y	616	LUT	C8-C7-C6	-3.59	117.42	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	p	617	LUT	C40-C33-C34	-3.59	117.00	122.82
43	B	619	BCR	C7-C8-C9	-3.59	120.93	126.23
35	4	615	RRX	C7-C8-C9	-3.59	120.93	126.23
34	a	416	LMG	O7-C10-C11	3.58	119.24	111.48
31	9	306	CLA	O2A-C1-C2	3.58	121.90	108.11
35	9	317	RRX	C7-C8-C9	-3.58	120.93	126.23
31	5	614	CLA	O2A-C1-C2	3.58	121.90	108.11
47	e	102	HEM	CHA-C4D-ND	3.58	128.80	124.37
30	q	311	CHL	C1A-CHA-C4D	3.58	124.95	118.98
31	b	608	CLA	C1-C2-C3	-3.58	120.33	126.20
31	p	604	CLA	C1-C2-C3	-3.57	120.98	126.76
31	5	615	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
30	G	623	CHL	C1A-CHA-C4D	3.57	124.94	118.98
30	G	608	CHL	C1A-CHA-C4D	3.57	124.94	118.98
30	Y	301	CHL	C1A-CHA-C4D	3.57	124.94	118.98
30	8	607	CHL	C1A-CHA-C4D	3.57	124.94	118.98
32	p	616	LUT	C39-C29-C30	-3.57	117.03	122.82
36	6	319	NEX	C27-C28-C29	-3.57	119.99	125.53
31	R	305	CLA	CBC-CAC-C3C	-3.57	102.74	112.42
32	6	318	LUT	C18-C5-C6	-3.57	120.59	124.48
31	y	610	CLA	C1-C2-C3	-3.57	120.35	126.20
31	y	602	CLA	O2A-C1-C2	3.57	121.83	108.11
31	s	315	CLA	O2A-C1-C2	3.57	121.38	109.44
30	g	308	CHL	C1A-CHA-C4D	3.57	124.93	118.98
36	0	618	NEX	C27-C28-C29	-3.57	120.00	125.53
31	p	611	CLA	C1-C2-C3	-3.57	120.36	126.20
31	3	305	CLA	C1-C2-C3	-3.56	120.36	126.20
30	9	303	CHL	C1A-CHA-C4D	3.56	124.93	118.98
36	N	318	NEX	C12-C13-C14	3.56	124.61	119.01
34	1	618	LMG	O7-C10-C11	3.56	119.19	111.48
32	Y	315	LUT	C8-C7-C6	-3.56	117.48	127.00
30	N	306	CHL	C1-C2-C3	-3.56	120.36	126.20
30	6	302	CHL	C1A-CHA-C4D	3.56	124.92	118.98
30	n	309	CHL	C1A-CHA-C4D	3.56	124.92	118.98
44	D	406	PL9	C7-C3-C4	3.56	119.84	116.91
43	B	618	BCR	C8-C7-C6	-3.56	117.49	127.00
30	6	307	CHL	C1A-CHA-C4D	3.56	124.92	118.98
32	8	616	LUT	C1-C6-C5	-3.56	117.77	122.64
30	6	309	CHL	C1A-CHA-C4D	3.56	124.92	118.98
32	5	617	LUT	C1-C6-C5	-3.56	117.78	122.64
34	9	301	LMG	C3-C4-C5	3.56	116.68	110.23
32	n	318	LUT	C1-C6-C5	-3.55	117.78	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	b	620	BCR	C38-C26-C25	-3.55	120.61	124.48
30	4	608	CHL	C3D-C4D-CHA	3.55	113.94	108.54
30	q	303	CHL	C1A-CHA-C4D	3.55	124.91	118.98
31	S	312	CLA	C1-O2A-CGA	3.55	125.25	116.65
31	q	304	CLA	C1-C2-C3	-3.55	120.38	126.20
34	A	418	LMG	O7-C10-C11	3.55	119.16	111.48
30	1	601	CHL	C3D-C4D-CHA	3.55	113.93	108.54
43	t	101	BCR	C34-C9-C10	-3.55	117.07	122.82
30	7	306	CHL	C1-C2-C3	-3.55	120.39	126.20
30	p	601	CHL	CHA-C1A-C2A	-3.55	124.98	133.31
31	3	315	CLA	O2A-C1-C2	3.54	121.75	108.11
31	b	608	CLA	O2A-C1-C2	3.54	121.75	108.11
31	G	603	CLA	C1-C2-C3	-3.54	120.39	126.20
32	n	318	LUT	C18-C5-C6	-3.54	120.62	124.48
31	G	609	CLA	O2A-C1-C2	3.54	121.74	108.11
31	2	602	CLA	C1-C2-C3	-3.54	120.39	126.20
32	g	316	LUT	C18-C5-C6	-3.54	120.62	124.48
30	s	309	CHL	CHA-C1A-C2A	-3.54	125.00	133.31
30	7	308	CHL	C1A-CHA-C4D	3.54	124.88	118.98
31	b	612	CLA	O2A-C1-C2	3.54	121.71	108.11
30	1	619	CHL	C1A-CHA-C4D	3.53	124.88	118.98
31	N	310	CLA	O2A-C1-C2	3.53	121.70	108.11
31	Y	314	CLA	O2A-C1-C2	3.53	121.70	108.11
43	T	101	BCR	C20-C19-C18	-3.53	116.68	126.36
30	q	309	CHL	CHA-C1A-C2A	-3.53	125.02	133.31
30	r	309	CHL	C1A-CHA-C4D	3.53	124.87	118.98
31	7	305	CLA	C1-C2-C3	-3.53	120.41	126.20
32	1	615	LUT	C7-C8-C9	-3.53	121.02	126.23
30	N	309	CHL	C1A-CHA-C4D	3.53	124.87	118.98
31	C	601	CLA	O2A-C1-C2	3.53	121.68	108.11
31	S	306	CLA	O2A-C1-C2	3.53	121.67	108.11
30	G	601	CHL	C1A-CHA-C4D	3.52	124.86	118.98
31	8	604	CLA	O2A-C1-C2	3.52	121.67	108.11
31	1	612	CLA	O2A-C1-C2	3.52	121.66	108.11
31	5	613	CLA	O2A-C1-C2	3.52	121.66	108.11
30	1	609	CHL	C1-C2-C3	-3.52	120.43	126.20
43	v	101	BCR	C24-C23-C22	-3.52	121.03	126.23
32	8	616	LUT	C18-C5-C6	-3.52	120.64	124.48
30	q	310	CHL	CHA-C1A-C2A	-3.52	125.05	133.31
30	R	309	CHL	C1A-CHA-C4D	3.52	124.85	118.98
31	B	602	CLA	C1-C2-C3	-3.52	120.44	126.20
31	9	305	CLA	C1-C2-C3	-3.52	120.44	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	n	310	CHL	C1-O2A-CGA	3.52	125.16	116.65
31	S	315	CLA	O2A-C1-C2	3.51	121.20	109.44
32	N	316	LUT	C21-C26-C27	-3.51	108.79	112.83
31	c	612	CLA	O2A-C1-C2	3.51	121.62	108.11
43	Z	101	BCR	C4-C5-C6	-3.51	117.96	122.70
31	C	610	CLA	C1-C2-C3	-3.51	120.45	126.20
31	0	611	CLA	O2A-C1-C2	3.51	121.61	108.11
30	p	607	CHL	C1A-CHA-C4D	3.51	124.84	118.98
37	R	318	XAT	C7-C8-C9	-3.51	120.09	125.53
30	N	308	CHL	C1A-CHA-C4D	3.51	124.83	118.98
36	3	319	NEX	C16-C1-C6	-3.51	107.33	110.47
32	3	317	LUT	C7-C8-C9	-3.51	121.05	126.23
32	3	317	LUT	C11-C10-C9	-3.51	122.36	127.28
31	p	614	CLA	O2A-C1-C2	3.51	121.60	108.11
30	0	605	CHL	C1-C2-C3	-3.51	120.45	126.20
30	s	308	CHL	C1A-CHA-C4D	3.50	124.83	118.98
32	N	317	LUT	C18-C5-C4	3.50	120.86	114.42
31	n	305	CLA	O2A-C1-C2	3.50	121.58	108.11
30	y	607	CHL	C1A-CHA-C4D	3.50	124.82	118.98
30	y	601	CHL	C1-C2-C3	-3.50	120.47	126.20
31	y	603	CLA	C1-C2-C3	-3.50	120.47	126.20
31	N	315	CLA	O2A-C1-C2	3.50	121.57	108.11
31	b	607	CLA	C1-C2-C3	-3.50	120.47	126.20
31	s	303	CLA	C1-C2-C3	-3.50	120.47	126.20
31	2	610	CLA	C1-C2-C3	-3.50	120.47	126.20
31	6	315	CLA	C1-C2-C3	-3.50	120.47	126.20
30	G	607	CHL	C1A-CHA-C4D	3.50	124.82	118.98
31	N	305	CLA	O2A-C1-C2	3.50	121.56	108.11
34	C	624	LMG	O7-C10-C11	3.49	119.03	111.48
30	0	605	CHL	C3C-C4C-NC	-3.49	106.12	114.65
31	p	603	CLA	C1-C2-C3	-3.49	120.48	126.20
31	9	305	CLA	O2A-C1-C2	3.49	121.54	108.11
43	D	405	BCR	C30-C25-C26	-3.49	117.87	122.64
31	R	304	CLA	C1-C2-C3	-3.49	120.48	126.20
32	N	317	LUT	C31-C30-C29	-3.49	122.38	127.28
32	1	615	LUT	C11-C10-C9	-3.49	122.39	127.28
31	A	406	CLA	O2A-C1-C2	3.49	121.53	108.11
31	8	602	CLA	C1-C2-C3	-3.49	120.48	126.20
30	8	601	CHL	C1A-CHA-C4D	3.49	124.80	118.98
31	b	616	CLA	O2A-C1-C2	3.49	121.53	108.11
32	6	318	LUT	C21-C26-C27	-3.49	108.82	112.83
32	R	317	LUT	C7-C8-C9	-3.49	121.08	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	t	101	BCR	C36-C18-C17	-3.49	117.17	122.82
31	D	403	CLA	O2A-C1-C2	3.49	121.52	108.11
30	3	310	CHL	C1A-CHA-C4D	3.48	124.80	118.98
30	N	306	CHL	C1-O2A-CGA	3.48	125.08	116.65
30	y	606	CHL	C1A-CHA-C4D	3.48	124.79	118.98
34	9	301	LMG	O8-C28-C29	3.48	122.45	111.83
35	9	317	RRX	C30-C25-C26	-3.48	117.88	122.64
30	9	311	CHL	C1A-CHA-C4D	3.48	124.79	118.98
30	n	302	CHL	C1A-CHA-C4D	3.48	124.79	118.98
33	e	101	LHG	O8-C23-C24	3.48	122.44	111.83
31	0	603	CLA	O2A-C1-C2	3.48	121.49	108.11
30	5	601	CHL	C1-C2-C3	-3.48	121.14	126.76
35	G	614	RRX	C30-C25-C26	-3.47	117.89	122.64
32	S	318	LUT	C15-C14-C13	-3.47	122.41	127.28
31	b	606	CLA	O2A-C1-C2	3.47	121.47	108.11
30	9	308	CHL	C1-C2-C3	-3.47	120.51	126.20
32	s	317	LUT	C15-C14-C13	-3.47	122.41	127.28
43	D	405	BCR	C2-C1-C6	3.47	115.48	110.44
31	b	610	CLA	O2A-C1-C2	3.47	121.47	108.11
31	2	613	CLA	O2A-C1-C2	3.47	121.47	108.11
31	5	612	CLA	O2A-C1-C2	3.47	121.46	108.11
31	N	303	CLA	C1-C2-C3	-3.47	120.51	126.20
30	Y	308	CHL	C1A-CHA-C4D	3.47	124.77	118.98
31	4	613	CLA	O2A-C1-C2	3.47	121.45	108.11
31	N	321	CLA	O2A-C1-C2	3.47	121.45	108.11
31	s	305	CLA	O2A-C1-C2	3.47	121.45	108.11
30	n	307	CHL	C1A-CHA-C4D	3.47	124.77	118.98
32	S	318	LUT	C18-C5-C4	3.47	120.80	114.42
30	r	310	CHL	C1A-CHA-C4D	3.47	124.77	118.98
31	p	604	CLA	O2A-C1-C2	3.47	121.45	108.11
30	1	601	CHL	CMA-C3A-C4A	3.47	122.08	114.61
31	7	312	CLA	O2A-C1-C2	3.47	121.44	108.11
43	D	405	BCR	C38-C26-C25	-3.47	120.70	124.48
47	e	102	HEM	CHB-C1B-NB	3.46	128.65	124.37
31	R	315	CLA	O2A-C1-C2	3.46	121.44	108.11
45	c	617	DGD	C1E-O6E-C5E	3.46	120.48	113.72
30	8	606	CHL	C1A-CHA-C4D	3.46	124.76	118.98
31	N	313	CLA	C1-C2-C3	-3.46	120.53	126.20
31	B	610	CLA	O2A-C1-C2	3.46	121.42	108.11
30	1	607	CHL	C1A-CHA-C4D	3.46	124.75	118.98
31	c	601	CLA	O2A-C1-C2	3.46	121.42	108.11
31	5	614	CLA	C1-C2-C3	-3.46	120.53	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	y	601	CHL	C1A-CHA-C4D	3.46	124.75	118.98
31	y	615	CLA	O2A-C1-C2	3.46	121.41	108.11
32	s	317	LUT	C7-C8-C9	-3.46	121.12	126.23
35	4	615	RRX	C30-C25-C26	-3.46	117.91	122.64
31	s	314	CLA	O2A-C1-C2	3.45	121.40	108.11
31	B	615	CLA	C2C-C1C-NC	3.45	113.61	109.98
43	V	101	BCR	C38-C26-C27	3.45	120.95	113.60
30	4	608	CHL	C1A-CHA-C4D	3.45	124.74	118.98
34	N	320	LMG	O7-C10-C11	3.45	118.94	111.48
30	N	307	CHL	C1A-CHA-C4D	3.45	124.74	118.98
30	n	310	CHL	CMA-C3A-C4A	3.45	122.04	114.61
36	G	616	NEX	C2-C1-C6	3.44	112.56	109.21
31	r	303	CLA	O2D-CGD-O1D	-3.44	117.14	123.85
43	A	410	BCR	C4-C5-C6	-3.44	118.05	122.70
31	n	311	CLA	O2A-C1-C2	3.44	121.36	108.11
31	y	604	CLA	O2A-C1-C2	3.44	121.36	108.11
30	S	308	CHL	C1A-CHA-C4D	3.44	124.72	118.98
31	C	606	CLA	O2A-C1-C2	3.44	121.33	108.11
30	p	608	CHL	C1A-CHA-C4D	3.44	124.72	118.98
47	E	101	HEM	CHA-C4D-ND	3.44	128.62	124.37
31	2	611	CLA	C1-C2-C3	-3.43	120.57	126.20
43	c	615	BCR	C20-C19-C18	-3.43	116.95	126.36
31	B	605	CLA	O2A-C1-C2	3.43	121.32	108.11
32	s	318	LUT	C8-C7-C6	-3.43	117.84	127.00
43	A	410	BCR	C20-C19-C18	-3.43	116.96	126.36
30	G	606	CHL	C1A-CHA-C4D	3.43	124.70	118.98
36	y	618	NEX	C17-C1-C6	-3.42	107.41	110.47
31	g	310	CLA	O2A-C1-C2	3.42	121.28	108.11
30	Y	302	CHL	C1A-CHA-C4D	3.42	124.69	118.98
30	p	607	CHL	CHA-C1A-C2A	-3.42	125.27	133.31
36	p	618	NEX	C38-C25-C26	-3.42	116.67	122.30
32	p	617	LUT	C39-C29-C30	-3.42	117.27	122.82
32	0	616	LUT	C8-C7-C6	-3.42	117.87	127.00
32	G	615	LUT	C7-C8-C9	-3.42	121.18	126.23
34	3	321	LMG	O7-C10-C11	3.42	118.87	111.48
31	S	312	CLA	C1-C2-C3	-3.42	120.60	126.20
42	D	401	PHO	CMB-C2B-C3B	3.42	131.51	124.68
30	g	302	CHL	C1-C2-C3	-3.42	120.60	126.20
31	B	608	CLA	O2A-C1-C2	3.41	121.25	108.11
31	1	603	CLA	O2A-C1-C2	3.41	121.24	108.11
32	y	616	LUT	C10-C11-C12	-3.41	113.31	123.20
31	G	604	CLA	C1-C2-C3	-3.41	120.61	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	3	309	CHL	C3C-C4C-NC	-3.41	106.32	114.65
30	g	302	CHL	C1A-CHA-C4D	3.41	124.67	118.98
31	6	303	CLA	O2A-C1-C2	3.41	121.22	108.11
31	s	306	CLA	O2A-C1-C2	3.41	121.21	108.11
32	6	318	LUT	C31-C30-C29	-3.40	122.50	127.28
32	Y	316	LUT	C1-C6-C5	-3.40	117.98	122.64
43	B	618	BCR	C30-C25-C26	-3.40	117.98	122.64
31	Y	304	CLA	C1-C2-C3	-3.40	120.62	126.20
31	Y	305	CLA	O2A-C1-C2	3.40	121.20	108.11
30	G	607	CHL	C1-C2-C3	-3.40	121.26	126.76
31	y	610	CLA	O2A-C1-C2	3.40	121.20	108.11
31	C	610	CLA	O2A-C1-C2	3.40	121.20	108.11
31	p	602	CLA	O2A-C1-C2	3.40	121.20	108.11
30	y	601	CHL	C1-O2A-CGA	3.40	124.88	116.65
31	7	311	CLA	C1-C2-C3	-3.40	120.63	126.20
30	s	302	CHL	CHA-C1A-C2A	-3.40	125.32	133.31
31	R	311	CLA	C1-C2-C3	-3.40	120.63	126.20
32	n	318	LUT	C11-C10-C9	-3.40	122.52	127.28
31	b	609	CLA	O2A-C1-C2	3.40	121.17	108.11
32	5	616	LUT	C11-C10-C9	-3.39	122.52	127.28
43	t	101	BCR	C35-C13-C14	-3.39	117.32	122.82
30	4	601	CHL	C1A-CHA-C4D	3.39	124.64	118.98
31	6	316	CLA	O2A-C1-C2	3.39	121.15	108.11
31	g	311	CLA	C1-C2-C3	-3.39	120.65	126.20
43	v	101	BCR	C15-C14-C13	-3.39	122.53	127.28
31	4	603	CLA	C1-C2-C3	-3.39	120.65	126.20
31	n	316	CLA	O2A-C1-C2	3.39	121.14	108.11
30	Y	302	CHL	C1-O2A-CGA	3.39	124.84	116.65
30	6	302	CHL	C1-C2-C3	-3.39	120.65	126.20
30	S	302	CHL	CHA-C1A-C2A	-3.38	125.36	133.31
31	a	407	CLA	O2A-C1-C2	3.38	121.13	108.11
31	q	305	CLA	O2A-C1-C2	3.38	121.12	108.11
30	4	606	CHL	C1A-CHA-C4D	3.38	124.62	118.98
32	s	317	LUT	C31-C30-C29	-3.38	122.54	127.28
37	9	322	XAT	C6-C7-C8	-3.38	118.85	125.99
37	q	321	XAT	C6-C7-C8	-3.38	118.85	125.99
43	h	101	BCR	C38-C26-C25	-3.38	120.80	124.48
30	2	607	CHL	C1A-CHA-C4D	3.38	124.62	118.98
30	2	601	CHL	C1A-CHA-C4D	3.38	124.62	118.98
30	q	308	CHL	C3D-C4D-CHA	3.38	113.67	108.54
32	8	615	LUT	C21-C26-C27	-3.38	108.94	112.83
31	Y	310	CLA	O2A-C1-C2	3.37	121.09	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	4	619	XAT	C6-C7-C8	-3.37	118.86	125.99
43	v	101	BCR	C4-C5-C6	-3.37	118.15	122.70
31	0	610	CLA	O2A-C1-C2	3.37	121.08	108.11
43	T	101	BCR	C23-C24-C25	-3.37	117.99	127.00
37	R	318	XAT	C38-C25-C26	-3.37	116.75	122.30
32	8	616	LUT	C11-C10-C9	-3.37	122.55	127.28
43	B	617	BCR	C21-C20-C19	-3.37	113.43	123.20
30	N	306	CHL	C1A-CHA-C4D	3.37	124.60	118.98
31	5	611	CLA	O2A-C1-C2	3.37	121.07	108.11
33	B	624	LHG	O7-C7-C8	3.37	118.77	111.48
31	S	305	CLA	O2A-C1-C2	3.37	121.07	108.11
32	3	317	LUT	C31-C30-C29	-3.37	122.56	127.28
37	2	619	XAT	C6-C7-C8	-3.37	118.87	125.99
31	a	409	CLA	O2A-C1-C2	3.37	121.06	108.11
37	g	321	XAT	C6-C7-C8	-3.37	118.88	125.99
30	q	308	CHL	C1-C2-C3	-3.37	121.32	126.76
31	A	409	CLA	O2A-C1-C2	3.37	121.06	108.11
31	q	312	CLA	O2A-C1-C2	3.37	121.06	108.11
37	G	620	XAT	C6-C7-C8	-3.36	118.88	125.99
30	q	308	CHL	C1-O2A-CGA	3.36	124.79	116.65
31	6	304	CLA	O2A-C1-C2	3.36	121.05	108.11
31	S	310	CLA	C1-C2-C3	-3.36	120.69	126.20
30	7	307	CHL	C1-O2A-CGA	3.36	124.79	116.65
31	7	316	CLA	O2A-C1-C2	3.36	121.04	108.11
31	1	602	CLA	C1-C2-C3	-3.36	120.69	126.20
32	S	318	LUT	C11-C10-C9	-3.36	122.57	127.28
32	y	617	LUT	C31-C30-C29	-3.36	122.57	127.28
43	c	615	BCR	C8-C7-C6	-3.36	118.03	127.00
31	5	602	CLA	O2A-C1-C2	3.36	121.03	108.11
32	n	317	LUT	C21-C26-C27	-3.36	108.97	112.83
31	G	603	CLA	O2A-C1-C2	3.36	121.02	108.11
31	n	314	CLA	O2A-C1-C2	3.36	121.02	108.11
30	0	606	CHL	CHA-C1A-C2A	-3.35	125.43	133.31
47	E	101	HEM	CHB-C1B-NB	3.35	128.51	124.37
32	s	317	LUT	C21-C26-C27	-3.35	108.97	112.83
31	5	603	CLA	O2A-C1-C2	3.35	120.99	108.11
31	8	612	CLA	O2A-C1-C2	3.35	120.99	108.11
32	r	317	LUT	C30-C31-C32	-3.35	113.50	123.20
30	q	310	CHL	C1-O2A-CGA	3.35	124.75	116.65
31	b	604	CLA	O2A-C1-C2	3.35	120.99	108.11
30	2	601	CHL	C1-O2A-CGA	3.35	124.75	116.65
30	G	608	CHL	CMA-C3A-C4A	3.34	121.81	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	607	CHL	C1-C2-C3	-3.34	121.35	126.76
32	9	318	LUT	C26-C27-C28	-3.34	119.38	124.58
35	q	317	RRX	C8-C7-C6	-3.34	118.09	127.00
31	0	614	CLA	O2A-C1-C2	3.33	120.94	108.11
31	8	614	CLA	O2A-C1-C2	3.33	120.94	108.11
31	8	609	CLA	O2A-C1-C2	3.33	120.93	108.11
30	p	607	CHL	C1-C2-C3	-3.33	121.37	126.76
30	S	308	CHL	C3C-C4C-NC	-3.33	106.50	114.65
30	1	601	CHL	C3C-C4C-NC	-3.33	106.51	114.65
43	b	618	BCR	C20-C21-C22	-3.33	122.61	127.28
30	4	607	CHL	C1A-CHA-C4D	3.33	124.54	118.98
31	5	611	CLA	C1-C2-C3	-3.33	120.74	126.20
36	G	616	NEX	C17-C1-C6	-3.33	107.49	110.47
31	3	305	CLA	O2A-C1-C2	3.33	120.91	108.11
31	7	313	CLA	C1-C2-C3	-3.33	120.75	126.20
31	4	602	CLA	O2A-C1-C2	3.33	120.91	108.11
31	r	305	CLA	O2A-C1-C2	3.33	120.91	108.11
32	6	317	LUT	C7-C8-C9	-3.33	121.31	126.23
32	5	616	LUT	C21-C26-C27	-3.32	109.00	112.83
31	S	303	CLA	O2A-C1-C2	3.32	120.90	108.11
31	y	614	CLA	O2A-C1-C2	3.32	120.90	108.11
30	9	310	CHL	C1A-CHA-C4D	3.32	124.53	118.98
31	p	611	CLA	O2A-C1-C2	3.32	120.89	108.11
30	3	302	CHL	C3C-C4C-NC	-3.32	106.53	114.65
30	s	309	CHL	C1A-CHA-C4D	3.32	124.52	118.98
31	3	311	CLA	O2A-C1-C2	3.32	120.87	108.11
32	N	316	LUT	C1-C6-C5	-3.32	118.11	122.64
30	1	619	CHL	C3C-C4C-NC	-3.31	106.55	114.65
32	2	615	LUT	C7-C8-C9	-3.31	121.33	126.23
30	p	601	CHL	C1A-CHA-C4D	3.31	124.51	118.98
36	n	319	NEX	C31-C30-C29	3.31	131.92	127.28
31	g	304	CLA	O2A-C1-C2	3.31	120.85	108.11
43	b	620	BCR	C30-C25-C26	-3.31	118.11	122.64
31	r	303	CLA	C3B-C4B-NB	-3.31	107.58	110.53
43	d	406	BCR	C30-C25-C26	-3.31	118.11	122.64
32	r	317	LUT	C31-C30-C29	-3.31	122.64	127.28
31	G	610	CLA	O2A-C1-C2	3.31	120.84	108.11
31	B	613	CLA	O2A-C1-C2	3.31	120.83	108.11
30	1	606	CHL	C1A-CHA-C4D	3.31	124.50	118.98
30	n	306	CHL	C1A-CHA-C4D	3.31	124.50	118.98
31	q	304	CLA	O2A-C1-C2	3.31	120.83	108.11
43	c	614	BCR	C1-C6-C5	-3.30	118.12	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	8	605	CHL	C1A-CHA-C4D	3.30	124.50	118.98
31	7	311	CLA	O2A-C1-C2	3.30	120.81	108.11
31	8	602	CLA	O2A-C1-C2	3.30	120.81	108.11
31	s	306	CLA	C1D-ND-C4D	-3.30	104.00	106.31
31	G	609	CLA	C1-C2-C3	-3.30	120.79	126.20
30	1	608	CHL	C1A-CHA-C4D	3.30	124.49	118.98
30	6	310	CHL	C1A-CHA-C4D	3.30	124.48	118.98
31	3	313	CLA	O2A-C1-C2	3.30	120.80	108.11
31	B	604	CLA	CMA-C3A-C4A	3.30	120.64	111.77
30	Y	302	CHL	C3C-C4C-NC	-3.30	106.59	114.65
32	7	317	LUT	C18-C5-C6	-3.30	120.89	124.48
31	B	609	CLA	O2A-C1-C2	3.30	120.79	108.11
30	n	302	CHL	C3C-C4C-NC	-3.30	106.60	114.65
31	b	604	CLA	C1-C2-C3	-3.29	120.80	126.20
30	8	601	CHL	C3C-C4C-NC	-3.29	106.61	114.65
36	r	319	NEX	C17-C1-C6	-3.29	107.53	110.47
43	z	101	BCR	C38-C26-C25	-3.29	120.89	124.48
30	G	608	CHL	C3C-C4C-NC	-3.29	106.61	114.65
31	p	615	CLA	C3B-C4B-NB	-3.29	107.60	110.53
30	1	619	CHL	CAA-C2A-C3A	-3.29	104.12	113.00
30	0	606	CHL	C1-C2-C3	-3.28	121.45	126.76
31	3	301	CLA	C3B-C4B-NB	-3.28	107.60	110.53
31	4	604	CLA	O2A-C1-C2	3.28	120.75	108.11
31	d	404	CLA	C1-C2-C3	-3.28	120.82	126.20
30	g	309	CHL	C3C-C4C-NC	-3.28	106.62	114.65
30	Y	306	CHL	C1A-CHA-C4D	3.28	124.46	118.98
43	t	101	BCR	C23-C24-C25	-3.28	118.23	127.00
30	R	310	CHL	C3C-C4C-NC	-3.28	106.63	114.65
30	7	310	CHL	C1-C2-C3	-3.28	120.82	126.20
32	S	317	LUT	C21-C26-C27	-3.28	109.06	112.83
30	N	309	CHL	C3C-C4C-NC	-3.28	106.64	114.65
32	Y	315	LUT	C30-C31-C32	-3.28	113.70	123.20
32	s	318	LUT	C18-C5-C4	3.28	120.45	114.42
32	R	317	LUT	C8-C7-C6	-3.28	118.24	127.00
36	R	319	NEX	C38-C25-C26	-3.28	116.91	122.30
44	d	407	PL9	C7-C3-C4	3.28	119.61	116.91
31	0	602	CLA	O2A-C1-C2	3.28	120.71	108.11
34	W	201	LMG	O8-C28-C29	3.28	121.82	111.83
31	b	605	CLA	O2D-CGD-O1D	-3.27	117.47	123.85
30	Y	309	CHL	C1-C2-C3	-3.27	120.83	126.20
30	y	606	CHL	C1-O2A-CGA	3.27	124.58	116.65
31	R	305	CLA	C1C-C2C-C3C	-3.27	103.54	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	S	308	CHL	C4D-CHA-CBD	-3.27	105.67	108.97
43	b	618	BCR	C16-C15-C14	-3.27	116.82	123.52
31	2	610	CLA	O2A-C1-C2	3.27	120.70	108.11
30	n	310	CHL	C3C-C4C-NC	-3.27	106.66	114.65
31	0	603	CLA	C1-C2-C3	-3.27	120.84	126.20
31	b	611	CLA	O2A-C1-C2	3.27	120.69	108.11
43	d	406	BCR	C1-C6-C5	-3.27	118.17	122.64
32	6	317	LUT	C8-C7-C6	-3.27	118.27	127.00
43	B	617	BCR	C16-C15-C14	-3.27	116.83	123.52
31	c	606	CLA	C2C-C1C-NC	3.27	113.42	109.98
31	g	310	CLA	C1-C2-C3	-3.27	120.84	126.20
30	3	308	CHL	C1A-CHA-C4D	3.27	124.43	118.98
30	7	309	CHL	C3C-C4C-NC	-3.27	106.67	114.65
36	q	319	NEX	O24-C25-C38	-3.27	111.40	115.05
30	y	605	CHL	C3C-C4C-NC	-3.27	106.67	114.65
34	g	322	LMG	O8-C28-C29	3.26	121.79	111.83
31	q	312	CLA	C1D-ND-C4D	-3.26	104.02	106.31
31	r	303	CLA	O1D-CGD-CBD	-3.26	118.08	124.52
31	N	313	CLA	O2A-C1-C2	3.26	120.66	108.11
31	1	611	CLA	O2A-C1-C2	3.26	120.66	108.11
35	g	315	RRX	C20-C19-C18	-3.26	117.42	126.36
31	p	610	CLA	C1-C2-C3	-3.26	120.86	126.20
43	a	410	BCR	C8-C7-C6	-3.26	118.29	127.00
43	v	101	BCR	C30-C25-C26	-3.26	118.18	122.64
30	4	607	CHL	C3C-C4C-NC	-3.26	106.69	114.65
32	1	615	LUT	C30-C31-C32	-3.26	113.76	123.20
31	B	612	CLA	C1-C2-C3	-3.26	120.86	126.20
31	2	604	CLA	O2A-C1-C2	3.26	120.64	108.11
31	R	303	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
30	6	309	CHL	C3C-C4C-NC	-3.26	106.69	114.65
32	R	317	LUT	C1-C6-C5	-3.25	118.19	122.64
31	r	304	CLA	C1-C2-C3	-3.25	120.87	126.20
43	H	101	BCR	C20-C21-C22	-3.25	122.72	127.28
30	0	607	CHL	C1-C2-C3	-3.25	120.87	126.20
30	S	309	CHL	C1A-CHA-C4D	3.25	124.41	118.98
30	Y	301	CHL	C1-C2-C3	-3.25	120.88	126.20
32	r	317	LUT	C10-C11-C12	-3.25	113.79	123.20
43	C	615	BCR	C33-C5-C4	3.25	120.52	113.60
31	4	610	CLA	C1-C2-C3	-3.25	120.88	126.20
36	4	617	NEX	O24-C25-C38	-3.25	111.42	115.05
30	r	310	CHL	C3C-C4C-NC	-3.25	106.72	114.65
31	2	612	CLA	O2A-C1-C2	3.25	120.60	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	0	616	LUT	C35-C15-C14	-3.24	116.88	123.52
30	2	607	CHL	C1-O2A-CGA	3.24	124.50	116.65
34	n	322	LMG	O1-C1-C2	3.24	113.20	108.27
31	b	616	CLA	C2C-C1C-NC	3.24	113.39	109.98
34	9	301	LMG	O7-C10-C11	3.24	118.49	111.48
32	S	318	LUT	C7-C8-C9	-3.24	121.44	126.23
31	7	315	CLA	C1-C2-C3	-3.24	120.89	126.20
32	0	617	LUT	C31-C30-C29	-3.24	122.74	127.28
32	n	317	LUT	C7-C8-C9	-3.24	121.45	126.23
31	8	603	CLA	O2A-C1-C2	3.24	120.56	108.11
31	n	304	CLA	O2A-C1-C2	3.24	120.56	108.11
30	Y	301	CHL	C3C-C4C-NC	-3.23	106.74	114.65
43	B	617	BCR	C8-C7-C6	-3.23	118.36	127.00
30	y	607	CHL	C1-O2A-CGA	3.23	124.48	116.65
43	C	615	BCR	C38-C26-C25	-3.23	120.96	124.48
31	C	602	CLA	C1-C2-C3	-3.23	120.90	126.20
46	d	403	BCT	O3-C-O1	-3.23	111.41	119.68
43	T	101	BCR	C2-C1-C6	3.23	115.13	110.44
30	4	608	CHL	C3C-C4C-NC	-3.23	106.75	114.65
42	A	408	PHO	O1D-CGD-CBD	3.23	129.62	124.72
36	S	319	NEX	C17-C1-C6	-3.23	107.58	110.47
30	y	609	CHL	C1-O2A-CGA	3.23	124.47	116.65
31	b	614	CLA	O2A-C1-C2	3.23	120.53	108.11
31	5	610	CLA	O2A-C1-C2	3.23	120.53	108.11
30	1	601	CHL	C1B-CHB-C4A	3.23	123.40	121.32
31	2	609	CLA	C1-C2-C3	-3.23	120.91	126.20
43	v	101	BCR	C8-C7-C6	-3.22	118.39	127.00
30	0	608	CHL	C3C-C4C-NC	-3.22	106.77	114.65
31	1	614	CLA	O2A-C1-C2	3.22	120.51	108.11
30	Y	306	CHL	C3C-C4C-NC	-3.22	106.78	114.65
32	8	615	LUT	C7-C8-C9	-3.22	121.47	126.23
32	S	318	LUT	C8-C7-C6	-3.22	118.40	127.00
30	R	310	CHL	CHA-C1A-C2A	-3.22	125.75	133.31
33	b	628	LHG	O8-C23-C24	3.22	121.64	111.83
31	p	603	CLA	C1-O2A-CGA	3.22	124.44	116.65
34	9	321	LMG	O8-C28-C29	3.22	121.64	111.83
30	7	306	CHL	C1A-CHA-C4D	3.22	124.35	118.98
31	C	609	CLA	C2C-C1C-NC	3.22	113.36	109.98
30	5	605	CHL	C1A-CHA-C4D	3.21	124.34	118.98
31	1	614	CLA	C1-C2-C3	-3.21	120.93	126.20
31	B	615	CLA	C1-C2-C3	-3.21	120.93	126.20
31	1	602	CLA	O2A-C1-C2	3.21	120.47	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1	615	LUT	C10-C11-C12	-3.21	113.89	123.20
31	b	613	CLA	C1-C2-C3	-3.21	120.93	126.20
31	G	604	CLA	O2A-C1-C2	3.21	120.47	108.11
43	T	101	BCR	C30-C25-C26	-3.21	118.25	122.64
31	B	615	CLA	O2A-C1-C2	3.21	120.47	108.11
32	S	318	LUT	C27-C28-C29	-3.21	119.42	126.32
31	n	303	CLA	C1-C2-C3	-3.21	120.94	126.20
43	c	614	BCR	C27-C26-C25	-3.21	118.37	122.70
30	y	605	CHL	C1A-CHA-C4D	3.21	124.34	118.98
30	G	623	CHL	C3C-C4C-NC	-3.21	106.81	114.65
32	S	318	LUT	C18-C5-C6	-3.21	120.98	124.48
30	S	309	CHL	C3C-C4C-NC	-3.21	106.81	114.65
30	r	308	CHL	C1-C2-C3	-3.21	120.94	126.20
31	1	612	CLA	C1-C2-C3	-3.21	120.94	126.20
32	S	317	LUT	C11-C10-C9	-3.21	122.78	127.28
32	8	616	LUT	C21-C26-C27	-3.21	109.14	112.83
31	n	303	CLA	O2A-C1-C2	3.21	120.44	108.11
38	b	627	SQD	O7-S-C6	-3.20	101.97	106.76
30	2	601	CHL	C3C-C4C-NC	-3.20	106.82	114.65
31	y	603	CLA	O2A-C1-C2	3.20	120.44	108.11
32	y	617	LUT	C8-C7-C6	-3.20	118.44	127.00
30	0	601	CHL	C1-C2-C3	-3.20	120.95	126.20
31	6	314	CLA	O2A-C1-C2	3.20	120.43	108.11
34	B	621	LMG	O8-C28-C29	3.20	121.59	111.83
32	n	318	LUT	C21-C26-C27	-3.20	109.15	112.83
43	T	101	BCR	C15-C14-C13	-3.20	122.79	127.28
43	h	101	BCR	C2-C1-C6	3.20	115.09	110.44
30	8	608	CHL	C3C-C4C-NC	-3.20	106.83	114.65
33	t	102	LHG	C5-O7-C7	-3.20	110.14	117.80
31	2	603	CLA	O2A-C1-C2	3.20	120.41	108.11
31	N	303	CLA	O2A-C1-C2	3.20	120.41	108.11
30	7	306	CHL	C1-O2A-CGA	3.20	124.39	116.65
30	g	308	CHL	C1-O2A-CGA	3.20	124.39	116.65
43	b	619	BCR	C8-C7-C6	-3.19	118.47	127.00
30	7	308	CHL	C3C-C4C-NC	-3.19	106.84	114.65
31	4	603	CLA	O2A-C1-C2	3.19	120.40	108.11
33	g	319	LHG	O8-C23-C24	3.19	121.57	111.83
30	7	302	CHL	C1-O2A-CGA	3.19	124.38	116.65
31	9	314	CLA	C3B-C4B-NB	-3.19	107.68	110.53
30	7	321	CHL	C3C-C4C-NC	-3.19	106.85	114.65
30	N	307	CHL	C3C-C4C-NC	-3.19	106.85	114.65
36	N	318	NEX	C20-C13-C14	-3.19	117.65	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	v	101	BCR	C10-C11-C12	-3.19	113.96	123.20
30	p	606	CHL	C1-C2-C3	-3.19	121.60	126.76
30	N	308	CHL	C3C-C4C-NC	-3.19	106.86	114.65
31	7	304	CLA	O2A-C1-C2	3.19	120.37	108.11
31	N	304	CLA	O2A-C1-C2	3.19	120.37	108.11
30	5	607	CHL	C3C-C4C-NC	-3.19	106.86	114.65
34	k	101	LMG	O8-C28-C29	3.18	121.55	111.83
30	4	609	CHL	C1-C2-C3	-3.18	120.98	126.20
32	3	318	LUT	C15-C35-C34	-3.18	117.00	123.52
30	N	302	CHL	C3C-C4C-NC	-3.18	106.87	114.65
30	g	302	CHL	C3C-C4C-NC	-3.18	106.87	114.65
30	y	608	CHL	C3C-C4C-NC	-3.18	106.87	114.65
30	q	310	CHL	C3C-C4C-NC	-3.18	106.87	114.65
43	a	410	BCR	C7-C8-C9	-3.18	121.53	126.23
30	n	308	CHL	C3C-C4C-NC	-3.18	106.87	114.65
31	R	316	CLA	O2A-C1-C2	3.18	120.35	108.11
30	7	302	CHL	C1-C2-C3	-3.18	120.98	126.20
30	2	607	CHL	C3C-C4C-NC	-3.18	106.88	114.65
31	p	610	CLA	O2A-C1-C2	3.18	120.35	108.11
31	p	614	CLA	C1-C2-C3	-3.18	120.99	126.20
32	0	616	LUT	C30-C31-C32	-3.18	113.99	123.20
42	A	408	PHO	C2B-C1B-NB	-3.18	107.13	109.43
43	b	619	BCR	C24-C23-C22	-3.18	121.53	126.23
30	G	601	CHL	C1-C2-C3	-3.18	120.99	126.20
31	6	312	CLA	C1-C2-C3	-3.18	120.99	126.20
31	b	613	CLA	O2A-C1-C2	3.18	120.34	108.11
30	S	302	CHL	C1A-CHA-C4D	3.18	124.28	118.98
31	p	614	CLA	C1D-ND-C4D	-3.18	104.08	106.31
43	B	619	BCR	C1-C6-C5	-3.18	118.30	122.64
31	6	311	CLA	O2A-C1-C2	3.18	120.33	108.11
31	6	312	CLA	CMA-C3A-C4A	3.17	120.31	111.77
31	9	314	CLA	O2A-C1-C2	3.17	120.32	108.11
42	D	401	PHO	O1D-CGD-CBD	3.17	129.54	124.72
30	1	607	CHL	C3C-C4C-NC	-3.17	106.89	114.65
46	D	402	BCT	O2-C-O1	-3.17	111.56	119.68
30	8	605	CHL	C3C-C4C-NC	-3.17	106.91	114.65
30	y	601	CHL	C3C-C4C-NC	-3.17	106.91	114.65
43	D	405	BCR	C12-C13-C14	3.17	123.99	119.01
30	n	306	CHL	C3C-C4C-NC	-3.17	106.91	114.65
30	6	310	CHL	C3C-C4C-NC	-3.17	106.91	114.65
36	g	317	NEX	C38-C25-C26	-3.17	117.09	122.30
30	p	607	CHL	C3C-C4C-NC	-3.17	106.91	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	n	318	LUT	C31-C30-C29	-3.17	122.84	127.28
43	c	615	BCR	C30-C25-C26	-3.17	118.31	122.64
43	B	618	BCR	C24-C23-C22	-3.16	121.55	126.23
47	e	102	HEM	C1B-NB-C4B	3.16	108.95	105.21
31	p	611	CLA	C3B-C4B-NB	-3.16	107.71	110.53
30	8	607	CHL	C3C-C4C-NC	-3.16	106.92	114.65
30	S	302	CHL	C3C-C4C-NC	-3.16	106.92	114.65
31	3	306	CLA	O2A-C1-C2	3.16	120.28	108.11
43	Z	101	BCR	C30-C25-C26	-3.16	118.31	122.64
31	7	313	CLA	O2A-C1-C2	3.16	120.27	108.11
42	A	408	PHO	O2D-CGD-O1D	-3.16	117.70	123.85
31	Y	313	CLA	CMA-C3A-C4A	3.16	120.27	111.77
31	R	306	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
32	8	616	LUT	C31-C30-C29	-3.16	122.85	127.28
30	g	307	CHL	C3C-C4C-NC	-3.16	106.93	114.65
31	b	613	CLA	C1D-ND-C4D	-3.16	104.10	106.31
30	1	608	CHL	C3C-C4C-NC	-3.16	106.93	114.65
30	0	609	CHL	C1-O2A-CGA	3.16	124.29	116.65
31	c	602	CLA	C1-C2-C3	-3.16	121.02	126.20
30	3	310	CHL	C3C-C4C-NC	-3.16	106.94	114.65
30	4	609	CHL	C3C-C4C-NC	-3.16	106.94	114.65
30	0	609	CHL	C3C-C4C-NC	-3.15	106.94	114.65
32	0	616	LUT	C1-C6-C5	-3.15	118.33	122.64
30	y	607	CHL	C3C-C4C-NC	-3.15	106.94	114.65
30	Y	306	CHL	CHA-C1A-C2A	-3.15	125.90	133.31
31	2	602	CLA	O2A-C1-C2	3.15	120.24	108.11
31	q	306	CLA	O2A-C1-C2	3.15	120.24	108.11
43	D	405	BCR	C38-C26-C27	3.15	120.31	113.60
31	R	304	CLA	O2A-C1-C2	3.15	120.23	108.11
31	5	603	CLA	C1-C2-C3	-3.15	121.03	126.20
31	2	612	CLA	CMA-C3A-C4A	3.15	120.24	111.77
30	4	606	CHL	C1-C2-C3	-3.15	121.67	126.76
30	s	308	CHL	C3C-C4C-NC	-3.15	106.95	114.65
30	q	309	CHL	C1A-CHA-C4D	3.15	124.23	118.98
30	5	606	CHL	C1-C2-C3	-3.15	121.67	126.76
31	0	613	CLA	O2A-C1-C2	3.15	120.21	108.11
32	4	616	LUT	C21-C26-C27	-3.14	109.21	112.83
31	G	612	CLA	O2A-C1-C2	3.14	120.21	108.11
30	6	302	CHL	C1-O2A-CGA	3.14	124.26	116.65
32	3	318	LUT	C21-C26-C27	-3.14	109.21	112.83
31	r	315	CLA	C1-O2A-CGA	3.14	124.26	116.65
31	Y	304	CLA	O2A-C1-C2	3.14	120.20	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	9	322	XAT	C7-C8-C9	-3.14	120.65	125.53
36	2	616	NEX	C38-C25-C26	-3.14	117.13	122.30
37	q	321	XAT	C7-C8-C9	-3.14	120.66	125.53
34	0	620	LMG	O1-C1-C2	3.14	113.04	108.27
30	N	302	CHL	C1-O2A-CGA	3.14	124.25	116.65
30	Y	309	CHL	CMA-C3A-C4A	3.14	121.37	114.61
30	5	608	CHL	C3C-C4C-NC	-3.14	106.98	114.65
30	6	302	CHL	C3C-C4C-NC	-3.14	106.98	114.65
43	B	619	BCR	C8-C7-C6	-3.14	118.62	127.00
30	G	623	CHL	C1-O2A-CGA	3.14	124.24	116.65
31	7	315	CLA	O2A-C1-C2	3.14	120.18	108.11
32	s	318	LUT	C18-C5-C6	-3.14	121.06	124.48
34	C	619	LMG	O8-C28-C29	3.14	121.40	111.83
31	7	304	CLA	C3B-C4B-NB	-3.14	107.73	110.53
31	y	611	CLA	C3B-C4B-NB	-3.14	107.73	110.53
33	A	415	LHG	O8-C23-C24	3.14	121.39	111.83
31	9	315	CLA	C1-C2-C3	-3.13	121.06	126.20
32	3	318	LUT	C18-C5-C4	3.13	120.18	114.42
30	9	311	CHL	C3C-C4C-NC	-3.13	106.99	114.65
31	g	314	CLA	C3B-C4B-NB	-3.13	107.73	110.53
31	c	608	CLA	O2A-C1-C2	3.13	120.17	108.11
30	8	605	CHL	C1-C2-C3	-3.13	121.06	126.20
32	y	617	LUT	C30-C31-C32	-3.13	114.12	123.20
31	2	602	CLA	C1D-ND-C4D	-3.13	104.11	106.31
30	5	609	CHL	C3C-C4C-NC	-3.13	106.99	114.65
33	K	102	LHG	O8-C23-C24	3.13	121.39	111.83
31	C	611	CLA	C1-C2-C3	-3.13	121.06	126.20
30	8	606	CHL	C1-C2-C3	-3.13	121.07	126.20
30	n	306	CHL	C1-C2-C3	-3.13	121.07	126.20
31	c	606	CLA	O2A-C1-C2	3.13	120.15	108.11
31	5	613	CLA	C1-C2-C3	-3.13	121.07	126.20
43	C	615	BCR	C27-C26-C25	-3.13	118.48	122.70
30	n	309	CHL	C3C-C4C-NC	-3.13	107.00	114.65
31	8	610	CLA	C3B-C4B-NB	-3.13	107.74	110.53
32	p	616	LUT	C31-C30-C29	3.13	131.66	127.28
30	3	307	CHL	C3C-C4C-NC	-3.13	107.01	114.65
37	2	619	XAT	C7-C8-C9	-3.12	120.68	125.53
37	G	620	XAT	C7-C8-C9	-3.12	120.68	125.53
37	g	321	XAT	C7-C8-C9	-3.12	120.68	125.53
31	s	303	CLA	O2A-C1-C2	3.12	120.13	108.11
30	s	309	CHL	C3C-C4C-NC	-3.12	107.02	114.65
36	5	618	NEX	C17-C1-C6	-3.12	107.68	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	g	303	CLA	C1-O2A-CGA	3.12	124.21	116.65
30	6	308	CHL	C3C-C4C-NC	-3.12	107.02	114.65
37	4	619	XAT	C7-C8-C9	-3.12	120.69	125.53
43	C	615	BCR	C19-C18-C17	3.12	123.92	119.01
31	r	307	CLA	C2C-C1C-NC	3.12	113.26	109.98
31	n	312	CLA	C3B-C4B-NB	-3.12	107.75	110.53
31	6	305	CLA	O2A-C1-C2	3.12	120.11	108.11
30	1	606	CHL	C3C-C4C-NC	-3.12	107.03	114.65
43	A	410	BCR	C23-C24-C25	-3.12	118.67	127.00
30	Y	306	CHL	C4D-CHA-CBD	-3.12	105.83	108.97
33	A	415	LHG	C5-O7-C7	-3.12	110.34	117.80
30	G	623	CHL	C1-C2-C3	-3.12	121.09	126.20
30	G	601	CHL	C3C-C4C-NC	-3.11	107.04	114.65
31	s	311	CLA	C1-C2-C3	-3.11	121.09	126.20
36	8	617	NEX	C38-C25-C26	-3.11	117.18	122.30
42	a	408	PHO	C2B-C1B-NB	-3.11	107.18	109.43
30	2	608	CHL	C3C-C4C-NC	-3.11	107.04	114.65
31	5	604	CLA	O2A-C1-C2	3.11	120.08	108.11
30	y	609	CHL	C3C-C4C-NC	-3.11	107.05	114.65
30	2	606	CHL	C1-C2-C3	-3.11	121.73	126.76
32	6	317	LUT	C15-C14-C13	-3.11	122.92	127.28
31	B	612	CLA	O2A-C1-C2	3.11	120.07	108.11
31	Y	311	CLA	O2A-C1-C2	3.11	120.07	108.11
32	Y	316	LUT	C30-C31-C32	-3.11	114.19	123.20
30	1	619	CHL	C4D-CHA-CBD	-3.11	105.83	108.97
32	s	318	LUT	C11-C10-C9	-3.11	122.92	127.28
30	3	303	CHL	C3C-C4C-NC	-3.11	107.06	114.65
30	p	605	CHL	C3C-C4C-NC	-3.11	107.06	114.65
34	0	622	LMG	O8-C28-C29	3.11	121.31	111.83
31	9	304	CLA	C1D-ND-C4D	-3.11	104.13	106.31
30	R	309	CHL	C3C-C4C-NC	-3.10	107.06	114.65
30	0	607	CHL	C3C-C4C-NC	-3.10	107.06	114.65
30	p	608	CHL	C3C-C4C-NC	-3.10	107.07	114.65
42	d	402	PHO	C2B-C1B-NB	-3.10	107.19	109.43
31	R	307	CLA	C2C-C1C-NC	3.10	113.24	109.98
30	6	306	CHL	C3C-C4C-NC	-3.10	107.07	114.65
30	G	605	CHL	C3C-C4C-NC	-3.10	107.07	114.65
30	5	609	CHL	C1-O2A-CGA	3.10	124.16	116.65
30	R	310	CHL	C1A-CHA-C4D	3.10	124.16	118.98
43	v	101	BCR	C23-C24-C25	-3.10	118.72	127.00
32	5	616	LUT	C31-C30-C29	-3.10	122.93	127.28
31	1	603	CLA	C1-C2-C3	-3.10	121.12	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	B	618	BCR	C27-C26-C25	-3.10	118.52	122.70
37	g	321	XAT	C38-C25-C26	-3.10	117.20	122.30
34	n	322	LMG	O8-C28-C29	3.10	121.28	111.83
31	3	312	CLA	C1-C2-C3	-3.10	121.12	126.20
30	Y	309	CHL	C3C-C4C-NC	-3.10	107.08	114.65
34	0	620	LMG	C8-O7-C10	-3.10	110.39	117.80
30	2	606	CHL	C3C-C4C-NC	-3.10	107.08	114.65
31	S	306	CLA	C1D-ND-C4D	-3.09	104.14	106.31
30	Y	308	CHL	C1-O2A-CGA	3.09	124.14	116.65
31	r	305	CLA	C1-C2-C3	-3.09	121.13	126.20
31	c	606	CLA	C1C-C2C-C3C	-3.09	103.73	106.98
31	C	612	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
30	n	307	CHL	C3C-C4C-NC	-3.09	107.09	114.65
30	8	606	CHL	C3C-C4C-NC	-3.09	107.09	114.65
30	y	606	CHL	C3C-C4C-NC	-3.09	107.09	114.65
31	c	601	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
34	b	622	LMG	O8-C28-C29	3.09	121.26	111.83
30	n	307	CHL	C1-C2-C3	-3.09	121.13	126.20
30	q	307	CHL	C3C-C4C-NC	-3.09	107.10	114.65
30	0	606	CHL	C4D-CHA-CBD	-3.09	105.85	108.97
30	1	609	CHL	C3C-C4C-NC	-3.09	107.10	114.65
32	9	318	LUT	C21-C26-C27	-3.09	109.28	112.83
30	9	310	CHL	C3C-C4C-NC	-3.09	107.10	114.65
34	c	621	LMG	O8-C28-C29	3.09	121.25	111.83
32	s	318	LUT	C7-C8-C9	-3.09	121.67	126.23
31	c	601	CLA	C3B-C4B-NB	-3.09	107.77	110.53
30	2	608	CHL	CMA-C3A-C4A	3.09	121.26	114.61
30	y	609	CHL	CMA-C3A-C4A	3.09	121.26	114.61
30	N	306	CHL	C3C-C4C-NC	-3.09	107.11	114.65
30	7	306	CHL	C3C-C4C-NC	-3.09	107.11	114.65
31	7	303	CLA	O2A-C1-C2	3.09	119.98	108.11
31	g	303	CLA	O2A-C1-C2	3.09	119.98	108.11
31	b	607	CLA	O2A-CGA-CBA	3.08	121.24	111.83
30	p	609	CHL	C3C-C4C-NC	-3.08	107.11	114.65
30	S	309	CHL	C1-O2A-CGA	3.08	124.12	116.65
30	8	608	CHL	CMA-C3A-C4A	3.08	121.26	114.61
31	r	311	CLA	O2A-CGA-CBA	3.08	121.24	111.83
30	4	601	CHL	C3C-C4C-NC	-3.08	107.11	114.65
32	g	316	LUT	C18-C5-C4	3.08	120.09	114.42
30	q	303	CHL	C3C-C4C-NC	-3.08	107.11	114.65
31	3	316	CLA	O2A-C1-C2	3.08	119.97	108.11
30	Y	307	CHL	C3C-C4C-NC	-3.08	107.12	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	R	310	CHL	C4D-CHA-CBD	-3.08	105.86	108.97
32	7	317	LUT	C1-C6-C5	-3.08	118.42	122.64
30	s	302	CHL	C3C-C4C-NC	-3.08	107.12	114.65
31	g	305	CLA	O2A-C1-C2	3.08	119.96	108.11
32	p	617	LUT	C18-C5-C4	3.08	120.08	114.42
31	1	613	CLA	O2A-C1-C2	3.08	119.95	108.11
31	q	305	CLA	CMA-C3A-C4A	3.08	120.05	111.77
37	q	321	XAT	C38-C25-C26	-3.08	117.24	122.30
30	g	308	CHL	C3C-C4C-NC	-3.08	107.13	114.65
30	g	309	CHL	C1-C2-C3	-3.08	121.16	126.20
30	6	307	CHL	C3C-C4C-NC	-3.07	107.14	114.65
31	B	604	CLA	C2C-C1C-NC	3.07	113.21	109.98
32	q	318	LUT	C18-C5-C4	3.07	120.07	114.42
37	2	619	XAT	C38-C25-C26	-3.07	117.24	122.30
30	R	310	CHL	C1-C2-C3	-3.07	121.17	126.20
31	1	611	CLA	C3B-C4B-NB	-3.07	107.79	110.53
32	6	317	LUT	C11-C10-C9	-3.07	122.97	127.28
43	V	101	BCR	C10-C11-C12	-3.07	114.31	123.20
33	A	417	LHG	O8-C23-C24	3.07	121.19	111.83
31	6	304	CLA	C3B-C4B-NB	-3.07	107.79	110.53
31	3	304	CLA	CMA-C3A-C4A	3.07	120.02	111.77
31	R	303	CLA	O1D-CGD-CBD	-3.07	118.47	124.52
31	S	314	CLA	O2A-C1-C2	3.07	119.91	108.11
37	r	318	XAT	C6-C7-C8	-3.07	119.51	125.99
35	g	315	RRX	C11-C12-C13	-3.07	117.95	126.36
30	7	302	CHL	C3C-C4C-NC	-3.07	107.16	114.65
33	5	619	LHG	C5-O7-C7	-3.06	110.46	117.80
33	e	101	LHG	C5-O7-C7	-3.06	110.46	117.80
32	R	317	LUT	C40-C33-C34	-3.06	117.85	122.82
30	g	309	CHL	CMA-C3A-C4A	3.06	121.21	114.61
30	g	306	CHL	C3C-C4C-NC	-3.06	107.17	114.65
30	r	309	CHL	C3C-C4C-NC	-3.06	107.17	114.65
37	4	619	XAT	C38-C25-C26	-3.06	117.26	122.30
31	r	312	CLA	C1-C2-C3	-3.06	121.18	126.20
31	4	612	CLA	C3B-C4B-NB	-3.06	107.80	110.53
32	1	615	LUT	C35-C15-C14	-3.06	117.26	123.52
31	q	315	CLA	C1-C2-C3	-3.06	121.18	126.20
43	C	614	BCR	C1-C6-C5	-3.06	118.45	122.64
30	p	601	CHL	C1-C2-C3	-3.06	121.81	126.76
31	2	611	CLA	O2A-C1-C2	3.06	119.88	108.11
30	7	307	CHL	C3C-C4C-NC	-3.06	107.18	114.65
43	T	101	BCR	C24-C23-C22	-3.06	121.71	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	s	322	LHG	O8-C23-C24	3.06	121.16	111.83
30	7	310	CHL	C3C-C4C-NC	-3.06	107.18	114.65
30	3	310	CHL	CMA-C3A-C4A	3.06	121.20	114.61
30	n	301	CHL	C3C-C4C-NC	-3.06	107.18	114.65
34	9	302	LMG	O8-C28-C29	3.06	121.15	111.83
32	s	318	LUT	C31-C30-C29	-3.05	122.99	127.28
37	9	322	XAT	C38-C25-C26	-3.05	117.28	122.30
30	5	605	CHL	C3C-C4C-NC	-3.05	107.19	114.65
31	A	406	CLA	C1C-C2C-C3C	-3.05	103.77	106.98
32	r	317	LUT	C35-C15-C14	-3.05	117.27	123.52
31	C	612	CLA	C2C-C1C-NC	3.05	113.19	109.98
30	N	302	CHL	C1-C2-C3	-3.05	121.20	126.20
30	0	601	CHL	C3C-C4C-NC	-3.05	107.19	114.65
31	6	313	CLA	O2A-C1-C2	3.05	119.85	108.11
31	2	610	CLA	C3B-C4B-NB	-3.05	107.81	110.53
31	5	611	CLA	C3B-C4B-NB	-3.05	107.81	110.53
43	a	410	BCR	C1-C6-C5	-3.05	118.47	122.64
31	0	613	CLA	CMA-C3A-C4A	3.05	119.97	111.77
43	V	101	BCR	C8-C7-C6	-3.05	118.85	127.00
31	S	313	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
30	Y	308	CHL	C3C-C4C-NC	-3.05	107.20	114.65
31	4	610	CLA	C3B-C4B-NB	-3.05	107.81	110.53
31	s	313	CLA	C2C-C1C-NC	3.05	113.18	109.98
30	r	308	CHL	C3C-C4C-NC	-3.05	107.20	114.65
31	n	304	CLA	CMA-C3A-C4A	3.05	119.96	111.77
31	y	615	CLA	C3B-C4B-NB	-3.04	107.81	110.53
30	5	607	CHL	C1A-CHA-C4D	3.04	124.06	118.98
31	c	603	CLA	CMA-C3A-C4A	3.04	119.95	111.77
31	N	312	CLA	C3B-C4B-NB	-3.04	107.81	110.53
31	q	304	CLA	CMA-C3A-C4A	3.04	119.95	111.77
32	0	616	LUT	C15-C14-C13	-3.04	123.01	127.28
32	N	317	LUT	C21-C26-C27	-3.04	109.33	112.83
31	9	315	CLA	CMA-C3A-C4A	3.04	119.95	111.77
30	5	609	CHL	CMA-C3A-C4A	3.04	121.16	114.61
34	b	626	LMG	O8-C28-C29	3.04	121.11	111.83
30	9	303	CHL	C3C-C4C-NC	-3.04	107.22	114.65
43	B	619	BCR	C15-C16-C17	-3.04	117.30	123.52
37	G	620	XAT	C38-C25-C26	-3.04	117.30	122.30
31	Y	313	CLA	O2A-C1-C2	3.04	119.80	108.11
31	S	311	CLA	C1-C2-C3	-3.04	121.22	126.20
31	c	612	CLA	C2C-C1C-NC	3.04	113.17	109.98
30	0	605	CHL	C1A-CHA-C4D	3.04	124.05	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	B	618	BCR	C16-C17-C18	-3.04	123.02	127.28
30	G	606	CHL	C3C-C4C-NC	-3.04	107.23	114.65
31	7	303	CLA	C1-C2-C3	-3.04	121.22	126.20
33	9	320	LHG	C5-O7-C7	-3.04	110.53	117.80
30	p	606	CHL	C3C-C4C-NC	-3.04	107.23	114.65
31	4	603	CLA	CMA-C3A-C4A	3.04	119.93	111.77
31	C	605	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
30	5	607	CHL	CHA-C1A-C2A	-3.03	126.18	133.31
30	N	301	CHL	C3C-C4C-NC	-3.03	107.24	114.65
30	6	307	CHL	C1-C2-C3	-3.03	121.86	126.76
34	2	620	LMG	O8-C28-C29	3.03	121.08	111.83
31	6	304	CLA	C1-C2-C3	-3.03	121.23	126.20
43	C	614	BCR	C21-C20-C19	-3.03	114.42	123.20
36	6	319	NEX	C38-C25-C26	-3.03	117.31	122.30
36	r	319	NEX	C38-C25-C26	-3.03	117.32	122.30
30	N	309	CHL	CMA-C3A-C4A	3.03	121.14	114.61
31	C	606	CLA	C3B-C4B-NB	-3.03	107.83	110.53
31	G	603	CLA	C3B-C4B-NB	-3.03	107.83	110.53
30	9	309	CHL	C3C-C4C-NC	-3.03	107.25	114.65
35	2	614	RRX	C20-C19-C18	-3.03	118.06	126.36
31	c	611	CLA	CMA-C3A-C4A	3.03	119.91	111.77
31	r	304	CLA	O2A-C1-C2	3.03	119.76	108.11
36	0	618	NEX	C17-C1-C6	-3.03	107.76	110.47
31	c	613	CLA	O2A-C1-C2	3.03	119.76	108.11
33	D	408	LHG	O8-C23-C24	3.03	121.06	111.83
31	3	314	CLA	O2A-C1-C2	3.03	119.75	108.11
43	a	410	BCR	C16-C17-C18	-3.03	123.03	127.28
30	2	605	CHL	C3C-C4C-NC	-3.03	107.25	114.65
30	4	606	CHL	C3C-C4C-NC	-3.03	107.25	114.65
31	6	313	CLA	CMA-C3A-C4A	3.03	119.91	111.77
31	6	311	CLA	CMA-C3A-C4A	3.03	119.91	111.77
31	8	603	CLA	CMA-C3A-C4A	3.02	119.90	111.77
34	C	619	LMG	C8-O7-C10	-3.02	110.56	117.80
43	B	617	BCR	C10-C11-C12	-3.02	114.44	123.20
30	q	311	CHL	C3C-C4C-NC	-3.02	107.26	114.65
31	D	404	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
31	c	605	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
31	B	610	CLA	CMA-C3A-C4A	3.02	119.90	111.77
31	Y	312	CLA	C3B-C4B-NB	-3.02	107.83	110.53
31	3	301	CLA	CMA-C3A-C4A	3.02	119.89	111.77
34	6	322	LMG	O8-C28-C29	3.02	121.05	111.83
31	5	612	CLA	CMA-C3A-C4A	3.02	119.89	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	N	321	CLA	C3B-C4B-NB	-3.02	107.83	110.53
31	q	305	CLA	C3B-C4B-NB	-3.02	107.83	110.53
36	Y	317	NEX	C17-C1-C6	-3.02	107.77	110.47
32	r	317	LUT	C15-C35-C34	-3.02	117.34	123.52
30	8	606	CHL	C1-O2A-CGA	3.02	123.96	116.65
31	y	614	CLA	C3B-C4B-NB	-3.02	107.84	110.53
31	q	314	CLA	C3B-C4B-NB	-3.02	107.84	110.53
31	0	615	CLA	O2A-C1-C2	3.02	119.72	108.11
31	c	610	CLA	O2A-CGA-CBA	3.02	121.03	111.83
32	6	317	LUT	C1-C6-C5	-3.02	118.52	122.64
36	0	618	NEX	C38-C25-C26	-3.02	117.34	122.30
34	b	624	LMG	O8-C28-C29	3.02	121.03	111.83
34	d	411	LMG	O8-C28-C29	3.02	121.03	111.83
37	r	318	XAT	C7-C8-C9	-3.01	120.85	125.53
31	6	313	CLA	C3B-C4B-NB	-3.01	107.84	110.53
31	C	609	CLA	C1C-C2C-C3C	-3.01	103.81	106.98
31	r	316	CLA	CMA-C3A-C4A	3.01	119.87	111.77
42	d	402	PHO	C4D-CHA-CBD	-3.01	107.01	108.45
31	Y	304	CLA	C3B-C4B-NB	-3.01	107.84	110.53
30	0	609	CHL	CMA-C3A-C4A	3.01	121.10	114.61
31	3	312	CLA	CMA-C3A-C4A	3.01	119.87	111.77
30	8	607	CHL	C1-O2A-CGA	3.01	123.94	116.65
31	N	311	CLA	C3B-C4B-NB	-3.01	107.84	110.53
31	3	305	CLA	CMA-C3A-C4A	3.01	119.86	111.77
31	2	609	CLA	O2A-C1-C2	3.01	119.69	108.11
36	9	319	NEX	C38-C25-C26	-3.01	117.35	122.30
33	d	408	LHG	C5-O7-C7	-3.01	110.60	117.80
34	Q1	101	LMG	O8-C28-C29	3.01	121.01	111.83
31	A	406	CLA	C2C-C1C-NC	3.01	113.14	109.98
31	7	312	CLA	C3B-C4B-NB	-3.01	107.85	110.53
30	0	605	CHL	CHA-C1A-C2A	-3.01	126.25	133.31
34	b	629	LMG	O8-C28-C29	3.01	121.00	111.83
34	c	620	LMG	C8-O7-C10	-3.01	110.60	117.80
31	B	616	CLA	C2C-C1C-NC	3.00	113.14	109.98
31	3	316	CLA	C1-C2-C3	-3.00	121.27	126.20
30	n	302	CHL	C1-O2A-CGA	3.00	123.92	116.65
31	D	403	CLA	C1-C2-C3	-3.00	121.28	126.20
31	2	603	CLA	CMA-C3A-C4A	3.00	119.84	111.77
31	p	612	CLA	C3B-C4B-NB	-3.00	107.85	110.53
30	9	307	CHL	C3C-C4C-NC	-3.00	107.31	114.65
31	3	315	CLA	C3B-C4B-NB	-3.00	107.85	110.53
31	q	315	CLA	C2C-C1C-NC	3.00	113.14	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	603	CLA	CMA-C3A-C4A	3.00	119.84	111.77
32	0	616	LUT	C7-C8-C9	-3.00	121.80	126.23
34	y	620	LMG	O8-C28-C29	3.00	120.99	111.83
30	p	601	CHL	C3C-C4C-NC	-3.00	107.31	114.65
31	S	304	CLA	C1C-C2C-C3C	-3.00	103.83	106.98
31	a	407	CLA	C1C-C2C-C3C	-3.00	103.83	106.98
31	7	311	CLA	C1D-ND-C4D	-3.00	104.21	106.31
30	n	307	CHL	C1-O2A-CGA	3.00	123.91	116.65
31	S	313	CLA	C2C-C1C-NC	3.00	113.13	109.98
34	B	625	LMG	O8-C28-C29	3.00	120.98	111.83
31	6	315	CLA	C1D-ND-C4D	-3.00	104.21	106.31
30	8	601	CHL	C1-O2A-CGA	3.00	123.91	116.65
31	b	605	CLA	C2C-C1C-NC	3.00	113.13	109.98
34	5	620	LMG	O8-C28-C29	3.00	120.97	111.83
31	C	611	CLA	CMA-C3A-C4A	3.00	119.83	111.77
31	1	610	CLA	C1D-ND-C4D	-3.00	104.21	106.31
31	5	610	CLA	C1D-ND-C4D	-3.00	104.21	106.31
30	9	308	CHL	C3C-C4C-NC	-3.00	107.33	114.65
43	V	101	BCR	C23-C24-C25	-2.99	119.00	127.00
45	c	618	DGD	O1G-C1A-C2A	2.99	120.97	111.83
43	B	619	BCR	C33-C5-C4	2.99	119.98	113.60
42	D	401	PHO	O2D-CGD-O1D	-2.99	118.02	123.85
32	G	615	LUT	C1-C6-C5	-2.99	118.54	122.64
47	E	101	HEM	C1B-NB-C4B	2.99	108.75	105.21
31	6	314	CLA	CMA-C3A-C4A	2.99	119.82	111.77
31	s	310	CLA	C2C-C1C-NC	2.99	113.13	109.98
30	5	606	CHL	C3C-C4C-NC	-2.99	107.33	114.65
31	p	614	CLA	C3B-C4B-NB	-2.99	107.86	110.53
43	B	619	BCR	C33-C5-C6	-2.99	121.22	124.48
30	4	605	CHL	C3C-C4C-NC	-2.99	107.33	114.65
30	3	302	CHL	C1A-CHA-C4D	2.99	123.97	118.98
30	q	309	CHL	C3C-C4C-NC	-2.99	107.34	114.65
32	5	616	LUT	C1-C6-C5	-2.99	118.55	122.64
31	N	310	CLA	CMA-C3A-C4A	2.99	119.81	111.77
43	B	618	BCR	C15-C16-C17	-2.99	117.40	123.52
31	R	307	CLA	C1C-C2C-C3C	-2.99	103.83	106.98
45	c	617	DGD	O1G-C1A-C2A	2.99	120.95	111.83
31	c	602	CLA	C2C-C1C-NC	2.99	113.12	109.98
31	b	603	CLA	C3B-C4B-NB	-2.99	107.86	110.53
31	1	612	CLA	O2A-CGA-CBA	2.99	120.95	111.83
31	4	614	CLA	CMA-C3A-C4A	2.99	119.80	111.77
31	7	314	CLA	O2A-C1-C2	2.99	119.61	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	607	CLA	O2A-C1-C2	2.99	119.60	108.11
34	I	101	LMG	O8-C28-C29	2.99	120.94	111.83
31	Y	310	CLA	C1D-ND-C4D	-2.99	104.22	106.31
31	g	313	CLA	C1-C2-C3	-2.99	121.31	126.20
30	q	303	CHL	C1-O2A-CGA	2.98	123.88	116.65
45	C	618	DGD	O2G-C1B-C2B	2.98	117.94	111.48
30	7	306	CHL	CMA-C3A-C4A	2.98	121.04	114.61
30	5	601	CHL	C3C-C4C-NC	-2.98	107.36	114.65
30	R	308	CHL	C3C-C4C-NC	-2.98	107.36	114.65
33	2	617	LHG	C5-O7-C7	-2.98	110.66	117.80
31	b	602	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
31	R	311	CLA	O2A-CGA-CBA	2.98	120.93	111.83
31	b	616	CLA	C1-C2-C3	-2.98	121.31	126.20
31	s	306	CLA	C3B-C4B-NB	-2.98	107.87	110.53
34	W	202	LMG	O8-C28-C29	2.98	120.92	111.83
31	r	316	CLA	C2C-C1C-NC	2.98	113.11	109.98
31	S	306	CLA	C3B-C4B-NB	-2.98	107.87	110.53
31	R	306	CLA	C2C-C1C-NC	2.98	113.11	109.98
36	6	319	NEX	C17-C1-C6	-2.98	107.81	110.47
31	B	607	CLA	C1C-C2C-C3C	-2.98	103.85	106.98
31	B	616	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
31	4	602	CLA	CMA-C3A-C4A	2.98	119.77	111.77
31	b	611	CLA	C3B-C4B-NB	-2.98	107.87	110.53
31	R	306	CLA	CAA-C2A-C3A	-2.98	104.96	113.00
31	8	609	CLA	CMA-C3A-C4A	2.98	119.77	111.77
31	C	601	CLA	C3B-C4B-NB	-2.98	107.87	110.53
31	b	602	CLA	C3B-C4B-NB	-2.98	107.87	110.53
31	n	303	CLA	CMA-C3A-C4A	2.97	119.77	111.77
31	B	615	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
31	9	304	CLA	CMA-C3A-C4A	2.97	119.77	111.77
45	C	617	DGD	O2G-C1B-C2B	2.97	117.92	111.48
37	g	321	XAT	C18-C5-C6	-2.97	117.41	122.30
31	3	311	CLA	C2C-C1C-NC	2.97	113.11	109.98
31	R	306	CLA	C1C-C2C-C3C	-2.97	103.85	106.98
31	C	601	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
33	8	618	LHG	O8-C23-C24	2.97	120.90	111.83
30	s	302	CHL	C1A-CHA-C4D	2.97	123.94	118.98
34	R	321	LMG	O8-C28-C29	2.97	120.90	111.83
31	0	610	CLA	C1D-ND-C4D	-2.97	104.23	106.31
31	r	304	CLA	CMA-C3A-C4A	2.97	119.76	111.77
43	C	615	BCR	C23-C24-C25	-2.97	119.06	127.00
37	G	620	XAT	C18-C5-C6	-2.97	117.41	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	1	611	CLA	CMA-C3A-C4A	2.97	119.75	111.77
31	g	313	CLA	O2A-C1-C2	2.97	119.53	108.11
31	p	613	CLA	C1C-C2C-C3C	-2.97	103.86	106.98
31	B	603	CLA	O2A-C1-C2	2.97	119.53	108.11
31	5	614	CLA	C3B-C4B-NB	-2.97	107.88	110.53
33	n	320	LHG	O8-C23-C24	2.97	120.88	111.83
31	8	602	CLA	CMA-C3A-C4A	2.97	119.75	111.77
31	y	610	CLA	C1D-ND-C4D	-2.97	104.23	106.31
31	c	602	CLA	C6-C5-C3	-2.97	106.24	113.47
30	1	605	CHL	C3C-C4C-NC	-2.97	107.40	114.65
43	C	615	BCR	C23-C22-C21	2.97	123.68	119.01
31	B	615	CLA	C1C-C2C-C3C	-2.97	103.86	106.98
31	2	609	CLA	C1D-ND-C4D	-2.97	104.23	106.31
34	a	401	LMG	C8-O7-C10	-2.97	110.70	117.80
33	j	102	LHG	C5-O7-C7	-2.97	110.70	117.80
31	A	406	CLA	CAA-C2A-C3A	-2.97	104.99	113.00
37	q	321	XAT	C18-C5-C6	-2.97	117.42	122.30
31	r	305	CLA	CMA-C3A-C4A	2.96	119.74	111.77
31	B	612	CLA	C3B-C4B-NB	-2.96	107.88	110.53
37	4	619	XAT	C18-C5-C6	-2.96	117.42	122.30
36	6	319	NEX	C26-C27-C28	-2.96	119.73	125.99
31	c	612	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
45	C	616	DGD	O1G-C1A-C2A	2.96	120.86	111.83
36	N	318	NEX	C17-C1-C6	-2.96	107.82	110.47
31	n	311	CLA	C1D-ND-C4D	-2.96	104.24	106.31
31	A	409	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
30	G	607	CHL	C3C-C4C-NC	-2.96	107.42	114.65
32	1	616	LUT	C31-C30-C29	-2.96	123.13	127.28
31	s	316	CLA	C1C-C2C-C3C	-2.96	103.87	106.98
45	c	616	DGD	O1G-C1A-C2A	2.96	120.85	111.83
31	4	613	CLA	C3B-C4B-NB	-2.96	107.89	110.53
36	0	618	NEX	C26-C27-C28	-2.96	119.74	125.99
31	5	602	CLA	C1D-ND-C4D	-2.95	104.24	106.31
31	C	602	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
31	0	604	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
31	2	604	CLA	C2C-C1C-NC	2.95	113.08	109.98
31	q	306	CLA	C2C-C1C-NC	2.95	113.08	109.98
31	C	610	CLA	O2A-CGA-CBA	2.95	120.84	111.83
32	6	317	LUT	C30-C31-C32	-2.95	114.64	123.20
30	1	609	CHL	CMA-C3A-C4A	2.95	120.97	114.61
31	c	609	CLA	C2C-C1C-NC	2.95	113.08	109.98
31	4	602	CLA	C1D-ND-C4D	-2.95	104.24	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	6	311	CLA	C1D-ND-C4D	-2.95	104.24	106.31
42	A	408	PHO	CMB-C2B-C3B	2.95	130.58	124.68
31	1	603	CLA	C2C-C1C-NC	2.95	113.08	109.98
36	6	319	NEX	C2-C1-C6	2.95	112.08	109.21
31	3	315	CLA	CMA-C3A-C4A	2.95	119.70	111.77
31	N	310	CLA	C1D-ND-C4D	-2.95	104.24	106.31
31	p	611	CLA	C1D-ND-C4D	-2.95	104.24	106.31
31	4	604	CLA	CMA-C3A-C4A	2.95	119.70	111.77
31	Y	303	CLA	CMA-C3A-C4A	2.95	119.70	111.77
31	s	304	CLA	C3B-C4B-NB	-2.95	107.90	110.53
31	y	602	CLA	CMA-C3A-C4A	2.95	119.69	111.77
31	1	603	CLA	C1C-C2C-C3C	-2.95	103.88	106.98
30	Y	307	CHL	C1-C2-C3	-2.95	121.37	126.20
37	9	322	XAT	C18-C5-C6	-2.95	117.45	122.30
30	r	310	CHL	C1-C2-C3	-2.95	121.37	126.20
43	C	614	BCR	C11-C12-C13	-2.95	118.28	126.36
31	C	602	CLA	C6-C5-C3	-2.95	106.29	113.47
31	9	315	CLA	O2A-C1-C2	2.95	119.44	108.11
31	6	313	CLA	C1-C2-C3	-2.94	121.37	126.20
31	R	316	CLA	C2C-C1C-NC	2.94	113.08	109.98
31	b	606	CLA	C1C-C2C-C3C	-2.94	103.88	106.98
31	6	303	CLA	CMA-C3A-C4A	2.94	119.69	111.77
31	C	605	CLA	O2A-C1-C2	2.94	119.44	108.11
31	6	316	CLA	C2C-C1C-NC	2.94	113.07	109.98
35	G	614	RRX	C20-C19-C18	-2.94	118.29	126.36
36	0	618	NEX	C2-C1-C6	2.94	112.07	109.21
30	2	601	CHL	C1-C2-C3	-2.94	121.37	126.20
31	C	612	CLA	C1C-C2C-C3C	-2.94	103.88	106.98
31	c	612	CLA	C1C-C2C-C3C	-2.94	103.89	106.98
31	p	612	CLA	CMA-C3A-C4A	2.94	119.68	111.77
30	g	308	CHL	C1-C2-C3	-2.94	122.00	126.76
30	1	601	CHL	C4D-CHA-CBD	-2.94	106.00	108.97
31	S	304	CLA	C3B-C4B-NB	-2.94	107.90	110.53
35	9	317	RRX	C38-C26-C27	2.94	119.83	114.42
35	9	317	RRX	C20-C19-C18	-2.94	118.30	126.36
32	s	317	LUT	C8-C7-C6	-2.94	119.14	127.00
31	q	306	CLA	CMA-C3A-C4A	2.94	119.68	111.77
43	h	101	BCR	C38-C26-C27	2.94	119.86	113.60
37	2	619	XAT	C18-C5-C6	-2.94	117.46	122.30
31	0	610	CLA	C3B-C4B-NB	-2.94	107.91	110.53
32	N	317	LUT	C18-C5-C6	-2.94	121.28	124.48
31	B	606	CLA	O2A-C1-C2	2.94	119.42	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	s	307	CHL	C3C-C4C-NC	-2.94	107.47	114.65
31	C	610	CLA	C1C-C2C-C3C	-2.94	103.89	106.98
31	S	303	CLA	C1D-ND-C4D	-2.94	104.25	106.31
35	4	615	RRX	C20-C19-C18	-2.94	118.31	126.36
31	N	313	CLA	CMA-C3A-C4A	2.94	119.67	111.77
30	3	308	CHL	C3C-C4C-NC	-2.94	107.47	114.65
43	h	101	BCR	C29-C30-C25	2.94	114.71	110.44
30	0	606	CHL	C3C-C4C-NC	-2.94	107.47	114.65
31	B	601	CLA	C3B-C4B-NB	-2.94	107.91	110.53
43	T	101	BCR	C11-C10-C9	-2.94	123.16	127.28
34	D	410	LMG	O8-C28-C29	2.94	120.79	111.83
31	s	303	CLA	C1D-ND-C4D	-2.94	104.25	106.31
31	a	409	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
31	Y	311	CLA	C1-C2-C3	-2.93	121.39	126.20
32	s	317	LUT	C11-C10-C9	-2.93	123.16	127.28
30	S	307	CHL	C3C-C4C-NC	-2.93	107.48	114.65
31	c	602	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
35	4	615	RRX	C38-C26-C27	2.93	119.82	114.42
31	s	304	CLA	CMA-C3A-C4A	2.93	119.66	111.77
31	y	613	CLA	O2A-CGA-CBA	2.93	120.78	111.83
31	B	605	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
43	d	406	BCR	C20-C21-C22	-2.93	123.17	127.28
31	5	614	CLA	CMA-C3A-C4A	2.93	119.66	111.77
35	G	614	RRX	C38-C26-C27	2.93	119.81	114.42
32	p	616	LUT	C7-C8-C9	-2.93	121.90	126.23
30	6	310	CHL	C1-C2-C3	-2.93	121.39	126.20
31	s	315	CLA	C1C-C2C-C3C	-2.93	103.90	106.98
31	3	314	CLA	C3B-C4B-NB	-2.93	107.91	110.53
32	3	318	LUT	C31-C30-C29	-2.93	123.17	127.28
31	3	313	CLA	C2C-C1C-NC	2.93	113.06	109.98
31	5	602	CLA	CMA-C3A-C4A	2.93	119.64	111.77
32	7	317	LUT	C30-C31-C32	-2.93	114.71	123.20
36	G	616	NEX	C5-C6-C1	2.93	122.60	119.70
31	N	314	CLA	CMA-C3A-C4A	2.93	119.64	111.77
31	R	315	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
34	X	202	LMG	O8-C28-C29	2.93	120.76	111.83
31	C	607	CLA	C1C-C2C-C3C	-2.93	103.90	106.98
31	7	303	CLA	CMA-C3A-C4A	2.93	119.64	111.77
37	9	322	XAT	C27-C28-C29	2.93	130.07	125.53
31	c	611	CLA	O2A-CGA-CBA	2.93	120.76	111.83
35	9	317	RRX	C33-C5-C4	2.93	119.84	113.60
31	2	603	CLA	C3B-C4B-NB	-2.93	107.92	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	605	CLA	CMA-C3A-C4A	2.93	119.64	111.77
32	2	615	LUT	C11-C10-C9	-2.93	123.17	127.28
43	Z	101	BCR	C11-C12-C13	-2.92	118.34	126.36
31	9	315	CLA	C2C-C1C-NC	2.92	113.05	109.98
35	4	615	RRX	C33-C5-C4	2.92	119.83	113.60
31	6	311	CLA	C1-C2-C3	-2.92	121.41	126.20
34	2	621	LMG	O8-C28-C29	2.92	120.75	111.83
31	N	311	CLA	CMA-C3A-C4A	2.92	119.63	111.77
33	q	320	LHG	O8-C23-C24	2.92	120.75	111.83
30	G	608	CHL	C1-O2A-CGA	2.92	123.73	116.65
31	3	306	CLA	C1D-ND-C4D	-2.92	104.26	106.31
30	3	302	CHL	CMA-C3A-C4A	2.92	120.91	114.61
31	s	312	CLA	CMA-C3A-C4A	2.92	119.62	111.77
31	4	612	CLA	C1D-ND-C4D	-2.92	104.26	106.31
43	C	614	BCR	C24-C23-C22	-2.92	121.92	126.23
37	q	321	XAT	C27-C28-C29	2.92	130.06	125.53
31	G	613	CLA	C3B-C4B-NB	-2.92	107.92	110.53
31	2	602	CLA	CMA-C3A-C4A	2.92	119.62	111.77
31	B	607	CLA	C2C-C1C-NC	2.92	113.05	109.98
31	n	315	CLA	CMA-C3A-C4A	2.92	119.62	111.77
30	Y	302	CHL	C1-C2-C3	-2.92	121.42	126.20
31	b	616	CLA	C1C-C2C-C3C	-2.92	103.91	106.98
31	3	316	CLA	C3B-C4B-NB	-2.91	107.93	110.53
31	8	613	CLA	CMA-C3A-C4A	2.91	119.61	111.77
31	r	304	CLA	C1D-ND-C4D	-2.91	104.27	106.31
31	C	605	CLA	C1-O2A-CGA	2.91	123.71	116.65
31	7	304	CLA	CMA-C3A-C4A	2.91	119.60	111.77
31	c	609	CLA	O2A-C1-C2	2.91	119.32	108.11
32	5	616	LUT	C7-C8-C9	-2.91	121.93	126.23
34	q	302	LMG	O8-C28-C29	2.91	120.71	111.83
31	R	305	CLA	C2C-C1C-NC	2.91	113.04	109.98
31	3	315	CLA	C1-C2-C3	-2.91	121.43	126.20
36	2	616	NEX	C17-C1-C6	-2.91	107.87	110.47
31	g	304	CLA	CMA-C3A-C4A	2.91	119.60	111.77
31	Y	314	CLA	CMA-C3A-C4A	2.91	119.59	111.77
31	r	314	CLA	C3B-C4B-NB	-2.91	107.93	110.53
31	y	612	CLA	C3B-C4B-NB	-2.91	107.93	110.53
31	0	611	CLA	C1-C2-C3	-2.91	121.43	126.20
31	N	304	CLA	CMA-C3A-C4A	2.91	119.59	111.77
30	9	309	CHL	CMA-C3A-C4A	2.91	120.88	114.61
31	G	603	CLA	CMA-C3A-C4A	2.91	119.59	111.77
31	2	602	CLA	C3B-C4B-NB	-2.91	107.94	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	611	CLA	CMA-C3A-C4A	2.91	119.58	111.77
32	R	317	LUT	C31-C32-C33	2.91	134.33	126.36
32	0	617	LUT	C10-C11-C12	-2.91	114.78	123.20
35	G	614	RRX	C33-C5-C4	2.91	119.79	113.60
31	B	601	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
36	9	319	NEX	C2-C1-C6	2.90	112.03	109.21
31	b	610	CLA	C1C-C2C-C3C	-2.90	103.92	106.98
31	N	311	CLA	C1D-ND-C4D	-2.90	104.27	106.31
37	r	318	XAT	C38-C25-C26	-2.90	117.52	122.30
31	C	605	CLA	C2C-C1C-NC	2.90	113.03	109.98
31	8	614	CLA	CMA-C3A-C4A	2.90	119.58	111.77
37	g	321	XAT	C27-C28-C29	2.90	130.03	125.53
31	8	612	CLA	CMA-C3A-C4A	2.90	119.57	111.77
31	N	303	CLA	CMA-C3A-C4A	2.90	119.57	111.77
32	q	318	LUT	C21-C26-C27	-2.90	109.49	112.83
31	Y	313	CLA	C2C-C1C-NC	2.90	113.03	109.98
31	2	609	CLA	CMA-C3A-C4A	2.90	119.57	111.77
32	Y	315	LUT	C35-C15-C14	-2.90	117.59	123.52
31	n	311	CLA	CMA-C3A-C4A	2.90	119.57	111.77
31	n	314	CLA	CMA-C3A-C4A	2.90	119.56	111.77
31	b	609	CLA	C1C-C2C-C3C	-2.90	103.93	106.98
31	N	314	CLA	O2A-CGA-CBA	2.90	120.67	111.83
31	R	316	CLA	C1C-C2C-C3C	-2.90	103.93	106.98
43	B	617	BCR	C38-C26-C27	2.90	119.77	113.60
30	s	309	CHL	C1-O2A-CGA	2.90	123.66	116.65
37	4	619	XAT	C27-C28-C29	2.90	130.03	125.53
31	q	312	CLA	CMA-C3A-C4A	2.90	119.56	111.77
31	y	603	CLA	CMA-C3A-C4A	2.90	119.56	111.77
30	n	302	CHL	C1-C2-C3	-2.90	121.45	126.20
31	5	611	CLA	C1D-ND-C4D	-2.90	104.28	106.31
31	8	609	CLA	C1D-ND-C4D	-2.90	104.28	106.31
31	4	612	CLA	C1C-C2C-C3C	-2.90	103.93	106.98
31	b	603	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
31	R	306	CLA	O1D-CGD-CBD	-2.89	118.81	124.52
31	R	313	CLA	C3B-C4B-NB	-2.89	107.95	110.53
31	s	306	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
32	n	317	LUT	C8-C7-C6	-2.89	119.27	127.00
30	8	601	CHL	C1-C2-C3	-2.89	121.46	126.20
43	C	615	BCR	C30-C25-C26	-2.89	118.68	122.64
31	C	611	CLA	O2A-CGA-CBA	2.89	120.65	111.83
32	y	616	LUT	C15-C14-C13	-2.89	123.22	127.28
30	y	608	CHL	C1-O2A-CGA	2.89	123.65	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	S	302	CHL	C4D-CHA-CBD	-2.89	106.05	108.97
31	b	604	CLA	O2A-CGA-CBA	2.89	120.65	111.83
34	b	622	LMG	O1-C1-C2	2.89	112.66	108.27
32	y	616	LUT	C35-C15-C14	-2.89	117.61	123.52
34	d	410	LMG	O8-C28-C29	2.89	120.64	111.83
43	T	101	BCR	C11-C12-C13	-2.89	118.44	126.36
32	3	317	LUT	C1-C6-C5	-2.89	118.69	122.64
30	N	309	CHL	C1-O2A-CGA	2.89	123.64	116.65
37	2	619	XAT	C27-C28-C29	2.89	130.01	125.53
31	8	610	CLA	CMA-C3A-C4A	2.89	119.53	111.77
31	g	304	CLA	C3B-C4B-NB	-2.89	107.95	110.53
31	S	306	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
31	B	602	CLA	C1C-C2C-C3C	-2.89	103.94	106.98
34	D	411	LMG	O8-C28-C29	2.89	120.64	111.83
34	S	321	LMG	O8-C28-C29	2.89	120.64	111.83
31	1	613	CLA	C2C-C1C-NC	2.89	113.01	109.98
31	p	613	CLA	C2C-C1C-NC	2.89	113.01	109.98
31	5	613	CLA	C3B-C4B-NB	-2.89	107.95	110.53
31	4	610	CLA	C1C-C2C-C3C	-2.89	103.94	106.98
32	y	617	LUT	C15-C35-C34	-2.88	117.62	123.52
31	b	607	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
31	p	603	CLA	C1C-C2C-C3C	-2.88	103.95	106.98
31	g	313	CLA	CMA-C3A-C4A	2.88	119.53	111.77
34	q1	101	LMG	O8-C28-C29	2.88	120.63	111.83
43	c	614	BCR	C20-C19-C18	2.88	134.27	126.36
31	N	312	CLA	C1D-ND-C4D	-2.88	104.29	106.31
31	S	310	CLA	C2C-C1C-NC	2.88	113.01	109.98
31	g	305	CLA	C2C-C1C-NC	2.88	113.01	109.98
31	y	613	CLA	C2C-C1C-NC	2.88	113.01	109.98
30	0	606	CHL	C1-O2A-CGA	2.88	123.62	116.65
31	R	307	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
31	c	605	CLA	O2A-C1-C2	2.88	119.19	108.11
30	4	609	CHL	C1-O2A-CGA	2.88	123.62	116.65
31	B	606	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
31	Y	310	CLA	CMA-C3A-C4A	2.88	119.51	111.77
31	y	613	CLA	C1C-C2C-C3C	-2.88	103.95	106.98
31	9	316	CLA	CMA-C3A-C4A	2.88	119.51	111.77
31	N	304	CLA	C1C-C2C-C3C	-2.88	103.95	106.98
31	C	608	CLA	O2A-C1-C2	2.88	119.18	108.11
31	r	313	CLA	C3B-C4B-NB	-2.88	107.96	110.53
31	s	314	CLA	CMA-C3A-C4A	2.88	119.51	111.77
31	S	316	CLA	C1C-C2C-C3C	-2.88	103.95	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	610	CLA	CMA-C3A-C4A	2.88	119.50	111.77
31	5	611	CLA	CMA-C3A-C4A	2.88	119.50	111.77
31	G	610	CLA	C2C-C1C-NC	2.88	113.00	109.98
31	R	304	CLA	O2A-CGA-CBA	2.87	120.60	111.83
31	r	315	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
31	s	314	CLA	C2C-C1C-NC	2.87	113.00	109.98
34	s	321	LMG	O8-C28-C29	2.87	120.60	111.83
31	B	614	CLA	CMA-C3A-C4A	2.87	119.50	111.77
31	p	610	CLA	CMA-C3A-C4A	2.87	119.50	111.77
31	p	614	CLA	CMD-C2D-C3D	-2.87	121.10	127.69
43	c	615	BCR	C24-C23-C22	-2.87	121.99	126.23
32	8	615	LUT	C8-C7-C6	-2.87	119.33	127.00
37	G	620	XAT	C27-C28-C29	2.87	129.99	125.53
30	G	608	CHL	C1-C2-C3	-2.87	121.49	126.20
30	n	301	CHL	C1-O2A-CGA	2.87	123.60	116.65
31	p	603	CLA	O2A-CGA-CBA	2.87	120.59	111.83
31	N	315	CLA	CMA-C3A-C4A	2.87	119.49	111.77
36	4	617	NEX	C17-C1-C6	-2.87	107.90	110.47
43	A	410	BCR	C1-C6-C5	-2.87	118.72	122.64
31	1	614	CLA	CMA-C3A-C4A	2.87	119.48	111.77
35	2	614	RRX	C38-C26-C27	2.87	119.69	114.42
32	9	318	LUT	C27-C28-C29	-2.87	120.16	126.32
31	3	316	CLA	C1C-C2C-C3C	-2.87	103.97	106.98
31	g	310	CLA	O2A-CGA-CBA	2.87	120.57	111.83
31	n	312	CLA	CMA-C3A-C4A	2.87	119.48	111.77
31	B	613	CLA	C1C-C2C-C3C	-2.87	103.97	106.98
30	s	302	CHL	C4D-CHA-CBD	-2.87	106.08	108.97
31	0	615	CLA	C3B-C4B-NB	-2.87	107.97	110.53
33	C	623	LHG	O8-C23-C24	2.87	120.57	111.83
31	3	301	CLA	C1D-ND-C4D	-2.86	104.30	106.31
32	r	317	LUT	C20-C13-C12	2.86	122.46	118.09
31	c	609	CLA	C1-C2-C3	-2.86	121.50	126.20
43	c	615	BCR	C23-C24-C25	-2.86	119.35	127.00
30	9	310	CHL	C1-O2A-CGA	2.86	123.58	116.65
31	7	313	CLA	C3B-C4B-NB	-2.86	107.97	110.53
34	a	413	LMG	O8-C28-C29	2.86	120.56	111.83
31	5	615	CLA	CMA-C3A-C4A	2.86	119.47	111.77
31	p	603	CLA	C2C-C1C-NC	2.86	112.99	109.98
32	7	318	LUT	C11-C10-C9	-2.86	123.27	127.28
31	S	315	CLA	C1C-C2C-C3C	-2.86	103.97	106.98
33	t	102	LHG	O8-C23-C24	2.86	120.56	111.83
30	N	308	CHL	CMA-C3A-C4A	2.86	120.78	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	314	CLA	CMA-C3A-C4A	2.86	119.46	111.77
31	C	606	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
31	p	611	CLA	CMA-C3A-C4A	2.86	119.46	111.77
31	c	611	CLA	CAA-CBA-CGA	-2.86	105.09	113.21
31	n	304	CLA	C1C-C2C-C3C	-2.86	103.97	106.98
31	g	312	CLA	CMA-C3A-C4A	2.86	119.46	111.77
33	z	102	LHG	O8-C23-C24	2.86	120.55	111.83
31	5	603	CLA	CMA-C3A-C4A	2.86	119.46	111.77
31	S	306	CLA	CMA-C3A-C4A	2.86	119.45	111.77
31	B	612	CLA	C1D-ND-C4D	-2.86	104.31	106.31
31	r	306	CLA	C1C-C2C-C3C	-2.86	103.98	106.98
32	r	317	LUT	C7-C8-C9	-2.86	122.01	126.23
31	y	615	CLA	C1D-ND-C4D	-2.85	104.31	106.31
31	b	610	CLA	O2A-CGA-CBA	2.85	120.54	111.83
31	9	306	CLA	CMA-C3A-C4A	2.85	119.44	111.77
31	4	604	CLA	C2C-C1C-NC	2.85	112.98	109.98
32	0	617	LUT	C1-C6-C5	-2.85	118.74	122.64
35	2	614	RRX	C33-C5-C4	2.85	119.68	113.60
31	G	604	CLA	C1D-ND-C4D	-2.85	104.31	106.31
31	q	304	CLA	C1D-ND-C4D	-2.85	104.31	106.31
30	q	310	CHL	C4D-CHA-CBD	-2.85	106.09	108.97
30	2	608	CHL	C1-C2-C3	-2.85	121.53	126.20
31	C	605	CLA	C1C-C2C-C3C	-2.85	103.98	106.98
31	9	305	CLA	C3B-C4B-NB	-2.85	107.98	110.53
31	r	312	CLA	O2A-CGA-CBA	2.85	120.53	111.83
31	n	314	CLA	C2C-C1C-NC	2.85	112.98	109.98
31	7	312	CLA	CMA-C3A-C4A	2.85	119.43	111.77
31	c	609	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
31	2	610	CLA	C1D-ND-C4D	-2.85	104.31	106.31
31	r	304	CLA	C1C-C2C-C3C	-2.85	103.98	106.98
31	r	305	CLA	C1C-C2C-C3C	-2.85	103.98	106.98
31	b	611	CLA	CMA-C3A-C4A	2.85	119.43	111.77
31	G	611	CLA	C2C-C1C-NC	2.85	112.97	109.98
31	a	407	CLA	C2C-C1C-NC	2.85	112.97	109.98
33	R	320	LHG	C5-O7-C7	-2.85	110.98	117.80
31	a	407	CLA	CMA-C3A-C4A	2.85	119.43	111.77
31	B	606	CLA	C1-C2-C3	-2.85	121.53	126.20
31	C	609	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
31	3	313	CLA	C3B-C4B-NB	-2.85	107.99	110.53
31	R	303	CLA	C3B-C4B-NB	-2.85	107.99	110.53
34	g	320	LMG	C8-O7-C10	-2.85	110.98	117.80
48	R	302	LMU	C1B-O1B-C4'	-2.85	111.23	117.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	607	CLA	C2C-C1C-NC	2.85	112.97	109.98
38	G	624	SQD	O7-S-C6	-2.85	102.51	106.76
31	B	610	CLA	C3B-C4B-NB	-2.85	107.99	110.53
31	7	314	CLA	CMA-C3A-C4A	2.85	119.42	111.77
31	G	604	CLA	C2C-C1C-NC	2.84	112.97	109.98
31	7	314	CLA	C2C-C1C-NC	2.84	112.97	109.98
31	p	610	CLA	C1D-ND-C4D	-2.84	104.32	106.31
31	q	305	CLA	C1C-C2C-C3C	-2.84	103.99	106.98
31	q	314	CLA	C1C-C2C-C3C	-2.84	103.99	106.98
31	0	614	CLA	CMA-C3A-C4A	2.84	119.42	111.77
31	A	407	CLA	C2C-C1C-NC	2.84	112.97	109.98
31	d	401	CLA	CMA-C3A-C4A	2.84	119.42	111.77
31	5	614	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
30	4	607	CHL	C1-C2-C3	-2.84	121.54	126.20
31	8	612	CLA	C2C-C1C-NC	2.84	112.97	109.98
31	g	313	CLA	C2C-C1C-NC	2.84	112.97	109.98
31	B	603	CLA	O2A-CGA-CBA	2.84	120.50	111.83
34	W	203	LMG	O8-C28-C29	2.84	120.50	111.83
35	g	315	RRX	C8-C7-C6	-2.84	119.41	127.00
31	C	605	CLA	CHA-C4D-ND	2.84	138.41	132.55
43	B	619	BCR	C23-C24-C25	-2.84	119.41	127.00
31	7	313	CLA	C4B-CHC-C1C	2.84	132.93	126.25
31	6	315	CLA	CMA-C3A-C4A	2.84	119.41	111.77
31	6	303	CLA	C1D-ND-C4D	-2.84	104.32	106.31
36	4	617	NEX	C26-C27-C28	-2.84	119.99	125.99
43	T	101	BCR	C16-C17-C18	-2.84	123.30	127.28
31	s	312	CLA	C2C-C1C-NC	2.84	112.96	109.98
31	3	312	CLA	C2C-C1C-NC	2.84	112.96	109.98
31	Y	314	CLA	C2C-C1C-NC	2.84	112.96	109.98
31	n	305	CLA	C2C-C1C-NC	2.84	112.96	109.98
31	s	312	CLA	C1C-C2C-C3C	-2.84	104.00	106.98
31	1	612	CLA	C3B-C4B-NB	-2.84	108.00	110.53
34	7	320	LMG	O8-C28-C29	2.84	120.49	111.83
31	y	604	CLA	C2C-C1C-NC	2.84	112.96	109.98
31	3	311	CLA	C1C-C2C-C3C	-2.84	104.00	106.98
31	B	608	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
31	n	303	CLA	C1D-ND-C4D	-2.84	104.32	106.31
31	G	602	CLA	CMA-C3A-C4A	2.84	119.39	111.77
31	p	614	CLA	CMA-C3A-C4A	2.84	119.39	111.77
31	0	613	CLA	C2C-C1C-NC	2.84	112.96	109.98
31	g	314	CLA	CMA-C3A-C4A	2.84	119.39	111.77
43	C	615	BCR	C35-C13-C12	-2.83	113.76	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	303	CLA	CMA-C3A-C4A	2.83	119.39	111.77
31	c	607	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
31	d	405	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
34	6	321	LMG	O8-C28-C29	2.83	120.47	111.83
31	3	316	CLA	CMD-C2D-C3D	-2.83	121.19	127.69
31	s	316	CLA	C2C-C1C-NC	2.83	112.96	109.98
31	b	617	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
31	g	305	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
31	b	612	CLA	C1D-ND-C4D	-2.83	104.33	106.31
31	b	615	CLA	C1D-ND-C4D	-2.83	104.33	106.31
30	r	310	CHL	C4D-CHA-CBD	-2.83	106.11	108.97
30	q	309	CHL	CMA-C3A-C4A	2.83	120.71	114.61
31	n	313	CLA	C1D-ND-C4D	-2.83	104.33	106.31
31	9	315	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
43	Z	101	BCR	C2-C1-C6	2.83	114.55	110.44
31	C	604	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
31	N	314	CLA	C3B-C4B-NB	-2.83	108.00	110.53
31	S	312	CLA	C3B-C4B-NB	-2.83	108.00	110.53
31	y	610	CLA	C3B-C4B-NB	-2.83	108.00	110.53
31	9	305	CLA	CMA-C3A-C4A	2.83	119.38	111.77
31	s	305	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
31	b	614	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
31	n	316	CLA	CMA-C3A-C4A	2.83	119.38	111.77
31	Y	311	CLA	C2C-C1C-NC	2.83	112.95	109.98
31	3	312	CLA	C1C-C2C-C3C	-2.83	104.01	106.98
31	r	316	CLA	C1C-C2C-C3C	-2.83	104.01	106.98
32	3	317	LUT	C8-C7-C6	-2.83	119.44	127.00
31	1	613	CLA	CMA-C3A-C4A	2.83	119.37	111.77
33	B	624	LHG	O8-C23-C24	2.83	120.45	111.83
31	7	316	CLA	C1C-C2C-C3C	-2.83	104.01	106.98
31	n	305	CLA	C1C-C2C-C3C	-2.83	104.01	106.98
31	R	311	CLA	C2C-C1C-NC	2.83	112.95	109.98
31	B	606	CLA	C1C-C2C-C3C	-2.83	104.01	106.98
31	2	613	CLA	CMA-C3A-C4A	2.83	119.37	111.77
31	s	303	CLA	CMA-C3A-C4A	2.82	119.36	111.77
31	d	401	CLA	C1C-C2C-C3C	-2.82	104.01	106.98
31	g	313	CLA	C1C-C2C-C3C	-2.82	104.01	106.98
31	6	313	CLA	C1D-ND-C4D	-2.82	104.33	106.31
31	B	611	CLA	C3B-C4B-NB	-2.82	108.01	110.53
31	8	612	CLA	C1C-C2C-C3C	-2.82	104.01	106.98
31	4	603	CLA	C3B-C4B-NB	-2.82	108.01	110.53
31	n	311	CLA	C3B-C4B-NB	-2.82	108.01	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	611	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
32	1	616	LUT	C30-C31-C32	-2.82	115.03	123.20
31	b	613	CLA	C3B-C4B-NB	-2.82	108.01	110.53
30	p	609	CHL	CMA-C3A-C4A	2.82	120.69	114.61
30	g	309	CHL	C1-O2A-CGA	2.82	123.47	116.65
31	b	610	CLA	C2C-C1C-NC	2.82	112.94	109.98
31	p	615	CLA	O1D-CGD-CBD	-2.82	118.96	124.52
31	C	601	CLA	C1C-C2C-C3C	-2.82	104.02	106.98
31	3	312	CLA	C3B-C4B-NB	-2.82	108.02	110.53
31	N	304	CLA	C2C-C1C-NC	2.82	112.94	109.98
31	7	313	CLA	C1C-C2C-C3C	-2.82	104.02	106.98
31	9	304	CLA	C1C-C2C-C3C	-2.82	104.02	106.98
34	W	202	LMG	O1-C1-C2	2.82	112.55	108.27
31	g	311	CLA	CAA-C2A-C3A	-2.82	105.39	113.00
31	g	311	CLA	C2C-C1C-NC	2.82	112.94	109.98
31	N	321	CLA	C1D-ND-C4D	-2.82	104.34	106.31
31	4	614	CLA	O2A-CGA-CBA	2.82	120.42	111.83
31	n	314	CLA	C1C-C2C-C3C	-2.82	104.02	106.98
31	8	611	CLA	C1D-ND-C4D	-2.81	104.34	106.31
31	N	310	CLA	C3B-C4B-NB	-2.81	108.02	110.53
31	q	312	CLA	O1D-CGD-CBD	-2.81	118.97	124.52
31	s	310	CLA	C1C-C2C-C3C	-2.81	104.02	106.98
31	B	604	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
31	c	608	CLA	CAA-C2A-C3A	-2.81	105.40	113.00
34	A	418	LMG	C8-O7-C10	-2.81	111.06	117.80
31	C	609	CLA	C1-C2-C3	-2.81	121.59	126.20
31	Y	303	CLA	C2C-C1C-NC	2.81	112.94	109.98
32	y	617	LUT	C10-C11-C12	-2.81	115.05	123.20
31	0	611	CLA	C3B-C4B-NB	-2.81	108.02	110.53
31	3	313	CLA	C1C-C2C-C3C	-2.81	104.02	106.98
31	p	612	CLA	C2C-C1C-NC	2.81	112.93	109.98
33	S	322	LHG	O8-C23-C24	2.81	120.40	111.83
31	d	404	CLA	O2A-CGA-CBA	2.81	120.40	111.83
31	p	610	CLA	C3B-C4B-NB	-2.81	108.02	110.53
31	5	613	CLA	CMA-C3A-C4A	2.81	119.32	111.77
31	B	611	CLA	CMA-C3A-C4A	2.81	119.32	111.77
31	y	614	CLA	CMA-C3A-C4A	2.81	119.32	111.77
31	C	602	CLA	C2C-C1C-NC	2.81	112.93	109.98
31	B	609	CLA	C1C-C2C-C3C	-2.81	104.03	106.98
31	c	601	CLA	CMA-C3A-C4A	2.81	119.32	111.77
30	q	308	CHL	CMA-C3A-C4A	2.81	120.66	114.61
30	q	308	CHL	C3C-C4C-NC	-2.81	107.79	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	601	CLA	CMA-C3A-C4A	2.81	119.32	111.77
31	7	311	CLA	CMA-C3A-C4A	2.81	119.32	111.77
31	2	603	CLA	C1D-ND-C4D	-2.81	104.34	106.31
31	N	314	CLA	C1D-ND-C4D	-2.81	104.34	106.31
36	3	319	NEX	C38-C25-C26	-2.81	117.69	122.30
31	7	311	CLA	C3B-C4B-NB	-2.80	108.03	110.53
31	3	314	CLA	C2C-C1C-NC	2.80	112.93	109.98
31	3	306	CLA	CMA-C3A-C4A	2.80	119.31	111.77
31	C	603	CLA	CHD-C1D-ND	-2.80	120.86	124.80
43	B	618	BCR	C20-C19-C18	-2.80	118.68	126.36
34	r	321	LMG	O1-C1-C2	2.80	112.53	108.27
31	C	610	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
31	8	604	CLA	C2C-C1C-NC	2.80	112.93	109.98
31	9	305	CLA	C1C-C2C-C3C	-2.80	104.03	106.98
31	1	604	CLA	C1C-C2C-C3C	-2.80	104.03	106.98
31	1	613	CLA	C1C-C2C-C3C	-2.80	104.03	106.98
31	9	314	CLA	O2A-CGA-CBA	2.80	120.38	111.83
34	w	204	LMG	O8-C28-C29	2.80	120.38	111.83
31	q	314	CLA	CMA-C3A-C4A	2.80	119.30	111.77
33	N	319	LHG	O8-C23-C24	2.80	120.38	111.83
31	1	614	CLA	C1D-ND-C4D	-2.80	104.35	106.31
31	c	605	CLA	C2C-C1C-NC	2.80	112.92	109.98
31	B	609	CLA	C2C-C1C-NC	2.80	112.92	109.98
31	R	305	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
31	b	610	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
32	5	616	LUT	C8-C7-C6	-2.80	119.52	127.00
31	Y	311	CLA	C1-O2A-CGA	2.80	123.42	116.65
31	a	409	CLA	C1C-C2C-C3C	-2.80	104.04	106.98
31	4	613	CLA	CMA-C3A-C4A	2.80	119.29	111.77
31	n	315	CLA	C3B-C4B-NB	-2.80	108.03	110.53
34	d	409	LMG	O8-C28-C29	2.80	120.36	111.83
42	D	401	PHO	C2B-C1B-NB	-2.80	107.41	109.43
31	R	314	CLA	C3B-C4B-NB	-2.80	108.03	110.53
31	0	615	CLA	CMA-C3A-C4A	2.80	119.29	111.77
31	6	314	CLA	C2C-C1C-NC	2.80	112.92	109.98
31	q	316	CLA	CMA-C3A-C4A	2.80	119.29	111.77
31	4	604	CLA	C1C-C2C-C3C	-2.80	104.04	106.98
31	s	316	CLA	C4B-CHC-C1C	2.80	132.82	126.25
31	8	610	CLA	C1D-ND-C4D	-2.79	104.35	106.31
34	q	301	LMG	O8-C28-C29	2.79	120.36	111.83
31	C	609	CLA	O2A-C1-C2	2.79	118.86	108.11
31	8	609	CLA	C3B-C4B-NB	-2.79	108.04	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	k	102	LMG	O8-C28-C29	2.79	120.35	111.83
31	7	316	CLA	C2C-C1C-NC	2.79	112.92	109.98
31	n	304	CLA	C2C-C1C-NC	2.79	112.92	109.98
31	d	401	CLA	C2C-C1C-NC	2.79	112.91	109.98
30	0	607	CHL	C1-O2A-CGA	2.79	123.41	116.65
31	B	608	CLA	C1C-C2C-C3C	-2.79	104.04	106.98
30	1	608	CHL	CMA-C3A-C4A	2.79	120.62	114.61
43	D	405	BCR	C4-C5-C6	-2.79	118.93	122.70
31	G	602	CLA	C1D-ND-C4D	-2.79	104.35	106.31
31	2	611	CLA	C1C-C2C-C3C	-2.79	104.05	106.98
31	S	310	CLA	C1C-C2C-C3C	-2.79	104.05	106.98
31	3	316	CLA	CMA-C3A-C4A	2.79	119.27	111.77
31	B	607	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
31	A	409	CLA	C2C-C1C-NC	2.79	112.91	109.98
30	y	607	CHL	C1-C2-C3	-2.79	121.63	126.20
31	9	312	CLA	C3B-C4B-NB	-2.79	108.04	110.53
31	6	316	CLA	CMA-C3A-C4A	2.79	119.27	111.77
31	R	303	CLA	C2C-C1C-NC	2.79	112.91	109.98
31	R	304	CLA	C1C-C2C-C3C	-2.79	104.05	106.98
30	Y	307	CHL	CMA-C3A-C4A	2.79	120.62	114.61
31	b	608	CLA	C2C-C1C-NC	2.79	112.91	109.98
31	C	603	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
38	X	201	SQD	O7-S-C6	-2.79	102.59	106.76
30	n	309	CHL	C1-O2A-CGA	2.79	123.40	116.65
31	g	303	CLA	CMA-C3A-C4A	2.79	119.26	111.77
31	R	312	CLA	O2A-C1-C2	2.79	118.83	108.11
31	b	617	CLA	C2C-C1C-NC	2.79	112.91	109.98
31	8	603	CLA	C1C-C2C-C3C	-2.79	104.05	106.98
31	2	611	CLA	C1D-ND-C4D	-2.79	104.36	106.31
32	g	316	LUT	C11-C12-C13	-2.79	118.72	126.36
31	b	616	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
31	s	306	CLA	CMA-C3A-C4A	2.79	119.26	111.77
31	5	604	CLA	C2C-C1C-NC	2.79	112.91	109.98
34	6	321	LMG	C8-O7-C10	-2.79	111.13	117.80
30	s	309	CHL	C4D-CHA-CBD	-2.79	106.16	108.97
31	b	608	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
31	D	404	CLA	C1D-ND-C4D	-2.78	104.36	106.31
31	b	606	CLA	C2C-C1C-NC	2.78	112.91	109.98
31	b	614	CLA	C2C-C1C-NC	2.78	112.91	109.98
31	g	304	CLA	C2C-C1C-NC	2.78	112.91	109.98
31	A	407	CLA	C1C-C2C-C3C	-2.78	104.05	106.98
31	a	409	CLA	C2C-C1C-NC	2.78	112.91	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	305	CLA	C2C-C1C-NC	2.78	112.91	109.98
30	2	608	CHL	C1-O2A-CGA	2.78	123.39	116.65
31	q	314	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
31	p	602	CLA	CMA-C3A-C4A	2.78	119.25	111.77
34	C	624	LMG	O8-C28-C29	2.78	120.32	111.83
32	1	615	LUT	C31-C30-C29	-2.78	123.38	127.28
31	B	602	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
30	S	309	CHL	C4D-CHA-CBD	-2.78	106.16	108.97
31	S	314	CLA	C2C-C1C-NC	2.78	112.90	109.98
31	r	312	CLA	O2A-C1-C2	2.78	118.81	108.11
36	8	617	NEX	C17-C1-C6	-2.78	107.98	110.47
31	N	314	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
31	8	613	CLA	C1D-ND-C4D	-2.78	104.36	106.31
31	s	314	CLA	O2A-CGA-CBA	2.78	120.31	111.83
31	3	316	CLA	C2C-C1C-NC	2.78	112.90	109.98
31	6	312	CLA	C2C-C1C-NC	2.78	112.90	109.98
31	y	603	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
31	y	613	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
31	c	603	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
43	A	410	BCR	C11-C12-C13	-2.78	118.75	126.36
31	C	607	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
31	N	303	CLA	C1D-ND-C4D	-2.78	104.36	106.31
31	5	604	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
31	N	312	CLA	CMA-C3A-C4A	2.78	119.24	111.77
34	s	321	LMG	O1-C1-C2	2.78	112.49	108.27
36	5	618	NEX	C26-C27-C28	-2.78	120.12	125.99
34	G	621	LMG	O8-C28-C29	2.78	120.30	111.83
31	B	614	CLA	C3B-C4B-NB	-2.78	108.05	110.53
31	r	304	CLA	C2C-C1C-NC	2.78	112.90	109.98
31	7	304	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
34	k	101	LMG	C8-O7-C10	-2.77	111.16	117.80
31	3	314	CLA	C1C-C2C-C3C	-2.77	104.06	106.98
31	c	610	CLA	C1C-C2C-C3C	-2.77	104.06	106.98
34	N	320	LMG	O8-C28-C29	2.77	120.29	111.83
30	1	605	CHL	CMA-C3A-C4A	2.77	120.59	114.61
32	y	616	LUT	C7-C8-C9	-2.77	122.13	126.23
31	R	311	CLA	C1C-C2C-C3C	-2.77	104.06	106.98
31	7	314	CLA	C1C-C2C-C3C	-2.77	104.06	106.98
31	s	304	CLA	C1C-C2C-C3C	-2.77	104.06	106.98
31	4	613	CLA	O2A-CGA-CBA	2.77	120.29	111.83
31	G	609	CLA	O2A-CGA-CBA	2.77	120.29	111.83
43	z	101	BCR	C4-C5-C6	-2.77	118.96	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	603	CLA	C2C-C1C-NC	2.77	112.89	109.98
31	5	603	CLA	C1C-C2C-C3C	-2.77	104.06	106.98
31	5	613	CLA	C1C-C2C-C3C	-2.77	104.06	106.98
43	B	617	BCR	C2-C1-C6	2.77	114.47	110.44
30	9	303	CHL	C1-O2A-CGA	2.77	123.36	116.65
31	3	315	CLA	C1D-ND-C4D	-2.77	104.37	106.31
31	0	615	CLA	C1D-ND-C4D	-2.77	104.37	106.31
31	n	315	CLA	C1D-ND-C4D	-2.77	104.37	106.31
31	g	304	CLA	C1C-C2C-C3C	-2.77	104.06	106.98
31	N	315	CLA	C3B-C4B-NB	-2.77	108.06	110.53
31	G	612	CLA	CMA-C3A-C4A	2.77	119.22	111.77
31	y	602	CLA	C1D-ND-C4D	-2.77	104.37	106.31
31	b	603	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
31	g	303	CLA	C2D-C1D-ND	2.77	112.87	110.13
31	8	612	CLA	O2A-CGA-CBA	2.77	120.28	111.83
37	R	318	XAT	C18-C5-C6	-2.77	117.74	122.30
31	2	604	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
34	x	202	LMG	O8-C28-C29	2.77	120.28	111.83
32	6	317	LUT	C35-C15-C14	-2.77	117.85	123.52
43	C	615	BCR	C24-C23-C22	-2.77	122.14	126.23
31	9	305	CLA	C2C-C1C-NC	2.77	112.89	109.98
31	c	611	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
31	3	314	CLA	C1D-ND-C4D	-2.77	104.37	106.31
31	9	306	CLA	C1D-ND-C4D	-2.77	104.37	106.31
31	p	612	CLA	C1D-ND-C4D	-2.77	104.37	106.31
31	n	316	CLA	C1D-ND-C4D	-2.77	104.37	106.31
31	R	314	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
31	g	312	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
31	Y	314	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
31	0	610	CLA	CMA-C3A-C4A	2.77	119.21	111.77
31	2	609	CLA	C3B-C4B-NB	-2.77	108.06	110.53
31	b	615	CLA	CMA-C3A-C4A	2.77	119.21	111.77
31	n	314	CLA	O2A-CGA-CBA	2.77	120.27	111.83
31	6	314	CLA	C1C-C2C-C3C	-2.76	104.07	106.98
31	b	607	CLA	C1C-C2C-C3C	-2.76	104.07	106.98
31	y	615	CLA	C1C-C2C-C3C	-2.76	104.07	106.98
31	r	306	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
33	j	102	LHG	O8-C23-C24	2.76	120.26	111.83
31	2	611	CLA	C2C-C1C-NC	2.76	112.89	109.98
33	b	625	LHG	O8-C23-C24	2.76	120.26	111.83
31	q	304	CLA	C3B-C4B-NB	-2.76	108.06	110.53
31	B	611	CLA	C1D-ND-C4D	-2.76	104.37	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	604	CLA	C1C-C2C-C3C	-2.76	104.07	106.98
31	b	606	CLA	O2A-CGA-CBA	2.76	120.26	111.83
34	b	601	LMG	O8-C28-C29	2.76	120.26	111.83
31	6	314	CLA	C1D-ND-C4D	-2.76	104.37	106.31
31	B	610	CLA	C2C-C1C-NC	2.76	112.88	109.98
31	r	306	CLA	C2C-C1C-NC	2.76	112.88	109.98
31	r	311	CLA	C2C-C1C-NC	2.76	112.88	109.98
31	S	316	CLA	CMA-C3A-C4A	2.76	119.19	111.77
31	N	321	CLA	CMA-C3A-C4A	2.76	119.19	111.77
34	D	412	LMG	O8-C28-C29	2.76	120.25	111.83
32	q	318	LUT	C11-C12-C13	-2.76	118.80	126.36
31	8	602	CLA	C1D-ND-C4D	-2.76	104.38	106.31
31	n	313	CLA	CMA-C3A-C4A	2.76	119.19	111.77
32	5	617	LUT	C15-C35-C34	-2.76	117.88	123.52
31	q	306	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
31	G	613	CLA	CMA-C3A-C4A	2.76	119.19	111.77
31	6	305	CLA	C1D-ND-C4D	-2.76	104.38	106.31
31	1	614	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
31	A	407	CLA	CMA-C3A-C4A	2.76	119.18	111.77
31	g	311	CLA	C3B-C4B-NB	-2.76	108.07	110.53
38	6	301	SQD	O7-S-C6	-2.76	102.64	106.76
31	9	316	CLA	C1D-ND-C4D	-2.76	104.38	106.31
31	A	409	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
31	B	605	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
31	Y	311	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
31	g	310	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
31	S	305	CLA	C2C-C1C-NC	2.76	112.88	109.98
31	0	610	CLA	C1-C2-C3	-2.76	121.68	126.20
31	b	602	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
31	7	305	CLA	C2C-C1C-NC	2.76	112.88	109.98
31	s	315	CLA	C2C-C1C-NC	2.76	112.88	109.98
34	A	414	LMG	O8-C28-C29	2.75	120.23	111.83
31	8	613	CLA	C3B-C4B-NB	-2.75	108.07	110.53
34	w	202	LMG	O8-C28-C29	2.75	120.23	111.83
31	4	612	CLA	CMA-C3A-C4A	2.75	119.17	111.77
32	7	318	LUT	C21-C26-C27	-2.75	109.66	112.83
32	1	615	LUT	C15-C14-C13	-2.75	123.42	127.28
31	p	613	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
31	g	312	CLA	C2C-C1C-NC	2.75	112.87	109.98
43	b	619	BCR	C23-C24-C25	-2.75	119.64	127.00
32	0	616	LUT	C11-C10-C9	-2.75	123.42	127.28
31	7	315	CLA	CMA-C3A-C4A	2.75	119.17	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y	305	CLA	C2C-C1C-NC	2.75	112.87	109.98
31	r	316	CLA	CHD-C1D-ND	-2.75	120.93	124.80
31	Y	310	CLA	C3B-C4B-NB	-2.75	108.07	110.53
34	n	322	LMG	O7-C10-O9	-2.75	117.27	123.70
31	c	609	CLA	C1C-C2C-C3C	-2.75	104.09	106.98
31	N	313	CLA	C2C-C1C-NC	2.75	112.87	109.98
31	7	315	CLA	C2C-C1C-NC	2.75	112.87	109.98
38	a	411	SQD	O7-S-C6	-2.75	102.65	106.76
31	2	613	CLA	C3B-C4B-NB	-2.75	108.07	110.53
31	2	610	CLA	C2C-C1C-NC	2.75	112.87	109.98
31	B	606	CLA	C2C-C1C-NC	2.75	112.87	109.98
31	G	603	CLA	C1C-C2C-C3C	-2.75	104.09	106.98
31	n	315	CLA	C1C-C2C-C3C	-2.75	104.09	106.98
31	9	313	CLA	C2C-C1C-NC	2.75	112.87	109.98
31	8	611	CLA	CMA-C3A-C4A	2.75	119.16	111.77
34	D	409	LMG	O8-C28-C29	2.75	120.22	111.83
31	g	312	CLA	C1D-ND-C4D	-2.75	104.38	106.31
31	6	304	CLA	C4B-CHC-C1C	2.75	132.71	126.25
31	Y	303	CLA	C1C-C2C-C3C	-2.75	104.09	106.98
31	0	604	CLA	C1C-C2C-C3C	-2.75	104.09	106.98
31	0	604	CLA	C2C-C1C-NC	2.75	112.87	109.98
43	b	619	BCR	C7-C8-C9	-2.75	122.17	126.23
31	b	604	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
31	g	311	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
31	C	607	CLA	C3B-C4B-NB	-2.75	108.08	110.53
31	p	613	CLA	C1D-ND-C4D	-2.75	104.39	106.31
31	q	315	CLA	CMA-C3A-C4A	2.75	119.15	111.77
31	Y	304	CLA	CMA-C3A-C4A	2.75	119.15	111.77
31	n	315	CLA	C2C-C1C-NC	2.75	112.87	109.98
31	B	613	CLA	C3B-C4B-NB	-2.75	108.08	110.53
35	g	315	RRX	C38-C26-C27	2.75	119.47	114.42
33	1	617	LHG	C5-O7-C7	-2.75	111.23	117.80
43	b	620	BCR	C11-C12-C13	-2.75	118.84	126.36
31	y	610	CLA	CMA-C3A-C4A	2.75	119.15	111.77
31	r	307	CLA	C1C-C2C-C3C	-2.74	104.09	106.98
31	c	613	CLA	C2C-C1C-NC	2.74	112.86	109.98
30	3	308	CHL	C4D-CHA-CBD	-2.74	106.20	108.97
31	1	610	CLA	CMA-C3A-C4A	2.74	119.15	111.77
31	2	610	CLA	C1C-C2C-C3C	-2.74	104.09	106.98
31	G	604	CLA	C1C-C2C-C3C	-2.74	104.09	106.98
31	A	407	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
33	9	320	LHG	O8-C23-C24	2.74	120.20	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	6	313	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
31	7	313	CLA	C2C-C1C-NC	2.74	112.86	109.98
31	r	303	CLA	C2C-C1C-NC	2.74	112.86	109.98
38	s	301	SQD	O7-S-C6	-2.74	102.66	106.76
31	R	315	CLA	C2C-C1C-NC	2.74	112.86	109.98
31	n	312	CLA	C1D-ND-C4D	-2.74	104.39	106.31
45	C	617	DGD	O1G-C1A-C2A	2.74	120.19	111.83
31	2	609	CLA	O1D-CGD-CBD	-2.74	119.11	124.52
31	6	316	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
31	c	611	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
31	g	310	CLA	C2C-C1C-NC	2.74	112.86	109.98
34	b	622	LMG	C8-O7-C10	-2.74	111.24	117.80
43	b	619	BCR	C38-C26-C27	2.74	119.44	113.60
31	b	609	CLA	C2C-C1C-NC	2.74	112.86	109.98
31	r	313	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
30	6	309	CHL	CMA-C3A-C4A	2.74	120.51	114.61
31	6	304	CLA	CMA-C3A-C4A	2.74	119.13	111.77
31	5	613	CLA	C2C-C1C-NC	2.74	112.86	109.98
32	2	615	LUT	C18-C5-C4	2.74	119.46	114.42
31	G	603	CLA	C1D-ND-C4D	-2.74	104.39	106.31
31	N	312	CLA	C4B-CHC-C1C	2.74	132.69	126.25
31	3	315	CLA	C2C-C1C-NC	2.74	112.86	109.98
31	c	606	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
31	3	304	CLA	C1D-ND-C4D	-2.74	104.39	106.31
31	9	306	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
33	c	622	LHG	O8-C23-C24	2.74	120.18	111.83
31	5	610	CLA	C3B-C4B-NB	-2.74	108.09	110.53
31	6	315	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
31	7	315	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
31	c	607	CLA	C2C-C1C-NC	2.74	112.86	109.98
34	n	321	LMG	O1-C1-C2	2.74	112.43	108.27
34	w	203	LMG	C9-C8-C7	-2.73	105.41	111.78
31	c	613	CLA	C1C-C2C-C3C	-2.73	104.10	106.98
31	S	316	CLA	C2C-C1C-NC	2.73	112.85	109.98
31	s	304	CLA	C2C-C1C-NC	2.73	112.85	109.98
43	c	614	BCR	C23-C22-C21	2.73	123.31	119.01
30	1	601	CHL	CMA-C3A-C2A	2.73	124.69	114.13
31	R	311	CLA	CAA-C2A-C3A	-2.73	105.61	113.00
33	6	320	LHG	O8-C23-C24	2.73	120.17	111.83
31	5	603	CLA	C1D-ND-C4D	-2.73	104.39	106.31
31	N	315	CLA	C1D-ND-C4D	-2.73	104.39	106.31
34	w	204	LMG	C8-O7-C10	-2.73	111.25	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	316	CLA	C3B-C4B-NB	-2.73	108.09	110.53
31	y	613	CLA	C3B-C4B-NB	-2.73	108.09	110.53
31	s	313	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
31	8	613	CLA	C2C-C1C-NC	2.73	112.85	109.98
31	d	405	CLA	C2C-C1C-NC	2.73	112.85	109.98
32	0	617	LUT	C18-C5-C4	2.73	119.44	114.42
31	n	304	CLA	C1D-ND-C4D	-2.73	104.39	106.31
32	8	615	LUT	C11-C10-C9	-2.73	123.45	127.28
43	t	101	BCR	C29-C30-C25	2.73	114.41	110.44
31	7	311	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
31	9	306	CLA	C2C-C1C-NC	2.73	112.85	109.98
33	M	101	LHG	O8-C23-C24	2.73	120.16	111.83
31	q	316	CLA	C2C-C1C-NC	2.73	112.85	109.98
31	4	613	CLA	C4B-CHC-C1C	2.73	132.67	126.25
30	q	308	CHL	C4D-CHA-CBD	-2.73	106.21	108.97
31	8	613	CLA	O2A-CGA-CBA	2.73	120.16	111.83
45	C	618	DGD	O1G-C1A-C2A	2.73	120.16	111.83
31	N	305	CLA	C2C-C1C-NC	2.73	112.85	109.98
37	R	318	XAT	C6-C7-C8	-2.73	120.22	125.99
31	p	612	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
31	r	311	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
30	4	607	CHL	C1-O2A-CGA	2.73	123.26	116.65
31	p	602	CLA	C2C-C1C-NC	2.73	112.85	109.98
31	r	306	CLA	CAA-C2A-C3A	-2.73	105.63	113.00
31	4	612	CLA	C4B-CHC-C1C	2.73	132.66	126.25
31	c	607	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
31	D	403	CLA	O2A-CGA-CBA	2.73	120.15	111.83
31	2	613	CLA	C1D-ND-C4D	-2.73	104.40	106.31
31	3	313	CLA	C1D-ND-C4D	-2.73	104.40	106.31
31	1	602	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
34	2	618	LMG	O8-C28-C29	2.73	120.15	111.83
31	R	312	CLA	CHD-C1D-ND	-2.73	120.97	124.80
38	R	322	SQD	O7-S-C6	-2.73	102.69	106.76
31	B	612	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
31	8	614	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
33	G	618	LHG	O8-C23-C24	2.73	120.15	111.83
33	M	101	LHG	C5-O7-C7	-2.73	111.27	117.80
31	8	614	CLA	C3B-C4B-NB	-2.73	108.10	110.53
31	R	316	CLA	CHD-C1D-ND	-2.73	120.97	124.80
31	q	305	CLA	C4B-CHC-C1C	2.72	132.65	126.25
38	r	322	SQD	O7-S-C6	-2.72	102.69	106.76
43	D	405	BCR	C35-C13-C14	-2.72	118.40	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	y	618	NEX	C38-C25-C26	-2.72	117.82	122.30
31	G	602	CLA	C1-C2-C3	-2.72	121.73	126.20
31	3	305	CLA	C1C-C2C-C3C	-2.72	104.11	106.98
31	4	603	CLA	C4B-CHC-C1C	2.72	132.65	126.25
31	Y	311	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
31	3	315	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
31	s	314	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
32	1	616	LUT	C10-C11-C12	-2.72	115.31	123.20
30	3	309	CHL	C1A-CHA-C4D	2.72	123.53	118.98
33	L	101	LHG	O8-C23-C24	2.72	120.14	111.83
32	n	318	LUT	C18-C5-C4	2.72	119.42	114.42
31	b	613	CLA	C6-C5-C3	-2.72	106.84	113.47
34	f	101	LMG	O8-C28-C29	2.72	120.13	111.83
30	Y	301	CHL	CMA-C3A-C4A	2.72	120.47	114.61
31	C	611	CLA	C2C-C1C-NC	2.72	112.84	109.98
31	p	615	CLA	C1D-ND-C4D	-2.72	104.40	106.31
31	C	603	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
31	8	613	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
31	2	602	CLA	C2C-C1C-NC	2.72	112.84	109.98
31	c	602	CLA	C1-O2A-CGA	2.72	123.23	116.65
32	n	317	LUT	C11-C10-C9	-2.72	123.46	127.28
31	7	303	CLA	C1D-ND-C4D	-2.72	104.40	106.31
31	y	613	CLA	CMA-C3A-C4A	2.72	119.08	111.77
31	c	607	CLA	O2A-CGA-CBA	2.72	120.12	111.83
48	K	101	LMU	O5'-C1'-C2'	2.72	115.96	110.37
31	R	312	CLA	C3B-C4B-NB	-2.72	108.10	110.53
31	N	305	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
31	R	311	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
31	0	611	CLA	C2C-C1C-NC	2.72	112.84	109.98
31	5	615	CLA	CHA-C1A-NA	-2.72	120.24	126.39
31	s	311	CLA	C6-C5-C3	-2.72	106.85	113.47
31	n	316	CLA	C3B-C4B-NB	-2.72	108.10	110.53
31	N	310	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
31	5	602	CLA	C2C-C1C-NC	2.72	112.84	109.98
38	G	617	SQD	O7-S-C6	-2.72	102.70	106.76
30	0	601	CHL	C1-O2A-CGA	2.72	123.23	116.65
32	2	615	LUT	C8-C7-C6	-2.72	119.74	127.00
31	N	321	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
31	4	611	CLA	C2C-C1C-NC	2.72	112.83	109.98
31	G	602	CLA	O2A-C1-C2	2.72	118.56	108.11
31	y	614	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
31	B	607	CLA	C3B-C4B-NB	-2.72	108.11	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	304	CLA	C2C-C1C-NC	2.72	112.83	109.98
33	7	319	LHG	O8-C23-C24	2.72	120.11	111.83
31	8	612	CLA	C1D-ND-C4D	-2.72	104.41	106.31
31	g	305	CLA	C1D-ND-C4D	-2.72	104.41	106.31
31	2	612	CLA	C1C-C2C-C3C	-2.71	104.12	106.98
31	S	305	CLA	C1C-C2C-C3C	-2.71	104.12	106.98
31	b	604	CLA	C1C-C2C-C3C	-2.71	104.12	106.98
31	3	306	CLA	C2C-C1C-NC	2.71	112.83	109.98
31	7	312	CLA	C2C-C1C-NC	2.71	112.83	109.98
31	9	314	CLA	C4B-CHC-C1C	2.71	132.63	126.25
38	A	411	SQD	O7-S-C6	-2.71	102.70	106.76
31	Y	310	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
31	c	607	CLA	C3B-C4B-NB	-2.71	108.11	110.53
42	A	408	PHO	C1-C2-C3	-2.71	121.75	126.20
30	g	302	CHL	C4D-CHA-CBD	-2.71	106.23	108.97
31	6	312	CLA	O2A-CGA-CBA	2.71	120.11	111.83
31	y	604	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
31	5	611	CLA	C2C-C1C-NC	2.71	112.83	109.98
31	7	312	CLA	C1D-ND-C4D	-2.71	104.41	106.31
31	8	602	CLA	C3B-C4B-NB	-2.71	108.11	110.53
31	6	303	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
31	S	311	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
31	0	612	CLA	C3B-C4B-NB	-2.71	108.11	110.53
31	6	304	CLA	C1D-ND-C4D	-2.71	104.41	106.31
31	1	610	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
31	5	615	CLA	CMD-C2D-C3D	-2.71	121.47	127.69
31	S	304	CLA	CHA-C4D-ND	2.71	138.14	132.55
30	1	619	CHL	CHA-C1A-C2A	-2.71	126.94	133.31
31	1	610	CLA	C3B-C4B-NB	-2.71	108.11	110.53
31	4	614	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
31	5	614	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
31	2	611	CLA	O2A-CGA-CBA	2.71	120.10	111.83
31	4	604	CLA	C1D-ND-C4D	-2.71	104.41	106.31
31	g	304	CLA	C1D-ND-C4D	-2.71	104.41	106.31
34	C	622	LMG	O8-C28-C29	2.71	120.09	111.83
31	5	610	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
43	C	615	BCR	C36-C18-C17	-2.71	118.43	122.82
31	R	303	CLA	CMA-C3A-C4A	2.71	119.05	111.77
31	C	611	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
36	r	301	NEX	C5-C6-C1	2.71	122.38	119.70
33	1	617	LHG	O8-C23-C24	2.71	120.09	111.83
31	p	603	CLA	CMA-C3A-C4A	2.71	119.05	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y	611	CLA	O2A-C1-C2	2.71	118.53	108.11
33	D	407	LHG	O8-C23-C24	2.71	120.09	111.83
34	6	323	LMG	O8-C28-C29	2.71	120.09	111.83
32	8	616	LUT	C18-C5-C4	2.71	119.40	114.42
31	1	611	CLA	C1D-ND-C4D	-2.71	104.41	106.31
31	N	303	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
31	6	303	CLA	C2C-C1C-NC	2.71	112.82	109.98
31	n	315	CLA	O2A-CGA-CBA	2.71	120.08	111.83
32	6	318	LUT	C1-C6-C5	-2.71	118.94	122.64
31	7	316	CLA	C3B-C4B-NB	-2.71	108.11	110.53
31	5	610	CLA	CMA-C3A-C4A	2.71	119.04	111.77
34	G	619	LMG	C8-O7-C10	-2.71	111.32	117.80
31	3	304	CLA	C2C-C1C-NC	2.70	112.82	109.98
31	8	610	CLA	C2C-C1C-NC	2.70	112.82	109.98
31	C	605	CLA	C3B-C4B-NB	-2.70	108.12	110.53
31	d	404	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
31	B	606	CLA	O2A-CGA-CBA	2.70	120.08	111.83
31	b	617	CLA	O2A-CGA-CBA	2.70	120.08	111.83
31	4	610	CLA	O2A-C1-C2	2.70	118.51	108.11
33	3	320	LHG	C6-C5-C4	-2.70	105.48	111.78
31	c	604	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
31	y	611	CLA	C1-O2A-CGA	2.70	123.19	116.65
31	2	603	CLA	C4B-CHC-C1C	2.70	132.60	126.25
31	b	604	CLA	CHA-C4D-ND	2.70	138.12	132.55
31	2	613	CLA	C2C-C1C-NC	2.70	112.82	109.98
30	4	608	CHL	C1-O2A-CGA	2.70	123.19	116.65
31	g	314	CLA	C1D-ND-C4D	-2.70	104.42	106.31
34	J	101	LMG	O8-C28-C29	2.70	120.07	111.83
38	g	301	SQD	O7-S-C6	-2.70	102.72	106.76
31	6	313	CLA	C2C-C1C-NC	2.70	112.82	109.98
31	N	314	CLA	C2C-C1C-NC	2.70	112.82	109.98
31	r	307	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
31	b	611	CLA	C1D-ND-C4D	-2.70	104.42	106.31
31	2	613	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
31	p	615	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
43	c	614	BCR	C38-C26-C27	2.70	119.35	113.60
31	3	306	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
31	4	603	CLA	C2C-C1C-NC	2.70	112.82	109.98
34	j	101	LMG	O8-C28-C29	2.70	120.06	111.83
31	B	602	CLA	C2C-C1C-NC	2.70	112.81	109.98
43	T	101	BCR	C29-C30-C25	2.70	114.36	110.44
31	d	404	CLA	O2D-CGD-O1D	-2.70	118.60	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	1	614	CLA	C2C-C1C-NC	2.70	112.81	109.98
31	4	604	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
31	a	407	CLA	CAA-C2A-C3A	-2.70	105.72	113.00
31	B	605	CLA	C2C-C1C-NC	2.70	112.81	109.98
31	S	312	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
31	6	312	CLA	C1-O2A-CGA	2.69	123.17	116.65
31	r	305	CLA	C2C-C1C-NC	2.69	112.81	109.98
38	m	101	SQD	O7-S-C6	-2.69	102.73	106.76
31	N	303	CLA	C3B-C4B-NB	-2.69	108.12	110.53
31	g	303	CLA	C3B-C4B-NB	-2.69	108.12	110.53
31	3	301	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
31	5	602	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
31	4	610	CLA	CMA-C3A-C4A	2.69	119.01	111.77
32	9	318	LUT	C31-C32-C33	-2.69	118.98	126.36
31	B	609	CLA	O2A-CGA-CBA	2.69	120.05	111.83
31	S	314	CLA	CMA-C3A-C4A	2.69	119.01	111.77
31	2	603	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
31	5	614	CLA	C2C-C1C-NC	2.69	112.81	109.98
38	M	102	SQD	O7-S-C6	-2.69	102.74	106.76
31	4	610	CLA	C1D-ND-C4D	-2.69	104.42	106.31
43	B	618	BCR	C23-C24-C25	-2.69	119.81	127.00
31	7	316	CLA	CMA-C3A-C4A	2.69	119.01	111.77
33	6	320	LHG	C5-O7-C7	-2.69	111.35	117.80
37	r	318	XAT	C26-C27-C28	-2.69	120.30	125.99
31	q	313	CLA	C2C-C1C-NC	2.69	112.81	109.98
31	b	612	CLA	CMA-C3A-C4A	2.69	119.01	111.77
31	7	305	CLA	O2A-C1-C2	2.69	118.46	108.11
31	5	615	CLA	CHA-C4D-ND	2.69	138.10	132.55
31	S	305	CLA	C1D-ND-C4D	-2.69	104.42	106.31
31	7	304	CLA	C1D-ND-C4D	-2.69	104.42	106.31
31	8	603	CLA	C1D-ND-C4D	-2.69	104.42	106.31
31	r	305	CLA	C1D-ND-C4D	-2.69	104.42	106.31
31	C	610	CLA	C2C-C1C-NC	2.69	112.81	109.98
31	R	314	CLA	CHD-C1D-ND	-2.69	121.02	124.80
31	1	611	CLA	C1-C2-C3	-2.69	121.79	126.20
31	0	614	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
31	Y	313	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
31	0	613	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
36	R	301	NEX	C40-C33-C34	-2.69	118.46	122.82
31	d	405	CLA	CAA-C2A-C3A	-2.69	105.73	113.00
31	2	602	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
31	C	613	CLA	C1C-C2C-C3C	-2.69	104.15	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	303	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
31	S	311	CLA	C2C-C1C-NC	2.69	112.81	109.98
31	q	314	CLA	C2C-C1C-NC	2.69	112.81	109.98
31	0	602	CLA	O2A-CGA-CBA	2.69	120.03	111.83
31	6	311	CLA	C3B-C4B-NB	-2.69	108.13	110.53
34	b	624	LMG	O1-C1-C2	2.69	112.35	108.27
43	t	101	BCR	C16-C15-C14	2.69	129.02	123.52
31	4	613	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
31	y	612	CLA	C2C-C1C-NC	2.69	112.80	109.98
31	c	610	CLA	C1-O2A-CGA	2.69	123.15	116.65
32	s	318	LUT	C30-C31-C32	-2.69	115.42	123.20
31	N	313	CLA	C1C-C2C-C3C	-2.69	104.16	106.98
30	9	307	CHL	C4D-CHA-CBD	-2.69	106.26	108.97
31	b	611	CLA	C4B-CHC-C1C	2.69	132.56	126.25
34	1	618	LMG	O8-C28-C29	2.69	120.02	111.83
31	R	312	CLA	CMD-C2D-C3D	-2.69	121.53	127.69
31	7	305	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
43	h	101	BCR	C8-C7-C6	-2.68	119.83	127.00
30	3	308	CHL	CMA-C3A-C4A	2.68	120.39	114.61
31	a	409	CLA	CAA-C2A-C3A	-2.68	105.75	113.00
31	b	617	CLA	CHD-C1D-ND	-2.68	121.03	124.80
31	3	306	CLA	C3B-C4B-NB	-2.68	108.13	110.53
31	G	603	CLA	C2C-C1C-NC	2.68	112.80	109.98
30	5	609	CHL	C4D-CHA-CBD	-2.68	106.26	108.97
31	s	305	CLA	C1D-ND-C4D	-2.68	104.43	106.31
36	G	616	NEX	C38-C25-C26	-2.68	117.89	122.30
43	c	615	BCR	C33-C5-C4	2.68	119.32	113.60
32	1	615	LUT	C1-C6-C5	-2.68	118.97	122.64
31	7	312	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
31	2	603	CLA	C2C-C1C-NC	2.68	112.80	109.98
31	8	603	CLA	CMD-C2D-C3D	-2.68	121.54	127.69
31	S	304	CLA	CHA-C1A-NA	-2.68	120.32	126.39
31	c	613	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
32	0	616	LUT	C18-C5-C4	2.68	119.35	114.42
31	b	611	CLA	C2C-C1C-NC	2.68	112.80	109.98
31	5	604	CLA	C1D-ND-C4D	-2.68	104.43	106.31
31	q	305	CLA	C1D-ND-C4D	-2.68	104.43	106.31
31	g	303	CLA	C4B-CHC-C1C	2.68	132.55	126.25
31	N	313	CLA	C3B-C4B-NB	-2.68	108.14	110.53
31	1	612	CLA	C4B-CHC-C1C	2.68	132.55	126.25
31	Y	312	CLA	C4B-CHC-C1C	2.68	132.55	126.25
33	C	623	LHG	C5-O7-C7	-2.68	111.38	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C	620	DGD	C2G-O2G-C1B	-2.68	111.38	117.80
31	5	613	CLA	C1D-ND-C4D	-2.68	104.43	106.31
31	G	611	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
31	b	615	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
31	9	304	CLA	C2C-C1C-NC	2.68	112.80	109.98
31	b	614	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
31	3	311	CLA	O2A-CGA-CBA	2.68	120.00	111.83
34	0	620	LMG	O8-C28-C29	2.68	120.00	111.83
31	n	303	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
31	4	602	CLA	C2C-C1C-NC	2.68	112.80	109.98
31	0	614	CLA	C2C-C1C-NC	2.68	112.80	109.98
31	8	614	CLA	C2C-C1C-NC	2.68	112.80	109.98
31	r	316	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
31	y	614	CLA	C1D-ND-C4D	-2.68	104.43	106.31
30	4	605	CHL	C4D-CHA-CBD	-2.68	106.27	108.97
31	s	312	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
38	B	620	SQD	O7-S-C6	-2.68	102.76	106.76
31	6	315	CLA	C2C-C1C-NC	2.68	112.79	109.98
34	C	621	LMG	O8-C28-C29	2.68	120.00	111.83
31	6	312	CLA	C3B-C4B-NB	-2.68	108.14	110.53
30	g	306	CHL	CMA-C3A-C4A	2.68	120.38	114.61
31	9	305	CLA	C4B-CHC-C1C	2.68	132.54	126.25
34	B	622	LMG	C8-O7-C10	-2.68	111.39	117.80
31	0	603	CLA	C2C-C1C-NC	2.68	112.79	109.98
31	9	304	CLA	O2A-CGA-CBA	2.68	119.99	111.83
31	p	615	CLA	C4B-CHC-C1C	2.67	132.54	126.25
31	B	603	CLA	C2C-C1C-NC	2.67	112.79	109.98
31	R	313	CLA	C2C-C1C-NC	2.67	112.79	109.98
38	y	621	SQD	O7-S-C6	-2.67	102.76	106.76
30	9	311	CHL	C1-O2A-CGA	2.67	123.12	116.65
32	7	317	LUT	C18-C5-C4	2.67	119.34	114.42
31	Y	303	CLA	C1D-ND-C4D	-2.67	104.44	106.31
43	b	618	BCR	C21-C20-C19	-2.67	115.45	123.20
31	p	614	CLA	C4B-CHC-C1C	2.67	132.53	126.25
31	y	611	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
31	6	305	CLA	C2C-C1C-NC	2.67	112.79	109.98
31	B	610	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
30	0	608	CHL	C1-O2A-CGA	2.67	123.12	116.65
31	n	312	CLA	C2C-C1C-NC	2.67	112.79	109.98
31	n	314	CLA	C1D-ND-C4D	-2.67	104.44	106.31
30	4	606	CHL	C4D-CHA-CBD	-2.67	106.27	108.97
30	q	311	CHL	C4D-CHA-CBD	-2.67	106.27	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	9	318	LUT	C11-C12-C13	-2.67	119.04	126.36
31	Y	305	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
31	r	314	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
43	A	410	BCR	C8-C7-C6	-2.67	119.86	127.00
31	s	304	CLA	C1D-ND-C4D	-2.67	104.44	106.31
31	G	602	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
31	A	409	CLA	CAA-C2A-C3A	-2.67	105.78	113.00
31	3	304	CLA	C3B-C4B-NB	-2.67	108.15	110.53
31	G	602	CLA	C3B-C4B-NB	-2.67	108.15	110.53
34	7	320	LMG	C7-O1-C1	-2.67	108.07	113.80
36	N	318	NEX	C2-C1-C6	2.67	111.81	109.21
32	g	316	LUT	C31-C32-C33	-2.67	119.04	126.36
31	p	610	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
31	8	604	CLA	C1D-ND-C4D	-2.67	104.44	106.31
31	r	312	CLA	C3B-C4B-NB	-2.67	108.15	110.53
31	c	603	CLA	O2A-CGA-CBA	2.67	119.97	111.83
31	s	304	CLA	C4B-CHC-C1C	2.67	132.52	126.25
31	0	612	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
31	S	315	CLA	C2C-C1C-NC	2.67	112.78	109.98
31	1	602	CLA	CMA-C3A-C4A	2.67	118.94	111.77
30	y	605	CHL	C4D-CHA-CBD	-2.67	106.28	108.97
34	c	620	LMG	O8-C28-C29	2.67	119.97	111.83
34	Y	319	LMG	O8-C28-C29	2.67	119.97	111.83
30	G	623	CHL	C4D-CHA-CBD	-2.67	106.28	108.97
31	4	603	CLA	C1C-C2C-C3C	-2.67	104.18	106.98
31	B	604	CLA	C1C-C2C-C3C	-2.67	104.18	106.98
31	8	609	CLA	C1C-C2C-C3C	-2.67	104.18	106.98
31	Y	305	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
31	B	610	CLA	C1D-ND-C4D	-2.67	104.44	106.31
30	G	601	CHL	C4D-CHA-CBD	-2.67	106.28	108.97
31	p	611	CLA	C2C-C1C-NC	2.66	112.78	109.98
31	c	603	CLA	C2C-C1C-NC	2.66	112.78	109.98
31	S	315	CLA	CMD-C2D-C3D	-2.66	121.58	127.69
31	Y	312	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
31	g	314	CLA	C4B-CHC-C1C	2.66	132.51	126.25
31	n	311	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
31	2	609	CLA	C2C-C1C-NC	2.66	112.78	109.98
31	4	614	CLA	C2C-C1C-NC	2.66	112.78	109.98
31	9	313	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
31	R	307	CLA	C3B-C4B-NB	-2.66	108.15	110.53
31	b	615	CLA	C3B-C4B-NB	-2.66	108.15	110.53
32	G	615	LUT	C10-C11-C12	-2.66	115.48	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	S	317	LUT	C8-C7-C6	-2.66	119.89	127.00
31	2	609	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
31	N	311	CLA	C2C-C1C-NC	2.66	112.78	109.98
31	B	603	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
31	0	603	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
31	q	304	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
31	0	612	CLA	C2C-C1C-NC	2.66	112.78	109.98
31	0	611	CLA	CMA-C3A-C4A	2.66	118.92	111.77
31	r	316	CLA	O2A-C1-C2	2.66	118.35	108.11
31	9	304	CLA	C3B-C4B-NB	-2.66	108.16	110.53
31	b	612	CLA	C3B-C4B-NB	-2.66	108.16	110.53
31	G	613	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
31	6	311	CLA	C2C-C1C-NC	2.66	112.78	109.98
31	y	615	CLA	CMA-C3A-C4A	2.66	118.92	111.77
31	4	611	CLA	C1D-ND-C4D	-2.66	104.45	106.31
31	D	403	CLA	C2C-C1C-NC	2.66	112.78	109.98
33	5	619	LHG	O8-C23-C24	2.66	119.94	111.83
31	c	608	CLA	C1-C2-C3	-2.66	121.84	126.20
31	C	606	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
31	9	316	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
31	N	303	CLA	C2C-C1C-NC	2.66	112.77	109.98
31	c	611	CLA	C2C-C1C-NC	2.66	112.77	109.98
30	6	308	CHL	C4D-CHA-CBD	-2.66	106.29	108.97
30	1	607	CHL	C1-C2-C3	-2.66	121.84	126.20
31	5	602	CLA	C3B-C4B-NB	-2.66	108.16	110.53
31	5	603	CLA	C3B-C4B-NB	-2.66	108.16	110.53
31	q	306	CLA	C3B-C4B-NB	-2.66	108.16	110.53
31	c	610	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
32	1	616	LUT	C11-C10-C9	-2.66	123.55	127.28
31	4	602	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
32	0	617	LUT	C30-C31-C32	-2.66	115.50	123.20
31	N	315	CLA	C2C-C1C-NC	2.66	112.77	109.98
31	s	303	CLA	C2C-C1C-NC	2.66	112.77	109.98
32	y	616	LUT	C39-C29-C28	2.66	122.14	118.09
38	b	621	SQD	O7-S-C6	-2.66	102.79	106.76
31	5	612	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
31	3	305	CLA	C2C-C1C-NC	2.66	112.77	109.98
31	6	304	CLA	C2C-C1C-NC	2.66	112.77	109.98
31	8	610	CLA	C4B-CHC-C1C	2.66	132.49	126.25
34	X	203	LMG	O8-C28-C29	2.66	119.93	111.83
31	4	602	CLA	C3B-C4B-NB	-2.65	108.16	110.53
30	5	606	CHL	CMA-C3A-C4A	2.65	120.33	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	611	CLA	C4B-CHC-C1C	2.65	132.49	126.25
31	S	303	CLA	C4B-CHC-C1C	2.65	132.49	126.25
32	1	616	LUT	C8-C7-C6	-2.65	119.91	127.00
31	N	315	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
31	p	614	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
31	B	610	CLA	C4B-CHC-C1C	2.65	132.49	126.25
31	7	304	CLA	C4B-CHC-C1C	2.65	132.49	126.25
31	r	313	CLA	C2C-C1C-NC	2.65	112.77	109.98
30	9	311	CHL	C1-C2-C3	-2.65	121.85	126.20
31	c	607	CLA	O2A-C1-C2	2.65	118.32	108.11
31	3	301	CLA	C4B-CHC-C1C	2.65	132.49	126.25
31	n	313	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
32	7	318	LUT	C1-C6-C5	-2.65	119.01	122.64
31	y	613	CLA	O2A-C1-C2	2.65	118.31	108.11
31	3	315	CLA	C4B-CHC-C1C	2.65	132.48	126.25
31	1	604	CLA	O2A-CGA-CBA	2.65	119.92	111.83
31	B	613	CLA	C2C-C1C-NC	2.65	112.77	109.98
31	1	611	CLA	C4B-CHC-C1C	2.65	132.48	126.25
44	A	416	PL9	C36-C34-C33	-2.65	115.22	121.17
31	r	316	CLA	O2A-CGA-CBA	2.65	119.92	111.83
31	p	612	CLA	C4B-CHC-C1C	2.65	132.48	126.25
33	s	320	LHG	C6-C5-C4	-2.65	105.60	111.78
31	r	307	CLA	CAA-C2A-C3A	-2.65	105.84	113.00
31	7	303	CLA	C2C-C1C-NC	2.65	112.77	109.98
31	Y	311	CLA	C3B-C4B-NB	-2.65	108.16	110.53
30	4	609	CHL	C4D-CHA-CBD	-2.65	106.30	108.97
43	b	619	BCR	C33-C5-C4	2.65	119.25	113.60
31	3	304	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
31	3	305	CLA	C3B-C4B-NB	-2.65	108.17	110.53
31	S	303	CLA	C3B-C4B-NB	-2.65	108.17	110.53
43	d	406	BCR	C11-C12-C13	2.65	133.63	126.36
31	q	305	CLA	C2C-C1C-NC	2.65	112.76	109.98
38	B	623	SQD	O7-S-C6	-2.65	102.80	106.76
31	Y	314	CLA	C1D-ND-C4D	-2.65	104.45	106.31
34	s	321	LMG	C7-O1-C1	-2.65	108.12	113.80
31	g	314	CLA	C2C-C1C-NC	2.65	112.76	109.98
47	E	101	HEM	CHD-C1D-C2D	-2.65	120.85	125.03
30	S	307	CHL	C4D-CHA-CBD	-2.65	106.30	108.97
30	9	311	CHL	C4D-CHA-CBD	-2.65	106.30	108.97
31	y	602	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
31	y	602	CLA	C2C-C1C-NC	2.65	112.76	109.98
31	D	404	CLA	C1C-C2C-C3C	-2.65	104.20	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	313	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
36	g	317	NEX	C17-C1-C6	-2.65	108.10	110.47
31	G	611	CLA	CHA-C4D-ND	2.65	138.01	132.55
31	7	315	CLA	C1D-ND-C4D	-2.65	104.46	106.31
34	G	622	LMG	O8-C28-C29	2.65	119.90	111.83
31	b	608	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
31	G	610	CLA	C3B-C4B-NB	-2.64	108.17	110.53
31	C	608	CLA	CAA-C2A-C3A	-2.64	105.85	113.00
31	G	612	CLA	C2C-C1C-NC	2.64	112.76	109.98
38	S	301	SQD	O7-S-C6	-2.64	102.81	106.76
43	D	405	BCR	C1-C6-C7	2.64	122.82	115.65
31	y	615	CLA	C4B-CHC-C1C	2.64	132.46	126.25
30	5	601	CHL	C4D-CHA-CBD	-2.64	106.30	108.97
31	7	303	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
31	p	611	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
31	b	613	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
33	d	408	LHG	O8-C23-C24	2.64	119.89	111.83
32	4	616	LUT	C1-C6-C5	-2.64	119.02	122.64
31	C	608	CLA	C2C-C1C-NC	2.64	112.76	109.98
31	0	615	CLA	C2C-C1C-NC	2.64	112.76	109.98
31	1	614	CLA	C3B-C4B-NB	-2.64	108.17	110.53
31	6	311	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
31	9	312	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
31	r	303	CLA	C1D-ND-C4D	-2.64	104.46	106.31
33	4	618	LHG	O8-C23-C24	2.64	119.89	111.83
31	a	409	CLA	O2A-CGA-CBA	2.64	119.89	111.83
30	N	309	CHL	C1-C2-C3	-2.64	121.87	126.20
31	y	612	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
31	7	316	CLA	C1D-ND-C4D	-2.64	104.46	106.31
31	p	613	CLA	C3B-C4B-NB	-2.64	108.17	110.53
43	H	101	BCR	C16-C15-C14	-2.64	118.12	123.52
31	1	604	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
31	A	409	CLA	O2A-CGA-CBA	2.64	119.88	111.83
31	1	604	CLA	C2C-C1C-NC	2.64	112.75	109.98
34	w	201	LMG	O8-C28-C29	2.64	119.88	111.83
31	8	610	CLA	C1C-C2C-C3C	-2.64	104.21	106.98
31	b	612	CLA	C4B-CHC-C1C	2.64	132.45	126.25
43	b	619	BCR	C30-C25-C26	-2.64	119.03	122.64
31	n	303	CLA	C3B-C4B-NB	-2.64	108.18	110.53
31	p	604	CLA	CHD-C1D-ND	-2.64	121.09	124.80
31	B	608	CLA	C2C-C1C-NC	2.64	112.75	109.98
38	g	318	SQD	O7-S-C6	-2.64	102.82	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y	602	CLA	C3B-C4B-NB	-2.64	108.18	110.53
31	0	602	CLA	C1C-C2C-C3C	-2.64	104.21	106.98
31	q	316	CLA	C1C-C2C-C3C	-2.64	104.21	106.98
38	Y	320	SQD	O7-S-C6	-2.64	102.82	106.76
30	3	303	CHL	C1-O2A-CGA	2.64	123.03	116.65
31	s	316	CLA	CMA-C3A-C4A	2.64	118.86	111.77
31	1	611	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
31	Y	304	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
31	n	316	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
31	3	304	CLA	C4B-CHC-C1C	2.63	132.44	126.25
30	N	307	CHL	CMA-C3A-C4A	2.63	120.29	114.61
31	5	612	CLA	C2C-C1C-NC	2.63	112.75	109.98
31	3	313	CLA	C4B-CHC-C1C	2.63	132.44	126.25
34	w	205	LMG	O8-C28-C29	2.63	119.86	111.83
31	C	612	CLA	O2A-CGA-CBA	2.63	119.86	111.83
31	C	604	CLA	C2C-C1C-NC	2.63	112.75	109.98
31	N	305	CLA	C1D-ND-C4D	-2.63	104.47	106.31
31	A	409	CLA	CMA-C3A-C4A	2.63	118.85	111.77
31	C	607	CLA	O2A-CGA-CBA	2.63	119.86	111.83
31	G	610	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
31	8	611	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
30	p	609	CHL	C4D-CHA-CBD	-2.63	106.31	108.97
34	n	321	LMG	O8-C28-C29	2.63	119.86	111.83
31	c	602	CLA	CMA-C3A-C4A	2.63	118.84	111.77
32	0	616	LUT	C39-C29-C28	2.63	122.11	118.09
31	4	611	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
31	8	602	CLA	C2C-C1C-NC	2.63	112.75	109.98
31	5	610	CLA	C4B-CHC-C1C	2.63	132.43	126.25
31	R	312	CLA	O2A-CGA-CBA	2.63	119.86	111.83
31	5	612	CLA	C3B-C4B-NB	-2.63	108.18	110.53
31	0	602	CLA	CMA-C3A-C4A	2.63	118.84	111.77
31	a	409	CLA	CMA-C3A-C4A	2.63	118.84	111.77
31	0	612	CLA	CHA-C4D-ND	2.63	137.97	132.55
31	5	602	CLA	C4B-CHC-C1C	2.63	132.43	126.25
33	3	320	LHG	O8-C23-C24	2.63	119.85	111.83
31	p	602	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
43	c	615	BCR	C19-C18-C17	2.63	123.14	119.01
31	N	321	CLA	C2C-C1C-NC	2.63	112.74	109.98
31	b	604	CLA	C2C-C1C-NC	2.63	112.74	109.98
31	p	615	CLA	CMA-C3A-C4A	2.63	118.84	111.77
31	N	312	CLA	C2C-C1C-NC	2.63	112.74	109.98
31	n	313	CLA	C2C-C1C-NC	2.63	112.74	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	610	CLA	O2A-CGA-CBA	2.63	119.85	111.83
31	y	611	CLA	C4B-CHC-C1C	2.63	132.43	126.25
31	g	311	CLA	CMA-C3A-C4A	2.63	118.83	111.77
32	6	317	LUT	C18-C5-C4	2.63	119.25	114.42
31	8	602	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
30	Y	301	CHL	C4D-CHA-CBD	-2.63	106.32	108.97
31	S	314	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
31	B	604	CLA	CHA-C4D-ND	2.63	137.97	132.55
31	n	303	CLA	C2C-C1C-NC	2.63	112.74	109.98
36	R	319	NEX	C17-C1-C6	-2.63	108.12	110.47
31	n	313	CLA	C3B-C4B-NB	-2.63	108.19	110.53
31	y	603	CLA	C3B-C4B-NB	-2.63	108.19	110.53
34	p	620	LMG	O8-C28-C29	2.63	119.84	111.83
32	Y	316	LUT	C18-C5-C4	2.63	119.25	114.42
31	b	603	CLA	C2C-C1C-NC	2.62	112.74	109.98
31	2	604	CLA	C3B-C4B-NB	-2.62	108.19	110.53
31	s	303	CLA	C3B-C4B-NB	-2.62	108.19	110.53
43	c	614	BCR	C1-C6-C7	2.62	122.77	115.65
32	1	616	LUT	C15-C35-C34	-2.62	118.15	123.52
31	G	612	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
31	N	312	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
32	0	617	LUT	C27-C28-C29	-2.62	120.68	126.32
31	B	604	CLA	CMD-C2D-C3D	-2.62	121.67	127.69
31	s	315	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
31	4	612	CLA	C2D-C1D-ND	2.62	112.72	110.13
31	n	311	CLA	C4B-CHC-C1C	2.62	132.41	126.25
31	3	313	CLA	O2A-CGA-CBA	2.62	119.83	111.83
43	b	618	BCR	C1-C6-C5	-2.62	119.05	122.64
31	B	602	CLA	C3B-C4B-NB	-2.62	108.19	110.53
31	d	405	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
31	n	312	CLA	C4B-CHC-C1C	2.62	132.41	126.25
30	6	307	CHL	C4D-CHA-CBD	-2.62	106.32	108.97
30	p	607	CHL	C1-O2A-CGA	2.62	123.00	116.65
31	9	314	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
31	8	611	CLA	C3B-C4B-NB	-2.62	108.19	110.53
31	C	613	CLA	C2C-C1C-NC	2.62	112.73	109.98
31	r	314	CLA	CHD-C1D-ND	-2.62	121.11	124.80
34	r	321	LMG	O8-C28-C29	2.62	119.83	111.83
31	r	303	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
31	G	602	CLA	C2C-C1C-NC	2.62	112.73	109.98
31	y	612	CLA	C4B-CHC-C1C	2.62	132.41	126.25
43	T	101	BCR	C38-C26-C27	2.62	119.18	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	602	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
31	3	311	CLA	CMA-C3A-C4A	2.62	118.81	111.77
30	Y	309	CHL	C1-O2A-CGA	2.62	122.99	116.65
31	B	616	CLA	O2A-CGA-CBA	2.62	119.82	111.83
31	0	612	CLA	C4B-CHC-C1C	2.62	132.41	126.25
31	7	312	CLA	C4B-CHC-C1C	2.62	132.41	126.25
31	R	316	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
43	V	101	BCR	C30-C25-C24	2.62	122.75	115.65
31	6	313	CLA	C4B-CHC-C1C	2.62	132.40	126.25
31	4	610	CLA	CHA-C4D-ND	2.62	137.95	132.55
31	g	314	CLA	C1C-C2C-C3C	-2.62	104.23	106.98
31	b	607	CLA	C2C-C1C-NC	2.62	112.73	109.98
31	D	403	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
30	p	601	CHL	C4D-CHA-CBD	-2.62	106.33	108.97
31	N	310	CLA	C2C-C1C-NC	2.62	112.73	109.98
31	S	312	CLA	C2C-C1C-NC	2.62	112.73	109.98
31	4	602	CLA	C4B-CHC-C1C	2.62	132.40	126.25
31	S	310	CLA	CMA-C3A-C4A	2.62	118.80	111.77
31	5	611	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
31	n	312	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
31	Y	313	CLA	O2A-CGA-CBA	2.61	119.81	111.83
31	s	303	CLA	C4B-CHC-C1C	2.61	132.40	126.25
31	8	611	CLA	C2C-C1C-NC	2.61	112.73	109.98
31	p	604	CLA	O2A-CGA-CBA	2.61	119.81	111.83
31	C	604	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
31	1	611	CLA	C2C-C1C-NC	2.61	112.73	109.98
43	z	101	BCR	C29-C30-C25	2.61	114.23	110.44
31	y	614	CLA	C4B-CHC-C1C	2.61	132.39	126.25
31	1	610	CLA	CHD-C1D-ND	-2.61	121.12	124.80
31	b	611	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
30	G	608	CHL	CMA-C3A-C2A	2.61	124.22	114.13
31	B	603	CLA	CMA-C3A-C4A	2.61	118.80	111.77
31	S	311	CLA	CAA-C2A-C3A	-2.61	105.94	113.00
31	4	613	CLA	C2C-C1C-NC	2.61	112.73	109.98
31	C	603	CLA	C2C-C1C-NC	2.61	112.73	109.98
31	8	609	CLA	C2C-C1C-NC	2.61	112.73	109.98
31	2	609	CLA	C4B-CHC-C1C	2.61	132.39	126.25
31	p	614	CLA	C2C-C1C-NC	2.61	112.72	109.98
31	q	304	CLA	C2C-C1C-NC	2.61	112.72	109.98
31	9	304	CLA	C4B-CHC-C1C	2.61	132.39	126.25
31	q	313	CLA	C1D-ND-C4D	-2.61	104.48	106.31
33	0	619	LHG	O8-C23-C24	2.61	119.80	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	0	611	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
31	G	612	CLA	O2A-CGA-CBA	2.61	119.80	111.83
31	R	314	CLA	C2C-C1C-NC	2.61	112.72	109.98
31	B	604	CLA	O1D-CGD-CBD	-2.61	119.37	124.52
34	B	622	LMG	O8-C28-C29	2.61	119.79	111.83
43	D	405	BCR	C33-C5-C4	2.61	119.16	113.60
31	C	601	CLA	O2A-CGA-CBA	2.61	119.79	111.83
31	s	313	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
31	Y	312	CLA	C2C-C1C-NC	2.61	112.72	109.98
31	0	602	CLA	C2C-C1C-NC	2.61	112.72	109.98
31	G	613	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
43	Z	101	BCR	C21-C20-C19	-2.61	115.64	123.20
31	n	311	CLA	C2C-C1C-NC	2.61	112.72	109.98
31	N	313	CLA	C1D-ND-C4D	-2.61	104.48	106.31
30	0	605	CHL	C4D-CHA-CBD	-2.61	106.34	108.97
31	g	303	CLA	CHD-C1D-ND	-2.61	121.14	124.80
31	Y	304	CLA	C4B-CHC-C1C	2.61	132.38	126.25
47	e	102	HEM	CHD-C1D-C2D	-2.61	120.91	125.03
31	8	603	CLA	C3B-C4B-NB	-2.61	108.20	110.53
31	N	321	CLA	C4B-CHC-C1C	2.61	132.37	126.25
31	5	612	CLA	C1D-ND-C4D	-2.61	104.48	106.31
31	5	614	CLA	C1D-ND-C4D	-2.61	104.48	106.31
31	p	604	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
31	b	615	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
31	y	610	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
30	q	310	CHL	CMA-C3A-C4A	2.61	120.22	114.61
34	3	321	LMG	O8-C28-C29	2.60	119.78	111.83
34	q	301	LMG	C8-O7-C10	-2.60	111.56	117.80
31	D	403	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
31	r	312	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
33	L	101	LHG	C5-O7-C7	-2.60	111.56	117.80
31	N	313	CLA	O2A-CGA-CBA	2.60	119.77	111.83
31	r	315	CLA	O2A-CGA-CBA	2.60	119.77	111.83
31	r	313	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
31	r	315	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
31	3	312	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
43	b	620	BCR	C23-C24-C25	-2.60	120.05	127.00
31	b	605	CLA	CHA-C4D-ND	2.60	137.92	132.55
33	r	320	LHG	C5-O7-C7	-2.60	111.57	117.80
43	h	101	BCR	C23-C24-C25	-2.60	120.05	127.00
31	6	305	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
31	B	614	CLA	C1C-C2C-C3C	-2.60	104.24	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	605	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
31	9	316	CLA	C2C-C1C-NC	2.60	112.72	109.98
31	R	305	CLA	CHD-C1D-ND	-2.60	121.14	124.80
31	3	314	CLA	C4B-CHC-C1C	2.60	132.37	126.25
30	7	310	CHL	C4D-CHA-CBD	-2.60	106.34	108.97
31	G	603	CLA	C4B-CHC-C1C	2.60	132.36	126.25
31	G	603	CLA	O2A-CGA-CBA	2.60	119.77	111.83
31	G	604	CLA	CMA-C3A-C4A	2.60	118.76	111.77
36	n	319	NEX	C38-C25-C26	-2.60	118.02	122.30
31	3	316	CLA	CHA-C4D-ND	2.60	137.91	132.55
31	Y	303	CLA	C4B-CHC-C1C	2.60	132.36	126.25
34	G	619	LMG	O8-C28-C29	2.60	119.76	111.83
31	B	614	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
34	a	416	LMG	C8-O7-C10	-2.60	111.57	117.80
30	2	608	CHL	C4D-CHA-CBD	-2.60	106.35	108.97
31	6	312	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
35	2	614	RRX	C8-C7-C6	-2.60	120.05	127.00
31	R	312	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
31	S	303	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
36	s	319	NEX	O24-C25-C38	-2.60	112.14	115.05
32	4	616	LUT	C27-C28-C29	-2.60	120.73	126.32
31	R	313	CLA	CMA-C3A-C4A	2.60	118.76	111.77
31	y	614	CLA	C2C-C1C-NC	2.60	112.71	109.98
30	n	306	CHL	C1-O2A-CGA	2.60	122.94	116.65
31	3	313	CLA	CMA-C3A-C4A	2.60	118.76	111.77
31	y	603	CLA	C2C-C1C-NC	2.60	112.71	109.98
31	9	312	CLA	C1D-ND-C4D	-2.60	104.49	106.31
31	b	609	CLA	CMA-C3A-C4A	2.60	118.76	111.77
31	p	611	CLA	C4B-CHC-C1C	2.60	132.36	126.25
43	B	619	BCR	C38-C26-C27	2.60	119.14	113.60
31	9	313	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
31	7	305	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
33	r	320	LHG	O8-C23-C24	2.60	119.75	111.83
31	n	305	CLA	C1D-ND-C4D	-2.60	104.49	106.31
43	h	101	BCR	C15-C16-C17	-2.60	118.21	123.52
30	9	308	CHL	C4D-CHA-CBD	-2.60	106.35	108.97
31	3	311	CLA	C4B-CHC-C1C	2.60	132.35	126.25
31	Y	310	CLA	C4B-CHC-C1C	2.60	132.35	126.25
31	s	311	CLA	CHD-C1D-ND	-2.60	121.15	124.80
31	1	602	CLA	C4B-CHC-C1C	2.60	132.35	126.25
30	p	609	CHL	C1-O2A-CGA	2.60	122.93	116.65
31	6	304	CLA	OBD-CAD-C3D	-2.60	122.35	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	313	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
33	D	408	LHG	C5-O7-C7	-2.59	111.59	117.80
31	G	611	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
31	p	604	CLA	C3B-C4B-NB	-2.59	108.21	110.53
34	J	102	LMG	O8-C28-C29	2.59	119.75	111.83
33	p	619	LHG	O8-C23-C24	2.59	119.74	111.83
30	n	309	CHL	CMA-C3A-C4A	2.59	120.20	114.61
31	C	601	CLA	C4B-CHC-C1C	2.59	132.34	126.25
31	N	305	CLA	C3B-C4B-NB	-2.59	108.22	110.53
31	9	306	CLA	C3B-C4B-NB	-2.59	108.22	110.53
38	A	413	SQD	O7-S-C6	-2.59	102.89	106.76
32	y	617	LUT	C11-C10-C9	-2.59	123.64	127.28
31	9	315	CLA	C3B-C4B-NB	-2.59	108.22	110.53
31	s	315	CLA	C3B-C4B-NB	-2.59	108.22	110.53
31	B	610	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
31	6	304	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
30	G	606	CHL	C1-O2A-CGA	2.59	122.92	116.65
31	6	311	CLA	C4B-CHC-C1C	2.59	132.34	126.25
34	g	320	LMG	O8-C28-C29	2.59	119.73	111.83
31	N	303	CLA	C4B-CHC-C1C	2.59	132.34	126.25
31	9	313	CLA	C3B-C4B-NB	-2.59	108.22	110.53
31	2	612	CLA	C2C-C1C-NC	2.59	112.70	109.98
31	2	604	CLA	CMA-C3A-C4A	2.59	118.73	111.77
31	1	610	CLA	CMD-C2D-C3D	-2.59	121.75	127.69
31	2	604	CLA	C1D-ND-C4D	-2.59	104.50	106.31
43	c	615	BCR	C29-C30-C25	2.59	114.20	110.44
31	9	314	CLA	CHA-C4D-ND	2.59	137.89	132.55
30	q	303	CHL	C4D-CHA-CBD	-2.59	106.36	108.97
31	2	610	CLA	C4B-CHC-C1C	2.59	132.33	126.25
31	c	601	CLA	CHA-C4D-ND	2.59	137.89	132.55
31	n	303	CLA	C4B-CHC-C1C	2.59	132.33	126.25
33	D	407	LHG	C5-O7-C7	-2.59	111.60	117.80
31	G	610	CLA	CMA-C3A-C4A	2.59	118.73	111.77
31	c	603	CLA	CHD-C1D-ND	-2.59	121.16	124.80
31	c	612	CLA	O2A-CGA-CBA	2.59	119.72	111.83
31	9	313	CLA	CMA-C3A-C4A	2.59	118.72	111.77
31	B	601	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
32	3	317	LUT	C18-C5-C4	2.59	119.18	114.42
30	g	307	CHL	CMA-C3A-C4A	2.59	120.18	114.61
31	R	315	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
30	2	606	CHL	C4D-CHA-CBD	-2.58	106.36	108.97
31	0	614	CLA	C3B-C4B-NB	-2.58	108.22	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	s	317	LUT	C30-C31-C32	-2.58	115.71	123.20
31	g	311	CLA	C1C-C2C-C3C	-2.58	104.26	106.98
32	p	617	LUT	C15-C14-C13	-2.58	123.65	127.28
31	7	305	CLA	CMD-C2D-C3D	-2.58	121.76	127.69
30	3	303	CHL	C4D-CHA-CBD	-2.58	106.36	108.97
31	y	613	CLA	C4B-CHC-C1C	2.58	132.32	126.25
31	c	605	CLA	C1C-C2C-C3C	-2.58	104.26	106.98
31	2	609	CLA	O2A-CGA-CBA	2.58	119.71	111.83
31	G	602	CLA	C4B-CHC-C1C	2.58	132.32	126.25
31	N	311	CLA	C1C-C2C-C3C	-2.58	104.26	106.98
37	R	318	XAT	C26-C27-C28	-2.58	120.53	125.99
31	q	313	CLA	CMA-C3A-C4A	2.58	118.71	111.77
31	s	306	CLA	C4B-CHC-C1C	2.58	132.32	126.25
31	6	312	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
31	5	603	CLA	C2C-C1C-NC	2.58	112.69	109.98
31	B	603	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
30	p	608	CHL	C1-O2A-CGA	2.58	122.90	116.65
31	S	306	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
35	q	317	RRX	C23-C24-C25	-2.58	120.11	127.00
32	8	616	LUT	C30-C31-C32	-2.58	115.72	123.20
30	8	605	CHL	C1-O2A-CGA	2.58	122.90	116.65
31	3	316	CLA	C4B-CHC-C1C	2.58	132.31	126.25
31	n	316	CLA	C4B-CHC-C1C	2.58	132.31	126.25
31	y	610	CLA	C4B-CHC-C1C	2.58	132.31	126.25
31	6	303	CLA	C3B-C4B-NB	-2.58	108.23	110.53
31	6	315	CLA	C3B-C4B-NB	-2.58	108.23	110.53
31	S	315	CLA	C3B-C4B-NB	-2.58	108.23	110.53
31	g	312	CLA	C3B-C4B-NB	-2.58	108.23	110.53
30	1	605	CHL	C4D-CHA-CBD	-2.58	106.37	108.97
34	2	618	LMG	C8-O7-C10	-2.58	111.62	117.80
31	9	305	CLA	C1D-ND-C4D	-2.58	104.50	106.31
31	R	313	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
31	B	605	CLA	O2A-CGA-CBA	2.58	119.70	111.83
31	q	312	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
31	7	315	CLA	C3B-C4B-NB	-2.58	108.23	110.53
31	q	316	CLA	C3B-C4B-NB	-2.58	108.23	110.53
33	0	619	LHG	C6-C5-C4	-2.58	105.77	111.78
32	n	318	LUT	C30-C31-C32	-2.58	115.73	123.20
31	N	310	CLA	C4B-CHC-C1C	2.58	132.31	126.25
43	b	619	BCR	C29-C30-C25	2.58	114.18	110.44
31	1	604	CLA	O1D-CGD-CBD	-2.58	119.43	124.52
31	7	305	CLA	CHA-C4D-ND	2.58	137.87	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	s	307	CHL	C4D-CHA-CBD	-2.58	106.37	108.97
36	R	301	NEX	C31-C30-C29	2.58	130.89	127.28
31	p	614	CLA	O2A-CGA-CBA	2.58	119.69	111.83
31	1	602	CLA	O2A-CGA-CBA	2.58	119.69	111.83
31	5	610	CLA	C2C-C1C-NC	2.58	112.69	109.98
31	p	603	CLA	CHD-C1D-ND	-2.58	121.18	124.80
37	r	318	XAT	C18-C5-C6	-2.58	118.06	122.30
31	8	609	CLA	C4B-CHC-C1C	2.58	132.30	126.25
31	g	311	CLA	CHA-C4D-ND	2.58	137.86	132.55
31	y	615	CLA	C2C-C1C-NC	2.58	112.69	109.98
36	p	618	NEX	C26-C27-C28	-2.58	120.55	125.99
30	n	310	CHL	CMA-C3A-C2A	2.58	124.08	114.13
31	R	316	CLA	O2A-CGA-CBA	2.58	119.69	111.83
30	g	302	CHL	C1-O2A-CGA	2.58	122.88	116.65
31	a	407	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
30	R	309	CHL	C4D-CHA-CBD	-2.57	106.37	108.97
36	p	618	NEX	C17-C1-C6	-2.57	108.17	110.47
31	1	610	CLA	O2A-CGA-CBA	2.57	119.68	111.83
31	s	306	CLA	C1C-C2C-C3C	-2.57	104.27	106.98
32	y	616	LUT	C19-C9-C8	2.57	122.02	118.09
31	B	608	CLA	CMA-C3A-C4A	2.57	118.69	111.77
31	G	609	CLA	CAA-C2A-C3A	-2.57	106.05	113.00
31	1	610	CLA	C4B-CHC-C1C	2.57	132.30	126.25
31	7	315	CLA	O2A-CGA-CBA	2.57	119.68	111.83
31	s	312	CLA	C3B-C4B-NB	-2.57	108.23	110.53
30	p	605	CHL	C4D-CHA-CBD	-2.57	106.37	108.97
31	n	316	CLA	C2C-C1C-NC	2.57	112.68	109.98
43	B	618	BCR	C38-C26-C25	-2.57	121.68	124.48
34	A	412	LMG	O8-C28-C29	2.57	119.67	111.83
31	r	307	CLA	C3B-C4B-NB	-2.57	108.23	110.53
31	6	305	CLA	CMA-C3A-C4A	2.57	118.68	111.77
31	G	613	CLA	C4B-CHC-C1C	2.57	132.29	126.25
31	B	607	CLA	O2A-CGA-CBA	2.57	119.67	111.83
31	q	315	CLA	O2A-C1-C2	2.57	117.99	108.11
31	Y	312	CLA	CHA-C4D-ND	2.57	137.85	132.55
32	p	617	LUT	C8-C7-C6	-2.57	120.14	127.00
31	C	606	CLA	C2C-C1C-NC	2.57	112.68	109.98
31	p	610	CLA	C2C-C1C-NC	2.57	112.68	109.98
31	8	602	CLA	C4B-CHC-C1C	2.57	132.29	126.25
31	C	602	CLA	CMA-C3A-C4A	2.57	118.67	111.77
31	G	609	CLA	C2C-C1C-NC	2.57	112.68	109.98
31	d	401	CLA	O2D-CGD-O1D	-2.57	118.85	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Y	315	LUT	C39-C29-C28	2.57	122.01	118.09
43	A	410	BCR	C33-C5-C4	2.57	119.07	113.60
32	6	318	LUT	C18-C5-C4	2.57	119.14	114.42
33	S	320	LHG	O8-C23-C24	2.57	119.66	111.83
36	s	319	NEX	C4-C3-C2	2.57	115.59	110.79
31	B	606	CLA	C3B-C4B-NB	-2.57	108.24	110.53
31	Y	313	CLA	O2D-CGD-O1D	-2.57	118.86	123.85
31	5	614	CLA	C4B-CHC-C1C	2.57	132.28	126.25
31	2	610	CLA	O2A-CGA-CBA	2.57	119.66	111.83
37	2	619	XAT	C26-C27-C28	-2.56	120.57	125.99
31	b	609	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
30	G	608	CHL	C4D-CHA-CBD	-2.56	106.38	108.97
31	R	306	CLA	CHA-C4D-ND	2.56	137.84	132.55
31	D	404	CLA	C2C-C1C-NC	2.56	112.67	109.98
31	5	604	CLA	C3B-C4B-NB	-2.56	108.24	110.53
36	s	319	NEX	C38-C25-C26	-2.56	118.08	122.30
31	b	613	CLA	C4B-CHC-C1C	2.56	132.27	126.25
31	q	316	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
31	C	613	CLA	CBA-CAA-C2A	2.56	121.42	113.79
31	y	602	CLA	C4B-CHC-C1C	2.56	132.27	126.25
31	1	612	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
31	y	612	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
31	s	311	CLA	C4B-CHC-C1C	2.56	132.27	126.25
31	0	603	CLA	CHD-C1D-ND	-2.56	121.20	124.80
43	B	618	BCR	C10-C11-C12	-2.56	115.78	123.20
31	9	305	CLA	O2A-CGA-CBA	2.56	119.64	111.83
31	b	613	CLA	O2A-CGA-CBA	2.56	119.64	111.83
31	N	315	CLA	C4B-CHC-C1C	2.56	132.27	126.25
31	7	304	CLA	CHA-C4D-ND	2.56	137.83	132.55
32	r	317	LUT	C19-C9-C8	2.56	122.00	118.09
31	q	312	CLA	C2C-C1C-NC	2.56	112.67	109.98
33	s	320	LHG	O8-C23-C24	2.56	119.64	111.83
34	c	624	LMG	O8-C28-C29	2.56	119.64	111.83
43	C	614	BCR	C15-C16-C17	-2.56	118.28	123.52
31	y	611	CLA	C1-C2-C3	-2.56	122.00	126.20
38	x	201	SQD	O7-S-C6	-2.56	102.94	106.76
31	5	604	CLA	CMA-C3A-C4A	2.56	118.65	111.77
31	y	604	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
31	b	615	CLA	C2C-C1C-NC	2.56	112.67	109.98
31	7	311	CLA	C4B-CHC-C1C	2.56	132.26	126.25
31	S	313	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
31	n	304	CLA	C3B-C4B-NB	-2.56	108.25	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	r	305	CLA	C3B-C4B-NB	-2.56	108.25	110.53
31	p	604	CLA	C2C-C1C-NC	2.56	112.67	109.98
31	p	615	CLA	CHD-C1D-ND	-2.56	121.20	124.80
36	N	318	NEX	C31-C30-C29	2.56	130.86	127.28
31	8	611	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
31	N	304	CLA	C1D-ND-C4D	-2.56	104.52	106.31
37	G	620	XAT	C26-C27-C28	-2.56	120.59	125.99
38	a	412	SQD	O7-S-C6	-2.56	102.94	106.76
31	N	305	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
31	7	313	CLA	CHA-C4D-ND	2.56	137.82	132.55
31	y	613	CLA	CHA-C4D-ND	2.56	137.82	132.55
31	Y	312	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
31	p	604	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
31	B	606	CLA	CHA-C4D-ND	2.56	137.82	132.55
31	S	305	CLA	C3B-C4B-NB	-2.56	108.25	110.53
31	n	314	CLA	C3B-C4B-NB	-2.56	108.25	110.53
31	B	612	CLA	C6-C5-C3	-2.56	107.24	113.47
33	S	320	LHG	C5-O7-C7	-2.55	111.68	117.80
31	Y	304	CLA	C2C-C1C-NC	2.55	112.67	109.98
31	b	606	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
30	N	307	CHL	C1-C2-C3	-2.55	122.01	126.20
45	c	617	DGD	C2G-O2G-C1B	-2.55	111.68	117.80
32	y	616	LUT	C15-C35-C34	-2.55	118.29	123.52
30	G	605	CHL	C4D-CHA-CBD	-2.55	106.39	108.97
31	R	314	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
31	B	607	CLA	CHA-C4D-ND	2.55	137.82	132.55
35	G	614	RRX	C8-C7-C6	-2.55	120.18	127.00
30	3	309	CHL	C1-O2A-CGA	2.55	122.83	116.65
31	0	603	CLA	C3B-C4B-NB	-2.55	108.25	110.53
31	Y	305	CLA	C1D-ND-C4D	-2.55	104.52	106.31
31	9	314	CLA	C1D-ND-C4D	-2.55	104.52	106.31
30	1	606	CHL	CMA-C3A-C4A	2.55	120.11	114.61
36	q	319	NEX	C17-C1-C6	-2.55	108.19	110.47
31	1	614	CLA	O2A-CGA-CBA	2.55	119.62	111.83
31	b	612	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
31	p	614	CLA	CHA-C4D-ND	2.55	137.81	132.55
31	Y	314	CLA	C3B-C4B-NB	-2.55	108.25	110.53
31	8	612	CLA	C3B-C4B-NB	-2.55	108.25	110.53
31	Y	310	CLA	C2C-C1C-NC	2.55	112.66	109.98
31	a	407	CLA	C4B-CHC-C1C	2.55	132.25	126.25
31	q	312	CLA	C2D-C1D-ND	2.55	112.65	110.13
43	b	618	BCR	C37-C22-C23	2.55	121.98	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y	613	CLA	C6-C5-C3	-2.55	107.25	113.47
31	7	314	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
31	S	303	CLA	C2C-C1C-NC	2.55	112.66	109.98
32	1	615	LUT	C20-C13-C12	2.55	121.98	118.09
31	B	612	CLA	O2A-CGA-CBA	2.55	119.61	111.83
31	5	613	CLA	C4B-CHC-C1C	2.55	132.24	126.25
31	R	304	CLA	C4B-CHC-C1C	2.55	132.24	126.25
35	4	615	RRX	C8-C7-C6	-2.55	120.19	127.00
31	q	313	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
30	R	308	CHL	C4D-CHA-CBD	-2.55	106.40	108.97
31	3	301	CLA	C2C-C1C-NC	2.55	112.66	109.98
32	Y	316	LUT	C18-C5-C6	-2.55	121.70	124.48
31	7	303	CLA	C3B-C4B-NB	-2.55	108.25	110.53
31	b	613	CLA	C2D-C1D-ND	2.55	112.65	110.13
31	s	306	CLA	C2D-C1D-ND	2.55	112.65	110.13
31	B	611	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
30	5	606	CHL	C4D-CHA-CBD	-2.55	106.40	108.97
31	N	311	CLA	C4B-CHC-C1C	2.55	132.24	126.25
36	r	301	NEX	C38-C25-C26	-2.55	118.11	122.30
31	b	611	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
30	7	307	CHL	C4D-CHA-CBD	-2.55	106.40	108.97
31	r	306	CLA	CHD-C1D-ND	-2.55	121.22	124.80
33	a	415	LHG	C5-O7-C7	-2.55	111.70	117.80
45	c	619	DGD	O1G-C1A-C2A	2.55	119.60	111.83
31	B	609	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
43	C	615	BCR	C34-C9-C8	-2.55	114.20	118.09
31	R	304	CLA	CHD-C1D-ND	-2.55	121.22	124.80
31	q	306	CLA	CHA-C4D-ND	2.55	137.80	132.55
31	9	315	CLA	C1D-ND-C4D	-2.55	104.53	106.31
31	S	311	CLA	CHD-C1D-ND	-2.55	121.22	124.80
31	n	313	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
31	4	612	CLA	C2C-C1C-NC	2.55	112.66	109.98
31	0	614	CLA	C1D-ND-C4D	-2.55	104.53	106.31
31	b	613	CLA	CMA-C3A-C4A	2.55	118.61	111.77
30	y	607	CHL	C4D-CHA-CBD	-2.54	106.40	108.97
33	y	619	LHG	O8-C23-C24	2.54	119.59	111.83
31	2	604	CLA	CHA-C4D-ND	2.54	137.80	132.55
30	g	307	CHL	C4D-CHA-CBD	-2.54	106.40	108.97
31	6	303	CLA	C4B-CHC-C1C	2.54	132.23	126.25
32	y	616	LUT	C31-C30-C29	-2.54	123.71	127.28
31	S	313	CLA	CHA-C4D-ND	2.54	137.80	132.55
35	9	317	RRX	C8-C7-C6	-2.54	120.20	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	8	615	LUT	C30-C31-C32	-2.54	115.83	123.20
32	n	317	LUT	C30-C31-C32	-2.54	115.83	123.20
37	q	321	XAT	C26-C27-C28	-2.54	120.62	125.99
31	2	611	CLA	C4B-CHC-C1C	2.54	132.23	126.25
34	B	621	LMG	C8-O7-C10	-2.54	111.71	117.80
31	s	305	CLA	CMA-C3A-C4A	2.54	118.61	111.77
31	c	605	CLA	CHA-C4D-ND	2.54	137.79	132.55
31	1	612	CLA	C2C-C1C-NC	2.54	112.65	109.98
30	3	307	CHL	C4D-CHA-CBD	-2.54	106.40	108.97
34	7	301	LMG	O8-C28-C29	2.54	119.58	111.83
31	G	613	CLA	C2C-C1C-NC	2.54	112.65	109.98
31	7	311	CLA	C2C-C1C-NC	2.54	112.65	109.98
30	g	309	CHL	C4D-CHA-CBD	-2.54	106.41	108.97
31	S	312	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
37	4	619	XAT	C26-C27-C28	-2.54	120.62	125.99
36	S	319	NEX	O24-C25-C38	-2.54	112.21	115.05
31	B	601	CLA	CHD-C1D-ND	-2.54	121.23	124.80
33	S	322	LHG	C5-O7-C7	-2.54	111.72	117.80
31	1	602	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
30	1	619	CHL	CMA-C3A-C2A	2.54	123.94	114.13
31	c	608	CLA	C2C-C1C-NC	2.54	112.65	109.98
31	c	605	CLA	C1-C2-C3	-2.54	122.04	126.20
31	b	608	CLA	CMA-C3A-C4A	2.54	118.60	111.77
31	d	401	CLA	CAA-C2A-C3A	-2.54	106.14	113.00
31	b	612	CLA	O2A-CGA-CBA	2.54	119.58	111.83
31	g	303	CLA	O2A-CGA-CBA	2.54	119.58	111.83
43	H	101	BCR	C30-C25-C26	-2.54	119.17	122.64
31	s	311	CLA	C3B-C4B-NB	-2.54	108.26	110.53
31	r	303	CLA	C4B-CHC-C1C	2.54	132.22	126.25
30	8	608	CHL	CMA-C3A-C2A	2.54	123.93	114.13
31	7	316	CLA	C4B-CHC-C1C	2.54	132.22	126.25
31	b	607	CLA	CHA-C4D-ND	2.54	137.78	132.55
32	G	615	LUT	C8-C7-C6	-2.54	120.22	127.00
30	g	309	CHL	CMA-C3A-C2A	2.54	123.93	114.13
31	8	604	CLA	C3B-C4B-NB	-2.54	108.27	110.53
31	d	401	CLA	CHD-C1D-ND	-2.54	121.23	124.80
30	4	606	CHL	C1-O2A-CGA	2.54	122.79	116.65
31	B	611	CLA	C4B-CHC-C1C	2.54	132.21	126.25
31	2	602	CLA	C4B-CHC-C1C	2.54	132.21	126.25
31	r	312	CLA	C4B-CHC-C1C	2.54	132.21	126.25
30	3	310	CHL	C4D-CHA-CBD	-2.54	106.41	108.97
31	b	607	CLA	CHD-C1D-ND	-2.54	121.23	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	614	CLA	C1D-ND-C4D	-2.54	104.53	106.31
30	0	606	CHL	CMA-C3A-C4A	2.54	120.07	114.61
31	0	615	CLA	C1C-C2C-C3C	-2.53	104.31	106.98
31	A	406	CLA	CMA-C3A-C4A	2.53	118.58	111.77
31	Y	314	CLA	C4B-CHC-C1C	2.53	132.21	126.25
31	0	602	CLA	C4B-CHC-C1C	2.53	132.21	126.25
30	0	608	CHL	C4D-CHA-CBD	-2.53	106.41	108.97
31	G	613	CLA	O2A-CGA-CBA	2.53	119.56	111.83
31	p	603	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
31	4	613	CLA	C1-O2A-CGA	2.53	122.78	116.65
31	B	607	CLA	CMA-C3A-C4A	2.53	118.58	111.77
31	7	304	CLA	CMD-C2D-C3D	-2.53	121.88	127.69
33	0	619	LHG	C5-O7-C7	-2.53	111.73	117.80
36	N	318	NEX	C38-C25-C26	-2.53	118.13	122.30
30	8	608	CHL	C4D-CHA-CBD	-2.53	106.41	108.97
31	3	304	CLA	O2A-CGA-CBA	2.53	119.56	111.83
31	R	303	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
33	2	617	LHG	O8-C23-C24	2.53	119.55	111.83
31	c	609	CLA	C6-C5-C3	-2.53	107.30	113.47
43	C	614	BCR	C2-C1-C6	2.53	114.11	110.44
31	r	304	CLA	C3B-C4B-NB	-2.53	108.27	110.53
31	A	407	CLA	C4B-CHC-C1C	2.53	132.19	126.25
37	9	322	XAT	C26-C27-C28	-2.53	120.64	125.99
31	g	304	CLA	O2A-CGA-CBA	2.53	119.55	111.83
30	p	608	CHL	C4D-CHA-CBD	-2.53	106.42	108.97
31	4	603	CLA	CHA-C4D-ND	2.53	137.77	132.55
31	B	614	CLA	CHA-C4D-ND	2.53	137.77	132.55
44	A	416	PL9	C32-C33-C34	-2.53	121.83	127.62
36	Y	317	NEX	C38-C25-C26	-2.53	118.14	122.30
30	7	308	CHL	C1-C2-C3	-2.53	122.05	126.20
31	y	612	CLA	CHA-C4D-ND	2.53	137.77	132.55
31	c	610	CLA	CHD-C1D-ND	-2.53	121.24	124.80
31	r	313	CLA	CAA-C2A-C3A	-2.53	106.17	113.00
31	S	305	CLA	CMA-C3A-C4A	2.53	118.57	111.77
37	g	321	XAT	C26-C27-C28	-2.53	120.65	125.99
31	b	602	CLA	C2C-C1C-NC	2.53	112.64	109.98
31	q	306	CLA	C6-C5-C3	-2.53	107.31	113.47
31	G	609	CLA	C4B-CHC-C1C	2.53	132.19	126.25
31	q	305	CLA	CHA-C4D-ND	2.53	137.76	132.55
30	N	301	CHL	C1-O2A-CGA	2.53	122.77	116.65
30	5	605	CHL	C4D-CHA-CBD	-2.53	106.42	108.97
31	8	614	CLA	C1D-ND-C4D	-2.53	104.54	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	305	CLA	C4B-CHC-C1C	2.53	132.19	126.25
31	s	311	CLA	O2A-CGA-CBA	2.53	119.54	111.83
33	G	618	LHG	C5-O7-C7	-2.53	111.75	117.80
31	c	613	CLA	C1-O2A-CGA	2.53	122.77	116.65
31	c	604	CLA	CHD-C1D-ND	-2.53	121.25	124.80
31	9	313	CLA	CHA-C4D-ND	2.53	137.76	132.55
31	s	305	CLA	C3B-C4B-NB	-2.52	108.28	110.53
36	N	318	NEX	C39-C29-C30	-2.52	118.73	122.82
31	s	315	CLA	CMD-C2D-C3D	-2.52	121.90	127.69
30	n	308	CHL	C4D-CHA-CBD	-2.52	106.42	108.97
31	d	404	CLA	C1D-ND-C4D	-2.52	104.54	106.31
31	B	612	CLA	CMA-C3A-C4A	2.52	118.56	111.77
31	1	610	CLA	C2C-C1C-NC	2.52	112.63	109.98
31	8	612	CLA	C1-C2-C3	-2.52	122.06	126.20
34	b	623	LMG	O8-C28-C29	2.52	119.53	111.83
31	d	405	CLA	CMA-C3A-C4A	2.52	118.56	111.77
31	B	603	CLA	CHA-C4D-ND	2.52	137.75	132.55
31	G	610	CLA	CHA-C4D-ND	2.52	137.75	132.55
31	q	314	CLA	CHA-C4D-ND	2.52	137.75	132.55
31	s	316	CLA	C3B-C4B-NB	-2.52	108.28	110.53
34	6	321	LMG	O1-C1-C2	2.52	112.10	108.27
30	9	311	CHL	CMA-C3A-C2A	2.52	123.87	114.13
31	B	605	CLA	CHA-C4D-ND	2.52	137.75	132.55
31	C	602	CLA	C1-O2A-CGA	2.52	122.75	116.65
31	q	315	CLA	C3B-C4B-NB	-2.52	108.28	110.53
31	2	613	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
31	2	613	CLA	C4B-CHC-C1C	2.52	132.18	126.25
34	w	201	LMG	C8-O7-C10	-2.52	111.76	117.80
30	7	321	CHL	C4D-CHA-CBD	-2.52	106.42	108.97
30	n	309	CHL	C4D-CHA-CBD	-2.52	106.42	108.97
34	a	401	LMG	O8-C28-C29	2.52	119.52	111.83
31	1	612	CLA	CHA-C4D-ND	2.52	137.75	132.55
31	S	306	CLA	C2C-C1C-NC	2.52	112.63	109.98
31	p	614	CLA	CHD-C1D-ND	-2.52	121.26	124.80
31	3	305	CLA	C1D-ND-C4D	-2.52	104.54	106.31
31	6	312	CLA	C4B-CHC-C1C	2.52	132.17	126.25
43	b	620	BCR	C38-C26-C27	2.52	118.97	113.60
31	0	610	CLA	C4B-CHC-C1C	2.52	132.17	126.25
31	g	304	CLA	C4B-CHC-C1C	2.52	132.17	126.25
30	8	607	CHL	CMA-C3A-C4A	2.52	120.04	114.61
31	R	315	CLA	CHA-C4D-ND	2.52	137.75	132.55
31	c	602	CLA	C4B-CHC-C1C	2.52	132.17	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	r	304	CLA	C4B-CHC-C1C	2.52	132.17	126.25
31	r	312	CLA	C2C-C1C-NC	2.52	112.63	109.98
31	q	316	CLA	CHA-C4D-ND	2.52	137.74	132.55
31	R	307	CLA	C4B-CHC-C1C	2.52	132.17	126.25
31	C	609	CLA	O2A-CGA-CBA	2.52	119.51	111.83
31	A	407	CLA	CAA-C2A-C3A	-2.52	106.20	113.00
31	3	315	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
31	s	310	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
34	4	621	LMG	O8-C28-C29	2.52	119.51	111.83
31	C	603	CLA	CMD-C2D-C3D	-2.52	121.92	127.69
31	6	305	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
30	n	301	CHL	C4D-CHA-CBD	-2.52	106.43	108.97
31	5	615	CLA	C3B-C4B-NB	-2.52	108.28	110.53
31	C	607	CLA	C1-C2-C3	-2.52	122.08	126.20
31	N	310	CLA	CHD-C1D-ND	-2.52	121.26	124.80
31	g	310	CLA	C4B-CHC-C1C	2.52	132.16	126.25
31	6	316	CLA	CHA-C4D-ND	2.52	137.74	132.55
31	g	311	CLA	C4B-CHC-C1C	2.52	132.16	126.25
31	0	612	CLA	CMA-C3A-C4A	2.51	118.53	111.77
31	7	303	CLA	C4B-CHC-C1C	2.51	132.16	126.25
43	H	101	BCR	C23-C24-C25	-2.51	120.28	127.00
31	n	313	CLA	C4B-CHC-C1C	2.51	132.16	126.25
31	c	610	CLA	C2C-C1C-NC	2.51	112.62	109.98
43	D	405	BCR	C20-C21-C22	-2.51	123.75	127.28
43	V	101	BCR	C15-C14-C13	-2.51	123.75	127.28
31	y	604	CLA	C1D-ND-C4D	-2.51	104.55	106.31
31	1	602	CLA	C2C-C1C-NC	2.51	112.62	109.98
30	2	605	CHL	C4D-CHA-CBD	-2.51	106.43	108.97
30	q	307	CHL	C4D-CHA-CBD	-2.51	106.43	108.97
31	6	304	CLA	O2A-CGA-CBA	2.51	119.50	111.83
34	4	620	LMG	O8-C28-C29	2.51	119.50	111.83
31	S	306	CLA	C4B-CHC-C1C	2.51	132.15	126.25
31	8	603	CLA	O2A-CGA-CBA	2.51	119.49	111.83
31	B	601	CLA	C2C-C1C-NC	2.51	112.62	109.98
31	g	313	CLA	C3B-C4B-NB	-2.51	108.29	110.53
32	Y	316	LUT	C8-C7-C6	-2.51	120.29	127.00
31	y	610	CLA	O2A-CGA-CBA	2.51	119.49	111.83
31	S	304	CLA	C2C-C1C-NC	2.51	112.62	109.98
31	s	306	CLA	C2C-C1C-NC	2.51	112.62	109.98
30	7	321	CHL	CMA-C3A-C4A	2.51	120.02	114.61
31	6	314	CLA	C3B-C4B-NB	-2.51	108.29	110.53
31	Y	303	CLA	C3B-C4B-NB	-2.51	108.29	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	608	CHL	CMA-C3A-C4A	2.51	120.02	114.61
31	q	314	CLA	C1D-ND-C4D	-2.51	104.55	106.31
44	A	416	PL9	C27-C28-C29	-2.51	121.88	127.62
31	2	602	CLA	CHA-C4D-ND	2.51	137.73	132.55
43	H	101	BCR	C38-C26-C27	2.51	118.95	113.60
31	8	603	CLA	CHA-C4D-ND	2.51	137.72	132.55
31	y	615	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
36	n	319	NEX	C39-C29-C30	-2.51	118.75	122.82
31	C	610	CLA	CHD-C1D-ND	-2.51	121.27	124.80
31	g	312	CLA	CHA-C4D-ND	2.51	137.72	132.55
32	G	615	LUT	C26-C27-C28	-2.51	120.68	124.58
31	r	303	CLA	CHA-C4D-ND	2.51	137.72	132.55
30	8	606	CHL	C4D-CHA-CBD	-2.51	106.44	108.97
33	a	415	LHG	O8-C23-C24	2.51	119.48	111.83
31	N	304	CLA	C3B-C4B-NB	-2.51	108.29	110.53
30	N	309	CHL	CMA-C3A-C2A	2.51	123.81	114.13
31	5	614	CLA	CHA-C4D-ND	2.51	137.72	132.55
31	3	316	CLA	CBA-CAA-C2A	-2.51	106.34	113.79
30	G	605	CHL	C1-O2A-CGA	2.51	123.79	116.67
31	0	610	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
31	r	314	CLA	C4B-CHC-C1C	2.51	132.14	126.25
31	6	316	CLA	C4B-CHC-C1C	2.50	132.14	126.25
30	7	302	CHL	C4D-CHA-CBD	-2.50	106.44	108.97
31	p	610	CLA	C4B-CHC-C1C	2.50	132.14	126.25
43	b	620	BCR	C21-C20-C19	-2.50	115.94	123.20
30	2	608	CHL	CMA-C3A-C2A	2.50	123.80	114.13
31	C	608	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
30	n	307	CHL	C4D-CHA-CBD	-2.50	106.44	108.97
31	c	607	CLA	CHA-C4D-ND	2.50	137.71	132.55
31	Y	304	CLA	C1D-ND-C4D	-2.50	104.56	106.31
31	y	602	CLA	O2A-CGA-CBA	2.50	119.47	111.83
34	A	418	LMG	O8-C28-C29	2.50	119.47	111.83
31	B	614	CLA	C2C-C1C-NC	2.50	112.61	109.98
31	G	603	CLA	CHA-C4D-ND	2.50	137.71	132.55
31	S	315	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
36	R	319	NEX	C26-C27-C28	-2.50	120.70	125.99
31	5	615	CLA	O1D-CGD-CBD	-2.50	119.58	124.52
31	C	611	CLA	CHA-C4D-ND	2.50	137.71	132.55
30	r	308	CHL	C4D-CHA-CBD	-2.50	106.44	108.97
31	b	614	CLA	C1D-ND-C4D	-2.50	104.56	106.31
30	n	308	CHL	CMA-C3A-C4A	2.50	120.00	114.61
31	S	315	CLA	CHD-C1D-ND	-2.50	121.28	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	p	604	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
31	5	603	CLA	O2A-CGA-CBA	2.50	119.46	111.83
30	5	608	CHL	C4D-CHA-CBD	-2.50	106.45	108.97
30	9	303	CHL	C4D-CHA-CBD	-2.50	106.45	108.97
31	S	303	CLA	O2A-CGA-CBA	2.50	119.46	111.83
31	9	305	CLA	CHA-C4D-ND	2.50	137.71	132.55
31	c	610	CLA	CAA-CBA-CGA	-2.50	106.11	113.21
31	3	305	CLA	CHA-C4D-ND	2.50	137.71	132.55
31	r	311	CLA	CAA-C2A-C3A	-2.50	106.25	113.00
31	9	316	CLA	C4B-CHC-C1C	2.50	132.12	126.25
31	a	409	CLA	C4B-CHC-C1C	2.50	132.12	126.25
31	G	610	CLA	CHA-C1A-NA	-2.50	120.73	126.39
31	c	613	CLA	CHA-C4D-ND	2.50	137.70	132.55
31	7	311	CLA	O2A-CGA-CBA	2.50	119.45	111.83
36	5	618	NEX	C38-C25-C26	-2.50	118.19	122.30
32	S	318	LUT	C35-C15-C14	-2.50	118.41	123.52
32	p	616	LUT	C8-C7-C6	-2.50	120.32	127.00
31	N	313	CLA	C4B-CHC-C1C	2.50	132.12	126.25
31	b	612	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
31	Y	305	CLA	C3B-C4B-NB	-2.50	108.30	110.53
31	S	305	CLA	C4B-CHC-C1C	2.50	132.12	126.25
31	S	316	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
31	6	314	CLA	O2A-CGA-CBA	2.50	119.45	111.83
31	Y	310	CLA	O2A-CGA-CBA	2.50	119.45	111.83
35	2	614	RRX	C27-C26-C25	-2.50	115.63	120.76
31	r	315	CLA	C1-C2-C3	-2.50	122.11	126.20
31	5	603	CLA	C4B-CHC-C1C	2.50	132.12	126.25
31	N	314	CLA	C4B-CHC-C1C	2.50	132.12	126.25
31	8	614	CLA	C4B-CHC-C1C	2.50	132.12	126.25
30	0	609	CHL	C4D-CHA-CBD	-2.50	106.45	108.97
31	7	304	CLA	C2C-C1C-NC	2.50	112.61	109.98
31	y	615	CLA	CHA-C4D-ND	2.50	137.70	132.55
32	N	316	LUT	C31-C30-C29	-2.50	123.78	127.28
30	N	307	CHL	C1-O2A-CGA	2.50	122.69	116.65
31	G	609	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
31	8	611	CLA	C4B-CHC-C1C	2.50	132.12	126.25
31	g	304	CLA	CMD-C2D-C3D	-2.50	121.96	127.69
30	G	607	CHL	C4D-CHA-CBD	-2.50	106.45	108.97
31	n	314	CLA	C1-C2-C3	-2.50	122.11	126.20
31	6	304	CLA	CHA-C4D-ND	2.50	137.70	132.55
31	c	611	CLA	CHA-C4D-ND	2.50	137.70	132.55
43	b	620	BCR	C33-C5-C4	2.50	118.92	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	A	416	PL9	C7-C8-C9	-2.50	122.53	126.83
32	N	317	LUT	C11-C12-C13	-2.50	119.52	126.36
31	r	314	CLA	C2C-C1C-NC	2.50	112.60	109.98
31	B	612	CLA	C4B-CHC-C1C	2.50	132.12	126.25
43	t	101	BCR	C1-C6-C5	-2.50	119.23	122.64
31	3	312	CLA	C4B-CHC-C1C	2.49	132.11	126.25
31	2	611	CLA	CMA-C3A-C4A	2.49	118.48	111.77
31	b	602	CLA	CHA-C4D-ND	2.49	137.70	132.55
31	s	315	CLA	CHA-C4D-ND	2.49	137.70	132.55
31	5	604	CLA	CHA-C4D-ND	2.49	137.69	132.55
31	g	304	CLA	CHA-C4D-ND	2.49	137.69	132.55
31	A	409	CLA	C4B-CHC-C1C	2.49	132.11	126.25
31	b	602	CLA	C4B-CHC-C1C	2.49	132.11	126.25
32	Y	315	LUT	C15-C35-C34	-2.49	118.42	123.52
44	a	414	PL9	O2-C1-C6	2.49	124.45	120.48
31	B	613	CLA	CHA-C4D-ND	2.49	137.69	132.55
31	C	610	CLA	CHA-C4D-ND	2.49	137.69	132.55
32	3	318	LUT	C8-C7-C6	-2.49	120.34	127.00
43	b	619	BCR	C15-C16-C17	-2.49	118.42	123.52
32	1	615	LUT	C39-C29-C28	2.49	121.90	118.09
31	6	313	CLA	CHA-C4D-ND	2.49	137.69	132.55
31	g	313	CLA	C1D-ND-C4D	-2.49	104.56	106.31
34	m	102	LMG	O8-C28-C29	2.49	119.44	111.83
31	S	314	CLA	C1-O2A-CGA	2.49	122.68	116.65
31	Y	303	CLA	O2A-CGA-CBA	2.49	119.43	111.83
32	1	615	LUT	C15-C35-C34	-2.49	118.42	123.52
33	p	619	LHG	C5-O7-C7	-2.49	111.83	117.80
33	l	101	LHG	O8-C23-C24	2.49	119.43	111.83
31	R	315	CLA	C4B-CHC-C1C	2.49	132.11	126.25
31	4	604	CLA	C3B-C4B-NB	-2.49	108.31	110.53
31	S	312	CLA	C4B-CHC-C1C	2.49	132.10	126.25
31	b	615	CLA	C4B-CHC-C1C	2.49	132.10	126.25
30	1	609	CHL	C4D-CHA-CBD	-2.49	106.46	108.97
31	C	602	CLA	C1C-C2C-C3C	-2.49	104.36	106.98
31	C	601	CLA	CHA-C4D-ND	2.49	137.69	132.55
31	n	304	CLA	O2A-CGA-CBA	2.49	119.43	111.83
31	B	605	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
31	c	605	CLA	C1-O2A-CGA	2.49	122.68	116.65
34	c	621	LMG	C8-O7-C10	-2.49	111.84	117.80
43	a	410	BCR	C19-C18-C17	-2.49	115.09	119.01
31	S	315	CLA	CHA-C4D-ND	2.49	137.68	132.55
31	p	612	CLA	CHA-C4D-ND	2.49	137.68	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	n	303	CLA	O2A-CGA-CBA	2.49	119.42	111.83
30	3	310	CHL	CMA-C3A-C2A	2.49	123.74	114.13
31	4	612	CLA	CHA-C4D-ND	2.49	137.68	132.55
31	s	304	CLA	CHA-C4D-ND	2.49	137.68	132.55
30	0	609	CHL	CMA-C3A-C2A	2.49	123.74	114.13
31	N	305	CLA	CHA-C4D-ND	2.49	137.68	132.55
31	d	401	CLA	C4B-CHC-C1C	2.49	132.10	126.25
31	G	603	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
34	r	321	LMG	O6-C1-C2	-2.49	105.26	110.37
30	5	607	CHL	C4D-CHA-CBD	-2.49	106.46	108.97
31	7	315	CLA	C4B-CHC-C1C	2.49	132.10	126.25
31	c	603	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
31	b	608	CLA	CHA-C4D-ND	2.49	137.68	132.55
31	1	614	CLA	C4B-CHC-C1C	2.49	132.09	126.25
31	4	610	CLA	C2C-C1C-NC	2.49	112.59	109.98
34	m	102	LMG	C4-C3-C2	-2.49	106.47	110.83
31	5	612	CLA	CHA-C4D-ND	2.49	137.68	132.55
31	Y	304	CLA	CHA-C4D-ND	2.49	137.68	132.55
30	1	605	CHL	C1-O2A-CGA	2.49	122.67	116.65
31	S	306	CLA	C2D-C1D-ND	2.49	112.59	110.13
31	q	312	CLA	O2A-CGA-CBA	2.49	119.41	111.83
31	r	316	CLA	CMD-C2D-C3D	-2.49	121.99	127.69
31	6	303	CLA	O2A-CGA-CBA	2.49	119.41	111.83
31	2	613	CLA	CHA-C4D-ND	2.48	137.68	132.55
31	p	613	CLA	CHA-C4D-ND	2.48	137.68	132.55
31	2	611	CLA	C3B-C4B-NB	-2.48	108.31	110.53
31	d	401	CLA	C3B-C4B-NB	-2.48	108.31	110.53
31	N	311	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
34	Y	319	LMG	C8-O7-C10	-2.48	111.85	117.80
31	b	608	CLA	O2A-CGA-CBA	2.48	119.41	111.83
30	6	306	CHL	CMA-C3A-C4A	2.48	119.96	114.61
31	8	613	CLA	C4B-CHC-C1C	2.48	132.09	126.25
31	6	315	CLA	CHD-C1D-ND	-2.48	121.31	124.80
31	Y	305	CLA	CHA-C4D-ND	2.48	137.67	132.55
31	Y	305	CLA	C4B-CHC-C1C	2.48	132.09	126.25
31	r	307	CLA	CHA-C4D-ND	2.48	137.67	132.55
33	3	320	LHG	C5-O7-C7	-2.48	111.85	117.80
31	C	604	CLA	CHD-C1D-ND	-2.48	121.31	124.80
32	Y	315	LUT	C20-C13-C12	2.48	121.88	118.09
44	a	414	PL9	C22-C23-C24	-2.48	121.94	127.62
31	C	612	CLA	CMA-C3A-C4A	2.48	118.44	111.77
31	q	315	CLA	O1D-CGD-CBD	-2.48	119.62	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	304	CLA	C2D-C1D-ND	2.48	112.58	110.13
30	6	302	CHL	C4D-CHA-CBD	-2.48	106.47	108.97
31	0	610	CLA	C1-O2A-CGA	2.48	122.66	116.65
31	B	611	CLA	C2C-C1C-NC	2.48	112.59	109.98
31	c	605	CLA	C3B-C4B-NB	-2.48	108.32	110.53
31	S	304	CLA	C4B-CHC-C1C	2.48	132.08	126.25
31	q	314	CLA	C4B-CHC-C1C	2.48	132.08	126.25
31	7	305	CLA	C1D-ND-C4D	-2.48	104.57	106.31
31	B	611	CLA	O2A-CGA-CBA	2.48	119.40	111.83
31	N	304	CLA	CHA-C4D-ND	2.48	137.66	132.55
31	R	312	CLA	C4B-CHC-C1C	2.48	132.08	126.25
31	r	312	CLA	CHD-C1D-ND	-2.48	121.31	124.80
30	N	306	CHL	C4D-CHA-CBD	-2.48	106.47	108.97
30	s	309	CHL	CMA-C3A-C4A	2.48	119.95	114.61
43	b	618	BCR	C8-C7-C6	-2.48	120.38	127.00
31	q	315	CLA	CHA-C4D-ND	2.48	137.66	132.55
31	b	615	CLA	CHA-C4D-ND	2.48	137.66	132.55
30	7	308	CHL	C4D-CHA-CBD	-2.48	106.47	108.97
31	D	403	CLA	C1D-ND-C4D	-2.48	104.57	106.31
31	b	614	CLA	C4B-CHC-C1C	2.48	132.07	126.25
31	R	303	CLA	CHA-C4D-ND	2.48	137.66	132.55
43	V	101	BCR	C7-C8-C9	-2.48	122.57	126.23
31	8	604	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
31	d	401	CLA	CMD-C2D-C3D	-2.48	122.01	127.69
30	Y	307	CHL	C4D-CHA-CBD	-2.48	106.47	108.97
31	g	313	CLA	C4B-CHC-C1C	2.48	132.07	126.25
31	7	316	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
31	1	604	CLA	CHA-C4D-ND	2.48	137.66	132.55
31	4	604	CLA	CHA-C4D-ND	2.48	137.66	132.55
31	G	604	CLA	C4B-CHC-C1C	2.48	132.07	126.25
31	C	612	CLA	C6-C5-C3	-2.48	107.43	113.47
31	N	303	CLA	C6-C5-C3	-2.48	107.43	113.47
31	2	612	CLA	C3B-C4B-NB	-2.48	108.32	110.53
30	N	308	CHL	C4D-CHA-CBD	-2.48	106.47	108.97
31	B	612	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
31	G	612	CLA	C4B-CHC-C1C	2.48	132.07	126.25
31	B	612	CLA	CHA-C4D-ND	2.48	137.66	132.55
30	y	609	CHL	C4D-CHA-CBD	-2.48	106.47	108.97
31	B	601	CLA	C4B-CHC-C1C	2.48	132.07	126.25
31	s	305	CLA	C4B-CHC-C1C	2.48	132.07	126.25
31	S	306	CLA	CHA-C4D-ND	2.48	137.66	132.55
31	s	313	CLA	CHD-C1D-ND	-2.48	121.32	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	0	611	CLA	O2A-CGA-CBA	2.48	119.38	111.83
30	p	601	CHL	CMA-C3A-C4A	2.48	119.94	114.61
31	s	311	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
31	2	610	CLA	CHA-C4D-ND	2.47	137.66	132.55
32	7	318	LUT	C30-C31-C32	-2.47	116.03	123.20
45	c	617	DGD	O6E-C1E-O5D	2.47	115.89	110.04
33	b	625	LHG	C5-O7-C7	-2.47	111.88	117.80
31	S	311	CLA	C4B-CHC-C1C	2.47	132.06	126.25
30	7	309	CHL	CMA-C3A-C4A	2.47	119.94	114.61
31	p	602	CLA	O2A-CGA-CBA	2.47	119.38	111.83
30	6	310	CHL	C4D-CHA-CBD	-2.47	106.47	108.97
31	0	603	CLA	O2A-CGA-CBA	2.47	119.37	111.83
31	b	614	CLA	CMA-C3A-C4A	2.47	118.42	111.77
43	c	615	BCR	C23-C22-C21	2.47	122.90	119.01
31	y	615	CLA	C6-C5-C3	-2.47	107.45	113.47
31	6	315	CLA	C4B-CHC-C1C	2.47	132.06	126.25
34	w	203	LMG	O8-C28-O10	-2.47	117.45	123.63
31	2	613	CLA	CMD-C2D-C3D	-2.47	122.02	127.69
31	g	311	CLA	O2A-CGA-CBA	2.47	119.37	111.83
31	R	314	CLA	C4B-CHC-C1C	2.47	132.06	126.25
31	7	305	CLA	C4B-CHC-C1C	2.47	132.06	126.25
31	b	607	CLA	CMD-C2D-C3D	-2.47	122.02	127.69
31	1	613	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
31	c	604	CLA	C3B-C4B-NB	-2.47	108.33	110.53
32	Y	316	LUT	C31-C30-C29	-2.47	123.81	127.28
36	Y	317	NEX	C31-C30-C29	2.47	130.74	127.28
36	S	319	NEX	C26-C27-C28	-2.47	120.77	125.99
31	G	613	CLA	CHA-C4D-ND	2.47	137.64	132.55
31	C	611	CLA	C4B-CHC-C1C	2.47	132.05	126.25
36	R	301	NEX	C38-C25-C26	-2.47	118.24	122.30
35	9	317	RRX	C27-C26-C25	-2.47	115.69	120.76
31	y	603	CLA	C4B-CHC-C1C	2.47	132.05	126.25
31	y	603	CLA	C1D-ND-C4D	-2.47	104.58	106.31
31	0	614	CLA	C6-C5-C3	-2.47	107.45	113.47
31	D	404	CLA	C2D-C1D-ND	2.47	112.57	110.13
31	4	602	CLA	O2A-CGA-CBA	2.47	119.36	111.83
31	r	307	CLA	CMA-C3A-C4A	2.47	118.41	111.77
31	3	316	CLA	CAA-C2A-C3A	-2.47	106.33	113.00
31	s	313	CLA	C3B-C4B-NB	-2.47	108.33	110.53
31	3	306	CLA	C4B-CHC-C1C	2.47	132.05	126.25
33	Y	318	LHG	O8-C23-C24	2.47	119.36	111.83
32	r	317	LUT	C40-C33-C32	2.47	121.86	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	601	CLA	C1C-C2C-C3C	-2.47	104.39	106.98
31	b	605	CLA	C4B-CHC-C1C	2.47	132.05	126.25
31	B	611	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
31	y	610	CLA	CMD-C2D-C3D	-2.47	122.03	127.69
30	1	609	CHL	CMA-C3A-C2A	2.47	123.65	114.13
31	3	311	CLA	O1D-CGD-CBD	-2.47	119.66	124.52
44	A	416	PL9	C22-C23-C24	-2.47	121.98	127.62
37	r	318	XAT	O4-C5-C18	-2.47	112.29	115.05
31	b	613	CLA	C2C-C1C-NC	2.46	112.57	109.98
31	p	610	CLA	O2A-CGA-CBA	2.46	119.35	111.83
43	z	101	BCR	C11-C12-C13	-2.46	119.61	126.36
31	G	604	CLA	CHA-C4D-ND	2.46	137.63	132.55
31	g	305	CLA	CHA-C4D-ND	2.46	137.63	132.55
32	0	616	LUT	C20-C13-C12	2.46	121.85	118.09
31	7	303	CLA	O2A-CGA-CBA	2.46	119.35	111.83
31	8	604	CLA	C4B-CHC-C1C	2.46	132.04	126.25
31	s	310	CLA	CMA-C3A-C4A	2.46	118.40	111.77
31	G	612	CLA	CHA-C4D-ND	2.46	137.63	132.55
31	R	304	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
31	3	316	CLA	O2A-CGA-CBA	2.46	119.35	111.83
31	q	315	CLA	C1C-C2C-C3C	-2.46	104.39	106.98
31	g	303	CLA	C1C-C2C-C3C	-2.46	104.39	106.98
31	A	406	CLA	CHD-C1D-ND	-2.46	121.34	124.80
31	A	407	CLA	CHD-C1D-ND	-2.46	121.34	124.80
31	3	315	CLA	CHA-C4D-ND	2.46	137.63	132.55
31	B	601	CLA	CHA-C4D-ND	2.46	137.63	132.55
31	9	306	CLA	CHA-C4D-ND	2.46	137.63	132.55
31	y	603	CLA	CHA-C4D-ND	2.46	137.63	132.55
30	1	607	CHL	C1-O2A-CGA	2.46	122.61	116.65
31	g	311	CLA	CHA-C1A-NA	-2.46	120.81	126.39
31	B	605	CLA	C4B-CHC-C1C	2.46	132.04	126.25
31	C	602	CLA	C4B-CHC-C1C	2.46	132.04	126.25
31	c	601	CLA	C4B-CHC-C1C	2.46	132.04	126.25
31	2	603	CLA	CHA-C4D-ND	2.46	137.63	132.55
31	c	604	CLA	C4B-CHC-C1C	2.46	132.04	126.25
31	N	313	CLA	CHA-C4D-ND	2.46	137.63	132.55
31	0	614	CLA	C4B-CHC-C1C	2.46	132.03	126.25
31	g	314	CLA	CHA-C4D-ND	2.46	137.63	132.55
31	n	312	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
36	2	616	NEX	C16-C1-C6	-2.46	108.27	110.47
31	G	613	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
31	q	313	CLA	O1D-CGD-CBD	-2.46	119.67	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	r	313	CLA	CMA-C3A-C4A	2.46	118.38	111.77
31	B	616	CLA	CHD-C1D-ND	-2.46	121.34	124.80
31	N	304	CLA	C4B-CHC-C1C	2.46	132.03	126.25
31	s	306	CLA	O1D-CGD-CBD	-2.46	119.67	124.52
31	q	312	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
31	5	611	CLA	CHA-C4D-ND	2.46	137.62	132.55
31	0	615	CLA	CHA-C4D-ND	2.46	137.62	132.55
31	7	303	CLA	CHA-C4D-ND	2.46	137.62	132.55
31	5	612	CLA	C4B-CHC-C1C	2.46	132.03	126.25
31	y	604	CLA	C3B-C4B-NB	-2.46	108.33	110.53
31	r	313	CLA	O2A-CGA-CBA	2.46	119.33	111.83
31	c	601	CLA	O2A-CGA-CBA	2.46	119.33	111.83
31	8	612	CLA	C4B-CHC-C1C	2.46	132.03	126.25
31	C	603	CLA	CHA-C4D-ND	2.46	137.62	132.55
31	R	313	CLA	C4B-CHC-C1C	2.46	132.03	126.25
31	b	603	CLA	CMA-C3A-C4A	2.46	118.38	111.77
34	7	322	LMG	O8-C28-C29	2.46	119.33	111.83
31	3	314	CLA	CHA-C4D-ND	2.46	137.62	132.55
31	n	312	CLA	CHA-C4D-ND	2.46	137.62	132.55
31	r	315	CLA	CHD-C1D-ND	-2.46	121.34	124.80
30	p	606	CHL	C4D-CHA-CBD	-2.46	106.49	108.97
30	n	306	CHL	C4D-CHA-CBD	-2.46	106.49	108.97
31	B	614	CLA	C4B-CHC-C1C	2.46	132.02	126.25
35	4	615	RRX	C27-C26-C25	-2.46	115.71	120.76
31	r	303	CLA	C2D-C1D-ND	2.46	112.56	110.13
36	3	319	NEX	C17-C1-C6	-2.46	108.27	110.47
31	b	609	CLA	C1D-ND-C4D	-2.46	104.59	106.31
31	g	313	CLA	CHA-C4D-ND	2.46	137.62	132.55
31	n	305	CLA	CHA-C4D-ND	2.46	137.62	132.55
31	a	406	CLA	C4B-CHC-C1C	2.46	132.02	126.25
31	G	609	CLA	CHD-C1D-ND	-2.46	121.35	124.80
35	G	614	RRX	C27-C26-C25	-2.46	115.71	120.76
31	q	312	CLA	CHA-C4D-ND	2.45	137.61	132.55
31	5	610	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
31	5	610	CLA	CMD-C2D-C3D	-2.45	122.06	127.69
31	n	314	CLA	C4B-CHC-C1C	2.45	132.02	126.25
31	r	311	CLA	C4B-CHC-C1C	2.45	132.02	126.25
31	7	312	CLA	CHA-C4D-ND	2.45	137.61	132.55
31	r	311	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
31	8	604	CLA	CMA-C3A-C4A	2.45	118.37	111.77
31	5	610	CLA	O2A-CGA-CBA	2.45	119.31	111.83
31	9	312	CLA	CHA-C4D-ND	2.45	137.61	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	306	CLA	C4B-CHC-C1C	2.45	132.01	126.25
31	6	305	CLA	C3B-C4B-NB	-2.45	108.34	110.53
31	d	404	CLA	CHA-C4D-ND	2.45	137.61	132.55
31	R	311	CLA	CHD-C1D-ND	-2.45	121.35	124.80
31	y	604	CLA	CHA-C4D-ND	2.45	137.61	132.55
32	N	317	LUT	C15-C35-C34	-2.45	118.50	123.52
43	b	618	BCR	C10-C11-C12	-2.45	116.10	123.20
31	N	305	CLA	C4B-CHC-C1C	2.45	132.01	126.25
31	Y	312	CLA	O2A-CGA-CBA	2.45	119.31	111.83
31	b	604	CLA	CMD-C2D-C3D	-2.45	122.07	127.69
31	y	604	CLA	C4B-CHC-C1C	2.45	132.01	126.25
31	y	610	CLA	CHD-C1D-ND	-2.45	121.36	124.80
31	3	313	CLA	CHA-C4D-ND	2.45	137.60	132.55
31	Y	313	CLA	CHA-C4D-ND	2.45	137.60	132.55
31	8	610	CLA	CHA-C4D-ND	2.45	137.60	132.55
31	Y	305	CLA	O2A-CGA-CBA	2.45	119.30	111.83
31	8	604	CLA	CHA-C4D-ND	2.45	137.60	132.55
32	7	318	LUT	C18-C5-C4	2.45	118.92	114.42
31	7	314	CLA	CHA-C4D-ND	2.45	137.60	132.55
31	5	604	CLA	C4B-CHC-C1C	2.45	132.00	126.25
31	9	312	CLA	C4B-CHC-C1C	2.45	132.00	126.25
31	n	315	CLA	C4B-CHC-C1C	2.45	132.00	126.25
31	r	314	CLA	CMA-C3A-C4A	2.45	118.35	111.77
36	p	618	NEX	C16-C1-C6	-2.45	108.28	110.47
31	8	613	CLA	CHA-C4D-ND	2.45	137.60	132.55
31	p	611	CLA	CHA-C4D-ND	2.45	137.60	132.55
31	G	602	CLA	CHA-C4D-ND	2.45	137.60	132.55
31	5	612	CLA	O2A-CGA-CBA	2.45	119.30	111.83
31	b	602	CLA	CHD-C1D-ND	-2.45	121.36	124.80
31	b	612	CLA	C2C-C1C-NC	2.45	112.55	109.98
32	p	616	LUT	C31-C32-C33	2.45	133.07	126.36
31	b	603	CLA	CHA-C4D-ND	2.45	137.60	132.55
44	a	414	PL9	C27-C28-C29	-2.45	122.02	127.62
31	Y	304	CLA	C6-C5-C3	-2.45	107.51	113.47
31	4	611	CLA	CHA-C4D-ND	2.45	137.60	132.55
32	S	317	LUT	C35-C15-C14	-2.45	118.52	123.52
31	G	604	CLA	C3B-C4B-NB	-2.45	108.35	110.53
31	p	610	CLA	CMD-C2D-C3D	-2.45	122.08	127.69
31	N	310	CLA	O2A-CGA-CBA	2.45	119.29	111.83
31	8	603	CLA	C4B-CHC-C1C	2.45	132.00	126.25
31	n	305	CLA	C4B-CHC-C1C	2.44	132.00	126.25
31	r	305	CLA	C4B-CHC-C1C	2.44	132.00	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	D	401	PHO	C4A-C3A-C2A	-2.44	100.51	102.84
31	g	305	CLA	C4B-CHC-C1C	2.44	132.00	126.25
31	C	604	CLA	CHA-C4D-ND	2.44	137.59	132.55
31	8	602	CLA	CHA-C4D-ND	2.44	137.59	132.55
30	Y	308	CHL	CMA-C3A-C4A	2.44	119.88	114.61
43	C	614	BCR	C29-C30-C25	2.44	113.99	110.44
43	H	101	BCR	C29-C30-C25	2.44	113.99	110.44
31	0	611	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
31	s	305	CLA	CHA-C4D-ND	2.44	137.59	132.55
30	3	302	CHL	C4D-CHA-CBD	-2.44	106.50	108.97
31	9	313	CLA	O2A-CGA-CBA	2.44	119.29	111.83
30	9	307	CHL	CMA-C3A-C4A	2.44	119.88	114.61
31	g	312	CLA	C4B-CHC-C1C	2.44	131.99	126.25
31	D	404	CLA	C3B-C4B-NB	-2.44	108.35	110.53
31	R	316	CLA	CMA-C3A-C4A	2.44	118.34	111.77
30	8	605	CHL	C4D-CHA-CBD	-2.44	106.50	108.97
32	7	317	LUT	C11-C12-C13	-2.44	119.67	126.36
31	7	313	CLA	O1D-CGD-CBD	-2.44	119.70	124.52
31	c	606	CLA	C4B-CHC-C1C	2.44	131.99	126.25
31	y	611	CLA	C1C-C2C-C3C	-2.44	104.41	106.98
31	N	315	CLA	CHA-C4D-ND	2.44	137.59	132.55
31	n	315	CLA	CHA-C4D-ND	2.44	137.59	132.55
31	8	610	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
31	B	613	CLA	CMA-C3A-C4A	2.44	118.34	111.77
31	1	604	CLA	C4B-CHC-C1C	2.44	131.99	126.25
32	7	317	LUT	C15-C35-C34	-2.44	118.52	123.52
31	C	609	CLA	CHD-C1D-ND	-2.44	121.37	124.80
31	q	315	CLA	C1D-ND-C4D	-2.44	104.60	106.31
31	7	316	CLA	CHA-C4D-ND	2.44	137.59	132.55
31	s	303	CLA	CMD-C2D-C3D	-2.44	122.09	127.69
43	C	615	BCR	C7-C6-C5	-2.44	115.93	121.56
30	5	609	CHL	CMA-C3A-C2A	2.44	123.56	114.13
34	7	322	LMG	C8-O7-C10	-2.44	111.95	117.80
31	N	303	CLA	O2A-CGA-CBA	2.44	119.28	111.83
31	r	315	CLA	CMA-C3A-C4A	2.44	118.33	111.77
30	6	310	CHL	CMA-C3A-C4A	2.44	119.87	114.61
30	7	307	CHL	CMA-C3A-C4A	2.44	119.87	114.61
31	s	316	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
31	s	312	CLA	CHA-C4D-ND	2.44	137.58	132.55
31	B	603	CLA	C4B-CHC-C1C	2.44	131.98	126.25
31	C	613	CLA	CHA-C4D-ND	2.44	137.58	132.55
31	R	312	CLA	CHA-C4D-ND	2.44	137.58	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	609	CLA	CHD-C1D-ND	-2.44	121.37	124.80
31	6	314	CLA	C4B-CHC-C1C	2.44	131.98	126.25
31	p	610	CLA	CHA-C4D-ND	2.44	137.58	132.55
31	N	310	CLA	CMD-C2D-C3D	-2.44	122.10	127.69
34	a	416	LMG	O8-C28-C29	2.44	119.27	111.83
31	R	303	CLA	C4B-CHC-C1C	2.44	131.98	126.25
48	R	302	LMU	O5'-C5'-C4'	-2.44	104.69	109.72
31	p	603	CLA	CHA-C4D-ND	2.44	137.58	132.55
31	0	611	CLA	C4B-CHC-C1C	2.44	131.98	126.25
31	p	611	CLA	O2D-CGD-O1D	-2.44	119.11	123.85
31	4	614	CLA	CMD-C2D-C3D	-2.44	122.10	127.69
31	N	303	CLA	CHA-C4D-ND	2.44	137.57	132.55
31	s	313	CLA	CHA-C4D-ND	2.44	137.57	132.55
31	9	315	CLA	C4B-CHC-C1C	2.43	131.97	126.25
31	5	603	CLA	CHD-C1D-ND	-2.43	121.38	124.80
31	4	614	CLA	CHA-C4D-ND	2.43	137.57	132.55
31	B	602	CLA	CHA-C4D-ND	2.43	137.57	132.55
31	B	601	CLA	O2A-CGA-CBA	2.43	119.26	111.83
31	9	312	CLA	C2C-C1C-NC	2.43	112.54	109.98
31	y	610	CLA	C2C-C1C-NC	2.43	112.54	109.98
32	0	617	LUT	C8-C7-C6	-2.43	120.50	127.00
34	w	202	LMG	C8-O7-C10	-2.43	111.97	117.80
31	7	305	CLA	C3B-C4B-NB	-2.43	108.36	110.53
31	4	614	CLA	C4B-CHC-C1C	2.43	131.97	126.25
31	6	312	CLA	CHA-C4D-ND	2.43	137.57	132.55
31	n	303	CLA	CHA-C4D-ND	2.43	137.57	132.55
30	r	309	CHL	C4D-CHA-CBD	-2.43	106.51	108.97
32	y	616	LUT	C27-C28-C29	-2.43	121.09	126.32
31	3	304	CLA	CHA-C4D-ND	2.43	137.57	132.55
31	p	604	CLA	CHA-C4D-ND	2.43	137.57	132.55
31	G	602	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
31	C	613	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
42	D	401	PHO	C1-C2-C3	-2.43	122.21	126.20
31	2	611	CLA	CHA-C4D-ND	2.43	137.57	132.55
31	3	312	CLA	CHA-C4D-ND	2.43	137.57	132.55
31	b	614	CLA	CHA-C4D-ND	2.43	137.57	132.55
31	1	603	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
31	B	616	CLA	C1C-C2C-C3C	-2.43	104.42	106.98
31	q	305	CLA	O2A-CGA-CBA	2.43	119.25	111.83
43	A	410	BCR	C29-C30-C25	2.43	113.97	110.44
30	0	607	CHL	C4D-CHA-CBD	-2.43	106.51	108.97
31	2	609	CLA	CHA-C4D-ND	2.43	137.57	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	n	317	LUT	C31-C30-C29	-2.43	123.87	127.28
31	N	321	CLA	CHA-C4D-ND	2.43	137.57	132.55
31	n	305	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
31	R	304	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
31	9	304	CLA	CHD-C1D-ND	-2.43	121.38	124.80
31	B	607	CLA	C4B-CHC-C1C	2.43	131.96	126.25
31	c	610	CLA	CHA-C4D-ND	2.43	137.56	132.55
31	8	602	CLA	O2A-CGA-CBA	2.43	119.25	111.83
34	c	624	LMG	C8-O7-C10	-2.43	111.98	117.80
31	9	315	CLA	CHA-C4D-ND	2.43	137.56	132.55
31	c	603	CLA	CHA-C4D-ND	2.43	137.56	132.55
31	7	313	CLA	O2A-CGA-CBA	2.43	119.24	111.83
31	G	610	CLA	C4B-CHC-C1C	2.43	131.96	126.25
31	3	316	CLA	CHD-C1D-ND	-2.43	121.38	124.80
31	s	303	CLA	CHD-C1D-ND	-2.43	121.38	124.80
31	c	607	CLA	C4B-CHC-C1C	2.43	131.96	126.25
32	5	617	LUT	C8-C7-C6	-2.43	120.51	127.00
31	C	608	CLA	C4B-CHC-C1C	2.43	131.96	126.25
31	n	315	CLA	C2D-C1D-ND	2.43	112.53	110.13
30	4	606	CHL	CMA-C3A-C4A	2.43	119.84	114.61
31	n	304	CLA	C4B-CHC-C1C	2.43	131.96	126.25
31	C	603	CLA	O2A-CGA-CBA	2.43	119.24	111.83
30	y	601	CHL	C4D-CHA-CBD	-2.43	106.52	108.97
32	8	615	LUT	C31-C30-C29	-2.43	123.87	127.28
31	0	611	CLA	CHA-C4D-ND	2.43	137.56	132.55
31	b	611	CLA	CHA-C4D-ND	2.43	137.56	132.55
31	0	603	CLA	C4B-CHC-C1C	2.43	131.95	126.25
31	p	602	CLA	C4B-CHC-C1C	2.43	131.95	126.25
31	b	612	CLA	CHA-C4D-ND	2.43	137.56	132.55
31	R	312	CLA	C1-C2-C3	-2.43	122.22	126.20
30	G	606	CHL	C4D-CHA-CBD	-2.43	106.52	108.97
30	N	302	CHL	C4D-CHA-CBD	-2.43	106.52	108.97
31	0	614	CLA	O2D-CGD-O1D	-2.43	119.13	123.85
43	z	101	BCR	C21-C20-C19	-2.43	116.17	123.20
31	S	312	CLA	CMA-C3A-C4A	2.43	118.29	111.77
31	7	313	CLA	CMD-C2D-C3D	-2.43	122.13	127.69
31	B	609	CLA	C3B-C4B-NB	-2.43	108.36	110.53
31	n	305	CLA	C3B-C4B-NB	-2.43	108.36	110.53
31	s	314	CLA	CHA-C4D-ND	2.42	137.55	132.55
31	g	314	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
31	6	311	CLA	CHD-C1D-ND	-2.42	121.39	124.80
32	6	317	LUT	C39-C29-C28	2.42	121.79	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	312	CLA	CMA-C3A-C4A	2.42	118.29	111.77
31	b	602	CLA	O2A-CGA-CBA	2.42	119.23	111.83
31	s	306	CLA	O2A-CGA-CBA	2.42	119.22	111.83
31	N	311	CLA	CHA-C4D-ND	2.42	137.55	132.55
31	n	311	CLA	CHD-C1D-ND	-2.42	121.39	124.80
31	s	315	CLA	CHD-C1D-ND	-2.42	121.39	124.80
33	S	320	LHG	C6-C5-C4	-2.42	106.14	111.78
43	D	405	BCR	C23-C24-C25	-2.42	120.53	127.00
45	C	620	DGD	O1G-C1A-C2A	2.42	119.22	111.83
30	y	606	CHL	C4D-CHA-CBD	-2.42	106.52	108.97
31	R	307	CLA	CAA-C2A-C3A	-2.42	106.45	113.00
31	7	311	CLA	CHD-C1D-ND	-2.42	121.39	124.80
31	B	610	CLA	CHA-C4D-ND	2.42	137.55	132.55
31	Y	311	CLA	C4B-CHC-C1C	2.42	131.94	126.25
30	1	607	CHL	C4D-CHA-CBD	-2.42	106.53	108.97
38	a	412	SQD	O5-C1-O6	-2.42	104.32	110.04
31	B	609	CLA	C1D-ND-C4D	-2.42	104.61	106.31
31	6	305	CLA	C6-C5-C3	-2.42	107.57	113.47
31	r	315	CLA	C2C-C1C-NC	2.42	112.53	109.98
34	w	203	LMG	C7-O1-C1	-2.42	108.61	113.80
31	R	303	CLA	CAA-CBA-CGA	-2.42	106.33	113.21
31	0	612	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
36	Y	317	NEX	C16-C1-C6	-2.42	108.31	110.47
31	c	609	CLA	CHA-C4D-ND	2.42	137.54	132.55
43	a	410	BCR	C29-C30-C25	2.42	113.95	110.44
31	1	603	CLA	O2A-CGA-CBA	2.42	119.21	111.83
31	b	604	CLA	CMA-C3A-C4A	2.42	118.28	111.77
31	n	304	CLA	CHA-C4D-ND	2.42	137.54	132.55
31	n	314	CLA	CHA-C4D-ND	2.42	137.54	132.55
43	c	615	BCR	C7-C8-C9	-2.42	122.66	126.23
31	R	304	CLA	C3B-C4B-NB	-2.42	108.37	110.53
31	b	604	CLA	C3B-C4B-NB	-2.42	108.37	110.53
31	p	615	CLA	C2C-C1C-NC	2.42	112.52	109.98
43	B	619	BCR	C21-C20-C19	-2.42	116.19	123.20
31	6	311	CLA	CHA-C4D-ND	2.42	137.54	132.55
31	C	602	CLA	CHA-C4D-ND	2.42	137.54	132.55
31	q	304	CLA	C4B-CHC-C1C	2.42	131.93	126.25
31	N	314	CLA	C2D-C1D-ND	2.42	112.52	110.13
31	c	604	CLA	C1C-C2C-C3C	-2.42	104.44	106.98
32	7	318	LUT	C15-C35-C34	-2.42	118.57	123.52
31	1	611	CLA	CHA-C4D-ND	2.42	137.54	132.55
31	4	604	CLA	C4B-CHC-C1C	2.42	131.93	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	6	305	CLA	C4B-CHC-C1C	2.42	131.93	126.25
31	B	609	CLA	C4B-CHC-C1C	2.42	131.93	126.25
30	N	309	CHL	C4D-CHA-CBD	-2.42	106.53	108.97
31	2	602	CLA	C2D-C1D-ND	2.42	112.52	110.13
31	g	314	CLA	O2A-CGA-CBA	2.42	119.20	111.83
34	d	409	LMG	C8-O7-C10	-2.42	112.01	117.80
31	R	307	CLA	CHA-C4D-ND	2.42	137.53	132.55
31	S	311	CLA	O2A-CGA-CBA	2.42	119.20	111.83
44	A	416	PL9	C37-C38-C39	-2.42	122.09	127.62
31	D	404	CLA	CMA-C3A-C4A	2.42	118.27	111.77
31	q	304	CLA	CHA-C4D-ND	2.42	137.53	132.55
30	Y	307	CHL	CMA-C3A-C2A	2.42	123.46	114.13
31	7	311	CLA	CMD-C2D-C3D	-2.42	122.15	127.69
31	s	311	CLA	CAA-C2A-C3A	-2.42	106.47	113.00
31	0	614	CLA	CHA-C4D-ND	2.42	137.53	132.55
30	1	609	CHL	C1-O2A-CGA	2.42	122.50	116.65
31	2	604	CLA	C4B-CHC-C1C	2.42	131.93	126.25
30	6	310	CHL	CMA-C3A-C2A	2.42	123.46	114.13
31	5	603	CLA	CHA-C4D-ND	2.42	137.53	132.55
31	5	610	CLA	CHA-C4D-ND	2.42	137.53	132.55
31	R	315	CLA	O2A-CGA-CBA	2.42	119.20	111.83
32	S	317	LUT	C30-C31-C32	-2.41	116.20	123.20
31	Y	313	CLA	C1-O2A-CGA	2.41	122.50	116.65
31	b	605	CLA	CHA-C1A-NA	-2.41	120.92	126.39
36	g	317	NEX	C39-C29-C30	-2.41	118.90	122.82
36	9	319	NEX	C17-C1-C6	-2.41	108.31	110.47
31	g	305	CLA	C3B-C4B-NB	-2.41	108.38	110.53
31	3	306	CLA	CHD-C1D-ND	-2.41	121.41	124.80
31	0	613	CLA	CHA-C4D-ND	2.41	137.53	132.55
31	9	316	CLA	CHA-C4D-ND	2.41	137.53	132.55
31	S	305	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
32	5	617	LUT	C21-C26-C27	-2.41	110.05	112.83
31	A	409	CLA	C1D-ND-C4D	-2.41	104.62	106.31
31	S	315	CLA	C4B-CHC-C1C	2.41	131.92	126.25
31	q	313	CLA	CHA-C4D-ND	2.41	137.53	132.55
31	6	303	CLA	CHD-C1D-ND	-2.41	121.41	124.80
34	a	413	LMG	O1-C1-C2	2.41	111.94	108.27
31	A	405	CLA	C2C-C1C-NC	2.41	112.52	109.98
31	R	306	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
31	G	602	CLA	O2A-CGA-CBA	2.41	119.19	111.83
30	Y	302	CHL	C4D-CHA-CBD	-2.41	106.53	108.97
31	d	404	CLA	C4B-CHC-C1C	2.41	131.92	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	306	CLA	O2A-CGA-CBA	2.41	119.19	111.83
31	q	314	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
31	Y	303	CLA	CHA-C4D-ND	2.41	137.53	132.55
31	r	304	CLA	C6-C5-C3	-2.41	107.59	113.47
44	a	414	PL9	C40-C39-C41	2.41	119.41	115.23
31	q	305	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
31	8	611	CLA	CHA-C4D-ND	2.41	137.52	132.55
32	n	318	LUT	C8-C7-C6	-2.41	120.56	127.00
32	S	317	LUT	C27-C28-C29	-2.41	121.14	126.32
33	R	320	LHG	O8-C23-C24	2.41	119.19	111.83
32	n	317	LUT	C35-C15-C14	-2.41	118.59	123.52
30	0	609	CHL	C1-C2-C3	-2.41	122.25	126.20
31	7	313	CLA	C1D-ND-C4D	-2.41	104.62	106.31
31	R	311	CLA	C4B-CHC-C1C	2.41	131.91	126.25
31	9	313	CLA	C4B-CHC-C1C	2.41	131.91	126.25
31	3	306	CLA	CHA-C4D-ND	2.41	137.52	132.55
31	b	606	CLA	CHA-C4D-ND	2.41	137.52	132.55
31	s	311	CLA	C2C-C1C-NC	2.41	112.51	109.98
31	r	316	CLA	C3B-C4B-NB	-2.41	108.38	110.53
31	y	614	CLA	CHA-C4D-ND	2.41	137.52	132.55
31	0	604	CLA	CHD-C1D-ND	-2.41	121.41	124.80
31	Y	313	CLA	C4B-CHC-C1C	2.41	131.91	126.25
31	q	306	CLA	C4B-CHC-C1C	2.41	131.91	126.25
31	S	314	CLA	CHA-C4D-ND	2.41	137.52	132.55
34	x	202	LMG	C8-O7-C10	-2.41	112.03	117.80
31	p	603	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
31	r	307	CLA	C4B-CHC-C1C	2.41	131.91	126.25
31	8	614	CLA	CHA-C4D-ND	2.41	137.52	132.55
31	1	603	CLA	C4B-CHC-C1C	2.41	131.91	126.25
31	1	602	CLA	C3B-C4B-NB	-2.41	108.38	110.53
34	x	202	LMG	O1-C7-C8	-2.41	104.96	110.82
31	r	312	CLA	CHA-C4D-ND	2.41	137.51	132.55
31	R	304	CLA	C1D-ND-C4D	-2.41	104.62	106.31
31	7	315	CLA	CHA-C4D-ND	2.41	137.51	132.55
31	r	316	CLA	CHA-C4D-ND	2.41	137.51	132.55
30	r	308	CHL	CMA-C3A-C4A	2.41	119.79	114.61
31	4	602	CLA	C6-C5-C3	-2.41	107.61	113.47
32	7	317	LUT	C8-C7-C6	-2.41	120.57	127.00
31	s	316	CLA	CHA-C4D-ND	2.41	137.51	132.55
31	B	606	CLA	CMD-C2D-C3D	-2.40	122.17	127.69
31	1	604	CLA	CHD-C1D-ND	-2.40	121.42	124.80
31	c	613	CLA	CHA-C1A-NA	-2.40	120.95	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	604	CLA	C2C-C1C-NC	2.40	112.51	109.98
31	N	315	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
31	G	610	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
30	q	303	CHL	C1-C2-C3	-2.40	122.26	126.20
31	3	314	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
43	C	615	BCR	C29-C30-C25	2.40	113.93	110.44
31	6	314	CLA	CHA-C4D-ND	2.40	137.50	132.55
31	B	615	CLA	CHD-C1D-ND	-2.40	121.42	124.80
31	p	613	CLA	C4B-CHC-C1C	2.40	131.90	126.25
30	1	606	CHL	C1-C2-C3	-2.40	122.26	126.20
34	p	620	LMG	C8-O7-C10	-2.40	112.05	117.80
43	H	101	BCR	C8-C7-C6	-2.40	120.58	127.00
31	6	303	CLA	CHA-C4D-ND	2.40	137.50	132.55
31	c	606	CLA	CHA-C4D-ND	2.40	137.50	132.55
31	B	613	CLA	C4B-CHC-C1C	2.40	131.89	126.25
31	S	314	CLA	C4B-CHC-C1C	2.40	131.89	126.25
31	r	305	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
31	n	313	CLA	CHA-C4D-ND	2.40	137.50	132.55
31	1	603	CLA	CHD-C1D-ND	-2.40	121.42	124.80
31	5	613	CLA	CHA-C4D-ND	2.40	137.50	132.55
31	b	613	CLA	CHA-C4D-ND	2.40	137.50	132.55
31	0	604	CLA	O2A-CGA-CBA	2.40	119.15	111.83
31	3	315	CLA	O2A-CGA-CBA	2.40	119.15	111.83
31	r	303	CLA	CMA-C3A-C4A	2.40	118.22	111.77
31	C	601	CLA	C2C-C1C-NC	2.40	112.50	109.98
31	8	612	CLA	CHA-C4D-ND	2.40	137.50	132.55
31	S	315	CLA	O2A-CGA-CBA	2.40	119.15	111.83
31	3	306	CLA	CMD-C2D-C3D	-2.40	122.19	127.69
31	1	610	CLA	CHA-C4D-ND	2.40	137.50	132.55
31	s	303	CLA	CHA-C4D-ND	2.40	137.50	132.55
31	5	614	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
31	d	404	CLA	C2C-C1C-NC	2.40	112.50	109.98
31	S	305	CLA	CHA-C4D-ND	2.40	137.50	132.55
31	Y	310	CLA	CHD-C1D-ND	-2.40	121.43	124.80
31	4	602	CLA	CHA-C4D-ND	2.40	137.49	132.55
31	C	606	CLA	CHA-C4D-ND	2.40	137.49	132.55
31	r	306	CLA	CHA-C4D-ND	2.40	137.49	132.55
31	S	316	CLA	CHD-C1D-ND	-2.40	121.43	124.80
32	S	317	LUT	C1-C6-C5	-2.40	119.36	122.64
31	6	305	CLA	CHA-C4D-ND	2.40	137.49	132.55
31	R	316	CLA	CHA-C4D-ND	2.40	137.49	132.55
31	S	310	CLA	CHA-C4D-ND	2.40	137.49	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	d	401	CLA	CHA-C4D-ND	2.40	137.49	132.55
31	r	304	CLA	CHA-C4D-ND	2.40	137.49	132.55
31	r	313	CLA	CHA-C4D-ND	2.40	137.49	132.55
31	s	306	CLA	CHA-C4D-ND	2.40	137.49	132.55
43	c	614	BCR	C35-C13-C14	-2.40	118.93	122.82
31	0	613	CLA	C4B-CHC-C1C	2.40	131.88	126.25
31	4	603	CLA	C1D-ND-C4D	-2.40	104.63	106.31
31	c	605	CLA	CMD-C2D-C3D	-2.40	122.20	127.69
31	s	311	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
32	8	616	LUT	C8-C7-C6	-2.40	120.60	127.00
31	0	610	CLA	O2A-CGA-CBA	2.39	119.14	111.83
31	b	614	CLA	O2A-CGA-CBA	2.39	119.14	111.83
31	c	602	CLA	CHA-C4D-ND	2.39	137.49	132.55
31	c	601	CLA	CHD-C1D-ND	-2.39	121.43	124.80
31	D	403	CLA	CHA-C4D-ND	2.39	137.49	132.55
31	5	602	CLA	CHD-C1D-ND	-2.39	121.43	124.80
31	5	611	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
31	N	321	CLA	O2A-CGA-CBA	2.39	119.13	111.83
31	G	611	CLA	CMA-C3A-C4A	2.39	118.20	111.77
36	Y	317	NEX	O24-C25-C38	-2.39	112.37	115.05
31	n	311	CLA	O2A-CGA-CBA	2.39	119.13	111.83
31	A	406	CLA	C4B-CHC-C1C	2.39	131.87	126.25
31	S	313	CLA	C4B-CHC-C1C	2.39	131.87	126.25
31	R	307	CLA	CMA-C3A-C4A	2.39	118.20	111.77
32	8	615	LUT	C35-C15-C14	-2.39	118.62	123.52
31	y	602	CLA	CHA-C4D-ND	2.39	137.48	132.55
31	R	313	CLA	CHA-C4D-ND	2.39	137.48	132.55
31	C	606	CLA	O2A-CGA-CBA	2.39	119.12	111.83
31	y	603	CLA	O2A-CGA-CBA	2.39	119.12	111.83
31	5	612	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
33	F1	301	LHG	O8-C23-C24	2.39	119.12	111.83
43	b	620	BCR	C8-C7-C6	-2.39	120.61	127.00
31	4	614	CLA	CHD-C1D-ND	-2.39	121.44	124.80
31	R	312	CLA	C2C-C1C-NC	2.39	112.49	109.98
31	A	405	CLA	O2A-CGA-CBA	2.39	119.12	111.83
32	0	616	LUT	C10-C11-C12	-2.39	116.28	123.20
34	9	302	LMG	C8-O7-C10	-2.39	112.08	117.80
31	r	313	CLA	C4B-CHC-C1C	2.39	131.86	126.25
31	r	315	CLA	C4B-CHC-C1C	2.39	131.86	126.25
31	B	616	CLA	CHA-C4D-ND	2.39	137.47	132.55
31	n	316	CLA	CHA-C4D-ND	2.39	137.47	132.55
31	r	315	CLA	CHA-C4D-ND	2.39	137.47	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	n	305	CLA	CMA-C3A-C4A	2.39	118.19	111.77
31	b	614	CLA	C3B-C4B-NB	-2.39	108.40	110.53
31	r	305	CLA	CHA-C4D-ND	2.39	137.47	132.55
31	S	314	CLA	O2A-CGA-CBA	2.39	119.11	111.83
31	y	610	CLA	CHA-C4D-ND	2.39	137.47	132.55
31	q	313	CLA	C2D-C1D-ND	2.39	112.49	110.13
31	0	615	CLA	C4B-CHC-C1C	2.39	131.86	126.25
30	0	608	CHL	CMA-C3A-C4A	2.39	119.75	114.61
31	R	314	CLA	CHA-C4D-ND	2.39	137.47	132.55
31	0	602	CLA	CHA-C4D-ND	2.39	137.47	132.55
31	1	611	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
31	q	316	CLA	CMD-C2D-C3D	-2.39	122.22	127.69
31	Y	304	CLA	O2A-CGA-CBA	2.39	119.11	111.83
35	q	317	RRX	C11-C10-C9	-2.39	123.93	127.28
31	B	604	CLA	C4B-CHC-C1C	2.38	131.85	126.25
31	1	613	CLA	CHA-C4D-ND	2.38	137.47	132.55
31	A	405	CLA	CHA-C4D-ND	2.38	137.47	132.55
31	N	310	CLA	CHA-C4D-ND	2.38	137.47	132.55
31	p	612	CLA	C2D-C1D-ND	2.38	112.49	110.13
31	r	304	CLA	C2D-C1D-ND	2.38	112.49	110.13
31	3	316	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
32	G	615	LUT	C20-C13-C12	2.38	121.73	118.09
31	S	313	CLA	C6-C5-C3	-2.38	107.66	113.47
31	c	604	CLA	CHA-C4D-ND	2.38	137.47	132.55
31	1	611	CLA	O2A-CGA-CBA	2.38	119.10	111.83
31	D	403	CLA	C4B-CHC-C1C	2.38	131.85	126.25
31	D	404	CLA	CAA-C2A-C3A	-2.38	106.56	113.00
31	c	609	CLA	C4B-CHC-C1C	2.38	131.85	126.25
31	B	612	CLA	C2C-C1C-NC	2.38	112.48	109.98
43	C	614	BCR	C8-C7-C6	-2.38	120.63	127.00
31	c	609	CLA	CHD-C1D-ND	-2.38	121.45	124.80
48	K	101	LMU	C1'-C2'-C3'	2.38	115.02	110.01
31	N	312	CLA	CHA-C4D-ND	2.38	137.47	132.55
43	h	101	BCR	C30-C25-C26	-2.38	119.38	122.64
30	2	607	CHL	CMA-C3A-C4A	2.38	119.74	114.61
36	r	319	NEX	C26-C27-C28	-2.38	120.96	125.99
31	B	613	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
31	c	608	CLA	C1C-C2C-C3C	-2.38	104.47	106.98
30	n	310	CHL	C4D-CHA-CBD	-2.38	106.57	108.97
31	S	310	CLA	C1-O2A-CGA	2.38	122.41	116.65
30	y	608	CHL	CMA-C3A-C4A	2.38	119.74	114.61
31	S	303	CLA	CHD-C1D-ND	-2.38	121.45	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	616	CLA	CHD-C1D-ND	-2.38	121.45	124.80
32	5	617	LUT	C27-C28-C29	-2.38	121.20	126.32
31	q	304	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
31	s	310	CLA	CHA-C4D-ND	2.38	137.46	132.55
43	t	101	BCR	C28-C27-C26	-2.38	109.81	114.06
31	s	305	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
31	s	314	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
31	C	607	CLA	C6-C5-C3	-2.38	107.67	113.47
31	0	604	CLA	CHA-C4D-ND	2.38	137.46	132.55
31	N	303	CLA	CHD-C1D-ND	-2.38	121.45	124.80
31	1	602	CLA	CHA-C4D-ND	2.38	137.46	132.55
31	b	617	CLA	CHA-C4D-ND	2.38	137.46	132.55
31	A	405	CLA	CAA-C2A-C1A	-2.38	104.18	111.97
31	A	406	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
31	2	612	CLA	C4B-CHC-C1C	2.38	131.84	126.25
31	s	312	CLA	C4B-CHC-C1C	2.38	131.84	126.25
32	S	318	LUT	C31-C32-C33	-2.38	119.84	126.36
31	S	311	CLA	C3B-C4B-NB	-2.38	108.41	110.53
31	d	405	CLA	C3B-C4B-NB	-2.38	108.41	110.53
31	5	613	CLA	O2A-CGA-CBA	2.38	119.09	111.83
36	S	319	NEX	C38-C25-C26	-2.38	118.39	122.30
31	5	615	CLA	CHD-C1D-ND	-2.38	121.46	124.80
31	1	614	CLA	CHA-C4D-ND	2.38	137.46	132.55
31	R	311	CLA	CHA-C4D-ND	2.38	137.46	132.55
31	4	613	CLA	CHA-C4D-ND	2.38	137.45	132.55
31	c	608	CLA	CHA-C4D-ND	2.38	137.45	132.55
30	N	301	CHL	C4D-CHA-CBD	-2.38	106.57	108.97
31	G	602	CLA	CHD-C1D-ND	-2.38	121.46	124.80
30	G	607	CHL	CMA-C3A-C4A	2.38	119.73	114.61
34	a	413	LMG	C3-C4-C5	2.38	114.54	110.23
43	B	618	BCR	C29-C30-C25	2.38	113.89	110.44
32	6	317	LUT	C10-C11-C12	-2.38	116.32	123.20
31	2	612	CLA	CHA-C4D-ND	2.38	137.45	132.55
31	c	605	CLA	C4B-CHC-C1C	2.38	131.83	126.25
31	5	610	CLA	CHD-C1D-ND	-2.38	121.46	124.80
34	6	323	LMG	O6-C5-C6	2.37	112.33	106.44
31	9	316	CLA	CMD-C2D-C3D	-2.37	122.24	127.69
31	r	312	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
31	S	310	CLA	CHD-C1D-ND	-2.37	121.46	124.80
30	s	308	CHL	C4D-CHA-CBD	-2.37	106.57	108.97
47	E	101	HEM	CBA-CAA-C2A	-2.37	105.97	112.53
30	p	609	CHL	CMA-C3A-C2A	2.37	123.30	114.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	0	617	LUT	C15-C35-C34	-2.37	118.66	123.52
31	3	314	CLA	C6-C5-C3	-2.37	107.69	113.47
31	3	314	CLA	O2A-CGA-CBA	2.37	119.07	111.83
31	b	611	CLA	O2A-CGA-CBA	2.37	119.07	111.83
31	C	607	CLA	CHD-C1D-ND	-2.37	121.46	124.80
31	C	606	CLA	C4B-CHC-C1C	2.37	131.83	126.25
31	N	321	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
31	g	305	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
31	S	303	CLA	CHA-C4D-ND	2.37	137.44	132.55
31	S	316	CLA	CHA-C4D-ND	2.37	137.44	132.55
31	b	613	CLA	C16-C15-C13	-2.37	108.08	115.97
31	0	603	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
31	4	610	CLA	C2D-C1D-ND	2.37	112.47	110.13
31	8	613	CLA	C2D-C1D-ND	2.37	112.47	110.13
31	G	610	CLA	O2A-CGA-CBA	2.37	119.06	111.83
31	g	310	CLA	C3B-C4B-NB	-2.37	108.41	110.53
38	0	621	SQD	O7-S-C6	-2.37	103.22	106.76
31	R	306	CLA	CHD-C1D-ND	-2.37	121.47	124.80
31	7	311	CLA	CHA-C4D-ND	2.37	137.44	132.55
31	q	312	CLA	C4B-CHC-C1C	2.37	132.56	125.21
31	6	305	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
31	C	604	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
30	8	607	CHL	C4D-CHA-CBD	-2.37	106.58	108.97
31	0	610	CLA	CHA-C4D-ND	2.37	137.44	132.55
31	G	603	CLA	CHD-C1D-ND	-2.37	121.47	124.80
31	N	314	CLA	CHA-C4D-ND	2.37	137.44	132.55
31	Y	314	CLA	CHA-C4D-ND	2.37	137.44	132.55
43	c	615	BCR	C36-C18-C17	-2.37	118.98	122.82
31	8	609	CLA	CHA-C4D-ND	2.37	137.44	132.55
31	8	609	CLA	O2A-CGA-CBA	2.37	119.06	111.83
31	a	406	CLA	CHA-C4D-ND	2.37	137.43	132.55
36	Y	317	NEX	C39-C29-C30	-2.37	118.98	122.82
31	r	311	CLA	CHD-C1D-ND	-2.37	121.47	124.80
30	4	601	CHL	C4D-CHA-CBD	-2.37	106.58	108.97
34	b	626	LMG	C8-O7-C10	-2.37	112.13	117.80
31	p	610	CLA	CHD-C1D-ND	-2.37	121.47	124.80
31	R	304	CLA	CHA-C4D-ND	2.36	137.43	132.55
31	A	406	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
31	b	610	CLA	CAA-CBA-CGA	-2.36	106.49	113.21
31	9	314	CLA	CMA-C3A-C4A	2.36	118.13	111.77
31	C	606	CLA	CHD-C1D-ND	-2.36	121.47	124.80
31	s	315	CLA	O2A-CGA-CBA	2.36	119.04	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	616	CLA	C3B-C4B-NB	-2.36	108.42	110.53
31	R	315	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
31	Y	311	CLA	CHA-C4D-ND	2.36	137.43	132.55
31	B	610	CLA	O2A-CGA-CBA	2.36	119.04	111.83
31	4	610	CLA	C4B-CHC-C1C	2.36	131.80	126.25
31	b	603	CLA	C4B-CHC-C1C	2.36	131.80	126.25
31	C	608	CLA	C6-C5-C3	-2.36	107.71	113.47
43	B	617	BCR	C3-C4-C5	-2.36	109.84	114.06
31	3	311	CLA	C3B-C4B-NB	-2.36	108.42	110.53
31	B	611	CLA	CHA-C4D-ND	2.36	137.42	132.55
31	B	602	CLA	C4B-CHC-C1C	2.36	131.80	126.25
31	4	611	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
31	5	602	CLA	CHA-C4D-ND	2.36	137.42	132.55
31	Y	310	CLA	CHA-C4D-ND	2.36	137.42	132.55
33	z	102	LHG	O7-C7-O9	-2.36	118.18	123.70
30	s	308	CHL	CMA-C3A-C4A	2.36	119.70	114.61
31	a	406	CLA	C3B-C4B-NB	-2.36	108.42	110.53
31	6	315	CLA	C2D-C1D-ND	2.36	112.46	110.13
43	B	618	BCR	C37-C22-C23	2.36	121.69	118.09
31	0	610	CLA	C2C-C1C-NC	2.36	112.46	109.98
31	4	612	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
31	b	602	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
32	r	317	LUT	C27-C28-C29	-2.36	121.25	126.32
31	5	615	CLA	C4B-CHC-C1C	2.36	131.80	126.25
31	c	612	CLA	CHA-C4D-ND	2.36	137.42	132.55
31	9	314	CLA	C2C-C1C-NC	2.36	112.46	109.98
31	Y	314	CLA	O2A-CGA-CBA	2.36	119.03	111.83
31	q	304	CLA	C6-C5-C3	-2.36	107.72	113.47
36	3	319	NEX	C26-C27-C28	-2.36	121.00	125.99
31	2	610	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
31	6	311	CLA	C2D-C1D-ND	2.36	112.46	110.13
31	A	405	CLA	C4B-CHC-C1C	2.36	131.79	126.25
31	b	605	CLA	O2A-CGA-CBA	2.36	119.02	111.83
31	6	303	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
36	2	616	NEX	C26-C27-C28	-2.36	121.01	125.99
31	y	611	CLA	CHA-C4D-ND	2.36	137.41	132.55
31	g	304	CLA	CHD-C1D-ND	-2.36	121.48	124.80
31	3	316	CLA	C1D-ND-C4D	-2.36	104.66	106.31
36	y	618	NEX	C2-C1-C6	2.36	111.50	109.21
36	G	616	NEX	C19-C9-C10	-2.36	119.00	122.82
31	1	613	CLA	C4B-CHC-C1C	2.36	131.79	126.25
31	S	312	CLA	CHA-C4D-ND	2.36	137.41	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	610	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
31	R	314	CLA	CMD-C2D-C3D	-2.36	122.29	127.69
43	V	101	BCR	C11-C10-C9	-2.36	123.97	127.28
31	C	607	CLA	CHA-C4D-ND	2.36	137.41	132.55
30	0	601	CHL	CMA-C3A-C2A	2.35	123.22	114.13
32	s	317	LUT	C35-C15-C14	-2.35	118.70	123.52
31	1	603	CLA	C3B-C4B-NB	-2.35	108.43	110.53
31	6	311	CLA	O1D-CGD-CBD	-2.35	119.87	124.52
30	9	311	CHL	CMA-C3A-C4A	2.35	119.68	114.61
30	7	309	CHL	C1-O2A-CGA	2.35	122.35	116.65
36	0	618	NEX	C31-C30-C29	2.35	130.58	127.28
30	6	309	CHL	C4D-CHA-CBD	-2.35	106.59	108.97
31	7	304	CLA	O2A-CGA-CBA	2.35	119.01	111.83
31	r	305	CLA	CHD-C1D-ND	-2.35	121.49	124.80
31	B	606	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
30	Y	308	CHL	C4D-CHA-CBD	-2.35	106.59	108.97
30	q	310	CHL	C3D-C4D-ND	-2.35	109.16	112.94
31	6	304	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
31	9	304	CLA	CHA-C4D-ND	2.35	137.40	132.55
31	3	301	CLA	C2D-C1D-ND	2.35	112.45	110.13
31	r	312	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
30	5	601	CHL	C1-O2A-CGA	2.35	122.34	116.65
31	g	310	CLA	CHA-C4D-ND	2.35	137.40	132.55
31	c	611	CLA	C4B-CHC-C1C	2.35	131.78	126.25
31	r	304	CLA	CHD-C1D-ND	-2.35	121.49	124.80
36	6	319	NEX	C31-C30-C29	2.35	130.57	127.28
31	4	603	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
31	7	304	CLA	CHD-C1D-ND	-2.35	121.50	124.80
31	N	304	CLA	O2A-CGA-CBA	2.35	119.00	111.83
31	N	311	CLA	C2D-C1D-ND	2.35	112.45	110.13
31	2	604	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
31	Y	303	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
31	B	602	CLA	CHD-C1D-ND	-2.35	121.50	124.80
30	G	607	CHL	C1-O2A-CGA	2.35	122.34	116.65
31	s	314	CLA	C4B-CHC-C1C	2.35	131.77	126.25
31	G	609	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
31	9	306	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
31	a	407	CLA	CHD-C1D-ND	-2.35	121.50	124.80
31	b	603	CLA	CHD-C1D-ND	-2.35	121.50	124.80
32	y	616	LUT	C18-C5-C4	2.35	118.74	114.42
31	6	316	CLA	C1D-ND-C4D	-2.35	104.66	106.31
31	q	313	CLA	C4B-CHC-C1C	2.35	132.50	125.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	603	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
31	R	316	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
30	S	309	CHL	CMA-C3A-C4A	2.35	119.67	114.61
31	C	604	CLA	C4B-CHC-C1C	2.35	131.77	126.25
31	n	304	CLA	CHD-C1D-ND	-2.35	121.50	124.80
31	8	612	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
31	b	613	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
31	n	303	CLA	C2D-C1D-ND	2.35	112.45	110.13
31	7	312	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
31	0	602	CLA	CHD-C1D-ND	-2.35	121.50	124.80
31	s	310	CLA	CHD-C1D-ND	-2.35	121.50	124.80
30	G	605	CHL	CMA-C3A-C4A	2.35	119.67	114.61
31	A	406	CLA	CHA-C4D-ND	2.35	137.39	132.55
32	y	617	LUT	C40-C33-C32	2.35	121.67	118.09
31	4	602	CLA	CHD-C1D-ND	-2.35	121.50	124.80
31	C	608	CLA	CHD-C1D-ND	-2.35	121.50	124.80
31	a	409	CLA	C1D-ND-C4D	-2.35	104.67	106.31
31	B	609	CLA	CHA-C4D-ND	2.35	137.39	132.55
31	S	316	CLA	C3B-C4B-NB	-2.35	108.44	110.53
31	B	609	CLA	C6-C5-C3	-2.35	107.75	113.47
30	N	307	CHL	C4D-CHA-CBD	-2.35	106.60	108.97
31	S	304	CLA	CHD-C1D-ND	-2.35	121.50	124.80
31	Y	304	CLA	O2D-CGD-O1D	-2.34	119.28	123.85
31	3	311	CLA	CHD-C1D-ND	-2.34	121.50	124.80
34	4	620	LMG	C8-O7-C10	-2.34	112.19	117.80
31	q	316	CLA	C4B-CHC-C1C	2.34	131.76	126.25
31	1	603	CLA	CMA-C3A-C4A	2.34	118.07	111.77
31	n	314	CLA	O2D-CGD-O1D	-2.34	119.28	123.85
31	y	603	CLA	O2D-CGD-O1D	-2.34	119.28	123.85
31	p	602	CLA	CHA-C4D-ND	2.34	137.38	132.55
31	8	603	CLA	CHD-C1D-ND	-2.34	121.50	124.80
31	8	614	CLA	CHD-C1D-ND	-2.34	121.50	124.80
31	S	310	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
30	Y	309	CHL	C4D-CHA-CBD	-2.34	106.60	108.97
30	g	306	CHL	C4D-CHA-CBD	-2.34	106.60	108.97
31	q	304	CLA	O2A-CGA-CBA	2.34	118.98	111.83
31	G	604	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
30	5	608	CHL	C1-O2A-CGA	2.34	122.32	116.65
31	R	313	CLA	O2A-CGA-CBA	2.34	118.98	111.83
31	b	615	CLA	O2A-CGA-CBA	2.34	118.98	111.83
34	9	301	LMG	O8-C9-C8	2.34	115.15	108.40
36	n	319	NEX	C20-C13-C14	-2.34	119.02	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	312	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
31	5	612	CLA	C2D-C1D-ND	2.34	112.44	110.13
31	b	610	CLA	CHA-C4D-ND	2.34	137.38	132.55
31	s	315	CLA	C4B-CHC-C1C	2.34	131.75	126.25
31	2	613	CLA	CHD-C1D-ND	-2.34	121.51	124.80
31	n	303	CLA	C6-C5-C3	-2.34	107.76	113.47
43	H	101	BCR	C33-C5-C4	2.34	118.59	113.60
35	q	317	RRX	C35-C13-C14	-2.34	119.02	122.82
31	n	304	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
31	y	615	CLA	C2D-C1D-ND	2.34	112.44	110.13
31	S	304	CLA	CMA-C3A-C4A	2.34	118.06	111.77
31	9	316	CLA	CHD-C1D-ND	-2.34	121.51	124.80
31	b	610	CLA	C4B-CHC-C1C	2.34	131.75	126.25
32	r	317	LUT	C39-C29-C28	2.34	121.66	118.09
31	y	603	CLA	CHD-C1D-ND	-2.34	121.51	124.80
30	3	303	CHL	CMA-C3A-C4A	2.34	119.65	114.61
31	9	305	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
31	g	313	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
30	g	308	CHL	C4D-CHA-CBD	-2.34	106.61	108.97
31	C	613	CLA	CMA-C3A-C4A	2.34	118.06	111.77
31	3	301	CLA	CHA-C4D-ND	2.34	137.37	132.55
31	C	612	CLA	CHA-C4D-ND	2.34	137.37	132.55
31	r	312	CLA	C1-O2A-CGA	2.34	122.31	116.65
43	z	101	BCR	C1-C6-C5	-2.34	119.44	122.64
31	c	608	CLA	C4B-CHC-C1C	2.34	131.74	126.25
31	c	608	CLA	C3B-C4B-NB	-2.34	108.44	110.53
31	g	305	CLA	CMA-C3A-C4A	2.34	118.05	111.77
31	r	304	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
31	5	611	CLA	O2A-CGA-CBA	2.34	118.96	111.83
31	a	406	CLA	C2C-C1C-NC	2.34	112.44	109.98
43	b	620	BCR	C1-C6-C5	-2.34	119.44	122.64
31	s	314	CLA	C1-O2A-CGA	2.34	122.31	116.65
34	b	624	LMG	C8-O7-C10	-2.34	112.20	117.80
31	y	611	CLA	C1D-ND-C4D	-2.34	104.67	106.31
31	G	609	CLA	CHA-C4D-ND	2.34	137.37	132.55
32	Y	316	LUT	C11-C12-C13	-2.34	119.96	126.36
31	g	312	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
31	N	312	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
31	y	614	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
36	r	301	NEX	C26-C27-C28	-2.34	121.06	125.99
36	n	319	NEX	C11-C10-C9	2.34	130.55	127.28
31	0	612	CLA	O2D-CGD-O1D	-2.33	119.30	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	315	CLA	CHD-C1D-ND	-2.33	121.52	124.80
31	y	612	CLA	O2A-CGA-CBA	2.33	118.95	111.83
31	B	615	CLA	CHA-C4D-ND	2.33	137.36	132.55
30	1	608	CHL	C4D-CHA-CBD	-2.33	106.61	108.97
32	9	318	LUT	C18-C5-C4	2.33	118.71	114.42
31	N	313	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
31	S	304	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
31	c	613	CLA	C2A-C1A-CHA	2.33	127.92	123.87
30	N	307	CHL	CMA-C3A-C2A	2.33	123.14	114.13
31	3	304	CLA	CHD-C1D-ND	-2.33	121.52	124.80
31	G	613	CLA	CHD-C1D-ND	-2.33	121.52	124.80
43	z	101	BCR	C2-C1-C6	2.33	113.83	110.44
36	G	616	NEX	C26-C27-C28	-2.33	121.06	125.99
31	d	405	CLA	C4B-CHC-C1C	2.33	131.73	126.25
34	D	409	LMG	O1-C7-C8	-2.33	105.15	110.82
31	3	301	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
31	S	311	CLA	CHA-C4D-ND	2.33	137.36	132.55
31	1	612	CLA	CHD-C1D-ND	-2.33	121.52	124.80
31	B	602	CLA	CHA-C1A-NA	-2.33	121.11	126.39
31	p	603	CLA	C3B-C4B-NB	-2.33	108.45	110.53
31	R	315	CLA	CMA-C3A-C4A	2.33	118.04	111.77
31	C	608	CLA	CHA-C4D-ND	2.33	137.36	132.55
31	a	407	CLA	CHA-C4D-ND	2.33	137.36	132.55
31	G	612	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
31	n	311	CLA	CHA-C4D-ND	2.33	137.36	132.55
31	c	608	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
31	d	405	CLA	C1D-ND-C4D	-2.33	104.68	106.31
31	R	303	CLA	O2A-CGA-CBA	2.33	118.94	111.83
31	6	315	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
31	8	614	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
31	2	609	CLA	C2D-C1D-ND	2.33	112.43	110.13
31	p	604	CLA	CMA-C3A-C4A	2.33	118.03	111.77
32	N	316	LUT	C30-C31-C32	-2.33	116.45	123.20
31	p	615	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
44	A	416	PL9	C40-C39-C41	2.33	119.27	115.23
30	3	309	CHL	C4D-CHA-CBD	-2.33	106.62	108.97
35	q	317	RRX	C32-C1-C6	2.33	113.89	110.24
31	S	305	CLA	O2A-CGA-CBA	2.33	118.93	111.83
44	A	416	PL9	O2-C1-C6	2.33	124.18	120.48
31	D	404	CLA	C1-O2A-CGA	2.33	122.28	116.65
31	D	403	CLA	C3B-C4B-NB	-2.33	108.45	110.53
31	0	603	CLA	CHA-C4D-ND	2.33	137.35	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	603	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
31	6	305	CLA	CHD-C1D-ND	-2.33	121.53	124.80
31	B	612	CLA	C2D-C1D-ND	2.33	112.43	110.13
31	y	615	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
31	3	311	CLA	CMD-C2D-C3D	-2.33	122.36	127.69
31	2	603	CLA	CHD-C1D-ND	-2.33	121.53	124.80
31	C	608	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
31	r	314	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
31	A	406	CLA	O2A-CGA-CBA	2.32	118.92	111.83
31	c	609	CLA	O2A-CGA-CBA	2.32	118.92	111.83
31	7	315	CLA	O2D-CGD-O1D	-2.32	119.32	123.85
31	y	602	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
31	y	614	CLA	O2A-CGA-CBA	2.32	118.92	111.83
31	q	305	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
34	W	202	LMG	O6-C1-O1	-2.32	104.55	110.04
31	n	316	CLA	CHD-C1D-ND	-2.32	121.53	124.80
43	b	618	BCR	C2-C1-C6	2.32	113.81	110.44
31	B	608	CLA	O2A-CGA-CBA	2.32	118.92	111.83
31	p	615	CLA	CHA-C4D-ND	2.32	137.34	132.55
31	g	303	CLA	C2C-C1C-NC	2.32	112.42	109.98
31	8	612	CLA	C6-C5-C3	-2.32	107.81	113.47
31	n	314	CLA	C6-C5-C3	-2.32	107.81	113.47
31	9	316	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
32	p	616	LUT	C18-C5-C4	2.32	118.69	114.42
31	2	609	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
31	0	604	CLA	C4B-CHC-C1C	2.32	131.71	126.25
31	r	316	CLA	C4B-CHC-C1C	2.32	131.71	126.25
31	7	303	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
30	5	606	CHL	CMA-C3A-C2A	2.32	123.09	114.13
43	b	620	BCR	C15-C16-C17	-2.32	118.77	123.52
30	6	306	CHL	C4D-CHA-CBD	-2.32	106.63	108.97
30	G	606	CHL	CMA-C3A-C4A	2.32	119.61	114.61
31	G	604	CLA	CHD-C1D-ND	-2.32	121.54	124.80
35	2	614	RRX	C1-C6-C7	2.32	121.94	115.65
31	y	603	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
31	9	314	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
35	g	315	RRX	C34-C9-C10	-2.32	119.06	122.82
31	3	304	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
31	5	602	CLA	C2D-C1D-ND	2.32	112.42	110.13
31	s	311	CLA	CHA-C4D-ND	2.32	137.33	132.55
31	p	604	CLA	C1D-ND-C4D	-2.32	104.69	106.31
31	2	602	CLA	CMD-C2D-C3D	-2.32	122.38	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	601	CHL	C1-O2A-CGA	2.32	122.26	116.65
31	N	312	CLA	CHD-C1D-ND	-2.32	121.54	124.80
31	d	404	CLA	CHD-C1D-ND	-2.32	121.54	124.80
31	y	615	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
31	R	316	CLA	C3B-C4B-NB	-2.32	108.46	110.53
31	p	612	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
43	B	618	BCR	C33-C5-C4	2.32	118.53	113.60
31	b	604	CLA	C4B-CHC-C1C	2.32	131.69	126.25
31	1	604	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
31	r	307	CLA	CHA-C1A-NA	-2.32	121.15	126.39
31	B	613	CLA	O2A-CGA-CBA	2.32	118.90	111.83
31	5	613	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
31	N	304	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
30	9	310	CHL	C4D-CHA-CBD	-2.32	106.63	108.97
31	B	604	CLA	CHA-C1A-NA	-2.32	121.15	126.39
31	b	607	CLA	C3B-C4B-NB	-2.32	108.46	110.53
31	c	611	CLA	C3B-C4B-NB	-2.32	108.46	110.53
31	Y	312	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
31	N	304	CLA	CHD-C1D-ND	-2.32	121.54	124.80
31	b	607	CLA	CAA-C2A-C3A	-2.32	106.74	113.00
31	Y	310	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
31	1	612	CLA	O2D-CGD-O1D	-2.31	119.34	123.85
31	3	311	CLA	CHA-C4D-ND	2.31	137.32	132.55
31	3	305	CLA	CMD-C2D-C3D	-2.31	122.38	127.69
31	R	313	CLA	CAA-C2A-C3A	-2.31	106.75	113.00
31	p	604	CLA	C4B-CHC-C1C	2.31	131.69	126.25
31	r	303	CLA	O2A-CGA-CBA	2.31	118.89	111.83
31	B	606	CLA	CHD-C1D-ND	-2.31	121.55	124.80
31	S	303	CLA	CMD-C2D-C3D	-2.31	122.38	127.69
31	0	603	CLA	CMD-C2D-C3D	-2.31	122.38	127.69
30	5	607	CHL	C1-O2A-CGA	2.31	122.25	116.65
32	s	318	LUT	C35-C15-C14	-2.31	118.79	123.52
30	4	606	CHL	CMA-C3A-C2A	2.31	123.06	114.13
31	0	611	CLA	CHD-C1D-ND	-2.31	121.55	124.80
31	y	614	CLA	CHD-C1D-ND	-2.31	121.55	124.80
31	r	306	CLA	C4B-CHC-C1C	2.31	131.69	126.25
36	N	318	NEX	C11-C10-C9	2.31	130.52	127.28
30	2	606	CHL	C1-O2A-CGA	2.31	122.25	116.65
31	2	609	CLA	CHD-C1D-ND	-2.31	121.55	124.80
31	y	602	CLA	CHD-C1D-ND	-2.31	121.55	124.80
31	S	310	CLA	C4B-CHC-C1C	2.31	131.68	126.25
31	s	310	CLA	C4B-CHC-C1C	2.31	131.68	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1	616	LUT	C1-C6-C5	-2.31	119.48	122.64
31	0	613	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
43	v	101	BCR	C38-C26-C27	2.31	118.52	113.60
31	n	316	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
31	7	313	CLA	CHD-C1D-ND	-2.31	121.55	124.80
30	s	307	CHL	CMA-C3A-C4A	2.31	119.59	114.61
43	B	619	BCR	C30-C25-C26	-2.31	119.48	122.64
31	s	303	CLA	C6-C5-C3	-2.31	107.84	113.47
30	8	601	CHL	C4D-CHA-CBD	-2.31	106.64	108.97
31	0	610	CLA	C2D-C1D-ND	2.31	112.41	110.13
31	1	614	CLA	CHD-C1D-ND	-2.31	121.55	124.80
31	g	310	CLA	CHD-C1D-ND	-2.31	121.55	124.80
36	N	318	NEX	O24-C25-C38	-2.31	112.47	115.05
31	S	316	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
31	N	315	CLA	O2A-CGA-CBA	2.31	118.88	111.83
31	r	305	CLA	O2A-CGA-CBA	2.31	118.88	111.83
31	0	614	CLA	CHD-C1D-ND	-2.31	121.55	124.80
31	8	609	CLA	C2D-C1D-ND	2.31	112.41	110.13
31	n	311	CLA	C2D-C1D-ND	2.31	112.41	110.13
31	3	301	CLA	C6-C5-C3	-2.31	107.84	113.47
31	7	314	CLA	C4B-CHC-C1C	2.31	131.68	126.25
30	N	302	CHL	CMA-C3A-C4A	2.31	119.58	114.61
31	7	305	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
31	4	610	CLA	CHA-C1A-NA	-2.31	121.16	126.39
35	9	317	RRX	C1-C6-C7	2.31	121.91	115.65
31	b	616	CLA	C1-O2A-CGA	2.31	122.24	116.65
34	A	414	LMG	C8-O7-C10	-2.31	112.27	117.80
30	4	609	CHL	CMA-C3A-C2A	2.31	123.04	114.13
31	p	613	CLA	C2D-C1D-ND	2.31	112.41	110.13
31	b	612	CLA	C2D-C1D-ND	2.31	112.41	110.13
35	4	615	RRX	C1-C6-C7	2.31	121.91	115.65
31	A	407	CLA	CHA-C4D-ND	2.31	137.31	132.55
36	3	319	NEX	C19-C9-C10	-2.31	119.08	122.82
32	N	316	LUT	C11-C12-C13	-2.31	120.04	126.36
31	Y	304	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
31	d	405	CLA	CHA-C4D-ND	2.31	137.31	132.55
33	e	101	LHG	O8-C23-O10	-2.31	117.86	123.63
31	5	604	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
31	6	316	CLA	O2A-CGA-CBA	2.30	118.86	111.83
31	3	306	CLA	O2D-CGD-O1D	-2.30	119.36	123.85
31	c	601	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
30	y	606	CHL	C1-C2-C3	-2.30	122.42	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	q	315	CLA	O2A-CGA-CBA	2.30	118.86	111.83
30	3	309	CHL	C4C-CHD-C1D	2.30	124.31	116.07
31	B	607	CLA	CAA-C2A-C1A	-2.30	104.43	111.97
32	q	318	LUT	C27-C28-C29	-2.30	121.37	126.32
31	9	312	CLA	CMA-C3A-C4A	2.30	117.96	111.77
31	B	615	CLA	C6-C5-C3	-2.30	107.86	113.47
31	b	616	CLA	CHA-C4D-ND	2.30	137.30	132.55
31	N	303	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
31	Y	305	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
31	9	306	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
31	c	603	CLA	C4B-CHC-C1C	2.30	131.66	126.25
31	n	303	CLA	CHD-C1D-ND	-2.30	121.56	124.80
31	g	304	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
30	2	607	CHL	C4D-CHA-CBD	-2.30	106.65	108.97
31	r	312	CLA	C1D-ND-C4D	-2.30	104.70	106.31
30	0	601	CHL	C4D-CHA-CBD	-2.30	106.65	108.97
31	S	311	CLA	CMA-C3A-C4A	2.30	117.96	111.77
31	n	316	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
31	N	321	CLA	CHD-C1D-ND	-2.30	121.57	124.80
31	5	603	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
31	6	311	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
31	7	316	CLA	O2A-CGA-CBA	2.30	118.85	111.83
31	R	315	CLA	CAA-C2A-C3A	-2.30	106.79	113.00
31	b	603	CLA	CHA-C1A-NA	-2.30	121.19	126.39
43	c	614	BCR	C19-C18-C17	2.30	122.62	119.01
31	8	609	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
38	B	620	SQD	O3-C3-C2	-2.30	104.96	110.38
31	N	321	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
31	1	603	CLA	CHA-C4D-ND	2.30	137.29	132.55
31	q	304	CLA	CHD-C1D-ND	-2.30	121.57	124.80
32	s	317	LUT	C1-C6-C5	-2.30	119.50	122.64
30	n	302	CHL	CMA-C3A-C4A	2.30	119.56	114.61
30	g	306	CHL	CMA-C3A-C2A	2.30	123.00	114.13
31	B	608	CLA	CHA-C4D-ND	2.30	137.29	132.55
31	r	311	CLA	CHA-C4D-ND	2.30	137.29	132.55
36	q	319	NEX	C38-C25-C26	-2.30	118.52	122.30
31	9	312	CLA	CHA-C1A-NA	-2.30	121.19	126.39
31	c	610	CLA	C4B-CHC-C1C	2.30	131.65	126.25
31	7	316	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
31	b	615	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
31	Y	311	CLA	CMA-C3A-C4A	2.30	117.95	111.77
30	N	308	CHL	CMA-C3A-C2A	2.30	123.00	114.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	s	318	LUT	C21-C26-C27	-2.30	110.18	112.83
31	C	613	CLA	C4B-CHC-C1C	2.30	131.65	126.25
31	8	611	CLA	CHD-C1D-ND	-2.30	121.57	124.80
31	q	315	CLA	CHA-C1A-NA	-2.30	121.19	126.39
31	4	602	CLA	C2D-C1D-ND	2.30	112.40	110.13
32	8	616	LUT	C15-C35-C34	-2.30	118.82	123.52
31	r	315	CLA	C3B-C4B-NB	-2.30	108.48	110.53
31	6	314	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
31	9	312	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
31	q	312	CLA	CHD-C1D-ND	-2.30	121.57	124.80
36	r	301	NEX	C16-C1-C6	-2.30	108.42	110.47
31	g	314	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
31	6	313	CLA	C2D-C1D-ND	2.30	112.40	110.13
31	n	313	CLA	CHD-C1D-ND	-2.30	121.57	124.80
31	2	604	CLA	O2A-CGA-CBA	2.29	118.83	111.83
30	p	601	CHL	C1-O2A-CGA	2.29	122.20	116.65
31	4	602	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
31	8	614	CLA	O2D-CGD-O1D	-2.29	119.38	123.85
36	r	319	NEX	O24-C25-C38	-2.29	112.48	115.05
31	d	404	CLA	C3B-C4B-NB	-2.29	108.48	110.53
31	b	606	CLA	CHD-C1D-ND	-2.29	121.57	124.80
30	g	307	CHL	CMA-C3A-C2A	2.29	122.99	114.13
31	Y	303	CLA	C6-C5-C3	-2.29	107.88	113.47
30	p	607	CHL	C4D-CHA-CBD	-2.29	106.65	108.97
43	z	101	BCR	C23-C24-C25	-2.29	120.87	127.00
31	c	611	CLA	CHD-C1D-ND	-2.29	121.58	124.80
31	D	404	CLA	C4B-CHC-C1C	2.29	131.64	126.25
38	Y	320	SQD	O3-C3-C2	-2.29	104.97	110.38
32	y	616	LUT	C20-C13-C12	2.29	121.59	118.09
31	B	608	CLA	C4B-CHC-C1C	2.29	131.64	126.25
31	4	614	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
31	r	304	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
34	b	624	LMG	O7-C10-O9	-2.29	118.35	123.70
31	6	315	CLA	O2A-CGA-CBA	2.29	118.82	111.83
30	0	601	CHL	CMA-C3A-C4A	2.29	119.55	114.61
32	y	616	LUT	C11-C10-C9	-2.29	124.06	127.28
31	G	602	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
31	0	610	CLA	CHD-C1D-ND	-2.29	121.58	124.80
31	0	602	CLA	C3B-C4B-NB	-2.29	108.48	110.53
31	b	614	CLA	CHD-C1D-ND	-2.29	121.58	124.80
31	6	304	CLA	C2D-C1D-ND	2.29	112.39	110.13
36	8	617	NEX	C26-C27-C28	-2.29	121.15	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	q	309	CHL	C4D-CHA-CBD	-2.29	106.66	108.97
31	G	611	CLA	C4B-CHC-C1C	2.29	131.63	126.25
31	b	616	CLA	C6-C5-C3	-2.29	107.89	113.47
31	Y	304	CLA	CHD-C1D-ND	-2.29	121.58	124.80
31	6	314	CLA	C6-C5-C3	-2.29	107.89	113.47
31	B	606	CLA	CAA-C2A-C3A	-2.29	106.81	113.00
31	b	606	CLA	C4B-CHC-C1C	2.29	131.63	126.25
31	0	615	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
35	G	614	RRX	C1-C6-C7	2.29	121.86	115.65
31	B	613	CLA	C1D-ND-C4D	-2.29	104.71	106.31
31	B	606	CLA	C6-C5-C3	-2.29	107.89	113.47
31	r	311	CLA	C3B-C4B-NB	-2.29	108.49	110.53
31	s	306	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
31	N	311	CLA	O2A-CGA-CBA	2.29	118.81	111.83
30	7	309	CHL	C4D-CHA-CBD	-2.29	106.66	108.97
31	R	306	CLA	CHA-C1A-NA	-2.29	121.21	126.39
31	B	603	CLA	C1-C2-C3	-2.29	122.45	126.20
31	y	612	CLA	O1D-CGD-CBD	-2.29	120.01	124.52
31	0	615	CLA	C2D-C1D-ND	2.29	112.39	110.13
31	2	612	CLA	O2A-CGA-CBA	2.29	118.81	111.83
31	1	614	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
30	7	308	CHL	C1-O2A-CGA	2.29	122.19	116.65
30	r	308	CHL	CMA-C3A-C2A	2.29	122.96	114.13
31	b	608	CLA	CMD-C2D-C3D	-2.29	122.45	127.69
38	s	301	SQD	O3-C3-C2	-2.29	104.99	110.38
31	B	611	CLA	C2D-C1D-ND	2.29	112.39	110.13
30	8	601	CHL	CMA-C3A-C4A	2.29	119.53	114.61
34	b	622	LMG	O7-C10-O9	-2.28	118.36	123.70
31	Y	303	CLA	CHD-C1D-ND	-2.28	121.59	124.80
31	s	316	CLA	CHD-C1D-ND	-2.28	121.59	124.80
31	r	311	CLA	C1-O2A-CGA	2.28	122.18	116.65
31	R	312	CLA	C1D-ND-C4D	-2.28	104.71	106.31
31	2	610	CLA	C2D-C1D-ND	2.28	112.39	110.13
31	p	611	CLA	C2D-C1D-ND	2.28	112.39	110.13
31	Y	303	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
31	c	603	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
31	5	614	CLA	O2A-CGA-CBA	2.28	118.80	111.83
32	5	616	LUT	C27-C28-C29	-2.28	121.41	126.32
31	B	607	CLA	CBC-CAC-C3C	-2.28	106.23	112.42
31	G	604	CLA	O2A-CGA-CBA	2.28	118.80	111.83
31	B	608	CLA	C3B-C4B-NB	-2.28	108.49	110.53
43	b	618	BCR	C38-C26-C27	2.28	118.46	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	y	608	CHL	C4D-CHA-CBD	-2.28	106.67	108.97
46	D	402	BCT	O3-C-O1	-2.28	113.84	119.68
31	g	305	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
31	y	613	CLA	C16-C15-C13	-2.28	108.38	115.97
43	Z	101	BCR	C23-C24-C25	-2.28	120.90	127.00
30	7	310	CHL	CMA-C3A-C2A	2.28	122.94	114.13
31	7	314	CLA	O2A-CGA-CBA	2.28	118.79	111.83
31	B	613	CLA	CHD-C1D-ND	-2.28	121.59	124.80
31	9	305	CLA	CHD-C1D-ND	-2.28	121.59	124.80
32	g	316	LUT	C39-C29-C30	-2.28	119.12	122.82
31	6	315	CLA	CHA-C4D-ND	2.28	137.25	132.55
32	n	317	LUT	C10-C11-C12	-2.28	116.59	123.20
31	6	316	CLA	C3B-C4B-NB	-2.28	108.49	110.53
30	N	306	CHL	CMA-C3A-C4A	2.28	119.53	114.61
31	R	314	CLA	CMA-C3A-C4A	2.28	117.90	111.77
32	0	616	LUT	C19-C9-C8	2.28	121.57	118.09
32	y	617	LUT	C39-C29-C28	2.28	121.57	118.09
38	B	623	SQD	O3-C3-C2	-2.28	105.00	110.38
31	r	305	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
31	r	312	CLA	C6-C5-C3	-2.28	107.92	113.47
30	9	309	CHL	C1-C2-C3	-2.28	122.46	126.20
31	C	607	CLA	C4B-CHC-C1C	2.28	131.60	126.25
31	n	313	CLA	C2D-C1D-ND	2.28	112.38	110.13
30	n	302	CHL	C4D-CHA-CBD	-2.28	106.67	108.97
30	5	609	CHL	C1-C2-C3	-2.28	122.47	126.20
31	6	316	CLA	CHA-C1A-NA	-2.28	121.23	126.39
30	N	302	CHL	CMA-C3A-C2A	2.28	122.93	114.13
31	6	315	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
31	N	303	CLA	O2D-CGD-O1D	-2.28	119.42	123.85
31	3	313	CLA	C2D-C1D-ND	2.28	112.38	110.13
31	b	610	CLA	CHA-C1A-NA	-2.28	121.23	126.39
31	y	611	CLA	C2C-C1C-NC	2.28	112.37	109.98
30	p	606	CHL	C1-O2A-CGA	2.28	122.16	116.65
31	8	602	CLA	CHD-C1D-ND	-2.28	121.60	124.80
31	4	604	CLA	O2A-CGA-CBA	2.28	118.78	111.83
38	b	621	SQD	O3-C3-C2	-2.28	105.01	110.38
31	S	303	CLA	C2D-C1D-ND	2.28	112.38	110.13
31	S	314	CLA	O2D-CGD-O1D	-2.28	119.42	123.85
31	9	315	CLA	O2D-CGD-O1D	-2.28	119.42	123.85
31	7	313	CLA	C6-C5-C3	-2.28	107.93	113.47
31	b	608	CLA	CHD-C1D-ND	-2.27	121.60	124.80
31	b	609	CLA	O2A-CGA-CBA	2.27	118.77	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	v	101	BCR	C16-C15-C14	-2.27	118.87	123.52
31	r	315	CLA	CMD-C2D-C3D	-2.27	122.47	127.69
31	B	605	CLA	C3B-C4B-NB	-2.27	108.50	110.53
31	R	311	CLA	C3B-C4B-NB	-2.27	108.50	110.53
31	c	606	CLA	O2A-CGA-CBA	2.27	118.77	111.83
31	5	614	CLA	CMD-C2D-C3D	-2.27	122.47	127.69
31	Y	314	CLA	CHD-C1D-ND	-2.27	121.60	124.80
31	R	311	CLA	C1-O2A-CGA	2.27	122.15	116.65
34	6	321	LMG	O7-C10-O9	-2.27	118.39	123.70
31	b	606	CLA	C1D-ND-C4D	-2.27	104.72	106.31
30	4	609	CHL	CMA-C3A-C4A	2.27	119.51	114.61
43	c	615	BCR	C11-C12-C13	-2.27	120.13	126.36
31	N	313	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
34	W	201	LMG	O8-C28-O10	-2.27	117.94	123.63
31	b	609	CLA	CHA-C4D-ND	2.27	137.24	132.55
43	V	101	BCR	C21-C20-C19	-2.27	116.62	123.20
31	3	315	CLA	C2D-C1D-ND	2.27	112.37	110.13
31	1	612	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
31	1	610	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
31	p	615	CLA	CHA-C1A-NA	-2.27	121.25	126.39
31	r	307	CLA	CHD-C1D-ND	-2.27	121.61	124.80
32	n	318	LUT	C15-C35-C34	-2.27	118.87	123.52
43	V	101	BCR	C16-C15-C14	-2.27	118.87	123.52
32	g	316	LUT	C27-C28-C29	-2.27	121.44	126.32
31	q	306	CLA	O2A-CGA-CBA	2.27	118.76	111.83
30	6	309	CHL	CMA-C3A-C2A	2.27	122.90	114.13
31	4	611	CLA	C2D-C1D-ND	2.27	112.37	110.13
31	0	615	CLA	CHA-C1A-NA	-2.27	121.25	126.39
31	C	605	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
31	n	304	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
32	1	616	LUT	C18-C5-C4	2.27	118.59	114.42
31	8	611	CLA	C2D-C1D-ND	2.27	112.37	110.13
31	g	305	CLA	CHD-C1D-ND	-2.27	121.61	124.80
31	r	304	CLA	O2A-CGA-CBA	2.27	118.75	111.83
32	3	317	LUT	C27-C28-C29	-2.27	121.44	126.32
43	z	101	BCR	C15-C16-C17	-2.27	118.88	123.52
31	9	315	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
38	R	322	SQD	O3-C3-C2	-2.27	105.03	110.38
38	S	301	SQD	O3-C3-C2	-2.27	105.03	110.38
31	r	314	CLA	CHA-C4D-ND	2.27	137.23	132.55
31	q	306	CLA	O1D-CGD-CBD	-2.27	120.05	124.52
31	s	312	CLA	O2A-CGA-CBA	2.27	118.75	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	w	203	LMG	C8-O7-C10	-2.27	112.37	117.80
31	R	316	CLA	C1D-ND-C4D	-2.27	104.72	106.31
31	1	614	CLA	C2D-C1D-ND	2.27	112.37	110.13
31	S	304	CLA	C2D-C1D-ND	2.27	112.37	110.13
32	8	615	LUT	C10-C11-C12	-2.27	116.63	123.20
31	c	607	CLA	CHA-C1A-NA	-2.27	121.26	126.39
30	7	309	CHL	CMA-C3A-C2A	2.27	122.88	114.13
31	a	406	CLA	C1D-ND-C4D	-2.27	104.72	106.31
31	6	304	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
31	n	313	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
31	C	604	CLA	CMA-C3A-C4A	2.27	117.86	111.77
32	G	615	LUT	C27-C28-C29	-2.27	121.45	126.32
38	6	301	SQD	O3-C3-C2	-2.27	105.04	110.38
38	m	101	SQD	O3-C3-C2	-2.27	105.04	110.38
32	4	616	LUT	C8-C7-C6	-2.27	120.95	127.00
31	p	613	CLA	CMA-C3A-C4A	2.27	117.86	111.77
31	q	304	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
31	q	316	CLA	CHD-C1D-ND	-2.26	121.61	124.80
31	C	609	CLA	C4B-CHC-C1C	2.26	131.57	126.25
31	p	603	CLA	C4B-CHC-C1C	2.26	131.57	126.25
31	6	303	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
31	4	604	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
31	g	314	CLA	C2D-C1D-ND	2.26	112.37	110.13
31	s	306	CLA	CHD-C1D-ND	-2.26	121.62	124.80
30	G	605	CHL	CMA-C3A-C2A	2.26	122.87	114.13
33	A	417	LHG	O8-C23-O10	-2.26	117.97	123.63
30	1	608	CHL	CMA-C3A-C2A	2.26	122.87	114.13
31	4	604	CLA	CHD-C1D-ND	-2.26	121.62	124.80
31	A	409	CLA	CHD-C1D-ND	-2.26	121.62	124.80
31	G	612	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
31	0	613	CLA	O2A-CGA-CBA	2.26	118.73	111.83
32	r	317	LUT	C8-C9-C10	-2.26	115.45	119.01
31	p	614	CLA	C2D-C1D-ND	2.26	112.36	110.13
31	a	406	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
31	s	303	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
31	B	614	CLA	O2A-CGA-CBA	2.26	118.73	111.83
31	g	313	CLA	O2A-CGA-CBA	2.26	118.73	111.83
33	4	618	LHG	C6-C5-C4	-2.26	106.51	111.78
31	4	614	CLA	C1D-ND-C4D	-2.26	104.72	106.31
34	W	201	LMG	C8-O7-C10	-2.26	112.38	117.80
31	Y	314	CLA	C2D-C1D-ND	2.26	112.36	110.13
32	7	317	LUT	C39-C29-C28	2.26	121.54	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	612	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
31	N	315	CLA	CHD-C1D-ND	-2.26	121.62	124.80
31	S	312	CLA	CHD-C1D-ND	-2.26	121.62	124.80
31	S	306	CLA	O2A-CGA-CBA	2.26	118.73	111.83
31	B	614	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
31	a	407	CLA	C6-C5-C3	-2.26	107.96	113.47
31	A	407	CLA	O2A-CGA-CBA	2.26	118.73	111.83
34	2	620	LMG	O8-C28-O10	-2.26	117.97	123.63
31	C	609	CLA	CHA-C4D-ND	2.26	137.21	132.55
31	3	312	CLA	C1-O2A-CGA	2.26	122.12	116.65
31	r	315	CLA	C1D-ND-C4D	-2.26	104.73	106.31
43	z	101	BCR	C8-C7-C6	-2.26	120.96	127.00
43	a	410	BCR	C33-C5-C4	2.26	118.41	113.60
31	C	611	CLA	CHD-C1D-ND	-2.26	121.62	124.80
31	b	615	CLA	CHD-C1D-ND	-2.26	121.62	124.80
38	X	201	SQD	O3-C3-C2	-2.26	105.05	110.38
31	G	604	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
30	9	309	CHL	C4D-CHA-CBD	-2.26	106.69	108.97
31	8	602	CLA	C2D-C1D-ND	2.26	112.36	110.13
43	a	410	BCR	C10-C11-C12	-2.26	116.66	123.20
31	6	313	CLA	O2A-CGA-CBA	2.26	118.72	111.83
30	S	307	CHL	CMA-C3A-C2A	2.26	122.85	114.13
34	k	102	LMG	C8-O7-C10	-2.26	112.39	117.80
31	C	613	CLA	CHA-C1A-NA	-2.26	121.28	126.39
31	A	405	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
30	R	308	CHL	CMA-C3A-C4A	2.26	119.48	114.61
31	s	310	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
34	C	621	LMG	O7-C10-O9	-2.26	118.43	123.70
31	7	303	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
31	b	615	CLA	C2D-C1D-ND	2.26	112.36	110.13
31	7	316	CLA	CHD-C1D-ND	-2.26	121.63	124.80
31	8	609	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
31	y	612	CLA	CHD-C1D-ND	-2.26	121.63	124.80
30	G	623	CHL	CMA-C3A-C2A	2.26	122.84	114.13
32	9	318	LUT	C8-C7-C6	-2.26	120.97	127.00
33	l	101	LHG	C5-O7-C7	-2.26	112.40	117.80
31	b	609	CLA	C4B-CHC-C1C	2.26	131.55	126.25
31	s	304	CLA	O2D-CGD-O1D	-2.26	119.46	123.85
31	g	303	CLA	CMD-C2D-C3D	-2.26	122.52	127.69
31	s	304	CLA	C2D-C1D-ND	2.26	112.36	110.13
31	s	310	CLA	C3B-C4B-NB	-2.25	108.52	110.53
31	3	305	CLA	O2D-CGD-O1D	-2.25	119.46	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	q	301	LMG	O7-C10-O9	-2.25	118.43	123.70
31	g	312	CLA	CHD-C1D-ND	-2.25	121.63	124.80
34	b	622	LMG	O6-C1-O1	-2.25	104.72	110.04
36	q	319	NEX	C26-C27-C28	-2.25	121.23	125.99
31	s	304	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
31	4	603	CLA	OBD-CAD-C3D	-2.25	123.15	128.42
31	g	312	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
31	R	315	CLA	CHD-C1D-ND	-2.25	121.63	124.80
31	c	612	CLA	CHD-C1D-ND	-2.25	121.63	124.80
31	3	314	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
31	b	617	CLA	C1-O2A-CGA	2.25	122.11	116.65
31	5	602	CLA	O2A-CGA-CBA	2.25	118.70	111.83
31	Y	305	CLA	CHD-C1D-ND	-2.25	121.63	124.80
31	3	313	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
31	R	305	CLA	CHA-C4D-ND	2.25	137.20	132.55
31	7	305	CLA	CHD-C1D-ND	-2.25	121.63	124.80
31	2	603	CLA	C2D-C1D-ND	2.25	112.36	110.13
31	d	405	CLA	C2D-C1D-ND	2.25	112.36	110.13
30	Y	308	CHL	CMA-C3A-C2A	2.25	122.83	114.13
30	6	309	CHL	C1-O2A-CGA	2.25	122.10	116.65
31	s	303	CLA	C6-C7-C8	-2.25	108.48	115.97
31	c	613	CLA	C1-C2-C3	-2.25	122.51	126.20
31	0	612	CLA	CHD-C1D-ND	-2.25	121.63	124.80
31	S	305	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
31	4	613	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
31	0	613	CLA	CHD-C1D-ND	-2.25	121.64	124.80
32	7	318	LUT	C8-C7-C6	-2.25	120.99	127.00
31	a	407	CLA	O2A-CGA-CBA	2.25	118.70	111.83
31	6	316	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
31	0	614	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
43	d	406	BCR	C33-C5-C4	2.25	118.39	113.60
31	s	313	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
31	9	312	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
31	C	608	CLA	CMA-C3A-C4A	2.25	117.82	111.77
36	s	319	NEX	C26-C27-C28	-2.25	121.24	125.99
31	b	608	CLA	C4B-CHC-C1C	2.25	131.53	126.25
45	c	617	DGD	C3G-O3G-C1D	-2.25	108.97	113.80
31	9	312	CLA	C1-O2A-CGA	2.25	122.09	116.65
31	c	603	CLA	C3B-C4B-NB	-2.25	108.52	110.53
31	8	602	CLA	C6-C5-C3	-2.25	107.99	113.47
31	8	611	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
31	y	614	CLA	CMD-C2D-C3D	-2.25	122.53	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	3	307	CHL	CMA-C3A-C4A	2.25	119.45	114.61
32	Y	316	LUT	C35-C15-C14	-2.25	118.92	123.52
31	D	404	CLA	CHA-C4D-ND	2.25	137.19	132.55
30	6	307	CHL	CMA-C3A-C4A	2.25	119.45	114.61
31	B	610	CLA	C2D-C1D-ND	2.25	112.35	110.13
31	b	617	CLA	C1C-C2C-C3C	-2.25	104.62	106.98
31	c	604	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
31	b	611	CLA	CHD-C1D-ND	-2.25	121.64	124.80
31	c	612	CLA	O1D-CGD-CBD	-2.25	120.09	124.52
31	S	310	CLA	C3B-C4B-NB	-2.25	108.53	110.53
31	R	305	CLA	C1-O2A-CGA	2.25	122.09	116.65
31	0	604	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
31	8	602	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
43	D	405	BCR	C11-C10-C9	2.25	130.43	127.28
45	c	619	DGD	C3G-O3G-C1D	-2.25	108.98	113.80
34	9	321	LMG	C8-O7-C10	-2.25	112.42	117.80
38	A	413	SQD	O3-C3-C2	-2.24	105.08	110.38
31	N	312	CLA	CMD-C2D-C3D	-2.24	122.54	127.69
31	S	306	CLA	CMD-C2D-C3D	-2.24	122.54	127.69
31	C	608	CLA	C3B-C4B-NB	-2.24	108.53	110.53
31	C	612	CLA	C4B-CHC-C1C	2.24	131.52	126.25
31	7	304	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
31	4	613	CLA	CMD-C2D-C3D	-2.24	122.54	127.69
31	8	603	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
31	g	305	CLA	O2A-CGA-CBA	2.24	118.67	111.83
31	s	304	CLA	CHD-C1D-ND	-2.24	121.65	124.80
32	6	318	LUT	C30-C31-C32	-2.24	116.70	123.20
31	n	311	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
36	9	319	NEX	C39-C29-C30	-2.24	119.18	122.82
31	9	313	CLA	CHD-C1D-ND	-2.24	121.65	124.80
31	A	409	CLA	CHA-C4D-ND	2.24	137.18	132.55
31	4	604	CLA	C2D-C1D-ND	2.24	112.34	110.13
31	Y	310	CLA	C2D-C1D-ND	2.24	112.34	110.13
32	1	615	LUT	C19-C9-C8	2.24	121.51	118.09
31	0	614	CLA	O2A-CGA-CBA	2.24	118.67	111.83
31	R	316	CLA	C4B-CHC-C1C	2.24	131.52	126.25
31	G	613	CLA	C1D-ND-C4D	-2.24	104.74	106.31
30	G	601	CHL	C1-O2A-CGA	2.24	122.08	116.65
32	r	317	LUT	C22-C23-C24	2.24	114.51	111.18
31	C	601	CLA	CHD-C1D-ND	-2.24	121.65	124.80
31	G	612	CLA	CHD-C1D-ND	-2.24	121.65	124.80
31	7	303	CLA	CHD-C1D-ND	-2.24	121.65	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	306	CLA	CHD-C1D-ND	-2.24	121.65	124.80
31	p	610	CLA	C6-C5-C3	-2.24	108.01	113.47
43	a	410	BCR	C38-C26-C27	2.24	118.38	113.60
34	B	621	LMG	O7-C10-O9	-2.24	118.47	123.70
31	y	613	CLA	CHA-C1A-NA	-2.24	121.32	126.39
31	c	613	CLA	C4B-CHC-C1C	2.24	131.52	126.25
31	5	604	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
34	s	321	LMG	C8-O7-C10	-2.24	112.43	117.80
32	y	617	LUT	C27-C28-C29	-2.24	121.50	126.32
30	p	605	CHL	CMA-C3A-C4A	2.24	119.44	114.61
32	g	316	LUT	C8-C7-C6	-2.24	121.01	127.00
31	7	303	CLA	C2D-C1D-ND	2.24	112.34	110.13
31	6	313	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
31	a	409	CLA	CHA-C4D-ND	2.24	137.17	132.55
31	2	603	CLA	O2A-CGA-CBA	2.24	118.66	111.83
31	R	314	CLA	O2A-CGA-CBA	2.24	118.66	111.83
31	B	612	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
31	1	614	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
31	b	606	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
31	s	303	CLA	C2D-C1D-ND	2.24	112.34	110.13
31	c	608	CLA	CHD-C1D-ND	-2.24	121.65	124.80
31	R	306	CLA	C2A-C1A-CHA	2.24	127.75	123.87
31	y	611	CLA	CHD-C1D-ND	-2.24	121.65	124.80
36	3	319	NEX	O24-C25-C38	-2.24	112.55	115.05
31	S	303	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
36	4	617	NEX	C38-C25-C26	-2.24	118.62	122.30
31	n	315	CLA	CHA-C1A-NA	-2.24	121.32	126.39
30	y	606	CHL	CMA-C3A-C4A	2.24	119.43	114.61
31	5	602	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
30	5	608	CHL	CMA-C3A-C2A	2.24	122.77	114.13
31	8	613	CLA	CHA-C1A-NA	-2.24	121.33	126.39
30	n	309	CHL	CMA-C3A-C2A	2.24	122.77	114.13
31	2	611	CLA	C2D-C1D-ND	2.24	112.34	110.13
31	B	613	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
36	S	319	NEX	C2-C1-C6	2.24	111.39	109.21
31	c	604	CLA	CMA-C3A-C4A	2.24	117.78	111.77
31	p	611	CLA	O2A-CGA-CBA	2.24	118.66	111.83
31	S	305	CLA	CHD-C1D-ND	-2.24	121.66	124.80
31	0	603	CLA	CMA-C3A-C4A	2.24	117.78	111.77
31	0	610	CLA	O1D-CGD-CBD	-2.24	120.11	124.52
30	G	606	CHL	CMA-C3A-C2A	2.24	122.77	114.13
31	2	612	CLA	O2D-CGD-O1D	-2.24	119.50	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	305	CLA	O2D-CGD-O1D	-2.24	119.50	123.85
31	g	303	CLA	C3D-C2D-C1D	-2.24	102.78	105.83
32	5	617	LUT	C18-C5-C4	2.24	118.53	114.42
31	N	305	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
31	c	612	CLA	C4B-CHC-C1C	2.24	131.50	126.25
36	5	618	NEX	O24-C25-C38	-2.24	112.55	115.05
31	d	405	CLA	C1-O2A-CGA	2.24	122.06	116.65
47	e	102	HEM	CHA-C4D-C3D	-2.24	121.11	125.23
30	s	307	CHL	CMA-C3A-C2A	2.24	122.76	114.13
31	s	314	CLA	C3B-C4B-NB	-2.23	108.53	110.53
31	n	305	CLA	CMD-C2D-C3D	-2.23	122.56	127.69
31	B	609	CLA	CHA-C1A-NA	-2.23	121.33	126.39
31	6	314	CLA	CHD-C1D-ND	-2.23	121.66	124.80
31	B	605	CLA	CHD-C1D-ND	-2.23	121.66	124.80
31	d	404	CLA	CMD-C2D-C3D	-2.23	122.56	127.69
32	7	318	LUT	C27-C28-C29	-2.23	121.52	126.32
30	p	606	CHL	CMA-C3A-C2A	2.23	122.76	114.13
31	a	409	CLA	C3B-C4B-NB	-2.23	108.54	110.53
31	n	303	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
36	p	618	NEX	C2-C1-C6	2.23	111.38	109.21
31	7	315	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
31	c	608	CLA	CMA-C3A-C4A	2.23	117.77	111.77
31	c	612	CLA	CMA-C3A-C4A	2.23	117.77	111.77
31	9	312	CLA	CAA-C2A-C3A	-2.23	106.97	113.00
31	q	316	CLA	O2A-CGA-CBA	2.23	118.64	111.83
43	d	406	BCR	C23-C24-C25	-2.23	121.04	127.00
31	9	312	CLA	O2A-CGA-CBA	2.23	118.64	111.83
31	s	310	CLA	O2A-CGA-CBA	2.23	118.64	111.83
31	B	601	CLA	CMA-C3A-C4A	2.23	117.77	111.77
31	C	610	CLA	CHA-C1A-NA	-2.23	121.34	126.39
31	6	303	CLA	C2D-C1D-ND	2.23	112.33	110.13
31	N	321	CLA	C2D-C1D-ND	2.23	112.33	110.13
31	C	612	CLA	CHD-C1D-ND	-2.23	121.66	124.80
32	5	617	LUT	C22-C23-C24	2.23	114.50	111.18
31	a	409	CLA	CHD-C1D-ND	-2.23	121.66	124.80
31	y	602	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
30	y	608	CHL	CMA-C3A-C2A	2.23	122.74	114.13
30	N	306	CHL	CMA-C3A-C2A	2.23	122.74	114.13
43	z	101	BCR	C16-C15-C14	-2.23	118.96	123.52
30	7	306	CHL	CMA-C3A-C2A	2.23	122.74	114.13
31	8	602	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
36	g	317	NEX	C26-C27-C28	-2.23	121.28	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	604	CLA	C2D-C1D-ND	2.23	112.33	110.13
31	4	613	CLA	CHD-C1D-ND	-2.23	121.67	124.80
31	6	316	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
32	s	317	LUT	C15-C35-C34	-2.23	118.96	123.52
31	R	306	CLA	C4B-CHC-C1C	2.23	131.49	126.25
34	Q1	101	LMG	O1-C1-C2	2.23	111.66	108.27
31	4	610	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
31	5	604	CLA	C2D-C1D-ND	2.23	112.33	110.13
31	b	612	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
31	N	310	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
31	g	310	CLA	CAA-C2A-C3A	-2.23	106.98	113.00
31	8	604	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
38	A	411	SQD	O3-C3-C2	-2.23	105.13	110.38
32	N	317	LUT	C27-C28-C29	-2.23	121.53	126.32
30	G	601	CHL	CMA-C3A-C4A	2.23	119.41	114.61
31	y	604	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
31	8	614	CLA	O2A-CGA-CBA	2.23	118.62	111.83
31	S	304	CLA	C1D-ND-C4D	-2.23	104.75	106.31
31	2	604	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
31	c	607	CLA	OBD-CAD-C3D	-2.23	123.21	128.42
36	8	617	NEX	C16-C1-C6	-2.23	108.48	110.47
31	R	307	CLA	CHA-C1A-NA	-2.23	121.35	126.39
31	N	314	CLA	CHA-C1A-NA	-2.23	121.35	126.39
31	2	609	CLA	CHA-C1A-NA	-2.22	121.35	126.39
31	s	316	CLA	C1D-ND-C4D	-2.22	104.75	106.31
31	B	616	CLA	C4B-CHC-C1C	2.22	131.48	126.25
31	r	305	CLA	O1D-CGD-CBD	-2.22	120.13	124.52
30	Y	301	CHL	CMA-C3A-C2A	2.22	122.72	114.13
30	7	310	CHL	C1-O2A-CGA	2.22	122.03	116.65
31	y	615	CLA	CHD-C1D-ND	-2.22	121.67	124.80
31	7	315	CLA	CHA-C1A-NA	-2.22	121.36	126.39
31	0	602	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
31	3	304	CLA	C2D-C1D-ND	2.22	112.33	110.13
31	7	312	CLA	C2D-C1D-ND	2.22	112.33	110.13
31	8	610	CLA	C2D-C1D-ND	2.22	112.33	110.13
31	p	612	CLA	O1D-CGD-CBD	-2.22	120.13	124.52
31	R	311	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
31	6	314	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
32	3	318	LUT	C27-C28-C29	-2.22	121.55	126.32
31	7	316	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
36	R	301	NEX	O24-C25-C38	-2.22	112.57	115.05
43	b	620	BCR	C16-C15-C14	-2.22	118.97	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	a	412	SQD	O3-C3-C2	-2.22	105.14	110.38
31	s	314	CLA	CHD-C1D-ND	-2.22	121.68	124.80
30	y	606	CHL	CMA-C3A-C2A	2.22	122.70	114.13
38	g	301	SQD	O3-C3-C2	-2.22	105.14	110.38
31	9	313	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
31	9	312	CLA	C2D-C1D-ND	2.22	112.32	110.13
32	3	318	LUT	C30-C31-C32	-2.22	116.77	123.20
34	Q1	101	LMG	C8-O7-C10	-2.22	112.48	117.80
31	q	305	CLA	CHD-C1D-ND	-2.22	121.68	124.80
44	a	414	PL9	C12-C13-C14	-2.22	122.54	127.62
43	C	615	BCR	C38-C26-C27	2.22	118.33	113.60
43	b	618	BCR	C33-C5-C4	2.22	118.33	113.60
31	q	312	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
31	3	315	CLA	CHD-C1D-ND	-2.22	121.68	124.80
34	w	203	LMG	O7-C10-O9	-2.22	118.52	123.70
31	g	303	CLA	CHA-C4D-ND	2.22	137.13	132.55
31	N	315	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
30	q	310	CHL	C4D-ND-C1D	2.22	106.90	105.22
32	7	317	LUT	C35-C15-C14	-2.22	118.98	123.52
32	1	616	LUT	C39-C29-C28	2.22	121.47	118.09
31	N	304	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
31	g	313	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
31	p	602	CLA	C3B-C4B-NB	-2.22	108.55	110.53
30	9	308	CHL	CMA-C3A-C4A	2.22	119.39	114.61
31	q	306	CLA	C1D-ND-C4D	-2.21	104.76	106.31
31	5	610	CLA	C2D-C1D-ND	2.21	112.32	110.13
31	5	614	CLA	C2D-C1D-ND	2.21	112.32	110.13
31	8	612	CLA	C2D-C1D-ND	2.21	112.32	110.13
31	c	610	CLA	C3B-C4B-NB	-2.21	108.55	110.53
43	b	618	BCR	C36-C18-C19	2.21	121.47	118.09
38	G	617	SQD	O3-C3-C2	-2.21	105.16	110.38
31	S	313	CLA	CHD-C1D-ND	-2.21	121.69	124.80
31	6	314	CLA	C2D-C1D-ND	2.21	112.32	110.13
31	s	311	CLA	C1D-ND-C4D	-2.21	104.76	106.31
31	S	316	CLA	C4B-CHC-C1C	2.21	131.45	126.25
43	H	101	BCR	C11-C12-C13	-2.21	120.30	126.36
31	S	310	CLA	CMD-C2D-C3D	-2.21	122.61	127.69
31	r	306	CLA	CHA-C1A-NA	-2.21	121.38	126.39
31	2	613	CLA	O2A-CGA-CBA	2.21	118.58	111.83
31	b	611	CLA	C2D-C1D-ND	2.21	112.32	110.13
30	1	606	CHL	CMA-C3A-C2A	2.21	122.67	114.13
43	D	405	BCR	C1-C6-C5	-2.21	119.61	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	304	CLA	CHA-C1A-NA	-2.21	121.38	126.39
31	G	610	CLA	C2A-C1A-CHA	2.21	127.70	123.87
36	N	318	NEX	C4-C3-C2	2.21	114.93	110.79
32	n	317	LUT	C39-C29-C28	2.21	121.47	118.09
43	b	618	BCR	C35-C13-C12	2.21	121.47	118.09
31	0	604	CLA	C3B-C4B-NB	-2.21	108.56	110.53
32	3	317	LUT	C30-C31-C32	-2.21	116.79	123.20
31	5	602	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
31	N	312	CLA	C2D-C1D-ND	2.21	112.31	110.13
31	2	603	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
31	Y	312	CLA	C6-C5-C3	-2.21	108.08	113.47
31	B	603	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
31	8	604	CLA	CHD-C1D-ND	-2.21	121.69	124.80
31	n	316	CLA	O2A-CGA-CBA	2.21	118.57	111.83
31	s	305	CLA	O2A-CGA-CBA	2.21	118.57	111.83
31	y	610	CLA	C2D-C1D-ND	2.21	112.31	110.13
31	y	614	CLA	C2D-C1D-ND	2.21	112.31	110.13
31	g	313	CLA	CHD-C1D-ND	-2.21	121.69	124.80
31	S	304	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
31	9	304	CLA	C1-O2A-CGA	2.21	122.00	116.65
37	G	620	XAT	O4-C6-C7	-2.21	110.55	116.88
36	n	319	NEX	C12-C13-C14	2.21	122.48	119.01
30	n	302	CHL	CMA-C3A-C2A	2.21	122.66	114.13
31	S	313	CLA	C3B-C4B-NB	-2.21	108.56	110.53
37	g	321	XAT	O4-C6-C7	-2.21	110.55	116.88
31	S	306	CLA	CHD-C1D-ND	-2.21	121.69	124.80
31	b	612	CLA	CHD-C1D-ND	-2.21	121.69	124.80
31	9	306	CLA	C2D-C1D-ND	2.21	112.31	110.13
30	r	310	CHL	C1-O2A-CGA	2.21	122.00	116.65
31	a	406	CLA	C1C-C2C-C3C	-2.21	104.66	106.98
31	5	613	CLA	CHD-C1D-ND	-2.21	121.69	124.80
31	1	602	CLA	CAA-C2A-C3A	-2.21	107.03	113.00
31	p	603	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
36	R	301	NEX	C17-C1-C6	-2.21	108.50	110.47
34	c	620	LMG	O7-C10-O9	-2.21	118.54	123.70
31	5	613	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
31	0	613	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
38	G	624	SQD	O3-C3-C2	-2.21	105.17	110.38
30	8	601	CHL	CMA-C3A-C2A	2.21	122.66	114.13
31	p	602	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
34	m	102	LMG	O7-C10-O9	-2.21	118.54	123.70
38	a	411	SQD	O3-C3-C2	-2.21	105.17	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G	613	CLA	CAA-C2A-C3A	-2.21	107.03	113.00
31	D	404	CLA	O2A-CGA-CBA	2.21	118.56	111.83
35	g	315	RRX	C35-C13-C14	-2.21	119.24	122.82
31	1	612	CLA	C1D-ND-C4D	-2.21	104.76	106.31
32	S	317	LUT	C15-C35-C34	-2.21	119.00	123.52
43	D	405	BCR	C20-C19-C18	-2.21	120.31	126.36
31	6	313	CLA	CHD-C1D-ND	-2.21	121.70	124.80
31	n	303	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
31	B	609	CLA	C2D-C1D-ND	2.21	112.31	110.13
31	5	603	CLA	O2D-CGD-O1D	-2.21	119.56	123.85
34	B	625	LMG	C9-C8-C7	-2.21	106.64	111.78
31	5	604	CLA	CHD-C1D-ND	-2.21	121.70	124.80
31	B	609	CLA	CHD-C1D-ND	-2.21	121.70	124.80
31	b	611	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
31	s	311	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
31	p	610	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
31	4	613	CLA	C1D-ND-C4D	-2.20	104.77	106.31
31	b	610	CLA	C1D-ND-C4D	-2.20	104.77	106.31
31	5	611	CLA	C2D-C1D-ND	2.20	112.31	110.13
31	N	310	CLA	C2D-C1D-ND	2.20	112.31	110.13
31	n	314	CLA	C2D-C1D-ND	2.20	112.31	110.13
31	4	603	CLA	O2A-CGA-CBA	2.20	118.56	111.83
31	G	609	CLA	C3B-C4B-NB	-2.20	108.56	110.53
31	A	405	CLA	CMD-C2D-C3D	-2.20	122.63	127.69
31	Y	304	CLA	CHA-C1A-NA	-2.20	121.40	126.39
37	9	322	XAT	O4-C6-C7	-2.20	110.56	116.88
31	S	310	CLA	O2A-CGA-CBA	2.20	118.56	111.83
31	B	615	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
31	1	611	CLA	C2D-C1D-ND	2.20	112.31	110.13
31	9	304	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
31	3	315	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
31	c	610	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
32	s	317	LUT	C20-C13-C12	2.20	121.45	118.09
37	q	321	XAT	O4-C6-C7	-2.20	110.57	116.88
31	N	305	CLA	C2D-C1D-ND	2.20	112.31	110.13
31	3	312	CLA	O2A-CGA-CBA	2.20	118.55	111.83
43	c	615	BCR	C37-C22-C21	-2.20	119.25	122.82
31	B	610	CLA	CHD-C1D-ND	-2.20	121.71	124.80
31	9	315	CLA	CHD-C1D-ND	-2.20	121.71	124.80
31	a	409	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
31	b	614	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
31	N	304	CLA	C2D-C1D-ND	2.20	112.30	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	315	CLA	C2D-C1D-ND	2.20	112.30	110.13
31	n	316	CLA	C2D-C1D-ND	2.20	112.30	110.13
31	2	612	CLA	CHD-C1D-ND	-2.20	121.71	124.80
31	S	304	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
33	t	102	LHG	O7-C7-O9	-2.20	118.56	123.70
31	n	305	CLA	CHD-C1D-ND	-2.20	121.71	124.80
31	6	311	CLA	O2A-CGA-CBA	2.20	118.54	111.83
31	N	303	CLA	C2D-C1D-ND	2.20	112.30	110.13
31	R	304	CLA	CMA-C3A-C4A	2.20	117.68	111.77
31	C	610	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
31	s	305	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
31	6	303	CLA	C6-C5-C3	-2.20	108.12	113.47
37	4	619	XAT	O4-C6-C7	-2.20	110.58	116.88
31	S	311	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
31	1	604	CLA	C1-O2A-CGA	2.20	121.97	116.65
36	R	301	NEX	C39-C29-C30	-2.20	119.26	122.82
36	Y	317	NEX	C40-C33-C34	-2.20	119.26	122.82
31	g	314	CLA	CHD-C1D-ND	-2.20	121.71	124.80
30	y	605	CHL	C4C-CHD-C1D	2.20	123.93	116.07
31	4	610	CLA	C6-C5-C3	-2.20	108.12	113.47
31	0	613	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
31	8	604	CLA	C2D-C1D-ND	2.20	112.30	110.13
43	C	614	BCR	C29-C28-C27	2.20	116.10	111.28
34	9	301	LMG	C4-C3-C2	2.20	114.68	110.83
31	4	610	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
31	c	607	CLA	CHD-C1D-ND	-2.20	121.71	124.80
38	0	621	SQD	O3-C3-C2	-2.20	105.20	110.38
37	2	619	XAT	O4-C6-C7	-2.20	110.59	116.88
32	s	317	LUT	C27-C28-C29	-2.19	121.60	126.32
43	c	614	BCR	C24-C25-C26	-2.19	116.50	121.56
31	g	312	CLA	C2D-C1D-ND	2.19	112.30	110.13
31	r	314	CLA	O2A-CGA-CBA	2.19	118.53	111.83
30	7	307	CHL	CMA-C3A-C2A	2.19	122.60	114.13
31	6	304	CLA	CHA-C1A-NA	-2.19	121.42	126.39
31	A	409	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
31	1	611	CLA	CAA-C2A-C3A	-2.19	107.07	113.00
43	h	101	BCR	C33-C5-C4	2.19	118.27	113.60
32	q	318	LUT	C15-C35-C34	-2.19	119.03	123.52
31	y	604	CLA	CHD-C1D-ND	-2.19	121.72	124.80
31	s	316	CLA	CHA-C1A-NA	-2.19	121.43	126.39
34	S	321	LMG	C8-O7-C10	-2.19	112.55	117.80
30	y	607	CHL	CMA-C3A-C2A	2.19	122.59	114.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	615	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
33	g	319	LHG	C5-O7-C7	-2.19	112.55	117.80
30	2	606	CHL	CMA-C3A-C2A	2.19	122.59	114.13
31	1	604	CLA	C3B-C4B-NB	-2.19	108.57	110.53
31	p	612	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
31	0	612	CLA	CHA-C1A-NA	-2.19	121.43	126.39
30	Y	302	CHL	CMA-C3A-C2A	2.19	122.59	114.13
31	5	603	CLA	C2D-C1D-ND	2.19	112.29	110.13
31	p	615	CLA	C2D-C1D-ND	2.19	112.29	110.13
31	c	605	CLA	C6-C5-C3	-2.19	108.13	113.47
31	c	608	CLA	CHA-C1A-NA	-2.19	121.43	126.39
35	g	315	RRX	C23-C24-C25	-2.19	121.15	127.00
31	4	612	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
32	6	318	LUT	C27-C28-C29	-2.19	121.61	126.32
31	y	614	CLA	CHA-C1A-NA	-2.19	121.43	126.39
30	q	309	CHL	CMD-C2D-C3D	2.19	129.06	124.68
31	g	310	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
31	s	312	CLA	CHD-C1D-ND	-2.19	121.72	124.80
31	b	617	CLA	CHA-C1A-NA	-2.19	121.43	126.39
31	q	314	CLA	CHD-C1D-ND	-2.19	121.72	124.80
31	p	604	CLA	C1-O2A-CGA	2.19	121.95	116.65
31	0	602	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
31	c	609	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
32	Y	315	LUT	C11-C10-C9	-2.19	124.21	127.28
31	7	314	CLA	C1-O2A-CGA	2.19	121.95	116.65
31	4	611	CLA	C4B-CHC-C1C	2.19	132.00	125.21
34	y	620	LMG	C9-C8-C7	-2.19	106.68	111.78
31	c	604	CLA	C1D-ND-C4D	-2.19	104.78	106.31
31	n	311	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
42	D	401	PHO	O2A-CGA-O1A	-2.19	118.16	123.63
31	2	613	CLA	C2D-C1D-ND	2.19	112.29	110.13
31	n	304	CLA	C2D-C1D-ND	2.19	112.29	110.13
38	r	322	SQD	O3-C3-C2	-2.19	105.22	110.38
32	5	616	LUT	C18-C5-C4	2.19	118.44	114.42
31	s	313	CLA	C4B-CHC-C1C	2.19	131.39	126.25
31	3	313	CLA	CHD-C1D-ND	-2.19	121.72	124.80
31	4	611	CLA	CHA-C1A-NA	-2.19	121.44	126.39
31	s	313	CLA	C1D-ND-C4D	-2.19	104.78	106.31
30	1	608	CHL	C4C-CHD-C1D	2.19	123.89	116.07
32	6	318	LUT	C15-C35-C34	-2.19	119.05	123.52
31	A	405	CLA	C3B-C4B-NB	-2.19	108.58	110.53
31	8	612	CLA	CMD-C2D-C3D	-2.19	122.68	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	606	CLA	C4B-CHC-C1C	2.18	131.38	126.25
33	4	618	LHG	C5-O7-C7	-2.18	112.57	117.80
43	V	101	BCR	C15-C16-C17	-2.18	119.05	123.52
31	6	304	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
31	c	613	CLA	CBA-CAA-C2A	2.18	120.29	113.79
31	y	602	CLA	C2D-C1D-ND	2.18	112.29	110.13
30	s	302	CHL	C4C-CHD-C1D	2.18	123.88	116.07
31	S	311	CLA	C6-C5-C3	-2.18	108.15	113.47
31	p	614	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
30	q	311	CHL	CMA-C3A-C2A	2.18	122.56	114.13
31	d	405	CLA	CHA-C1A-NA	-2.18	121.45	126.39
30	7	321	CHL	C1-O2A-CGA	2.18	121.93	116.65
31	0	603	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
31	b	616	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
31	A	405	CLA	CAA-CBA-CGA	-2.18	107.01	113.21
30	3	303	CHL	CMA-C3A-C2A	2.18	122.55	114.13
31	g	314	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
31	C	611	CLA	CAA-CBA-CGA	-2.18	107.02	113.21
31	N	305	CLA	CHA-C1A-NA	-2.18	121.45	126.39
31	A	409	CLA	C3B-C4B-NB	-2.18	108.58	110.53
31	C	605	CLA	CHA-C1A-NA	-2.18	121.45	126.39
31	9	305	CLA	CHA-C1A-NA	-2.18	121.45	126.39
31	p	602	CLA	CHD-C1D-ND	-2.18	121.73	124.80
31	R	313	CLA	C2D-C1D-ND	2.18	112.28	110.13
31	p	612	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
31	C	611	CLA	CHA-C1A-NA	-2.18	121.45	126.39
32	8	615	LUT	C39-C29-C28	2.18	121.42	118.09
43	b	619	BCR	C10-C11-C12	-2.18	116.88	123.20
31	r	313	CLA	CHD-C1D-ND	-2.18	121.73	124.80
31	0	602	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
30	R	310	CHL	C4C-CHD-C1D	2.18	123.87	116.07
31	N	305	CLA	CMA-C3A-C4A	2.18	117.63	111.77
31	D	403	CLA	C2D-C1D-ND	2.18	112.28	110.13
31	G	604	CLA	C2D-C1D-ND	2.18	112.28	110.13
31	N	315	CLA	C2D-C1D-ND	2.18	112.28	110.13
31	p	610	CLA	C2D-C1D-ND	2.18	112.28	110.13
34	0	622	LMG	C8-O7-C10	-2.18	112.58	117.80
31	5	615	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
30	p	606	CHL	CMA-C3A-C4A	2.18	119.31	114.61
31	B	613	CLA	CHA-C1A-NA	-2.18	121.46	126.39
31	S	311	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
32	G	615	LUT	C39-C29-C30	-2.18	119.29	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	607	CLA	CMA-C3A-C4A	2.18	117.63	111.77
31	G	602	CLA	CHA-C1A-NA	-2.18	121.46	126.39
30	7	306	CHL	C4D-CHA-CBD	-2.18	106.77	108.97
32	s	317	LUT	C18-C5-C4	2.18	118.42	114.42
31	C	606	CLA	CMA-C3A-C4A	2.18	117.62	111.77
31	s	314	CLA	CHA-C1A-NA	-2.18	121.46	126.39
43	h	101	BCR	C31-C1-C6	-2.18	106.83	110.24
31	R	315	CLA	C6-C5-C3	-2.18	108.17	113.47
31	s	316	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
31	7	316	CLA	CHA-C1A-NA	-2.18	121.46	126.39
31	c	602	CLA	CHA-C1A-NA	-2.18	121.46	126.39
31	N	305	CLA	CHD-C1D-ND	-2.18	121.74	124.80
32	r	317	LUT	C12-C13-C14	-2.18	115.59	119.01
36	0	618	NEX	C19-C9-C10	-2.18	119.29	122.82
31	Y	314	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
31	s	305	CLA	C2D-C1D-ND	2.18	112.28	110.13
31	3	315	CLA	CHA-C1A-NA	-2.18	121.47	126.39
32	N	317	LUT	C30-C31-C32	-2.18	116.90	123.20
31	0	612	CLA	O1D-CGD-CBD	-2.18	120.23	124.52
31	2	604	CLA	CHA-C1A-NA	-2.17	121.47	126.39
31	7	311	CLA	C2D-C1D-ND	2.17	112.28	110.13
34	w	203	LMG	C30-C29-C28	-2.17	105.73	113.69
31	3	304	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
31	S	315	CLA	C1D-ND-C4D	-2.17	104.79	106.31
31	S	313	CLA	C3D-C2D-C1D	-2.17	102.86	105.83
35	g	315	RRX	C33-C5-C4	2.17	118.23	113.60
31	9	305	CLA	C2D-C1D-ND	2.17	112.28	110.13
31	9	312	CLA	CHD-C1D-ND	-2.17	121.74	124.80
31	1	611	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
31	b	606	CLA	CAA-C2A-C3A	-2.17	107.13	113.00
31	y	612	CLA	CHA-C1A-NA	-2.17	121.47	126.39
30	4	601	CHL	CMA-C3A-C4A	2.17	119.29	114.61
31	0	610	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
31	9	304	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
31	2	610	CLA	CHD-C1D-ND	-2.17	121.75	124.80
32	N	316	LUT	C15-C35-C34	-2.17	119.08	123.52
30	0	607	CHL	CMA-C3A-C2A	2.17	122.52	114.13
31	b	613	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
31	q	316	CLA	CHA-C1A-NA	-2.17	121.47	126.39
31	y	611	CLA	C2D-C1D-ND	2.17	112.28	110.13
43	B	619	BCR	C29-C30-C25	2.17	113.59	110.44
31	B	601	CLA	CMD-C2D-C3D	-2.17	122.71	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	0	615	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
30	6	310	CHL	C1-O2A-CGA	2.17	121.91	116.65
31	C	607	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
31	n	312	CLA	C2D-C1D-ND	2.17	112.27	110.13
30	n	306	CHL	CMA-C3A-C2A	2.17	122.51	114.13
31	r	303	CLA	CAA-CBA-CGA	-2.17	107.05	113.21
30	g	308	CHL	CMA-C3A-C4A	2.17	119.29	114.61
31	b	609	CLA	C3B-C4B-NB	-2.17	108.59	110.53
32	1	615	LUT	C12-C13-C14	-2.17	115.60	119.01
32	3	318	LUT	C11-C10-C9	-2.17	124.23	127.28
32	S	317	LUT	C20-C13-C12	2.17	121.40	118.09
31	2	610	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
31	n	314	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
31	0	614	CLA	C2D-C1D-ND	2.17	112.27	110.13
31	1	611	CLA	CHD-C1D-ND	-2.17	121.75	124.80
32	p	617	LUT	C15-C35-C34	2.17	127.96	123.52
34	m	102	LMG	C8-O7-C10	-2.17	112.61	117.80
31	C	610	CLA	C4B-CHC-C1C	2.17	131.35	126.25
31	N	305	CLA	O2A-CGA-CBA	2.17	118.45	111.83
36	8	617	NEX	O24-C25-C38	-2.17	112.62	115.05
31	s	311	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
31	y	604	CLA	O2A-CGA-CBA	2.17	118.44	111.83
30	5	605	CHL	CMA-C3A-C4A	2.17	119.28	114.61
31	d	401	CLA	C1-O2A-CGA	2.17	121.90	116.65
31	B	607	CLA	C16-C15-C13	-2.17	108.76	115.97
31	s	305	CLA	CHD-C1D-ND	-2.17	121.75	124.80
31	Y	314	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
31	n	305	CLA	O2A-CGA-CBA	2.17	118.44	111.83
31	q	315	CLA	C4B-CHC-C1C	2.17	131.34	126.25
43	h	101	BCR	C20-C19-C18	-2.17	120.42	126.36
36	q	319	NEX	C40-C33-C34	-2.17	119.31	122.82
31	2	604	CLA	CHD-C1D-ND	-2.17	121.75	124.80
32	y	617	LUT	C19-C9-C8	2.17	121.40	118.09
31	B	611	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
31	C	608	CLA	O2A-CGA-CBA	2.17	118.44	111.83
31	0	602	CLA	C1D-ND-C4D	-2.17	104.79	106.31
30	n	308	CHL	C1-O2A-CGA	2.17	121.89	116.65
31	1	614	CLA	CHA-C1A-NA	-2.17	121.49	126.39
43	d	406	BCR	C21-C20-C19	-2.17	116.92	123.20
31	4	603	CLA	CHD-C1D-ND	-2.17	121.75	124.80
31	B	611	CLA	CHD-C1D-ND	-2.17	121.75	124.80
31	B	610	CLA	CMD-C2D-C3D	-2.17	122.72	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	313	CLA	O1D-CGD-CBD	-2.17	120.25	124.52
31	p	602	CLA	O1D-CGD-CBD	-2.17	120.25	124.52
31	6	304	CLA	C3D-C2D-C1D	-2.17	102.88	105.83
31	c	609	CLA	CMA-C3A-C4A	2.16	117.59	111.77
31	C	601	CLA	CMD-C2D-C3D	-2.16	122.72	127.69
30	5	605	CHL	CMA-C3A-C2A	2.16	122.49	114.13
31	D	404	CLA	CHD-C1D-ND	-2.16	121.76	124.80
31	3	306	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
31	1	612	CLA	CHA-C1A-NA	-2.16	121.49	126.39
31	a	406	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
43	Z	101	BCR	C16-C15-C14	-2.16	119.09	123.52
31	4	602	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
30	2	601	CHL	CMA-C3A-C2A	2.16	122.48	114.13
31	g	310	CLA	CMA-C3A-C4A	2.16	117.59	111.77
32	s	318	LUT	C15-C35-C34	-2.16	119.09	123.52
31	Y	314	CLA	CHA-C1A-NA	-2.16	121.49	126.39
31	4	611	CLA	CHD-C1D-ND	-2.16	121.76	124.80
32	Y	315	LUT	C31-C30-C29	-2.16	124.25	127.28
36	y	618	NEX	C31-C30-C29	2.16	130.31	127.28
31	S	316	CLA	CHA-C1A-NA	-2.16	121.49	126.39
31	5	612	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
31	c	607	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
31	n	303	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
34	W	202	LMG	C8-O7-C10	-2.16	112.62	117.80
31	S	305	CLA	C2D-C1D-ND	2.16	112.27	110.13
31	q	304	CLA	C2D-C1D-ND	2.16	112.27	110.13
31	C	604	CLA	C3B-C4B-NB	-2.16	108.60	110.53
31	2	611	CLA	CHD-C1D-ND	-2.16	121.76	124.80
31	r	311	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
31	6	305	CLA	O2A-CGA-CBA	2.16	118.43	111.83
43	d	406	BCR	C29-C30-C25	2.16	113.58	110.44
33	y	619	LHG	C6-C5-C4	-2.16	106.75	111.78
30	7	302	CHL	CMA-C3A-C2A	2.16	122.48	114.13
31	d	401	CLA	O2A-CGA-CBA	2.16	118.42	111.83
31	1	610	CLA	C2D-C1D-ND	2.16	112.27	110.13
31	b	614	CLA	C2D-C1D-ND	2.16	112.27	110.13
30	g	302	CHL	CMA-C3A-C2A	2.16	122.48	114.13
31	5	612	CLA	CHA-C1A-NA	-2.16	121.50	126.39
31	q	306	CLA	CHA-C1A-NA	-2.16	121.50	126.39
31	r	306	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
38	M	102	SQD	O3-C3-C2	-2.16	105.28	110.38
31	B	602	CLA	CMA-C3A-C4A	2.16	117.58	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	A	414	LMG	C1-O6-C5	-2.16	109.50	113.72
31	y	615	CLA	O2A-CGA-CBA	2.16	118.42	111.83
30	p	601	CHL	C4C-CHD-C1D	2.16	123.80	116.07
36	n	319	NEX	C16-C1-C6	-2.16	108.54	110.47
31	C	607	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
31	B	603	CLA	C3B-C4B-NB	-2.16	108.60	110.53
30	3	302	CHL	CMA-C3A-C2A	2.16	122.47	114.13
31	2	612	CLA	C1D-ND-C4D	-2.16	104.80	106.31
31	3	316	CLA	C2D-C1D-ND	2.16	112.26	110.13
32	0	616	LUT	C31-C30-C29	-2.16	124.25	127.28
31	7	304	CLA	CHA-C1A-NA	-2.16	121.50	126.39
36	n	319	NEX	C28-C29-C30	2.16	122.41	119.01
31	S	313	CLA	O2A-CGA-CBA	2.16	118.42	111.83
31	9	313	CLA	CHA-C1A-NA	-2.16	121.50	126.39
31	D	403	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
31	3	314	CLA	C2D-C1D-ND	2.16	112.26	110.13
31	n	305	CLA	C2D-C1D-ND	2.16	112.26	110.13
31	3	305	CLA	CHA-C1A-NA	-2.16	121.50	126.39
31	c	612	CLA	CHA-C1A-NA	-2.16	121.50	126.39
31	A	407	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
45	C	620	DGD	O2G-C1B-O1B	-2.16	118.66	123.70
30	1	605	CHL	CMA-C3A-C2A	2.16	122.46	114.13
31	b	617	CLA	C4B-CHC-C1C	2.16	131.32	126.25
31	n	305	CLA	CHA-C1A-NA	-2.16	121.50	126.39
34	6	323	LMG	C1-O6-C5	2.16	117.93	113.72
33	Y	318	LHG	C6-C5-C4	-2.16	106.75	111.78
31	3	301	CLA	CHD-C1D-ND	-2.16	121.77	124.80
34	G	621	LMG	C8-O7-C10	-2.16	112.63	117.80
31	3	313	CLA	O2D-CGD-O1D	-2.16	119.65	123.85
31	r	303	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
34	C	619	LMG	O8-C28-O10	-2.16	118.23	123.63
30	4	601	CHL	CMA-C3A-C2A	2.16	122.46	114.13
30	8	605	CHL	CMA-C3A-C2A	2.16	122.46	114.13
30	8	605	CHL	CMA-C3A-C4A	2.16	119.26	114.61
31	B	602	CLA	O2A-CGA-CBA	2.16	118.41	111.83
31	D	404	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
31	A	407	CLA	C1-O2A-CGA	2.16	121.87	116.65
31	r	313	CLA	C1-O2A-CGA	2.16	121.87	116.65
31	7	314	CLA	CHD-C1D-ND	-2.16	121.77	124.80
31	b	610	CLA	C2D-C1D-ND	2.16	112.26	110.13
31	5	602	CLA	CHA-C1A-NA	-2.16	121.51	126.39
31	N	315	CLA	O1D-CGD-CBD	-2.15	120.27	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	c	614	BCR	C33-C5-C4	2.15	118.19	113.60
31	S	313	CLA	CMA-C3A-C4A	2.15	117.56	111.77
31	1	602	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
31	8	614	CLA	CHA-C1A-NA	-2.15	121.51	126.39
31	C	613	CLA	C3B-C4B-NB	-2.15	108.61	110.53
31	R	315	CLA	C3B-C4B-NB	-2.15	108.61	110.53
31	2	611	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
31	G	603	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
30	S	307	CHL	CMA-C3A-C4A	2.15	119.25	114.61
31	N	313	CLA	CHD-C1D-ND	-2.15	121.77	124.80
30	7	321	CHL	CMD-C2D-C3D	2.15	128.99	124.68
31	N	313	CLA	CHA-C1A-NA	-2.15	121.52	126.39
31	b	603	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
31	c	607	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
32	G	615	LUT	C31-C32-C33	-2.15	120.46	126.36
31	9	316	CLA	C2D-C1D-ND	2.15	112.26	110.13
32	Y	316	LUT	C27-C28-C29	-2.15	121.69	126.32
31	N	304	CLA	CHA-C1A-NA	-2.15	121.52	126.39
31	N	313	CLA	C2D-C1D-ND	2.15	112.26	110.13
31	b	602	CLA	C1D-ND-C4D	-2.15	104.80	106.31
31	2	611	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
32	y	617	LUT	C35-C15-C14	-2.15	119.12	123.52
31	1	602	CLA	CHD-C1D-ND	-2.15	121.78	124.80
30	3	308	CHL	C4C-CHD-C1D	2.15	123.76	116.07
31	Y	303	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
31	C	607	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
30	5	605	CHL	C4C-CHD-C1D	2.15	123.76	116.07
31	5	604	CLA	O2A-CGA-CBA	2.15	118.39	111.83
31	7	312	CLA	O2A-CGA-CBA	2.15	118.39	111.83
31	G	609	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
31	3	316	CLA	CHA-C1A-NA	-2.15	121.52	126.39
31	8	602	CLA	CHA-C1A-NA	-2.15	121.52	126.39
31	p	602	CLA	C1D-ND-C4D	-2.15	104.80	106.31
34	D	410	LMG	C8-O7-C10	-2.15	112.65	117.80
31	q	313	CLA	CHA-C1A-NA	-2.15	121.53	126.39
31	y	612	CLA	C1-O2A-CGA	2.15	121.85	116.65
31	4	613	CLA	CAA-C2A-C3A	-2.15	107.19	113.00
31	r	314	CLA	C2D-C1D-ND	2.15	112.25	110.13
31	7	312	CLA	CHD-C1D-ND	-2.15	121.78	124.80
31	s	303	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
31	S	314	CLA	CHA-C1A-NA	-2.15	121.53	126.39
30	2	601	CHL	C4D-CHA-CBD	-2.15	106.80	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y	303	CLA	C2D-C1D-ND	2.15	112.25	110.13
31	r	315	CLA	CAA-C2A-C3A	-2.15	107.20	113.00
31	R	307	CLA	CHD-C1D-ND	-2.15	121.78	124.80
36	R	301	NEX	C20-C13-C14	-2.15	119.34	122.82
43	v	101	BCR	C30-C25-C24	2.15	121.47	115.65
43	v	101	BCR	C35-C13-C12	2.15	121.37	118.09
31	B	608	CLA	C1D-ND-C4D	-2.15	104.81	106.31
31	4	614	CLA	C1-O2A-CGA	2.15	121.85	116.65
31	R	306	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
31	r	314	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
31	n	314	CLA	CHA-C1A-NA	-2.15	121.53	126.39
30	1	606	CHL	C4D-CHA-CBD	-2.15	106.80	108.97
30	4	608	CHL	C4D-CHA-CBD	-2.15	106.80	108.97
31	C	613	CLA	C2D-C1D-ND	2.15	112.25	110.13
31	8	612	CLA	CHD-C1D-ND	-2.15	121.78	124.80
36	6	319	NEX	C19-C9-C10	-2.15	119.34	122.82
31	p	614	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
31	G	611	CLA	CHA-C1A-NA	-2.15	121.53	126.39
31	s	303	CLA	O2A-CGA-CBA	2.15	118.38	111.83
31	1	612	CLA	O1D-CGD-CBD	-2.15	120.29	124.52
34	g	320	LMG	O7-C10-O9	-2.14	118.69	123.70
43	c	614	BCR	C29-C30-C25	2.14	113.55	110.44
31	2	602	CLA	O2D-CGD-O1D	-2.14	119.67	123.85
43	t	101	BCR	C3-C4-C5	-2.14	110.23	114.06
31	G	611	CLA	C3B-C4B-NB	-2.14	108.62	110.53
45	C	618	DGD	C1D-O6D-C5D	-2.14	109.53	113.72
31	6	304	CLA	CHD-C1D-ND	-2.14	121.79	124.80
31	9	312	CLA	C6-C5-C3	-2.14	108.25	113.47
44	a	414	PL9	C32-C33-C34	-2.14	122.72	127.62
31	c	613	CLA	CMA-C3A-C4A	2.14	117.53	111.77
30	n	306	CHL	CMA-C3A-C4A	2.14	119.23	114.61
31	3	311	CLA	CHA-C1A-NA	-2.14	121.54	126.39
30	7	306	CHL	C4C-CHD-C1D	2.14	123.73	116.07
31	5	612	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
31	N	310	CLA	C11-C10-C8	-2.14	108.85	115.97
32	4	616	LUT	C11-C12-C13	-2.14	120.49	126.36
31	B	607	CLA	CHD-C1D-ND	-2.14	121.79	124.80
31	G	613	CLA	CHA-C1A-NA	-2.14	121.54	126.39
43	V	101	BCR	C35-C13-C12	2.14	121.36	118.09
31	S	311	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
31	B	607	CLA	CBA-CAA-C2A	-2.14	107.42	113.79
31	B	614	CLA	CHD-C1D-ND	-2.14	121.79	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	606	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
31	Y	305	CLA	CMA-C3A-C4A	2.14	117.53	111.77
34	j	101	LMG	C8-O7-C10	-2.14	112.67	117.80
31	9	306	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
31	8	604	CLA	CHA-C1A-NA	-2.14	121.55	126.39
30	N	301	CHL	CMA-C3A-C4A	2.14	119.22	114.61
31	7	312	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
31	r	307	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
31	q	313	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
30	r	308	CHL	C1-O2A-CGA	2.14	121.83	116.65
31	B	606	CLA	CBC-CAC-C3C	-2.14	106.62	112.42
31	S	316	CLA	CBC-CAC-C3C	-2.14	106.62	112.42
31	c	603	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
31	B	614	CLA	C2D-C1D-ND	2.14	112.24	110.13
31	G	602	CLA	C2D-C1D-ND	2.14	112.24	110.13
31	4	611	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
32	p	616	LUT	C19-C9-C10	-2.14	119.35	122.82
31	4	603	CLA	CHA-C1A-NA	-2.14	121.55	126.39
31	b	613	CLA	CHD-C1D-ND	-2.14	121.79	124.80
31	1	613	CLA	C3B-C4B-NB	-2.14	108.62	110.53
30	G	601	CHL	CMA-C3A-C2A	2.14	122.39	114.13
31	9	314	CLA	C2D-C1D-ND	2.14	112.24	110.13
31	p	612	CLA	CHD-C1D-ND	-2.14	121.79	124.80
34	d	411	LMG	O7-C10-O9	-2.14	118.71	123.70
31	C	603	CLA	C4B-CHC-C1C	2.14	131.27	126.25
31	s	311	CLA	CMA-C3A-C4A	2.14	117.52	111.77
31	9	304	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
31	7	314	CLA	C3B-C4B-NB	-2.14	108.62	110.53
32	N	316	LUT	C18-C5-C4	2.14	118.35	114.42
31	3	301	CLA	O2A-CGA-CBA	2.14	118.35	111.83
31	3	314	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
31	5	604	CLA	CHA-C1A-NA	-2.14	121.55	126.39
32	p	616	LUT	C15-C35-C34	2.14	127.89	123.52
31	4	610	CLA	CMC-C2C-C1C	2.14	128.37	125.03
31	n	312	CLA	O2A-CGA-CBA	2.14	118.35	111.83
43	T	101	BCR	C8-C7-C6	-2.14	121.29	127.00
30	q	309	CHL	CMA-C3A-C2A	2.14	122.38	114.13
31	A	407	CLA	C3B-C4B-NB	-2.14	108.62	110.53
31	n	311	CLA	CHA-C1A-NA	-2.14	121.55	126.39
31	d	404	CLA	C2D-C1D-ND	2.14	112.24	110.13
32	n	317	LUT	C18-C5-C4	2.14	118.35	114.42
31	8	610	CLA	O2A-CGA-CBA	2.14	118.35	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	n	315	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
31	G	612	CLA	C3B-C4B-NB	-2.14	108.62	110.53
36	9	319	NEX	C26-C27-C28	-2.13	121.48	125.99
30	S	308	CHL	C3D-C4D-ND	-2.13	109.51	112.94
31	R	313	CLA	CHA-C1A-NA	-2.13	121.56	126.39
31	q	305	CLA	CHA-C1A-NA	-2.13	121.56	126.39
31	C	608	CLA	C1D-ND-C4D	-2.13	104.81	106.31
32	Y	315	LUT	C19-C9-C8	2.13	121.35	118.09
30	9	310	CHL	CMA-C3A-C2A	2.13	122.37	114.13
31	Y	312	CLA	CHD-C1D-ND	-2.13	121.80	124.80
31	p	613	CLA	CHD-C1D-ND	-2.13	121.80	124.80
30	q	303	CHL	CMD-C2D-C3D	2.13	128.94	124.68
33	b	628	LHG	C5-O7-C7	-2.13	112.69	117.80
31	C	606	CLA	C1D-ND-C4D	-2.13	104.82	106.31
31	8	612	CLA	CHA-C1A-NA	-2.13	121.56	126.39
31	a	406	CLA	C2D-C1D-ND	2.13	112.24	110.13
32	1	615	LUT	C18-C5-C4	2.13	118.34	114.42
43	v	101	BCR	C33-C5-C4	2.13	118.14	113.60
43	B	617	BCR	C30-C25-C26	-2.13	119.72	122.64
31	9	314	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
38	b	627	SQD	O3-C3-C2	-2.13	105.35	110.38
30	6	306	CHL	CMD-C2D-C3D	2.13	128.94	124.68
31	d	405	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
31	2	603	CLA	CHA-C1A-NA	-2.13	121.57	126.39
31	3	311	CLA	C1D-ND-C4D	-2.13	104.82	106.31
32	4	616	LUT	C15-C35-C34	-2.13	119.16	123.52
31	0	611	CLA	CHA-C1A-NA	-2.13	121.57	126.39
30	7	310	CHL	CMA-C3A-C4A	2.13	119.20	114.61
31	3	316	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
31	g	313	CLA	C2D-C1D-ND	2.13	112.23	110.13
30	R	308	CHL	CMA-C3A-C2A	2.13	122.35	114.13
31	9	315	CLA	CHA-C1A-NA	-2.13	121.57	126.39
31	S	311	CLA	CHA-C1A-NA	-2.13	121.57	126.39
31	S	313	CLA	C2D-C1D-ND	2.13	112.23	110.13
30	8	607	CHL	CMA-C3A-C2A	2.13	122.35	114.13
30	N	307	CHL	C1C-C2C-CMC	2.13	130.64	126.80
31	3	305	CLA	CHD-C1D-ND	-2.13	121.81	124.80
31	7	311	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
32	7	318	LUT	C10-C11-C12	-2.13	117.03	123.20
31	3	311	CLA	O2D-CGD-O1D	-2.13	119.71	123.85
31	Y	305	CLA	C2D-C1D-ND	2.13	112.23	110.13
32	7	317	LUT	C31-C30-C29	-2.13	124.29	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	608	CLA	C1-C2-C3	-2.13	122.71	126.20
31	C	610	CLA	C3B-C4B-NB	-2.13	108.63	110.53
31	1	611	CLA	CHA-C1A-NA	-2.13	121.57	126.39
31	3	304	CLA	CHA-C1A-NA	-2.13	121.57	126.39
31	b	605	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
32	8	615	LUT	C18-C5-C4	2.13	118.33	114.42
31	p	603	CLA	CHA-C1A-NA	-2.13	121.58	126.39
30	Y	306	CHL	C4C-CHD-C1D	2.13	123.68	116.07
31	3	313	CLA	CHA-C1A-NA	-2.13	121.58	126.39
30	n	308	CHL	CMD-C2D-C3D	2.13	128.93	124.68
33	C	623	LHG	O7-C7-O9	-2.13	118.73	123.70
31	r	314	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
31	y	604	CLA	CAA-C2A-C3A	-2.13	107.25	113.00
43	Z	101	BCR	C15-C16-C17	-2.13	119.17	123.52
31	R	316	CLA	C2D-C1D-ND	2.13	112.23	110.13
31	5	612	CLA	CHD-C1D-ND	-2.13	121.81	124.80
34	6	322	LMG	C8-O7-C10	-2.13	112.71	117.80
31	C	602	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
31	b	610	CLA	CHD-C1D-ND	-2.13	121.81	124.80
31	n	314	CLA	CHD-C1D-ND	-2.13	121.81	124.80
31	6	312	CLA	CHA-C1A-NA	-2.13	121.58	126.39
30	0	608	CHL	CMA-C3A-C2A	2.12	122.34	114.13
36	0	618	NEX	C4-C3-C2	2.12	114.76	110.79
44	a	414	PL9	C37-C38-C39	-2.12	122.76	127.62
31	C	611	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
33	A	415	LHG	O8-C23-O10	-2.12	118.31	123.63
32	y	616	LUT	C40-C33-C32	2.12	121.33	118.09
31	g	305	CLA	C2D-C1D-ND	2.12	112.23	110.13
31	a	406	CLA	CHD-C1D-ND	-2.12	121.81	124.80
31	r	307	CLA	O2A-CGA-CBA	2.12	118.31	111.83
31	c	601	CLA	C2C-C1C-NC	2.12	112.21	109.98
31	C	605	CLA	C7-C6-C5	-2.12	107.60	113.26
31	g	310	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
43	c	614	BCR	C10-C11-C12	2.12	129.35	123.20
30	q	310	CHL	CMA-C3A-C2A	2.12	122.33	114.13
31	9	315	CLA	O2A-CGA-CBA	2.12	118.31	111.83
31	R	314	CLA	C1-O2A-CGA	2.12	121.79	116.65
31	0	614	CLA	CHA-C1A-NA	-2.12	121.59	126.39
31	7	314	CLA	CHA-C1A-NA	-2.12	121.59	126.39
31	2	612	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
31	6	313	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
32	G	615	LUT	C15-C35-C34	2.12	127.86	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	a	414	PL9	O1-C4-C3	-2.12	118.49	120.73
30	2	601	CHL	C4C-CHD-C1D	2.12	123.66	116.07
31	5	603	CLA	CHA-C1A-NA	-2.12	121.59	126.39
31	p	602	CLA	CHA-C1A-NA	-2.12	121.59	126.39
31	g	313	CLA	CHA-C1A-NA	-2.12	121.59	126.39
31	A	405	CLA	C1D-ND-C4D	-2.12	104.82	106.31
31	g	314	CLA	CHA-C1A-NA	-2.12	121.59	126.39
36	6	319	NEX	C4-C3-C2	2.12	114.76	110.79
31	G	611	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
38	g	318	SQD	O3-C3-C2	-2.12	105.38	110.38
31	7	305	CLA	CHA-C1A-NA	-2.12	121.59	126.39
31	S	314	CLA	C2D-C1D-ND	2.12	112.22	110.13
31	2	602	CLA	CHA-C1A-NA	-2.12	121.59	126.39
31	4	602	CLA	CHA-C1A-NA	-2.12	121.59	126.39
31	s	311	CLA	CHA-C1A-NA	-2.12	121.59	126.39
43	c	614	BCR	C8-C7-C6	-2.12	121.34	127.00
31	3	305	CLA	O2A-CGA-CBA	2.12	118.30	111.83
31	0	603	CLA	CHA-C1A-NA	-2.12	121.59	126.39
31	y	610	CLA	CHA-C1A-NA	-2.12	121.59	126.39
32	y	617	LUT	C1-C6-C5	-2.12	119.74	122.64
31	5	613	CLA	CHA-C1A-NA	-2.12	121.59	126.39
31	y	603	CLA	CHA-C1A-NA	-2.12	121.59	126.39
31	7	316	CLA	C2D-C1D-ND	2.12	112.22	110.13
31	G	611	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
31	3	314	CLA	CHD-C1D-ND	-2.12	121.82	124.80
31	Y	313	CLA	CHD-C1D-ND	-2.12	121.82	124.80
31	8	604	CLA	O2A-CGA-CBA	2.12	118.29	111.83
31	Y	304	CLA	C2D-C1D-ND	2.12	112.22	110.13
30	g	302	CHL	CMD-C2D-C3D	2.12	128.91	124.68
30	s	307	CHL	CMD-C2D-C3D	2.12	128.91	124.68
31	B	610	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
34	D	409	LMG	C8-O7-C10	-2.12	112.73	117.80
43	d	406	BCR	C38-C26-C27	2.12	118.11	113.60
36	y	618	NEX	C26-C27-C28	-2.12	121.52	125.99
36	9	319	NEX	C4-C3-C2	2.12	114.75	110.79
31	G	602	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
44	a	414	PL9	C36-C34-C33	-2.12	116.42	121.17
37	r	318	XAT	O4-C6-C7	-2.12	110.82	116.88
36	y	618	NEX	O24-C25-C38	-2.12	112.68	115.05
31	B	612	CLA	CHD-C1D-ND	-2.12	121.83	124.80
31	R	306	CLA	O2A-CGA-CBA	2.12	118.28	111.83
31	6	305	CLA	C2D-C1D-ND	2.11	112.22	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	614	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
31	y	614	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
31	C	602	CLA	CHA-C1A-NA	-2.11	121.60	126.39
32	S	317	LUT	C10-C11-C12	-2.11	117.07	123.20
31	q	306	CLA	O2D-CGD-O1D	-2.11	119.73	123.85
31	7	304	CLA	OBD-CAD-C3D	-2.11	123.48	128.42
31	s	306	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
31	3	314	CLA	CHA-C1A-NA	-2.11	121.61	126.39
32	G	615	LUT	C11-C10-C9	-2.11	124.31	127.28
31	C	607	CLA	CHA-C1A-NA	-2.11	121.61	126.39
31	S	303	CLA	C11-C10-C8	-2.11	108.94	115.97
30	S	308	CHL	CMD-C2D-C3D	2.11	128.90	124.68
31	R	307	CLA	O2A-CGA-CBA	2.11	118.28	111.83
32	6	318	LUT	C8-C7-C6	-2.11	121.36	127.00
31	c	608	CLA	C1-O2A-CGA	2.11	121.76	116.65
30	4	606	CHL	C4C-CHD-C1D	2.11	123.62	116.07
31	r	316	CLA	C1-C2-C3	-2.11	122.74	126.20
30	p	605	CHL	CMD-C2D-C3D	2.11	128.90	124.68
36	y	618	NEX	C39-C29-C30	-2.11	119.40	122.82
31	7	303	CLA	CHA-C1A-NA	-2.11	121.61	126.39
36	G	616	NEX	C20-C13-C14	-2.11	119.40	122.82
30	y	607	CHL	CMD-C2D-C3D	2.11	128.90	124.68
30	s	309	CHL	C4C-CHD-C1D	2.11	123.62	116.07
31	G	611	CLA	CHD-C1D-ND	-2.11	121.83	124.80
30	G	605	CHL	CMD-C2D-C3D	2.11	128.90	124.68
30	n	301	CHL	CMD-C2D-C3D	2.11	128.90	124.68
31	q	305	CLA	C2D-C1D-ND	2.11	112.21	110.13
31	C	601	CLA	CAA-C2A-C3A	-2.11	107.30	113.00
47	E	101	HEM	C1A-CHA-C4D	-2.11	121.29	126.25
31	R	314	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
31	A	405	CLA	CMA-C3A-C4A	2.11	117.44	111.77
31	S	314	CLA	CHD-C1D-ND	-2.11	121.83	124.80
31	C	601	CLA	C1D-ND-C4D	-2.11	104.83	106.31
31	b	617	CLA	CMA-C3A-C4A	2.11	117.44	111.77
32	r	317	LUT	C11-C10-C9	-2.11	124.32	127.28
31	G	610	CLA	CAA-C2A-C3A	-2.11	107.30	113.00
31	7	313	CLA	C2D-C1D-ND	2.11	112.21	110.13
43	v	101	BCR	C21-C20-C19	-2.11	117.09	123.20
36	4	617	NEX	C39-C29-C30	-2.11	119.40	122.82
36	R	319	NEX	C16-C1-C6	-2.11	108.58	110.47
31	y	603	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
31	A	405	CLA	CHD-C1D-ND	-2.11	121.84	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	611	CLA	CMD-C2D-C3D	-2.11	122.86	127.69
31	q	306	CLA	CMD-C2D-C3D	-2.11	122.86	127.69
31	Y	310	CLA	CHA-C1A-NA	-2.11	121.62	126.39
37	R	318	XAT	C24-C23-C22	-2.11	106.85	110.79
31	5	612	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
31	0	613	CLA	CHA-C1A-NA	-2.11	121.62	126.39
30	q	311	CHL	CMD-C2D-C3D	2.11	128.89	124.68
32	1	616	LUT	C20-C13-C12	2.11	121.31	118.09
31	Y	304	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
31	A	405	CLA	C1C-C2C-C3C	-2.11	104.76	106.98
31	r	304	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
31	A	407	CLA	C1D-ND-C4D	-2.11	104.83	106.31
30	N	302	CHL	CMD-C2D-C3D	2.11	128.89	124.68
31	c	604	CLA	O2A-CGA-CBA	2.11	118.26	111.83
31	R	316	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
31	c	612	CLA	C3B-C4B-NB	-2.11	108.65	110.53
31	B	615	CLA	C4B-CHC-C1C	2.11	131.20	126.25
30	0	606	CHL	C4C-CHD-C1D	2.11	123.60	116.07
31	c	613	CLA	C2D-C1D-ND	2.11	112.21	110.13
34	G	622	LMG	C8-O7-C10	-2.11	112.76	117.80
30	y	601	CHL	CMD-C2D-C3D	2.11	128.89	124.68
31	B	609	CLA	CMD-C2D-C3D	-2.11	122.86	127.69
31	B	602	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
32	6	317	LUT	C20-C13-C12	2.10	121.30	118.09
31	s	314	CLA	CMD-C2D-C3D	-2.10	122.86	127.69
30	9	307	CHL	CMD-C2D-C3D	2.10	128.89	124.68
30	G	607	CHL	CMA-C3A-C2A	2.10	122.26	114.13
36	N	318	NEX	C15-C14-C13	-2.10	124.33	127.28
32	G	615	LUT	C18-C5-C4	2.10	118.29	114.42
31	G	609	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
31	c	604	CLA	C1-O2A-CGA	2.10	121.74	116.65
30	g	308	CHL	CMA-C3A-C2A	2.10	122.25	114.13
31	c	602	CLA	CHD-C1D-ND	-2.10	121.84	124.80
36	3	319	NEX	C8-C7-C6	-2.10	175.18	177.66
31	1	604	CLA	CHA-C1A-NA	-2.10	121.63	126.39
31	2	612	CLA	C1-O2A-CGA	2.10	121.74	116.65
31	p	611	CLA	CHD-C1D-ND	-2.10	121.84	124.80
32	9	318	LUT	C40-C33-C34	-2.10	119.41	122.82
31	q	313	CLA	O2D-CGD-O1D	-2.10	119.75	123.85
31	1	602	CLA	CMD-C2D-C3D	-2.10	122.87	127.69
31	R	313	CLA	CHD-C1D-ND	-2.10	121.84	124.80
31	N	303	CLA	O1D-CGD-CBD	-2.10	120.37	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	604	CLA	C6-C5-C3	-2.10	108.35	113.47
31	R	303	CLA	C2D-C1D-ND	2.10	112.21	110.13
31	r	306	CLA	C3B-C4B-NB	-2.10	108.65	110.53
42	d	402	PHO	CMA-C3A-C4A	-2.10	110.08	114.61
31	7	304	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
30	n	308	CHL	CMA-C3A-C2A	2.10	122.24	114.13
34	c	621	LMG	O8-C28-O10	-2.10	118.37	123.63
31	y	604	CLA	C2D-C1D-ND	2.10	112.20	110.13
43	C	615	BCR	C37-C22-C21	-2.10	119.41	122.82
30	6	308	CHL	CMD-C2D-C3D	2.10	128.88	124.68
31	C	613	CLA	CHD-C1D-ND	-2.10	121.85	124.80
31	9	312	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
31	7	311	CLA	CHA-C1A-NA	-2.10	121.64	126.39
32	s	318	LUT	C39-C29-C28	2.10	121.30	118.09
32	s	317	LUT	C10-C11-C12	-2.10	117.12	123.20
32	9	318	LUT	C38-C25-C24	-2.10	118.39	123.36
31	8	609	CLA	CHA-C1A-NA	-2.10	121.64	126.39
31	b	606	CLA	C2D-C1D-ND	2.10	112.20	110.13
44	a	414	PL9	O2-C1-C2	-2.10	117.06	121.83
31	r	313	CLA	CHA-C1A-NA	-2.10	121.64	126.39
30	4	601	CHL	C4C-CHD-C1D	2.10	123.58	116.07
31	Y	312	CLA	C1D-ND-C4D	-2.10	104.84	106.31
43	H	101	BCR	C21-C20-C19	-2.10	117.12	123.20
31	9	316	CLA	CHA-C1A-NA	-2.10	121.64	126.39
31	8	614	CLA	C2D-C1D-ND	2.10	112.20	110.13
31	r	305	CLA	C2D-C1D-ND	2.10	112.20	110.13
32	s	318	LUT	C20-C13-C12	2.10	121.29	118.09
31	2	609	CLA	C6-C7-C8	-2.10	108.99	115.97
31	G	610	CLA	C1-C2-C3	-2.10	122.76	126.20
31	8	613	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
31	c	611	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
31	p	610	CLA	CHA-C1A-NA	-2.10	121.64	126.39
30	7	321	CHL	CMA-C3A-C2A	2.10	122.23	114.13
31	9	304	CLA	CHA-C1A-NA	-2.10	121.64	126.39
30	0	606	CHL	C3D-C4D-ND	-2.10	109.58	112.94
31	1	613	CLA	O2A-CGA-CBA	2.10	118.23	111.83
31	D	403	CLA	CHD-C1D-ND	-2.10	121.85	124.80
31	C	611	CLA	C3B-C4B-NB	-2.10	108.66	110.53
31	b	610	CLA	C3B-C4B-NB	-2.10	108.66	110.53
31	N	315	CLA	CHA-C1A-NA	-2.10	121.64	126.39
31	S	310	CLA	CHA-C1A-NA	-2.10	121.64	126.39
30	n	307	CHL	CMD-C2D-C3D	2.10	128.87	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	y	606	CHL	CMD-C2D-C3D	2.10	128.87	124.68
31	n	316	CLA	C6-C5-C3	-2.10	108.36	113.47
31	N	312	CLA	O1D-CGD-CBD	-2.10	120.39	124.52
43	B	617	BCR	C37-C22-C23	2.10	121.29	118.09
31	B	604	CLA	O2A-CGA-CBA	2.10	118.22	111.83
30	G	607	CHL	CMD-C2D-C3D	2.10	128.87	124.68
31	g	310	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
31	n	303	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
31	3	313	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
43	Z	101	BCR	C8-C7-C6	-2.09	121.40	127.00
34	2	621	LMG	O7-C10-O9	-2.09	118.81	123.70
34	w	204	LMG	O7-C10-O9	-2.09	118.81	123.70
31	p	602	CLA	C2D-C1D-ND	2.09	112.20	110.13
31	S	303	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
30	S	308	CHL	C4C-CHD-C1D	2.09	123.56	116.07
30	S	307	CHL	CMD-C2D-C3D	2.09	128.87	124.68
31	3	306	CLA	OBD-CAD-C3D	-2.09	123.52	128.42
31	6	316	CLA	CHD-C1D-ND	-2.09	121.86	124.80
31	d	401	CLA	C1D-ND-C4D	-2.09	104.84	106.31
31	C	602	CLA	C3B-C4B-NB	-2.09	108.66	110.53
30	2	605	CHL	CMD-C2D-C3D	2.09	128.87	124.68
30	R	308	CHL	CMD-C2D-C3D	2.09	128.87	124.68
30	p	607	CHL	CMD-C2D-C3D	2.09	128.87	124.68
31	s	313	CLA	CMA-C3A-C4A	2.09	117.40	111.77
31	5	614	CLA	CHA-C1A-NA	-2.09	121.65	126.39
31	8	610	CLA	CHD-C1D-ND	-2.09	121.86	124.80
34	q	301	LMG	O6-C5-C6	2.09	111.63	106.44
31	Y	311	CLA	CHD-C1D-ND	-2.09	121.86	124.80
30	8	606	CHL	CMD-C2D-C3D	2.09	128.86	124.68
36	y	618	NEX	C4-C3-C2	2.09	114.70	110.79
30	y	601	CHL	CMA-C3A-C2A	2.09	122.21	114.13
32	1	615	LUT	C27-C28-C29	-2.09	121.82	126.32
31	p	610	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
31	0	615	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
31	c	607	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
30	n	307	CHL	CMA-C3A-C4A	2.09	119.12	114.61
31	R	305	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
32	s	317	LUT	C19-C9-C8	2.09	121.28	118.09
31	S	316	CLA	C1D-ND-C4D	-2.09	104.84	106.31
30	7	302	CHL	CMD-C2D-C3D	2.09	128.86	124.68
31	b	611	CLA	CHA-C1A-NA	-2.09	121.66	126.39
31	S	315	CLA	CHA-C1A-NA	-2.09	121.66	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	9	310	CHL	C4C-CHD-C1D	2.09	123.55	116.07
31	2	604	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
31	c	609	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
31	c	607	CLA	CMA-C3A-C4A	2.09	117.39	111.77
31	3	306	CLA	C2D-C1D-ND	2.09	112.19	110.13
31	5	613	CLA	C2D-C1D-ND	2.09	112.19	110.13
31	5	604	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
31	3	301	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
30	p	608	CHL	C4C-CHD-C1D	2.09	123.54	116.07
30	N	301	CHL	CMD-C2D-C3D	2.09	128.86	124.68
30	9	309	CHL	CMD-C2D-C3D	2.09	128.86	124.68
36	8	617	NEX	C2-C1-C6	2.09	111.24	109.21
31	n	315	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
31	c	612	CLA	C2D-C1D-ND	2.09	112.19	110.13
31	b	606	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
30	r	309	CHL	CMD-C2D-C3D	2.09	128.86	124.68
31	8	613	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
31	N	311	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
30	G	623	CHL	CMD-C2D-C3D	2.09	128.85	124.68
30	7	302	CHL	CMA-C3A-C4A	2.09	119.11	114.61
32	Y	316	LUT	C39-C29-C28	2.09	121.28	118.09
31	3	312	CLA	CHD-C1D-ND	-2.09	121.86	124.80
30	Y	307	CHL	CMD-C2D-C3D	2.09	128.85	124.68
30	0	609	CHL	CMD-C2D-C3D	2.09	128.85	124.68
31	G	602	CLA	C1-O2A-CGA	2.09	121.70	116.65
38	y	621	SQD	O3-C3-C2	-2.09	105.46	110.38
36	n	319	NEX	C11-C12-C13	2.09	132.09	126.36
31	g	304	CLA	CHA-C1A-NA	-2.09	121.67	126.39
31	S	306	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
30	8	606	CHL	CMA-C3A-C4A	2.09	119.11	114.61
30	s	308	CHL	CMD-C2D-C3D	2.09	128.85	124.68
30	y	609	CHL	CMD-C2D-C3D	2.09	128.85	124.68
31	9	305	CLA	OBD-CAD-C3D	-2.09	123.54	128.42
35	g	315	RRX	C8-C9-C10	2.09	122.29	119.01
31	6	316	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
30	2	608	CHL	CMD-C2D-C3D	2.09	128.85	124.68
30	g	306	CHL	CMD-C2D-C3D	2.09	128.85	124.68
47	e	102	HEM	C3B-C4B-NB	-2.09	107.97	109.47
36	p	618	NEX	C20-C13-C14	-2.09	119.44	122.82
36	s	319	NEX	C2-C1-C6	2.08	111.24	109.21
31	s	316	CLA	CBC-CAC-C3C	-2.08	106.77	112.42
43	b	618	BCR	C30-C25-C24	2.08	121.30	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	605	CHL	CMD-C2D-C3D	2.08	128.85	124.68
30	Y	309	CHL	CMD-C2D-C3D	2.08	128.85	124.68
30	q	310	CHL	CMD-C2D-C3D	2.08	128.85	124.68
31	g	311	CLA	C2A-C1A-CHA	2.08	127.48	123.87
30	S	308	CHL	CMA-C3A-C2A	2.08	122.18	114.13
31	c	611	CLA	CHA-C1A-NA	-2.08	121.67	126.39
31	7	303	CLA	C6-C5-C3	-2.08	108.39	113.47
30	0	606	CHL	CMD-C2D-C3D	2.08	128.85	124.68
36	r	301	NEX	C31-C30-C29	2.08	130.20	127.28
31	3	304	CLA	C6-C5-C3	-2.08	108.39	113.47
34	J	101	LMG	C8-O7-C10	-2.08	112.81	117.80
31	6	315	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
30	Y	302	CHL	CMD-C2D-C3D	2.08	128.85	124.68
31	0	610	CLA	CHA-C1A-NA	-2.08	121.67	126.39
31	S	313	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
34	7	322	LMG	O7-C10-O9	-2.08	118.83	123.70
32	n	317	LUT	C20-C13-C12	2.08	121.27	118.09
30	3	307	CHL	CMA-C3A-C2A	2.08	122.17	114.13
44	A	416	PL9	O2-C1-C2	-2.08	117.09	121.83
31	A	406	CLA	CHA-C1A-NA	-2.08	121.68	126.39
36	g	317	NEX	C31-C30-C29	2.08	130.20	127.28
45	c	617	DGD	O2G-C1B-O1B	-2.08	118.84	123.70
31	C	608	CLA	CHA-C1A-NA	-2.08	121.68	126.39
31	b	607	CLA	C4B-CHC-C1C	2.08	131.14	126.25
31	c	606	CLA	C3B-C4B-NB	-2.08	108.67	110.53
31	6	314	CLA	CHA-C1A-NA	-2.08	121.68	126.39
30	9	303	CHL	CMD-C2D-C3D	2.08	128.84	124.68
31	b	616	CLA	C4B-CHC-C1C	2.08	131.14	126.25
31	R	312	CLA	C1-O2A-CGA	2.08	121.69	116.65
30	9	308	CHL	CMD-C2D-C3D	2.08	128.84	124.68
36	n	319	NEX	C19-C9-C10	-2.08	119.44	122.82
31	B	602	CLA	C6-C7-C8	-2.08	109.05	115.97
31	Y	313	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
31	7	314	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
31	7	313	CLA	CHA-C1A-NA	-2.08	121.68	126.39
31	g	312	CLA	CHA-C1A-NA	-2.08	121.68	126.39
31	0	602	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	C	602	CLA	CHD-C1D-ND	-2.08	121.88	124.80
30	6	310	CHL	CMD-C2D-C3D	2.08	128.84	124.68
31	S	314	CLA	C3B-C4B-NB	-2.08	108.67	110.53
31	b	606	CLA	C3B-C4B-NB	-2.08	108.67	110.53
36	r	319	NEX	C39-C29-C30	-2.08	119.45	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	q	307	CHL	CMA-C3A-C2A	2.08	122.16	114.13
30	1	601	CHL	CMD-C2D-C3D	2.08	128.84	124.68
30	0	601	CHL	CMD-C2D-C3D	2.08	128.84	124.68
31	B	615	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	C	609	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	S	314	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	b	604	CLA	CHA-C1A-NA	-2.08	121.68	126.39
30	5	606	CHL	CMD-C2D-C3D	2.08	128.84	124.68
31	s	315	CLA	CHA-C1A-NA	-2.08	121.68	126.39
48	c	623	LMU	O5B-C1B-C2B	2.08	114.64	110.37
30	G	606	CHL	C4C-CHD-C1D	2.08	123.50	116.07
31	b	609	CLA	C2D-C1D-ND	2.08	112.18	110.13
31	y	602	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
31	r	303	CLA	CHA-C1A-NA	-2.08	121.69	126.39
31	R	303	CLA	CHD-C1D-ND	-2.08	121.88	124.80
30	Y	301	CHL	CMD-C2D-C3D	2.08	128.84	124.68
30	9	309	CHL	CMA-C3A-C2A	2.08	122.15	114.13
31	0	610	CLA	O2D-CGD-O1D	-2.08	119.80	123.85
30	N	307	CHL	C4C-CHD-C1D	2.08	123.50	116.07
30	g	307	CHL	C4C-CHD-C1D	2.08	123.50	116.07
31	Y	303	CLA	CHA-C1A-NA	-2.08	121.69	126.39
30	Y	306	CHL	CMD-C2D-C3D	2.08	128.83	124.68
31	Y	310	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
33	A	415	LHG	O7-C7-O9	-2.08	118.85	123.70
34	G	622	LMG	O7-C10-O9	-2.08	118.85	123.70
36	q	319	NEX	C20-C13-C14	-2.08	119.45	122.82
30	S	302	CHL	CMD-C2D-C3D	2.08	128.83	124.68
31	9	314	CLA	CHD-C1D-ND	-2.08	121.88	124.80
32	n	317	LUT	C15-C35-C34	-2.08	119.27	123.52
32	8	615	LUT	C20-C13-C12	2.08	121.26	118.09
34	b	624	LMG	O6-C1-C2	-2.08	106.10	110.37
35	g	315	RRX	C2-C1-C6	2.08	113.45	110.44
31	p	604	CLA	CAA-C2A-C3A	-2.08	107.39	113.00
31	3	313	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
30	r	310	CHL	CMD-C2D-C3D	2.08	128.83	124.68
31	6	303	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
31	9	305	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
31	q	305	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
37	2	619	XAT	O24-C26-C27	-2.08	110.93	116.88
31	3	301	CLA	CHA-C1A-NA	-2.08	121.69	126.39
31	q	315	CLA	O2D-CGD-O1D	-2.08	119.81	123.85
30	4	605	CHL	CMD-C2D-C3D	2.07	128.83	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	304	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
31	g	310	CLA	CHA-C1A-NA	-2.07	121.69	126.39
31	y	610	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
31	B	608	CLA	C6-C5-C3	-2.07	108.42	113.47
31	B	614	CLA	CHA-C1A-NA	-2.07	121.69	126.39
30	2	601	CHL	CMD-C2D-C3D	2.07	128.83	124.68
31	N	304	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
31	a	407	CLA	C3B-C4B-NB	-2.07	108.68	110.53
30	g	302	CHL	C4C-CHD-C1D	2.07	123.49	116.07
31	7	312	CLA	CHA-C1A-NA	-2.07	121.70	126.39
34	B	622	LMG	O7-C10-O9	-2.07	118.86	123.70
31	8	602	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
31	A	406	CLA	C6-C5-C3	-2.07	108.42	113.47
31	n	303	CLA	CHA-C1A-NA	-2.07	121.70	126.39
33	s	322	LHG	O7-C7-O9	-2.07	118.86	123.70
30	p	606	CHL	CMD-C2D-C3D	2.07	128.82	124.68
30	q	307	CHL	CMD-C2D-C3D	2.07	128.82	124.68
30	s	309	CHL	CMD-C2D-C3D	2.07	128.82	124.68
31	3	304	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
31	s	313	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
30	G	623	CHL	C4C-CHD-C1D	2.07	123.48	116.07
31	N	303	CLA	CHA-C1A-NA	-2.07	121.70	126.39
31	8	603	CLA	CHA-C1A-NA	-2.07	121.70	126.39
30	g	307	CHL	CMD-C2D-C3D	2.07	128.82	124.68
37	G	620	XAT	O24-C26-C27	-2.07	110.94	116.88
31	2	611	CLA	CHA-C1A-NA	-2.07	121.70	126.39
30	S	302	CHL	C4C-CHD-C1D	2.07	123.48	116.07
31	4	611	CLA	CHB-C1B-C2B	-2.07	126.12	130.51
47	E	101	HEM	CHA-C4D-C3D	-2.07	121.41	125.23
32	3	317	LUT	C35-C15-C14	-2.07	119.28	123.52
31	p	611	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
31	s	305	CLA	CHA-C1A-NA	-2.07	121.70	126.39
34	2	621	LMG	C9-C8-C7	-2.07	106.95	111.78
30	1	606	CHL	C4C-CHD-C1D	2.07	123.48	116.07
31	p	612	CLA	CHA-C1A-NA	-2.07	121.70	126.39
31	6	311	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
31	6	313	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
30	3	307	CHL	CMD-C2D-C3D	2.07	128.82	124.68
30	4	609	CHL	CMD-C2D-C3D	2.07	128.82	124.68
31	1	610	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
31	S	315	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
31	r	314	CLA	CHA-C1A-NA	-2.07	121.70	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	6	302	CHL	CMD-C2D-C3D	2.07	128.82	124.68
30	8	605	CHL	C4C-CHD-C1D	2.07	123.47	116.07
30	7	308	CHL	CMD-C2D-C3D	2.07	128.82	124.68
30	9	303	CHL	CMA-C3A-C2A	2.07	122.12	114.13
31	5	610	CLA	CHA-C1A-NA	-2.07	121.71	126.39
31	6	311	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
30	6	307	CHL	CMD-C2D-C3D	2.07	128.82	124.68
31	R	303	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
31	6	315	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
31	C	607	CLA	C2D-C1D-ND	2.07	112.17	110.13
30	n	302	CHL	CMD-C2D-C3D	2.07	128.82	124.68
31	N	311	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
31	b	615	CLA	CHA-C1A-NA	-2.07	121.71	126.39
31	y	602	CLA	CHA-C1A-NA	-2.07	121.71	126.39
32	8	615	LUT	C19-C9-C8	2.07	121.25	118.09
43	A	410	BCR	C38-C26-C27	2.07	118.00	113.60
31	S	305	CLA	CHA-C1A-NA	-2.07	121.71	126.39
37	4	619	XAT	O24-C26-C27	-2.07	110.95	116.88
31	2	612	CLA	C2D-C1D-ND	2.07	112.17	110.13
31	R	311	CLA	CHA-C1A-NA	-2.07	121.71	126.39
31	y	604	CLA	CMA-C3A-C4A	2.07	117.33	111.77
30	N	307	CHL	CMD-C2D-C3D	2.07	128.81	124.68
31	b	607	CLA	C1D-ND-C4D	-2.07	104.86	106.31
31	9	304	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
31	B	609	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
31	Y	314	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
31	G	603	CLA	CHA-C1A-NA	-2.07	121.71	126.39
30	1	605	CHL	CMD-C2D-C3D	2.07	128.81	124.68
30	p	609	CHL	CMD-C2D-C3D	2.07	128.81	124.68
30	n	310	CHL	CMD-C2D-C3D	2.07	128.81	124.68
30	R	309	CHL	C4C-CHD-C1D	2.07	123.46	116.07
31	G	610	CLA	CHD-C1D-ND	-2.07	121.89	124.80
34	9	321	LMG	O8-C28-O10	-2.07	118.46	123.63
30	y	605	CHL	CMD-C2D-C3D	2.07	128.81	124.68
34	2	618	LMG	O7-C10-O9	-2.07	118.88	123.70
31	B	611	CLA	CHA-C1A-NA	-2.07	121.71	126.39
32	8	615	LUT	C15-C35-C34	-2.07	119.29	123.52
31	n	312	CLA	CHD-C1D-ND	-2.07	121.90	124.80
45	C	617	DGD	O1G-C1A-O1A	-2.07	118.46	123.63
31	9	315	CLA	C2D-C1D-ND	2.07	112.17	110.13
37	9	322	XAT	O24-C26-C27	-2.07	110.96	116.88
31	N	321	CLA	CHA-C1A-NA	-2.06	121.72	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	407	CLA	CHA-C1A-NA	-2.06	121.72	126.39
31	S	314	CLA	C6-C5-C3	-2.06	108.44	113.47
37	g	321	XAT	O24-C26-C27	-2.06	110.96	116.88
31	C	601	CLA	C2D-C1D-ND	2.06	112.17	110.13
31	7	303	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
30	n	306	CHL	C4C-CHD-C1D	2.06	123.45	116.07
30	0	607	CHL	CMD-C2D-C3D	2.06	128.81	124.68
33	g	319	LHG	O8-C23-O10	-2.06	118.47	123.63
31	C	611	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
32	5	616	LUT	C35-C15-C14	-2.06	119.30	123.52
31	2	602	CLA	CHD-C1D-ND	-2.06	121.90	124.80
31	R	312	CLA	CAA-CBA-CGA	-2.06	107.35	113.21
31	G	609	CLA	C1D-ND-C4D	-2.06	104.86	106.31
31	1	610	CLA	CHA-C1A-NA	-2.06	121.72	126.39
31	C	612	CLA	CHA-C1A-NA	-2.06	121.72	126.39
30	G	601	CHL	CMD-C2D-C3D	2.06	128.80	124.68
31	1	612	CLA	C2D-C1D-ND	2.06	112.17	110.13
31	g	310	CLA	C2D-C1D-ND	2.06	112.17	110.13
31	s	316	CLA	C2D-C1D-ND	2.06	112.17	110.13
32	n	317	LUT	C19-C9-C8	2.06	121.24	118.09
48	r	302	LMU	C1B-O1B-C4'	-2.06	113.09	117.98
35	q	317	RRX	C19-C18-C17	2.06	122.25	119.01
31	N	314	CLA	O2D-CGD-O1D	-2.06	119.83	123.85
34	k	101	LMG	O8-C28-O10	-2.06	118.47	123.63
30	2	601	CHL	CMA-C3A-C4A	2.06	119.05	114.61
30	S	309	CHL	C4C-CHD-C1D	2.06	123.44	116.07
32	6	317	LUT	C19-C9-C8	2.06	121.24	118.09
31	r	315	CLA	CAA-C2A-C1A	-2.06	105.22	111.97
30	5	607	CHL	CMD-C2D-C3D	2.06	128.80	124.68
30	G	608	CHL	CMD-C2D-C3D	2.06	128.80	124.68
30	R	309	CHL	CMD-C2D-C3D	2.06	128.80	124.68
31	b	617	CLA	C3B-C4B-NB	-2.06	108.69	110.53
31	S	313	CLA	CHA-C1A-NA	-2.06	121.72	126.39
31	N	313	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
31	S	311	CLA	C1D-ND-C4D	-2.06	104.87	106.31
31	y	613	CLA	C1D-ND-C4D	-2.06	104.87	106.31
30	Y	308	CHL	C4C-CHD-C1D	2.06	123.44	116.07
30	4	601	CHL	CMD-C2D-C3D	2.06	128.80	124.68
31	n	316	CLA	CHA-C1A-NA	-2.06	121.72	126.39
31	c	611	CLA	C2D-C1D-ND	2.06	112.17	110.13
31	1	613	CLA	CHA-C1A-NA	-2.06	121.73	126.39
31	Y	312	CLA	CHA-C1A-NA	-2.06	121.73	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	1	603	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
31	q	316	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
30	3	310	CHL	C4C-CHD-C1D	2.06	123.44	116.07
30	6	302	CHL	CMA-C3A-C2A	2.06	122.08	114.13
31	5	603	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
47	E	101	HEM	CHA-C1A-NA	2.06	127.59	123.86
32	8	616	LUT	C27-C28-C29	-2.06	121.89	126.32
31	N	311	CLA	CHD-C1D-ND	-2.06	121.91	124.80
36	R	319	NEX	C2-C1-C6	2.06	111.21	109.21
34	c	620	LMG	O8-C28-O10	-2.06	118.48	123.63
31	B	616	CLA	CHA-C1A-NA	-2.06	121.73	126.39
34	C	619	LMG	O7-C10-O9	-2.06	118.89	123.70
31	G	609	CLA	CHA-C1A-NA	-2.06	121.73	126.39
34	d	410	LMG	O8-C28-O10	-2.06	118.48	123.63
31	b	612	CLA	CHA-C1A-NA	-2.06	121.73	126.39
30	n	309	CHL	CMD-C2D-C3D	2.06	128.79	124.68
31	c	601	CLA	C2D-C1D-ND	2.06	112.16	110.13
31	5	613	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
30	N	309	CHL	CMD-C2D-C3D	2.06	128.79	124.68
31	C	612	CLA	C3B-C4B-NB	-2.06	108.69	110.53
43	C	614	BCR	C38-C26-C27	2.06	117.98	113.60
31	1	602	CLA	C1D-ND-C4D	-2.06	104.87	106.31
31	g	310	CLA	C1D-ND-C4D	-2.06	104.87	106.31
31	6	303	CLA	CHA-C1A-NA	-2.06	121.73	126.39
30	2	605	CHL	CMA-C3A-C2A	2.06	122.07	114.13
30	r	308	CHL	CMD-C2D-C3D	2.06	128.79	124.68
32	s	317	LUT	C39-C29-C28	2.06	121.23	118.09
31	N	310	CLA	CHA-C1A-NA	-2.06	121.73	126.39
32	Y	316	LUT	C15-C35-C34	-2.06	119.31	123.52
31	B	604	CLA	CAA-C2A-C3A	-2.06	107.44	113.00
30	9	311	CHL	CMD-C2D-C3D	2.06	128.79	124.68
31	B	601	CLA	CHA-C1A-NA	-2.06	121.74	126.39
31	p	614	CLA	CHA-C1A-NA	-2.06	121.74	126.39
31	A	406	CLA	C1D-ND-C4D	-2.06	104.87	106.31
31	p	612	CLA	O2A-CGA-CBA	2.06	119.90	112.14
34	B	625	LMG	O8-C28-O10	-2.05	118.49	123.63
30	n	307	CHL	CMA-C3A-C2A	2.05	122.06	114.13
32	g	316	LUT	C19-C9-C10	-2.05	119.49	122.82
30	3	302	CHL	CMD-C2D-C3D	2.05	128.79	124.68
31	c	611	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
30	q	309	CHL	C4C-CHD-C1D	2.05	123.42	116.07
31	B	615	CLA	CMA-C3A-C4A	2.05	117.29	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	606	CLA	C6-C7-C8	-2.05	109.14	115.97
31	B	602	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
30	1	619	CHL	C1C-C2C-CMC	2.05	130.50	126.80
31	c	601	CLA	C1D-ND-C4D	-2.05	104.87	106.31
38	x	201	SQD	O5-C1-O6	-2.05	105.19	110.04
31	C	606	CLA	CHA-C1A-NA	-2.05	121.74	126.39
31	4	603	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
31	c	603	CLA	CHA-C1A-NA	-2.05	121.74	126.39
31	8	604	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
30	Y	306	CHL	CMA-C3A-C4A	2.05	119.03	114.61
31	s	303	CLA	C11-C10-C8	-2.05	109.14	115.97
30	5	601	CHL	CMD-C2D-C3D	2.05	128.78	124.68
30	5	608	CHL	CMD-C2D-C3D	2.05	128.78	124.68
31	3	315	CLA	C1-O2A-CGA	2.05	121.62	116.65
30	5	609	CHL	CMD-C2D-C3D	2.05	128.78	124.68
31	0	613	CLA	C3B-C4B-NB	-2.05	108.70	110.53
31	q	314	CLA	CAA-CBA-CGA	-2.05	107.38	113.21
30	g	306	CHL	C1-O2A-CGA	2.05	122.50	116.67
31	G	613	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
31	b	617	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
30	R	310	CHL	CMD-C2D-C3D	2.05	128.78	124.68
30	8	601	CHL	CMD-C2D-C3D	2.05	128.78	124.68
31	N	311	CLA	CHA-C1A-NA	-2.05	121.75	126.39
31	7	305	CLA	O2A-CGA-CBA	2.05	118.09	111.83
30	q	307	CHL	CMA-C3A-C4A	2.05	119.03	114.61
31	C	610	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
30	g	308	CHL	CMD-C2D-C3D	2.05	128.78	124.68
31	C	608	CLA	C2D-C1D-ND	2.05	112.16	110.13
31	G	603	CLA	C2D-C1D-ND	2.05	112.16	110.13
31	7	305	CLA	C2D-C1D-ND	2.05	112.16	110.13
31	3	315	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
43	T	101	BCR	C1-C6-C5	-2.05	119.83	122.64
31	b	614	CLA	CHA-C1A-NA	-2.05	121.75	126.39
31	n	304	CLA	CHA-C1A-NA	-2.05	121.75	126.39
48	K	101	LMU	C1-O1'-C1'	-2.05	110.18	113.68
30	q	309	CHL	C1C-C2C-CMC	2.05	130.50	126.80
31	b	612	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
30	6	310	CHL	C4C-CHD-C1D	2.05	123.40	116.07
37	r	318	XAT	C24-C23-C22	-2.05	106.96	110.79
31	5	611	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
31	p	604	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
31	Y	314	CLA	CAA-C2A-C3A	-2.05	107.46	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y	612	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
37	q	321	XAT	O24-C26-C27	-2.05	111.01	116.88
31	2	604	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
31	g	311	CLA	CHD-C1D-ND	-2.05	121.92	124.80
31	C	605	CLA	C4B-CHC-C1C	2.05	131.06	126.25
30	g	309	CHL	CMD-C2D-C3D	2.05	128.78	124.68
32	y	616	LUT	C8-C9-C10	-2.05	115.79	119.01
30	4	606	CHL	CMD-C2D-C3D	2.05	128.78	124.68
30	7	307	CHL	CMD-C2D-C3D	2.05	128.78	124.68
30	7	310	CHL	CMD-C2D-C3D	2.05	128.78	124.68
31	5	602	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
30	8	606	CHL	CMA-C3A-C2A	2.05	122.04	114.13
31	N	312	CLA	CHA-C1A-NA	-2.05	121.75	126.39
31	6	315	CLA	C6-C5-C3	-2.05	108.48	113.47
32	s	318	LUT	C22-C23-C24	2.05	114.22	111.18
31	R	305	CLA	C4B-CHC-C1C	2.05	131.06	126.25
31	8	614	CLA	C6-C5-C3	-2.05	108.48	113.47
31	c	604	CLA	C2D-C1D-ND	2.05	112.15	110.13
31	d	405	CLA	CMD-C2D-C3D	-2.05	123.00	127.69
31	r	304	CLA	CHA-C1A-NA	-2.05	121.76	126.39
30	1	609	CHL	CMD-C2D-C3D	2.05	128.77	124.68
37	R	318	XAT	O4-C5-C18	-2.05	112.76	115.05
32	0	617	LUT	C20-C13-C12	2.05	121.21	118.09
30	8	608	CHL	CMD-C2D-C3D	2.05	128.77	124.68
31	A	405	CLA	C2D-C1D-ND	2.05	112.15	110.13
30	N	308	CHL	C1-O2A-CGA	2.05	121.60	116.65
31	1	614	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
31	c	610	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
30	n	301	CHL	CMA-C3A-C2A	2.05	122.03	114.13
30	G	606	CHL	CMD-C2D-C3D	2.05	128.77	124.68
36	8	617	NEX	C31-C30-C29	2.05	130.15	127.28
34	n	321	LMG	C8-O7-C10	-2.05	112.90	117.80
36	8	617	NEX	C39-C29-C30	-2.05	119.50	122.82
31	B	610	CLA	CHA-C1A-NA	-2.05	121.76	126.39
31	6	312	CLA	CHD-C1D-ND	-2.05	121.92	124.80
31	8	610	CLA	CMD-C2D-C3D	-2.05	123.00	127.69
43	z	101	BCR	C34-C9-C10	-2.04	119.50	122.82
32	n	318	LUT	C10-C11-C12	-2.04	117.28	123.20
31	Y	310	CLA	O2D-CGD-O1D	-2.04	119.87	123.85
31	S	314	CLA	CMD-C2D-C3D	-2.04	123.00	127.69
31	R	305	CLA	O2A-CGA-CBA	2.04	118.07	111.83
31	r	316	CLA	C6-C5-C3	-2.04	108.49	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	304	CLA	C2D-C1D-ND	2.04	112.15	110.13
32	Y	315	LUT	C28-C29-C30	-2.04	115.79	119.01
31	b	605	CLA	C2A-C1A-CHA	2.04	127.41	123.87
31	0	613	CLA	C1D-ND-C4D	-2.04	104.88	106.31
31	5	611	CLA	CHA-C1A-NA	-2.04	121.76	126.39
31	y	604	CLA	CHA-C1A-NA	-2.04	121.76	126.39
32	n	318	LUT	C27-C28-C29	-2.04	121.93	126.32
31	0	610	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
30	S	302	CHL	CMA-C3A-C4A	2.04	119.01	114.61
31	n	312	CLA	CMD-C2D-C3D	-2.04	123.00	127.69
31	4	614	CLA	CHA-C1A-NA	-2.04	121.76	126.39
31	S	312	CLA	CHA-C1A-NA	-2.04	121.76	126.39
31	B	615	CLA	C3B-C4B-NB	-2.04	108.71	110.53
31	R	305	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
34	b	601	LMG	C9-C8-C7	-2.04	107.02	111.78
31	s	313	CLA	CHA-C1A-NA	-2.04	121.77	126.39
31	Y	312	CLA	CMA-C3A-C4A	2.04	117.26	111.77
31	3	312	CLA	C1D-ND-C4D	-2.04	104.88	106.31
31	s	314	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
31	4	614	CLA	C3B-C4B-NB	-2.04	108.71	110.53
31	2	612	CLA	CHA-C1A-NA	-2.04	121.77	126.39
31	c	608	CLA	O2A-CGA-CBA	2.04	118.06	111.83
30	2	606	CHL	CMD-C2D-C3D	2.04	128.76	124.68
30	4	605	CHL	CMA-C3A-C4A	2.04	119.01	114.61
31	d	405	CLA	O2A-CGA-CBA	2.04	118.06	111.83
33	K	102	LHG	O7-C7-O9	-2.04	118.93	123.70
31	g	310	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
36	p	618	NEX	C40-C33-C34	-2.04	119.51	122.82
31	5	614	CLA	CHD-C1D-ND	-2.04	121.93	124.80
31	2	603	CLA	C6-C5-C3	-2.04	108.50	113.47
31	4	613	CLA	C2D-C1D-ND	2.04	112.15	110.13
31	C	611	CLA	C2D-C1D-ND	2.04	112.15	110.13
31	0	602	CLA	C2D-C1D-ND	2.04	112.15	110.13
31	s	311	CLA	C2D-C1D-ND	2.04	112.15	110.13
31	R	313	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	c	601	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
30	7	306	CHL	CMD-C2D-C3D	2.04	128.76	124.68
43	A	410	BCR	C35-C13-C14	-2.04	119.51	122.82
31	C	607	CLA	C6-C7-C8	-2.04	109.18	115.97
34	D	411	LMG	O8-C28-O10	-2.04	118.53	123.63
31	y	615	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	Y	305	CLA	CHA-C1A-NA	-2.04	121.77	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	3	303	CHL	CMD-C2D-C3D	2.04	128.76	124.68
31	r	304	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
31	c	613	CLA	O2A-CGA-CBA	2.04	118.05	111.83
31	q	312	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
33	9	320	LHG	O7-C7-O9	-2.04	118.94	123.70
31	6	305	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
31	c	601	CLA	CAA-C2A-C3A	-2.04	107.49	113.00
31	y	614	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	5	610	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
30	1	607	CHL	CMA-C3A-C2A	2.04	122.00	114.13
31	2	602	CLA	C6-C5-C3	-2.04	108.50	113.47
31	b	610	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
30	9	311	CHL	C3D-C4D-ND	-2.04	109.67	112.94
31	1	603	CLA	CHA-C1A-NA	-2.04	121.78	126.39
31	G	604	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
31	4	602	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	0	612	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	0	614	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
30	0	605	CHL	C3D-C4D-ND	-2.04	109.67	112.94
31	C	605	CLA	CHD-C1D-ND	-2.04	121.94	124.80
30	1	607	CHL	CMD-C2D-C3D	2.04	128.75	124.68
30	p	608	CHL	CMD-C2D-C3D	2.04	128.75	124.68
31	3	301	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
48	c	623	LMU	O5'-C1'-C2'	2.04	114.55	110.37
31	4	614	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	A	407	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	G	612	CLA	CHA-C1A-NA	-2.04	121.78	126.39
31	4	614	CLA	C2D-C1D-ND	2.04	112.14	110.13
44	A	416	PL9	C12-C13-C14	-2.04	122.96	127.62
31	C	613	CLA	C2A-C1A-CHA	2.04	127.40	123.87
31	2	609	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	B	601	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	7	313	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
32	8	616	LUT	C35-C15-C14	-2.04	119.35	123.52
34	b	624	LMG	O6-C5-C4	2.04	113.37	109.70
31	q	306	CLA	CHD-C1D-ND	-2.04	121.94	124.80
31	n	315	CLA	CHD-C1D-ND	-2.04	121.94	124.80
36	n	319	NEX	C1-C2-C3	2.04	118.06	113.59
31	B	605	CLA	C1D-ND-C4D	-2.04	104.88	106.31
31	r	311	CLA	C1D-ND-C4D	-2.04	104.88	106.31
31	g	304	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
44	a	414	PL9	C42-C43-C44	-2.03	122.97	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	r	315	CLA	C2D-C1D-ND	2.03	112.14	110.13
31	b	604	CLA	CHD-C1D-ND	-2.03	121.94	124.80
30	6	309	CHL	CMD-C2D-C3D	2.03	128.75	124.68
31	n	305	CLA	O1D-CGD-CBD	-2.03	120.50	124.52
31	B	610	CLA	C6-C5-C3	-2.03	108.51	113.47
31	B	612	CLA	CMD-C2D-C3D	-2.03	123.02	127.69
31	b	617	CLA	CMD-C2D-C3D	-2.03	123.02	127.69
31	8	609	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
32	8	616	LUT	C10-C11-C12	-2.03	117.31	123.20
30	3	310	CHL	CMD-C2D-C3D	2.03	128.75	124.68
33	D	408	LHG	O8-C23-O10	-2.03	118.54	123.63
31	C	603	CLA	CHA-C1A-NA	-2.03	121.79	126.39
31	R	314	CLA	CHA-C1A-NA	-2.03	121.79	126.39
31	8	602	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	S	312	CLA	CMD-C2D-C3D	-2.03	123.03	127.69
34	1	618	LMG	C8-O7-C10	-2.03	112.93	117.80
31	4	602	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
31	r	312	CLA	CMA-C3A-C4A	2.03	117.24	111.77
31	N	310	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
34	b	626	LMG	O8-C28-O10	-2.03	118.54	123.63
36	q	319	NEX	C19-C9-C10	-2.03	119.52	122.82
34	D	410	LMG	O8-C28-O10	-2.03	118.54	123.63
31	C	613	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	N	314	CLA	CHD-C1D-ND	-2.03	121.94	124.80
31	c	613	CLA	CHD-C1D-ND	-2.03	121.94	124.80
30	Y	308	CHL	CMD-C2D-C3D	2.03	128.74	124.68
31	y	613	CLA	C1-O2A-CGA	2.03	121.57	116.65
30	7	308	CHL	C4C-CHD-C1D	2.03	123.34	116.07
31	r	316	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
36	Y	317	NEX	C1-C2-C3	2.03	118.05	113.59
30	p	609	CHL	C1-C2-C3	-2.03	122.87	126.20
30	n	301	CHL	CMA-C3A-C4A	2.03	118.99	114.61
30	6	308	CHL	CMA-C3A-C2A	2.03	121.97	114.13
31	D	404	CLA	CMD-C2D-C3D	-2.03	123.03	127.69
30	8	606	CHL	C4C-CHD-C1D	2.03	123.33	116.07
31	c	612	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	n	315	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	B	603	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
31	Y	311	CLA	CHA-C1A-NA	-2.03	121.80	126.39
35	q	317	RRX	C38-C26-C27	2.03	118.15	114.42
31	B	601	CLA	C1D-ND-C4D	-2.03	104.89	106.31
31	r	306	CLA	O2A-CGA-CBA	2.03	118.02	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	b	618	BCR	C1-C6-C7	2.03	121.16	115.65
36	R	319	NEX	O24-C25-C38	-2.03	112.78	115.05
31	S	303	CLA	CHA-C1A-NA	-2.03	121.80	126.39
31	8	610	CLA	CHA-C1A-NA	-2.03	121.80	126.39
31	N	314	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	r	312	CLA	CAA-CBA-CGA	-2.03	107.45	113.21
30	Y	302	CHL	C4C-CHD-C1D	2.03	123.33	116.07
34	W	202	LMG	O7-C10-O9	-2.03	118.96	123.70
33	F1	301	LHG	C5-O7-C7	-2.03	112.94	117.80
31	R	303	CLA	CMD-C2D-C3D	-2.03	123.04	127.69
43	c	614	BCR	C2-C1-C6	2.03	113.39	110.44
31	r	312	CLA	C2D-C1D-ND	2.03	112.13	110.13
31	7	315	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	2	613	CLA	CHA-C1A-NA	-2.03	121.80	126.39
30	s	302	CHL	CMD-C2D-C3D	2.03	128.73	124.68
31	d	405	CLA	CHD-C1D-ND	-2.03	121.95	124.80
31	R	316	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
30	n	307	CHL	C4C-CHD-C1D	2.03	123.32	116.07
32	1	616	LUT	C19-C9-C8	2.03	121.18	118.09
30	n	306	CHL	CMD-C2D-C3D	2.03	128.73	124.68
30	R	308	CHL	C1-O2A-CGA	2.03	121.56	116.65
43	z	101	BCR	C36-C18-C19	2.03	121.18	118.09
47	e	102	HEM	C1A-CHA-C4D	-2.03	121.48	126.25
31	y	603	CLA	C2D-C1D-ND	2.03	112.13	110.13
30	N	308	CHL	CMD-C2D-C3D	2.03	128.73	124.68
31	s	310	CLA	CHA-C1A-NA	-2.03	121.80	126.39
31	c	613	CLA	CBC-CAC-C3C	-2.03	106.93	112.42
31	4	603	CLA	C6-C5-C3	-2.03	108.53	113.47
31	a	406	CLA	C3D-C2D-C1D	-2.03	103.07	105.83
31	0	612	CLA	C1D-ND-C4D	-2.03	104.89	106.31
31	c	608	CLA	C1D-ND-C4D	-2.03	104.89	106.31
36	r	301	NEX	C20-C13-C14	-2.03	119.53	122.82
31	C	609	CLA	C6-C5-C3	-2.03	108.53	113.47
30	3	309	CHL	CMA-C3A-C2A	2.03	121.95	114.13
31	s	313	CLA	O2A-CGA-CBA	2.02	118.01	111.83
34	G	619	LMG	O7-C10-O9	-2.02	118.97	123.70
34	9	302	LMG	O7-C10-O9	-2.02	118.97	123.70
31	0	615	CLA	CAA-CBA-CGA	-2.02	107.46	113.21
31	6	313	CLA	C6-C5-C3	-2.02	108.54	113.47
31	A	405	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
38	x	201	SQD	O3-C3-C2	-2.02	105.60	110.38
31	4	613	CLA	CHA-C1A-NA	-2.02	121.81	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	613	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
44	a	414	PL9	C20-C19-C21	2.02	118.74	115.23
30	9	308	CHL	CMA-C3A-C2A	2.02	121.94	114.13
31	D	404	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
31	c	604	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
32	y	616	LUT	C12-C13-C14	-2.02	115.83	119.01
31	C	611	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
31	8	612	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
31	S	311	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
34	S	321	LMG	O7-C10-O9	-2.02	118.98	123.70
36	r	301	NEX	C40-C33-C34	-2.02	119.54	122.82
31	g	304	CLA	C2D-C1D-ND	2.02	112.13	110.13
31	7	303	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
30	9	303	CHL	C4C-CHD-C1D	2.02	123.30	116.07
31	c	606	CLA	CHA-C1A-NA	-2.02	121.81	126.39
31	y	611	CLA	CHA-C1A-NA	-2.02	121.81	126.39
30	y	607	CHL	C4C-CHD-C1D	2.02	123.30	116.07
32	s	318	LUT	C10-C11-C12	-2.02	117.34	123.20
31	S	304	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
36	G	616	NEX	C39-C29-C30	-2.02	119.54	122.82
30	Y	306	CHL	C3D-C4D-ND	-2.02	109.70	112.94
31	b	603	CLA	O2A-CGA-CBA	2.02	118.00	111.83
31	Y	313	CLA	CHA-C1A-NA	-2.02	121.82	126.39
31	6	311	CLA	C1-O2A-CGA	2.02	121.54	116.65
31	0	613	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
31	B	602	CLA	CMD-C2D-C3D	-2.02	123.06	127.69
32	7	318	LUT	C20-C13-C12	2.02	121.17	118.09
31	b	607	CLA	CBC-CAC-C3C	-2.02	106.94	112.42
31	c	605	CLA	O2A-CGA-CBA	2.02	117.99	111.83
30	8	605	CHL	CMD-C2D-C3D	2.02	128.72	124.68
31	c	613	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	6	313	CLA	CHA-C1A-NA	-2.02	121.82	126.39
31	B	615	CLA	CHA-C1A-NA	-2.02	121.82	126.39
45	c	618	DGD	O1G-C1A-O1A	-2.02	118.58	123.63
31	B	607	CLA	C1D-ND-C4D	-2.02	104.90	106.31
31	9	305	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
34	g	322	LMG	C1-O6-C5	-2.02	109.78	113.72
31	3	311	CLA	C6-C5-C3	-2.02	108.55	113.47
31	q	312	CLA	CHA-C1A-NA	-2.02	121.82	126.39
31	B	607	CLA	CMD-C2D-C3D	-2.02	123.06	127.69
31	3	304	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	4	612	CLA	CHA-C1A-NA	-2.02	121.82	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	6	320	LHG	O7-C7-O9	-2.02	118.99	123.70
31	B	603	CLA	CHD-C1D-ND	-2.02	121.96	124.80
47	E	101	HEM	CHB-C1B-C2B	-2.02	121.22	126.95
30	Y	301	CHL	C4C-CHD-C1D	2.02	123.28	116.07
44	A	416	PL9	C42-C43-C44	-2.02	123.01	127.62
31	4	604	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	s	304	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
30	r	309	CHL	C4C-CHD-C1D	2.02	123.28	116.07
30	2	607	CHL	CMD-C2D-C3D	2.02	128.71	124.68
31	a	406	CLA	O2A-CGA-CBA	2.02	117.98	111.83
31	c	609	CLA	CHA-C1A-NA	-2.02	121.83	126.39
31	b	608	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	s	311	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	s	316	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
30	q	303	CHL	CMA-C3A-C2A	2.02	121.91	114.13
31	R	313	CLA	C1-O2A-CGA	2.01	121.53	116.65
31	9	316	CLA	O1D-CGD-CBD	-2.01	120.54	124.52
31	n	316	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
31	r	306	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
31	C	604	CLA	C6-C7-C8	-2.01	109.27	115.97
30	4	608	CHL	CMA-C3A-C4A	2.01	118.95	114.61
30	1	606	CHL	CMD-C2D-C3D	2.01	128.71	124.68
30	r	308	CHL	C4C-CHD-C1D	2.01	123.28	116.07
31	c	609	CLA	C3B-C4B-NB	-2.01	108.73	110.53
36	S	319	NEX	C4-C3-C2	2.01	114.56	110.79
34	9	301	LMG	O8-C28-O10	-2.01	118.59	123.63
44	d	407	PL9	C7-C3-C2	-2.01	121.01	123.39
30	1	619	CHL	C3D-C4D-ND	-2.01	109.71	112.94
32	N	317	LUT	C8-C7-C6	-2.01	121.62	127.00
33	7	319	LHG	C5-O7-C7	-2.01	112.98	117.80
30	G	607	CHL	C4C-CHD-C1D	2.01	123.27	116.07
31	n	314	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
31	C	611	CLA	C1-O2A-CGA	2.01	121.52	116.65
32	n	318	LUT	C35-C15-C14	-2.01	119.40	123.52
43	b	620	BCR	C2-C1-C6	2.01	113.36	110.44
31	7	314	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
31	1	613	CLA	CHD-C1D-ND	-2.01	121.97	124.80
30	3	302	CHL	C3D-C4D-ND	-2.01	109.71	112.94
31	A	409	CLA	C2D-C1D-ND	2.01	112.12	110.13
31	8	610	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
36	r	301	NEX	C39-C29-C30	-2.01	119.56	122.82
31	b	614	CLA	C3D-C2D-C1D	-2.01	103.08	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	c	621	LMG	O7-C10-O9	-2.01	119.00	123.70
31	3	305	CLA	C6-C5-C3	-2.01	108.57	113.47
34	w	202	LMG	C9-C8-C7	-2.01	107.09	111.78
31	1	611	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
30	9	310	CHL	CMD-C2D-C3D	2.01	128.70	124.68
31	n	316	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
31	8	613	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	s	313	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	b	616	CLA	CHA-C1A-NA	-2.01	121.84	126.39
30	p	606	CHL	C4C-CHD-C1D	2.01	123.26	116.07
32	1	615	LUT	C40-C33-C32	2.01	121.16	118.09
31	4	612	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
31	b	613	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
30	8	607	CHL	CMD-C2D-C3D	2.01	128.70	124.68
30	q	308	CHL	CMD-C2D-C3D	2.01	128.70	124.68
30	6	302	CHL	C4C-CHD-C1D	2.01	123.26	116.07
31	n	312	CLA	CHA-C1A-NA	-2.01	121.84	126.39
31	c	609	CLA	C16-C15-C13	-2.01	109.28	115.97
30	N	306	CHL	CMD-C2D-C3D	2.01	128.70	124.68
30	G	608	CHL	C4C-CHD-C1D	2.01	123.26	116.07
34	6	322	LMG	O8-C28-O10	-2.01	118.60	123.63
34	W	202	LMG	O8-C28-O10	-2.01	118.60	123.63
32	1	616	LUT	C35-C15-C14	-2.01	119.41	123.52
31	r	316	CLA	C1D-ND-C4D	-2.01	104.90	106.31
30	4	605	CHL	CMA-C3A-C2A	2.01	121.89	114.13
34	b	622	LMG	C7-O1-C1	2.01	118.10	113.80
30	0	605	CHL	CMD-C2D-C3D	2.01	128.70	124.68
34	9	301	LMG	O7-C10-O9	-2.01	119.01	123.70
30	1	607	CHL	C4C-CHD-C1D	2.01	123.26	116.07
31	B	613	CLA	C2D-C1D-ND	2.01	112.11	110.13
31	c	603	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
34	X	203	LMG	C8-O7-C10	-2.01	112.99	117.80
31	b	605	CLA	C3B-C4B-NB	-2.01	108.74	110.53
31	C	604	CLA	O2A-CGA-CBA	2.01	117.96	111.83
32	7	317	LUT	C20-C13-C12	2.01	121.16	118.09
30	r	310	CHL	C4C-CHD-C1D	2.01	123.25	116.07
31	c	601	CLA	CHA-C1A-NA	-2.01	121.84	126.39
31	r	305	CLA	CHA-C1A-NA	-2.01	121.84	126.39
31	c	608	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	g	314	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	6	313	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
33	s	320	LHG	C5-O7-C7	-2.01	112.99	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	619	CHL	CMD-C2D-C3D	2.01	128.69	124.68
31	C	605	CLA	O2A-CGA-CBA	2.01	117.95	111.83
31	B	610	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	C	602	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	N	303	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	c	602	CLA	CMD-C2D-C3D	-2.01	123.09	127.69
30	3	308	CHL	CMD-C2D-C3D	2.01	128.69	124.68
31	c	610	CLA	C2D-C1D-ND	2.01	112.11	110.13
31	a	407	CLA	CMD-C2D-C3D	-2.01	123.09	127.69
31	3	312	CLA	CHA-C1A-NA	-2.01	121.85	126.39
30	7	309	CHL	C4C-CHD-C1D	2.01	123.25	116.07
31	5	615	CLA	C2A-C1A-CHA	2.01	127.35	123.87
31	q	313	CLA	CHD-C1D-ND	-2.01	121.98	124.80
31	q	315	CLA	C2D-C1D-ND	2.01	112.11	110.13
31	c	607	CLA	C2D-C1D-ND	2.01	112.11	110.13
31	n	311	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	B	616	CLA	C1-O2A-CGA	2.01	121.50	116.65
31	D	404	CLA	CHA-C1A-NA	-2.01	121.85	126.39
32	0	617	LUT	C35-C15-C14	-2.00	119.42	123.52
31	d	401	CLA	O1D-CGD-CBD	-2.00	120.56	124.52
30	q	309	CHL	C3D-C4D-ND	-2.00	109.72	112.94
31	2	602	CLA	O2A-CGA-CBA	2.00	117.95	111.83
34	b	629	LMG	C9-C8-C7	-2.00	107.11	111.78
31	2	613	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
31	N	312	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
31	r	316	CLA	C1-O2A-CGA	2.00	121.50	116.65
31	n	311	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
31	G	602	CLA	C6-C5-C3	-2.00	108.59	113.47
45	c	617	DGD	O1G-C1A-O1A	-2.00	118.62	123.63
32	R	317	LUT	C40-C33-C32	-2.00	115.03	118.09
36	y	618	NEX	C40-C33-C34	-2.00	119.57	122.82
31	8	613	CLA	CHD-C1D-ND	-2.00	121.98	124.80
31	y	602	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
43	A	410	BCR	C1-C6-C7	2.00	121.08	115.65
32	3	317	LUT	C11-C12-C13	-2.00	120.87	126.36
30	N	308	CHL	C4C-CHD-C1D	2.00	123.23	116.07
31	g	312	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
31	r	306	CLA	C1-O2A-CGA	2.00	121.50	116.65
30	s	302	CHL	CMA-C3A-C4A	2.00	118.92	114.61
31	q	315	CLA	CAC-C3C-C4C	2.00	127.39	124.79
34	q	301	LMG	C1-O6-C5	-2.00	109.81	113.72
30	2	605	CHL	CMA-C3A-C4A	2.00	118.92	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	607	CHL	CMA-C3A-C2A	2.00	121.86	114.13
31	1	613	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
31	2	603	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
31	9	316	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
31	n	312	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
31	0	604	CLA	C1D-ND-C4D	-2.00	104.91	106.31
31	C	609	CLA	CMA-C3A-C4A	2.00	117.15	111.77
30	y	608	CHL	CMD-C2D-C3D	2.00	128.68	124.68
31	p	602	CLA	CMD-C2D-C3D	-2.00	123.10	127.69
31	g	313	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
30	1	608	CHL	CMD-C2D-C3D	2.00	128.68	124.68
31	9	313	CLA	O1D-CGD-CBD	-2.00	120.57	124.52

All (636) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	1	601	CHL	ND
30	1	601	CHL	NA
30	1	601	CHL	NC
30	1	605	CHL	ND
30	1	605	CHL	NA
30	1	605	CHL	NC
30	1	606	CHL	ND
30	1	606	CHL	NA
30	1	606	CHL	NC
30	1	607	CHL	ND
30	1	607	CHL	NA
30	1	607	CHL	NC
30	1	608	CHL	ND
30	1	608	CHL	NA
30	1	608	CHL	NC
30	1	609	CHL	ND
30	1	609	CHL	NA
30	1	609	CHL	NC
30	1	619	CHL	ND
30	1	619	CHL	NA
30	1	619	CHL	NC
30	2	601	CHL	ND
30	2	601	CHL	NA
30	2	601	CHL	NC
30	2	605	CHL	ND
30	2	605	CHL	NA

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Mol	Chain	Res	Type	Atom
30	2	605	CHL	NC
30	2	606	CHL	ND
30	2	606	CHL	NA
30	2	606	CHL	NC
30	2	607	CHL	ND
30	2	607	CHL	NA
30	2	607	CHL	NC
30	2	608	CHL	ND
30	2	608	CHL	NA
30	2	608	CHL	NC
30	3	302	CHL	ND
30	3	302	CHL	NA
30	3	302	CHL	NC
30	3	303	CHL	ND
30	3	303	CHL	NA
30	3	303	CHL	NC
30	3	307	CHL	ND
30	3	307	CHL	NA
30	3	307	CHL	NC
30	3	308	CHL	ND
30	3	308	CHL	NA
30	3	308	CHL	NC
30	3	309	CHL	ND
30	3	309	CHL	NA
30	3	309	CHL	NC
30	3	310	CHL	ND
30	3	310	CHL	NA
30	3	310	CHL	NC
30	4	601	CHL	ND
30	4	601	CHL	NA
30	4	601	CHL	NC
30	4	605	CHL	ND
30	4	605	CHL	NA
30	4	605	CHL	NC
30	4	606	CHL	ND
30	4	606	CHL	NA
30	4	606	CHL	NC
30	4	607	CHL	ND
30	4	607	CHL	NA
30	4	607	CHL	NC
30	4	608	CHL	ND
30	4	608	CHL	NA

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Mol	Chain	Res	Type	Atom
30	4	608	CHL	NC
30	4	609	CHL	ND
30	4	609	CHL	NA
30	4	609	CHL	NC
30	5	601	CHL	ND
30	5	601	CHL	NA
30	5	601	CHL	NC
30	5	605	CHL	ND
30	5	605	CHL	NA
30	5	605	CHL	NC
30	5	606	CHL	ND
30	5	606	CHL	NA
30	5	606	CHL	NC
30	5	607	CHL	ND
30	5	607	CHL	NA
30	5	607	CHL	NC
30	5	608	CHL	ND
30	5	608	CHL	NA
30	5	608	CHL	NC
30	5	609	CHL	ND
30	5	609	CHL	NA
30	5	609	CHL	NC
30	6	302	CHL	ND
30	6	302	CHL	NA
30	6	302	CHL	NC
30	6	306	CHL	ND
30	6	306	CHL	NA
30	6	306	CHL	NC
30	6	307	CHL	ND
30	6	307	CHL	NA
30	6	307	CHL	NC
30	6	308	CHL	ND
30	6	308	CHL	NA
30	6	308	CHL	NC
30	6	309	CHL	ND
30	6	309	CHL	NA
30	6	309	CHL	NC
30	6	310	CHL	ND
30	6	310	CHL	NA
30	6	310	CHL	NC
30	G	601	CHL	ND
30	G	601	CHL	NA

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Mol	Chain	Res	Type	Atom
30	G	601	CHL	NC
30	G	605	CHL	ND
30	G	605	CHL	NA
30	G	605	CHL	NC
30	G	606	CHL	ND
30	G	606	CHL	NA
30	G	606	CHL	NC
30	G	607	CHL	ND
30	G	607	CHL	NA
30	G	607	CHL	NC
30	G	608	CHL	ND
30	G	608	CHL	NA
30	G	608	CHL	NC
30	G	623	CHL	ND
30	G	623	CHL	NA
30	G	623	CHL	NC
30	N	301	CHL	ND
30	N	301	CHL	NA
30	N	301	CHL	NC
30	N	302	CHL	ND
30	N	302	CHL	NA
30	N	302	CHL	NC
30	N	306	CHL	ND
30	N	306	CHL	NA
30	N	306	CHL	NC
30	N	307	CHL	ND
30	N	307	CHL	NA
30	N	307	CHL	NC
30	N	308	CHL	ND
30	N	308	CHL	NA
30	N	308	CHL	NC
30	N	309	CHL	ND
30	N	309	CHL	NA
30	N	309	CHL	NC
30	R	308	CHL	ND
30	R	308	CHL	NA
30	R	308	CHL	NC
30	R	309	CHL	ND
30	R	309	CHL	NA
30	R	309	CHL	NC
30	R	310	CHL	ND
30	R	310	CHL	NA

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Mol	Chain	Res	Type	Atom
30	R	310	CHL	NC
30	S	302	CHL	ND
30	S	302	CHL	NA
30	S	302	CHL	NC
30	S	307	CHL	ND
30	S	307	CHL	NA
30	S	307	CHL	NC
30	S	308	CHL	ND
30	S	308	CHL	NA
30	S	308	CHL	NC
30	S	309	CHL	ND
30	S	309	CHL	NA
30	S	309	CHL	NC
30	Y	301	CHL	ND
30	Y	301	CHL	NA
30	Y	301	CHL	NC
30	Y	302	CHL	ND
30	Y	302	CHL	NA
30	Y	302	CHL	NC
30	Y	306	CHL	ND
30	Y	306	CHL	NA
30	Y	306	CHL	NC
30	Y	307	CHL	ND
30	Y	307	CHL	NA
30	Y	307	CHL	NC
30	Y	308	CHL	ND
30	Y	308	CHL	NA
30	Y	308	CHL	NC
30	Y	309	CHL	ND
30	Y	309	CHL	NA
30	Y	309	CHL	NC
30	0	601	CHL	ND
30	0	601	CHL	NA
30	0	601	CHL	NC
30	0	605	CHL	ND
30	0	605	CHL	NA
30	0	605	CHL	NC
30	0	606	CHL	ND
30	0	606	CHL	NA
30	0	606	CHL	NC
30	0	607	CHL	ND
30	0	607	CHL	NA

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Mol	Chain	Res	Type	Atom
30	0	607	CHL	NC
30	0	608	CHL	ND
30	0	608	CHL	NA
30	0	608	CHL	NC
30	0	609	CHL	ND
30	0	609	CHL	NA
30	0	609	CHL	NC
30	7	302	CHL	ND
30	7	302	CHL	NA
30	7	302	CHL	NC
30	7	306	CHL	ND
30	7	306	CHL	NA
30	7	306	CHL	NC
30	7	307	CHL	ND
30	7	307	CHL	NA
30	7	307	CHL	NC
30	7	308	CHL	ND
30	7	308	CHL	NA
30	7	308	CHL	NC
30	7	309	CHL	ND
30	7	309	CHL	NA
30	7	309	CHL	NC
30	7	310	CHL	ND
30	7	310	CHL	NA
30	7	310	CHL	NC
30	7	321	CHL	ND
30	7	321	CHL	NA
30	7	321	CHL	NC
30	8	601	CHL	ND
30	8	601	CHL	NA
30	8	601	CHL	NC
30	8	605	CHL	ND
30	8	605	CHL	NA
30	8	605	CHL	NC
30	8	606	CHL	ND
30	8	606	CHL	NA
30	8	606	CHL	NC
30	8	607	CHL	ND
30	8	607	CHL	NA
30	8	607	CHL	NC
30	8	608	CHL	ND
30	8	608	CHL	NA

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Mol	Chain	Res	Type	Atom
30	8	608	CHL	NC
30	9	303	CHL	ND
30	9	303	CHL	NA
30	9	303	CHL	NC
30	9	307	CHL	ND
30	9	307	CHL	NA
30	9	307	CHL	NC
30	9	308	CHL	ND
30	9	308	CHL	NA
30	9	308	CHL	NC
30	9	309	CHL	ND
30	9	309	CHL	NA
30	9	309	CHL	NC
30	9	310	CHL	ND
30	9	310	CHL	NA
30	9	310	CHL	NC
30	9	311	CHL	ND
30	9	311	CHL	NA
30	9	311	CHL	NC
30	p	601	CHL	ND
30	p	601	CHL	NA
30	p	601	CHL	NC
30	p	605	CHL	ND
30	p	605	CHL	NA
30	p	605	CHL	NC
30	p	606	CHL	ND
30	p	606	CHL	NA
30	p	606	CHL	NC
30	p	607	CHL	ND
30	p	607	CHL	NA
30	p	607	CHL	NC
30	p	608	CHL	ND
30	p	608	CHL	NA
30	p	608	CHL	NC
30	p	609	CHL	ND
30	p	609	CHL	NA
30	p	609	CHL	NC
30	q	303	CHL	ND
30	q	303	CHL	NA
30	q	303	CHL	NC
30	q	307	CHL	ND
30	q	307	CHL	NA

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Mol	Chain	Res	Type	Atom
30	q	307	CHL	NC
30	q	308	CHL	ND
30	q	308	CHL	NA
30	q	308	CHL	NC
30	q	309	CHL	ND
30	q	309	CHL	NA
30	q	309	CHL	NC
30	q	310	CHL	ND
30	q	310	CHL	NA
30	q	310	CHL	NC
30	q	311	CHL	ND
30	q	311	CHL	NA
30	q	311	CHL	NC
30	g	302	CHL	ND
30	g	302	CHL	NA
30	g	302	CHL	NC
30	g	306	CHL	ND
30	g	306	CHL	NA
30	g	306	CHL	NC
30	g	307	CHL	ND
30	g	307	CHL	NA
30	g	307	CHL	NC
30	g	308	CHL	ND
30	g	308	CHL	NA
30	g	308	CHL	NC
30	g	309	CHL	ND
30	g	309	CHL	NA
30	g	309	CHL	NC
30	n	301	CHL	ND
30	n	301	CHL	NA
30	n	301	CHL	NC
30	n	302	CHL	ND
30	n	302	CHL	NA
30	n	302	CHL	NC
30	n	306	CHL	ND
30	n	306	CHL	NA
30	n	306	CHL	NC
30	n	307	CHL	ND
30	n	307	CHL	NA
30	n	307	CHL	NC
30	n	308	CHL	ND
30	n	308	CHL	NA

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Mol	Chain	Res	Type	Atom
30	n	308	CHL	NC
30	n	309	CHL	ND
30	n	309	CHL	NA
30	n	309	CHL	NC
30	n	310	CHL	ND
30	n	310	CHL	NA
30	n	310	CHL	NC
30	r	308	CHL	ND
30	r	308	CHL	NA
30	r	308	CHL	NC
30	r	309	CHL	ND
30	r	309	CHL	NA
30	r	309	CHL	NC
30	r	310	CHL	ND
30	r	310	CHL	NA
30	r	310	CHL	NC
30	s	302	CHL	ND
30	s	302	CHL	NA
30	s	302	CHL	NC
30	s	307	CHL	ND
30	s	307	CHL	NA
30	s	307	CHL	NC
30	s	308	CHL	ND
30	s	308	CHL	NA
30	s	308	CHL	NC
30	s	309	CHL	ND
30	s	309	CHL	NA
30	s	309	CHL	NC
30	y	601	CHL	ND
30	y	601	CHL	NA
30	y	601	CHL	NC
30	y	605	CHL	ND
30	y	605	CHL	NA
30	y	605	CHL	NC
30	y	606	CHL	ND
30	y	606	CHL	NA
30	y	606	CHL	NC
30	y	607	CHL	ND
30	y	607	CHL	NA
30	y	607	CHL	NC
30	y	608	CHL	ND
30	y	608	CHL	NA

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Mol	Chain	Res	Type	Atom
30	y	608	CHL	NC
30	y	609	CHL	ND
30	y	609	CHL	NA
30	y	609	CHL	NC
31	1	602	CLA	ND
31	1	603	CLA	ND
31	1	604	CLA	ND
31	1	610	CLA	ND
31	1	611	CLA	ND
31	1	612	CLA	ND
31	1	613	CLA	ND
31	1	614	CLA	ND
31	2	602	CLA	ND
31	2	603	CLA	ND
31	2	604	CLA	ND
31	2	609	CLA	ND
31	2	610	CLA	ND
31	2	611	CLA	ND
31	2	612	CLA	ND
31	2	613	CLA	ND
31	3	301	CLA	ND
31	3	304	CLA	ND
31	3	305	CLA	ND
31	3	306	CLA	ND
31	3	311	CLA	ND
31	3	312	CLA	ND
31	3	313	CLA	ND
31	3	314	CLA	ND
31	3	315	CLA	ND
31	3	316	CLA	ND
31	4	602	CLA	ND
31	4	603	CLA	ND
31	4	604	CLA	ND
31	4	610	CLA	ND
31	4	611	CLA	ND
31	4	612	CLA	ND
31	4	613	CLA	ND
31	4	614	CLA	ND
31	5	602	CLA	ND
31	5	603	CLA	ND
31	5	604	CLA	ND
31	5	610	CLA	ND

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Mol	Chain	Res	Type	Atom
31	5	611	CLA	ND
31	5	612	CLA	ND
31	5	613	CLA	ND
31	5	614	CLA	ND
31	5	615	CLA	ND
31	6	303	CLA	ND
31	6	304	CLA	ND
31	6	305	CLA	ND
31	6	311	CLA	ND
31	6	312	CLA	ND
31	6	313	CLA	ND
31	6	314	CLA	ND
31	6	315	CLA	ND
31	6	316	CLA	ND
31	A	405	CLA	ND
31	A	406	CLA	ND
31	A	407	CLA	ND
31	A	409	CLA	ND
31	B	601	CLA	ND
31	B	602	CLA	ND
31	B	603	CLA	ND
31	B	604	CLA	ND
31	B	605	CLA	ND
31	B	606	CLA	ND
31	B	607	CLA	ND
31	B	608	CLA	ND
31	B	609	CLA	ND
31	B	610	CLA	ND
31	B	611	CLA	ND
31	B	612	CLA	ND
31	B	613	CLA	ND
31	B	614	CLA	ND
31	B	615	CLA	ND
31	B	616	CLA	ND
31	C	601	CLA	ND
31	C	602	CLA	ND
31	C	603	CLA	ND
31	C	604	CLA	ND
31	C	605	CLA	ND
31	C	606	CLA	ND
31	C	607	CLA	ND
31	C	608	CLA	ND

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Mol	Chain	Res	Type	Atom
31	C	609	CLA	ND
31	C	610	CLA	ND
31	C	611	CLA	ND
31	C	612	CLA	ND
31	C	613	CLA	ND
31	D	403	CLA	ND
31	D	404	CLA	ND
31	G	602	CLA	ND
31	G	603	CLA	ND
31	G	604	CLA	ND
31	G	609	CLA	ND
31	G	610	CLA	ND
31	G	611	CLA	ND
31	G	612	CLA	ND
31	G	613	CLA	ND
31	N	303	CLA	ND
31	N	304	CLA	ND
31	N	305	CLA	ND
31	N	310	CLA	ND
31	N	311	CLA	ND
31	N	312	CLA	ND
31	N	313	CLA	ND
31	N	314	CLA	ND
31	N	315	CLA	ND
31	N	321	CLA	ND
31	R	303	CLA	ND
31	R	304	CLA	ND
31	R	305	CLA	ND
31	R	306	CLA	ND
31	R	307	CLA	ND
31	R	311	CLA	ND
31	R	312	CLA	ND
31	R	313	CLA	ND
31	R	314	CLA	ND
31	R	315	CLA	ND
31	R	316	CLA	ND
31	S	303	CLA	ND
31	S	304	CLA	ND
31	S	305	CLA	ND
31	S	306	CLA	ND
31	S	310	CLA	ND
31	S	311	CLA	ND

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Mol	Chain	Res	Type	Atom
31	S	312	CLA	ND
31	S	313	CLA	ND
31	S	314	CLA	ND
31	S	315	CLA	ND
31	S	316	CLA	ND
31	Y	303	CLA	ND
31	Y	304	CLA	ND
31	Y	305	CLA	ND
31	Y	310	CLA	ND
31	Y	311	CLA	ND
31	Y	312	CLA	ND
31	Y	313	CLA	ND
31	Y	314	CLA	ND
31	0	602	CLA	ND
31	0	603	CLA	ND
31	0	604	CLA	ND
31	0	610	CLA	ND
31	0	611	CLA	ND
31	0	612	CLA	ND
31	0	613	CLA	ND
31	0	614	CLA	ND
31	0	615	CLA	ND
31	7	303	CLA	ND
31	7	304	CLA	ND
31	7	305	CLA	ND
31	7	311	CLA	ND
31	7	312	CLA	ND
31	7	313	CLA	ND
31	7	314	CLA	ND
31	7	315	CLA	ND
31	7	316	CLA	ND
31	8	602	CLA	ND
31	8	603	CLA	ND
31	8	604	CLA	ND
31	8	609	CLA	ND
31	8	610	CLA	ND
31	8	611	CLA	ND
31	8	612	CLA	ND
31	8	613	CLA	ND
31	8	614	CLA	ND
31	9	304	CLA	ND
31	9	305	CLA	ND

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Mol	Chain	Res	Type	Atom
31	9	306	CLA	ND
31	9	312	CLA	ND
31	9	313	CLA	ND
31	9	314	CLA	ND
31	9	315	CLA	ND
31	9	316	CLA	ND
31	p	602	CLA	ND
31	p	603	CLA	ND
31	p	604	CLA	ND
31	p	610	CLA	ND
31	p	611	CLA	ND
31	p	612	CLA	ND
31	p	613	CLA	ND
31	p	614	CLA	ND
31	p	615	CLA	ND
31	q	304	CLA	ND
31	q	305	CLA	ND
31	q	306	CLA	ND
31	q	312	CLA	ND
31	q	313	CLA	ND
31	q	314	CLA	ND
31	q	315	CLA	ND
31	q	316	CLA	ND
31	a	406	CLA	ND
31	a	407	CLA	ND
31	a	409	CLA	ND
31	b	602	CLA	ND
31	b	603	CLA	ND
31	b	604	CLA	ND
31	b	605	CLA	ND
31	b	606	CLA	ND
31	b	607	CLA	ND
31	b	608	CLA	ND
31	b	609	CLA	ND
31	b	610	CLA	ND
31	b	611	CLA	ND
31	b	612	CLA	ND
31	b	613	CLA	ND
31	b	614	CLA	ND
31	b	615	CLA	ND
31	b	616	CLA	ND
31	b	617	CLA	ND

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Mol	Chain	Res	Type	Atom
31	c	601	CLA	ND
31	c	602	CLA	ND
31	c	603	CLA	ND
31	c	604	CLA	ND
31	c	605	CLA	ND
31	c	606	CLA	ND
31	c	607	CLA	ND
31	c	608	CLA	ND
31	c	609	CLA	ND
31	c	610	CLA	ND
31	c	611	CLA	ND
31	c	612	CLA	ND
31	c	613	CLA	ND
31	d	401	CLA	ND
31	d	404	CLA	ND
31	d	405	CLA	ND
31	g	303	CLA	ND
31	g	304	CLA	ND
31	g	305	CLA	ND
31	g	310	CLA	ND
31	g	311	CLA	ND
31	g	312	CLA	ND
31	g	313	CLA	ND
31	g	314	CLA	ND
31	n	303	CLA	ND
31	n	304	CLA	ND
31	n	305	CLA	ND
31	n	311	CLA	ND
31	n	312	CLA	ND
31	n	313	CLA	ND
31	n	314	CLA	ND
31	n	315	CLA	ND
31	n	316	CLA	ND
31	r	303	CLA	ND
31	r	304	CLA	ND
31	r	305	CLA	ND
31	r	306	CLA	ND
31	r	307	CLA	ND
31	r	311	CLA	ND
31	r	312	CLA	ND
31	r	313	CLA	ND
31	r	314	CLA	ND

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Mol	Chain	Res	Type	Atom
31	r	315	CLA	ND
31	r	316	CLA	ND
31	s	303	CLA	ND
31	s	304	CLA	ND
31	s	305	CLA	ND
31	s	306	CLA	ND
31	s	310	CLA	ND
31	s	311	CLA	ND
31	s	312	CLA	ND
31	s	313	CLA	ND
31	s	314	CLA	ND
31	s	315	CLA	ND
31	s	316	CLA	ND
31	y	602	CLA	ND
31	y	603	CLA	ND
31	y	604	CLA	ND
31	y	610	CLA	ND
31	y	611	CLA	ND
31	y	612	CLA	ND
31	y	613	CLA	ND
31	y	614	CLA	ND
31	y	615	CLA	ND

All (7524) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	1	606	CHL	CAD-CBD-CGD-O1D
30	1	606	CHL	CAD-CBD-CGD-O2D
30	1	607	CHL	C3A-C2A-CAA-CBA
30	1	609	CHL	C11-C12-C13-C14
30	2	601	CHL	C1A-C2A-CAA-CBA
30	2	601	CHL	C3A-C2A-CAA-CBA
30	3	302	CHL	C2-C1-O2A-CGA
30	3	302	CHL	CAD-CBD-CGD-O1D
30	3	302	CHL	CAD-CBD-CGD-O2D
30	3	307	CHL	CAD-CBD-CGD-O1D
30	3	307	CHL	CAD-CBD-CGD-O2D
30	4	601	CHL	C3A-C2A-CAA-CBA
30	4	607	CHL	C2-C1-O2A-CGA
30	5	605	CHL	CHA-CBD-CGD-O1D
30	6	302	CHL	C3A-C2A-CAA-CBA
30	6	307	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	G	601	CHL	C11-C12-C13-C14
30	G	605	CHL	C1A-C2A-CAA-CBA
30	G	608	CHL	C11-C12-C13-C14
30	Y	302	CHL	C1A-C2A-CAA-CBA
30	Y	302	CHL	C3A-C2A-CAA-CBA
30	0	605	CHL	C2-C1-O2A-CGA
30	0	605	CHL	C4-C3-C5-C6
30	7	302	CHL	C1A-C2A-CAA-CBA
30	7	302	CHL	C3A-C2A-CAA-CBA
30	7	306	CHL	C1A-C2A-CAA-CBA
30	7	306	CHL	CAD-CBD-CGD-O1D
30	7	306	CHL	CAD-CBD-CGD-O2D
30	7	307	CHL	CBD-CGD-O2D-CED
30	8	608	CHL	C3A-C2A-CAA-CBA
30	9	308	CHL	C2-C3-C5-C6
30	9	308	CHL	C4-C3-C5-C6
30	9	309	CHL	CBD-CGD-O2D-CED
30	9	310	CHL	C3A-C2A-CAA-CBA
30	p	601	CHL	C1A-C2A-CAA-CBA
30	p	601	CHL	C3A-C2A-CAA-CBA
30	p	607	CHL	CAD-CBD-CGD-O1D
30	p	607	CHL	CAD-CBD-CGD-O2D
30	q	303	CHL	C3A-C2A-CAA-CBA
30	q	309	CHL	C2-C1-O2A-CGA
30	q	309	CHL	CAD-CBD-CGD-O1D
30	q	309	CHL	CAD-CBD-CGD-O2D
30	g	302	CHL	C11-C12-C13-C14
30	g	306	CHL	C1A-C2A-CAA-CBA
30	g	309	CHL	C11-C12-C13-C14
30	r	310	CHL	CHA-CBD-CGD-O1D
30	r	310	CHL	CHA-CBD-CGD-O2D
30	s	302	CHL	CHA-CBD-CGD-O1D
30	s	302	CHL	CHA-CBD-CGD-O2D
30	y	601	CHL	C1A-C2A-CAA-CBA
30	y	601	CHL	C3A-C2A-CAA-CBA
31	1	602	CLA	CHA-CBD-CGD-O1D
31	1	602	CLA	CHA-CBD-CGD-O2D
31	1	603	CLA	CBD-CGD-O2D-CED
31	1	604	CLA	CHA-CBD-CGD-O1D
31	1	604	CLA	CHA-CBD-CGD-O2D
31	1	610	CLA	CBD-CGD-O2D-CED
31	1	610	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
31	1	611	CLA	C2-C1-O2A-CGA
31	1	612	CLA	C2-C1-O2A-CGA
31	1	612	CLA	CHA-CBD-CGD-O1D
31	1	612	CLA	CHA-CBD-CGD-O2D
31	1	613	CLA	CBD-CGD-O2D-CED
31	1	614	CLA	C1A-C2A-CAA-CBA
31	1	614	CLA	C2-C1-O2A-CGA
31	1	614	CLA	CBD-CGD-O2D-CED
31	2	602	CLA	CBD-CGD-O2D-CED
31	2	603	CLA	CHA-CBD-CGD-O1D
31	2	603	CLA	CHA-CBD-CGD-O2D
31	2	604	CLA	CHA-CBD-CGD-O1D
31	2	604	CLA	CHA-CBD-CGD-O2D
31	2	609	CLA	C2-C1-O2A-CGA
31	2	609	CLA	CBD-CGD-O2D-CED
31	2	610	CLA	C1A-C2A-CAA-CBA
31	2	611	CLA	C2-C1-O2A-CGA
31	2	613	CLA	C1A-C2A-CAA-CBA
31	2	613	CLA	C3A-C2A-CAA-CBA
31	2	613	CLA	C2-C1-O2A-CGA
31	2	613	CLA	CBD-CGD-O2D-CED
31	3	304	CLA	CHA-CBD-CGD-O1D
31	3	304	CLA	CHA-CBD-CGD-O2D
31	3	305	CLA	C1A-C2A-CAA-CBA
31	3	305	CLA	CHA-CBD-CGD-O1D
31	3	305	CLA	CHA-CBD-CGD-O2D
31	3	305	CLA	CBD-CGD-O2D-CED
31	3	306	CLA	C3A-C2A-CAA-CBA
31	3	306	CLA	CHA-CBD-CGD-O1D
31	3	306	CLA	CHA-CBD-CGD-O2D
31	3	312	CLA	C1A-C2A-CAA-CBA
31	3	312	CLA	C3A-C2A-CAA-CBA
31	3	312	CLA	C2-C1-O2A-CGA
31	3	312	CLA	CBD-CGD-O2D-CED
31	3	313	CLA	C2-C1-O2A-CGA
31	3	313	CLA	CHA-CBD-CGD-O1D
31	3	313	CLA	CHA-CBD-CGD-O2D
31	3	316	CLA	C2-C1-O2A-CGA
31	3	316	CLA	CBD-CGD-O2D-CED
31	4	603	CLA	CHA-CBD-CGD-O1D
31	4	603	CLA	CHA-CBD-CGD-O2D
31	4	604	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	4	604	CLA	CAD-CBD-CGD-O1D
31	4	604	CLA	CAD-CBD-CGD-O2D
31	4	604	CLA	C2-C3-C5-C6
31	4	610	CLA	C2-C1-O2A-CGA
31	4	612	CLA	CHA-CBD-CGD-O1D
31	4	612	CLA	CHA-CBD-CGD-O2D
31	4	614	CLA	CBA-CGA-O2A-C1
31	4	614	CLA	O1A-CGA-O2A-C1
31	5	602	CLA	CHA-CBD-CGD-O2D
31	5	602	CLA	CBD-CGD-O2D-CED
31	5	603	CLA	CBA-CGA-O2A-C1
31	5	603	CLA	O1A-CGA-O2A-C1
31	5	603	CLA	CHA-CBD-CGD-O1D
31	5	603	CLA	CHA-CBD-CGD-O2D
31	5	604	CLA	CHA-CBD-CGD-O1D
31	5	604	CLA	CHA-CBD-CGD-O2D
31	5	611	CLA	C3A-C2A-CAA-CBA
31	5	612	CLA	CBA-CGA-O2A-C1
31	5	612	CLA	O1A-CGA-O2A-C1
31	5	612	CLA	CHA-CBD-CGD-O1D
31	5	612	CLA	CHA-CBD-CGD-O2D
31	5	613	CLA	C2-C1-O2A-CGA
31	5	614	CLA	C1A-C2A-CAA-CBA
31	5	614	CLA	CHA-CBD-CGD-O1D
31	5	614	CLA	CHA-CBD-CGD-O2D
31	5	614	CLA	CBD-CGD-O2D-CED
31	5	615	CLA	C1A-C2A-CAA-CBA
31	5	615	CLA	C2B-C3B-CAB-CBB
31	5	615	CLA	C4B-C3B-CAB-CBB
31	5	615	CLA	CBD-CGD-O2D-CED
31	6	303	CLA	CHA-CBD-CGD-O1D
31	6	303	CLA	CHA-CBD-CGD-O2D
31	6	304	CLA	C1A-C2A-CAA-CBA
31	6	304	CLA	C2-C1-O2A-CGA
31	6	304	CLA	CHA-CBD-CGD-O1D
31	6	304	CLA	CHA-CBD-CGD-O2D
31	6	305	CLA	C1A-C2A-CAA-CBA
31	6	305	CLA	C3A-C2A-CAA-CBA
31	6	305	CLA	CAD-CBD-CGD-O2D
31	6	311	CLA	C1A-C2A-CAA-CBA
31	6	311	CLA	C3A-C2A-CAA-CBA
31	6	312	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
31	6	313	CLA	CHA-CBD-CGD-O1D
31	6	313	CLA	CHA-CBD-CGD-O2D
31	6	316	CLA	C1A-C2A-CAA-CBA
31	6	316	CLA	C3A-C2A-CAA-CBA
31	6	316	CLA	C2-C1-O2A-CGA
31	6	316	CLA	CBD-CGD-O2D-CED
31	A	406	CLA	C1A-C2A-CAA-CBA
31	A	406	CLA	C3A-C2A-CAA-CBA
31	B	602	CLA	C1A-C2A-CAA-CBA
31	B	602	CLA	CBA-CGA-O2A-C1
31	B	603	CLA	CBD-CGD-O2D-CED
31	B	604	CLA	C1A-C2A-CAA-CBA
31	B	605	CLA	CBD-CGD-O2D-CED
31	B	606	CLA	C4B-C3B-CAB-CBB
31	B	606	CLA	CBD-CGD-O2D-CED
31	B	607	CLA	C1A-C2A-CAA-CBA
31	B	607	CLA	C3A-C2A-CAA-CBA
31	B	607	CLA	CAD-CBD-CGD-O1D
31	B	607	CLA	CAD-CBD-CGD-O2D
31	B	609	CLA	C1A-C2A-CAA-CBA
31	B	609	CLA	C3A-C2A-CAA-CBA
31	B	609	CLA	CBD-CGD-O2D-CED
31	B	609	CLA	C11-C10-C8-C9
31	B	610	CLA	C2-C1-O2A-CGA
31	B	610	CLA	C11-C12-C13-C14
31	B	612	CLA	C1A-C2A-CAA-CBA
31	B	612	CLA	C3A-C2A-CAA-CBA
31	B	612	CLA	C2-C1-O2A-CGA
31	B	613	CLA	CBD-CGD-O2D-CED
31	B	613	CLA	C4-C3-C5-C6
31	B	614	CLA	CBD-CGD-O2D-CED
31	B	614	CLA	C6-C7-C8-C9
31	B	616	CLA	CHA-CBD-CGD-O2D
31	C	601	CLA	CAD-CBD-CGD-O1D
31	C	601	CLA	CAD-CBD-CGD-O2D
31	C	602	CLA	CAD-CBD-CGD-O1D
31	C	602	CLA	CAD-CBD-CGD-O2D
31	C	604	CLA	CAD-CBD-CGD-O2D
31	C	605	CLA	CAD-CBD-CGD-O2D
31	C	606	CLA	C1A-C2A-CAA-CBA
31	C	606	CLA	C3A-C2A-CAA-CBA
31	C	606	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	C	606	CLA	CAD-CBD-CGD-O2D
31	C	607	CLA	C4B-C3B-CAB-CBB
31	C	607	CLA	CHA-CBD-CGD-O1D
31	C	607	CLA	CHA-CBD-CGD-O2D
31	C	609	CLA	C2-C1-O2A-CGA
31	C	610	CLA	C1A-C2A-CAA-CBA
31	C	612	CLA	CBA-CGA-O2A-C1
31	C	612	CLA	O1A-CGA-O2A-C1
31	C	613	CLA	C1A-C2A-CAA-CBA
31	D	403	CLA	C6-C7-C8-C9
31	D	404	CLA	C1A-C2A-CAA-CBA
31	G	602	CLA	CHA-CBD-CGD-O1D
31	G	602	CLA	CHA-CBD-CGD-O2D
31	G	603	CLA	C1A-C2A-CAA-CBA
31	G	603	CLA	CBA-CGA-O2A-C1
31	G	604	CLA	C1A-C2A-CAA-CBA
31	G	604	CLA	C3A-C2A-CAA-CBA
31	G	610	CLA	C1A-C2A-CAA-CBA
31	G	610	CLA	C3A-C2A-CAA-CBA
31	G	610	CLA	C2-C3-C5-C6
31	G	610	CLA	C4-C3-C5-C6
31	G	611	CLA	CHA-CBD-CGD-O2D
31	G	612	CLA	CBD-CGD-O2D-CED
31	G	613	CLA	C2-C1-O2A-CGA
31	N	303	CLA	CHA-CBD-CGD-O1D
31	N	303	CLA	CHA-CBD-CGD-O2D
31	N	304	CLA	CHA-CBD-CGD-O1D
31	N	304	CLA	CHA-CBD-CGD-O2D
31	N	305	CLA	C1A-C2A-CAA-CBA
31	N	305	CLA	CAD-CBD-CGD-O1D
31	N	305	CLA	CAD-CBD-CGD-O2D
31	N	305	CLA	C11-C10-C8-C9
31	N	310	CLA	C1A-C2A-CAA-CBA
31	N	310	CLA	C3A-C2A-CAA-CBA
31	N	311	CLA	C1A-C2A-CAA-CBA
31	N	311	CLA	C3A-C2A-CAA-CBA
31	N	313	CLA	C6-C7-C8-C9
31	N	314	CLA	C1A-C2A-CAA-CBA
31	N	314	CLA	C3A-C2A-CAA-CBA
31	N	321	CLA	C2-C1-O2A-CGA
31	N	321	CLA	CBD-CGD-O2D-CED
31	R	303	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	R	303	CLA	CHA-CBD-CGD-O1D
31	R	303	CLA	CHA-CBD-CGD-O2D
31	R	306	CLA	C1A-C2A-CAA-CBA
31	R	306	CLA	C3A-C2A-CAA-CBA
31	R	306	CLA	CHA-CBD-CGD-O1D
31	R	306	CLA	CHA-CBD-CGD-O2D
31	R	312	CLA	C1A-C2A-CAA-CBA
31	R	312	CLA	C3A-C2A-CAA-CBA
31	R	313	CLA	CBD-CGD-O2D-CED
31	R	314	CLA	C2-C1-O2A-CGA
31	R	314	CLA	CBD-CGD-O2D-CED
31	R	315	CLA	C2-C1-O2A-CGA
31	R	316	CLA	C1A-C2A-CAA-CBA
31	R	316	CLA	C3A-C2A-CAA-CBA
31	S	303	CLA	C1A-C2A-CAA-CBA
31	S	303	CLA	C3A-C2A-CAA-CBA
31	S	304	CLA	C1A-C2A-CAA-CBA
31	S	304	CLA	C3A-C2A-CAA-CBA
31	S	306	CLA	C2-C1-O2A-CGA
31	S	306	CLA	CAD-CBD-CGD-O2D
31	S	310	CLA	C1A-C2A-CAA-CBA
31	S	310	CLA	C3A-C2A-CAA-CBA
31	S	310	CLA	CBD-CGD-O2D-CED
31	S	312	CLA	C1A-C2A-CAA-CBA
31	S	312	CLA	C3A-C2A-CAA-CBA
31	S	312	CLA	C2-C1-O2A-CGA
31	S	314	CLA	CBD-CGD-O2D-CED
31	S	314	CLA	C11-C10-C8-C9
31	S	315	CLA	C3A-C2A-CAA-CBA
31	S	316	CLA	CBA-CGA-O2A-C1
31	S	316	CLA	CBD-CGD-O2D-CED
31	Y	303	CLA	CHA-CBD-CGD-O1D
31	Y	303	CLA	CHA-CBD-CGD-O2D
31	Y	304	CLA	CHA-CBD-CGD-O1D
31	Y	304	CLA	CHA-CBD-CGD-O2D
31	Y	305	CLA	CAD-CBD-CGD-O1D
31	Y	305	CLA	CAD-CBD-CGD-O2D
31	Y	311	CLA	C1A-C2A-CAA-CBA
31	Y	311	CLA	C3A-C2A-CAA-CBA
31	Y	313	CLA	CBD-CGD-O2D-CED
31	0	602	CLA	CHA-CBD-CGD-O1D
31	0	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	0	603	CLA	C1A-C2A-CAA-CBA
31	0	603	CLA	C3A-C2A-CAA-CBA
31	0	603	CLA	C2-C1-O2A-CGA
31	0	603	CLA	CHA-CBD-CGD-O1D
31	0	603	CLA	CHA-CBD-CGD-O2D
31	0	604	CLA	C1A-C2A-CAA-CBA
31	0	604	CLA	C3A-C2A-CAA-CBA
31	0	604	CLA	CAD-CBD-CGD-O1D
31	0	604	CLA	CAD-CBD-CGD-O2D
31	0	610	CLA	C1A-C2A-CAA-CBA
31	0	610	CLA	C3A-C2A-CAA-CBA
31	0	610	CLA	C11-C10-C8-C9
31	0	611	CLA	C2-C1-O2A-CGA
31	0	612	CLA	CBA-CGA-O2A-C1
31	0	612	CLA	O1A-CGA-O2A-C1
31	0	612	CLA	CHA-CBD-CGD-O1D
31	0	612	CLA	CHA-CBD-CGD-O2D
31	0	613	CLA	CBD-CGD-O2D-CED
31	0	614	CLA	C1A-C2A-CAA-CBA
31	0	614	CLA	C3A-C2A-CAA-CBA
31	0	614	CLA	CBD-CGD-O2D-CED
31	0	614	CLA	O1D-CGD-O2D-CED
31	0	615	CLA	C1A-C2A-CAA-CBA
31	0	615	CLA	C3A-C2A-CAA-CBA
31	7	303	CLA	CHA-CBD-CGD-O1D
31	7	303	CLA	CHA-CBD-CGD-O2D
31	7	304	CLA	CHA-CBD-CGD-O1D
31	7	304	CLA	CHA-CBD-CGD-O2D
31	7	305	CLA	CHA-CBD-CGD-O1D
31	7	305	CLA	CHA-CBD-CGD-O2D
31	7	312	CLA	C1A-C2A-CAA-CBA
31	7	312	CLA	C3A-C2A-CAA-CBA
31	7	313	CLA	CHA-CBD-CGD-O1D
31	7	313	CLA	CHA-CBD-CGD-O2D
31	7	314	CLA	CBD-CGD-O2D-CED
31	7	315	CLA	C1A-C2A-CAA-CBA
31	7	315	CLA	C2-C1-O2A-CGA
31	7	315	CLA	CBD-CGD-O2D-CED
31	7	316	CLA	C1A-C2A-CAA-CBA
31	7	316	CLA	C2-C1-O2A-CGA
31	8	602	CLA	CHA-CBD-CGD-O1D
31	8	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	8	603	CLA	CBA-CGA-O2A-C1
31	8	603	CLA	O1A-CGA-O2A-C1
31	8	603	CLA	CHA-CBD-CGD-O1D
31	8	603	CLA	CHA-CBD-CGD-O2D
31	8	604	CLA	C1A-C2A-CAA-CBA
31	8	604	CLA	CAD-CBD-CGD-O2D
31	8	609	CLA	C1A-C2A-CAA-CBA
31	8	609	CLA	C3A-C2A-CAA-CBA
31	8	609	CLA	C6-C7-C8-C9
31	8	610	CLA	C1A-C2A-CAA-CBA
31	8	610	CLA	C3A-C2A-CAA-CBA
31	8	612	CLA	C2-C1-O2A-CGA
31	8	612	CLA	CBD-CGD-O2D-CED
31	8	612	CLA	C6-C7-C8-C9
31	8	613	CLA	C1A-C2A-CAA-CBA
31	8	613	CLA	C3A-C2A-CAA-CBA
31	8	613	CLA	C2-C1-O2A-CGA
31	8	614	CLA	CBD-CGD-O2D-CED
31	9	304	CLA	C1A-C2A-CAA-CBA
31	9	304	CLA	C2-C1-O2A-CGA
31	9	304	CLA	CHA-CBD-CGD-O1D
31	9	304	CLA	CHA-CBD-CGD-O2D
31	9	305	CLA	CHA-CBD-CGD-O1D
31	9	305	CLA	CHA-CBD-CGD-O2D
31	9	306	CLA	C1A-C2A-CAA-CBA
31	9	306	CLA	C3A-C2A-CAA-CBA
31	9	306	CLA	CHA-CBD-CGD-O1D
31	9	306	CLA	CHA-CBD-CGD-O2D
31	9	312	CLA	C1A-C2A-CAA-CBA
31	9	314	CLA	C2-C1-O2A-CGA
31	9	314	CLA	CBD-CGD-O2D-CED
31	9	315	CLA	CBD-CGD-O2D-CED
31	p	604	CLA	CHA-CBD-CGD-O1D
31	p	604	CLA	CHA-CBD-CGD-O2D
31	p	610	CLA	CBD-CGD-O2D-CED
31	p	611	CLA	C1A-C2A-CAA-CBA
31	p	611	CLA	C3A-C2A-CAA-CBA
31	p	611	CLA	C11-C10-C8-C7
31	p	612	CLA	CHA-CBD-CGD-O1D
31	p	612	CLA	CHA-CBD-CGD-O2D
31	p	613	CLA	CHA-CBD-CGD-O1D
31	p	613	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	p	613	CLA	CBD-CGD-O2D-CED
31	p	614	CLA	CBD-CGD-O2D-CED
31	p	614	CLA	O1D-CGD-O2D-CED
31	q	304	CLA	CHA-CBD-CGD-O1D
31	q	304	CLA	CHA-CBD-CGD-O2D
31	q	305	CLA	CHA-CBD-CGD-O1D
31	q	305	CLA	CHA-CBD-CGD-O2D
31	q	312	CLA	O1A-CGA-O2A-C1
31	q	312	CLA	CBD-CGD-O2D-CED
31	q	314	CLA	CAD-CBD-CGD-O1D
31	q	314	CLA	CAD-CBD-CGD-O2D
31	q	316	CLA	C1A-C2A-CAA-CBA
31	q	316	CLA	C3A-C2A-CAA-CBA
31	q	316	CLA	CBD-CGD-O2D-CED
31	a	407	CLA	C1A-C2A-CAA-CBA
31	b	602	CLA	C1A-C2A-CAA-CBA
31	b	602	CLA	C3A-C2A-CAA-CBA
31	b	603	CLA	C1A-C2A-CAA-CBA
31	b	603	CLA	CBA-CGA-O2A-C1
31	b	603	CLA	O1A-CGA-O2A-C1
31	b	604	CLA	CBD-CGD-O2D-CED
31	b	605	CLA	C1A-C2A-CAA-CBA
31	b	605	CLA	CAD-CBD-CGD-O1D
31	b	605	CLA	CAD-CBD-CGD-O2D
31	b	606	CLA	CBD-CGD-O2D-CED
31	b	607	CLA	CBD-CGD-O2D-CED
31	b	608	CLA	C1A-C2A-CAA-CBA
31	b	608	CLA	C3A-C2A-CAA-CBA
31	b	608	CLA	CAD-CBD-CGD-O1D
31	b	608	CLA	CAD-CBD-CGD-O2D
31	b	609	CLA	C1A-C2A-CAA-CBA
31	b	610	CLA	C1A-C2A-CAA-CBA
31	b	610	CLA	C3A-C2A-CAA-CBA
31	b	610	CLA	CAD-CBD-CGD-O1D
31	b	610	CLA	CAD-CBD-CGD-O2D
31	b	610	CLA	CBD-CGD-O2D-CED
31	b	610	CLA	C11-C10-C8-C9
31	b	611	CLA	CHA-CBD-CGD-O1D
31	b	611	CLA	CHA-CBD-CGD-O2D
31	b	613	CLA	C1A-C2A-CAA-CBA
31	b	613	CLA	C3A-C2A-CAA-CBA
31	b	613	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	b	613	CLA	CHA-CBD-CGD-O2D
31	b	614	CLA	CBD-CGD-O2D-CED
31	b	614	CLA	C2-C3-C5-C6
31	b	614	CLA	C4-C3-C5-C6
31	b	615	CLA	C6-C7-C8-C9
31	b	617	CLA	CBA-CGA-O2A-C1
31	b	617	CLA	O1A-CGA-O2A-C1
31	c	601	CLA	CAD-CBD-CGD-O1D
31	c	601	CLA	CAD-CBD-CGD-O2D
31	c	602	CLA	CAD-CBD-CGD-O1D
31	c	602	CLA	CAD-CBD-CGD-O2D
31	c	603	CLA	CBD-CGD-O2D-CED
31	c	604	CLA	CAD-CBD-CGD-O2D
31	c	605	CLA	CAD-CBD-CGD-O1D
31	c	605	CLA	CAD-CBD-CGD-O2D
31	c	606	CLA	C1A-C2A-CAA-CBA
31	c	606	CLA	C3A-C2A-CAA-CBA
31	c	606	CLA	CAD-CBD-CGD-O1D
31	c	606	CLA	CAD-CBD-CGD-O2D
31	c	607	CLA	CHA-CBD-CGD-O1D
31	c	607	CLA	CHA-CBD-CGD-O2D
31	c	609	CLA	C2-C1-O2A-CGA
31	c	609	CLA	C6-C7-C8-C9
31	c	610	CLA	CBA-CGA-O2A-C1
31	c	610	CLA	O1A-CGA-O2A-C1
31	c	612	CLA	CBA-CGA-O2A-C1
31	c	612	CLA	O1A-CGA-O2A-C1
31	c	613	CLA	C1A-C2A-CAA-CBA
31	d	404	CLA	C2-C3-C5-C6
31	d	404	CLA	C4-C3-C5-C6
31	d	405	CLA	C1A-C2A-CAA-CBA
31	d	405	CLA	C3A-C2A-CAA-CBA
31	d	405	CLA	CBD-CGD-O2D-CED
31	g	303	CLA	C2-C1-O2A-CGA
31	g	303	CLA	CHA-CBD-CGD-O1D
31	g	303	CLA	CHA-CBD-CGD-O2D
31	g	304	CLA	C1A-C2A-CAA-CBA
31	g	304	CLA	C3A-C2A-CAA-CBA
31	g	304	CLA	CHA-CBD-CGD-O1D
31	g	304	CLA	CHA-CBD-CGD-O2D
31	g	305	CLA	C1A-C2A-CAA-CBA
31	g	305	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	g	311	CLA	C1A-C2A-CAA-CBA
31	g	311	CLA	C3A-C2A-CAA-CBA
31	g	311	CLA	C6-C7-C8-C10
31	g	314	CLA	CBD-CGD-O2D-CED
31	n	303	CLA	CHA-CBD-CGD-O1D
31	n	303	CLA	CHA-CBD-CGD-O2D
31	n	304	CLA	CBA-CGA-O2A-C1
31	n	304	CLA	O1A-CGA-O2A-C1
31	n	304	CLA	CHA-CBD-CGD-O1D
31	n	304	CLA	CHA-CBD-CGD-O2D
31	n	305	CLA	C1A-C2A-CAA-CBA
31	n	311	CLA	C1A-C2A-CAA-CBA
31	n	311	CLA	C3A-C2A-CAA-CBA
31	n	312	CLA	C1A-C2A-CAA-CBA
31	n	312	CLA	C3A-C2A-CAA-CBA
31	n	314	CLA	C2-C1-O2A-CGA
31	n	314	CLA	CBD-CGD-O2D-CED
31	n	314	CLA	C6-C7-C8-C9
31	n	315	CLA	C1A-C2A-CAA-CBA
31	n	315	CLA	C3A-C2A-CAA-CBA
31	n	315	CLA	C2-C1-O2A-CGA
31	r	303	CLA	C1A-C2A-CAA-CBA
31	r	303	CLA	C3A-C2A-CAA-CBA
31	r	303	CLA	CHA-CBD-CGD-O1D
31	r	303	CLA	CHA-CBD-CGD-O2D
31	r	305	CLA	CHA-CBD-CGD-O1D
31	r	305	CLA	CHA-CBD-CGD-O2D
31	r	306	CLA	C1A-C2A-CAA-CBA
31	r	306	CLA	C3A-C2A-CAA-CBA
31	r	311	CLA	CBD-CGD-O2D-CED
31	r	312	CLA	C1A-C2A-CAA-CBA
31	r	312	CLA	C3A-C2A-CAA-CBA
31	r	313	CLA	CBD-CGD-O2D-CED
31	r	314	CLA	C2-C1-O2A-CGA
31	r	315	CLA	C1A-C2A-CAA-CBA
31	r	315	CLA	C3A-C2A-CAA-CBA
31	r	315	CLA	C2-C1-O2A-CGA
31	r	316	CLA	C1A-C2A-CAA-CBA
31	r	316	CLA	C3A-C2A-CAA-CBA
31	s	303	CLA	C3A-C2A-CAA-CBA
31	s	303	CLA	CBA-CGA-O2A-C1
31	s	303	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	s	304	CLA	C1A-C2A-CAA-CBA
31	s	304	CLA	CHA-CBD-CGD-O1D
31	s	304	CLA	CHA-CBD-CGD-O2D
31	s	305	CLA	CHA-CBD-CGD-O1D
31	s	305	CLA	CHA-CBD-CGD-O2D
31	s	306	CLA	CHA-CBD-CGD-O1D
31	s	306	CLA	CHA-CBD-CGD-O2D
31	s	310	CLA	C1A-C2A-CAA-CBA
31	s	310	CLA	C3A-C2A-CAA-CBA
31	s	312	CLA	C1A-C2A-CAA-CBA
31	s	312	CLA	C3A-C2A-CAA-CBA
31	s	314	CLA	CBD-CGD-O2D-CED
31	s	315	CLA	C3A-C2A-CAA-CBA
31	s	316	CLA	C1A-C2A-CAA-CBA
31	s	316	CLA	CBA-CGA-O2A-C1
31	s	316	CLA	CBD-CGD-O2D-CED
31	y	602	CLA	CHA-CBD-CGD-O1D
31	y	602	CLA	CHA-CBD-CGD-O2D
31	y	603	CLA	CHA-CBD-CGD-O1D
31	y	603	CLA	CHA-CBD-CGD-O2D
31	y	604	CLA	CAD-CBD-CGD-O1D
31	y	604	CLA	CAD-CBD-CGD-O2D
31	y	612	CLA	C6-C7-C8-C9
31	y	614	CLA	CBA-CGA-O2A-C1
31	y	614	CLA	O1A-CGA-O2A-C1
31	y	615	CLA	C1A-C2A-CAA-CBA
31	y	615	CLA	C3A-C2A-CAA-CBA
31	y	615	CLA	CHA-CBD-CGD-O1D
31	y	615	CLA	CHA-CBD-CGD-O2D
32	1	616	LUT	C7-C8-C9-C10
32	3	317	LUT	C11-C12-C13-C14
32	3	318	LUT	C11-C12-C13-C14
32	3	318	LUT	C11-C12-C13-C20
32	4	616	LUT	C7-C8-C9-C10
32	4	616	LUT	C7-C8-C9-C19
32	4	616	LUT	C31-C32-C33-C34
32	5	616	LUT	C11-C12-C13-C14
32	5	616	LUT	C31-C32-C33-C34
32	5	617	LUT	C7-C8-C9-C10
32	5	617	LUT	C7-C8-C9-C19
32	5	617	LUT	C31-C32-C33-C34
32	6	317	LUT	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	6	317	LUT	C31-C32-C33-C34
32	6	318	LUT	C7-C8-C9-C10
32	6	318	LUT	C7-C8-C9-C19
32	6	318	LUT	C31-C32-C33-C34
32	G	615	LUT	C21-C26-C27-C28
32	G	615	LUT	C25-C26-C27-C28
32	G	615	LUT	C31-C32-C33-C40
32	G	615	LUT	C33-C34-C35-C15
32	N	316	LUT	C11-C12-C13-C14
32	N	317	LUT	C31-C32-C33-C34
32	R	317	LUT	C11-C12-C13-C14
32	S	317	LUT	C7-C8-C9-C10
32	S	317	LUT	C7-C8-C9-C19
32	S	317	LUT	C11-C12-C13-C14
32	S	317	LUT	C11-C12-C13-C20
32	S	317	LUT	C31-C32-C33-C34
32	S	318	LUT	C11-C12-C13-C14
32	S	318	LUT	C21-C26-C27-C28
32	S	318	LUT	C25-C26-C27-C28
32	S	318	LUT	C31-C32-C33-C34
32	0	616	LUT	C11-C12-C13-C14
32	7	317	LUT	C11-C12-C13-C14
32	7	318	LUT	C7-C8-C9-C10
32	7	318	LUT	C7-C8-C9-C19
32	8	615	LUT	C7-C8-C9-C10
32	8	615	LUT	C7-C8-C9-C19
32	8	615	LUT	C11-C12-C13-C14
32	8	615	LUT	C31-C32-C33-C34
32	8	616	LUT	C31-C32-C33-C34
32	p	617	LUT	C7-C8-C9-C10
32	q	318	LUT	C11-C12-C13-C14
32	q	318	LUT	C31-C32-C33-C34
32	g	316	LUT	C21-C26-C27-C28
32	g	316	LUT	C25-C26-C27-C28
32	g	316	LUT	C31-C32-C33-C34
32	n	317	LUT	C7-C8-C9-C10
32	n	317	LUT	C7-C8-C9-C19
32	n	317	LUT	C11-C12-C13-C14
32	n	317	LUT	C31-C32-C33-C34
32	n	318	LUT	C31-C32-C33-C34
32	r	317	LUT	C11-C12-C13-C14
32	s	317	LUT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
32	s	317	LUT	C11-C12-C13-C14
32	s	317	LUT	C11-C12-C13-C20
32	s	317	LUT	C31-C32-C33-C34
32	s	317	LUT	C31-C32-C33-C40
32	s	318	LUT	C11-C12-C13-C14
32	s	318	LUT	C11-C12-C13-C20
32	y	617	LUT	C7-C8-C9-C10
32	y	617	LUT	C7-C8-C9-C19
33	1	617	LHG	O1-C1-C2-C3
33	1	617	LHG	C1-C2-C3-O3
33	1	617	LHG	C3-O3-P-O4
33	1	617	LHG	C3-O3-P-O6
33	1	617	LHG	C4-O6-P-O3
33	1	617	LHG	C4-O6-P-O4
33	2	617	LHG	C3-O3-P-O4
33	2	617	LHG	C3-O3-P-O6
33	2	617	LHG	C4-O6-P-O3
33	2	617	LHG	C4-O6-P-O4
33	2	617	LHG	C4-O6-P-O5
33	3	320	LHG	C4-O6-P-O3
33	3	320	LHG	C4-O6-P-O4
33	3	320	LHG	C4-O6-P-O5
33	3	320	LHG	O7-C5-C6-O8
33	4	618	LHG	C1-C2-C3-O3
33	4	618	LHG	C4-O6-P-O3
33	4	618	LHG	C4-O6-P-O4
33	4	618	LHG	C4-O6-P-O5
33	4	618	LHG	O9-C7-O7-C5
33	4	618	LHG	C8-C7-O7-C5
33	5	619	LHG	O1-C1-C2-O2
33	5	619	LHG	C3-O3-P-O5
33	5	619	LHG	C3-O3-P-O6
33	5	619	LHG	C4-O6-P-O3
33	5	619	LHG	C4-O6-P-O5
33	5	619	LHG	O9-C7-O7-C5
33	6	320	LHG	C4-O6-P-O3
33	6	320	LHG	C4-O6-P-O4
33	6	320	LHG	C4-O6-P-O5
33	A	415	LHG	O1-C1-C2-C3
33	A	415	LHG	C3-O3-P-O6
33	A	415	LHG	C4-O6-P-O3
33	A	415	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
33	A	415	LHG	O7-C5-C6-O8
33	A	417	LHG	C3-O3-P-O5
33	A	417	LHG	C4-O6-P-O3
33	A	417	LHG	C4-O6-P-O4
33	A	417	LHG	O6-C4-C5-O7
33	C	623	LHG	O1-C1-C2-C3
33	C	623	LHG	C1-C2-C3-O3
33	C	623	LHG	C4-O6-P-O5
33	C	623	LHG	C8-C7-O7-C5
33	D	407	LHG	O1-C1-C2-C3
33	D	407	LHG	C1-C2-C3-O3
33	D	407	LHG	C3-O3-P-O5
33	D	407	LHG	C4-O6-P-O5
33	D	408	LHG	O1-C1-C2-C3
33	D	408	LHG	C1-C2-C3-O3
33	D	408	LHG	C3-O3-P-O6
33	D	408	LHG	C4-O6-P-O5
33	G	618	LHG	C4-O6-P-O3
33	G	618	LHG	C4-O6-P-O4
33	G	618	LHG	C4-O6-P-O5
33	K	102	LHG	O1-C1-C2-O2
33	K	102	LHG	O1-C1-C2-C3
33	K	102	LHG	C1-C2-C3-O3
33	K	102	LHG	C3-O3-P-O4
33	K	102	LHG	C3-O3-P-O5
33	K	102	LHG	C3-O3-P-O6
33	K	102	LHG	C4-O6-P-O5
33	K	102	LHG	O9-C7-O7-C5
33	K	102	LHG	C8-C7-O7-C5
33	L	101	LHG	C4-O6-P-O3
33	L	101	LHG	C4-O6-P-O5
33	M	101	LHG	C3-O3-P-O5
33	M	101	LHG	C3-O3-P-O6
33	M	101	LHG	O7-C5-C6-O8
33	M	101	LHG	C8-C7-O7-C5
33	N	319	LHG	O1-C1-C2-O2
33	N	319	LHG	O1-C1-C2-C3
33	N	319	LHG	C3-O3-P-O5
33	N	319	LHG	C3-O3-P-O6
33	N	319	LHG	C4-O6-P-O3
33	N	319	LHG	C4-O6-P-O4
33	R	320	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
33	R	320	LHG	C4-O6-P-O3
33	R	320	LHG	C4-O6-P-O4
33	S	320	LHG	O1-C1-C2-O2
33	S	320	LHG	O1-C1-C2-C3
33	S	320	LHG	C1-C2-C3-O3
33	S	320	LHG	C3-O3-P-O5
33	S	320	LHG	C4-O6-P-O3
33	S	320	LHG	C4-O6-P-O4
33	S	320	LHG	C4-O6-P-O5
33	S	322	LHG	C1-C2-C3-O3
33	S	322	LHG	O2-C2-C3-O3
33	S	322	LHG	C3-O3-P-O6
33	S	322	LHG	C4-O6-P-O3
33	Y	318	LHG	C1-C2-C3-O3
33	Y	318	LHG	C3-O3-P-O4
33	Y	318	LHG	C3-O3-P-O6
33	Y	318	LHG	C4-O6-P-O3
33	0	619	LHG	O1-C1-C2-C3
33	0	619	LHG	C4-O6-P-O3
33	0	619	LHG	C4-O6-P-O5
33	0	619	LHG	O7-C5-C6-O8
33	0	619	LHG	C8-C7-O7-C5
33	7	319	LHG	C1-C2-C3-O3
33	7	319	LHG	C4-O6-P-O3
33	7	319	LHG	C4-O6-P-O4
33	8	618	LHG	O1-C1-C2-O2
33	8	618	LHG	C1-C2-C3-O3
33	8	618	LHG	O2-C2-C3-O3
33	8	618	LHG	C4-O6-P-O3
33	8	618	LHG	C4-O6-P-O4
33	8	618	LHG	C4-C5-O7-C7
33	9	320	LHG	O1-C1-C2-C3
33	9	320	LHG	C1-C2-C3-O3
33	9	320	LHG	C4-O6-P-O5
33	p	619	LHG	O1-C1-C2-O2
33	p	619	LHG	C1-C2-C3-O3
33	p	619	LHG	C4-O6-P-O3
33	p	619	LHG	C4-O6-P-O4
33	p	619	LHG	C4-O6-P-O5
33	p	619	LHG	C8-C7-O7-C5
33	q	320	LHG	O1-C1-C2-C3
33	q	320	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
33	q	320	LHG	C3-O3-P-O4
33	q	320	LHG	C3-O3-P-O6
33	q	320	LHG	C4-O6-P-O3
33	q	320	LHG	C4-O6-P-O4
33	a	415	LHG	C1-C2-C3-O3
33	a	415	LHG	C3-O3-P-O6
33	a	415	LHG	C4-O6-P-O4
33	a	415	LHG	O6-C4-C5-O7
33	b	625	LHG	C4-O6-P-O3
33	b	625	LHG	C4-O6-P-O5
33	b	628	LHG	C3-O3-P-O5
33	b	628	LHG	C4-O6-P-O3
33	b	628	LHG	C4-O6-P-O4
33	c	622	LHG	O1-C1-C2-C3
33	c	622	LHG	C3-O3-P-O5
33	c	622	LHG	C3-O3-P-O6
33	c	622	LHG	C4-O6-P-O3
33	c	622	LHG	C4-O6-P-O4
33	d	408	LHG	O1-C1-C2-C3
33	d	408	LHG	C1-C2-C3-O3
33	d	408	LHG	C4-O6-P-O3
33	d	408	LHG	C4-O6-P-O5
33	e	101	LHG	C3-O3-P-O6
33	e	101	LHG	C4-O6-P-O3
33	e	101	LHG	C4-O6-P-O4
33	g	319	LHG	O1-C1-C2-C3
33	g	319	LHG	C3-O3-P-O5
33	g	319	LHG	C4-O6-P-O3
33	j	102	LHG	C3-O3-P-O4
33	j	102	LHG	C3-O3-P-O5
33	j	102	LHG	C3-O3-P-O6
33	j	102	LHG	C4-O6-P-O3
33	j	102	LHG	O7-C5-C6-O8
33	l	101	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O4
33	l	101	LHG	C4-O6-P-O5
33	n	320	LHG	O1-C1-C2-O2
33	n	320	LHG	C1-C2-C3-O3
33	n	320	LHG	O2-C2-C3-O3
33	n	320	LHG	C4-O6-P-O3
33	n	320	LHG	C4-O6-P-O4
33	r	320	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
33	r	320	LHG	C4-O6-P-O3
33	r	320	LHG	C4-O6-P-O4
33	r	320	LHG	C4-O6-P-O5
33	s	320	LHG	C1-C2-C3-O3
33	s	320	LHG	C4-O6-P-O3
33	s	320	LHG	C4-O6-P-O4
33	s	320	LHG	C4-O6-P-O5
33	s	320	LHG	O7-C5-C6-O8
33	s	322	LHG	C4-O6-P-O3
33	s	322	LHG	C4-O6-P-O4
33	s	322	LHG	C8-C7-O7-C5
33	t	102	LHG	O1-C1-C2-C3
33	t	102	LHG	C1-C2-C3-O3
33	t	102	LHG	C3-O3-P-O6
33	t	102	LHG	C4-O6-P-O3
33	t	102	LHG	C4-O6-P-O4
33	y	619	LHG	C1-C2-C3-O3
33	y	619	LHG	C3-O3-P-O4
33	y	619	LHG	C3-O3-P-O5
33	y	619	LHG	C3-O3-P-O6
33	y	619	LHG	C4-O6-P-O3
33	z	102	LHG	O1-C1-C2-C3
33	z	102	LHG	C1-C2-C3-O3
33	z	102	LHG	C4-O6-P-O3
33	z	102	LHG	C4-O6-P-O5
33	z	102	LHG	O6-C4-C5-O7
33	z	102	LHG	O9-C7-O7-C5
33	z	102	LHG	C8-C7-O7-C5
33	F1	301	LHG	O2-C2-C3-O3
33	F1	301	LHG	C3-O3-P-O5
33	F1	301	LHG	C3-O3-P-O6
33	F1	301	LHG	O7-C5-C6-O8
34	4	620	LMG	O6-C1-O1-C7
34	4	620	LMG	C11-C10-O7-C8
34	4	621	LMG	O6-C1-O1-C7
34	4	621	LMG	C11-C10-O7-C8
34	5	620	LMG	C11-C10-O7-C8
34	6	321	LMG	O6-C1-O1-C7
34	6	322	LMG	C2-C1-O1-C7
34	6	322	LMG	O6-C1-O1-C7
34	6	322	LMG	O9-C10-O7-C8
34	6	322	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
34	6	323	LMG	O10-C28-O8-C9
34	A	412	LMG	O6-C1-O1-C7
34	A	412	LMG	C9-C8-O7-C10
34	A	414	LMG	O9-C10-O7-C8
34	A	414	LMG	C11-C10-O7-C8
34	A	418	LMG	C11-C10-O7-C8
34	B	622	LMG	C11-C10-O7-C8
34	B	625	LMG	O10-C28-O8-C9
34	C	621	LMG	O9-C10-O7-C8
34	C	621	LMG	C11-C10-O7-C8
34	C	622	LMG	C11-C10-O7-C8
34	G	622	LMG	C11-C10-O7-C8
34	I	101	LMG	C11-C10-O7-C8
34	J	102	LMG	C11-C10-O7-C8
34	N	320	LMG	C11-C10-O7-C8
34	W	202	LMG	O6-C1-O1-C7
34	W	203	LMG	O1-C7-C8-O7
34	W	203	LMG	C11-C10-O7-C8
34	X	202	LMG	C11-C10-O7-C8
34	X	203	LMG	O7-C8-C9-O8
34	Y	319	LMG	O6-C1-O1-C7
34	0	620	LMG	C2-C1-O1-C7
34	0	620	LMG	O6-C1-O1-C7
34	0	620	LMG	C11-C10-O7-C8
34	7	301	LMG	C11-C10-O7-C8
34	7	322	LMG	C11-C10-O7-C8
34	9	301	LMG	O9-C10-O7-C8
34	9	301	LMG	C11-C10-O7-C8
34	9	302	LMG	O6-C1-O1-C7
34	9	321	LMG	O6-C1-O1-C7
34	9	321	LMG	C11-C10-O7-C8
34	p	620	LMG	C11-C10-O7-C8
34	q	301	LMG	C2-C1-O1-C7
34	q	302	LMG	O9-C10-O7-C8
34	a	401	LMG	O9-C10-O7-C8
34	a	401	LMG	C11-C10-O7-C8
34	a	413	LMG	C11-C10-O7-C8
34	b	601	LMG	O6-C1-O1-C7
34	b	601	LMG	C11-C10-O7-C8
34	b	622	LMG	O6-C1-O1-C7
34	b	623	LMG	C11-C10-O7-C8
34	b	624	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
34	b	624	LMG	C8-C9-O8-C28
34	b	624	LMG	C11-C10-O7-C8
34	b	624	LMG	O10-C28-O8-C9
34	b	629	LMG	C11-C10-O7-C8
34	c	620	LMG	O6-C1-O1-C7
34	c	621	LMG	C11-C10-O7-C8
34	c	624	LMG	C11-C10-O7-C8
34	f	101	LMG	C11-C10-O7-C8
34	g	322	LMG	O6-C1-O1-C7
34	j	101	LMG	O10-C28-O8-C9
34	k	101	LMG	C11-C10-O7-C8
34	k	102	LMG	C11-C10-O7-C8
34	m	102	LMG	O6-C1-O1-C7
34	m	102	LMG	C11-C10-O7-C8
34	n	321	LMG	O6-C1-O1-C7
34	n	322	LMG	O6-C1-O1-C7
34	w	201	LMG	O6-C1-O1-C7
34	w	201	LMG	O1-C7-C8-O7
34	w	203	LMG	C11-C10-O7-C8
34	w	204	LMG	C2-C1-O1-C7
34	w	204	LMG	O6-C1-O1-C7
34	w	204	LMG	O9-C10-O7-C8
34	w	204	LMG	C11-C10-O7-C8
34	w	205	LMG	C2-C1-O1-C7
34	w	205	LMG	O6-C1-O1-C7
34	w	205	LMG	O9-C10-O7-C8
34	x	202	LMG	O9-C10-O7-C8
34	x	202	LMG	C11-C10-O7-C8
34	y	620	LMG	C11-C10-O7-C8
34	Q1	101	LMG	O6-C1-O1-C7
34	Q1	101	LMG	O9-C10-O7-C8
34	Q1	101	LMG	C11-C10-O7-C8
34	q1	101	LMG	C11-C10-O7-C8
35	2	614	RRX	C23-C24-C25-C30
35	2	614	RRX	C23-C24-C25-C26
35	2	614	RRX	C21-C22-C23-C24
35	2	614	RRX	C36-C18-C19-C20
35	2	614	RRX	C17-C18-C19-C20
35	2	614	RRX	C11-C12-C13-C14
35	2	614	RRX	C7-C8-C9-C10
35	2	614	RRX	C7-C8-C9-C34
35	4	615	RRX	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
35	4	615	RRX	C23-C24-C25-C26
35	4	615	RRX	C21-C22-C23-C24
35	4	615	RRX	C36-C18-C19-C20
35	4	615	RRX	C17-C18-C19-C20
35	4	615	RRX	C11-C12-C13-C14
35	4	615	RRX	C9-C10-C11-C12
35	4	615	RRX	C7-C8-C9-C10
35	4	615	RRX	C7-C8-C9-C34
35	G	614	RRX	C23-C24-C25-C30
35	G	614	RRX	C23-C24-C25-C26
35	G	614	RRX	C21-C22-C23-C24
35	G	614	RRX	C36-C18-C19-C20
35	G	614	RRX	C17-C18-C19-C20
35	G	614	RRX	C11-C12-C13-C14
35	G	614	RRX	C9-C10-C11-C12
35	G	614	RRX	C7-C8-C9-C10
35	G	614	RRX	C7-C8-C9-C34
35	9	317	RRX	C23-C24-C25-C30
35	9	317	RRX	C23-C24-C25-C26
35	9	317	RRX	C21-C22-C23-C24
35	9	317	RRX	C36-C18-C19-C20
35	9	317	RRX	C17-C18-C19-C20
35	9	317	RRX	C11-C12-C13-C14
35	9	317	RRX	C9-C10-C11-C12
35	9	317	RRX	C7-C8-C9-C10
35	9	317	RRX	C7-C8-C9-C34
35	q	317	RRX	C23-C24-C25-C30
35	q	317	RRX	C37-C22-C23-C24
35	q	317	RRX	C21-C22-C23-C24
35	q	317	RRX	C7-C8-C9-C10
35	g	315	RRX	C37-C22-C23-C24
35	g	315	RRX	C7-C8-C9-C10
36	2	616	NEX	C10-C11-C12-C13
36	2	616	NEX	C12-C13-C14-C15
36	2	616	NEX	C20-C13-C14-C15
36	2	616	NEX	C28-C29-C30-C31
36	2	616	NEX	C39-C29-C30-C31
36	2	616	NEX	C31-C32-C33-C34
36	2	616	NEX	C31-C32-C33-C40
36	3	319	NEX	C32-C33-C34-C35
36	3	319	NEX	C40-C33-C34-C35
36	4	617	NEX	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
36	4	617	NEX	C26-C27-C28-C29
36	4	617	NEX	C39-C29-C30-C31
36	5	618	NEX	C10-C11-C12-C13
36	5	618	NEX	C11-C12-C13-C14
36	5	618	NEX	C14-C15-C35-C34
36	5	618	NEX	C30-C31-C32-C33
36	6	319	NEX	C28-C29-C30-C31
36	6	319	NEX	C39-C29-C30-C31
36	6	319	NEX	C29-C30-C31-C32
36	6	319	NEX	C30-C31-C32-C33
36	N	318	NEX	C10-C11-C12-C13
36	N	318	NEX	C11-C12-C13-C14
36	N	318	NEX	C32-C33-C34-C35
36	N	318	NEX	C40-C33-C34-C35
36	0	618	NEX	C28-C29-C30-C31
36	0	618	NEX	C39-C29-C30-C31
36	0	618	NEX	C29-C30-C31-C32
36	0	618	NEX	C30-C31-C32-C33
36	8	617	NEX	C11-C12-C13-C14
36	9	319	NEX	C9-C10-C11-C12
36	9	319	NEX	C10-C11-C12-C13
36	9	319	NEX	C14-C15-C35-C34
36	p	618	NEX	C11-C10-C9-C8
36	p	618	NEX	C11-C10-C9-C19
36	q	319	NEX	C10-C11-C12-C13
36	q	319	NEX	C11-C12-C13-C14
36	q	319	NEX	C11-C12-C13-C20
36	q	319	NEX	C14-C15-C35-C34
36	q	319	NEX	C32-C33-C34-C35
36	q	319	NEX	C40-C33-C34-C35
36	g	317	NEX	C10-C11-C12-C13
36	g	317	NEX	C11-C12-C13-C14
36	g	317	NEX	C11-C12-C13-C20
36	g	317	NEX	C12-C13-C14-C15
36	g	317	NEX	C20-C13-C14-C15
36	g	317	NEX	C28-C29-C30-C31
36	g	317	NEX	C39-C29-C30-C31
36	n	319	NEX	C11-C10-C9-C8
36	n	319	NEX	C11-C10-C9-C19
36	n	319	NEX	C10-C11-C12-C13
36	n	319	NEX	C11-C12-C13-C14
36	n	319	NEX	C11-C12-C13-C20

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Mol	Chain	Res	Type	Atoms
36	r	319	NEX	C7-C8-C9-C10
36	r	319	NEX	C28-C29-C30-C31
37	2	619	XAT	C21-C26-C27-C28
37	2	619	XAT	C25-C26-C27-C28
37	2	619	XAT	O24-C26-C27-C28
37	2	619	XAT	C26-C27-C28-C29
37	4	619	XAT	C21-C26-C27-C28
37	4	619	XAT	C25-C26-C27-C28
37	4	619	XAT	O24-C26-C27-C28
37	4	619	XAT	C26-C27-C28-C29
37	G	620	XAT	C21-C26-C27-C28
37	G	620	XAT	C25-C26-C27-C28
37	G	620	XAT	O24-C26-C27-C28
37	G	620	XAT	C26-C27-C28-C29
37	9	322	XAT	C21-C26-C27-C28
37	9	322	XAT	C25-C26-C27-C28
37	9	322	XAT	O24-C26-C27-C28
37	9	322	XAT	C26-C27-C28-C29
37	q	321	XAT	C21-C26-C27-C28
37	q	321	XAT	C25-C26-C27-C28
37	q	321	XAT	O24-C26-C27-C28
37	q	321	XAT	C26-C27-C28-C29
37	g	321	XAT	C21-C26-C27-C28
37	g	321	XAT	C25-C26-C27-C28
37	g	321	XAT	O24-C26-C27-C28
37	g	321	XAT	C26-C27-C28-C29
38	6	301	SQD	O5-C5-C6-S
38	A	411	SQD	O47-C45-C46-O48
38	A	413	SQD	C2-C1-O6-C44
38	A	413	SQD	O5-C1-O6-C44
38	A	413	SQD	O5-C5-C6-S
38	B	620	SQD	O5-C1-O6-C44
38	B	620	SQD	O49-C7-O47-C45
38	B	620	SQD	C8-C7-O47-C45
38	B	623	SQD	O5-C5-C6-S
38	G	617	SQD	C2-C1-O6-C44
38	G	617	SQD	C8-C7-O47-C45
38	G	617	SQD	O5-C5-C6-S
38	R	322	SQD	O5-C5-C6-S
38	S	301	SQD	O6-C44-C45-O47
38	Y	320	SQD	O5-C1-O6-C44
38	Y	320	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
38	0	621	SQD	C2-C1-O6-C44
38	0	621	SQD	O5-C1-O6-C44
38	0	621	SQD	C8-C7-O47-C45
38	0	621	SQD	O5-C5-C6-S
38	a	412	SQD	C2-C1-O6-C44
38	a	412	SQD	O5-C1-O6-C44
38	a	412	SQD	O5-C5-C6-S
38	b	621	SQD	C8-C7-O47-C45
38	b	621	SQD	O5-C5-C6-S
38	b	627	SQD	O5-C5-C6-S
38	g	301	SQD	O5-C1-O6-C44
38	g	301	SQD	O5-C5-C6-S
38	g	318	SQD	O5-C1-O6-C44
38	r	322	SQD	C2-C1-O6-C44
38	r	322	SQD	O5-C1-O6-C44
38	r	322	SQD	O49-C7-O47-C45
38	r	322	SQD	C8-C7-O47-C45
38	r	322	SQD	O5-C5-C6-S
38	s	301	SQD	O5-C1-O6-C44
38	s	301	SQD	O5-C5-C6-S
38	x	201	SQD	O5-C5-C6-S
38	y	621	SQD	O6-C44-C45-O47
38	y	621	SQD	C8-C7-O47-C45
42	A	408	PHO	C11-C10-C8-C9
43	B	617	BCR	C7-C8-C9-C10
43	B	617	BCR	C7-C8-C9-C34
43	B	617	BCR	C11-C12-C13-C14
43	B	618	BCR	C7-C8-C9-C10
43	B	618	BCR	C7-C8-C9-C34
43	B	618	BCR	C11-C12-C13-C14
43	B	618	BCR	C11-C12-C13-C35
43	B	618	BCR	C17-C18-C19-C20
43	B	618	BCR	C36-C18-C19-C20
43	B	619	BCR	C7-C8-C9-C34
43	B	619	BCR	C11-C12-C13-C14
43	B	619	BCR	C11-C12-C13-C35
43	C	614	BCR	C11-C12-C13-C14
43	C	614	BCR	C11-C12-C13-C35
43	C	614	BCR	C17-C18-C19-C20
43	C	614	BCR	C36-C18-C19-C20
43	C	614	BCR	C21-C22-C23-C24
43	C	614	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
43	C	615	BCR	C11-C12-C13-C14
43	C	615	BCR	C11-C12-C13-C35
43	D	405	BCR	C11-C12-C13-C14
43	D	405	BCR	C11-C12-C13-C35
43	D	405	BCR	C17-C18-C19-C20
43	D	405	BCR	C36-C18-C19-C20
43	D	405	BCR	C19-C20-C21-C22
43	H	101	BCR	C7-C8-C9-C10
43	H	101	BCR	C7-C8-C9-C34
43	T	101	BCR	C9-C10-C11-C12
43	T	101	BCR	C21-C22-C23-C24
43	T	101	BCR	C37-C22-C23-C24
43	V	101	BCR	C11-C12-C13-C14
43	V	101	BCR	C11-C12-C13-C35
43	V	101	BCR	C37-C22-C23-C24
43	Z	101	BCR	C11-C12-C13-C14
43	Z	101	BCR	C11-C12-C13-C35
43	b	618	BCR	C5-C6-C7-C8
43	b	618	BCR	C11-C12-C13-C14
43	b	618	BCR	C11-C12-C13-C35
43	b	618	BCR	C13-C14-C15-C16
43	b	618	BCR	C37-C22-C23-C24
43	b	619	BCR	C7-C8-C9-C10
43	b	619	BCR	C7-C8-C9-C34
43	b	619	BCR	C9-C10-C11-C12
43	b	619	BCR	C17-C18-C19-C20
43	b	619	BCR	C36-C18-C19-C20
43	b	620	BCR	C11-C12-C13-C14
43	b	620	BCR	C11-C12-C13-C35
43	b	620	BCR	C17-C18-C19-C20
43	c	614	BCR	C5-C6-C7-C8
43	c	614	BCR	C17-C18-C19-C20
43	c	614	BCR	C36-C18-C19-C20
43	c	614	BCR	C21-C22-C23-C24
43	c	614	BCR	C23-C24-C25-C26
43	c	615	BCR	C7-C8-C9-C10
43	c	615	BCR	C7-C8-C9-C34
43	c	615	BCR	C11-C12-C13-C14
43	c	615	BCR	C11-C12-C13-C35
43	d	406	BCR	C17-C18-C19-C20
43	d	406	BCR	C23-C24-C25-C26
43	h	101	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
43	h	101	BCR	C7-C8-C9-C34
43	t	101	BCR	C5-C6-C7-C8
43	t	101	BCR	C11-C12-C13-C14
43	t	101	BCR	C11-C12-C13-C35
43	v	101	BCR	C11-C12-C13-C14
43	v	101	BCR	C11-C12-C13-C35
43	z	101	BCR	C7-C8-C9-C10
43	z	101	BCR	C7-C8-C9-C34
44	A	416	PL9	C7-C8-C9-C11
44	A	416	PL9	C12-C13-C14-C16
44	A	416	PL9	C17-C18-C19-C21
44	A	416	PL9	C32-C33-C34-C36
44	a	414	PL9	C7-C8-C9-C10
44	a	414	PL9	C7-C8-C9-C11
44	a	414	PL9	C27-C28-C29-C31
44	a	414	PL9	C32-C33-C34-C35
44	a	414	PL9	C32-C33-C34-C36
44	a	414	PL9	C37-C38-C39-C40
44	a	414	PL9	C37-C38-C39-C41
45	C	616	DGD	C2A-C1A-O1G-C1G
45	C	616	DGD	O1A-C1A-O1G-C1G
45	C	618	DGD	C2D-C1D-O3G-C3G
45	C	618	DGD	O6D-C1D-O3G-C3G
45	C	620	DGD	C2A-C1A-O1G-C1G
45	C	620	DGD	O1A-C1A-O1G-C1G
45	C	620	DGD	C2B-C1B-O2G-C2G
45	c	616	DGD	O1B-C1B-O2G-C2G
45	c	617	DGD	O1B-C1B-O2G-C2G
45	c	617	DGD	O6E-C1E-O5D-C6D
45	c	618	DGD	C2B-C1B-O2G-C2G
45	c	619	DGD	C2B-C1B-O2G-C2G
48	R	302	LMU	O5'-C1'-O1'-C1
31	1	614	CLA	O1D-CGD-O2D-CED
31	3	316	CLA	O1D-CGD-O2D-CED
31	5	615	CLA	O1D-CGD-O2D-CED
31	6	316	CLA	O1D-CGD-O2D-CED
31	N	315	CLA	O1D-CGD-O2D-CED
31	8	614	CLA	O1D-CGD-O2D-CED
31	9	315	CLA	O1D-CGD-O2D-CED
31	p	613	CLA	O1D-CGD-O2D-CED
31	p	615	CLA	O1D-CGD-O2D-CED
31	g	305	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	n	316	CLA	O1D-CGD-O2D-CED
31	r	314	CLA	O1D-CGD-O2D-CED
31	s	314	CLA	O1D-CGD-O2D-CED
31	2	609	CLA	O1D-CGD-O2D-CED
31	6	314	CLA	O1D-CGD-O2D-CED
31	A	405	CLA	O1D-CGD-O2D-CED
31	N	321	CLA	O1D-CGD-O2D-CED
31	7	315	CLA	O1D-CGD-O2D-CED
31	8	611	CLA	O1D-CGD-O2D-CED
31	n	313	CLA	O1D-CGD-O2D-CED
30	2	607	CHL	CBD-CGD-O2D-CED
30	4	606	CHL	CBD-CGD-O2D-CED
30	0	605	CHL	CBD-CGD-O2D-CED
30	p	608	CHL	CBD-CGD-O2D-CED
31	1	611	CLA	CBD-CGD-O2D-CED
31	2	604	CLA	CBD-CGD-O2D-CED
31	2	611	CLA	CBD-CGD-O2D-CED
31	2	612	CLA	CBD-CGD-O2D-CED
31	3	304	CLA	CBD-CGD-O2D-CED
31	3	314	CLA	CBD-CGD-O2D-CED
31	3	315	CLA	CBD-CGD-O2D-CED
31	4	602	CLA	CBD-CGD-O2D-CED
31	4	610	CLA	CBD-CGD-O2D-CED
31	4	613	CLA	CBD-CGD-O2D-CED
31	4	614	CLA	CBD-CGD-O2D-CED
31	5	603	CLA	CBD-CGD-O2D-CED
31	5	613	CLA	CBD-CGD-O2D-CED
31	6	303	CLA	CBD-CGD-O2D-CED
31	6	304	CLA	CBD-CGD-O2D-CED
31	6	311	CLA	CBD-CGD-O2D-CED
31	6	314	CLA	CBD-CGD-O2D-CED
31	A	405	CLA	CBD-CGD-O2D-CED
31	A	409	CLA	CBD-CGD-O2D-CED
31	B	602	CLA	CBD-CGD-O2D-CED
31	B	608	CLA	CBD-CGD-O2D-CED
31	B	616	CLA	CBD-CGD-O2D-CED
31	C	602	CLA	CBD-CGD-O2D-CED
31	C	603	CLA	CBD-CGD-O2D-CED
31	C	604	CLA	CBD-CGD-O2D-CED
31	C	606	CLA	CBD-CGD-O2D-CED
31	C	611	CLA	CBD-CGD-O2D-CED
31	C	612	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	D	404	CLA	CBD-CGD-O2D-CED
31	G	611	CLA	CBD-CGD-O2D-CED
31	G	613	CLA	CBD-CGD-O2D-CED
31	N	313	CLA	CBD-CGD-O2D-CED
31	N	315	CLA	CBD-CGD-O2D-CED
31	R	303	CLA	CBD-CGD-O2D-CED
31	R	305	CLA	CBD-CGD-O2D-CED
31	R	311	CLA	CBD-CGD-O2D-CED
31	R	312	CLA	CBD-CGD-O2D-CED
31	S	304	CLA	CBD-CGD-O2D-CED
31	S	305	CLA	CBD-CGD-O2D-CED
31	S	315	CLA	CBD-CGD-O2D-CED
31	Y	305	CLA	CBD-CGD-O2D-CED
31	Y	310	CLA	CBD-CGD-O2D-CED
31	0	603	CLA	CBD-CGD-O2D-CED
31	0	604	CLA	CBD-CGD-O2D-CED
31	0	611	CLA	CBD-CGD-O2D-CED
31	7	304	CLA	CBD-CGD-O2D-CED
31	7	305	CLA	CBD-CGD-O2D-CED
31	8	609	CLA	CBD-CGD-O2D-CED
31	8	611	CLA	CBD-CGD-O2D-CED
31	8	613	CLA	CBD-CGD-O2D-CED
31	9	306	CLA	CBD-CGD-O2D-CED
31	9	313	CLA	CBD-CGD-O2D-CED
31	p	602	CLA	CBD-CGD-O2D-CED
31	p	603	CLA	CBD-CGD-O2D-CED
31	p	604	CLA	CBD-CGD-O2D-CED
31	p	615	CLA	CBD-CGD-O2D-CED
31	q	304	CLA	CBD-CGD-O2D-CED
31	q	305	CLA	CBD-CGD-O2D-CED
31	q	314	CLA	CBD-CGD-O2D-CED
31	q	315	CLA	CBD-CGD-O2D-CED
31	a	406	CLA	CBD-CGD-O2D-CED
31	a	409	CLA	CBD-CGD-O2D-CED
31	b	602	CLA	CBD-CGD-O2D-CED
31	b	608	CLA	CBD-CGD-O2D-CED
31	b	609	CLA	CBD-CGD-O2D-CED
31	b	615	CLA	CBD-CGD-O2D-CED
31	b	617	CLA	CBD-CGD-O2D-CED
31	c	602	CLA	CBD-CGD-O2D-CED
31	c	606	CLA	CBD-CGD-O2D-CED
31	c	610	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	c	611	CLA	CBD-CGD-O2D-CED
31	g	305	CLA	CBD-CGD-O2D-CED
31	g	311	CLA	CBD-CGD-O2D-CED
31	g	312	CLA	CBD-CGD-O2D-CED
31	g	313	CLA	CBD-CGD-O2D-CED
31	n	313	CLA	CBD-CGD-O2D-CED
31	n	315	CLA	CBD-CGD-O2D-CED
31	n	316	CLA	CBD-CGD-O2D-CED
31	r	305	CLA	CBD-CGD-O2D-CED
31	r	306	CLA	CBD-CGD-O2D-CED
31	r	312	CLA	CBD-CGD-O2D-CED
31	r	314	CLA	CBD-CGD-O2D-CED
31	r	315	CLA	CBD-CGD-O2D-CED
31	r	316	CLA	CBD-CGD-O2D-CED
31	s	304	CLA	CBD-CGD-O2D-CED
31	s	311	CLA	CBD-CGD-O2D-CED
31	y	603	CLA	CBD-CGD-O2D-CED
31	1	604	CLA	O1A-CGA-O2A-C1
31	1	611	CLA	O1A-CGA-O2A-C1
31	2	610	CLA	O1A-CGA-O2A-C1
31	5	604	CLA	O1A-CGA-O2A-C1
31	5	610	CLA	O1A-CGA-O2A-C1
31	5	614	CLA	O1A-CGA-O2A-C1
31	6	313	CLA	O1A-CGA-O2A-C1
31	6	315	CLA	O1A-CGA-O2A-C1
31	B	601	CLA	O1A-CGA-O2A-C1
31	B	602	CLA	O1A-CGA-O2A-C1
31	B	614	CLA	O1A-CGA-O2A-C1
31	B	616	CLA	O1A-CGA-O2A-C1
31	G	603	CLA	O1A-CGA-O2A-C1
31	N	304	CLA	O1A-CGA-O2A-C1
31	R	316	CLA	O1A-CGA-O2A-C1
31	S	306	CLA	O1A-CGA-O2A-C1
31	p	610	CLA	O1A-CGA-O2A-C1
31	b	615	CLA	O1A-CGA-O2A-C1
31	g	304	CLA	O1A-CGA-O2A-C1
31	r	312	CLA	O1A-CGA-O2A-C1
31	r	313	CLA	O1A-CGA-O2A-C1
33	K	102	LHG	O10-C23-O8-C6
34	4	620	LMG	O10-C28-O8-C9
34	A	418	LMG	O10-C28-O8-C9
34	B	621	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
34	C	624	LMG	O10-C28-O8-C9
34	D	410	LMG	O10-C28-O8-C9
34	G	621	LMG	O10-C28-O8-C9
34	0	620	LMG	O10-C28-O8-C9
34	a	416	LMG	O10-C28-O8-C9
34	b	629	LMG	O10-C28-O8-C9
34	f	101	LMG	O10-C28-O8-C9
34	w	203	LMG	O10-C28-O8-C9
38	0	621	SQD	O10-C23-O48-C46
38	g	301	SQD	O10-C23-O48-C46
31	4	612	CLA	O1A-CGA-O2A-C1
31	5	615	CLA	O1A-CGA-O2A-C1
31	S	316	CLA	O1A-CGA-O2A-C1
31	q	314	CLA	O1A-CGA-O2A-C1
31	S	314	CLA	O1D-CGD-O2D-CED
31	9	306	CLA	C5-C6-C7-C8
48	r	302	LMU	O5B-C1B-O1B-C4'
31	4	612	CLA	CBA-CGA-O2A-C1
31	5	615	CLA	CBA-CGA-O2A-C1
31	9	316	CLA	CBA-CGA-O2A-C1
31	q	314	CLA	CBA-CGA-O2A-C1
48	c	623	LMU	C4B-C5B-C6B-O6B
31	2	612	CLA	O1D-CGD-O2D-CED
31	4	613	CLA	O1D-CGD-O2D-CED
31	6	311	CLA	O1D-CGD-O2D-CED
31	q	312	CLA	O1D-CGD-O2D-CED
31	q	314	CLA	O1D-CGD-O2D-CED
31	q	315	CLA	O1D-CGD-O2D-CED
31	a	406	CLA	O1D-CGD-O2D-CED
31	g	313	CLA	O1D-CGD-O2D-CED
31	1	604	CLA	CBA-CGA-O2A-C1
31	1	611	CLA	CBA-CGA-O2A-C1
31	2	610	CLA	CBA-CGA-O2A-C1
31	5	604	CLA	CBA-CGA-O2A-C1
31	5	610	CLA	CBA-CGA-O2A-C1
31	5	614	CLA	CBA-CGA-O2A-C1
31	6	313	CLA	CBA-CGA-O2A-C1
31	6	315	CLA	CBA-CGA-O2A-C1
31	B	616	CLA	CBA-CGA-O2A-C1
31	S	306	CLA	CBA-CGA-O2A-C1
31	0	611	CLA	CBA-CGA-O2A-C1
31	p	610	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	q	312	CLA	CBA-CGA-O2A-C1
31	b	615	CLA	CBA-CGA-O2A-C1
31	g	304	CLA	CBA-CGA-O2A-C1
31	r	312	CLA	CBA-CGA-O2A-C1
31	r	313	CLA	CBA-CGA-O2A-C1
33	K	102	LHG	C24-C23-O8-C6
34	A	418	LMG	C29-C28-O8-C9
34	B	621	LMG	C29-C28-O8-C9
34	D	410	LMG	C29-C28-O8-C9
34	G	621	LMG	C29-C28-O8-C9
34	a	416	LMG	C29-C28-O8-C9
34	f	101	LMG	C29-C28-O8-C9
34	w	203	LMG	C29-C28-O8-C9
34	x	202	LMG	C29-C28-O8-C9
38	B	620	SQD	C24-C23-O48-C46
38	g	301	SQD	C24-C23-O48-C46
31	2	603	CLA	CBD-CGD-O2D-CED
31	4	611	CLA	CBD-CGD-O2D-CED
31	5	610	CLA	CBD-CGD-O2D-CED
31	6	312	CLA	CBD-CGD-O2D-CED
31	G	609	CLA	CBD-CGD-O2D-CED
31	7	311	CLA	CBD-CGD-O2D-CED
31	y	604	CLA	CBD-CGD-O2D-CED
31	3	315	CLA	O1A-CGA-O2A-C1
31	5	611	CLA	O1A-CGA-O2A-C1
31	5	613	CLA	O1A-CGA-O2A-C1
31	6	312	CLA	O1A-CGA-O2A-C1
31	6	314	CLA	O1A-CGA-O2A-C1
31	B	610	CLA	O1A-CGA-O2A-C1
31	R	303	CLA	O1A-CGA-O2A-C1
31	R	311	CLA	O1A-CGA-O2A-C1
31	R	312	CLA	O1A-CGA-O2A-C1
31	R	313	CLA	O1A-CGA-O2A-C1
31	R	315	CLA	O1A-CGA-O2A-C1
31	S	303	CLA	O1A-CGA-O2A-C1
31	Y	304	CLA	O1A-CGA-O2A-C1
31	Y	305	CLA	O1A-CGA-O2A-C1
31	0	611	CLA	O1A-CGA-O2A-C1
31	0	615	CLA	O1A-CGA-O2A-C1
31	7	304	CLA	O1A-CGA-O2A-C1
31	7	305	CLA	O1A-CGA-O2A-C1
31	7	316	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	9	305	CLA	O1A-CGA-O2A-C1
31	9	313	CLA	O1A-CGA-O2A-C1
31	9	314	CLA	O1A-CGA-O2A-C1
31	p	603	CLA	O1A-CGA-O2A-C1
31	p	604	CLA	O1A-CGA-O2A-C1
31	p	614	CLA	O1A-CGA-O2A-C1
31	q	306	CLA	O1A-CGA-O2A-C1
31	g	314	CLA	O1A-CGA-O2A-C1
31	r	303	CLA	O1A-CGA-O2A-C1
31	r	311	CLA	O1A-CGA-O2A-C1
31	y	603	CLA	O1A-CGA-O2A-C1
33	p	619	LHG	O10-C23-O8-C6
33	q	320	LHG	O10-C23-O8-C6
33	z	102	LHG	O10-C23-O8-C6
34	1	618	LMG	O10-C28-O8-C9
34	2	618	LMG	O10-C28-O8-C9
34	6	321	LMG	O10-C28-O8-C9
34	6	322	LMG	O10-C28-O8-C9
34	D	409	LMG	O10-C28-O8-C9
34	G	619	LMG	O10-C28-O8-C9
34	G	622	LMG	O10-C28-O8-C9
34	I	101	LMG	O10-C28-O8-C9
34	J	101	LMG	O10-C28-O8-C9
34	N	320	LMG	O10-C28-O8-C9
34	R	321	LMG	O10-C28-O8-C9
34	W	201	LMG	O10-C28-O8-C9
34	W	202	LMG	O10-C28-O8-C9
34	X	202	LMG	O10-C28-O8-C9
34	7	320	LMG	O10-C28-O8-C9
34	7	322	LMG	O10-C28-O8-C9
34	9	302	LMG	O10-C28-O8-C9
34	9	321	LMG	O10-C28-O8-C9
34	p	620	LMG	O10-C28-O8-C9
34	q	301	LMG	O10-C28-O8-C9
34	q	302	LMG	O10-C28-O8-C9
34	a	401	LMG	O10-C28-O8-C9
34	b	601	LMG	O10-C28-O8-C9
34	b	626	LMG	O10-C28-O8-C9
34	c	620	LMG	O10-C28-O8-C9
34	c	624	LMG	O10-C28-O8-C9
34	g	320	LMG	O10-C28-O8-C9
34	g	322	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
34	m	102	LMG	O10-C28-O8-C9
34	n	322	LMG	O10-C28-O8-C9
34	x	202	LMG	O10-C28-O8-C9
34	Q1	101	LMG	O10-C28-O8-C9
34	q1	101	LMG	O10-C28-O8-C9
38	B	620	SQD	O10-C23-O48-C46
38	G	624	SQD	O10-C23-O48-C46
38	R	322	SQD	O10-C23-O48-C46
38	X	201	SQD	O10-C23-O48-C46
31	9	316	CLA	O1A-CGA-O2A-C1
31	s	316	CLA	O1A-CGA-O2A-C1
30	4	606	CHL	O1D-CGD-O2D-CED
30	7	307	CHL	O1D-CGD-O2D-CED
30	9	309	CHL	O1D-CGD-O2D-CED
31	2	602	CLA	O1D-CGD-O2D-CED
31	5	614	CLA	O1D-CGD-O2D-CED
31	C	603	CLA	O1D-CGD-O2D-CED
31	R	314	CLA	O1D-CGD-O2D-CED
31	S	316	CLA	O1D-CGD-O2D-CED
31	0	613	CLA	O1D-CGD-O2D-CED
31	9	314	CLA	O1D-CGD-O2D-CED
31	c	603	CLA	O1D-CGD-O2D-CED
31	n	314	CLA	O1D-CGD-O2D-CED
31	s	316	CLA	O1D-CGD-O2D-CED
31	1	610	CLA	O1D-CGD-O2D-CED
31	1	613	CLA	O1D-CGD-O2D-CED
31	2	613	CLA	O1D-CGD-O2D-CED
31	3	305	CLA	O1D-CGD-O2D-CED
31	3	312	CLA	O1D-CGD-O2D-CED
31	B	605	CLA	O1D-CGD-O2D-CED
31	S	310	CLA	O1D-CGD-O2D-CED
31	Y	313	CLA	O1D-CGD-O2D-CED
31	7	314	CLA	O1D-CGD-O2D-CED
31	8	612	CLA	O1D-CGD-O2D-CED
31	p	610	CLA	O1D-CGD-O2D-CED
31	q	316	CLA	O1D-CGD-O2D-CED
31	b	606	CLA	O1D-CGD-O2D-CED
31	b	607	CLA	O1D-CGD-O2D-CED
31	r	313	CLA	O1D-CGD-O2D-CED
31	2	610	CLA	CBD-CGD-O2D-CED
31	4	603	CLA	CBD-CGD-O2D-CED
31	B	601	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	N	312	CLA	CBD-CGD-O2D-CED
31	q	306	CLA	CBD-CGD-O2D-CED
31	c	613	CLA	CBD-CGD-O2D-CED
33	1	617	LHG	O9-C7-O7-C5
33	C	623	LHG	O9-C7-O7-C5
33	0	619	LHG	O9-C7-O7-C5
33	7	319	LHG	O9-C7-O7-C5
33	p	619	LHG	O9-C7-O7-C5
33	s	322	LHG	O9-C7-O7-C5
34	2	621	LMG	O9-C10-O7-C8
34	4	620	LMG	O9-C10-O7-C8
34	4	621	LMG	O9-C10-O7-C8
34	A	412	LMG	O9-C10-O7-C8
34	B	622	LMG	O9-C10-O7-C8
34	C	622	LMG	O9-C10-O7-C8
34	G	622	LMG	O9-C10-O7-C8
34	I	101	LMG	O9-C10-O7-C8
34	J	102	LMG	O9-C10-O7-C8
34	N	320	LMG	O9-C10-O7-C8
34	W	203	LMG	O9-C10-O7-C8
34	0	620	LMG	O9-C10-O7-C8
34	7	301	LMG	O9-C10-O7-C8
34	9	321	LMG	O9-C10-O7-C8
34	p	620	LMG	O9-C10-O7-C8
34	a	413	LMG	O9-C10-O7-C8
34	a	416	LMG	O9-C10-O7-C8
34	b	601	LMG	O9-C10-O7-C8
34	b	623	LMG	O9-C10-O7-C8
34	b	624	LMG	O9-C10-O7-C8
34	b	629	LMG	O9-C10-O7-C8
34	c	620	LMG	O9-C10-O7-C8
34	c	621	LMG	O9-C10-O7-C8
34	c	624	LMG	O9-C10-O7-C8
34	f	101	LMG	O9-C10-O7-C8
34	g	320	LMG	O9-C10-O7-C8
34	k	101	LMG	O9-C10-O7-C8
34	k	102	LMG	O9-C10-O7-C8
34	m	102	LMG	O9-C10-O7-C8
34	w	203	LMG	O9-C10-O7-C8
34	y	620	LMG	O9-C10-O7-C8
34	q1	101	LMG	O9-C10-O7-C8
38	G	617	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
38	0	621	SQD	O49-C7-O47-C45
38	b	621	SQD	O49-C7-O47-C45
38	y	621	SQD	O49-C7-O47-C45
45	C	620	DGD	O1B-C1B-O2G-C2G
45	c	619	DGD	O1B-C1B-O2G-C2G
31	p	612	CLA	O1A-CGA-O2A-C1
31	p	615	CLA	O1A-CGA-O2A-C1
48	K	101	LMU	C4B-C5B-C6B-O6B
31	1	613	CLA	C3-C5-C6-C7
31	2	603	CLA	C3-C5-C6-C7
31	2	611	CLA	C3-C5-C6-C7
31	2	612	CLA	C3-C5-C6-C7
31	2	613	CLA	C3-C5-C6-C7
31	3	301	CLA	C3-C5-C6-C7
31	4	602	CLA	C3-C5-C6-C7
31	6	304	CLA	C3-C5-C6-C7
31	6	305	CLA	C3-C5-C6-C7
31	6	311	CLA	C3-C5-C6-C7
31	6	313	CLA	C3-C5-C6-C7
31	6	314	CLA	C3-C5-C6-C7
31	A	409	CLA	C3-C5-C6-C7
31	B	602	CLA	C3-C5-C6-C7
31	B	604	CLA	C3-C5-C6-C7
31	C	604	CLA	C3-C5-C6-C7
31	C	609	CLA	C3-C5-C6-C7
31	D	403	CLA	C3-C5-C6-C7
31	G	603	CLA	C3-C5-C6-C7
31	G	612	CLA	C3-C5-C6-C7
31	N	304	CLA	C3-C5-C6-C7
31	R	312	CLA	C3-C5-C6-C7
31	S	311	CLA	C3-C5-C6-C7
31	S	313	CLA	C3-C5-C6-C7
31	Y	305	CLA	C3-C5-C6-C7
31	0	604	CLA	C3-C5-C6-C7
31	0	610	CLA	C3-C5-C6-C7
31	0	613	CLA	C3-C5-C6-C7
31	8	612	CLA	C3-C5-C6-C7
31	p	603	CLA	C3-C5-C6-C7
31	q	315	CLA	C3-C5-C6-C7
31	a	409	CLA	C3-C5-C6-C7
31	b	605	CLA	C3-C5-C6-C7
31	b	608	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	b	615	CLA	C3-C5-C6-C7
31	b	617	CLA	C3-C5-C6-C7
31	c	606	CLA	C3-C5-C6-C7
31	c	608	CLA	C3-C5-C6-C7
31	c	613	CLA	C3-C5-C6-C7
31	d	405	CLA	C3-C5-C6-C7
31	n	314	CLA	C3-C5-C6-C7
31	r	315	CLA	C3-C5-C6-C7
31	s	311	CLA	C3-C5-C6-C7
31	s	313	CLA	C3-C5-C6-C7
31	y	612	CLA	C3-C5-C6-C7
31	y	614	CLA	C3-C5-C6-C7
42	D	401	PHO	C3-C5-C6-C7
42	d	402	PHO	C3-C5-C6-C7
31	B	613	CLA	O1D-CGD-O2D-CED
31	b	610	CLA	O1D-CGD-O2D-CED
31	b	614	CLA	O1D-CGD-O2D-CED
31	d	405	CLA	O1D-CGD-O2D-CED
30	5	607	CHL	CBA-CGA-O2A-C1
31	3	315	CLA	CBA-CGA-O2A-C1
31	4	613	CLA	CBA-CGA-O2A-C1
31	5	613	CLA	CBA-CGA-O2A-C1
31	6	304	CLA	CBA-CGA-O2A-C1
31	6	312	CLA	CBA-CGA-O2A-C1
31	6	314	CLA	CBA-CGA-O2A-C1
31	A	409	CLA	CBA-CGA-O2A-C1
31	B	601	CLA	CBA-CGA-O2A-C1
31	B	610	CLA	CBA-CGA-O2A-C1
31	B	614	CLA	CBA-CGA-O2A-C1
31	N	304	CLA	CBA-CGA-O2A-C1
31	R	303	CLA	CBA-CGA-O2A-C1
31	R	311	CLA	CBA-CGA-O2A-C1
31	R	313	CLA	CBA-CGA-O2A-C1
31	R	316	CLA	CBA-CGA-O2A-C1
31	S	303	CLA	CBA-CGA-O2A-C1
31	Y	304	CLA	CBA-CGA-O2A-C1
31	0	615	CLA	CBA-CGA-O2A-C1
31	7	305	CLA	CBA-CGA-O2A-C1
31	9	305	CLA	CBA-CGA-O2A-C1
31	9	313	CLA	CBA-CGA-O2A-C1
31	p	614	CLA	CBA-CGA-O2A-C1
31	q	306	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	a	409	CLA	CBA-CGA-O2A-C1
31	c	609	CLA	CBA-CGA-O2A-C1
31	y	603	CLA	CBA-CGA-O2A-C1
33	q	320	LHG	C24-C23-O8-C6
33	z	102	LHG	C24-C23-O8-C6
34	1	618	LMG	C29-C28-O8-C9
34	2	618	LMG	C29-C28-O8-C9
34	4	620	LMG	C29-C28-O8-C9
34	6	323	LMG	C29-C28-O8-C9
34	B	625	LMG	C29-C28-O8-C9
34	C	624	LMG	C29-C28-O8-C9
34	D	409	LMG	C29-C28-O8-C9
34	G	619	LMG	C29-C28-O8-C9
34	I	101	LMG	C29-C28-O8-C9
34	J	101	LMG	C29-C28-O8-C9
34	N	320	LMG	C29-C28-O8-C9
34	R	321	LMG	C29-C28-O8-C9
34	0	620	LMG	C29-C28-O8-C9
34	7	320	LMG	C29-C28-O8-C9
34	7	322	LMG	C29-C28-O8-C9
34	9	321	LMG	C29-C28-O8-C9
34	q	301	LMG	C29-C28-O8-C9
34	b	601	LMG	C29-C28-O8-C9
34	b	624	LMG	C29-C28-O8-C9
34	b	626	LMG	C29-C28-O8-C9
34	b	629	LMG	C29-C28-O8-C9
34	c	620	LMG	C29-C28-O8-C9
34	j	101	LMG	C29-C28-O8-C9
34	m	102	LMG	C29-C28-O8-C9
34	n	322	LMG	C29-C28-O8-C9
34	Q1	101	LMG	C29-C28-O8-C9
34	q1	101	LMG	C29-C28-O8-C9
38	G	624	SQD	C24-C23-O48-C46
38	X	201	SQD	C24-C23-O48-C46
38	0	621	SQD	C24-C23-O48-C46
30	1	607	CHL	CBD-CGD-O2D-CED
30	q	307	CHL	CBD-CGD-O2D-CED
30	q	309	CHL	CBD-CGD-O2D-CED
30	q	310	CHL	CBD-CGD-O2D-CED
30	g	308	CHL	CBD-CGD-O2D-CED
30	n	301	CHL	CBD-CGD-O2D-CED
31	1	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	1	604	CLA	CBD-CGD-O2D-CED
31	3	311	CLA	CBD-CGD-O2D-CED
31	B	607	CLA	CBD-CGD-O2D-CED
31	C	610	CLA	CBD-CGD-O2D-CED
31	C	613	CLA	CBD-CGD-O2D-CED
31	G	603	CLA	CBD-CGD-O2D-CED
31	G	604	CLA	CBD-CGD-O2D-CED
31	G	610	CLA	CBD-CGD-O2D-CED
31	N	303	CLA	CBD-CGD-O2D-CED
31	N	310	CLA	CBD-CGD-O2D-CED
31	R	307	CLA	CBD-CGD-O2D-CED
31	R	315	CLA	CBD-CGD-O2D-CED
31	R	316	CLA	CBD-CGD-O2D-CED
31	S	312	CLA	CBD-CGD-O2D-CED
31	Y	304	CLA	CBD-CGD-O2D-CED
31	Y	311	CLA	CBD-CGD-O2D-CED
31	Y	312	CLA	CBD-CGD-O2D-CED
31	0	602	CLA	CBD-CGD-O2D-CED
31	0	610	CLA	CBD-CGD-O2D-CED
31	7	303	CLA	CBD-CGD-O2D-CED
31	8	602	CLA	CBD-CGD-O2D-CED
31	8	603	CLA	CBD-CGD-O2D-CED
31	8	604	CLA	CBD-CGD-O2D-CED
31	9	304	CLA	CBD-CGD-O2D-CED
31	9	312	CLA	CBD-CGD-O2D-CED
31	9	316	CLA	CBD-CGD-O2D-CED
31	b	603	CLA	CBD-CGD-O2D-CED
31	b	612	CLA	CBD-CGD-O2D-CED
31	b	616	CLA	CBD-CGD-O2D-CED
31	c	604	CLA	CBD-CGD-O2D-CED
31	c	612	CLA	CBD-CGD-O2D-CED
31	d	404	CLA	CBD-CGD-O2D-CED
31	g	303	CLA	CBD-CGD-O2D-CED
31	g	304	CLA	CBD-CGD-O2D-CED
31	g	310	CLA	CBD-CGD-O2D-CED
31	n	303	CLA	CBD-CGD-O2D-CED
31	n	304	CLA	CBD-CGD-O2D-CED
31	n	305	CLA	CBD-CGD-O2D-CED
31	n	311	CLA	CBD-CGD-O2D-CED
31	r	303	CLA	CBD-CGD-O2D-CED
31	r	307	CLA	CBD-CGD-O2D-CED
31	s	310	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	s	312	CLA	CBD-CGD-O2D-CED
31	s	315	CLA	CBD-CGD-O2D-CED
31	y	615	CLA	CBD-CGD-O2D-CED
33	1	617	LHG	C8-C7-O7-C5
33	5	619	LHG	C8-C7-O7-C5
33	7	319	LHG	C8-C7-O7-C5
34	2	621	LMG	C11-C10-O7-C8
34	6	321	LMG	C11-C10-O7-C8
34	q	302	LMG	C11-C10-O7-C8
34	a	416	LMG	C11-C10-O7-C8
34	c	620	LMG	C11-C10-O7-C8
34	g	320	LMG	C11-C10-O7-C8
34	w	205	LMG	C11-C10-O7-C8
45	c	616	DGD	C2B-C1B-O2G-C2G
45	c	617	DGD	C2B-C1B-O2G-C2G
31	1	603	CLA	O1D-CGD-O2D-CED
31	5	602	CLA	O1D-CGD-O2D-CED
31	B	603	CLA	O1D-CGD-O2D-CED
31	B	606	CLA	O1D-CGD-O2D-CED
31	B	609	CLA	O1D-CGD-O2D-CED
31	B	614	CLA	O1D-CGD-O2D-CED
31	G	612	CLA	O1D-CGD-O2D-CED
31	N	313	CLA	O1D-CGD-O2D-CED
31	R	311	CLA	O1D-CGD-O2D-CED
31	R	313	CLA	O1D-CGD-O2D-CED
31	S	315	CLA	O1D-CGD-O2D-CED
31	g	314	CLA	O1D-CGD-O2D-CED
31	r	311	CLA	O1D-CGD-O2D-CED
31	N	310	CLA	O1A-CGA-O2A-C1
31	9	313	CLA	C2-C1-O2A-CGA
31	b	604	CLA	O1D-CGD-O2D-CED
31	s	311	CLA	O1D-CGD-O2D-CED
31	4	610	CLA	C4-C3-C5-C6
31	A	409	CLA	C4-C3-C5-C6
31	B	602	CLA	C4-C3-C5-C6
31	B	603	CLA	C4-C3-C5-C6
31	B	604	CLA	C4-C3-C5-C6
31	D	403	CLA	C4-C3-C5-C6
31	D	404	CLA	C4-C3-C5-C6
31	S	310	CLA	C4-C3-C5-C6
31	0	602	CLA	C4-C3-C5-C6
31	0	610	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	a	409	CLA	C4-C3-C5-C6
31	b	603	CLA	C4-C3-C5-C6
31	b	605	CLA	C4-C3-C5-C6
31	b	606	CLA	C4-C3-C5-C6
31	b	609	CLA	C4-C3-C5-C6
44	A	416	PL9	C45-C44-C46-C47
31	4	610	CLA	C2-C3-C5-C6
31	A	409	CLA	C2-C3-C5-C6
31	B	602	CLA	C2-C3-C5-C6
31	B	603	CLA	C2-C3-C5-C6
31	B	604	CLA	C2-C3-C5-C6
31	S	310	CLA	C2-C3-C5-C6
31	0	602	CLA	C2-C3-C5-C6
31	0	610	CLA	C2-C3-C5-C6
31	a	409	CLA	C2-C3-C5-C6
31	b	609	CLA	C2-C3-C5-C6
31	p	612	CLA	CBA-CGA-O2A-C1
31	p	615	CLA	CBA-CGA-O2A-C1
31	0	612	CLA	CBD-CGD-O2D-CED
31	3	314	CLA	O1D-CGD-O2D-CED
31	3	315	CLA	O1D-CGD-O2D-CED
31	4	602	CLA	O1D-CGD-O2D-CED
31	C	606	CLA	O1D-CGD-O2D-CED
31	S	304	CLA	O1D-CGD-O2D-CED
31	9	313	CLA	O1D-CGD-O2D-CED
31	n	315	CLA	O1D-CGD-O2D-CED
48	c	623	LMU	O5B-C5B-C6B-O6B
31	p	610	CLA	C2A-CAA-CBA-CGA
31	q	312	CLA	C2A-CAA-CBA-CGA
31	A	409	CLA	O1A-CGA-O2A-C1
31	a	409	CLA	O1A-CGA-O2A-C1
30	4	607	CHL	C3-C5-C6-C7
30	7	302	CHL	C3-C5-C6-C7
31	1	602	CLA	C3-C5-C6-C7
31	1	604	CLA	C3-C5-C6-C7
31	1	610	CLA	C3-C5-C6-C7
31	3	304	CLA	C3-C5-C6-C7
31	3	316	CLA	C3-C5-C6-C7
31	B	614	CLA	C3-C5-C6-C7
31	C	612	CLA	C3-C5-C6-C7
31	R	315	CLA	C3-C5-C6-C7
31	R	316	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	Y	303	CLA	C3-C5-C6-C7
31	0	614	CLA	C3-C5-C6-C7
31	9	312	CLA	C3-C5-C6-C7
31	q	306	CLA	C3-C5-C6-C7
31	a	406	CLA	C3-C5-C6-C7
31	b	603	CLA	C3-C5-C6-C7
31	c	603	CLA	C3-C5-C6-C7
31	c	604	CLA	C3-C5-C6-C7
31	g	304	CLA	C3-C5-C6-C7
31	s	312	CLA	C3-C5-C6-C7
31	y	602	CLA	C3-C5-C6-C7
31	y	613	CLA	C3-C5-C6-C7
31	1	612	CLA	CBA-CGA-O2A-C1
31	2	603	CLA	CBA-CGA-O2A-C1
31	2	609	CLA	CBA-CGA-O2A-C1
31	2	611	CLA	CBA-CGA-O2A-C1
31	2	613	CLA	CBA-CGA-O2A-C1
31	5	611	CLA	CBA-CGA-O2A-C1
31	C	609	CLA	CBA-CGA-O2A-C1
31	N	314	CLA	CBA-CGA-O2A-C1
31	R	312	CLA	CBA-CGA-O2A-C1
31	R	315	CLA	CBA-CGA-O2A-C1
31	Y	305	CLA	CBA-CGA-O2A-C1
31	0	610	CLA	CBA-CGA-O2A-C1
31	7	304	CLA	CBA-CGA-O2A-C1
31	7	316	CLA	CBA-CGA-O2A-C1
31	8	613	CLA	CBA-CGA-O2A-C1
31	9	314	CLA	CBA-CGA-O2A-C1
31	p	603	CLA	CBA-CGA-O2A-C1
31	p	604	CLA	CBA-CGA-O2A-C1
31	b	613	CLA	CBA-CGA-O2A-C1
31	c	611	CLA	CBA-CGA-O2A-C1
31	g	314	CLA	CBA-CGA-O2A-C1
31	n	311	CLA	CBA-CGA-O2A-C1
31	n	315	CLA	CBA-CGA-O2A-C1
31	r	303	CLA	CBA-CGA-O2A-C1
31	r	311	CLA	CBA-CGA-O2A-C1
31	r	316	CLA	CBA-CGA-O2A-C1
33	p	619	LHG	C24-C23-O8-C6
34	4	621	LMG	C29-C28-O8-C9
34	6	321	LMG	C29-C28-O8-C9
34	6	322	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
34	D	411	LMG	C29-C28-O8-C9
34	G	622	LMG	C29-C28-O8-C9
34	W	201	LMG	C29-C28-O8-C9
34	W	202	LMG	C29-C28-O8-C9
34	X	202	LMG	C29-C28-O8-C9
34	9	302	LMG	C29-C28-O8-C9
34	p	620	LMG	C29-C28-O8-C9
34	q	302	LMG	C29-C28-O8-C9
34	a	401	LMG	C29-C28-O8-C9
34	c	624	LMG	C29-C28-O8-C9
34	d	410	LMG	C29-C28-O8-C9
34	g	320	LMG	C29-C28-O8-C9
34	g	322	LMG	C29-C28-O8-C9
38	R	322	SQD	C24-C23-O48-C46
42	A	408	PHO	CBA-CGA-O2A-C1
34	B	621	LMG	C20-C21-C22-C23
34	D	411	LMG	C17-C18-C19-C20
34	G	621	LMG	C20-C21-C22-C23
34	J	101	LMG	C35-C36-C37-C38
34	b	626	LMG	C20-C21-C22-C23
34	d	410	LMG	C17-C18-C19-C20
34	d	411	LMG	C38-C39-C40-C41
34	g	322	LMG	C38-C39-C40-C41
34	s	321	LMG	C17-C18-C19-C20
45	c	616	DGD	CEB-CFB-CGB-CHB
45	c	618	DGD	CBB-CCB-CDB-CEB
44	A	416	PL9	C32-C33-C34-C35
34	J	101	LMG	C20-C21-C22-C23
45	C	617	DGD	CBB-CCB-CDB-CEB
45	C	620	DGD	CBA-CCA-CDA-CEA
34	2	620	LMG	C35-C36-C37-C38
34	4	620	LMG	C35-C36-C37-C38
34	C	619	LMG	C20-C21-C22-C23
34	D	410	LMG	C20-C21-C22-C23
34	D	411	LMG	C20-C21-C22-C23
34	d	410	LMG	C20-C21-C22-C23
45	c	616	DGD	C8A-C9A-CAA-CBA
45	c	616	DGD	CBB-CCB-CDB-CEB
45	c	618	DGD	C8A-C9A-CAA-CBA
35	2	614	RRX	C19-C20-C21-C22
35	4	615	RRX	C19-C20-C21-C22
35	G	614	RRX	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
35	9	317	RRX	C19-C20-C21-C22
43	C	614	BCR	C19-C20-C21-C22
43	D	405	BCR	C13-C14-C15-C16
43	T	101	BCR	C15-C16-C17-C18
43	V	101	BCR	C13-C14-C15-C16
30	5	607	CHL	O1A-CGA-O2A-C1
31	1	603	CLA	O1A-CGA-O2A-C1
31	2	603	CLA	O1A-CGA-O2A-C1
31	2	604	CLA	O1A-CGA-O2A-C1
31	2	609	CLA	O1A-CGA-O2A-C1
31	4	613	CLA	O1A-CGA-O2A-C1
31	6	304	CLA	O1A-CGA-O2A-C1
31	6	316	CLA	O1A-CGA-O2A-C1
31	C	609	CLA	O1A-CGA-O2A-C1
31	N	314	CLA	O1A-CGA-O2A-C1
31	8	609	CLA	O1A-CGA-O2A-C1
31	n	311	CLA	O1A-CGA-O2A-C1
31	r	316	CLA	O1A-CGA-O2A-C1
34	2	621	LMG	O10-C28-O8-C9
34	4	621	LMG	O10-C28-O8-C9
38	a	411	SQD	O10-C23-O48-C46
33	M	101	LHG	O9-C7-O7-C5
34	5	620	LMG	O9-C10-O7-C8
34	6	321	LMG	O9-C10-O7-C8
34	6	323	LMG	O9-C10-O7-C8
34	A	418	LMG	O9-C10-O7-C8
34	X	202	LMG	O9-C10-O7-C8
34	7	322	LMG	O9-C10-O7-C8
38	Y	320	SQD	O49-C7-O47-C45
45	c	618	DGD	O1B-C1B-O2G-C2G
30	0	605	CHL	O1D-CGD-O2D-CED
31	2	611	CLA	O1D-CGD-O2D-CED
31	5	603	CLA	O1D-CGD-O2D-CED
31	b	615	CLA	O1D-CGD-O2D-CED
34	D	410	LMG	C17-C18-C19-C20
34	D	412	LMG	C38-C39-C40-C41
34	c	624	LMG	C35-C36-C37-C38
45	C	620	DGD	CBB-CCB-CDB-CEB
31	1	610	CLA	C5-C6-C7-C8
48	R	302	LMU	C3'-C4'-O1B-C1B
33	G	618	LHG	C13-C14-C15-C16
34	2	620	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
34	2	620	LMG	C38-C39-C40-C41
34	4	620	LMG	C17-C18-C19-C20
34	4	620	LMG	C38-C39-C40-C41
34	B	621	LMG	C17-C18-C19-C20
34	C	619	LMG	C35-C36-C37-C38
34	C	624	LMG	C17-C18-C19-C20
34	D	411	LMG	C35-C36-C37-C38
34	D	412	LMG	C35-C36-C37-C38
34	G	621	LMG	C35-C36-C37-C38
34	G	621	LMG	C38-C39-C40-C41
34	S	321	LMG	C17-C18-C19-C20
34	9	301	LMG	C20-C21-C22-C23
34	9	301	LMG	C35-C36-C37-C38
34	9	301	LMG	C38-C39-C40-C41
34	q	301	LMG	C17-C18-C19-C20
34	q	301	LMG	C35-C36-C37-C38
34	q	301	LMG	C38-C39-C40-C41
34	b	622	LMG	C17-C18-C19-C20
34	b	622	LMG	C20-C21-C22-C23
34	b	626	LMG	C17-C18-C19-C20
34	c	624	LMG	C38-C39-C40-C41
34	d	410	LMG	C35-C36-C37-C38
34	d	411	LMG	C35-C36-C37-C38
34	k	101	LMG	C17-C18-C19-C20
34	k	101	LMG	C35-C36-C37-C38
34	w	201	LMG	C35-C36-C37-C38
45	C	618	DGD	CEA-CFA-CGA-CHA
45	C	618	DGD	C8B-C9B-CAB-CBB
45	C	618	DGD	CBB-CCB-CDB-CEB
45	C	620	DGD	CEB-CFB-CGB-CHB
45	c	617	DGD	C8B-C9B-CAB-CBB
45	c	617	DGD	CBB-CCB-CDB-CEB
45	c	619	DGD	CEA-CFA-CGA-CHA
45	c	619	DGD	CBB-CCB-CDB-CEB
45	c	619	DGD	CEB-CFB-CGB-CHB
31	D	404	CLA	O1D-CGD-O2D-CED
31	R	305	CLA	O1D-CGD-O2D-CED
31	S	305	CLA	O1D-CGD-O2D-CED
31	Y	305	CLA	O1D-CGD-O2D-CED
31	0	611	CLA	O1D-CGD-O2D-CED
31	7	304	CLA	O1D-CGD-O2D-CED
31	p	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	g	311	CLA	O1D-CGD-O2D-CED
31	2	604	CLA	C3-C5-C6-C7
31	B	609	CLA	C3-C5-C6-C7
31	Y	312	CLA	C3-C5-C6-C7
31	Y	314	CLA	C3-C5-C6-C7
31	0	602	CLA	C3-C5-C6-C7
31	0	615	CLA	C3-C5-C6-C7
31	7	312	CLA	C3-C5-C6-C7
31	7	314	CLA	C3-C5-C6-C7
31	8	602	CLA	C3-C5-C6-C7
31	8	604	CLA	C3-C5-C6-C7
31	b	610	CLA	C3-C5-C6-C7
31	b	612	CLA	C3-C5-C6-C7
31	n	303	CLA	C3-C5-C6-C7
31	n	305	CLA	C3-C5-C6-C7
31	r	304	CLA	C3-C5-C6-C7
30	4	609	CHL	CBD-CGD-O2D-CED
30	N	301	CHL	CBD-CGD-O2D-CED
30	Y	308	CHL	CBD-CGD-O2D-CED
31	5	612	CLA	CBD-CGD-O2D-CED
31	6	305	CLA	CBD-CGD-O2D-CED
31	C	601	CLA	CBD-CGD-O2D-CED
31	N	305	CLA	CBD-CGD-O2D-CED
31	7	313	CLA	CBD-CGD-O2D-CED
31	c	601	CLA	CBD-CGD-O2D-CED
31	c	607	CLA	CBD-CGD-O2D-CED
34	W	201	LMG	C38-C39-C40-C41
34	W	201	LMG	C41-C42-C43-C44
34	g	322	LMG	C35-C36-C37-C38
34	w	202	LMG	C38-C39-C40-C41
34	w	202	LMG	C41-C42-C43-C44
33	1	617	LHG	O2-C2-C3-O3
33	3	320	LHG	O2-C2-C3-O3
33	5	619	LHG	O2-C2-C3-O3
33	A	417	LHG	O2-C2-C3-O3
33	B	624	LHG	O2-C2-C3-O3
33	C	623	LHG	O2-C2-C3-O3
33	K	102	LHG	O2-C2-C3-O3
33	N	319	LHG	O2-C2-C3-O3
33	R	320	LHG	O2-C2-C3-O3
33	Y	318	LHG	O2-C2-C3-O3
33	9	320	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
33	p	619	LHG	O2-C2-C3-O3
33	b	628	LHG	O2-C2-C3-O3
33	j	102	LHG	O2-C2-C3-O3
33	s	322	LHG	O2-C2-C3-O3
33	z	102	LHG	O2-C2-C3-O3
30	2	607	CHL	O1D-CGD-O2D-CED
31	2	604	CLA	O1D-CGD-O2D-CED
31	4	610	CLA	O1D-CGD-O2D-CED
31	4	614	CLA	O1D-CGD-O2D-CED
31	5	613	CLA	O1D-CGD-O2D-CED
31	6	304	CLA	O1D-CGD-O2D-CED
31	G	613	CLA	O1D-CGD-O2D-CED
31	R	312	CLA	O1D-CGD-O2D-CED
31	Y	310	CLA	O1D-CGD-O2D-CED
31	9	306	CLA	O1D-CGD-O2D-CED
31	p	603	CLA	O1D-CGD-O2D-CED
31	q	305	CLA	O1D-CGD-O2D-CED
31	c	610	CLA	O1D-CGD-O2D-CED
31	c	611	CLA	O1D-CGD-O2D-CED
31	g	312	CLA	O1D-CGD-O2D-CED
31	r	306	CLA	O1D-CGD-O2D-CED
31	r	312	CLA	O1D-CGD-O2D-CED
31	s	304	CLA	O1D-CGD-O2D-CED
31	1	614	CLA	CBA-CGA-O2A-C1
31	2	604	CLA	CBA-CGA-O2A-C1
31	3	313	CLA	CBA-CGA-O2A-C1
31	4	610	CLA	CBA-CGA-O2A-C1
31	6	311	CLA	CBA-CGA-O2A-C1
31	G	613	CLA	CBA-CGA-O2A-C1
31	N	310	CLA	CBA-CGA-O2A-C1
31	N	315	CLA	CBA-CGA-O2A-C1
31	S	310	CLA	CBA-CGA-O2A-C1
31	7	315	CLA	CBA-CGA-O2A-C1
31	8	609	CLA	CBA-CGA-O2A-C1
31	g	305	CLA	CBA-CGA-O2A-C1
31	r	307	CLA	CBA-CGA-O2A-C1
31	s	314	CLA	CBA-CGA-O2A-C1
33	5	619	LHG	C24-C23-O8-C6
38	a	411	SQD	C24-C23-O48-C46
31	0	610	CLA	O1A-CGA-O2A-C1
31	b	613	CLA	O1A-CGA-O2A-C1
31	c	609	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	s	314	CLA	O1A-CGA-O2A-C1
42	A	408	PHO	O1A-CGA-O2A-C1
31	B	602	CLA	O1D-CGD-O2D-CED
31	C	602	CLA	O1D-CGD-O2D-CED
31	C	611	CLA	O1D-CGD-O2D-CED
31	b	608	CLA	O1D-CGD-O2D-CED
31	y	603	CLA	O1D-CGD-O2D-CED
30	7	310	CHL	CBD-CGD-O2D-CED
31	3	313	CLA	CBD-CGD-O2D-CED
31	C	609	CLA	CBD-CGD-O2D-CED
31	y	602	CLA	CBD-CGD-O2D-CED
31	y	610	CLA	CBD-CGD-O2D-CED
33	N	319	LHG	C8-C7-O7-C5
33	8	618	LHG	C8-C7-O7-C5
33	n	320	LHG	C8-C7-O7-C5
34	1	618	LMG	C11-C10-O7-C8
34	2	618	LMG	C11-C10-O7-C8
34	6	323	LMG	C11-C10-O7-C8
34	A	412	LMG	C11-C10-O7-C8
34	B	621	LMG	C11-C10-O7-C8
34	J	101	LMG	C11-C10-O7-C8
34	7	320	LMG	C11-C10-O7-C8
34	s	321	LMG	C11-C10-O7-C8
31	8	609	CLA	O1D-CGD-O2D-CED
31	b	617	CLA	O1D-CGD-O2D-CED
31	1	614	CLA	O1A-CGA-O2A-C1
31	2	611	CLA	O1A-CGA-O2A-C1
31	G	613	CLA	O1A-CGA-O2A-C1
34	D	411	LMG	O10-C28-O8-C9
34	d	410	LMG	O10-C28-O8-C9
36	N	318	NEX	C14-C15-C35-C34
31	3	304	CLA	O1D-CGD-O2D-CED
31	6	303	CLA	O1D-CGD-O2D-CED
31	B	616	CLA	O1D-CGD-O2D-CED
31	C	604	CLA	O1D-CGD-O2D-CED
31	b	602	CLA	O1D-CGD-O2D-CED
31	b	609	CLA	O1D-CGD-O2D-CED
31	c	602	CLA	O1D-CGD-O2D-CED
31	c	606	CLA	O1D-CGD-O2D-CED
31	1	614	CLA	C3-C5-C6-C7
31	3	314	CLA	C3-C5-C6-C7
31	5	611	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	N	305	CLA	C3-C5-C6-C7
31	7	311	CLA	C3-C5-C6-C7
34	x	202	LMG	C8-C9-O8-C28
38	M	102	SQD	C45-C46-O48-C23
45	c	616	DGD	C2G-C1G-O1G-C1A
30	R	309	CHL	CBD-CGD-O2D-CED
30	0	607	CHL	CBD-CGD-O2D-CED
31	1	612	CLA	CBD-CGD-O2D-CED
31	B	611	CLA	CBD-CGD-O2D-CED
31	p	611	CLA	CBD-CGD-O2D-CED
31	p	612	CLA	CBD-CGD-O2D-CED
31	b	611	CLA	CBD-CGD-O2D-CED
31	c	609	CLA	CBD-CGD-O2D-CED
30	p	608	CHL	O1D-CGD-O2D-CED
31	1	611	CLA	O1D-CGD-O2D-CED
31	2	603	CLA	O1D-CGD-O2D-CED
31	B	608	CLA	O1D-CGD-O2D-CED
31	C	612	CLA	O1D-CGD-O2D-CED
31	G	609	CLA	O1D-CGD-O2D-CED
31	G	611	CLA	O1D-CGD-O2D-CED
31	0	604	CLA	O1D-CGD-O2D-CED
31	7	305	CLA	O1D-CGD-O2D-CED
31	7	311	CLA	O1D-CGD-O2D-CED
31	8	613	CLA	O1D-CGD-O2D-CED
31	p	602	CLA	O1D-CGD-O2D-CED
31	q	304	CLA	O1D-CGD-O2D-CED
31	r	305	CLA	O1D-CGD-O2D-CED
31	r	315	CLA	O1D-CGD-O2D-CED
31	r	316	CLA	O1D-CGD-O2D-CED
31	1	603	CLA	CBA-CGA-O2A-C1
31	6	316	CLA	CBA-CGA-O2A-C1
33	t	102	LHG	C24-C23-O8-C6
34	2	621	LMG	C29-C28-O8-C9
33	l	101	LHG	C11-C12-C13-C14
30	1	619	CHL	C4-C3-C5-C6
30	2	608	CHL	C4-C3-C5-C6
30	5	609	CHL	C4-C3-C5-C6
30	6	308	CHL	C4-C3-C5-C6
30	Y	302	CHL	C4-C3-C5-C6
30	0	609	CHL	C4-C3-C5-C6
30	y	606	CHL	C4-C3-C5-C6
31	B	605	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	p	602	CLA	C4-C3-C5-C6
31	s	310	CLA	C4-C3-C5-C6
30	1	619	CHL	C2-C3-C5-C6
30	2	608	CHL	C2-C3-C5-C6
30	5	609	CHL	C2-C3-C5-C6
30	Y	302	CHL	C2-C3-C5-C6
30	0	609	CHL	C2-C3-C5-C6
30	y	606	CHL	C2-C3-C5-C6
31	B	605	CLA	C2-C3-C5-C6
31	B	613	CLA	C2-C3-C5-C6
31	D	404	CLA	C2-C3-C5-C6
31	7	311	CLA	C5-C6-C7-C8
31	4	610	CLA	O1A-CGA-O2A-C1
31	7	315	CLA	O1A-CGA-O2A-C1
31	8	613	CLA	O1A-CGA-O2A-C1
31	c	611	CLA	O1A-CGA-O2A-C1
31	g	305	CLA	O1A-CGA-O2A-C1
33	8	618	LHG	O9-C7-O7-C5
33	n	320	LHG	O9-C7-O7-C5
48	K	101	LMU	O5B-C5B-C6B-O6B
48	R	302	LMU	O5B-C5B-C6B-O6B
44	A	416	PL9	C19-C21-C22-C23
44	a	414	PL9	C9-C11-C12-C13
30	N	306	CHL	CBD-CGD-O2D-CED
31	A	407	CLA	CBD-CGD-O2D-CED
31	B	610	CLA	CBD-CGD-O2D-CED
31	G	602	CLA	CBD-CGD-O2D-CED
31	d	401	CLA	CBD-CGD-O2D-CED
31	s	306	CLA	CBD-CGD-O2D-CED
31	y	612	CLA	CBD-CGD-O2D-CED
31	0	603	CLA	O1D-CGD-O2D-CED
33	K	102	LHG	C2-C3-O3-P
48	r	302	LMU	C4B-C5B-C6B-O6B
30	9	309	CHL	C3-C5-C6-C7
31	3	312	CLA	C2A-CAA-CBA-CGA
31	7	312	CLA	C2A-CAA-CBA-CGA
31	s	312	CLA	C2A-CAA-CBA-CGA
31	4	611	CLA	O1D-CGD-O2D-CED
31	5	610	CLA	O1D-CGD-O2D-CED
31	6	312	CLA	O1D-CGD-O2D-CED
31	1	612	CLA	O1A-CGA-O2A-C1
31	2	613	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	3	312	CLA	O1A-CGA-O2A-C1
31	3	313	CLA	O1A-CGA-O2A-C1
31	6	311	CLA	O1A-CGA-O2A-C1
31	N	315	CLA	O1A-CGA-O2A-C1
31	S	310	CLA	O1A-CGA-O2A-C1
31	n	315	CLA	O1A-CGA-O2A-C1
31	r	307	CLA	O1A-CGA-O2A-C1
31	s	310	CLA	O1A-CGA-O2A-C1
34	G	622	LMG	O6-C1-O1-C7
34	0	622	LMG	O6-C1-O1-C7
34	7	301	LMG	O6-C1-O1-C7
34	q	301	LMG	O6-C1-O1-C7
34	k	102	LMG	O6-C1-O1-C7
38	B	623	SQD	O5-C1-O6-C44
38	G	617	SQD	O5-C1-O6-C44
38	M	102	SQD	O5-C1-O6-C44
38	S	301	SQD	O5-C1-O6-C44
38	b	621	SQD	O5-C1-O6-C44
38	b	627	SQD	O5-C1-O6-C44
31	0	610	CLA	C5-C6-C7-C8
31	A	409	CLA	O1D-CGD-O2D-CED
31	a	409	CLA	O1D-CGD-O2D-CED
31	3	312	CLA	CBA-CGA-O2A-C1
31	B	605	CLA	CBA-CGA-O2A-C1
31	B	612	CLA	CBA-CGA-O2A-C1
31	C	611	CLA	CBA-CGA-O2A-C1
31	R	307	CLA	CBA-CGA-O2A-C1
31	Y	313	CLA	CBA-CGA-O2A-C1
31	c	607	CLA	CBA-CGA-O2A-C1
31	s	310	CLA	CBA-CGA-O2A-C1
31	y	604	CLA	CBA-CGA-O2A-C1
45	C	618	DGD	C2A-C1A-O1G-C1G
45	c	619	DGD	C2A-C1A-O1G-C1G
33	2	617	LHG	C13-C14-C15-C16
30	1	606	CHL	CBD-CGD-O2D-CED
30	5	601	CHL	CBD-CGD-O2D-CED
30	G	607	CHL	CBD-CGD-O2D-CED
30	Y	307	CHL	CBD-CGD-O2D-CED
30	8	607	CHL	CBD-CGD-O2D-CED
30	q	308	CHL	CBD-CGD-O2D-CED
30	n	309	CHL	CBD-CGD-O2D-CED
31	4	612	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	B	615	CLA	CBD-CGD-O2D-CED
31	C	607	CLA	CBD-CGD-O2D-CED
31	D	403	CLA	CBD-CGD-O2D-CED
31	N	311	CLA	CBD-CGD-O2D-CED
31	S	311	CLA	CBD-CGD-O2D-CED
31	Y	303	CLA	CBD-CGD-O2D-CED
44	A	416	PL9	C12-C13-C14-C15
33	t	102	LHG	O10-C23-O8-C6
33	2	617	LHG	C11-C12-C13-C14
48	r	302	LMU	O5B-C5B-C6B-O6B
31	N	312	CLA	O1D-CGD-O2D-CED
31	R	303	CLA	O1D-CGD-O2D-CED
31	8	603	CLA	O1D-CGD-O2D-CED
31	g	304	CLA	O1D-CGD-O2D-CED
33	2	617	LHG	C28-C29-C30-C31
33	S	320	LHG	C28-C29-C30-C31
33	s	322	LHG	C28-C29-C30-C31
30	3	303	CHL	CBD-CGD-O2D-CED
30	4	607	CHL	CBD-CGD-O2D-CED
31	q	313	CLA	CBD-CGD-O2D-CED
33	R	320	LHG	C8-C7-O7-C5
34	2	620	LMG	C11-C10-O7-C8
34	0	622	LMG	C11-C10-O7-C8
34	w	202	LMG	C11-C10-O7-C8
33	5	619	LHG	C7-C8-C9-C10
31	6	311	CLA	C5-C6-C7-C8
31	2	610	CLA	O1D-CGD-O2D-CED
31	q	306	CLA	O1D-CGD-O2D-CED
33	l	101	LHG	C9-C10-C11-C12
35	2	614	RRX	C9-C10-C11-C12
36	5	618	NEX	C29-C30-C31-C32
36	N	318	NEX	C13-C14-C15-C35
43	B	618	BCR	C19-C20-C21-C22
43	B	619	BCR	C9-C10-C11-C12
43	T	101	BCR	C19-C20-C21-C22
43	c	615	BCR	C9-C10-C11-C12
31	3	311	CLA	O1A-CGA-O2A-C1
31	A	406	CLA	O1A-CGA-O2A-C1
31	B	612	CLA	O1A-CGA-O2A-C1
31	C	611	CLA	O1A-CGA-O2A-C1
31	R	307	CLA	O1A-CGA-O2A-C1
31	p	611	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	5	619	LHG	O10-C23-O8-C6
45	C	618	DGD	O1A-C1A-O1G-C1G
31	9	304	CLA	C2C-C3C-CAC-CBC
33	N	319	LHG	O9-C7-O7-C5
34	1	618	LMG	O9-C10-O7-C8
34	2	618	LMG	O9-C10-O7-C8
34	J	101	LMG	O9-C10-O7-C8
34	s	321	LMG	O9-C10-O7-C8
33	2	617	LHG	C1-C2-C3-O3
33	5	619	LHG	C1-C2-C3-O3
33	6	320	LHG	C1-C2-C3-O3
33	A	417	LHG	C1-C2-C3-O3
33	G	618	LHG	C1-C2-C3-O3
33	L	101	LHG	C1-C2-C3-O3
33	N	319	LHG	C1-C2-C3-O3
33	b	625	LHG	C1-C2-C3-O3
33	c	622	LHG	C1-C2-C3-O3
33	g	319	LHG	C1-C2-C3-O3
33	j	102	LHG	C1-C2-C3-O3
33	l	101	LHG	C1-C2-C3-O3
33	F1	301	LHG	C1-C2-C3-O3
31	4	603	CLA	O1D-CGD-O2D-CED
31	1	602	CLA	CBA-CGA-O2A-C1
31	3	311	CLA	CBA-CGA-O2A-C1
31	3	316	CLA	CBA-CGA-O2A-C1
31	A	406	CLA	CBA-CGA-O2A-C1
31	C	607	CLA	CBA-CGA-O2A-C1
31	C	610	CLA	CBA-CGA-O2A-C1
31	G	604	CLA	CBA-CGA-O2A-C1
31	G	610	CLA	CBA-CGA-O2A-C1
31	N	305	CLA	CBA-CGA-O2A-C1
31	N	321	CLA	CBA-CGA-O2A-C1
31	R	314	CLA	CBA-CGA-O2A-C1
31	0	603	CLA	CBA-CGA-O2A-C1
31	8	604	CLA	CBA-CGA-O2A-C1
31	8	614	CLA	CBA-CGA-O2A-C1
31	9	304	CLA	CBA-CGA-O2A-C1
31	9	312	CLA	CBA-CGA-O2A-C1
31	p	611	CLA	CBA-CGA-O2A-C1
31	q	316	CLA	CBA-CGA-O2A-C1
31	a	407	CLA	CBA-CGA-O2A-C1
31	b	606	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	b	612	CLA	CBA-CGA-O2A-C1
31	d	405	CLA	CBA-CGA-O2A-C1
31	g	311	CLA	CBA-CGA-O2A-C1
31	n	305	CLA	CBA-CGA-O2A-C1
31	n	316	CLA	CBA-CGA-O2A-C1
33	G	618	LHG	C24-C23-O8-C6
38	M	102	SQD	C24-C23-O48-C46
38	m	101	SQD	C24-C23-O48-C46
42	a	408	PHO	CBA-CGA-O2A-C1
45	c	618	DGD	C2A-C1A-O1G-C1G
33	c	622	LHG	C33-C34-C35-C36
31	N	304	CLA	C5-C6-C7-C8
30	9	311	CHL	CBD-CGD-O2D-CED
31	s	305	CLA	CBD-CGD-O2D-CED
33	r	320	LHG	C11-C12-C13-C14
33	s	320	LHG	C28-C29-C30-C31
31	B	601	CLA	O1D-CGD-O2D-CED
31	B	607	CLA	O1D-CGD-O2D-CED
31	C	613	CLA	O1D-CGD-O2D-CED
31	N	303	CLA	O1D-CGD-O2D-CED
31	Y	304	CLA	O1D-CGD-O2D-CED
31	9	304	CLA	O1D-CGD-O2D-CED
31	9	312	CLA	O1D-CGD-O2D-CED
31	c	612	CLA	O1D-CGD-O2D-CED
31	c	613	CLA	O1D-CGD-O2D-CED
31	d	404	CLA	O1D-CGD-O2D-CED
31	n	311	CLA	O1D-CGD-O2D-CED
31	s	310	CLA	O1D-CGD-O2D-CED
31	y	604	CLA	O1D-CGD-O2D-CED
33	G	618	LHG	C11-C10-C9-C8
33	q	320	LHG	C26-C27-C28-C29
33	b	625	LHG	C25-C26-C27-C28
33	g	319	LHG	C26-C27-C28-C29
31	4	602	CLA	C8-C10-C11-C12
30	6	308	CHL	C2-C3-C5-C6
30	G	601	CHL	C2-C3-C5-C6
30	7	310	CHL	C2-C3-C5-C6
31	D	403	CLA	C2-C3-C5-C6
31	p	602	CLA	C2-C3-C5-C6
31	b	603	CLA	C2-C3-C5-C6
31	b	605	CLA	C2-C3-C5-C6
31	b	606	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	s	310	CLA	C2-C3-C5-C6
44	A	416	PL9	C43-C44-C46-C47
31	B	607	CLA	C3-C5-C6-C7
31	c	611	CLA	C3-C5-C6-C7
30	6	308	CHL	CBD-CGD-O2D-CED
30	1	605	CHL	C6-C7-C8-C9
30	1	605	CHL	C11-C10-C8-C9
30	1	607	CHL	C14-C13-C15-C16
30	3	310	CHL	C11-C10-C8-C9
30	6	308	CHL	C11-C10-C8-C9
30	6	308	CHL	C14-C13-C15-C16
30	6	310	CHL	C11-C10-C8-C9
30	G	623	CHL	C11-C10-C8-C9
30	G	623	CHL	C14-C13-C15-C16
30	N	306	CHL	C11-C10-C8-C9
30	N	309	CHL	C11-C10-C8-C9
30	Y	309	CHL	C11-C10-C8-C9
30	0	607	CHL	C11-C10-C8-C9
30	0	607	CHL	C14-C13-C15-C16
30	7	306	CHL	C11-C10-C8-C9
30	7	307	CHL	C11-C10-C8-C9
30	7	308	CHL	C14-C13-C15-C16
30	8	605	CHL	C11-C10-C8-C9
30	9	303	CHL	C14-C13-C15-C16
30	9	311	CHL	C6-C7-C8-C9
30	9	311	CHL	C11-C10-C8-C9
30	g	302	CHL	C11-C10-C8-C9
30	n	306	CHL	C11-C10-C8-C9
30	y	601	CHL	C11-C10-C8-C9
30	y	607	CHL	C14-C13-C15-C16
31	1	604	CLA	C6-C7-C8-C9
31	2	602	CLA	C11-C10-C8-C9
31	2	610	CLA	C6-C7-C8-C9
31	3	316	CLA	C6-C7-C8-C9
31	5	602	CLA	C6-C7-C8-C9
31	5	610	CLA	C6-C7-C8-C9
31	5	611	CLA	C6-C7-C8-C9
31	6	303	CLA	C6-C7-C8-C9
31	6	303	CLA	C11-C10-C8-C9
31	6	312	CLA	C11-C10-C8-C9
31	A	406	CLA	C14-C13-C15-C16
31	A	409	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	B	605	CLA	C11-C10-C8-C9
31	B	607	CLA	C11-C12-C13-C14
31	C	601	CLA	C11-C12-C13-C14
31	C	607	CLA	C14-C13-C15-C16
31	C	608	CLA	C11-C10-C8-C9
31	C	613	CLA	C11-C12-C13-C14
31	D	404	CLA	C6-C7-C8-C9
31	N	303	CLA	C11-C10-C8-C9
31	N	303	CLA	C11-C12-C13-C14
31	N	310	CLA	C6-C7-C8-C9
31	R	304	CLA	C6-C7-C8-C9
31	R	311	CLA	C11-C10-C8-C9
31	R	316	CLA	C14-C13-C15-C16
31	S	305	CLA	C6-C7-C8-C9
31	Y	311	CLA	C11-C12-C13-C14
31	Y	312	CLA	C11-C12-C13-C14
31	7	311	CLA	C11-C10-C8-C9
31	7	313	CLA	C11-C10-C8-C9
31	9	304	CLA	C11-C10-C8-C9
31	p	602	CLA	C6-C7-C8-C9
31	p	610	CLA	C6-C7-C8-C9
31	a	409	CLA	C6-C7-C8-C9
31	b	605	CLA	C6-C7-C8-C9
31	b	606	CLA	C14-C13-C15-C16
31	b	609	CLA	C14-C13-C15-C16
31	b	611	CLA	C6-C7-C8-C9
31	b	611	CLA	C11-C12-C13-C14
31	b	612	CLA	C6-C7-C8-C9
31	b	612	CLA	C11-C12-C13-C14
31	b	614	CLA	C6-C7-C8-C9
31	b	616	CLA	C11-C10-C8-C9
31	c	608	CLA	C6-C7-C8-C9
31	c	613	CLA	C14-C13-C15-C16
31	d	404	CLA	C6-C7-C8-C9
31	g	313	CLA	C6-C7-C8-C9
31	n	311	CLA	C6-C7-C8-C9
31	r	304	CLA	C6-C7-C8-C9
31	r	311	CLA	C11-C10-C8-C9
31	s	310	CLA	C6-C7-C8-C9
31	s	312	CLA	C6-C7-C8-C9
31	y	613	CLA	C11-C10-C8-C9
33	b	625	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
48	R	302	LMU	C4B-C5B-C6B-O6B
31	1	604	CLA	O1D-CGD-O2D-CED
31	3	311	CLA	O1D-CGD-O2D-CED
31	C	610	CLA	O1D-CGD-O2D-CED
31	G	610	CLA	O1D-CGD-O2D-CED
31	R	316	CLA	O1D-CGD-O2D-CED
31	7	303	CLA	O1D-CGD-O2D-CED
31	b	616	CLA	O1D-CGD-O2D-CED
31	c	604	CLA	O1D-CGD-O2D-CED
31	g	303	CLA	O1D-CGD-O2D-CED
34	4	621	LMG	C2-C1-O1-C7
34	G	622	LMG	C2-C1-O1-C7
34	0	622	LMG	C2-C1-O1-C7
34	7	301	LMG	C2-C1-O1-C7
34	9	301	LMG	C2-C1-O1-C7
34	b	624	LMG	C2-C1-O1-C7
34	k	102	LMG	C2-C1-O1-C7
34	n	321	LMG	C2-C1-O1-C7
38	B	620	SQD	C2-C1-O6-C44
38	B	623	SQD	C2-C1-O6-C44
38	g	318	SQD	C2-C1-O6-C44
38	s	301	SQD	C2-C1-O6-C44
31	G	603	CLA	C5-C6-C7-C8
33	d	408	LHG	C23-C24-C25-C26
33	e	101	LHG	C7-C8-C9-C10
33	4	618	LHG	O2-C2-C3-O3
33	6	320	LHG	O2-C2-C3-O3
33	A	415	LHG	O2-C2-C3-O3
33	D	407	LHG	O2-C2-C3-O3
33	L	101	LHG	O2-C2-C3-O3
33	S	320	LHG	O2-C2-C3-O3
33	7	319	LHG	O2-C2-C3-O3
33	a	415	LHG	O2-C2-C3-O3
33	d	408	LHG	O2-C2-C3-O3
33	l	101	LHG	O2-C2-C3-O3
33	t	102	LHG	O2-C2-C3-O3
33	y	619	LHG	O2-C2-C3-O3
30	n	301	CHL	O1D-CGD-O2D-CED
31	s	312	CLA	O1D-CGD-O2D-CED
31	s	315	CLA	O1D-CGD-O2D-CED
45	c	617	DGD	C2A-C1A-O1G-C1G
31	1	602	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	G	610	CLA	O1A-CGA-O2A-C1
31	N	305	CLA	O1A-CGA-O2A-C1
31	8	604	CLA	O1A-CGA-O2A-C1
31	8	614	CLA	O1A-CGA-O2A-C1
31	a	407	CLA	O1A-CGA-O2A-C1
31	d	405	CLA	O1A-CGA-O2A-C1
31	n	305	CLA	O1A-CGA-O2A-C1
30	1	608	CHL	CBD-CGD-O2D-CED
31	9	305	CLA	CBD-CGD-O2D-CED
31	N	310	CLA	O1D-CGD-O2D-CED
31	Y	312	CLA	O1D-CGD-O2D-CED
31	0	602	CLA	O1D-CGD-O2D-CED
31	8	602	CLA	O1D-CGD-O2D-CED
31	b	612	CLA	O1D-CGD-O2D-CED
31	n	304	CLA	O1D-CGD-O2D-CED
31	r	303	CLA	O1D-CGD-O2D-CED
32	1	616	LUT	C7-C8-C9-C19
32	3	317	LUT	C11-C12-C13-C20
32	3	318	LUT	C7-C8-C9-C19
32	4	616	LUT	C31-C32-C33-C40
32	5	616	LUT	C11-C12-C13-C20
32	5	616	LUT	C31-C32-C33-C40
32	5	617	LUT	C11-C12-C13-C20
32	5	617	LUT	C31-C32-C33-C40
32	6	317	LUT	C11-C12-C13-C20
32	6	317	LUT	C31-C32-C33-C40
32	6	318	LUT	C31-C32-C33-C40
32	G	615	LUT	C7-C8-C9-C19
32	N	316	LUT	C7-C8-C9-C19
32	N	316	LUT	C11-C12-C13-C20
32	N	317	LUT	C31-C32-C33-C40
32	R	317	LUT	C7-C8-C9-C19
32	R	317	LUT	C11-C12-C13-C20
32	R	317	LUT	C31-C32-C33-C40
32	S	317	LUT	C31-C32-C33-C40
32	S	318	LUT	C11-C12-C13-C20
32	S	318	LUT	C27-C28-C29-C39
32	S	318	LUT	C31-C32-C33-C40
32	0	616	LUT	C11-C12-C13-C20
32	7	317	LUT	C11-C12-C13-C20
32	8	615	LUT	C11-C12-C13-C20
32	8	615	LUT	C31-C32-C33-C40

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Mol	Chain	Res	Type	Atoms
32	8	616	LUT	C7-C8-C9-C19
32	8	616	LUT	C31-C32-C33-C40
32	p	616	LUT	C7-C8-C9-C19
32	q	318	LUT	C11-C12-C13-C20
32	q	318	LUT	C31-C32-C33-C40
32	g	316	LUT	C11-C12-C13-C20
32	g	316	LUT	C27-C28-C29-C39
32	g	316	LUT	C31-C32-C33-C40
32	n	317	LUT	C11-C12-C13-C20
32	n	317	LUT	C31-C32-C33-C40
32	n	318	LUT	C7-C8-C9-C19
32	n	318	LUT	C31-C32-C33-C40
32	r	317	LUT	C11-C12-C13-C20
32	s	317	LUT	C7-C8-C9-C19
35	2	614	RRX	C37-C22-C23-C24
35	2	614	RRX	C11-C12-C13-C35
35	4	615	RRX	C37-C22-C23-C24
35	4	615	RRX	C11-C12-C13-C35
35	G	614	RRX	C37-C22-C23-C24
35	G	614	RRX	C11-C12-C13-C35
35	9	317	RRX	C37-C22-C23-C24
35	9	317	RRX	C11-C12-C13-C35
35	q	317	RRX	C7-C8-C9-C34
36	5	618	NEX	C11-C12-C13-C20
36	6	319	NEX	C31-C32-C33-C40
36	N	318	NEX	C11-C12-C13-C20
36	0	618	NEX	C31-C32-C33-C40
36	8	617	NEX	C11-C12-C13-C20
37	2	619	XAT	C27-C28-C29-C39
37	4	619	XAT	C27-C28-C29-C39
37	G	620	XAT	C27-C28-C29-C39
37	9	322	XAT	C27-C28-C29-C39
37	q	321	XAT	C27-C28-C29-C39
37	g	321	XAT	C27-C28-C29-C39
43	B	617	BCR	C11-C12-C13-C35
43	B	617	BCR	C36-C18-C19-C20
43	B	617	BCR	C37-C22-C23-C24
43	C	614	BCR	C7-C8-C9-C34
43	V	101	BCR	C36-C18-C19-C20
43	Z	101	BCR	C7-C8-C9-C34
43	b	618	BCR	C36-C18-C19-C20
43	b	619	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
43	b	619	BCR	C37-C22-C23-C24
43	b	620	BCR	C36-C18-C19-C20
43	c	614	BCR	C11-C12-C13-C35
43	c	614	BCR	C37-C22-C23-C24
43	d	406	BCR	C36-C18-C19-C20
43	d	406	BCR	C37-C22-C23-C24
43	h	101	BCR	C11-C12-C13-C35
43	v	101	BCR	C7-C8-C9-C34
43	v	101	BCR	C36-C18-C19-C20
43	v	101	BCR	C37-C22-C23-C24
32	3	318	LUT	C7-C8-C9-C10
32	5	617	LUT	C11-C12-C13-C14
32	G	615	LUT	C7-C8-C9-C10
32	N	316	LUT	C7-C8-C9-C10
32	R	317	LUT	C31-C32-C33-C34
32	S	318	LUT	C27-C28-C29-C30
32	Y	316	LUT	C7-C8-C9-C10
32	7	317	LUT	C7-C8-C9-C10
32	8	616	LUT	C7-C8-C9-C10
32	p	616	LUT	C7-C8-C9-C10
32	p	616	LUT	C31-C32-C33-C34
32	g	316	LUT	C27-C28-C29-C30
32	n	318	LUT	C7-C8-C9-C10
35	g	315	RRX	C21-C22-C23-C24
36	6	319	NEX	C31-C32-C33-C34
36	0	618	NEX	C31-C32-C33-C34
37	2	619	XAT	C27-C28-C29-C30
37	4	619	XAT	C27-C28-C29-C30
37	G	620	XAT	C27-C28-C29-C30
37	9	322	XAT	C27-C28-C29-C30
37	q	321	XAT	C27-C28-C29-C30
37	g	321	XAT	C27-C28-C29-C30
43	B	617	BCR	C17-C18-C19-C20
43	C	614	BCR	C7-C8-C9-C10
43	V	101	BCR	C17-C18-C19-C20
43	b	618	BCR	C21-C22-C23-C24
43	b	619	BCR	C11-C12-C13-C14
43	c	614	BCR	C11-C12-C13-C14
43	d	406	BCR	C21-C22-C23-C24
43	h	101	BCR	C11-C12-C13-C14
43	v	101	BCR	C17-C18-C19-C20
33	q	320	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
33	g	319	LHG	C11-C10-C9-C8
30	R	310	CHL	C2A-CAA-CBA-CGA
31	2	613	CLA	C2A-CAA-CBA-CGA
31	5	603	CLA	C3-C5-C6-C7
31	B	614	CLA	C2A-CAA-CBA-CGA
31	S	312	CLA	C2A-CAA-CBA-CGA
31	p	614	CLA	C2A-CAA-CBA-CGA
31	s	314	CLA	C2A-CAA-CBA-CGA
33	3	320	LHG	C7-C8-C9-C10
33	S	322	LHG	C23-C24-C25-C26
33	p	619	LHG	C7-C8-C9-C10
33	b	625	LHG	C23-C24-C25-C26
33	F1	301	LHG	C23-C24-C25-C26
31	N	315	CLA	C5-C6-C7-C8
48	r	302	LMU	C5-C6-C7-C8
31	3	316	CLA	O1A-CGA-O2A-C1
31	N	321	CLA	O1A-CGA-O2A-C1
31	9	304	CLA	O1A-CGA-O2A-C1
31	q	316	CLA	O1A-CGA-O2A-C1
31	b	606	CLA	O1A-CGA-O2A-C1
31	n	316	CLA	O1A-CGA-O2A-C1
42	a	408	PHO	O1A-CGA-O2A-C1
30	9	307	CHL	CBD-CGD-O2D-CED
34	3	321	LMG	C11-C10-O7-C8
34	B	625	LMG	C11-C10-O7-C8
34	W	201	LMG	C11-C10-O7-C8
34	X	203	LMG	C11-C10-O7-C8
34	n	321	LMG	C11-C10-O7-C8
33	d	408	LHG	C31-C32-C33-C34
31	2	602	CLA	C2C-C3C-CAC-CBC
33	4	618	LHG	O7-C5-C6-O8
33	R	320	LHG	O7-C5-C6-O8
33	8	618	LHG	O7-C5-C6-O8
33	9	320	LHG	O7-C5-C6-O8
33	e	101	LHG	O7-C5-C6-O8
33	n	320	LHG	O7-C5-C6-O8
31	r	307	CLA	O1D-CGD-O2D-CED
31	c	608	CLA	CBA-CGA-O2A-C1
33	g	319	LHG	C24-C23-O8-C6
34	A	412	LMG	C29-C28-O8-C9
31	c	612	CLA	C5-C6-C7-C8
31	g	304	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	s	303	CLA	C8-C10-C11-C12
31	1	603	CLA	C2-C1-O2A-CGA
31	1	604	CLA	C2-C1-O2A-CGA
31	3	315	CLA	C2-C1-O2A-CGA
31	6	315	CLA	C2-C1-O2A-CGA
31	A	407	CLA	C2-C1-O2A-CGA
31	B	601	CLA	C2-C1-O2A-CGA
31	C	602	CLA	C2-C1-O2A-CGA
31	0	614	CLA	C2-C1-O2A-CGA
31	7	305	CLA	C2-C1-O2A-CGA
31	9	312	CLA	C2-C1-O2A-CGA
31	p	604	CLA	C2-C1-O2A-CGA
31	p	614	CLA	C2-C1-O2A-CGA
31	q	306	CLA	C2-C1-O2A-CGA
31	a	407	CLA	C2-C1-O2A-CGA
31	b	605	CLA	C2-C1-O2A-CGA
31	b	613	CLA	C2-C1-O2A-CGA
31	b	614	CLA	C2-C1-O2A-CGA
31	b	616	CLA	C2-C1-O2A-CGA
31	c	602	CLA	C2-C1-O2A-CGA
31	d	401	CLA	C2-C1-O2A-CGA
31	d	405	CLA	C2-C1-O2A-CGA
31	5	613	CLA	C5-C6-C7-C8
33	j	102	LHG	C24-C25-C26-C27
30	q	310	CHL	O1D-CGD-O2D-CED
31	1	602	CLA	O1D-CGD-O2D-CED
31	S	312	CLA	O1D-CGD-O2D-CED
31	Y	311	CLA	O1D-CGD-O2D-CED
31	g	310	CLA	O1D-CGD-O2D-CED
31	y	615	CLA	O1D-CGD-O2D-CED
31	7	312	CLA	CBD-CGD-O2D-CED
31	y	611	CLA	CBD-CGD-O2D-CED
36	g	317	NEX	C14-C15-C35-C34
31	A	409	CLA	C8-C10-C11-C12
31	B	606	CLA	C13-C15-C16-C17
31	a	409	CLA	C8-C10-C11-C12
33	C	623	LHG	O1-C1-C2-O2
33	D	407	LHG	O1-C1-C2-O2
33	S	322	LHG	O1-C1-C2-O2
33	7	319	LHG	O1-C1-C2-O2
33	9	320	LHG	O1-C1-C2-O2
33	b	628	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
33	l	101	LHG	O1-C1-C2-O2
33	z	102	LHG	O1-C1-C2-O2
31	G	610	CLA	C3-C5-C6-C7
31	N	313	CLA	C3-C5-C6-C7
31	g	303	CLA	C3-C5-C6-C7
33	M	101	LHG	C23-C24-C25-C26
30	1	607	CHL	O1D-CGD-O2D-CED
30	g	308	CHL	O1D-CGD-O2D-CED
31	n	303	CLA	O1D-CGD-O2D-CED
30	N	309	CHL	CBD-CGD-O2D-CED
31	4	604	CLA	CBD-CGD-O2D-CED
30	Y	309	CHL	C11-C12-C13-C15
30	q	309	CHL	C6-C7-C8-C10
31	1	611	CLA	C11-C10-C8-C7
31	3	316	CLA	C11-C10-C8-C7
31	4	613	CLA	C11-C10-C8-C7
31	6	314	CLA	C11-C10-C8-C7
31	7	312	CLA	C11-C10-C8-C7
31	a	406	CLA	C11-C10-C8-C7
31	b	613	CLA	C6-C7-C8-C10
31	b	614	CLA	C11-C12-C13-C15
31	c	603	CLA	C6-C7-C8-C10
31	3	306	CLA	CBA-CGA-O2A-C1
31	B	603	CLA	CBA-CGA-O2A-C1
31	R	304	CLA	CBA-CGA-O2A-C1
31	S	305	CLA	CBA-CGA-O2A-C1
31	b	614	CLA	CBA-CGA-O2A-C1
33	p	619	LHG	C24-C25-C26-C27
31	3	301	CLA	C4-C3-C5-C6
33	M	101	LHG	C34-C35-C36-C37
31	C	603	CLA	C8-C10-C11-C12
31	C	610	CLA	C13-C15-C16-C17
31	S	312	CLA	C10-C11-C12-C13
31	c	610	CLA	C15-C16-C17-C18
42	A	408	PHO	C8-C10-C11-C12
31	G	603	CLA	O1D-CGD-O2D-CED
31	G	604	CLA	O1D-CGD-O2D-CED
34	n	322	LMG	C28-C29-C30-C31
32	3	318	LUT	C9-C10-C11-C12
32	4	616	LUT	C9-C10-C11-C12
36	g	317	NEX	C13-C14-C15-C35
36	n	319	NEX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
43	B	618	BCR	C9-C10-C11-C12
43	D	405	BCR	C15-C16-C17-C18
43	V	101	BCR	C15-C16-C17-C18
43	b	620	BCR	C9-C10-C11-C12
43	c	614	BCR	C15-C16-C17-C18
34	2	620	LMG	O9-C10-O7-C8
34	B	621	LMG	O9-C10-O7-C8
34	W	201	LMG	O9-C10-O7-C8
34	0	622	LMG	O9-C10-O7-C8
34	7	320	LMG	O9-C10-O7-C8
31	R	315	CLA	O1D-CGD-O2D-CED
31	6	312	CLA	C5-C6-C7-C8
31	B	616	CLA	C5-C6-C7-C8
33	6	320	LHG	C11-C10-C9-C8
33	M	101	LHG	C26-C27-C28-C29
33	b	628	LHG	C29-C30-C31-C32
45	C	616	DGD	O6E-C5E-C6E-O5E
33	C	623	LHG	C26-C27-C28-C29
33	y	619	LHG	C29-C30-C31-C32
33	2	617	LHG	C7-C8-C9-C10
33	3	320	LHG	C23-C24-C25-C26
33	4	618	LHG	C23-C24-C25-C26
33	6	320	LHG	C23-C24-C25-C26
33	B	624	LHG	C23-C24-C25-C26
33	D	407	LHG	C23-C24-C25-C26
33	N	319	LHG	C23-C24-C25-C26
33	9	320	LHG	C7-C8-C9-C10
33	b	628	LHG	C7-C8-C9-C10
33	b	628	LHG	C23-C24-C25-C26
33	s	320	LHG	C7-C8-C9-C10
33	t	102	LHG	C7-C8-C9-C10
33	F1	301	LHG	C7-C8-C9-C10
34	n	321	LMG	C28-C29-C30-C31
31	C	607	CLA	O1A-CGA-O2A-C1
31	C	610	CLA	O1A-CGA-O2A-C1
31	G	604	CLA	O1A-CGA-O2A-C1
31	Y	313	CLA	O1A-CGA-O2A-C1
31	0	603	CLA	O1A-CGA-O2A-C1
31	b	612	CLA	O1A-CGA-O2A-C1
38	m	101	SQD	O10-C23-O48-C46
34	G	619	LMG	C11-C10-O7-C8
34	Y	319	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
31	R	307	CLA	O1D-CGD-O2D-CED
31	9	316	CLA	O1D-CGD-O2D-CED
31	n	305	CLA	O1D-CGD-O2D-CED
31	C	608	CLA	CBA-CGA-O2A-C1
33	b	625	LHG	C24-C23-O8-C6
31	1	613	CLA	C15-C16-C17-C18
31	B	603	CLA	C15-C16-C17-C18
31	R	311	CLA	C5-C6-C7-C8
31	0	602	CLA	C5-C6-C7-C8
31	a	407	CLA	C13-C15-C16-C17
31	b	607	CLA	C13-C15-C16-C17
31	b	612	CLA	C8-C10-C11-C12
31	c	601	CLA	C8-C10-C11-C12
31	c	606	CLA	C8-C10-C11-C12
31	s	310	CLA	C5-C6-C7-C8
34	x	202	LMG	O6-C5-C6-O5
30	0	601	CHL	C2A-CAA-CBA-CGA
30	0	607	CHL	C2A-CAA-CBA-CGA
30	y	605	CHL	C2A-CAA-CBA-CGA
31	2	609	CLA	C2A-CAA-CBA-CGA
31	3	306	CLA	C2A-CAA-CBA-CGA
31	6	314	CLA	C2A-CAA-CBA-CGA
31	B	604	CLA	C2A-CAA-CBA-CGA
31	B	606	CLA	C2A-CAA-CBA-CGA
31	D	404	CLA	C2A-CAA-CBA-CGA
31	R	316	CLA	C2A-CAA-CBA-CGA
31	S	303	CLA	C2A-CAA-CBA-CGA
31	9	316	CLA	C2A-CAA-CBA-CGA
31	p	603	CLA	C2A-CAA-CBA-CGA
31	a	406	CLA	C2A-CAA-CBA-CGA
31	r	312	CLA	C2A-CAA-CBA-CGA
30	y	607	CHL	C5-C6-C7-C8
31	1	612	CLA	C8-C10-C11-C12
31	B	606	CLA	C8-C10-C11-C12
31	B	609	CLA	C8-C10-C11-C12
31	C	613	CLA	C5-C6-C7-C8
31	G	604	CLA	C5-C6-C7-C8
31	S	303	CLA	C5-C6-C7-C8
31	S	314	CLA	C13-C15-C16-C17
31	7	313	CLA	C13-C15-C16-C17
31	8	612	CLA	C5-C6-C7-C8
31	q	306	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	a	406	CLA	C15-C16-C17-C18
31	b	606	CLA	C13-C15-C16-C17
31	n	314	CLA	C5-C6-C7-C8
31	y	610	CLA	C8-C10-C11-C12
31	y	613	CLA	C8-C10-C11-C12
33	B	624	LHG	C7-C8-C9-C10
33	C	623	LHG	C7-C8-C9-C10
33	G	618	LHG	C23-C24-C25-C26
33	K	102	LHG	C7-C8-C9-C10
33	S	320	LHG	C23-C24-C25-C26
33	7	319	LHG	C7-C8-C9-C10
33	q	320	LHG	C7-C8-C9-C10
33	g	319	LHG	C23-C24-C25-C26
33	s	320	LHG	C23-C24-C25-C26
33	z	102	LHG	C23-C24-C25-C26
34	J	101	LMG	C10-C11-C12-C13
45	c	618	DGD	C1B-C2B-C3B-C4B
31	0	612	CLA	O1D-CGD-O2D-CED
31	8	604	CLA	O1D-CGD-O2D-CED
31	b	603	CLA	O1D-CGD-O2D-CED
31	B	605	CLA	O1A-CGA-O2A-C1
31	R	314	CLA	O1A-CGA-O2A-C1
31	c	607	CLA	O1A-CGA-O2A-C1
33	G	618	LHG	O10-C23-O8-C6
38	M	102	SQD	O10-C23-O48-C46
31	N	321	CLA	C3-C5-C6-C7
31	Y	304	CLA	C3-C5-C6-C7
31	7	315	CLA	C3-C5-C6-C7
30	7	306	CHL	CBD-CGD-O2D-CED
34	j	101	LMG	O6-C1-O1-C7
38	X	201	SQD	O5-C1-O6-C44
31	2	613	CLA	C5-C6-C7-C8
33	A	417	LHG	C31-C32-C33-C34
34	r	321	LMG	C11-C12-C13-C14
31	0	610	CLA	O1D-CGD-O2D-CED
30	1	601	CHL	C10-C11-C12-C13
30	y	607	CHL	C8-C10-C11-C12
31	A	409	CLA	C5-C6-C7-C8
31	R	305	CLA	C8-C10-C11-C12
31	p	602	CLA	C5-C6-C7-C8
31	a	409	CLA	C5-C6-C7-C8
31	s	311	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	s	311	CLA	C10-C11-C12-C13
31	s	312	CLA	C13-C15-C16-C17
31	y	611	CLA	C13-C15-C16-C17
33	C	623	LHG	C33-C34-C35-C36
33	2	617	LHG	O2-C2-C3-O3
33	D	408	LHG	O2-C2-C3-O3
33	G	618	LHG	O2-C2-C3-O3
33	0	619	LHG	O2-C2-C3-O3
33	q	320	LHG	O2-C2-C3-O3
33	b	625	LHG	O2-C2-C3-O3
33	c	622	LHG	O2-C2-C3-O3
33	e	101	LHG	O2-C2-C3-O3
33	g	319	LHG	O2-C2-C3-O3
33	s	320	LHG	O2-C2-C3-O3
31	4	604	CLA	CBA-CGA-O2A-C1
31	G	612	CLA	CBA-CGA-O2A-C1
34	A	418	LMG	C35-C36-C37-C38
34	C	621	LMG	C35-C36-C37-C38
34	X	203	LMG	C35-C36-C37-C38
34	Y	319	LMG	C35-C36-C37-C38
34	0	622	LMG	C35-C36-C37-C38
34	a	416	LMG	C35-C36-C37-C38
34	f	101	LMG	C35-C36-C37-C38
34	g	320	LMG	C35-C36-C37-C38
34	w	204	LMG	C35-C36-C37-C38
34	q	302	LMG	C31-C32-C33-C34
31	N	304	CLA	CBD-CGD-O2D-CED
31	9	312	CLA	O1A-CGA-O2A-C1
31	y	604	CLA	O1A-CGA-O2A-C1
45	c	619	DGD	O1A-C1A-O1G-C1G
33	4	618	LHG	C7-C8-C9-C10
33	A	415	LHG	C7-C8-C9-C10
33	0	619	LHG	C7-C8-C9-C10
33	0	619	LHG	C23-C24-C25-C26
33	7	319	LHG	C23-C24-C25-C26
38	b	627	SQD	C7-C8-C9-C10
48	r	302	LMU	C1-C2-C3-C4
31	2	602	CLA	C13-C15-C16-C17
31	B	602	CLA	C15-C16-C17-C18
31	B	614	CLA	C8-C10-C11-C12
31	G	610	CLA	C5-C6-C7-C8
31	S	303	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	R	320	LHG	O9-C7-O7-C5
34	3	321	LMG	O9-C10-O7-C8
34	B	625	LMG	O9-C10-O7-C8
34	X	203	LMG	O9-C10-O7-C8
34	2	618	LMG	C35-C36-C37-C38
34	6	321	LMG	C35-C36-C37-C38
34	G	619	LMG	C35-C36-C37-C38
34	W	203	LMG	C35-C36-C37-C38
34	0	620	LMG	C35-C36-C37-C38
34	7	301	LMG	C17-C18-C19-C20
45	C	616	DGD	C8B-C9B-CAB-CBB
34	6	322	LMG	C17-C18-C19-C20
34	6	323	LMG	C35-C36-C37-C38
34	W	202	LMG	C35-C36-C37-C38
34	c	620	LMG	C35-C36-C37-C38
34	w	203	LMG	C35-C36-C37-C38
34	x	202	LMG	C35-C36-C37-C38
34	y	620	LMG	C35-C36-C37-C38
34	Q1	101	LMG	C35-C36-C37-C38
48	R	302	LMU	O1'-C1-C2-C3
31	2	602	CLA	C3-C5-C6-C7
31	3	311	CLA	C3-C5-C6-C7
30	q	307	CHL	O1D-CGD-O2D-CED
31	7	313	CLA	O1D-CGD-O2D-CED
31	c	601	CLA	O1D-CGD-O2D-CED
31	c	607	CLA	O1D-CGD-O2D-CED
31	4	613	CLA	C8-C10-C11-C12
31	6	312	CLA	C10-C11-C12-C13
31	B	608	CLA	C15-C16-C17-C18
31	D	403	CLA	C15-C16-C17-C18
31	S	312	CLA	C5-C6-C7-C8
31	7	313	CLA	C8-C10-C11-C12
31	b	607	CLA	C10-C11-C12-C13
31	b	613	CLA	C8-C10-C11-C12
31	b	617	CLA	C5-C6-C7-C8
31	y	612	CLA	C15-C16-C17-C18
31	6	315	CLA	CBD-CGD-O2D-CED
42	d	402	PHO	CBD-CGD-O2D-CED
30	G	601	CHL	C4-C3-C5-C6
34	g	322	LMG	C20-C21-C22-C23
31	g	311	CLA	O1A-CGA-O2A-C1
45	c	617	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
45	c	618	DGD	O1A-C1A-O1G-C1G
33	C	623	LHG	C23-C24-C25-C26
33	M	101	LHG	C7-C8-C9-C10
30	4	609	CHL	O1D-CGD-O2D-CED
30	N	301	CHL	O1D-CGD-O2D-CED
30	q	309	CHL	O1D-CGD-O2D-CED
31	5	612	CLA	O1D-CGD-O2D-CED
31	6	305	CLA	O1D-CGD-O2D-CED
31	C	601	CLA	O1D-CGD-O2D-CED
31	y	610	CLA	O1D-CGD-O2D-CED
34	w	202	LMG	C29-C30-C31-C32
34	W	203	LMG	O6-C5-C6-O5
31	C	603	CLA	C10-C11-C12-C13
31	S	313	CLA	C5-C6-C7-C8
31	8	612	CLA	C8-C10-C11-C12
31	b	607	CLA	C8-C10-C11-C12
31	c	611	CLA	C5-C6-C7-C8
31	n	314	CLA	C8-C10-C11-C12
31	s	310	CLA	C8-C10-C11-C12
31	y	611	CLA	C15-C16-C17-C18
31	Y	314	CLA	CBA-CGA-O2A-C1
31	0	602	CLA	CBA-CGA-O2A-C1
31	a	406	CLA	CBA-CGA-O2A-C1
31	c	605	CLA	CBA-CGA-O2A-C1
31	c	613	CLA	CBA-CGA-O2A-C1
31	r	314	CLA	CBA-CGA-O2A-C1
34	0	622	LMG	C29-C28-O8-C9
30	G	606	CHL	CBD-CGD-O2D-CED
30	r	309	CHL	CBD-CGD-O2D-CED
31	7	316	CLA	CBD-CGD-O2D-CED
33	r	320	LHG	C8-C7-O7-C5
34	9	302	LMG	C11-C10-O7-C8
31	B	603	CLA	O1A-CGA-O2A-C1
31	b	614	CLA	O1A-CGA-O2A-C1
31	y	602	CLA	O1D-CGD-O2D-CED
33	L	101	LHG	C23-C24-C25-C26
31	g	310	CLA	C8-C10-C11-C12
31	C	601	CLA	C3-C5-C6-C7
31	8	614	CLA	C3-C5-C6-C7
31	p	613	CLA	C3-C5-C6-C7
31	n	316	CLA	C3-C5-C6-C7
31	C	609	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
38	s	301	SQD	C30-C31-C32-C33
43	h	101	BCR	C9-C10-C11-C12
43	v	101	BCR	C13-C14-C15-C16
33	D	407	LHG	C7-C8-C9-C10
33	b	625	LHG	C7-C8-C9-C10
33	l	101	LHG	C7-C8-C9-C10
33	r	320	LHG	O9-C7-O7-C5
34	G	619	LMG	O9-C10-O7-C8
34	Y	319	LMG	O9-C10-O7-C8
34	9	302	LMG	O9-C10-O7-C8
34	n	321	LMG	O9-C10-O7-C8
34	n	322	LMG	O9-C10-O7-C8
34	w	202	LMG	O9-C10-O7-C8
33	3	320	LHG	C1-C2-C3-O3
33	A	415	LHG	C1-C2-C3-O3
33	B	624	LHG	C1-C2-C3-O3
33	R	320	LHG	C1-C2-C3-O3
33	0	619	LHG	C1-C2-C3-O3
33	b	628	LHG	C1-C2-C3-O3
33	e	101	LHG	C1-C2-C3-O3
33	s	322	LHG	C1-C2-C3-O3
31	5	610	CLA	C2A-CAA-CBA-CGA
31	B	610	CLA	C2A-CAA-CBA-CGA
31	9	312	CLA	C2A-CAA-CBA-CGA
30	Y	308	CHL	O1D-CGD-O2D-CED
31	N	303	CLA	CBA-CGA-O2A-C1
31	S	314	CLA	CBA-CGA-O2A-C1
31	7	303	CLA	CBA-CGA-O2A-C1
33	9	320	LHG	C24-C25-C26-C27
30	1	607	CHL	C5-C6-C7-C8
31	1	604	CLA	C8-C10-C11-C12
31	1	610	CLA	C8-C10-C11-C12
31	A	406	CLA	C13-C15-C16-C17
31	B	604	CLA	C8-C10-C11-C12
31	C	605	CLA	C5-C6-C7-C8
31	C	611	CLA	C13-C15-C16-C17
31	D	403	CLA	C13-C15-C16-C17
31	G	612	CLA	C5-C6-C7-C8
31	Y	313	CLA	C10-C11-C12-C13
31	Y	313	CLA	C13-C15-C16-C17
31	b	604	CLA	C5-C6-C7-C8
31	c	608	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	r	305	CLA	C8-C10-C11-C12
31	s	305	CLA	C8-C10-C11-C12
31	y	610	CLA	C5-C6-C7-C8
34	5	620	LMG	C12-C13-C14-C15
44	D	406	PL9	C47-C48-C49-C51
31	3	313	CLA	O1D-CGD-O2D-CED
30	N	308	CHL	CBD-CGD-O2D-CED
30	y	607	CHL	CBD-CGD-O2D-CED
30	7	321	CHL	C3-C5-C6-C7
30	n	308	CHL	C3-C5-C6-C7
33	8	618	LHG	C23-C24-C25-C26
33	c	622	LHG	C7-C8-C9-C10
33	n	320	LHG	C23-C24-C25-C26
30	G	623	CHL	C8-C10-C11-C12
31	2	602	CLA	C15-C16-C17-C18
31	2	610	CLA	C8-C10-C11-C12
31	5	602	CLA	C5-C6-C7-C8
31	C	605	CLA	C13-C15-C16-C17
31	C	610	CLA	C15-C16-C17-C18
31	Y	310	CLA	C5-C6-C7-C8
31	9	304	CLA	C5-C6-C7-C8
31	b	611	CLA	C5-C6-C7-C8
31	b	612	CLA	C13-C15-C16-C17
31	b	614	CLA	C5-C6-C7-C8
31	b	614	CLA	C8-C10-C11-C12
31	b	615	CLA	C8-C10-C11-C12
31	r	305	CLA	C5-C6-C7-C8
31	r	316	CLA	C5-C6-C7-C8
31	s	311	CLA	C15-C16-C17-C18
30	4	607	CHL	C5-C6-C7-C8
31	B	611	CLA	C8-C10-C11-C12
31	B	613	CLA	C5-C6-C7-C8
31	C	610	CLA	C8-C10-C11-C12
31	S	311	CLA	C8-C10-C11-C12
31	Y	312	CLA	C10-C11-C12-C13
31	0	602	CLA	C13-C15-C16-C17
31	p	610	CLA	C5-C6-C7-C8
31	b	617	CLA	C10-C11-C12-C13
31	s	314	CLA	C13-C15-C16-C17
31	B	611	CLA	O1D-CGD-O2D-CED
31	N	305	CLA	O1D-CGD-O2D-CED
31	b	610	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	c	604	CLA	CBA-CGA-O2A-C1
33	K	102	LHG	C23-C24-C25-C26
33	N	319	LHG	C7-C8-C9-C10
33	r	320	LHG	C23-C24-C25-C26
38	6	301	SQD	C23-C24-C25-C26
38	B	620	SQD	C7-C8-C9-C10
38	a	412	SQD	C7-C8-C9-C10
30	3	310	CHL	C4-C3-C5-C6
30	7	310	CHL	C4-C3-C5-C6
30	y	601	CHL	C4-C3-C5-C6
31	7	311	CLA	C4-C3-C5-C6
30	3	310	CHL	C2-C3-C5-C6
31	G	602	CLA	O1D-CGD-O2D-CED
31	p	611	CLA	O1D-CGD-O2D-CED
30	y	609	CHL	C5-C6-C7-C8
31	C	602	CLA	C13-C15-C16-C17
31	s	310	CLA	C3-C5-C6-C7
30	8	601	CHL	CBD-CGD-O2D-CED
30	n	302	CHL	CBD-CGD-O2D-CED
33	6	320	LHG	C8-C7-O7-C5
33	D	407	LHG	C8-C7-O7-C5
33	9	320	LHG	C8-C7-O7-C5
33	j	102	LHG	C8-C7-O7-C5
34	C	619	LMG	C11-C10-O7-C8
34	W	202	LMG	C11-C10-O7-C8
34	n	322	LMG	C11-C10-O7-C8
34	w	201	LMG	C11-C10-O7-C8
31	p	612	CLA	O1D-CGD-O2D-CED
31	y	612	CLA	O1D-CGD-O2D-CED
31	3	306	CLA	O1A-CGA-O2A-C1
33	6	320	LHG	O9-C7-O7-C5
33	D	407	LHG	O9-C7-O7-C5
33	9	320	LHG	O9-C7-O7-C5
33	j	102	LHG	O9-C7-O7-C5
34	C	619	LMG	O9-C10-O7-C8
34	G	621	LMG	O9-C10-O7-C8
34	W	202	LMG	O9-C10-O7-C8
34	w	201	LMG	O9-C10-O7-C8
34	R	321	LMG	C2-C1-O1-C7
34	q	302	LMG	C2-C1-O1-C7
34	a	413	LMG	C2-C1-O1-C7
34	j	101	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
34	n	322	LMG	C2-C1-O1-C7
38	6	301	SQD	C2-C1-O6-C44
38	M	102	SQD	C2-C1-O6-C44
38	R	322	SQD	C2-C1-O6-C44
38	X	201	SQD	C2-C1-O6-C44
45	C	617	DGD	C2E-C1E-O5D-C6D
45	c	617	DGD	C2E-C1E-O5D-C6D
33	L	101	LHG	C7-C8-C9-C10
44	A	416	PL9	C44-C46-C47-C48
44	D	406	PL9	C44-C46-C47-C48
33	4	618	LHG	C16-C17-C18-C19
33	7	319	LHG	C10-C11-C12-C13
30	7	310	CHL	O1D-CGD-O2D-CED
31	r	315	CLA	CBA-CGA-O2A-C1
31	3	314	CLA	C6-C7-C8-C9
31	4	603	CLA	C6-C7-C8-C9
31	p	603	CLA	C6-C7-C8-C10
31	G	612	CLA	O1A-CGA-O2A-C1
31	c	613	CLA	O1A-CGA-O2A-C1
36	2	616	NEX	C40-C33-C34-C35
36	3	319	NEX	C11-C10-C9-C19
36	4	617	NEX	C20-C13-C14-C15
36	N	318	NEX	C20-C13-C14-C15
36	N	318	NEX	C39-C29-C30-C31
36	R	319	NEX	C39-C29-C30-C31
36	R	319	NEX	C40-C33-C34-C35
36	8	617	NEX	C11-C10-C9-C19
36	8	617	NEX	C40-C33-C34-C35
36	p	618	NEX	C39-C29-C30-C31
36	n	319	NEX	C40-C33-C34-C35
36	r	301	NEX	C39-C29-C30-C31
36	r	319	NEX	C39-C29-C30-C31
37	R	318	XAT	C20-C13-C14-C15
31	6	315	CLA	C3-C5-C6-C7
31	c	601	CLA	C3-C5-C6-C7
33	a	415	LHG	C7-C8-C9-C10
34	A	414	LMG	C28-C29-C30-C31
31	Y	310	CLA	C8-C10-C11-C12
32	G	615	LUT	C27-C28-C29-C39
32	N	316	LUT	C31-C32-C33-C40
32	N	317	LUT	C11-C12-C13-C20
32	Y	316	LUT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
32	7	317	LUT	C7-C8-C9-C19
32	9	318	LUT	C7-C8-C9-C19
32	p	616	LUT	C11-C12-C13-C20
32	p	616	LUT	C31-C32-C33-C40
32	p	617	LUT	C7-C8-C9-C19
32	q	318	LUT	C7-C8-C9-C19
35	g	315	RRX	C7-C8-C9-C34
36	R	319	NEX	C31-C32-C33-C40
36	p	618	NEX	C11-C12-C13-C20
43	T	101	BCR	C11-C12-C13-C35
43	c	614	BCR	C7-C8-C9-C34
43	c	615	BCR	C37-C22-C23-C24
43	d	406	BCR	C11-C12-C13-C35
38	B	623	SQD	C14-C15-C16-C17
32	G	615	LUT	C27-C28-C29-C30
32	N	317	LUT	C7-C8-C9-C10
32	R	317	LUT	C7-C8-C9-C10
32	9	318	LUT	C7-C8-C9-C10
32	q	318	LUT	C7-C8-C9-C10
32	g	316	LUT	C11-C12-C13-C14
43	B	617	BCR	C21-C22-C23-C24
43	B	619	BCR	C7-C8-C9-C10
43	T	101	BCR	C11-C12-C13-C14
43	V	101	BCR	C21-C22-C23-C24
43	Z	101	BCR	C7-C8-C9-C10
43	b	618	BCR	C17-C18-C19-C20
43	b	619	BCR	C21-C22-C23-C24
43	c	614	BCR	C7-C8-C9-C10
43	c	615	BCR	C21-C22-C23-C24
43	d	406	BCR	C11-C12-C13-C14
43	v	101	BCR	C7-C8-C9-C10
43	v	101	BCR	C21-C22-C23-C24
31	N	303	CLA	O1A-CGA-O2A-C1
31	S	305	CLA	O1A-CGA-O2A-C1
34	0	622	LMG	O10-C28-O8-C9
33	G	618	LHG	C24-C25-C26-C27
33	K	102	LHG	C25-C26-C27-C28
30	1	619	CHL	C2A-CAA-CBA-CGA
30	3	309	CHL	C2A-CAA-CBA-CGA
30	4	608	CHL	C2A-CAA-CBA-CGA
30	5	608	CHL	C2A-CAA-CBA-CGA
30	G	623	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	N	306	CHL	C2A-CAA-CBA-CGA
30	Y	301	CHL	C2A-CAA-CBA-CGA
30	Y	302	CHL	C2A-CAA-CBA-CGA
30	Y	307	CHL	C2A-CAA-CBA-CGA
30	7	302	CHL	C2A-CAA-CBA-CGA
30	8	601	CHL	C2A-CAA-CBA-CGA
30	9	307	CHL	C2A-CAA-CBA-CGA
30	9	308	CHL	C2A-CAA-CBA-CGA
30	q	310	CHL	C2A-CAA-CBA-CGA
30	n	302	CHL	C2A-CAA-CBA-CGA
30	y	601	CHL	C2A-CAA-CBA-CGA
30	y	607	CHL	C2A-CAA-CBA-CGA
31	1	614	CLA	C2A-CAA-CBA-CGA
31	2	604	CLA	C2A-CAA-CBA-CGA
31	4	610	CLA	C2A-CAA-CBA-CGA
31	4	613	CLA	C2A-CAA-CBA-CGA
31	5	603	CLA	C2A-CAA-CBA-CGA
31	G	612	CLA	C2A-CAA-CBA-CGA
31	R	312	CLA	C2A-CAA-CBA-CGA
31	7	315	CLA	C2A-CAA-CBA-CGA
31	r	315	CLA	C2A-CAA-CBA-CGA
31	r	316	CLA	C2A-CAA-CBA-CGA
31	y	615	CLA	C2A-CAA-CBA-CGA
31	C	609	CLA	C13-C15-C16-C17
31	p	611	CLA	C8-C10-C11-C12
31	g	310	CLA	C5-C6-C7-C8
33	L	101	LHG	C30-C31-C32-C33
33	0	619	LHG	C9-C10-C11-C12
33	2	617	LHG	O1-C1-C2-C3
33	3	320	LHG	O1-C1-C2-C3
33	5	619	LHG	O1-C1-C2-C3
33	6	320	LHG	O1-C1-C2-C3
33	A	417	LHG	O1-C1-C2-C3
33	B	624	LHG	O1-C1-C2-C3
33	G	618	LHG	O1-C1-C2-C3
33	L	101	LHG	O1-C1-C2-C3
33	S	322	LHG	O1-C1-C2-C3
33	Y	318	LHG	O1-C1-C2-C3
33	7	319	LHG	O1-C1-C2-C3
33	8	618	LHG	O1-C1-C2-C3
33	p	619	LHG	O1-C1-C2-C3
33	b	625	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
33	b	628	LHG	O1-C1-C2-C3
33	e	101	LHG	O1-C1-C2-C3
33	j	102	LHG	O1-C1-C2-C3
33	l	101	LHG	O1-C1-C2-C3
33	n	320	LHG	O1-C1-C2-C3
33	s	320	LHG	O1-C1-C2-C3
33	s	322	LHG	O1-C1-C2-C3
33	y	619	LHG	O1-C1-C2-C3
33	F1	301	LHG	O1-C1-C2-C3
34	7	301	LMG	C28-C29-C30-C31
30	0	607	CHL	O1D-CGD-O2D-CED
31	1	612	CLA	O1D-CGD-O2D-CED
31	c	609	CLA	O1D-CGD-O2D-CED
33	n	320	LHG	C4-C5-O7-C7
34	q1	101	LMG	C7-C8-O7-C10
31	2	611	CLA	C6-C7-C8-C9
31	6	305	CLA	C6-C7-C8-C10
31	0	604	CLA	C6-C7-C8-C9
31	0	615	CLA	C6-C7-C8-C10
31	c	612	CLA	C6-C7-C8-C9
31	g	305	CLA	C6-C7-C8-C9
31	r	315	CLA	C6-C7-C8-C9
31	r	316	CLA	C16-C17-C18-C20
48	c	623	LMU	O1'-C1-C2-C3
31	A	407	CLA	O1D-CGD-O2D-CED
31	S	311	CLA	O1D-CGD-O2D-CED
31	b	611	CLA	O1D-CGD-O2D-CED
31	d	401	CLA	O1D-CGD-O2D-CED
31	C	608	CLA	O1A-CGA-O2A-C1
31	R	304	CLA	O1A-CGA-O2A-C1
31	S	314	CLA	O1A-CGA-O2A-C1
31	0	602	CLA	O1A-CGA-O2A-C1
31	c	608	CLA	O1A-CGA-O2A-C1
31	r	314	CLA	O1A-CGA-O2A-C1
33	b	625	LHG	O10-C23-O8-C6
33	g	319	LHG	O10-C23-O8-C6
34	A	412	LMG	O10-C28-O8-C9
31	3	315	CLA	C3-C5-C6-C7
31	5	602	CLA	C3-C5-C6-C7
31	R	304	CLA	C3-C5-C6-C7
31	y	603	CLA	C3-C5-C6-C7
31	D	404	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
36	2	616	NEX	C32-C33-C34-C35
36	3	319	NEX	C11-C10-C9-C8
36	4	617	NEX	C12-C13-C14-C15
36	4	617	NEX	C28-C29-C30-C31
36	N	318	NEX	C12-C13-C14-C15
36	N	318	NEX	C28-C29-C30-C31
36	R	319	NEX	C28-C29-C30-C31
36	R	319	NEX	C32-C33-C34-C35
36	8	617	NEX	C11-C10-C9-C8
36	8	617	NEX	C32-C33-C34-C35
36	p	618	NEX	C28-C29-C30-C31
36	q	319	NEX	C28-C29-C30-C31
36	n	319	NEX	C32-C33-C34-C35
36	r	301	NEX	C28-C29-C30-C31
37	R	318	XAT	C12-C13-C14-C15
33	B	624	LHG	C29-C30-C31-C32
34	B	621	LMG	O6-C1-O1-C7
34	q	302	LMG	O6-C1-O1-C7
38	6	301	SQD	O5-C1-O6-C44
38	R	322	SQD	O5-C1-O6-C44
45	C	617	DGD	O6E-C1E-O5D-C6D
31	B	610	CLA	O1D-CGD-O2D-CED
34	G	621	LMG	C11-C10-O7-C8
34	b	626	LMG	C11-C10-O7-C8
34	b	623	LMG	C28-C29-C30-C31
33	8	618	LHG	C24-C25-C26-C27
31	b	605	CLA	C8-C10-C11-C12
33	n	320	LHG	C24-C25-C26-C27
34	d	409	LMG	O6-C5-C6-O5
33	A	417	LHG	C29-C30-C31-C32
31	C	606	CLA	CBA-CGA-O2A-C1
31	c	603	CLA	CBA-CGA-O2A-C1
45	C	617	DGD	C2A-C1A-O1G-C1G
44	d	407	PL9	C47-C48-C49-C51
30	9	303	CHL	C8-C10-C11-C12
31	2	602	CLA	C5-C6-C7-C8
31	r	312	CLA	C8-C10-C11-C12
33	A	417	LHG	C7-C8-C9-C10
31	2	604	CLA	C2-C1-O2A-CGA
31	3	314	CLA	C2-C1-O2A-CGA
31	5	604	CLA	C2-C1-O2A-CGA
31	A	406	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
31	B	604	CLA	C2-C1-O2A-CGA
31	B	613	CLA	C2-C1-O2A-CGA
31	B	616	CLA	C2-C1-O2A-CGA
31	C	613	CLA	C2-C1-O2A-CGA
31	D	404	CLA	C2-C1-O2A-CGA
31	G	610	CLA	C2-C1-O2A-CGA
31	R	303	CLA	C2-C1-O2A-CGA
31	S	315	CLA	C2-C1-O2A-CGA
31	Y	304	CLA	C2-C1-O2A-CGA
31	Y	314	CLA	C2-C1-O2A-CGA
31	q	316	CLA	C2-C1-O2A-CGA
31	b	602	CLA	C2-C1-O2A-CGA
31	g	305	CLA	C2-C1-O2A-CGA
31	r	305	CLA	C2-C1-O2A-CGA
31	r	307	CLA	C2-C1-O2A-CGA
31	s	306	CLA	C2-C1-O2A-CGA
31	s	310	CLA	C2-C1-O2A-CGA
31	s	315	CLA	C2-C1-O2A-CGA
31	1	602	CLA	C11-C12-C13-C15
31	2	603	CLA	C6-C7-C8-C10
31	2	611	CLA	C6-C7-C8-C10
31	4	603	CLA	C6-C7-C8-C10
31	g	305	CLA	C6-C7-C8-C10
31	r	315	CLA	C6-C7-C8-C10
31	r	316	CLA	C16-C17-C18-C19
31	s	311	CLA	C16-C17-C18-C19
31	c	605	CLA	O1A-CGA-O2A-C1
31	C	602	CLA	C15-C16-C17-C18
31	b	616	CLA	C13-C15-C16-C17
31	g	313	CLA	C8-C10-C11-C12
31	r	312	CLA	C5-C6-C7-C8
34	b	626	LMG	C8-C9-O8-C28
33	5	619	LHG	C11-C10-C9-C8
31	a	407	CLA	CBD-CGD-O2D-CED
36	2	616	NEX	C14-C15-C35-C34
37	R	318	XAT	C14-C15-C35-C34
33	1	617	LHG	C11-C12-C13-C14
33	S	320	LHG	C29-C30-C31-C32
33	S	322	LHG	C13-C14-C15-C16
33	8	618	LHG	C31-C32-C33-C34
33	b	628	LHG	C11-C12-C13-C14
33	n	320	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
33	s	322	LHG	C13-C14-C15-C16
34	D	409	LMG	C32-C33-C34-C35
34	W	203	LMG	C30-C31-C32-C33
34	q	301	LMG	C16-C17-C18-C19
30	N	306	CHL	O1D-CGD-O2D-CED
30	R	309	CHL	O1D-CGD-O2D-CED
31	B	615	CLA	O1D-CGD-O2D-CED
33	q	320	LHG	C23-C24-C25-C26
30	Y	302	CHL	C10-C11-C12-C13
31	C	611	CLA	C15-C16-C17-C18
31	R	316	CLA	C13-C15-C16-C17
33	7	319	LHG	C11-C12-C13-C14
33	g	319	LHG	C11-C12-C13-C14
31	9	306	CLA	CBA-CGA-O2A-C1
31	r	306	CLA	CBA-CGA-O2A-C1
33	L	101	LHG	C11-C10-C9-C8
33	S	320	LHG	C9-C10-C11-C12
33	b	625	LHG	C13-C14-C15-C16
33	c	622	LHG	C11-C12-C13-C14
33	g	319	LHG	C28-C29-C30-C31
33	l	101	LHG	C13-C14-C15-C16
38	a	411	SQD	C10-C11-C12-C13
38	s	301	SQD	C11-C10-C9-C8
34	b	626	LMG	O9-C10-O7-C8
33	1	617	LHG	O1-C1-C2-O2
33	2	617	LHG	O1-C1-C2-O2
33	6	320	LHG	O1-C1-C2-O2
33	A	415	LHG	O1-C1-C2-O2
33	D	408	LHG	O1-C1-C2-O2
33	G	618	LHG	O1-C1-C2-O2
33	0	619	LHG	O1-C1-C2-O2
33	q	320	LHG	O1-C1-C2-O2
33	b	625	LHG	O1-C1-C2-O2
33	c	622	LHG	O1-C1-C2-O2
33	d	408	LHG	O1-C1-C2-O2
33	j	102	LHG	O1-C1-C2-O2
33	r	320	LHG	O1-C1-C2-O2
33	s	322	LHG	O1-C1-C2-O2
33	t	102	LHG	O1-C1-C2-O2
33	F1	301	LHG	O1-C1-C2-O2
31	S	305	CLA	C3-C5-C6-C7
31	7	304	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
33	D	408	LHG	C13-C14-C15-C16
33	N	319	LHG	C13-C14-C15-C16
33	R	320	LHG	C13-C14-C15-C16
33	c	622	LHG	C13-C14-C15-C16
38	B	620	SQD	C31-C32-C33-C34
30	G	607	CHL	O1D-CGD-O2D-CED
30	Y	307	CHL	O1D-CGD-O2D-CED
30	8	607	CHL	O1D-CGD-O2D-CED
31	Y	303	CLA	O1D-CGD-O2D-CED
31	s	306	CLA	O1D-CGD-O2D-CED
31	c	603	CLA	C8-C10-C11-C12
31	B	601	CLA	C4B-C3B-CAB-CBB
31	C	606	CLA	C4B-C3B-CAB-CBB
31	R	303	CLA	C4B-C3B-CAB-CBB
33	1	617	LHG	C23-C24-C25-C26
33	p	619	LHG	C23-C24-C25-C26
34	D	410	LMG	C10-C11-C12-C13
33	B	624	LHG	C11-C12-C13-C14
33	C	623	LHG	C11-C10-C9-C8
33	c	622	LHG	C29-C30-C31-C32
33	g	319	LHG	C34-C35-C36-C37
34	X	202	LMG	C8-C9-O8-C28
30	1	619	CHL	C11-C12-C13-C14
30	1	619	CHL	C11-C12-C13-C15
31	N	304	CLA	C6-C7-C8-C9
31	Y	304	CLA	C6-C7-C8-C9
31	Y	305	CLA	C6-C7-C8-C9
31	0	604	CLA	C6-C7-C8-C10
31	q	306	CLA	C6-C7-C8-C10
30	q	308	CHL	O1D-CGD-O2D-CED
31	4	604	CLA	O1A-CGA-O2A-C1
30	3	307	CHL	C2A-CAA-CBA-CGA
30	4	605	CHL	C2A-CAA-CBA-CGA
30	5	601	CHL	C2A-CAA-CBA-CGA
30	5	605	CHL	C2A-CAA-CBA-CGA
30	G	606	CHL	C2A-CAA-CBA-CGA
30	N	302	CHL	C2A-CAA-CBA-CGA
30	7	309	CHL	C2A-CAA-CBA-CGA
30	8	605	CHL	C2A-CAA-CBA-CGA
30	p	605	CHL	C2A-CAA-CBA-CGA
30	p	607	CHL	C2A-CAA-CBA-CGA
30	p	608	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	n	306	CHL	C2A-CAA-CBA-CGA
31	3	311	CLA	C2A-CAA-CBA-CGA
31	Y	311	CLA	C2A-CAA-CBA-CGA
31	b	605	CLA	C2A-CAA-CBA-CGA
33	r	320	LHG	C26-C27-C28-C29
33	s	320	LHG	C29-C30-C31-C32
31	6	313	CLA	C5-C6-C7-C8
31	S	311	CLA	C10-C11-C12-C13
31	q	315	CLA	C8-C10-C11-C12
31	d	404	CLA	C15-C16-C17-C18
42	a	408	PHO	C5-C6-C7-C8
33	A	415	LHG	C8-C7-O7-C5
34	C	624	LMG	C11-C10-O7-C8
34	D	411	LMG	C11-C10-O7-C8
34	q	301	LMG	C11-C10-O7-C8
34	b	622	LMG	C11-C10-O7-C8
34	d	410	LMG	C11-C10-O7-C8
33	Y	318	LHG	C11-C10-C9-C8
38	r	322	SQD	C27-C28-C29-C30
31	2	602	CLA	C12-C13-C15-C16
31	2	610	CLA	C11-C10-C8-C7
31	5	611	CLA	C11-C10-C8-C7
31	B	602	CLA	C11-C10-C8-C7
31	S	314	CLA	C6-C7-C8-C10
31	y	611	CLA	C11-C10-C8-C7
42	a	408	PHO	C11-C12-C13-C15
33	B	624	LHG	C15-C16-C17-C18
33	8	618	LHG	C28-C29-C30-C31
33	9	320	LHG	C25-C26-C27-C28
33	p	619	LHG	C26-C27-C28-C29
33	c	622	LHG	C9-C10-C11-C12
33	n	320	LHG	C28-C29-C30-C31
34	4	620	LMG	C16-C17-C18-C19
34	D	411	LMG	C32-C33-C34-C35
38	A	411	SQD	C12-C13-C14-C15
38	y	621	SQD	C25-C26-C27-C28
33	5	619	LHG	C23-C24-C25-C26
33	D	408	LHG	C7-C8-C9-C10
33	R	320	LHG	C23-C24-C25-C26
33	9	320	LHG	C23-C24-C25-C26
33	d	408	LHG	C7-C8-C9-C10
31	s	305	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	G	601	CHL	C8-C10-C11-C12
31	c	610	CLA	C13-C15-C16-C17
33	4	618	LHG	C28-C29-C30-C31
33	M	101	LHG	C30-C31-C32-C33
33	N	319	LHG	C31-C32-C33-C34
33	Y	318	LHG	C28-C29-C30-C31
33	e	101	LHG	C26-C27-C28-C29
33	z	102	LHG	C9-C10-C11-C12
33	z	102	LHG	C11-C12-C13-C14
34	b	601	LMG	C30-C31-C32-C33
34	d	410	LMG	C32-C33-C34-C35
31	Y	314	CLA	O1A-CGA-O2A-C1
31	b	610	CLA	O1A-CGA-O2A-C1
31	B	616	CLA	C3-C5-C6-C7
31	a	407	CLA	C3-C5-C6-C7
30	3	303	CHL	C3A-C2A-CAA-CBA
30	4	608	CHL	C3A-C2A-CAA-CBA
30	6	302	CHL	C4-C3-C5-C6
30	6	307	CHL	C3A-C2A-CAA-CBA
30	G	601	CHL	C3A-C2A-CAA-CBA
30	0	606	CHL	C3A-C2A-CAA-CBA
30	7	306	CHL	C3A-C2A-CAA-CBA
30	7	308	CHL	C3A-C2A-CAA-CBA
30	g	302	CHL	C3A-C2A-CAA-CBA
30	n	310	CHL	C3A-C2A-CAA-CBA
31	1	603	CLA	C3A-C2A-CAA-CBA
31	1	614	CLA	C3A-C2A-CAA-CBA
31	2	603	CLA	C3A-C2A-CAA-CBA
31	3	305	CLA	C3A-C2A-CAA-CBA
31	4	603	CLA	C3A-C2A-CAA-CBA
31	5	603	CLA	C3A-C2A-CAA-CBA
31	5	615	CLA	C3A-C2A-CAA-CBA
31	6	304	CLA	C3A-C2A-CAA-CBA
31	6	313	CLA	C3A-C2A-CAA-CBA
31	B	604	CLA	C3A-C2A-CAA-CBA
31	B	610	CLA	C3A-C2A-CAA-CBA
31	C	612	CLA	C3A-C2A-CAA-CBA
31	C	613	CLA	C3A-C2A-CAA-CBA
31	G	603	CLA	C3A-C2A-CAA-CBA
31	N	304	CLA	C3A-C2A-CAA-CBA
31	R	307	CLA	C3A-C2A-CAA-CBA
31	Y	304	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	0	612	CLA	C3A-C2A-CAA-CBA
31	7	304	CLA	C3A-C2A-CAA-CBA
31	7	315	CLA	C3A-C2A-CAA-CBA
31	8	603	CLA	C3A-C2A-CAA-CBA
31	9	305	CLA	C3A-C2A-CAA-CBA
31	p	603	CLA	C3A-C2A-CAA-CBA
31	q	305	CLA	C3A-C2A-CAA-CBA
31	a	407	CLA	C3A-C2A-CAA-CBA
31	b	605	CLA	C3A-C2A-CAA-CBA
31	c	610	CLA	C3A-C2A-CAA-CBA
31	c	612	CLA	C3A-C2A-CAA-CBA
31	c	613	CLA	C3A-C2A-CAA-CBA
31	n	304	CLA	C3A-C2A-CAA-CBA
31	r	307	CLA	C3A-C2A-CAA-CBA
31	y	603	CLA	C3A-C2A-CAA-CBA
30	1	606	CHL	O1D-CGD-O2D-CED
31	D	403	CLA	O1D-CGD-O2D-CED
33	4	618	LHG	C11-C10-C9-C8
33	D	407	LHG	C9-C10-C11-C12
33	R	320	LHG	C11-C12-C13-C14
33	S	322	LHG	C11-C12-C13-C14
33	8	618	LHG	C26-C27-C28-C29
33	n	320	LHG	C26-C27-C28-C29
30	y	601	CHL	C2-C3-C5-C6
31	9	304	CLA	C4C-C3C-CAC-CBC
48	c	623	LMU	C1-C2-C3-C4
33	y	619	LHG	C28-C29-C30-C31
31	1	612	CLA	C15-C16-C17-C18
31	B	611	CLA	C13-C15-C16-C17
31	Y	312	CLA	C15-C16-C17-C18
31	q	305	CLA	C5-C6-C7-C8
31	c	610	CLA	C8-C10-C11-C12
34	W	203	LMG	C4-C5-C6-O5
34	B	621	LMG	C8-C9-O8-C28
31	4	612	CLA	O1D-CGD-O2D-CED
33	s	322	LHG	C23-C24-C25-C26
38	0	621	SQD	C11-C12-C13-C14
35	g	315	RRX	C19-C20-C21-C22
36	8	617	NEX	C9-C10-C11-C12
43	b	618	BCR	C15-C16-C17-C18
31	1	602	CLA	C11-C12-C13-C14
31	3	305	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	6	305	CLA	C6-C7-C8-C9
31	Y	304	CLA	C6-C7-C8-C10
31	y	603	CLA	C6-C7-C8-C9
31	7	303	CLA	O1A-CGA-O2A-C1
31	a	406	CLA	O1A-CGA-O2A-C1
33	D	408	LHG	C9-C10-C11-C12
33	L	101	LHG	C11-C12-C13-C14
33	l	101	LHG	C34-C35-C36-C37
33	s	320	LHG	C26-C27-C28-C29
34	b	624	LMG	C13-C14-C15-C16
31	0	603	CLA	C5-C6-C7-C8
30	p	609	CHL	CBD-CGD-O2D-CED
31	C	608	CLA	CBD-CGD-O2D-CED
31	8	610	CLA	CBD-CGD-O2D-CED
31	n	312	CLA	CBD-CGD-O2D-CED
33	R	320	LHG	C26-C27-C28-C29
34	0	620	LMG	C13-C14-C15-C16
38	X	201	SQD	C25-C26-C27-C28
30	1	619	CHL	CBA-CGA-O2A-C1
30	G	605	CHL	CBA-CGA-O2A-C1
31	G	602	CLA	CBA-CGA-O2A-C1
31	R	306	CLA	CBA-CGA-O2A-C1
31	y	612	CLA	CBA-CGA-O2A-C1
31	y	613	CLA	CBA-CGA-O2A-C1
33	S	320	LHG	C4-C5-C6-O8
34	D	409	LMG	O1-C7-C8-C9
38	B	620	SQD	O6-C44-C45-C46
38	M	102	SQD	C44-C45-C46-O48
33	K	102	LHG	C13-C14-C15-C16
33	p	619	LHG	C11-C12-C13-C14
33	b	625	LHG	C10-C11-C12-C13
33	b	625	LHG	C28-C29-C30-C31
33	d	408	LHG	C11-C12-C13-C14
33	e	101	LHG	C25-C26-C27-C28
33	F1	301	LHG	C11-C10-C9-C8
30	7	308	CHL	C3-C5-C6-C7
31	G	602	CLA	C3-C5-C6-C7
31	8	603	CLA	C3-C5-C6-C7
31	9	315	CLA	C3-C5-C6-C7
31	g	313	CLA	C3-C5-C6-C7
31	s	305	CLA	C3-C5-C6-C7
33	2	617	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
33	A	415	LHG	C23-C24-C25-C26
33	8	618	LHG	C7-C8-C9-C10
33	j	102	LHG	C23-C24-C25-C26
33	n	320	LHG	C7-C8-C9-C10
34	9	302	LMG	C10-C11-C12-C13
38	G	624	SQD	C23-C24-C25-C26
45	C	616	DGD	C1A-C2A-C3A-C4A
31	c	609	CLA	C10-C11-C12-C13
31	r	316	CLA	C8-C10-C11-C12
31	C	607	CLA	O1D-CGD-O2D-CED
33	5	619	LHG	C9-C10-C11-C12
33	D	407	LHG	C13-C14-C15-C16
33	D	407	LHG	C34-C35-C36-C37
33	D	408	LHG	C11-C12-C13-C14
33	D	408	LHG	C26-C27-C28-C29
33	M	101	LHG	C28-C29-C30-C31
33	8	618	LHG	C15-C16-C17-C18
33	b	625	LHG	C9-C10-C11-C12
33	b	625	LHG	C26-C27-C28-C29
33	e	101	LHG	C28-C29-C30-C31
33	n	320	LHG	C15-C16-C17-C18
34	D	409	LMG	C18-C19-C20-C21
31	c	604	CLA	O1A-CGA-O2A-C1
31	r	315	CLA	O1A-CGA-O2A-C1
45	C	617	DGD	O1A-C1A-O1G-C1G
33	M	101	LHG	C33-C34-C35-C36
33	8	618	LHG	C13-C14-C15-C16
33	8	618	LHG	C33-C34-C35-C36
33	n	320	LHG	C33-C34-C35-C36
33	s	320	LHG	C25-C26-C27-C28
33	y	619	LHG	C11-C10-C9-C8
33	p	619	LHG	C5-C6-O8-C23
30	4	607	CHL	O1D-CGD-O2D-CED
34	6	321	LMG	C32-C33-C34-C35
34	n	321	LMG	C11-C12-C13-C14
30	n	309	CHL	O1D-CGD-O2D-CED
33	M	101	LHG	C31-C32-C33-C34
33	n	320	LHG	C13-C14-C15-C16
34	B	625	LMG	C33-C34-C35-C36
31	9	315	CLA	C6-C7-C8-C9
31	c	603	CLA	O1A-CGA-O2A-C1
31	B	601	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	B	606	CLA	C2B-C3B-CAB-CBB
31	C	606	CLA	C2B-C3B-CAB-CBB
31	C	607	CLA	C2B-C3B-CAB-CBB
31	R	303	CLA	C2B-C3B-CAB-CBB
31	r	313	CLA	C2B-C3B-CAB-CBB
31	s	312	CLA	C2B-C3B-CAB-CBB
32	5	616	LUT	C5-C6-C7-C8
32	p	617	LUT	C1-C6-C7-C8
35	q	317	RRX	C23-C24-C25-C26
43	A	410	BCR	C1-C6-C7-C8
43	A	410	BCR	C23-C24-C25-C26
43	B	617	BCR	C1-C6-C7-C8
43	B	619	BCR	C1-C6-C7-C8
43	V	101	BCR	C1-C6-C7-C8
43	V	101	BCR	C23-C24-C25-C30
43	a	410	BCR	C1-C6-C7-C8
43	b	618	BCR	C1-C6-C7-C8
43	b	618	BCR	C23-C24-C25-C26
43	b	619	BCR	C1-C6-C7-C8
43	c	614	BCR	C1-C6-C7-C8
43	c	615	BCR	C5-C6-C7-C8
43	d	406	BCR	C23-C24-C25-C30
43	t	101	BCR	C1-C6-C7-C8
43	v	101	BCR	C1-C6-C7-C8
43	v	101	BCR	C23-C24-C25-C30
33	M	101	LHG	C9-C10-C11-C12
33	q	320	LHG	C24-C25-C26-C27
33	a	415	LHG	C33-C34-C35-C36
34	D	412	LMG	C16-C17-C18-C19
34	d	409	LMG	C11-C10-O7-C8
30	2	606	CHL	CBA-CGA-O2A-C1
31	B	609	CLA	CBA-CGA-O2A-C1
30	g	302	CHL	C5-C6-C7-C8
31	7	311	CLA	C8-C10-C11-C12
31	3	301	CLA	C6-C7-C8-C9
31	1	612	CLA	C3-C5-C6-C7
31	p	602	CLA	C3-C5-C6-C7
31	N	321	CLA	C5-C6-C7-C8
33	5	619	LHG	C11-C12-C13-C14
33	D	407	LHG	C11-C12-C13-C14
33	e	101	LHG	C13-C14-C15-C16
33	y	619	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	6	320	LHG	C11-C12-C13-C14
33	G	618	LHG	C11-C12-C13-C14
33	q	320	LHG	C28-C29-C30-C31
33	g	319	LHG	C13-C14-C15-C16
33	t	102	LHG	C9-C10-C11-C12
34	b	624	LMG	C33-C34-C35-C36
30	5	607	CHL	C2A-CAA-CBA-CGA
30	6	307	CHL	C2A-CAA-CBA-CGA
30	6	308	CHL	C2A-CAA-CBA-CGA
30	R	308	CHL	C2A-CAA-CBA-CGA
30	7	321	CHL	C2A-CAA-CBA-CGA
30	9	310	CHL	C2A-CAA-CBA-CGA
30	p	606	CHL	C2A-CAA-CBA-CGA
30	n	308	CHL	C2A-CAA-CBA-CGA
30	r	308	CHL	C2A-CAA-CBA-CGA
31	3	315	CLA	C2A-CAA-CBA-CGA
31	9	304	CLA	C2A-CAA-CBA-CGA
31	b	615	CLA	C2A-CAA-CBA-CGA
31	c	610	CLA	C2A-CAA-CBA-CGA
33	l	101	LHG	C23-C24-C25-C26
38	s	301	SQD	C7-C8-C9-C10
31	Y	304	CLA	C5-C6-C7-C8
33	3	320	LHG	C26-C27-C28-C29
33	4	618	LHG	C26-C27-C28-C29
33	q	320	LHG	C11-C12-C13-C14
33	b	625	LHG	C11-C12-C13-C14
33	b	628	LHG	C31-C32-C33-C34
34	C	619	LMG	C19-C20-C21-C22
34	x	202	LMG	C33-C34-C35-C36
34	y	620	LMG	C30-C31-C32-C33
30	1	619	CHL	O1A-CGA-O2A-C1
31	G	602	CLA	O1A-CGA-O2A-C1
31	9	306	CLA	O1A-CGA-O2A-C1
31	y	612	CLA	O1A-CGA-O2A-C1
31	y	613	CLA	O1A-CGA-O2A-C1
44	a	414	PL9	C4-C3-C7-C8
44	d	407	PL9	C4-C3-C7-C8
33	z	102	LHG	C13-C14-C15-C16
34	C	624	LMG	O9-C10-O7-C8
34	D	411	LMG	O9-C10-O7-C8
34	q	301	LMG	O9-C10-O7-C8
34	b	622	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
34	d	410	LMG	O9-C10-O7-C8
30	4	601	CHL	C4-C3-C5-C6
30	0	601	CHL	C4-C3-C5-C6
30	q	303	CHL	C4-C3-C5-C6
33	A	415	LHG	C29-C30-C31-C32
33	D	407	LHG	C10-C11-C12-C13
33	Y	318	LHG	C11-C12-C13-C14
33	a	415	LHG	C28-C29-C30-C31
34	6	321	LMG	C29-C30-C31-C32
36	8	617	NEX	C10-C11-C12-C13
36	p	618	NEX	C30-C31-C32-C33
36	q	319	NEX	C30-C31-C32-C33
37	R	318	XAT	C10-C11-C12-C13
37	r	318	XAT	C10-C11-C12-C13
31	C	608	CLA	C5-C6-C7-C8
30	q	303	CHL	C2-C3-C5-C6
31	3	301	CLA	C2-C3-C5-C6
34	D	409	LMG	O6-C5-C6-O5
31	8	603	CLA	C6-C7-C8-C9
31	c	612	CLA	C6-C7-C8-C10
31	7	315	CLA	C5-C6-C7-C8
33	1	617	LHG	C25-C26-C27-C28
33	4	618	LHG	C11-C12-C13-C14
33	5	619	LHG	C25-C26-C27-C28
33	M	101	LHG	C11-C10-C9-C8
33	S	320	LHG	C25-C26-C27-C28
33	S	322	LHG	C33-C34-C35-C36
33	t	102	LHG	C30-C31-C32-C33
31	B	613	CLA	CBA-CGA-O2A-C1
31	1	613	CLA	C14-C13-C15-C16
31	4	610	CLA	C6-C7-C8-C9
31	S	312	CLA	C6-C7-C8-C9
33	z	102	LHG	C25-C26-C27-C28
33	t	102	LHG	C35-C36-C37-C38
33	B	624	LHG	C13-C14-C15-C16
33	p	619	LHG	C10-C11-C12-C13
33	q	320	LHG	C13-C14-C15-C16
34	R	321	LMG	O6-C1-O1-C7
33	N	319	LHG	C11-C10-C9-C8
33	S	320	LHG	C13-C14-C15-C16
33	b	628	LHG	C28-C29-C30-C31
31	q	313	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
34	W	202	LMG	C2-C1-O1-C7
34	m	102	LMG	C2-C1-O1-C7
34	r	321	LMG	C2-C1-O1-C7
34	Q1	101	LMG	C2-C1-O1-C7
38	b	627	SQD	C2-C1-O6-C44
31	4	602	CLA	C5-C6-C7-C8
31	0	610	CLA	C8-C10-C11-C12
31	7	314	CLA	C13-C15-C16-C17
31	C	606	CLA	O1A-CGA-O2A-C1
31	r	306	CLA	O1A-CGA-O2A-C1
31	s	305	CLA	O1A-CGA-O2A-C1
33	K	102	LHG	C11-C12-C13-C14
33	d	408	LHG	C13-C14-C15-C16
33	t	102	LHG	C26-C27-C28-C29
33	S	320	LHG	C11-C10-C9-C8
34	m	102	LMG	C30-C31-C32-C33
45	c	616	DGD	CAA-CBA-CCA-CDA
48	r	302	LMU	C6-C7-C8-C9
33	L	101	LHG	C33-C34-C35-C36
45	c	617	DGD	C3B-C4B-C5B-C6B
31	y	612	CLA	C8-C10-C11-C12
43	C	614	BCR	C9-C10-C11-C12
43	c	614	BCR	C13-C14-C15-C16
43	v	101	BCR	C9-C10-C11-C12
31	3	314	CLA	C6-C7-C8-C10
31	9	305	CLA	C6-C7-C8-C9
31	n	304	CLA	C6-C7-C8-C9
34	B	622	LMG	C33-C34-C35-C36
33	3	320	LHG	C8-C7-O7-C5
33	S	320	LHG	C8-C7-O7-C5
33	b	628	LHG	C8-C7-O7-C5
33	s	320	LHG	C8-C7-O7-C5
33	t	102	LHG	C8-C7-O7-C5
34	D	409	LMG	C11-C10-O7-C8
34	D	410	LMG	C11-C10-O7-C8
34	S	321	LMG	C11-C10-O7-C8
34	g	322	LMG	C11-C10-O7-C8
34	r	321	LMG	C11-C10-O7-C8
38	a	412	SQD	C8-C7-O47-C45
45	C	616	DGD	C2B-C1B-O2G-C2G
31	3	316	CLA	C8-C10-C11-C12
33	j	102	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
34	b	622	LMG	C10-C11-C12-C13
33	e	101	LHG	C33-C34-C35-C36
45	c	619	DGD	CCA-CDA-CEA-CFA
33	z	102	LHG	C5-C6-O8-C23
33	S	320	LHG	O9-C7-O7-C5
34	D	410	LMG	O9-C10-O7-C8
34	g	322	LMG	O9-C10-O7-C8
38	a	412	SQD	O49-C7-O47-C45
31	2	602	CLA	C4C-C3C-CAC-CBC
33	D	407	LHG	C31-C32-C33-C34
33	y	619	LHG	C27-C28-C29-C30
30	9	310	CHL	CBD-CGD-O2D-CED
32	2	615	LUT	C31-C32-C33-C40
32	6	318	LUT	C11-C12-C13-C20
32	N	317	LUT	C7-C8-C9-C19
43	T	101	BCR	C7-C8-C9-C34
43	a	410	BCR	C36-C18-C19-C20
33	A	417	LHG	C25-C26-C27-C28
33	s	322	LHG	C7-C8-C9-C10
38	a	411	SQD	C9-C10-C11-C12
31	6	312	CLA	C3-C5-C6-C7
31	g	305	CLA	C3-C5-C6-C7
32	N	317	LUT	C11-C12-C13-C14
43	T	101	BCR	C7-C8-C9-C10
38	s	301	SQD	C24-C23-O48-C46
34	G	619	LMG	C8-C7-O1-C1
34	I	101	LMG	C8-C7-O1-C1
34	J	102	LMG	C8-C7-O1-C1
34	W	202	LMG	C8-C7-O1-C1
34	Y	319	LMG	C8-C7-O1-C1
34	b	622	LMG	C8-C7-O1-C1
34	c	621	LMG	C8-C7-O1-C1
34	f	101	LMG	C8-C7-O1-C1
34	Q1	101	LMG	C8-C7-O1-C1
38	R	322	SQD	C45-C44-O6-C1
38	X	201	SQD	C45-C44-O6-C1
45	c	619	DGD	C5D-C6D-O5D-C1E
31	B	610	CLA	C5-C6-C7-C8
30	q	308	CHL	C2A-CAA-CBA-CGA
31	Y	313	CLA	C2A-CAA-CBA-CGA
31	b	613	CLA	C2A-CAA-CBA-CGA
31	C	603	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
31	N	304	CLA	C6-C7-C8-C10
31	7	304	CLA	C6-C7-C8-C9
31	7	304	CLA	C6-C7-C8-C10
31	8	603	CLA	C6-C7-C8-C10
31	9	315	CLA	C6-C7-C8-C10
31	q	312	CLA	C6-C7-C8-C9
31	q	312	CLA	C6-C7-C8-C10
31	n	304	CLA	C6-C7-C8-C10
31	y	603	CLA	C6-C7-C8-C10
33	s	320	LHG	C13-C14-C15-C16
34	a	416	LMG	C11-C12-C13-C14
30	1	607	CHL	C4-C3-C5-C6
30	R	309	CHL	C4-C3-C5-C6
30	7	302	CHL	C4-C3-C5-C6
30	9	311	CHL	C4-C3-C5-C6
30	r	309	CHL	C4-C3-C5-C6
31	B	609	CLA	C4-C3-C5-C6
31	s	314	CLA	C4-C3-C5-C6
33	4	618	LHG	C13-C14-C15-C16
33	q	320	LHG	C11-C10-C9-C8
34	a	416	LMG	C30-C31-C32-C33
31	B	608	CLA	C13-C15-C16-C17
33	t	102	LHG	C28-C29-C30-C31
33	F1	301	LHG	C11-C12-C13-C14
30	5	601	CHL	O1D-CGD-O2D-CED
31	N	311	CLA	O1D-CGD-O2D-CED
34	b	601	LMG	C15-C16-C17-C18
34	f	101	LMG	C32-C33-C34-C35
34	y	620	LMG	C12-C13-C14-C15
34	y	620	LMG	C29-C30-C31-C32
38	B	620	SQD	C25-C26-C27-C28
31	R	306	CLA	O1A-CGA-O2A-C1
34	7	322	LMG	O6-C5-C6-O5
31	3	312	CLA	C13-C15-C16-C17
31	4	602	CLA	C13-C15-C16-C17
31	b	608	CLA	C15-C16-C17-C18
31	s	305	CLA	O1D-CGD-O2D-CED
33	j	102	LHG	C26-C27-C28-C29
33	A	415	LHG	O9-C7-O7-C5
34	S	321	LMG	O9-C10-O7-C8
34	d	409	LMG	O9-C10-O7-C8
34	r	321	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
34	g	320	LMG	O6-C5-C6-O5
34	w	202	LMG	O6-C5-C6-O5
34	Q1	101	LMG	O6-C5-C6-O5
33	B	624	LHG	C16-C17-C18-C19
34	B	625	LMG	C8-C9-O8-C28
33	b	625	LHG	C8-C7-O7-C5
30	7	307	CHL	C5-C6-C7-C8
31	C	605	CLA	C8-C10-C11-C12
31	D	404	CLA	C13-C15-C16-C17
31	R	311	CLA	C8-C10-C11-C12
31	b	608	CLA	C13-C15-C16-C17
31	c	601	CLA	C15-C16-C17-C18
48	r	302	LMU	O1'-C1-C2-C3
48	R	302	LMU	C6-C7-C8-C9
31	B	609	CLA	O1A-CGA-O2A-C1
33	l	101	LHG	C25-C26-C27-C28
34	m	102	LMG	C29-C30-C31-C32
38	a	412	SQD	C11-C10-C9-C8
45	c	616	DGD	C6A-C7A-C8A-C9A
33	1	617	LHG	C7-C8-C9-C10
34	m	102	LMG	C10-C11-C12-C13
31	s	312	CLA	C8-C10-C11-C12
30	3	303	CHL	O1D-CGD-O2D-CED
33	N	319	LHG	C33-C34-C35-C36
34	B	622	LMG	O6-C5-C6-O5
34	R	321	LMG	O6-C5-C6-O5
34	w	201	LMG	O6-C5-C6-O5
45	C	620	DGD	O6E-C5E-C6E-O5E
31	G	604	CLA	C3-C5-C6-C7
31	S	310	CLA	C3-C5-C6-C7
31	q	305	CLA	C3-C5-C6-C7
31	n	304	CLA	C3-C5-C6-C7
30	y	606	CHL	CBD-CGD-O2D-CED
33	1	617	LHG	O7-C5-C6-O8
33	S	320	LHG	O7-C5-C6-O8
33	7	319	LHG	O7-C5-C6-O8
33	b	625	LHG	O7-C5-C6-O8
33	r	320	LHG	O7-C5-C6-O8
33	s	322	LHG	O7-C5-C6-O8
34	A	418	LMG	O1-C7-C8-O7
34	D	412	LMG	O7-C8-C9-O8
34	R	321	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
34	a	416	LMG	O1-C7-C8-O7
34	n	321	LMG	O7-C8-C9-O8
38	6	301	SQD	O47-C45-C46-O48
38	G	624	SQD	O47-C45-C46-O48
48	R	302	LMU	C5'-C4'-O1B-C1B
33	B	624	LHG	C28-C29-C30-C31
33	D	408	LHG	C27-C28-C29-C30
34	c	621	LMG	C32-C33-C34-C35
31	C	605	CLA	CBA-CGA-O2A-C1
31	g	310	CLA	CBA-CGA-O2A-C1
33	B	624	LHG	C24-C23-O8-C6
30	G	605	CHL	O1A-CGA-O2A-C1
33	1	617	LHG	C26-C27-C28-C29
33	2	617	LHG	C9-C10-C11-C12
33	A	415	LHG	C28-C29-C30-C31
33	L	101	LHG	C31-C32-C33-C34
33	j	102	LHG	C28-C29-C30-C31
34	2	620	LMG	C18-C19-C20-C21
34	B	622	LMG	C32-C33-C34-C35
45	c	616	DGD	CCB-CDB-CEB-CFB
31	B	605	CLA	C5-C6-C7-C8
33	4	618	LHG	C30-C31-C32-C33
45	C	617	DGD	C2A-C3A-C4A-C5A
30	n	310	CHL	CBD-CGD-O2D-CED
33	D	408	LHG	C28-C29-C30-C31
31	N	315	CLA	C2-C1-O2A-CGA
31	R	307	CLA	C2-C1-O2A-CGA
31	8	604	CLA	C2-C1-O2A-CGA
31	g	314	CLA	C2-C1-O2A-CGA
31	C	612	CLA	C6-C7-C8-C9
31	p	611	CLA	C11-C12-C13-C15
31	q	305	CLA	C6-C7-C8-C9
33	A	417	LHG	C26-C27-C28-C29
33	S	320	LHG	C11-C12-C13-C14
33	0	619	LHG	C11-C12-C13-C14
33	d	408	LHG	C28-C29-C30-C31
33	j	102	LHG	C13-C14-C15-C16
45	c	618	DGD	CCA-CDA-CEA-CFA
48	r	302	LMU	C2-C3-C4-C5
34	G	619	LMG	O6-C5-C6-O5
33	d	408	LHG	C26-C27-C28-C29
30	G	623	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	Y	311	CLA	C4-C3-C5-C6
31	a	406	CLA	C4-C3-C5-C6
31	b	610	CLA	C4-C3-C5-C6
31	s	313	CLA	C4-C3-C5-C6
30	q	309	CHL	C2-C3-C5-C6
31	s	314	CLA	C2-C3-C5-C6
33	b	628	LHG	O9-C7-O7-C5
34	D	409	LMG	O9-C10-O7-C8
34	d	411	LMG	C13-C14-C15-C16
30	9	309	CHL	C2A-CAA-CBA-CGA
30	q	309	CHL	C2A-CAA-CBA-CGA
31	A	405	CLA	C2A-CAA-CBA-CGA
31	C	601	CLA	C2A-CAA-CBA-CGA
31	N	305	CLA	C2A-CAA-CBA-CGA
31	N	311	CLA	C2A-CAA-CBA-CGA
31	0	602	CLA	C2A-CAA-CBA-CGA
31	q	316	CLA	C2A-CAA-CBA-CGA
31	n	305	CLA	C2A-CAA-CBA-CGA
31	r	307	CLA	C2A-CAA-CBA-CGA
31	9	305	CLA	O1D-CGD-O2D-CED
30	N	307	CHL	CBA-CGA-O2A-C1
45	c	616	DGD	C2A-C1A-O1G-C1G
34	W	201	LMG	O6-C5-C6-O5
34	c	620	LMG	O6-C5-C6-O5
31	1	614	CLA	C5-C6-C7-C8
33	4	618	LHG	C14-C15-C16-C17
33	c	622	LHG	C34-C35-C36-C37
38	R	322	SQD	C11-C12-C13-C14
45	C	620	DGD	C4B-C5B-C6B-C7B
34	w	205	LMG	C8-C9-O8-C28
31	y	611	CLA	O1D-CGD-O2D-CED
31	G	612	CLA	C13-C15-C16-C17
31	c	605	CLA	C5-C6-C7-C8
34	C	621	LMG	O6-C5-C6-O5
38	a	412	SQD	C23-C24-C25-C26
31	0	614	CLA	C5-C6-C7-C8
33	A	415	LHG	C31-C32-C33-C34
33	s	322	LHG	C26-C27-C28-C29
44	D	406	PL9	C47-C48-C49-C50
34	k	102	LMG	O6-C5-C6-O5
33	3	320	LHG	O1-C1-C2-O2
33	L	101	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
33	R	320	LHG	O1-C1-C2-O2
33	Y	318	LHG	O1-C1-C2-O2
33	g	319	LHG	O1-C1-C2-O2
30	2	606	CHL	O1A-CGA-O2A-C1
31	B	613	CLA	O1A-CGA-O2A-C1
31	C	605	CLA	O1A-CGA-O2A-C1
30	1	606	CHL	C3-C5-C6-C7
31	y	604	CLA	C3-C5-C6-C7
34	n	321	LMG	C12-C13-C14-C15
33	s	322	LHG	C33-C34-C35-C36
31	1	602	CLA	C1A-C2A-CAA-CBA
31	1	603	CLA	C1A-C2A-CAA-CBA
31	1	610	CLA	C1A-C2A-CAA-CBA
31	2	602	CLA	C1A-C2A-CAA-CBA
31	2	603	CLA	C1A-C2A-CAA-CBA
31	2	604	CLA	C1A-C2A-CAA-CBA
31	2	609	CLA	C1A-C2A-CAA-CBA
31	3	304	CLA	C1A-C2A-CAA-CBA
31	3	306	CLA	C1A-C2A-CAA-CBA
31	3	315	CLA	C1A-C2A-CAA-CBA
31	3	316	CLA	C1A-C2A-CAA-CBA
31	4	602	CLA	C1A-C2A-CAA-CBA
31	4	603	CLA	C1A-C2A-CAA-CBA
31	4	604	CLA	C1A-C2A-CAA-CBA
31	4	610	CLA	C1A-C2A-CAA-CBA
31	4	611	CLA	C1A-C2A-CAA-CBA
31	5	602	CLA	C1A-C2A-CAA-CBA
31	5	603	CLA	C1A-C2A-CAA-CBA
31	5	604	CLA	C1A-C2A-CAA-CBA
31	5	611	CLA	C1A-C2A-CAA-CBA
31	6	303	CLA	C1A-C2A-CAA-CBA
31	6	313	CLA	C1A-C2A-CAA-CBA
31	6	314	CLA	C1A-C2A-CAA-CBA
31	6	315	CLA	C1A-C2A-CAA-CBA
31	A	407	CLA	C1A-C2A-CAA-CBA
31	B	610	CLA	C1A-C2A-CAA-CBA
31	C	601	CLA	C1A-C2A-CAA-CBA
31	C	603	CLA	C1A-C2A-CAA-CBA
31	C	608	CLA	C1A-C2A-CAA-CBA
31	C	611	CLA	C1A-C2A-CAA-CBA
31	C	612	CLA	C1A-C2A-CAA-CBA
31	G	602	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	G	609	CLA	C1A-C2A-CAA-CBA
31	N	304	CLA	C1A-C2A-CAA-CBA
31	R	303	CLA	C1A-C2A-CAA-CBA
31	R	307	CLA	C1A-C2A-CAA-CBA
31	S	311	CLA	C1A-C2A-CAA-CBA
31	S	315	CLA	C1A-C2A-CAA-CBA
31	S	316	CLA	C1A-C2A-CAA-CBA
31	Y	303	CLA	C1A-C2A-CAA-CBA
31	Y	304	CLA	C1A-C2A-CAA-CBA
31	Y	310	CLA	C1A-C2A-CAA-CBA
31	Y	314	CLA	C1A-C2A-CAA-CBA
31	0	612	CLA	C1A-C2A-CAA-CBA
31	7	303	CLA	C1A-C2A-CAA-CBA
31	7	304	CLA	C1A-C2A-CAA-CBA
31	7	305	CLA	C1A-C2A-CAA-CBA
31	7	311	CLA	C1A-C2A-CAA-CBA
31	8	602	CLA	C1A-C2A-CAA-CBA
31	8	603	CLA	C1A-C2A-CAA-CBA
31	9	305	CLA	C1A-C2A-CAA-CBA
31	9	313	CLA	C1A-C2A-CAA-CBA
31	p	602	CLA	C1A-C2A-CAA-CBA
31	p	603	CLA	C1A-C2A-CAA-CBA
31	p	604	CLA	C1A-C2A-CAA-CBA
31	p	610	CLA	C1A-C2A-CAA-CBA
31	p	613	CLA	C1A-C2A-CAA-CBA
31	p	614	CLA	C1A-C2A-CAA-CBA
31	q	304	CLA	C1A-C2A-CAA-CBA
31	q	305	CLA	C1A-C2A-CAA-CBA
31	q	312	CLA	C1A-C2A-CAA-CBA
31	b	604	CLA	C1A-C2A-CAA-CBA
31	b	607	CLA	C1A-C2A-CAA-CBA
31	b	615	CLA	C1A-C2A-CAA-CBA
31	c	601	CLA	C1A-C2A-CAA-CBA
31	c	603	CLA	C1A-C2A-CAA-CBA
31	c	608	CLA	C1A-C2A-CAA-CBA
31	c	610	CLA	C1A-C2A-CAA-CBA
31	c	611	CLA	C1A-C2A-CAA-CBA
31	d	401	CLA	C1A-C2A-CAA-CBA
31	g	303	CLA	C1A-C2A-CAA-CBA
31	g	310	CLA	C1A-C2A-CAA-CBA
31	n	303	CLA	C1A-C2A-CAA-CBA
31	n	304	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	r	304	CLA	C1A-C2A-CAA-CBA
31	r	307	CLA	C1A-C2A-CAA-CBA
31	r	313	CLA	C1A-C2A-CAA-CBA
31	s	303	CLA	C1A-C2A-CAA-CBA
31	s	311	CLA	C1A-C2A-CAA-CBA
31	s	315	CLA	C1A-C2A-CAA-CBA
31	y	602	CLA	C1A-C2A-CAA-CBA
31	y	603	CLA	C1A-C2A-CAA-CBA
31	y	604	CLA	C1A-C2A-CAA-CBA
31	y	610	CLA	C1A-C2A-CAA-CBA
31	y	614	CLA	C1A-C2A-CAA-CBA
30	6	308	CHL	O1D-CGD-O2D-CED
33	j	102	LHG	C24-C23-O8-C6
31	C	601	CLA	C8-C10-C11-C12
33	B	624	LHG	C31-C32-C33-C34
33	Y	318	LHG	C33-C34-C35-C36
33	e	101	LHG	C24-C25-C26-C27
33	y	619	LHG	C13-C14-C15-C16
34	Q1	101	LMG	C31-C32-C33-C34
33	N	319	LHG	C28-C29-C30-C31
33	A	415	LHG	C11-C12-C13-C14
33	D	407	LHG	C30-C31-C32-C33
31	N	310	CLA	C5-C6-C7-C8
33	1	617	LHG	O6-C4-C5-C6
33	2	617	LHG	O6-C4-C5-C6
33	6	320	LHG	O6-C4-C5-C6
33	A	417	LHG	O6-C4-C5-C6
33	G	618	LHG	O6-C4-C5-C6
33	N	319	LHG	O6-C4-C5-C6
33	R	320	LHG	O6-C4-C5-C6
33	8	618	LHG	O6-C4-C5-C6
33	9	320	LHG	O6-C4-C5-C6
33	a	415	LHG	O6-C4-C5-C6
33	n	320	LHG	O6-C4-C5-C6
33	z	102	LHG	O6-C4-C5-C6
33	F1	301	LHG	O6-C4-C5-C6
34	b	626	LMG	O6-C5-C6-O5
33	3	320	LHG	O9-C7-O7-C5
45	C	616	DGD	O1B-C1B-O2G-C2G
33	s	322	LHG	C11-C12-C13-C14
33	s	322	LHG	C34-C35-C36-C37
38	S	301	SQD	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
30	1	605	CHL	C11-C10-C8-C7
30	1	605	CHL	C12-C13-C15-C16
30	1	606	CHL	C11-C10-C8-C7
30	1	606	CHL	C11-C12-C13-C15
30	1	607	CHL	C12-C13-C15-C16
30	2	601	CHL	C11-C10-C8-C7
30	2	608	CHL	C6-C7-C8-C10
30	6	310	CHL	C11-C10-C8-C7
30	G	623	CHL	C12-C13-C15-C16
30	N	306	CHL	C11-C10-C8-C7
30	Y	301	CHL	C12-C13-C15-C16
30	Y	307	CHL	C11-C10-C8-C7
30	Y	309	CHL	C12-C13-C15-C16
30	7	302	CHL	C11-C12-C13-C15
30	7	302	CHL	C12-C13-C15-C16
30	7	306	CHL	C6-C7-C8-C10
30	7	306	CHL	C11-C12-C13-C15
30	7	306	CHL	C12-C13-C15-C16
30	7	307	CHL	C12-C13-C15-C16
30	7	308	CHL	C12-C13-C15-C16
30	8	605	CHL	C11-C10-C8-C7
30	8	605	CHL	C11-C12-C13-C15
30	8	605	CHL	C12-C13-C15-C16
30	8	606	CHL	C11-C10-C8-C7
30	9	311	CHL	C11-C10-C8-C7
30	g	302	CHL	C11-C10-C8-C7
30	n	306	CHL	C11-C10-C8-C7
30	n	306	CHL	C11-C12-C13-C15
30	n	306	CHL	C12-C13-C15-C16
30	n	307	CHL	C11-C10-C8-C7
30	y	607	CHL	C11-C12-C13-C15
31	1	613	CLA	C6-C7-C8-C10
31	4	602	CLA	C6-C7-C8-C10
31	6	311	CLA	C6-C7-C8-C10
31	6	314	CLA	C6-C7-C8-C10
31	B	607	CLA	C11-C12-C13-C15
31	B	609	CLA	C6-C7-C8-C10
31	B	615	CLA	C6-C7-C8-C10
31	C	601	CLA	C11-C12-C13-C15
31	C	602	CLA	C6-C7-C8-C10
31	C	603	CLA	C11-C12-C13-C15
31	C	605	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
31	C	610	CLA	C12-C13-C15-C16
31	D	403	CLA	C11-C12-C13-C15
31	N	313	CLA	C6-C7-C8-C10
31	R	304	CLA	C6-C7-C8-C10
31	R	304	CLA	C11-C10-C8-C7
31	R	311	CLA	C11-C10-C8-C7
31	R	316	CLA	C6-C7-C8-C10
31	Y	311	CLA	C11-C10-C8-C7
31	Y	311	CLA	C11-C12-C13-C15
31	0	602	CLA	C6-C7-C8-C10
31	0	603	CLA	C6-C7-C8-C10
31	0	610	CLA	C11-C10-C8-C7
31	7	312	CLA	C6-C7-C8-C10
31	8	612	CLA	C6-C7-C8-C10
31	9	304	CLA	C11-C10-C8-C7
31	9	306	CLA	C6-C7-C8-C10
31	9	306	CLA	C11-C10-C8-C7
31	p	611	CLA	C6-C7-C8-C10
31	b	606	CLA	C12-C13-C15-C16
31	c	603	CLA	C11-C12-C13-C15
31	c	613	CLA	C12-C13-C15-C16
31	d	405	CLA	C6-C7-C8-C10
31	n	314	CLA	C6-C7-C8-C10
31	r	305	CLA	C6-C7-C8-C10
31	r	311	CLA	C6-C7-C8-C10
31	y	602	CLA	C6-C7-C8-C10
42	D	401	PHO	C11-C10-C8-C7
33	C	623	LHG	C9-C10-C11-C12
31	b	603	CLA	C16-C17-C18-C20
31	g	304	CLA	C6-C7-C8-C9
31	4	610	CLA	C10-C11-C12-C13
48	R	302	LMU	C1-C2-C3-C4
34	C	624	LMG	O6-C5-C6-O5
33	4	618	LHG	C24-C25-C26-C27
31	s	304	CLA	C3A-C2A-CAA-CBA
30	g	306	CHL	CBA-CGA-O2A-C1
33	b	628	LHG	C13-C14-C15-C16
33	s	322	LHG	C31-C32-C33-C34
31	B	603	CLA	C10-C11-C12-C13
31	b	609	CLA	C5-C6-C7-C8
31	c	602	CLA	C8-C10-C11-C12
31	c	603	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
34	k	101	LMG	C18-C19-C20-C21
30	1	605	CHL	C4-C3-C5-C6
30	1	609	CHL	C4-C3-C5-C6
30	N	302	CHL	C4-C3-C5-C6
30	8	601	CHL	C4-C3-C5-C6
30	q	309	CHL	C4-C3-C5-C6
30	g	302	CHL	C4-C3-C5-C6
30	n	302	CHL	C4-C3-C5-C6
30	r	308	CHL	C4-C3-C5-C6
31	C	610	CLA	C4-C3-C5-C6
31	b	608	CLA	C4-C3-C5-C6
30	N	302	CHL	C2-C3-C5-C6
30	0	607	CHL	C2-C3-C5-C6
30	8	601	CHL	C2-C3-C5-C6
30	g	302	CHL	C2-C3-C5-C6
30	n	302	CHL	C2-C3-C5-C6
31	Y	311	CLA	C2-C3-C5-C6
31	0	603	CLA	C2-C3-C5-C6
31	7	314	CLA	C2-C3-C5-C6
31	a	406	CLA	C2-C3-C5-C6
31	b	608	CLA	C2-C3-C5-C6
31	b	610	CLA	C2-C3-C5-C6
31	y	604	CLA	C2-C3-C5-C6
31	y	611	CLA	C2-C3-C5-C6
44	a	414	PL9	C12-C11-C9-C8
33	Y	318	LHG	C9-C10-C11-C12
34	I	101	LMG	O6-C5-C6-O5
34	p	620	LMG	O6-C5-C6-O5
34	d	411	LMG	O6-C5-C6-O5
33	L	101	LHG	C29-C30-C31-C32
33	9	320	LHG	C26-C27-C28-C29
30	y	606	CHL	C2A-CAA-CBA-CGA
31	R	306	CLA	C2A-CAA-CBA-CGA
31	8	604	CLA	C2A-CAA-CBA-CGA
31	b	602	CLA	C2A-CAA-CBA-CGA
31	d	405	CLA	C2A-CAA-CBA-CGA
30	1	606	CHL	C11-C10-C8-C9
31	2	602	CLA	C6-C7-C8-C9
31	3	304	CLA	C6-C7-C8-C9
31	4	602	CLA	C6-C7-C8-C9
31	6	304	CLA	C6-C7-C8-C9
31	B	609	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	B	615	CLA	C6-C7-C8-C9
31	C	608	CLA	C6-C7-C8-C9
31	C	610	CLA	C14-C13-C15-C16
31	D	403	CLA	C11-C12-C13-C14
31	R	311	CLA	C6-C7-C8-C9
31	R	316	CLA	C6-C7-C8-C9
31	Y	303	CLA	C6-C7-C8-C9
31	0	602	CLA	C6-C7-C8-C9
31	0	602	CLA	C11-C10-C8-C9
31	8	612	CLA	C11-C12-C13-C14
31	9	306	CLA	C6-C7-C8-C9
31	p	611	CLA	C6-C7-C8-C9
31	b	605	CLA	C14-C13-C15-C16
31	b	616	CLA	C11-C12-C13-C14
31	c	607	CLA	C11-C12-C13-C14
31	g	303	CLA	C6-C7-C8-C9
31	g	303	CLA	C14-C13-C15-C16
31	n	314	CLA	C11-C12-C13-C14
33	Y	318	LHG	C30-C31-C32-C33
34	6	323	LMG	C29-C30-C31-C32
38	s	301	SQD	C9-C10-C11-C12
45	c	616	DGD	C9B-CAB-CBB-CCB
34	2	618	LMG	O6-C5-C6-O5
45	C	618	DGD	O6E-C5E-C6E-O5E
38	x	201	SQD	C23-C24-C25-C26
48	K	101	LMU	C1-C2-C3-C4
33	8	618	LHG	C34-C35-C36-C37
33	n	320	LHG	C34-C35-C36-C37
34	k	101	LMG	C30-C31-C32-C33
30	9	311	CHL	O1D-CGD-O2D-CED
31	7	313	CLA	CBA-CGA-O2A-C1
31	q	304	CLA	CBA-CGA-O2A-C1
33	M	101	LHG	C24-C23-O8-C6
33	F1	301	LHG	C24-C23-O8-C6
34	r	321	LMG	C29-C28-O8-C9
34	s	321	LMG	O6-C5-C6-O5
33	C	623	LHG	C35-C36-C37-C38
31	7	312	CLA	O1D-CGD-O2D-CED
34	A	414	LMG	C2-C1-O1-C7
34	D	410	LMG	C2-C1-O1-C7
34	W	201	LMG	C2-C1-O1-C7
34	b	601	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
34	b	629	LMG	C2-C1-O1-C7
34	w	202	LMG	C2-C1-O1-C7
45	c	619	DGD	C2D-C1D-O3G-C3G
31	0	604	CLA	C5-C6-C7-C8
34	x	202	LMG	C28-C29-C30-C31
30	1	608	CHL	O1D-CGD-O2D-CED
33	1	617	LHG	C4-C5-C6-O8
33	5	619	LHG	C4-C5-C6-O8
33	D	408	LHG	C4-C5-C6-O8
33	R	320	LHG	C4-C5-C6-O8
33	0	619	LHG	C4-C5-C6-O8
33	e	101	LHG	C4-C5-C6-O8
33	j	102	LHG	C4-C5-C6-O8
33	r	320	LHG	C4-C5-C6-O8
34	A	414	LMG	O1-C7-C8-C9
34	A	418	LMG	O1-C7-C8-C9
34	B	621	LMG	C7-C8-C9-O8
34	B	625	LMG	C7-C8-C9-O8
34	C	621	LMG	C7-C8-C9-O8
34	N	320	LMG	O1-C7-C8-C9
34	W	203	LMG	O1-C7-C8-C9
34	X	203	LMG	C7-C8-C9-O8
34	7	322	LMG	O1-C7-C8-C9
34	9	301	LMG	O1-C7-C8-C9
34	b	629	LMG	C7-C8-C9-O8
34	g	320	LMG	O1-C7-C8-C9
38	6	301	SQD	O6-C44-C45-C46
38	A	411	SQD	C44-C45-C46-O48
38	A	413	SQD	C44-C45-C46-O48
38	B	623	SQD	O6-C44-C45-C46
38	G	617	SQD	C44-C45-C46-O48
38	R	322	SQD	O6-C44-C45-C46
38	S	301	SQD	C44-C45-C46-O48
38	b	627	SQD	C44-C45-C46-O48
38	r	322	SQD	O6-C44-C45-C46
38	y	621	SQD	C44-C45-C46-O48
33	G	618	LHG	C33-C34-C35-C36
33	L	101	LHG	C13-C14-C15-C16
33	7	319	LHG	C24-C25-C26-C27
38	m	101	SQD	C26-C27-C28-C29
45	c	618	DGD	C3A-C4A-C5A-C6A
48	R	302	LMU	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
31	N	304	CLA	O1D-CGD-O2D-CED
33	b	628	LHG	C30-C31-C32-C33
31	B	607	CLA	C10-C11-C12-C13
31	B	611	CLA	C15-C16-C17-C18
31	c	611	CLA	C8-C10-C11-C12
33	6	320	LHG	C9-C10-C11-C12
33	D	408	LHG	C17-C18-C19-C20
33	b	628	LHG	C15-C16-C17-C18
38	b	621	SQD	C26-C27-C28-C29
31	4	604	CLA	O1D-CGD-O2D-CED
30	4	607	CHL	CBA-CGA-O2A-C1
31	2	612	CLA	CBA-CGA-O2A-C1
31	B	611	CLA	CBA-CGA-O2A-C1
31	8	602	CLA	CBA-CGA-O2A-C1
31	y	611	CLA	CBA-CGA-O2A-C1
34	S	321	LMG	O6-C5-C6-O5
45	c	618	DGD	O6E-C5E-C6E-O5E
31	C	612	CLA	C6-C7-C8-C10
31	0	615	CLA	C6-C7-C8-C9
31	c	603	CLA	C16-C17-C18-C20
31	g	304	CLA	C6-C7-C8-C10
31	3	301	CLA	C5-C6-C7-C8
33	A	417	LHG	C33-C34-C35-C36
33	D	408	LHG	C16-C17-C18-C19
33	n	320	LHG	C11-C10-C9-C8
34	c	624	LMG	C29-C30-C31-C32
34	n	322	LMG	C33-C34-C35-C36
38	a	412	SQD	C9-C10-C11-C12
34	3	321	LMG	C8-C9-O8-C28
34	b	629	LMG	C8-C9-O8-C28
31	b	610	CLA	C13-C15-C16-C17
33	8	618	LHG	C11-C10-C9-C8
33	b	628	LHG	C9-C10-C11-C12
33	j	102	LHG	C31-C32-C33-C34
34	S	321	LMG	C14-C15-C16-C17
34	q	302	LMG	C11-C12-C13-C14
30	1	619	CHL	CHA-CBD-CGD-O1D
30	2	608	CHL	CHA-CBD-CGD-O1D
30	4	606	CHL	CHA-CBD-CGD-O1D
30	5	605	CHL	CHA-CBD-CGD-O2D
30	G	608	CHL	CHA-CBD-CGD-O1D
30	R	310	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
30	Y	308	CHL	CHA-CBD-CGD-O1D
30	7	310	CHL	CHA-CBD-CGD-O1D
30	8	605	CHL	CHA-CBD-CGD-O1D
30	8	605	CHL	CHA-CBD-CGD-O2D
30	g	307	CHL	CHA-CBD-CGD-O1D
30	g	307	CHL	CHA-CBD-CGD-O2D
30	n	306	CHL	CHA-CBD-CGD-O1D
30	n	306	CHL	CHA-CBD-CGD-O2D
30	n	309	CHL	CHA-CBD-CGD-O1D
36	2	616	NEX	C11-C10-C9-C19
36	3	319	NEX	C39-C29-C30-C31
36	N	318	NEX	C11-C10-C9-C19
36	R	301	NEX	C39-C29-C30-C31
36	q	319	NEX	C39-C29-C30-C31
36	g	317	NEX	C40-C33-C34-C35
37	2	619	XAT	C20-C13-C14-C15
37	4	619	XAT	C20-C13-C14-C15
37	G	620	XAT	C20-C13-C14-C15
37	9	322	XAT	C20-C13-C14-C15
37	q	321	XAT	C20-C13-C14-C15
37	g	321	XAT	C20-C13-C14-C15
42	d	402	PHO	CHA-CBD-CGD-O1D
42	d	402	PHO	CHA-CBD-CGD-O2D
31	1	604	CLA	C13-C15-C16-C17
31	r	316	CLA	C13-C15-C16-C17
33	r	320	LHG	C7-C8-C9-C10
34	0	620	LMG	C28-C29-C30-C31
31	7	313	CLA	O1A-CGA-O2A-C1
45	c	616	DGD	O1A-C1A-O1G-C1G
34	B	621	LMG	C29-C30-C31-C32
30	Y	307	CHL	C4-C3-C5-C6
30	9	303	CHL	C4-C3-C5-C6
31	0	603	CLA	C4-C3-C5-C6
31	7	314	CLA	C4-C3-C5-C6
31	s	305	CLA	C4-C3-C5-C6
31	y	611	CLA	C4-C3-C5-C6
30	1	605	CHL	C2-C3-C5-C6
30	1	607	CHL	C2-C3-C5-C6
30	1	609	CHL	C2-C3-C5-C6
30	6	302	CHL	C2-C3-C5-C6
30	G	623	CHL	C2-C3-C5-C6
30	Y	307	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	9	303	CHL	C2-C3-C5-C6
30	r	308	CHL	C2-C3-C5-C6
31	B	609	CLA	C2-C3-C5-C6
31	c	605	CLA	C2-C3-C5-C6
31	s	305	CLA	C2-C3-C5-C6
31	5	610	CLA	C5-C6-C7-C8
31	7	313	CLA	C5-C6-C7-C8
31	8	609	CLA	C5-C6-C7-C8
31	9	305	CLA	C5-C6-C7-C8
43	A	410	BCR	C7-C8-C9-C34
43	C	615	BCR	C37-C22-C23-C24
43	D	405	BCR	C37-C22-C23-C24
43	T	101	BCR	C36-C18-C19-C20
34	5	620	LMG	C8-C9-O8-C28
31	p	611	CLA	C11-C12-C13-C14
31	r	304	CLA	C11-C12-C13-C15
34	d	411	LMG	C12-C13-C14-C15
34	g	322	LMG	C12-C13-C14-C15
34	4	620	LMG	O6-C5-C6-O5
32	2	615	LUT	C31-C32-C33-C34
32	G	615	LUT	C31-C32-C33-C34
31	g	310	CLA	O1A-CGA-O2A-C1
31	R	315	CLA	C5-C6-C7-C8
31	S	312	CLA	C13-C15-C16-C17
31	b	603	CLA	C15-C16-C17-C18
31	c	609	CLA	C13-C15-C16-C17
42	A	408	PHO	C5-C6-C7-C8
33	2	617	LHG	C27-C28-C29-C30
33	r	320	LHG	C13-C14-C15-C16
30	4	609	CHL	C2A-CAA-CBA-CGA
30	r	310	CHL	C2A-CAA-CBA-CGA
31	3	305	CLA	C2A-CAA-CBA-CGA
31	6	315	CLA	C2A-CAA-CBA-CGA
31	c	601	CLA	C2A-CAA-CBA-CGA
48	K	101	LMU	O5'-C5'-C6'-O6'
33	2	617	LHG	C26-C27-C28-C29
31	9	306	CLA	C8-C10-C11-C12
31	c	603	CLA	C10-C11-C12-C13
33	D	408	LHG	C33-C34-C35-C36
34	b	622	LMG	C19-C20-C21-C22
33	A	417	LHG	C23-C24-C25-C26
34	b	623	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	N	307	CHL	O1A-CGA-O2A-C1
38	s	301	SQD	O10-C23-O48-C46
33	B	624	LHG	C10-C11-C12-C13
33	B	624	LHG	C12-C13-C14-C15
33	G	618	LHG	C30-C31-C32-C33
33	S	322	LHG	C26-C27-C28-C29
33	j	102	LHG	C34-C35-C36-C37
30	9	307	CHL	O1D-CGD-O2D-CED
31	C	601	CLA	CBA-CGA-O2A-C1
31	Y	311	CLA	CBA-CGA-O2A-C1
33	N	319	LHG	C4-C5-O7-C7
34	3	321	LMG	C9-C8-O7-C10
34	7	320	LMG	C9-C8-O7-C10
45	c	619	DGD	C1G-C2G-O2G-C1B
30	1	619	CHL	C5-C6-C7-C8
30	g	309	CHL	C5-C6-C7-C8
30	y	609	CHL	C8-C10-C11-C12
31	B	614	CLA	C10-C11-C12-C13
44	d	407	PL9	C47-C48-C49-C50
33	g	319	LHG	C30-C31-C32-C33
33	l	101	LHG	C16-C17-C18-C19
38	B	623	SQD	C25-C26-C27-C28
38	r	322	SQD	C10-C11-C12-C13
36	R	319	NEX	C13-C14-C15-C35
36	q	319	NEX	C29-C30-C31-C32
43	b	618	BCR	C19-C20-C21-C22
43	d	406	BCR	C19-C20-C21-C22
43	h	101	BCR	C19-C20-C21-C22
31	6	316	CLA	C6-C7-C8-C9
31	r	305	CLA	C11-C12-C13-C15
38	x	201	SQD	C27-C28-C29-C30
38	B	620	SQD	C23-C24-C25-C26
31	b	604	CLA	C3-C5-C6-C7
45	c	619	DGD	C4D-C5D-C6D-O5D
33	A	415	LHG	C33-C34-C35-C36
33	N	319	LHG	C11-C12-C13-C14
34	b	626	LMG	C31-C32-C33-C34
30	N	309	CHL	O1D-CGD-O2D-CED
36	6	319	NEX	C32-C33-C34-C35
36	0	618	NEX	C32-C33-C34-C35
37	2	619	XAT	C12-C13-C14-C15
33	S	322	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	b	625	LHG	C29-C30-C31-C32
33	5	619	LHG	O6-C4-C5-O7
33	g	319	LHG	O6-C4-C5-O7
33	r	320	LHG	O6-C4-C5-O7
33	y	619	LHG	O6-C4-C5-O7
30	1	606	CHL	C5-C6-C7-C8
31	2	602	CLA	C10-C11-C12-C13
31	n	311	CLA	C5-C6-C7-C8
33	S	320	LHG	C26-C27-C28-C29
33	a	415	LHG	C31-C32-C33-C34
30	9	309	CHL	CBA-CGA-O2A-C1
31	C	603	CLA	CBA-CGA-O2A-C1
31	7	314	CLA	CBA-CGA-O2A-C1
31	c	606	CLA	CBA-CGA-O2A-C1
33	3	320	LHG	C24-C23-O8-C6
33	C	623	LHG	C24-C23-O8-C6
34	3	321	LMG	C29-C28-O8-C9
33	B	624	LHG	C35-C36-C37-C38
34	q1	101	LMG	C8-C9-O8-C28
31	n	316	CLA	C5-C6-C7-C8
33	2	617	LHG	C10-C11-C12-C13
34	D	409	LMG	C12-C13-C14-C15
45	c	617	DGD	C7A-C8A-C9A-CAA
33	1	617	LHG	C11-C10-C9-C8
33	l	101	LHG	C31-C32-C33-C34
34	2	621	LMG	C31-C32-C33-C34
30	R	308	CHL	C4-C3-C5-C6
30	0	607	CHL	C4-C3-C5-C6
30	9	309	CHL	C4-C3-C5-C6
31	1	610	CLA	C4-C3-C5-C6
31	y	604	CLA	C4-C3-C5-C6
30	N	306	CHL	C2-C3-C5-C6
31	C	610	CLA	C2-C3-C5-C6
33	9	320	LHG	C28-C29-C30-C31
33	0	619	LHG	C12-C13-C14-C15
33	b	628	LHG	C11-C10-C9-C8
33	s	320	LHG	C11-C12-C13-C14
34	D	409	LMG	C11-C12-C13-C14
34	D	412	LMG	C36-C37-C38-C39
33	q	320	LHG	C33-C34-C35-C36
33	e	101	LHG	C11-C12-C13-C14
33	s	320	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
38	B	623	SQD	C12-C13-C14-C15
31	Y	314	CLA	C6-C7-C8-C9
44	A	416	PL9	C37-C38-C39-C41
33	6	320	LHG	O7-C5-C6-O8
34	2	620	LMG	O1-C7-C8-O7
34	2	620	LMG	O7-C8-C9-O8
34	5	620	LMG	O1-C7-C8-O7
34	D	409	LMG	O1-C7-C8-O7
34	G	621	LMG	O1-C7-C8-O7
34	I	101	LMG	O1-C7-C8-O7
34	0	620	LMG	O1-C7-C8-O7
34	7	322	LMG	O7-C8-C9-O8
34	w	205	LMG	O1-C7-C8-O7
34	x	202	LMG	O1-C7-C8-O7
45	C	617	DGD	O2G-C2G-C3G-O3G
45	C	620	DGD	O2G-C2G-C3G-O3G
33	t	102	LHG	C11-C12-C13-C14
34	x	202	LMG	C34-C35-C36-C37
33	6	320	LHG	C13-C14-C15-C16
33	F1	301	LHG	C13-C14-C15-C16
34	b	629	LMG	C33-C34-C35-C36
45	c	616	DGD	CDB-CEB-CFB-CGB
31	7	315	CLA	C6-C7-C8-C9
33	s	320	LHG	C31-C32-C33-C34
33	y	619	LHG	C35-C36-C37-C38
34	2	618	LMG	O7-C10-C11-C12
34	6	323	LMG	O7-C10-C11-C12
33	F1	301	LHG	C9-C10-C11-C12
38	s	301	SQD	C25-C26-C27-C28
30	1	608	CHL	C2A-CAA-CBA-CGA
31	R	304	CLA	C2A-CAA-CBA-CGA
30	N	307	CHL	C3-C5-C6-C7
31	C	611	CLA	C3-C5-C6-C7
31	9	305	CLA	C3-C5-C6-C7
31	N	313	CLA	C2-C1-O2A-CGA
33	A	417	LHG	C28-C29-C30-C31
33	p	619	LHG	C25-C26-C27-C28
34	w	205	LMG	C31-C32-C33-C34
30	g	306	CHL	O1A-CGA-O2A-C1
34	r	321	LMG	O10-C28-O8-C9
33	s	322	LHG	C29-C30-C31-C32
34	D	411	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
34	d	410	LMG	C37-C38-C39-C40
31	a	407	CLA	O1D-CGD-O2D-CED
30	3	302	CHL	CBA-CGA-O2A-C1
30	3	309	CHL	CBA-CGA-O2A-C1
31	6	303	CLA	CBA-CGA-O2A-C1
31	6	305	CLA	CBA-CGA-O2A-C1
31	7	312	CLA	CBA-CGA-O2A-C1
30	g	302	CHL	CAA-CBA-CGA-O2A
33	r	320	LHG	C25-C26-C27-C28
31	3	306	CLA	CBD-CGD-O2D-CED
33	p	619	LHG	C28-C29-C30-C31
33	l	101	LHG	C30-C31-C32-C33
38	s	301	SQD	C28-C29-C30-C31
31	4	603	CLA	C3-C5-C6-C7
31	S	303	CLA	C3-C5-C6-C7
33	9	320	LHG	C11-C10-C9-C8
33	b	628	LHG	C33-C34-C35-C36
33	c	622	LHG	C30-C31-C32-C33
38	b	627	SQD	C16-C17-C18-C19
30	G	606	CHL	O1D-CGD-O2D-CED
30	7	306	CHL	O1D-CGD-O2D-CED
34	6	322	LMG	C10-C11-C12-C13
38	b	621	SQD	C17-C18-C19-C20
48	K	101	LMU	C6-C7-C8-C9
33	S	322	LHG	C35-C36-C37-C38
31	A	405	CLA	C5-C6-C7-C8
31	B	608	CLA	C8-C10-C11-C12
31	C	601	CLA	C10-C11-C12-C13
31	7	305	CLA	C5-C6-C7-C8
31	b	604	CLA	C13-C15-C16-C17
42	A	408	PHO	C10-C11-C12-C13
31	6	315	CLA	O1D-CGD-O2D-CED
32	5	617	LUT	C9-C10-C11-C12
30	2	608	CHL	C11-C10-C8-C9
30	q	309	CHL	C11-C10-C8-C9
31	6	304	CLA	C11-C10-C8-C9
30	3	310	CHL	C11-C12-C13-C14
31	G	603	CLA	C6-C7-C8-C9
31	Y	312	CLA	C16-C17-C18-C19
31	c	601	CLA	C16-C17-C18-C20
31	r	304	CLA	C11-C12-C13-C14
30	8	608	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	3	302	CHL	C4-C3-C5-C6
30	4	609	CHL	C4-C3-C5-C6
31	0	613	CLA	C4-C3-C5-C6
31	c	605	CLA	C4-C3-C5-C6
30	3	302	CHL	C2-C3-C5-C6
33	c	622	LHG	C12-C13-C14-C15
34	2	620	LMG	C34-C35-C36-C37
34	W	201	LMG	C39-C40-C41-C42
31	7	316	CLA	O1D-CGD-O2D-CED
30	7	321	CHL	CBA-CGA-O2A-C1
30	n	308	CHL	CBA-CGA-O2A-C1
31	C	604	CLA	CBA-CGA-O2A-C1
31	b	608	CLA	CBA-CGA-O2A-C1
31	n	303	CLA	CBA-CGA-O2A-C1
34	k	102	LMG	C29-C28-O8-C9
30	2	601	CHL	C8-C10-C11-C12
33	a	415	LHG	C23-C24-C25-C26
34	q	301	LMG	C18-C19-C20-C21
33	8	618	LHG	C11-C12-C13-C14
33	t	102	LHG	O9-C7-O7-C5
33	e	101	LHG	O1-C1-C2-O2
30	1	606	CHL	C11-C12-C13-C14
30	Y	301	CHL	C14-C13-C15-C16
30	Y	309	CHL	C14-C13-C15-C16
30	7	302	CHL	C11-C12-C13-C14
30	7	307	CHL	C14-C13-C15-C16
30	7	310	CHL	C11-C12-C13-C14
30	8	605	CHL	C14-C13-C15-C16
30	8	606	CHL	C11-C10-C8-C9
30	n	306	CHL	C14-C13-C15-C16
30	n	307	CHL	C11-C10-C8-C9
31	1	613	CLA	C6-C7-C8-C9
31	2	609	CLA	C6-C7-C8-C9
31	6	311	CLA	C6-C7-C8-C9
31	6	313	CLA	C6-C7-C8-C9
31	6	314	CLA	C6-C7-C8-C9
31	B	602	CLA	C11-C12-C13-C14
31	B	603	CLA	C6-C7-C8-C9
31	B	603	CLA	C11-C12-C13-C14
31	B	605	CLA	C14-C13-C15-C16
31	B	614	CLA	C11-C10-C8-C9
31	B	616	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	C	601	CLA	C6-C7-C8-C9
31	C	603	CLA	C11-C12-C13-C14
31	C	605	CLA	C11-C10-C8-C9
31	R	304	CLA	C11-C10-C8-C9
31	R	312	CLA	C11-C10-C8-C9
31	Y	303	CLA	C11-C10-C8-C9
31	0	603	CLA	C6-C7-C8-C9
31	0	613	CLA	C6-C7-C8-C9
31	7	312	CLA	C6-C7-C8-C9
31	7	314	CLA	C11-C12-C13-C14
31	8	604	CLA	C11-C10-C8-C9
31	q	315	CLA	C11-C10-C8-C9
31	b	604	CLA	C11-C12-C13-C14
31	b	605	CLA	C11-C12-C13-C14
31	b	613	CLA	C6-C7-C8-C9
31	c	603	CLA	C11-C12-C13-C14
31	d	405	CLA	C6-C7-C8-C9
31	n	305	CLA	C11-C10-C8-C9
31	n	305	CLA	C14-C13-C15-C16
31	r	311	CLA	C6-C7-C8-C9
31	s	313	CLA	C6-C7-C8-C9
31	y	602	CLA	C6-C7-C8-C9
31	y	612	CLA	C14-C13-C15-C16
42	D	401	PHO	C11-C12-C13-C14
33	n	320	LHG	C11-C12-C13-C14
33	s	322	LHG	C27-C28-C29-C30
33	y	619	LHG	C9-C10-C11-C12
31	C	608	CLA	O1D-CGD-O2D-CED
31	N	305	CLA	C5-C6-C7-C8
31	r	315	CLA	C5-C6-C7-C8
31	y	604	CLA	C5-C6-C7-C8
33	N	319	LHG	C2-C3-O3-P
33	8	618	LHG	C5-C4-O6-P
33	n	320	LHG	C5-C4-O6-P
38	a	411	SQD	C32-C33-C34-C35
31	2	612	CLA	O1A-CGA-O2A-C1
31	2	602	CLA	C4B-C3B-CAB-CBB
31	B	615	CLA	C4B-C3B-CAB-CBB
31	S	310	CLA	C4B-C3B-CAB-CBB
31	Y	311	CLA	C4B-C3B-CAB-CBB
31	0	615	CLA	C4B-C3B-CAB-CBB
31	b	602	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	b	603	CLA	C4B-C3B-CAB-CBB
31	b	616	CLA	C4B-C3B-CAB-CBB
31	r	313	CLA	C4B-C3B-CAB-CBB
31	r	316	CLA	C4B-C3B-CAB-CBB
31	s	312	CLA	C4B-C3B-CAB-CBB
33	2	617	LHG	C16-C17-C18-C19
33	q	320	LHG	C30-C31-C32-C33
33	j	102	LHG	C11-C12-C13-C14
34	G	619	LMG	O7-C10-C11-C12
34	c	620	LMG	O7-C10-C11-C12
38	R	322	SQD	C12-C13-C14-C15
31	6	316	CLA	C5-C6-C7-C8
31	R	304	CLA	C10-C11-C12-C13
31	0	611	CLA	C5-C6-C7-C8
31	8	612	CLA	C15-C16-C17-C18
31	d	405	CLA	C10-C11-C12-C13
31	n	314	CLA	C15-C16-C17-C18
45	c	619	DGD	O6D-C5D-C6D-O5D
33	R	320	LHG	C28-C29-C30-C31
31	B	603	CLA	C2A-CAA-CBA-CGA
31	p	615	CLA	C2A-CAA-CBA-CGA
34	q	301	LMG	C11-C12-C13-C14
34	w	204	LMG	O6-C5-C6-O5
34	4	620	LMG	C2-C1-O1-C7
34	B	625	LMG	C2-C1-O1-C7
34	C	621	LMG	C2-C1-O1-C7
34	C	624	LMG	C2-C1-O1-C7
34	9	302	LMG	C2-C1-O1-C7
34	9	321	LMG	C2-C1-O1-C7
34	b	626	LMG	C2-C1-O1-C7
45	C	617	DGD	C2D-C1D-O3G-C3G
45	C	620	DGD	C2D-C1D-O3G-C3G
42	a	408	PHO	C8-C10-C11-C12
33	B	624	LHG	C17-C18-C19-C20
33	S	320	LHG	C30-C31-C32-C33
33	j	102	LHG	C11-C10-C9-C8
34	X	203	LMG	C11-C12-C13-C14
31	9	312	CLA	C6-C7-C8-C9
31	n	316	CLA	C6-C7-C8-C9
33	A	415	LHG	O6-C4-C5-C6
33	D	408	LHG	O6-C4-C5-C6
33	K	102	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
33	S	320	LHG	O6-C4-C5-C6
33	j	102	LHG	O6-C4-C5-C6
33	r	320	LHG	O6-C4-C5-C6
33	s	320	LHG	O6-C4-C5-C6
33	y	619	LHG	O6-C4-C5-C6
31	2	604	CLA	C6-C7-C8-C9
31	8	614	CLA	C6-C7-C8-C9
30	5	601	CHL	CAA-CBA-CGA-O2A
34	g	320	LMG	O7-C10-C11-C12
30	1	607	CHL	C11-C10-C8-C7
30	G	601	CHL	C11-C12-C13-C15
30	G	623	CHL	C11-C12-C13-C15
30	g	302	CHL	C11-C12-C13-C15
30	g	309	CHL	C11-C12-C13-C15
30	y	606	CHL	C11-C10-C8-C7
31	1	610	CLA	C11-C10-C8-C7
31	2	602	CLA	C6-C7-C8-C10
31	3	304	CLA	C6-C7-C8-C10
31	6	304	CLA	C6-C7-C8-C10
31	6	312	CLA	C6-C7-C8-C10
31	6	313	CLA	C6-C7-C8-C10
31	B	602	CLA	C11-C12-C13-C15
31	B	603	CLA	C6-C7-C8-C10
31	B	603	CLA	C11-C12-C13-C15
31	B	605	CLA	C11-C10-C8-C7
31	B	607	CLA	C11-C10-C8-C7
31	B	609	CLA	C11-C10-C8-C7
31	B	610	CLA	C11-C12-C13-C15
31	B	613	CLA	C11-C12-C13-C15
31	B	614	CLA	C6-C7-C8-C10
31	B	616	CLA	C6-C7-C8-C10
31	C	608	CLA	C6-C7-C8-C10
31	C	608	CLA	C11-C10-C8-C7
31	D	403	CLA	C6-C7-C8-C10
31	D	404	CLA	C6-C7-C8-C10
31	G	602	CLA	C6-C7-C8-C10
31	N	313	CLA	C11-C12-C13-C15
31	R	311	CLA	C6-C7-C8-C10
31	R	312	CLA	C11-C10-C8-C7
31	S	314	CLA	C11-C10-C8-C7
31	Y	303	CLA	C6-C7-C8-C10
31	0	613	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	8	612	CLA	C11-C12-C13-C15
31	q	315	CLA	C11-C10-C8-C7
31	b	604	CLA	C11-C12-C13-C15
31	b	605	CLA	C11-C12-C13-C15
31	b	605	CLA	C12-C13-C15-C16
31	b	608	CLA	C11-C12-C13-C15
31	b	610	CLA	C11-C10-C8-C7
31	b	612	CLA	C11-C12-C13-C15
31	b	613	CLA	C11-C12-C13-C15
31	b	615	CLA	C6-C7-C8-C10
31	b	616	CLA	C11-C12-C13-C15
31	c	607	CLA	C11-C12-C13-C15
31	c	609	CLA	C6-C7-C8-C10
31	c	611	CLA	C11-C10-C8-C7
31	g	303	CLA	C6-C7-C8-C10
31	g	310	CLA	C11-C12-C13-C15
31	n	305	CLA	C12-C13-C15-C16
31	n	314	CLA	C11-C12-C13-C15
31	r	304	CLA	C6-C7-C8-C10
31	s	314	CLA	C11-C10-C8-C7
31	s	314	CLA	C12-C13-C15-C16
31	y	610	CLA	C11-C12-C13-C15
31	y	612	CLA	C6-C7-C8-C10
31	y	612	CLA	C12-C13-C15-C16
30	1	609	CHL	C10-C11-C12-C13
30	0	607	CHL	C8-C10-C11-C12
30	8	605	CHL	C8-C10-C11-C12
30	n	306	CHL	C8-C10-C11-C12
31	B	603	CLA	C8-C10-C11-C12
31	C	613	CLA	C8-C10-C11-C12
31	C	613	CLA	C13-C15-C16-C17
31	b	610	CLA	C8-C10-C11-C12
33	L	101	LHG	C35-C36-C37-C38
33	D	407	LHG	C26-C27-C28-C29
38	m	101	SQD	C23-C24-C25-C26
33	2	617	LHG	C34-C35-C36-C37
31	7	305	CLA	C8-C10-C11-C12
31	s	305	CLA	C5-C6-C7-C8
31	2	603	CLA	C6-C7-C8-C9
31	s	311	CLA	C16-C17-C18-C20
33	D	407	LHG	C35-C36-C37-C38
33	M	101	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	t	102	LHG	C11-C10-C9-C8
33	B	624	LHG	O10-C23-O8-C6
33	j	102	LHG	O10-C23-O8-C6
38	R	322	SQD	C26-C27-C28-C29
33	1	617	LHG	C28-C29-C30-C31
30	1	601	CHL	C3A-C2A-CAA-CBA
30	4	607	CHL	C3A-C2A-CAA-CBA
30	6	310	CHL	C3A-C2A-CAA-CBA
30	N	306	CHL	C4-C3-C5-C6
30	0	608	CHL	C3A-C2A-CAA-CBA
30	q	309	CHL	C3A-C2A-CAA-CBA
30	q	311	CHL	C3A-C2A-CAA-CBA
30	r	310	CHL	C4-C3-C5-C6
31	2	610	CLA	C3A-C2A-CAA-CBA
31	3	301	CLA	C3A-C2A-CAA-CBA
31	3	313	CLA	C3A-C2A-CAA-CBA
31	B	608	CLA	C3A-C2A-CAA-CBA
31	7	316	CLA	C3A-C2A-CAA-CBA
31	p	613	CLA	C3A-C2A-CAA-CBA
31	b	609	CLA	C3A-C2A-CAA-CBA
31	c	603	CLA	C4-C3-C5-C6
31	c	606	CLA	C4-C3-C5-C6
31	c	610	CLA	C4-C3-C5-C6
31	r	316	CLA	C4-C3-C5-C6
31	y	611	CLA	C3A-C2A-CAA-CBA
31	s	313	CLA	C5-C6-C7-C8
31	3	313	CLA	CAA-CBA-CGA-O2A
31	7	311	CLA	C2-C3-C5-C6
31	c	610	CLA	C2-C3-C5-C6
31	r	316	CLA	C2-C3-C5-C6
34	a	413	LMG	O6-C1-O1-C7
34	B	622	LMG	C12-C13-C14-C15
30	4	607	CHL	O1A-CGA-O2A-C1
31	C	601	CLA	O1A-CGA-O2A-C1
31	7	314	CLA	O1A-CGA-O2A-C1
31	8	602	CLA	O1A-CGA-O2A-C1
33	F1	301	LHG	O10-C23-O8-C6
34	3	321	LMG	O10-C28-O8-C9
38	b	621	SQD	C35-C36-C37-C38
31	b	602	CLA	CBA-CGA-O2A-C1
43	H	101	BCR	C19-C20-C21-C22
43	T	101	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
43	a	410	BCR	C15-C16-C17-C18
43	b	619	BCR	C15-C16-C17-C18
43	b	619	BCR	C19-C20-C21-C22
43	b	620	BCR	C19-C20-C21-C22
43	c	614	BCR	C9-C10-C11-C12
43	c	614	BCR	C19-C20-C21-C22
43	h	101	BCR	C13-C14-C15-C16
31	5	613	CLA	C3-C5-C6-C7
31	G	603	CLA	C6-C7-C8-C10
31	G	604	CLA	C6-C7-C8-C9
30	7	302	CHL	C8-C10-C11-C12
32	3	318	LUT	C31-C32-C33-C40
32	s	318	LUT	C31-C32-C33-C40
43	V	101	BCR	C7-C8-C9-C34
43	a	410	BCR	C7-C8-C9-C34
43	z	101	BCR	C36-C18-C19-C20
34	w	204	LMG	C11-C12-C13-C14
31	4	604	CLA	C4-C3-C5-C6
31	B	611	CLA	O1A-CGA-O2A-C1
31	q	304	CLA	O1A-CGA-O2A-C1
31	y	611	CLA	O1A-CGA-O2A-C1
33	M	101	LHG	O10-C23-O8-C6
30	N	308	CHL	O1D-CGD-O2D-CED
30	n	302	CHL	O1D-CGD-O2D-CED
34	C	624	LMG	C15-C16-C17-C18
36	R	319	NEX	C31-C32-C33-C34
43	C	615	BCR	C21-C22-C23-C24
43	D	405	BCR	C21-C22-C23-C24
33	K	102	LHG	C26-C27-C28-C29
33	e	101	LHG	C23-C24-C25-C26
34	C	622	LMG	C28-C29-C30-C31
33	Y	318	LHG	C35-C36-C37-C38
30	4	607	CHL	C2A-CAA-CBA-CGA
30	8	607	CHL	C2A-CAA-CBA-CGA
30	n	309	CHL	C2A-CAA-CBA-CGA
31	b	608	CLA	C2A-CAA-CBA-CGA
31	s	303	CLA	C2A-CAA-CBA-CGA
31	3	315	CLA	C6-C7-C8-C9
30	8	601	CHL	O1D-CGD-O2D-CED
38	x	201	SQD	C24-C23-O48-C46
31	N	313	CLA	C15-C16-C17-C18
33	4	618	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
33	6	320	LHG	C4-C5-C6-O8
33	A	415	LHG	C4-C5-C6-O8
33	C	623	LHG	C4-C5-C6-O8
33	L	101	LHG	C4-C5-C6-O8
33	M	101	LHG	C4-C5-C6-O8
33	7	319	LHG	C4-C5-C6-O8
33	8	618	LHG	C4-C5-C6-O8
33	9	320	LHG	C4-C5-C6-O8
33	b	625	LHG	C4-C5-C6-O8
33	c	622	LHG	C4-C5-C6-O8
33	n	320	LHG	C4-C5-C6-O8
34	2	618	LMG	O1-C7-C8-C9
34	2	620	LMG	O1-C7-C8-C9
34	A	412	LMG	C7-C8-C9-O8
34	D	412	LMG	C7-C8-C9-O8
34	G	619	LMG	O1-C7-C8-C9
34	G	621	LMG	O1-C7-C8-C9
34	I	101	LMG	O1-C7-C8-C9
34	R	321	LMG	C7-C8-C9-O8
34	0	622	LMG	O1-C7-C8-C9
34	7	322	LMG	C7-C8-C9-O8
34	a	416	LMG	O1-C7-C8-C9
34	b	624	LMG	C7-C8-C9-O8
34	n	321	LMG	C7-C8-C9-O8
34	r	321	LMG	O1-C7-C8-C9
34	s	321	LMG	C7-C8-C9-O8
34	w	201	LMG	O1-C7-C8-C9
34	w	205	LMG	O1-C7-C8-C9
34	w	205	LMG	C7-C8-C9-O8
38	A	411	SQD	O6-C44-C45-C46
38	G	624	SQD	O6-C44-C45-C46
38	Y	320	SQD	C44-C45-C46-O48
38	a	412	SQD	C44-C45-C46-O48
38	x	201	SQD	O6-C44-C45-C46
44	a	414	PL9	C39-C41-C42-C43
33	0	619	LHG	C13-C14-C15-C16
30	5	609	CHL	C3-C5-C6-C7
31	B	606	CLA	C3-C5-C6-C7
33	G	618	LHG	C28-C29-C30-C31
34	0	620	LMG	C29-C30-C31-C32
33	S	322	LHG	C7-C8-C9-C10
30	6	310	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	9	305	CLA	C6-C7-C8-C10
31	q	305	CLA	C6-C7-C8-C10
31	1	611	CLA	C5-C6-C7-C8
31	1	612	CLA	C5-C6-C7-C8
31	B	606	CLA	C10-C11-C12-C13
31	s	303	CLA	C10-C11-C12-C13
33	j	102	LHG	C30-C31-C32-C33
38	b	621	SQD	C30-C31-C32-C33
31	Y	311	CLA	O1A-CGA-O2A-C1
31	8	614	CLA	C5-C6-C7-C8
33	B	624	LHG	C25-C26-C27-C28
33	q	320	LHG	C25-C26-C27-C28
33	b	628	LHG	C34-C35-C36-C37
34	9	301	LMG	C11-C12-C13-C14
30	1	607	CHL	C1A-C2A-CAA-CBA
30	3	303	CHL	C1A-C2A-CAA-CBA
30	4	601	CHL	C1A-C2A-CAA-CBA
30	4	608	CHL	C1A-C2A-CAA-CBA
30	4	609	CHL	C1A-C2A-CAA-CBA
30	6	302	CHL	C1A-C2A-CAA-CBA
30	G	601	CHL	C1A-C2A-CAA-CBA
30	0	606	CHL	C1A-C2A-CAA-CBA
30	7	308	CHL	C1A-C2A-CAA-CBA
30	9	310	CHL	C1A-C2A-CAA-CBA
30	q	303	CHL	C1A-C2A-CAA-CBA
30	g	302	CHL	C1A-C2A-CAA-CBA
31	c	605	CLA	CBD-CGD-O2D-CED
45	C	616	DGD	C5B-C6B-C7B-C8B
30	2	601	CHL	C4-C3-C5-C6
31	2	602	CLA	C4-C3-C5-C6
31	2	612	CLA	C4-C3-C5-C6
31	A	405	CLA	C4-C3-C5-C6
31	S	303	CLA	C4-C3-C5-C6
31	9	304	CLA	C4-C3-C5-C6
31	5	615	CLA	C2C-C3C-CAC-CBC
33	y	619	LHG	C34-C35-C36-C37
31	0	613	CLA	C2-C3-C5-C6
31	c	603	CLA	C2-C3-C5-C6
31	c	606	CLA	C2-C3-C5-C6
33	L	101	LHG	C34-C35-C36-C37
34	C	624	LMG	C11-C12-C13-C14
30	y	607	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
34	B	621	LMG	C37-C38-C39-C40
34	9	302	LMG	C31-C32-C33-C34
31	Y	312	CLA	C16-C17-C18-C20
31	c	601	CLA	C16-C17-C18-C19
31	2	609	CLA	C5-C6-C7-C8
33	1	617	LHG	O6-C4-C5-O7
33	C	623	LHG	O6-C4-C5-O7
33	D	408	LHG	O6-C4-C5-O7
33	M	101	LHG	O6-C4-C5-O7
33	R	320	LHG	O6-C4-C5-O7
33	8	618	LHG	O6-C4-C5-O7
33	q	320	LHG	O6-C4-C5-O7
33	n	320	LHG	O6-C4-C5-O7
33	s	320	LHG	O6-C4-C5-O7
33	b	628	LHG	C25-C26-C27-C28
38	S	301	SQD	C27-C28-C29-C30
31	n	312	CLA	O1D-CGD-O2D-CED
31	b	602	CLA	C2B-C3B-CAB-CBB
35	4	615	RRX	C1-C6-C7-C8
35	G	614	RRX	C1-C6-C7-C8
35	9	317	RRX	C1-C6-C7-C8
43	B	618	BCR	C1-C6-C7-C8
43	C	614	BCR	C23-C24-C25-C26
43	D	405	BCR	C23-C24-C25-C30
43	T	101	BCR	C23-C24-C25-C26
34	4	620	LMG	C32-C33-C34-C35
34	4	620	LMG	C34-C35-C36-C37
34	G	621	LMG	C34-C35-C36-C37
31	2	613	CLA	CAA-CBA-CGA-O2A
33	3	320	LHG	C2-C3-O3-P
33	7	319	LHG	C5-C4-O6-P
33	b	628	LHG	C2-C3-O3-P
33	z	102	LHG	C2-C3-O3-P
33	F1	301	LHG	C2-C3-O3-P
45	c	617	DGD	CFB-CGB-CHB-CIB
30	3	302	CHL	C11-C10-C8-C9
33	R	320	LHG	C7-C8-C9-C10
45	c	616	DGD	C1B-C2B-C3B-C4B
33	S	322	LHG	C24-C25-C26-C27
33	0	619	LHG	C26-C27-C28-C29
38	A	413	SQD	C10-C11-C12-C13
31	4	610	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	b	616	CLA	C10-C11-C12-C13
33	s	322	LHG	C35-C36-C37-C38
33	D	407	LHG	C25-C26-C27-C28
33	G	618	LHG	C9-C10-C11-C12
34	C	624	LMG	C18-C19-C20-C21
31	6	312	CLA	C11-C12-C13-C15
31	p	603	CLA	C6-C7-C8-C9
33	R	320	LHG	O8-C23-C24-C25
34	5	620	LMG	O7-C10-C11-C12
30	2	606	CHL	C2A-CAA-CBA-CGA
31	8	610	CLA	O1D-CGD-O2D-CED
34	d	409	LMG	C10-C11-C12-C13
31	3	312	CLA	C15-C16-C17-C18
33	2	617	LHG	O7-C5-C6-O8
33	5	619	LHG	O7-C5-C6-O8
33	C	623	LHG	O7-C5-C6-O8
33	N	319	LHG	O7-C5-C6-O8
33	q	320	LHG	O7-C5-C6-O8
33	c	622	LHG	O7-C5-C6-O8
33	y	619	LHG	O7-C5-C6-O8
34	A	412	LMG	O7-C8-C9-O8
34	A	414	LMG	O1-C7-C8-O7
34	B	625	LMG	O7-C8-C9-O8
34	C	621	LMG	O7-C8-C9-O8
34	X	203	LMG	O1-C7-C8-O7
34	0	622	LMG	O1-C7-C8-O7
34	7	322	LMG	O1-C7-C8-O7
34	b	624	LMG	O7-C8-C9-O8
38	B	620	SQD	O6-C44-C45-O47
38	R	322	SQD	O6-C44-C45-O47
38	y	621	SQD	O47-C45-C46-O48
33	y	619	LHG	C26-C27-C28-C29
44	D	406	PL9	C4-C3-C7-C8
33	3	320	LHG	C9-C10-C11-C12
33	6	320	LHG	C28-C29-C30-C31
33	D	408	LHG	C34-C35-C36-C37
31	p	610	CLA	C3-C5-C6-C7
33	q	320	LHG	C29-C30-C31-C32
34	x	202	LMG	C11-C12-C13-C14
45	C	616	DGD	C4A-C5A-C6A-C7A
31	y	612	CLA	C5-C6-C7-C8
33	l	101	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
33	b	625	LHG	O9-C7-O7-C5
33	s	320	LHG	O9-C7-O7-C5
33	g	319	LHG	C35-C36-C37-C38
30	7	307	CHL	C8-C10-C11-C12
31	2	602	CLA	C2-C3-C5-C6
31	A	405	CLA	C2-C3-C5-C6
31	2	613	CLA	C6-C7-C8-C9
33	Y	318	LHG	C31-C32-C33-C34
30	9	311	CHL	C11-C12-C13-C14
31	3	306	CLA	C6-C7-C8-C9
31	Y	305	CLA	C6-C7-C8-C10
33	g	319	LHG	C33-C34-C35-C36
33	G	618	LHG	C7-C8-C9-C10
34	B	622	LMG	C28-C29-C30-C31
34	n	322	LMG	C10-C11-C12-C13
38	M	102	SQD	C23-C24-C25-C26
31	B	615	CLA	C3-C5-C6-C7
31	r	311	CLA	C3-C5-C6-C7
31	1	614	CLA	C6-C7-C8-C9
30	2	608	CHL	C6-C7-C8-C9
30	G	623	CHL	C11-C12-C13-C14
30	Y	307	CHL	C11-C10-C8-C9
30	Y	309	CHL	C11-C12-C13-C14
30	7	306	CHL	C11-C12-C13-C14
30	8	605	CHL	C11-C12-C13-C14
30	n	306	CHL	C11-C12-C13-C14
30	y	601	CHL	C11-C12-C13-C14
30	y	607	CHL	C11-C12-C13-C14
31	4	610	CLA	C11-C10-C8-C9
31	b	613	CLA	C11-C12-C13-C14
31	c	605	CLA	C6-C7-C8-C9
31	g	313	CLA	C11-C10-C8-C9
42	a	408	PHO	C11-C10-C8-C9
33	e	101	LHG	C11-C10-C9-C8
33	e	101	LHG	C31-C32-C33-C34
45	C	620	DGD	C5A-C6A-C7A-C8A
31	y	614	CLA	C6-C7-C8-C9
33	K	102	LHG	C11-C10-C9-C8
34	4	620	LMG	C18-C19-C20-C21
34	A	418	LMG	C12-C13-C14-C15
45	c	618	DGD	O6D-C1D-O3G-C3G
33	3	320	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
30	p	609	CHL	O1D-CGD-O2D-CED
45	C	618	DGD	CAB-CBB-CCB-CDB
30	9	311	CHL	C11-C12-C13-C15
31	C	603	CLA	C16-C17-C18-C19
31	S	310	CLA	C11-C12-C13-C15
34	6	321	LMG	C2-C1-O1-C7
34	b	622	LMG	C2-C1-O1-C7
34	c	620	LMG	C2-C1-O1-C7
30	9	309	CHL	O1A-CGA-O2A-C1
33	R	320	LHG	C25-C26-C27-C28
38	y	621	SQD	C13-C14-C15-C16
45	c	618	DGD	C6B-C7B-C8B-C9B
33	7	319	LHG	C28-C29-C30-C31
44	A	416	PL9	C9-C11-C12-C13
33	N	319	LHG	C29-C30-C31-C32
38	B	623	SQD	C19-C20-C21-C22
30	4	606	CHL	C2A-CAA-CBA-CGA
30	6	309	CHL	C2A-CAA-CBA-CGA
30	N	308	CHL	C2A-CAA-CBA-CGA
30	0	605	CHL	C2A-CAA-CBA-CGA
30	0	608	CHL	C2A-CAA-CBA-CGA
33	G	618	LHG	C34-C35-C36-C37
33	a	415	LHG	C9-C10-C11-C12
33	2	617	LHG	C35-C36-C37-C38
33	g	319	LHG	C7-C8-C9-C10
33	b	628	LHG	C19-C20-C21-C22
30	4	601	CHL	CBA-CGA-O2A-C1
31	Y	312	CLA	CBA-CGA-O2A-C1
31	b	605	CLA	CBA-CGA-O2A-C1
33	A	415	LHG	C24-C23-O8-C6
38	B	623	SQD	C24-C23-O48-C46
33	Y	318	LHG	C29-C30-C31-C32
31	6	304	CLA	CAA-CBA-CGA-O2A
34	W	202	LMG	O7-C10-C11-C12
45	c	619	DGD	O1G-C1A-C2A-C3A
30	7	302	CHL	C2-C3-C5-C6
31	3	305	CLA	C6-C7-C8-C9
31	q	306	CLA	C6-C7-C8-C9
31	c	603	CLA	C16-C17-C18-C19
30	1	609	CHL	C8-C10-C11-C12
31	s	312	CLA	C5-C6-C7-C8
33	N	319	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
31	c	601	CLA	C5-C6-C7-C8
30	n	310	CHL	O1D-CGD-O2D-CED
33	B	624	LHG	C9-C10-C11-C12
33	a	415	LHG	C24-C25-C26-C27
38	B	623	SQD	C26-C27-C28-C29
38	R	322	SQD	C9-C10-C11-C12
36	6	319	NEX	C40-C33-C34-C35
36	0	618	NEX	C40-C33-C34-C35
31	C	603	CLA	O1A-CGA-O2A-C1
31	n	303	CLA	O1A-CGA-O2A-C1
31	g	311	CLA	C3-C5-C6-C7
31	B	604	CLA	CBA-CGA-O2A-C1
31	r	305	CLA	CBA-CGA-O2A-C1
33	S	322	LHG	O6-C4-C5-C6
33	q	320	LHG	O6-C4-C5-C6
33	c	622	LHG	O6-C4-C5-C6
30	3	310	CHL	C11-C12-C13-C15
31	b	603	CLA	C16-C17-C18-C19
31	r	305	CLA	C11-C12-C13-C14
33	y	619	LHG	C16-C17-C18-C19
31	7	304	CLA	C5-C6-C7-C8
31	s	303	CLA	C13-C15-C16-C17
42	A	408	PHO	C15-C16-C17-C18
32	6	317	LUT	C27-C28-C29-C39
32	p	617	LUT	C31-C32-C33-C40
32	g	316	LUT	C7-C8-C9-C19
43	b	620	BCR	C7-C8-C9-C34
33	b	625	LHG	C11-C10-C9-C8
30	1	609	CHL	C11-C12-C13-C15
30	G	608	CHL	C11-C12-C13-C15
30	G	608	CHL	C12-C13-C15-C16
30	0	607	CHL	C12-C13-C15-C16
30	8	608	CHL	C12-C13-C15-C16
30	9	303	CHL	C11-C10-C8-C7
30	g	309	CHL	C11-C10-C8-C7
31	4	602	CLA	C11-C10-C8-C7
31	4	610	CLA	C11-C10-C8-C7
31	5	610	CLA	C6-C7-C8-C10
31	6	303	CLA	C6-C7-C8-C10
31	A	409	CLA	C6-C7-C8-C10
31	B	611	CLA	C6-C7-C8-C10
31	B	614	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
31	B	616	CLA	C11-C10-C8-C7
31	C	611	CLA	C11-C12-C13-C15
31	D	403	CLA	C11-C10-C8-C7
31	G	612	CLA	C11-C12-C13-C15
31	N	305	CLA	C6-C7-C8-C10
31	S	305	CLA	C6-C7-C8-C10
31	S	311	CLA	C11-C10-C8-C7
31	S	313	CLA	C6-C7-C8-C10
31	Y	312	CLA	C12-C13-C15-C16
31	7	305	CLA	C11-C10-C8-C7
31	8	602	CLA	C11-C10-C8-C7
31	8	604	CLA	C12-C13-C15-C16
31	a	409	CLA	C6-C7-C8-C10
31	b	610	CLA	C6-C7-C8-C10
31	b	612	CLA	C6-C7-C8-C10
31	b	616	CLA	C6-C7-C8-C10
31	c	605	CLA	C6-C7-C8-C10
31	c	608	CLA	C6-C7-C8-C10
31	g	313	CLA	C6-C7-C8-C10
31	g	313	CLA	C11-C10-C8-C7
31	n	303	CLA	C11-C10-C8-C7
31	r	311	CLA	C11-C10-C8-C7
31	s	305	CLA	C11-C12-C13-C15
31	s	311	CLA	C11-C10-C8-C7
31	s	312	CLA	C12-C13-C15-C16
31	s	313	CLA	C6-C7-C8-C10
31	y	613	CLA	C12-C13-C15-C16
33	8	618	LHG	C27-C28-C29-C30
34	J	102	LMG	C33-C34-C35-C36
38	B	623	SQD	C16-C17-C18-C19
33	G	618	LHG	C26-C27-C28-C29
33	G	618	LHG	C29-C30-C31-C32
33	n	320	LHG	C27-C28-C29-C30
33	z	102	LHG	C26-C27-C28-C29
32	6	318	LUT	C11-C12-C13-C14
32	N	316	LUT	C31-C32-C33-C34
32	p	616	LUT	C11-C12-C13-C14
32	p	617	LUT	C31-C32-C33-C34
32	g	316	LUT	C7-C8-C9-C10
36	p	618	NEX	C11-C12-C13-C14
43	A	410	BCR	C7-C8-C9-C10
43	T	101	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
43	b	620	BCR	C7-C8-C9-C10
43	z	101	BCR	C17-C18-C19-C20
31	b	616	CLA	CBA-CGA-O2A-C1
33	C	623	LHG	C28-C29-C30-C31
34	a	416	LMG	C12-C13-C14-C15
38	B	620	SQD	C18-C19-C20-C21
45	C	617	DGD	C6B-C7B-C8B-C9B
30	3	302	CHL	O1A-CGA-O2A-C1
31	C	604	CLA	O1A-CGA-O2A-C1
31	7	312	CLA	O1A-CGA-O2A-C1
31	b	608	CLA	O1A-CGA-O2A-C1
31	r	305	CLA	O1A-CGA-O2A-C1
33	C	623	LHG	O10-C23-O8-C6
34	k	102	LMG	O10-C28-O8-C9
34	2	618	LMG	C8-C7-O1-C1
34	2	621	LMG	C8-C7-O1-C1
34	5	620	LMG	C8-C7-O1-C1
34	6	323	LMG	C8-C7-O1-C1
34	D	411	LMG	C8-C7-O1-C1
34	G	622	LMG	C8-C7-O1-C1
34	N	320	LMG	C8-C7-O1-C1
34	R	321	LMG	C8-C7-O1-C1
34	X	203	LMG	C8-C7-O1-C1
34	7	322	LMG	C8-C7-O1-C1
34	9	321	LMG	C8-C7-O1-C1
34	q	302	LMG	C8-C7-O1-C1
34	d	410	LMG	C8-C7-O1-C1
34	g	320	LMG	C8-C7-O1-C1
34	g	322	LMG	C8-C7-O1-C1
34	j	101	LMG	C8-C7-O1-C1
34	w	205	LMG	C8-C7-O1-C1
34	y	620	LMG	C8-C7-O1-C1
38	6	301	SQD	C45-C44-O6-C1
38	A	411	SQD	C45-C44-O6-C1
38	A	411	SQD	C5-C6-S-O8
38	G	617	SQD	C45-C44-O6-C1
38	s	301	SQD	C5-C6-S-O8
38	x	201	SQD	C45-C44-O6-C1
45	C	617	DGD	C5D-C6D-O5D-C1E
45	c	617	DGD	C5D-C6D-O5D-C1E
38	B	623	SQD	C23-C24-C25-C26
30	8	605	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	n	306	CHL	C13-C15-C16-C17
31	b	605	CLA	C15-C16-C17-C18
31	r	304	CLA	C8-C10-C11-C12
30	1	606	CHL	C2A-CAA-CBA-CGA
30	6	306	CHL	C2A-CAA-CBA-CGA
30	G	607	CHL	C2A-CAA-CBA-CGA
30	g	308	CHL	C2A-CAA-CBA-CGA
31	1	602	CLA	C2A-CAA-CBA-CGA
31	C	612	CLA	C2A-CAA-CBA-CGA
31	G	602	CLA	C2A-CAA-CBA-CGA
31	6	316	CLA	C6-C7-C8-C10
31	b	605	CLA	CBD-CGD-O2D-CED
34	j	101	LMG	C11-C10-O7-C8
38	R	322	SQD	C31-C32-C33-C34
30	3	309	CHL	O1A-CGA-O2A-C1
31	6	303	CLA	O1A-CGA-O2A-C1
31	Y	312	CLA	O1A-CGA-O2A-C1
31	c	606	CLA	O1A-CGA-O2A-C1
30	r	310	CHL	C2-C3-C5-C6
31	2	612	CLA	C2-C3-C5-C6
31	S	303	CLA	C2-C3-C5-C6
47	E	101	HEM	C2B-C3B-CAB-CBB
47	e	102	HEM	C2B-C3B-CAB-CBB
31	1	602	CLA	C5-C6-C7-C8
31	4	603	CLA	C5-C6-C7-C8
31	B	609	CLA	C15-C16-C17-C18
31	S	305	CLA	C5-C6-C7-C8
33	a	415	LHG	C26-C27-C28-C29
34	w	201	LMG	C33-C34-C35-C36
34	y	620	LMG	C10-C11-C12-C13
31	3	305	CLA	C3-C5-C6-C7
33	l	101	LHG	C26-C27-C28-C29
34	c	624	LMG	C32-C33-C34-C35
30	r	309	CHL	O1D-CGD-O2D-CED
31	3	306	CLA	C5-C6-C7-C8
33	7	319	LHG	C4-C5-O7-C7
34	1	618	LMG	C9-C8-O7-C10
34	I	101	LMG	C7-C8-O7-C10
34	f	101	LMG	C9-C8-O7-C10
45	c	616	DGD	C1G-C2G-O2G-C1B
31	6	305	CLA	O1A-CGA-O2A-C1
34	a	413	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
36	3	319	NEX	C14-C15-C35-C34
33	D	407	LHG	C33-C34-C35-C36
31	G	604	CLA	C6-C7-C8-C10
33	3	320	LHG	C28-C29-C30-C31
30	9	310	CHL	O1D-CGD-O2D-CED
31	6	304	CLA	C5-C6-C7-C8
30	N	309	CHL	CBA-CGA-O2A-C1
33	s	322	LHG	C9-C10-C11-C12
34	w	202	LMG	C39-C40-C41-C42
36	2	616	NEX	C11-C10-C9-C8
36	3	319	NEX	C28-C29-C30-C31
36	N	318	NEX	C11-C10-C9-C8
36	g	317	NEX	C32-C33-C34-C35
37	4	619	XAT	C12-C13-C14-C15
37	G	620	XAT	C12-C13-C14-C15
37	9	322	XAT	C12-C13-C14-C15
37	q	321	XAT	C12-C13-C14-C15
37	g	321	XAT	C12-C13-C14-C15
30	Y	301	CHL	C5-C6-C7-C8
31	3	304	CLA	C8-C10-C11-C12
31	G	609	CLA	C5-C6-C7-C8
31	0	611	CLA	C10-C11-C12-C13
33	6	320	LHG	O6-C4-C5-O7
33	D	407	LHG	O6-C4-C5-O7
33	L	101	LHG	O6-C4-C5-O7
33	S	320	LHG	O6-C4-C5-O7
33	b	628	LHG	O6-C4-C5-O7
33	c	622	LHG	O6-C4-C5-O7
33	j	102	LHG	O6-C4-C5-O7
33	l	101	LHG	O6-C4-C5-O7
45	c	616	DGD	CAB-CBB-CCB-CDB
30	y	606	CHL	O1D-CGD-O2D-CED
31	c	605	CLA	O1D-CGD-O2D-CED
38	a	411	SQD	C31-C32-C33-C34
33	2	617	LHG	C4-C5-C6-O8
33	3	320	LHG	C4-C5-C6-O8
33	S	322	LHG	C4-C5-C6-O8
33	s	320	LHG	C4-C5-C6-O8
33	s	322	LHG	C4-C5-C6-O8
33	y	619	LHG	C4-C5-C6-O8
33	F1	301	LHG	C4-C5-C6-O8
34	J	101	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
34	X	203	LMG	O1-C7-C8-C9
34	Y	319	LMG	O1-C7-C8-C9
34	0	620	LMG	O1-C7-C8-C9
34	c	621	LMG	O1-C7-C8-C9
34	f	101	LMG	C7-C8-C9-O8
34	n	322	LMG	O1-C7-C8-C9
38	6	301	SQD	C44-C45-C46-O48
38	S	301	SQD	O6-C44-C45-C46
38	Y	320	SQD	O6-C44-C45-C46
38	a	412	SQD	O6-C44-C45-C46
38	b	621	SQD	C44-C45-C46-O48
38	y	621	SQD	O6-C44-C45-C46
47	E	101	HEM	C4C-C3C-CAC-CBC
47	e	102	HEM	C4C-C3C-CAC-CBC
33	2	617	LHG	C30-C31-C32-C33
33	5	619	LHG	C26-C27-C28-C29
33	0	619	LHG	C27-C28-C29-C30
33	6	320	LHG	C26-C27-C28-C29
33	d	408	LHG	C9-C10-C11-C12
31	G	612	CLA	C4-C3-C5-C6
31	7	315	CLA	C4-C3-C5-C6
30	1	605	CHL	C2A-CAA-CBA-CGA
30	2	607	CHL	C2A-CAA-CBA-CGA
31	R	307	CLA	C2A-CAA-CBA-CGA
31	S	314	CLA	C2A-CAA-CBA-CGA
31	p	611	CLA	C2A-CAA-CBA-CGA
33	B	624	LHG	O7-C7-C8-C9
30	0	601	CHL	C2-C3-C5-C6
30	9	311	CHL	C2-C3-C5-C6
30	r	309	CHL	C2-C3-C5-C6
44	a	414	PL9	C13-C14-C16-C17
33	C	623	LHG	C31-C32-C33-C34
34	B	625	LMG	C31-C32-C33-C34
34	b	622	LMG	C34-C35-C36-C37
36	r	319	NEX	C7-C8-C9-C19
36	s	319	NEX	C7-C8-C9-C19
31	N	310	CLA	C15-C16-C17-C18
31	b	610	CLA	C15-C16-C17-C18
31	b	616	CLA	O1A-CGA-O2A-C1
31	3	306	CLA	C2C-C3C-CAC-CBC
33	D	408	LHG	O7-C5-C6-O8
33	Y	318	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
34	4	621	LMG	O1-C7-C8-O7
34	c	621	LMG	O1-C7-C8-O7
34	r	321	LMG	O1-C7-C8-O7
34	s	321	LMG	O7-C8-C9-O8
34	w	205	LMG	O7-C8-C9-O8
38	6	301	SQD	O6-C44-C45-O47
38	A	413	SQD	O6-C44-C45-O47
38	G	624	SQD	O6-C44-C45-O47
38	M	102	SQD	O47-C45-C46-O48
38	Y	320	SQD	O47-C45-C46-O48
38	g	318	SQD	O6-C44-C45-O47
38	s	301	SQD	O6-C44-C45-O47
38	x	201	SQD	O6-C44-C45-O47
45	C	620	DGD	O1G-C1G-C2G-O2G
45	c	618	DGD	O2G-C2G-C3G-O3G
30	1	601	CHL	C11-C12-C13-C14
30	Y	301	CHL	C11-C12-C13-C14
31	4	602	CLA	C11-C10-C8-C9
31	6	312	CLA	C6-C7-C8-C9
31	G	602	CLA	C6-C7-C8-C9
31	N	310	CLA	C11-C12-C13-C14
31	S	303	CLA	C6-C7-C8-C9
31	7	305	CLA	C6-C7-C8-C9
31	7	305	CLA	C11-C10-C8-C9
31	b	606	CLA	C6-C7-C8-C9
31	b	616	CLA	C6-C7-C8-C9
31	c	601	CLA	C6-C7-C8-C9
31	c	601	CLA	C11-C12-C13-C14
31	c	603	CLA	C14-C13-C15-C16
31	n	303	CLA	C11-C10-C8-C9
31	s	305	CLA	C6-C7-C8-C9
31	s	311	CLA	C11-C10-C8-C9
31	s	312	CLA	C14-C13-C15-C16
31	y	610	CLA	C6-C7-C8-C9
42	D	401	PHO	C6-C7-C8-C9
34	W	202	LMG	O6-C5-C6-O5
31	D	404	CLA	CBA-CGA-O2A-C1
34	j	101	LMG	O9-C10-O7-C8
48	R	302	LMU	C5-C6-C7-C8
30	4	601	CHL	O1A-CGA-O2A-C1
38	x	201	SQD	O10-C23-O48-C46
31	9	312	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	b	625	LHG	C30-C31-C32-C33
34	b	623	LMG	C31-C32-C33-C34
30	0	609	CHL	C8-C10-C11-C12
31	C	605	CLA	C10-C11-C12-C13
31	C	612	CLA	C5-C6-C7-C8
33	g	319	LHG	C9-C10-C11-C12
38	b	627	SQD	C12-C13-C14-C15
45	C	617	DGD	C2B-C3B-C4B-C5B
31	B	607	CLA	C8-C10-C11-C12
31	b	602	CLA	O1A-CGA-O2A-C1
31	C	604	CLA	C2-C1-O2A-CGA
31	N	311	CLA	C2-C1-O2A-CGA
43	v	101	BCR	C15-C16-C17-C18
31	y	615	CLA	CBA-CGA-O2A-C1
31	A	409	CLA	C11-C12-C13-C15
31	a	409	CLA	C11-C12-C13-C15
33	9	320	LHG	C5-C4-O6-P
33	S	322	LHG	C30-C31-C32-C33
34	I	101	LMG	C31-C32-C33-C34
34	2	618	LMG	C8-C9-O8-C28
33	q	320	LHG	C31-C32-C33-C34
34	j	101	LMG	C11-C12-C13-C14
31	B	614	CLA	C4-C3-C5-C6
31	A	406	CLA	C3-C5-C6-C7
34	b	622	LMG	C16-C17-C18-C19
30	7	308	CHL	C5-C6-C7-C8
30	q	303	CHL	C5-C6-C7-C8
31	1	613	CLA	C13-C15-C16-C17
31	5	602	CLA	C8-C10-C11-C12
31	b	611	CLA	C8-C10-C11-C12
38	B	623	SQD	O10-C23-O48-C46
31	3	301	CLA	CBA-CGA-O2A-C1
33	0	619	LHG	C24-C23-O8-C6
38	S	301	SQD	C24-C23-O48-C46
33	A	417	LHG	C11-C10-C9-C8
31	2	602	CLA	C16-C17-C18-C19
31	B	611	CLA	C16-C17-C18-C19
31	y	613	CLA	C5-C6-C7-C8
30	7	321	CHL	O1A-CGA-O2A-C1
30	n	308	CHL	O1A-CGA-O2A-C1
31	B	604	CLA	O1A-CGA-O2A-C1
34	x	202	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
33	3	320	LHG	C11-C10-C9-C8
33	M	101	LHG	C29-C30-C31-C32
33	c	622	LHG	C35-C36-C37-C38
31	B	609	CLA	C13-C15-C16-C17
31	s	314	CLA	C3-C5-C6-C7
30	3	302	CHL	C4C-C3C-CAC-CBC
30	8	608	CHL	C4C-C3C-CAC-CBC
30	q	311	CHL	C4C-C3C-CAC-CBC
30	g	309	CHL	C4C-C3C-CAC-CBC
30	n	310	CHL	C4C-C3C-CAC-CBC
38	6	301	SQD	C4-C5-C6-S
38	A	413	SQD	C4-C5-C6-S
38	B	623	SQD	C4-C5-C6-S
38	R	322	SQD	C4-C5-C6-S
38	0	621	SQD	C4-C5-C6-S
38	b	627	SQD	C4-C5-C6-S
38	r	322	SQD	C4-C5-C6-S
34	b	622	LMG	C18-C19-C20-C21
48	K	101	LMU	C2-C3-C4-C5
31	b	605	CLA	O1A-CGA-O2A-C1
31	y	615	CLA	O1A-CGA-O2A-C1
30	y	609	CHL	C10-C11-C12-C13
31	g	313	CLA	C15-C16-C17-C18
38	M	102	SQD	C25-C26-C27-C28
33	6	320	LHG	C29-C30-C31-C32
33	A	415	LHG	C27-C28-C29-C30
31	3	306	CLA	C6-C7-C8-C10
31	6	312	CLA	C11-C12-C13-C14
34	W	203	LMG	C10-C11-C12-C13
33	y	619	LHG	O1-C1-C2-O2
34	1	618	LMG	C11-C12-C13-C14
33	j	102	LHG	C9-C10-C11-C12
34	a	401	LMG	C11-C12-C13-C14
33	A	415	LHG	C34-C35-C36-C37
31	1	603	CLA	C4B-C3B-CAB-CBB
31	1	611	CLA	C1A-C2A-CAA-CBA
31	3	313	CLA	C1A-C2A-CAA-CBA
31	5	610	CLA	C1A-C2A-CAA-CBA
31	6	312	CLA	C4B-C3B-CAB-CBB
31	B	608	CLA	C1A-C2A-CAA-CBA
31	G	613	CLA	C4B-C3B-CAB-CBB
31	N	303	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	R	307	CLA	C4B-C3B-CAB-CBB
31	R	313	CLA	C4B-C3B-CAB-CBB
31	Y	305	CLA	C1A-C2A-CAA-CBA
31	0	602	CLA	C1A-C2A-CAA-CBA
31	0	611	CLA	C4B-C3B-CAB-CBB
31	9	313	CLA	C4B-C3B-CAB-CBB
31	q	306	CLA	C1A-C2A-CAA-CBA
31	c	601	CLA	C4B-C3B-CAB-CBB
31	c	612	CLA	C1A-C2A-CAA-CBA
31	g	311	CLA	C4B-C3B-CAB-CBB
31	r	307	CLA	C4B-C3B-CAB-CBB
30	Y	309	CHL	CBA-CGA-O2A-C1
31	y	614	CLA	C5-C6-C7-C8
38	R	322	SQD	C32-C33-C34-C35
45	C	618	DGD	C1B-C2B-C3B-C4B
31	4	614	CLA	C4-C3-C5-C6
31	C	613	CLA	C4-C3-C5-C6
31	y	613	CLA	C4-C3-C5-C6
44	D	406	PL9	C15-C14-C16-C17
31	c	606	CLA	C5-C6-C7-C8
30	p	601	CHL	CAA-CBA-CGA-O2A
31	N	314	CLA	CAA-CBA-CGA-O2A
45	c	617	DGD	O1G-C1A-C2A-C3A
32	7	318	LUT	C11-C12-C13-C14
32	s	318	LUT	C31-C32-C33-C34
43	a	410	BCR	C7-C8-C9-C10
36	p	618	NEX	C13-C14-C15-C35
33	S	322	LHG	C11-C10-C9-C8
33	7	319	LHG	C26-C27-C28-C29
33	t	102	LHG	C34-C35-C36-C37
33	5	619	LHG	C28-C29-C30-C31
31	p	611	CLA	C5-C6-C7-C8
31	N	311	CLA	O1A-CGA-O2A-C1
30	y	608	CHL	C2A-CAA-CBA-CGA
31	c	606	CLA	C2A-CAA-CBA-CGA
31	y	611	CLA	C2A-CAA-CBA-CGA
34	2	620	LMG	C37-C38-C39-C40
34	W	201	LMG	C12-C13-C14-C15
31	3	306	CLA	O1D-CGD-O2D-CED
33	4	618	LHG	O6-C4-C5-C6
33	5	619	LHG	O6-C4-C5-C6
33	C	623	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
33	D	407	LHG	O6-C4-C5-C6
33	L	101	LHG	O6-C4-C5-C6
33	M	101	LHG	O6-C4-C5-C6
33	b	628	LHG	O6-C4-C5-C6
33	e	101	LHG	O6-C4-C5-C6
33	g	319	LHG	O6-C4-C5-C6
33	l	101	LHG	O6-C4-C5-C6
33	t	102	LHG	O6-C4-C5-C6
38	B	620	SQD	C10-C11-C12-C13
38	x	201	SQD	C10-C11-C12-C13
33	b	628	LHG	C12-C13-C14-C15
33	s	322	LHG	C10-C11-C12-C13
30	0	605	CHL	C2-C3-C5-C6
38	A	411	SQD	C5-C6-S-O7
33	A	417	LHG	C24-C25-C26-C27
33	y	619	LHG	C14-C15-C16-C17
38	a	412	SQD	C11-C12-C13-C14
42	d	402	PHO	O1D-CGD-O2D-CED
30	1	601	CHL	C6-C7-C8-C10
30	1	601	CHL	C12-C13-C15-C16
30	1	619	CHL	C11-C10-C8-C7
30	3	310	CHL	C11-C10-C8-C7
30	4	601	CHL	C6-C7-C8-C10
30	6	308	CHL	C11-C10-C8-C7
30	6	308	CHL	C12-C13-C15-C16
30	G	601	CHL	C12-C13-C15-C16
30	G	623	CHL	C11-C10-C8-C7
30	N	307	CHL	C11-C10-C8-C7
30	N	309	CHL	C11-C10-C8-C7
30	Y	309	CHL	C11-C10-C8-C7
30	0	607	CHL	C11-C10-C8-C7
30	7	307	CHL	C11-C10-C8-C7
30	7	310	CHL	C12-C13-C15-C16
30	7	321	CHL	C12-C13-C15-C16
30	9	303	CHL	C12-C13-C15-C16
30	g	302	CHL	C12-C13-C15-C16
30	g	309	CHL	C12-C13-C15-C16
30	n	308	CHL	C12-C13-C15-C16
30	n	310	CHL	C12-C13-C15-C16
30	y	601	CHL	C11-C10-C8-C7
30	y	607	CHL	C12-C13-C15-C16
31	1	604	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	2	609	CLA	C11-C10-C8-C7
31	2	610	CLA	C6-C7-C8-C10
31	5	602	CLA	C6-C7-C8-C10
31	5	602	CLA	C11-C10-C8-C7
31	5	610	CLA	C11-C10-C8-C7
31	6	311	CLA	C11-C12-C13-C15
31	6	313	CLA	C11-C10-C8-C7
31	A	409	CLA	C11-C10-C8-C7
31	B	606	CLA	C6-C7-C8-C10
31	B	614	CLA	C11-C12-C13-C15
31	B	615	CLA	C11-C12-C13-C15
31	C	602	CLA	C11-C12-C13-C15
31	C	606	CLA	C6-C7-C8-C10
31	G	602	CLA	C11-C12-C13-C15
31	G	609	CLA	C11-C12-C13-C15
31	N	313	CLA	C11-C10-C8-C7
31	S	303	CLA	C11-C10-C8-C7
31	S	312	CLA	C11-C10-C8-C7
31	Y	310	CLA	C11-C12-C13-C15
31	7	313	CLA	C11-C10-C8-C7
31	p	610	CLA	C6-C7-C8-C10
31	q	304	CLA	C11-C10-C8-C7
31	a	409	CLA	C11-C10-C8-C7
31	b	615	CLA	C11-C12-C13-C15
31	c	607	CLA	C11-C10-C8-C7
31	c	611	CLA	C12-C13-C15-C16
31	d	404	CLA	C6-C7-C8-C10
31	d	404	CLA	C11-C10-C8-C7
31	s	303	CLA	C11-C10-C8-C7
31	s	312	CLA	C6-C7-C8-C10
42	A	408	PHO	C6-C7-C8-C10
31	2	612	CLA	C16-C17-C18-C19
31	S	310	CLA	C11-C12-C13-C14
31	S	311	CLA	C16-C17-C18-C19
31	7	303	CLA	C11-C12-C13-C15
33	A	415	LHG	O10-C23-O8-C6
31	N	311	CLA	CBA-CGA-O2A-C1
33	D	407	LHG	C11-C10-C9-C8
34	d	409	LMG	C32-C33-C34-C35
33	j	102	LHG	C18-C19-C20-C21
30	N	309	CHL	O1A-CGA-O2A-C1
33	0	619	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
30	2	608	CHL	C5-C6-C7-C8
34	b	629	LMG	C10-C11-C12-C13
33	C	623	LHG	C2-C3-O3-P
33	N	319	LHG	C5-C4-O6-P
33	S	322	LHG	C2-C3-O3-P
33	c	622	LHG	C2-C3-O3-P
33	F1	301	LHG	C5-C4-O6-P
31	1	613	CLA	C4-C3-C5-C6
31	B	602	CLA	C3A-C2A-CAA-CBA
31	p	615	CLA	C3A-C2A-CAA-CBA
31	S	311	CLA	C16-C17-C18-C20
33	3	320	LHG	C10-C11-C12-C13
48	c	623	LMU	C2-C3-C4-C5
34	5	620	LMG	C31-C32-C33-C34
38	A	411	SQD	C9-C10-C11-C12
45	c	616	DGD	C4B-C5B-C6B-C7B
38	b	621	SQD	C9-C10-C11-C12
33	2	617	LHG	O6-C4-C5-O7
33	4	618	LHG	O6-C4-C5-O7
33	A	415	LHG	O6-C4-C5-O7
33	B	624	LHG	O6-C4-C5-O7
33	G	618	LHG	O6-C4-C5-O7
33	K	102	LHG	O6-C4-C5-O7
33	N	319	LHG	O6-C4-C5-O7
33	S	322	LHG	O6-C4-C5-O7
33	7	319	LHG	O6-C4-C5-O7
33	9	320	LHG	O6-C4-C5-O7
33	e	101	LHG	O6-C4-C5-O7
33	t	102	LHG	O6-C4-C5-O7
34	6	322	LMG	C11-C12-C13-C14
30	Y	308	CHL	C2A-CAA-CBA-CGA
30	s	309	CHL	C2A-CAA-CBA-CGA
31	b	617	CLA	C2A-CAA-CBA-CGA
31	r	306	CLA	C2A-CAA-CBA-CGA
30	0	607	CHL	C11-C12-C13-C14
31	B	607	CLA	C11-C10-C8-C9
31	B	611	CLA	C6-C7-C8-C9
31	B	616	CLA	C11-C10-C8-C9
31	C	602	CLA	C11-C12-C13-C14
31	C	611	CLA	C11-C12-C13-C14
31	D	403	CLA	C11-C10-C8-C9
31	G	612	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	N	313	CLA	C11-C12-C13-C14
31	S	313	CLA	C6-C7-C8-C9
31	8	602	CLA	C11-C10-C8-C9
31	8	604	CLA	C14-C13-C15-C16
31	b	610	CLA	C6-C7-C8-C9
31	s	305	CLA	C11-C12-C13-C14
31	s	314	CLA	C11-C10-C8-C9
34	X	203	LMG	O7-C10-C11-C12
31	2	609	CLA	C10-C11-C12-C13
34	C	619	LMG	C12-C13-C14-C15
45	C	618	DGD	C6A-C7A-C8A-C9A
36	3	319	NEX	C13-C14-C15-C35
36	g	317	NEX	C9-C10-C11-C12
43	B	617	BCR	C9-C10-C11-C12
43	B	617	BCR	C13-C14-C15-C16
43	B	617	BCR	C19-C20-C21-C22
43	V	101	BCR	C9-C10-C11-C12
30	6	307	CHL	CBD-CGD-O2D-CED
33	s	322	LHG	C30-C31-C32-C33
30	1	608	CHL	C1-C2-C3-C4
30	2	607	CHL	C1-C2-C3-C4
30	3	303	CHL	C1-C2-C3-C4
30	3	309	CHL	C1-C2-C3-C4
30	5	608	CHL	C1-C2-C3-C4
30	6	309	CHL	C1-C2-C3-C4
30	G	606	CHL	C1-C2-C3-C4
30	N	301	CHL	C1-C2-C3-C4
30	N	308	CHL	C1-C2-C3-C4
30	Y	308	CHL	C1-C2-C3-C4
30	0	608	CHL	C1-C2-C3-C4
30	7	309	CHL	C1-C2-C3-C4
30	8	607	CHL	C1-C2-C3-C4
30	9	310	CHL	C1-C2-C3-C4
30	p	608	CHL	C1-C2-C3-C4
30	q	310	CHL	C1-C2-C3-C4
30	g	307	CHL	C1-C2-C3-C4
30	n	301	CHL	C1-C2-C3-C4
30	n	309	CHL	C1-C2-C3-C4
30	y	608	CHL	C1-C2-C3-C4
31	B	601	CLA	C1-C2-C3-C4
31	G	613	CLA	C1-C2-C3-C4
31	R	313	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
31	b	602	CLA	C1-C2-C3-C4
31	g	314	CLA	C1-C2-C3-C4
31	r	313	CLA	C1-C2-C3-C4
38	B	620	SQD	O5-C5-C6-S
38	a	411	SQD	O5-C5-C6-S
30	8	608	CHL	O1D-CGD-O2D-CED
31	b	605	CLA	O1D-CGD-O2D-CED
33	2	617	LHG	C12-C13-C14-C15
34	D	410	LMG	C16-C17-C18-C19
38	A	411	SQD	C27-C28-C29-C30
38	m	101	SQD	C32-C33-C34-C35
47	e	102	HEM	C4D-C3D-CAD-CBD
31	3	301	CLA	O1A-CGA-O2A-C1
38	S	301	SQD	O10-C23-O48-C46
33	L	101	LHG	O7-C5-C6-O8
34	A	412	LMG	O1-C7-C8-O7
34	B	621	LMG	O7-C8-C9-O8
34	N	320	LMG	O1-C7-C8-O7
34	Y	319	LMG	O1-C7-C8-O7
34	9	301	LMG	O1-C7-C8-O7
34	b	629	LMG	O7-C8-C9-O8
34	f	101	LMG	O7-C8-C9-O8
34	g	320	LMG	O1-C7-C8-O7
34	w	202	LMG	O1-C7-C8-O7
34	w	204	LMG	O1-C7-C8-O7
38	A	411	SQD	O6-C44-C45-O47
38	A	413	SQD	O47-C45-C46-O48
38	B	623	SQD	O6-C44-C45-O47
38	B	623	SQD	O47-C45-C46-O48
38	G	617	SQD	O47-C45-C46-O48
38	a	411	SQD	O47-C45-C46-O48
38	a	412	SQD	O6-C44-C45-O47
38	a	412	SQD	O47-C45-C46-O48
38	b	627	SQD	O47-C45-C46-O48
38	m	101	SQD	O6-C44-C45-O47
38	r	322	SQD	O6-C44-C45-O47
38	r	322	SQD	O47-C45-C46-O48
31	2	603	CLA	C5-C6-C7-C8
31	r	316	CLA	C15-C16-C17-C18
33	p	619	LHG	C11-C10-C9-C8
30	4	609	CHL	C11-C10-C8-C9
34	2	620	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
34	4	621	LMG	O1-C7-C8-C9
34	5	620	LMG	O1-C7-C8-C9
34	w	202	LMG	O1-C7-C8-C9
34	x	202	LMG	O1-C7-C8-C9
38	A	413	SQD	O6-C44-C45-C46
38	B	623	SQD	C44-C45-C46-O48
38	X	201	SQD	C44-C45-C46-O48
38	a	411	SQD	C44-C45-C46-O48
38	m	101	SQD	O6-C44-C45-C46
38	r	322	SQD	C44-C45-C46-O48
45	C	618	DGD	O1G-C1G-C2G-C3G
45	C	620	DGD	O1G-C1G-C2G-C3G
45	c	619	DGD	O1G-C1G-C2G-C3G
33	r	320	LHG	O8-C23-C24-C25
34	g	322	LMG	O7-C10-C11-C12
30	4	601	CHL	CAD-CBD-CGD-O2D
30	4	607	CHL	CAD-CBD-CGD-O2D
30	5	601	CHL	CAD-CBD-CGD-O2D
30	0	601	CHL	CAD-CBD-CGD-O2D
30	8	601	CHL	CAD-CBD-CGD-O2D
30	9	303	CHL	CAD-CBD-CGD-O2D
30	p	601	CHL	CAD-CBD-CGD-O2D
30	q	303	CHL	CAD-CBD-CGD-O2D
30	n	302	CHL	CAD-CBD-CGD-O2D
30	s	308	CHL	CAD-CBD-CGD-O2D
30	y	601	CHL	CAD-CBD-CGD-O2D
31	B	605	CLA	CAD-CBD-CGD-O2D
31	B	609	CLA	CAD-CBD-CGD-O2D
31	C	603	CLA	CAD-CBD-CGD-O2D
31	C	612	CLA	CAD-CBD-CGD-O2D
31	0	615	CLA	CAD-CBD-CGD-O2D
31	b	606	CLA	CAD-CBD-CGD-O2D
31	n	305	CLA	CAD-CBD-CGD-O2D
33	4	618	LHG	C29-C30-C31-C32
31	1	604	CLA	C10-C11-C12-C13
31	y	604	CLA	C6-C7-C8-C10
42	a	408	PHO	C16-C17-C18-C19
31	B	603	CLA	C3-C5-C6-C7
31	N	315	CLA	C3-C5-C6-C7
30	6	310	CHL	C2A-CAA-CBA-CGA
30	p	601	CHL	C2A-CAA-CBA-CGA
31	8	610	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	p	602	CLA	C2A-CAA-CBA-CGA
31	g	305	CLA	C2A-CAA-CBA-CGA
31	n	312	CLA	C2A-CAA-CBA-CGA
31	y	613	CLA	C2A-CAA-CBA-CGA
33	S	322	LHG	C31-C32-C33-C34
38	b	621	SQD	C14-C15-C16-C17
31	B	605	CLA	C13-C15-C16-C17
31	C	613	CLA	C15-C16-C17-C18
31	q	315	CLA	C13-C15-C16-C17
30	Y	309	CHL	O1A-CGA-O2A-C1
31	D	404	CLA	O1A-CGA-O2A-C1
33	B	624	LHG	C14-C15-C16-C17
33	a	415	LHG	C29-C30-C31-C32
34	D	412	LMG	O7-C10-C11-C12
30	Y	302	CHL	O1A-CGA-O2A-C1
33	L	101	LHG	C26-C27-C28-C29
30	1	608	CHL	CHA-CBD-CGD-O1D
30	1	608	CHL	CHA-CBD-CGD-O2D
30	1	609	CHL	CHA-CBD-CGD-O1D
30	1	609	CHL	CHA-CBD-CGD-O2D
30	1	619	CHL	CHA-CBD-CGD-O2D
30	2	606	CHL	CHA-CBD-CGD-O1D
30	2	606	CHL	CHA-CBD-CGD-O2D
30	2	608	CHL	CHA-CBD-CGD-O2D
30	3	310	CHL	CHA-CBD-CGD-O1D
30	3	310	CHL	CHA-CBD-CGD-O2D
30	4	601	CHL	CAD-CBD-CGD-O1D
30	4	606	CHL	CHA-CBD-CGD-O2D
30	4	607	CHL	CAD-CBD-CGD-O1D
30	4	608	CHL	CHA-CBD-CGD-O2D
30	4	609	CHL	CHA-CBD-CGD-O1D
30	4	609	CHL	CHA-CBD-CGD-O2D
30	5	601	CHL	CAD-CBD-CGD-O1D
30	5	606	CHL	CHA-CBD-CGD-O2D
30	6	307	CHL	CHA-CBD-CGD-O2D
30	6	309	CHL	CHA-CBD-CGD-O1D
30	6	309	CHL	CHA-CBD-CGD-O2D
30	G	608	CHL	CHA-CBD-CGD-O2D
30	N	308	CHL	CHA-CBD-CGD-O1D
30	N	308	CHL	CHA-CBD-CGD-O2D
30	N	309	CHL	CHA-CBD-CGD-O1D
30	N	309	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	R	308	CHL	CHA-CBD-CGD-O1D
30	R	308	CHL	CHA-CBD-CGD-O2D
30	R	309	CHL	CHA-CBD-CGD-O2D
30	R	310	CHL	CHA-CBD-CGD-O2D
30	S	307	CHL	CHA-CBD-CGD-O2D
30	Y	301	CHL	CHA-CBD-CGD-O1D
30	Y	301	CHL	CHA-CBD-CGD-O2D
30	Y	306	CHL	CHA-CBD-CGD-O1D
30	Y	306	CHL	CHA-CBD-CGD-O2D
30	Y	308	CHL	CHA-CBD-CGD-O2D
30	Y	309	CHL	CHA-CBD-CGD-O1D
30	Y	309	CHL	CHA-CBD-CGD-O2D
30	0	601	CHL	CAD-CBD-CGD-O1D
30	0	608	CHL	CHA-CBD-CGD-O1D
30	0	608	CHL	CHA-CBD-CGD-O2D
30	7	302	CHL	CHA-CBD-CGD-O1D
30	7	302	CHL	CHA-CBD-CGD-O2D
30	7	308	CHL	CHA-CBD-CGD-O1D
30	7	308	CHL	CHA-CBD-CGD-O2D
30	7	309	CHL	CHA-CBD-CGD-O1D
30	7	309	CHL	CHA-CBD-CGD-O2D
30	7	310	CHL	CHA-CBD-CGD-O2D
30	7	321	CHL	CHA-CBD-CGD-O2D
30	8	601	CHL	CAD-CBD-CGD-O1D
30	8	607	CHL	CHA-CBD-CGD-O1D
30	8	607	CHL	CHA-CBD-CGD-O2D
30	8	608	CHL	CHA-CBD-CGD-O1D
30	8	608	CHL	CHA-CBD-CGD-O2D
30	9	303	CHL	CAD-CBD-CGD-O1D
30	9	310	CHL	CHA-CBD-CGD-O1D
30	9	310	CHL	CHA-CBD-CGD-O2D
30	p	601	CHL	CAD-CBD-CGD-O1D
30	p	606	CHL	CHA-CBD-CGD-O1D
30	p	606	CHL	CHA-CBD-CGD-O2D
30	p	609	CHL	CHA-CBD-CGD-O1D
30	p	609	CHL	CHA-CBD-CGD-O2D
30	q	303	CHL	CAD-CBD-CGD-O1D
30	q	308	CHL	CHA-CBD-CGD-O2D
30	q	311	CHL	CHA-CBD-CGD-O1D
30	q	311	CHL	CHA-CBD-CGD-O2D
30	g	308	CHL	CHA-CBD-CGD-O1D
30	g	308	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	g	309	CHL	CHA-CBD-CGD-O1D
30	g	309	CHL	CHA-CBD-CGD-O2D
30	n	302	CHL	CAD-CBD-CGD-O1D
30	n	308	CHL	CHA-CBD-CGD-O2D
30	n	309	CHL	CHA-CBD-CGD-O2D
30	n	310	CHL	CHA-CBD-CGD-O2D
30	r	309	CHL	CHA-CBD-CGD-O2D
30	s	307	CHL	CHA-CBD-CGD-O1D
30	s	307	CHL	CHA-CBD-CGD-O2D
30	s	308	CHL	CAD-CBD-CGD-O1D
30	y	601	CHL	CAD-CBD-CGD-O1D
30	y	607	CHL	CHA-CBD-CGD-O1D
30	y	607	CHL	CHA-CBD-CGD-O2D
30	y	608	CHL	CHA-CBD-CGD-O1D
30	y	608	CHL	CHA-CBD-CGD-O2D
30	y	609	CHL	CHA-CBD-CGD-O1D
30	y	609	CHL	CHA-CBD-CGD-O2D
31	4	602	CLA	CHA-CBD-CGD-O1D
31	4	602	CLA	CHA-CBD-CGD-O2D
31	5	602	CLA	CHA-CBD-CGD-O1D
31	6	305	CLA	CAD-CBD-CGD-O1D
31	B	605	CLA	CAD-CBD-CGD-O1D
31	B	609	CLA	CAD-CBD-CGD-O1D
31	B	610	CLA	CHA-CBD-CGD-O1D
31	B	610	CLA	CHA-CBD-CGD-O2D
31	B	616	CLA	CHA-CBD-CGD-O1D
31	C	603	CLA	CAD-CBD-CGD-O1D
31	C	604	CLA	CAD-CBD-CGD-O1D
31	C	605	CLA	CAD-CBD-CGD-O1D
31	C	612	CLA	CAD-CBD-CGD-O1D
31	G	603	CLA	CHA-CBD-CGD-O1D
31	G	604	CLA	CHA-CBD-CGD-O1D
31	G	604	CLA	CHA-CBD-CGD-O2D
31	G	611	CLA	CHA-CBD-CGD-O1D
31	S	304	CLA	CHA-CBD-CGD-O1D
31	S	304	CLA	CHA-CBD-CGD-O2D
31	S	306	CLA	CAD-CBD-CGD-O1D
31	0	615	CLA	CAD-CBD-CGD-O1D
31	8	604	CLA	CAD-CBD-CGD-O1D
31	p	602	CLA	CHA-CBD-CGD-O1D
31	p	602	CLA	CHA-CBD-CGD-O2D
31	p	603	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	p	603	CLA	CHA-CBD-CGD-O2D
31	b	606	CLA	CAD-CBD-CGD-O1D
31	c	604	CLA	CAD-CBD-CGD-O1D
31	c	612	CLA	CHA-CBD-CGD-O1D
31	c	612	CLA	CHA-CBD-CGD-O2D
31	g	312	CLA	CHA-CBD-CGD-O1D
31	g	312	CLA	CHA-CBD-CGD-O2D
31	n	305	CLA	CAD-CBD-CGD-O1D
31	y	612	CLA	CHA-CBD-CGD-O1D
31	y	612	CLA	CHA-CBD-CGD-O2D
32	Y	316	LUT	C29-C30-C31-C32
33	5	619	LHG	C4-O6-P-O4
33	A	415	LHG	C3-O3-P-O5
33	A	415	LHG	C4-O6-P-O5
33	B	624	LHG	C3-O3-P-O4
33	B	624	LHG	C4-O6-P-O5
33	D	407	LHG	C3-O3-P-O6
33	D	407	LHG	C4-O6-P-O3
33	D	407	LHG	C4-O6-P-O4
33	D	408	LHG	C3-O3-P-O5
33	L	101	LHG	C4-O6-P-O4
33	M	101	LHG	C3-O3-P-O4
33	N	319	LHG	C3-O3-P-O4
33	S	322	LHG	C3-O3-P-O5
33	S	322	LHG	C4-O6-P-O5
33	Y	318	LHG	C3-O3-P-O5
33	Y	318	LHG	C4-O6-P-O5
33	0	619	LHG	C3-O3-P-O5
33	0	619	LHG	C4-O6-P-O4
33	a	415	LHG	C3-O3-P-O5
33	a	415	LHG	C4-O6-P-O3
33	b	625	LHG	C4-O6-P-O4
33	c	622	LHG	C3-O3-P-O4
33	d	408	LHG	C3-O3-P-O5
33	d	408	LHG	C4-O6-P-O4
33	e	101	LHG	C3-O3-P-O5
33	e	101	LHG	C4-O6-P-O5
33	g	319	LHG	C4-O6-P-O5
33	j	102	LHG	C4-O6-P-O5
33	t	102	LHG	C3-O3-P-O5
33	y	619	LHG	C4-O6-P-O5
33	F1	301	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
36	R	301	NEX	C13-C14-C15-C35
36	8	617	NEX	C13-C14-C15-C35
42	D	401	PHO	CHA-CBD-CGD-O1D
42	D	401	PHO	CHA-CBD-CGD-O2D
43	H	101	BCR	C9-C10-C11-C12
43	b	618	BCR	C9-C10-C11-C12
43	c	615	BCR	C19-C20-C21-C22
31	b	613	CLA	C3-C5-C6-C7
33	F1	301	LHG	C26-C27-C28-C29
31	7	313	CLA	C4-C3-C5-C6
31	b	604	CLA	C4-C3-C5-C6
44	a	414	PL9	C30-C29-C31-C32
31	1	603	CLA	C2B-C3B-CAB-CBB
31	2	602	CLA	C2B-C3B-CAB-CBB
31	6	312	CLA	C2B-C3B-CAB-CBB
31	r	307	CLA	C2B-C3B-CAB-CBB
35	2	614	RRX	C1-C6-C7-C8
35	q	317	RRX	C1-C6-C7-C8
33	1	617	LHG	C9-C10-C11-C12
34	2	620	LMG	C16-C17-C18-C19
34	r	321	LMG	C13-C14-C15-C16
48	r	302	LMU	C7-C8-C9-C10
31	G	612	CLA	C2-C3-C5-C6
31	6	311	CLA	C8-C10-C11-C12
31	n	304	CLA	C5-C6-C7-C8
32	7	318	LUT	C11-C12-C13-C20
33	A	417	LHG	C2-C3-O3-P
33	S	322	LHG	C5-C4-O6-P
33	9	320	LHG	C2-C3-O3-P
33	p	619	LHG	C5-C4-O6-P
33	j	102	LHG	C2-C3-O3-P
33	y	619	LHG	C2-C3-O3-P
38	A	411	SQD	C29-C30-C31-C32
31	d	404	CLA	C3-C5-C6-C7
33	4	618	LHG	C33-C34-C35-C36
31	5	611	CLA	O1D-CGD-O2D-CED
31	2	609	CLA	C11-C12-C13-C14
31	B	608	CLA	C16-C17-C18-C20
33	L	101	LHG	C25-C26-C27-C28
31	1	614	CLA	CAA-CBA-CGA-O2A
34	b	629	LMG	O7-C10-C11-C12
31	b	604	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	Y	301	CHL	CBA-CGA-O2A-C1
33	g	319	LHG	C25-C26-C27-C28
38	A	413	SQD	C28-C29-C30-C31
33	A	417	LHG	O1-C1-C2-O2
33	B	624	LHG	O1-C1-C2-O2
31	q	312	CLA	C3-C5-C6-C7
31	B	612	CLA	C13-C15-C16-C17
33	L	101	LHG	C10-C11-C12-C13
33	d	408	LHG	C11-C10-C9-C8
34	5	620	LMG	C29-C30-C31-C32
31	B	605	CLA	C15-C16-C17-C18
30	2	608	CHL	C11-C10-C8-C7
30	3	302	CHL	C11-C10-C8-C7
30	q	309	CHL	C11-C10-C8-C7
31	Y	310	CLA	C3-C5-C6-C7
34	W	201	LMG	C16-C17-C18-C19
34	6	323	LMG	C9-C8-O7-C10
34	D	411	LMG	C9-C8-O7-C10
34	a	413	LMG	C7-C8-O7-C10
34	b	624	LMG	C7-C8-O7-C10
34	d	410	LMG	C9-C8-O7-C10
34	w	203	LMG	C9-C8-O7-C10
38	r	322	SQD	C46-C45-O47-C7
33	S	320	LHG	C24-C25-C26-C27
33	d	408	LHG	C34-C35-C36-C37
33	r	320	LHG	C28-C29-C30-C31
43	a	410	BCR	C18-C19-C20-C21
43	c	614	BCR	C18-C19-C20-C21
31	G	609	CLA	C8-C10-C11-C12
31	N	313	CLA	C8-C10-C11-C12
31	c	606	CLA	C15-C16-C17-C18
30	4	601	CHL	C2-C3-C5-C6
31	s	313	CLA	C2-C3-C5-C6
33	A	415	LHG	C13-C14-C15-C16
43	a	410	BCR	C13-C14-C15-C16
31	2	612	CLA	C16-C17-C18-C20
31	3	304	CLA	C11-C12-C13-C15
31	N	303	CLA	C16-C17-C18-C20
31	B	616	CLA	C13-C15-C16-C17
33	B	624	LHG	O6-C4-C5-C6
33	7	319	LHG	O6-C4-C5-C6
31	c	601	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	6	306	CHL	CBD-CGD-O2D-CED
31	6	315	CLA	C6-C7-C8-C9
33	7	319	LHG	C12-C13-C14-C15
33	c	622	LHG	C17-C18-C19-C20
44	d	407	PL9	C16-C17-C18-C19
30	1	601	CHL	C6-C7-C8-C9
30	4	601	CHL	C6-C7-C8-C9
30	7	321	CHL	C11-C12-C13-C14
30	q	303	CHL	C11-C12-C13-C14
30	q	309	CHL	C6-C7-C8-C9
30	n	308	CHL	C11-C12-C13-C14
31	2	609	CLA	C11-C10-C8-C9
31	3	304	CLA	C11-C10-C8-C9
31	3	312	CLA	C6-C7-C8-C9
31	B	614	CLA	C11-C12-C13-C14
31	D	404	CLA	C14-C13-C15-C16
31	G	609	CLA	C11-C12-C13-C14
31	G	612	CLA	C11-C10-C8-C9
31	N	305	CLA	C6-C7-C8-C9
31	N	313	CLA	C11-C10-C8-C9
31	S	303	CLA	C11-C10-C8-C9
31	8	602	CLA	C6-C7-C8-C9
31	8	604	CLA	C6-C7-C8-C9
31	b	608	CLA	C11-C12-C13-C14
31	b	615	CLA	C11-C12-C13-C14
31	c	607	CLA	C14-C13-C15-C16
31	c	611	CLA	C11-C10-C8-C9
31	g	310	CLA	C11-C12-C13-C14
31	n	303	CLA	C6-C7-C8-C9
31	n	305	CLA	C6-C7-C8-C9
31	r	316	CLA	C14-C13-C15-C16
31	s	314	CLA	C14-C13-C15-C16
31	y	610	CLA	C11-C12-C13-C14
30	3	302	CHL	C6-C7-C8-C10
30	7	306	CHL	C11-C10-C8-C7
31	A	406	CLA	C12-C13-C15-C16
31	C	613	CLA	C11-C12-C13-C15
31	S	311	CLA	C12-C13-C15-C16
31	8	602	CLA	C6-C7-C8-C10
31	8	604	CLA	C6-C7-C8-C10
31	b	611	CLA	C11-C10-C8-C7
31	n	303	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	n	305	CLA	C6-C7-C8-C10
31	y	612	CLA	C11-C10-C8-C7
36	R	301	NEX	C28-C29-C30-C31
36	n	319	NEX	C28-C29-C30-C31
36	y	618	NEX	C28-C29-C30-C31
34	b	622	LMG	C29-C30-C31-C32
33	F1	301	LHG	O6-C4-C5-O7
34	r	321	LMG	O6-C1-O1-C7
31	4	602	CLA	C16-C17-C18-C20
31	a	409	CLA	C11-C12-C13-C14
33	D	408	LHG	C31-C32-C33-C34
31	9	304	CLA	CAA-CBA-CGA-O2A
34	C	619	LMG	O7-C10-C11-C12
34	S	321	LMG	O7-C10-C11-C12
33	B	624	LHG	C30-C31-C32-C33
45	c	618	DGD	C2D-C1D-O3G-C3G
42	D	401	PHO	C4-C3-C5-C6
31	7	315	CLA	C2-C3-C5-C6
30	Y	302	CHL	CBA-CGA-O2A-C1
30	9	303	CHL	C10-C11-C12-C13
31	c	603	CLA	C5-C6-C7-C8
34	A	414	LMG	C29-C30-C31-C32
38	B	620	SQD	C14-C15-C16-C17
31	N	303	CLA	C13-C15-C16-C17
33	Y	318	LHG	C2-C3-O3-P
38	m	101	SQD	C24-C25-C26-C27
33	S	322	LHG	O7-C5-C6-O8
34	2	618	LMG	O1-C7-C8-O7
34	J	101	LMG	O1-C7-C8-O7
34	W	201	LMG	O1-C7-C8-O7
34	n	322	LMG	O1-C7-C8-O7
38	S	301	SQD	O47-C45-C46-O48
38	Y	320	SQD	O6-C44-C45-O47
31	8	613	CLA	CAA-CBA-CGA-O2A
34	9	301	LMG	C30-C31-C32-C33
31	B	607	CLA	CBA-CGA-O2A-C1
34	n	321	LMG	C10-C11-C12-C13
33	7	319	LHG	C9-C10-C11-C12
34	b	623	LMG	C33-C34-C35-C36
31	A	409	CLA	C11-C12-C13-C14
34	6	321	LMG	C4-C5-C6-O5
33	L	101	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
34	b	626	LMG	C29-C30-C31-C32
31	7	305	CLA	C15-C16-C17-C18
31	7	315	CLA	CAA-CBA-CGA-O2A
31	g	314	CLA	CAA-CBA-CGA-O2A
31	n	315	CLA	CAA-CBA-CGA-O2A
30	7	306	CHL	C2A-CAA-CBA-CGA
34	W	201	LMG	C11-C12-C13-C14
34	c	624	LMG	C31-C32-C33-C34
31	8	614	CLA	C2-C1-O2A-CGA
31	p	611	CLA	C2-C1-O2A-CGA
31	c	604	CLA	C2-C1-O2A-CGA
31	n	316	CLA	C2-C1-O2A-CGA
44	A	416	PL9	C40-C39-C41-C42
34	d	411	LMG	O7-C10-C11-C12
34	s	321	LMG	O7-C10-C11-C12
30	R	308	CHL	C2-C3-C5-C6
33	4	618	LHG	C9-C10-C11-C12
33	q	320	LHG	C4-C5-C6-O8
34	W	201	LMG	O1-C7-C8-C9
38	G	624	SQD	C44-C45-C46-O48
45	C	620	DGD	C1G-C2G-C3G-O3G
31	4	613	CLA	C3-C5-C6-C7
31	y	615	CLA	C3-C5-C6-C7
34	w	201	LMG	C29-C28-O8-C9
34	B	625	LMG	O7-C10-C11-C12
31	8	603	CLA	C5-C6-C7-C8
33	d	408	LHG	C29-C30-C31-C32
34	f	101	LMG	C31-C32-C33-C34
31	2	602	CLA	C16-C17-C18-C20
30	3	309	CHL	CBD-CGD-O2D-CED
31	b	615	CLA	C15-C16-C17-C18
34	6	322	LMG	C31-C32-C33-C34
32	3	318	LUT	C31-C32-C33-C34
32	6	317	LUT	C27-C28-C29-C30
31	s	312	CLA	CBA-CGA-O2A-C1
34	0	620	LMG	C32-C33-C34-C35
34	2	620	LMG	C8-C7-O1-C1
34	G	621	LMG	C8-C7-O1-C1
34	0	622	LMG	C8-C7-O1-C1
34	7	301	LMG	C8-C7-O1-C1
38	M	102	SQD	C45-C44-O6-C1
38	b	621	SQD	C45-C44-O6-C1

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Mol	Chain	Res	Type	Atoms
31	b	603	CLA	C13-C15-C16-C17
31	2	612	CLA	C2A-CAA-CBA-CGA
31	6	305	CLA	C2A-CAA-CBA-CGA
31	B	607	CLA	C2A-CAA-CBA-CGA
31	c	605	CLA	C2A-CAA-CBA-CGA
30	6	307	CHL	O1D-CGD-O2D-CED
36	N	318	NEX	C33-C34-C35-C15
37	R	318	XAT	C13-C14-C15-C35
33	D	408	LHG	C30-C31-C32-C33
38	G	624	SQD	O5-C1-O6-C44
33	7	319	LHG	C25-C26-C27-C28
33	e	101	LHG	C10-C11-C12-C13
31	N	315	CLA	C4-C3-C5-C6
31	7	313	CLA	C2-C3-C5-C6
38	b	627	SQD	C13-C14-C15-C16
31	s	311	CLA	C5-C6-C7-C8
44	D	406	PL9	C2-C3-C7-C8
31	4	610	CLA	CAA-CBA-CGA-O2A
31	6	311	CLA	C11-C12-C13-C14
31	B	615	CLA	C11-C12-C13-C14
31	C	607	CLA	C11-C12-C13-C14
31	S	312	CLA	C11-C10-C8-C9
31	Y	310	CLA	C11-C12-C13-C14
31	7	313	CLA	C6-C7-C8-C9
31	q	304	CLA	C6-C7-C8-C9
31	q	304	CLA	C11-C10-C8-C9
31	c	606	CLA	C6-C7-C8-C9
31	s	312	CLA	C11-C12-C13-C14
33	c	622	LHG	C24-C23-O8-C6
38	6	301	SQD	C24-C23-O48-C46
31	C	611	CLA	C8-C10-C11-C12
33	b	628	LHG	C24-C25-C26-C27
31	3	312	CLA	C4B-C3B-CAB-CBB
31	C	601	CLA	C4B-C3B-CAB-CBB
31	0	603	CLA	C4B-C3B-CAB-CBB
31	b	607	CLA	C4B-C3B-CAB-CBB
31	c	604	CLA	C4B-C3B-CAB-CBB
33	8	618	LHG	C17-C18-C19-C20
33	B	624	LHG	C26-C27-C28-C29
34	2	621	LMG	C30-C31-C32-C33
33	n	320	LHG	C17-C18-C19-C20
30	6	306	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	7	312	CLA	C10-C11-C12-C13
31	4	610	CLA	C11-C12-C13-C14
30	r	308	CHL	CBA-CGA-O2A-C1
31	c	601	CLA	CBA-CGA-O2A-C1
45	c	618	DGD	C1A-C2A-C3A-C4A
30	2	605	CHL	CAA-CBA-CGA-O2A
30	3	307	CHL	CAA-CBA-CGA-O2A
30	5	605	CHL	CAA-CBA-CGA-O2A
34	w	201	LMG	O10-C28-O8-C9
31	7	314	CLA	C2A-CAA-CBA-CGA
30	R	310	CHL	C4-C3-C5-C6
31	q	305	CLA	C4-C3-C5-C6
31	p	612	CLA	CAA-CBA-CGA-O2A
30	R	309	CHL	C2-C3-C5-C6
34	7	320	LMG	C33-C34-C35-C36
30	9	307	CHL	CAA-CBA-CGA-O2A
45	C	617	DGD	C3B-C4B-C5B-C6B
30	Y	301	CHL	O1A-CGA-O2A-C1
31	S	313	CLA	O1A-CGA-O2A-C1
38	6	301	SQD	O10-C23-O48-C46
34	6	322	LMG	C8-C9-O8-C28
47	E	101	HEM	C4B-C3B-CAB-CBB
47	e	102	HEM	C4B-C3B-CAB-CBB
31	y	613	CLA	C16-C17-C18-C19
34	6	323	LMG	O9-C10-C11-C12
33	t	102	LHG	C29-C30-C31-C32
38	r	322	SQD	C25-C26-C27-C28
30	3	310	CHL	C6-C7-C8-C10
31	1	612	CLA	C6-C7-C8-C10
31	6	303	CLA	C11-C12-C13-C15
31	B	605	CLA	C11-C12-C13-C15
31	B	610	CLA	C11-C10-C8-C7
31	B	611	CLA	C11-C10-C8-C7
31	0	610	CLA	C6-C7-C8-C10
31	7	314	CLA	C11-C10-C8-C7
31	q	315	CLA	C11-C12-C13-C15
31	b	608	CLA	C11-C10-C8-C7
31	b	617	CLA	C11-C12-C13-C15
31	y	613	CLA	C11-C10-C8-C7
31	3	301	CLA	C2C-C3C-CAC-CBC
31	s	312	CLA	O1A-CGA-O2A-C1
31	Y	314	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	t	102	LHG	C24-C25-C26-C27
33	g	319	LHG	C31-C32-C33-C34
33	1	617	LHG	C27-C28-C29-C30
33	S	322	LHG	C25-C26-C27-C28
34	2	618	LMG	O9-C10-C11-C12
45	C	617	DGD	C1A-C2A-C3A-C4A
33	D	408	LHG	C25-C26-C27-C28
38	S	301	SQD	C30-C31-C32-C33
31	d	404	CLA	CAA-CBA-CGA-O2A
31	2	609	CLA	C11-C12-C13-C15
31	3	304	CLA	C11-C12-C13-C14
31	y	602	CLA	C11-C12-C13-C15
31	y	604	CLA	C6-C7-C8-C9
34	B	622	LMG	C29-C30-C31-C32
30	g	302	CHL	CAA-CBA-CGA-O1A
34	c	620	LMG	O1-C7-C8-O7
38	b	621	SQD	O47-C45-C46-O48
31	R	311	CLA	C2C-C3C-CAC-CBC
34	d	409	LMG	C11-C12-C13-C14
30	3	309	CHL	C3A-C2A-CAA-CBA
30	5	607	CHL	C3A-C2A-CAA-CBA
30	7	309	CHL	C3A-C2A-CAA-CBA
30	9	309	CHL	C3A-C2A-CAA-CBA
30	p	608	CHL	C3A-C2A-CAA-CBA
31	1	612	CLA	C3A-C2A-CAA-CBA
31	6	315	CLA	C4-C3-C5-C6
31	C	610	CLA	C3A-C2A-CAA-CBA
31	b	603	CLA	C3A-C2A-CAA-CBA
31	3	315	CLA	C5-C6-C7-C8
33	A	415	LHG	C11-C10-C9-C8
31	y	613	CLA	C2-C3-C5-C6
33	G	618	LHG	C31-C32-C33-C34
33	e	101	LHG	C12-C13-C14-C15
33	l	101	LHG	C29-C30-C31-C32
34	C	619	LMG	C32-C33-C34-C35
32	2	615	LUT	C39-C29-C30-C31
32	G	615	LUT	C40-C33-C34-C35
32	R	317	LUT	C39-C29-C30-C31
32	9	318	LUT	C40-C33-C34-C35
32	p	616	LUT	C39-C29-C30-C31
32	p	617	LUT	C39-C29-C30-C31
35	2	614	RRX	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
35	4	615	RRX	C16-C17-C18-C36
35	G	614	RRX	C16-C17-C18-C36
35	9	317	RRX	C16-C17-C18-C36
35	q	317	RRX	C16-C17-C18-C36
35	g	315	RRX	C16-C17-C18-C36
36	5	618	NEX	C39-C29-C30-C31
36	n	319	NEX	C39-C29-C30-C31
36	s	319	NEX	C39-C29-C30-C31
36	y	618	NEX	C39-C29-C30-C31
37	4	619	XAT	C40-C33-C34-C35
37	g	321	XAT	C40-C33-C34-C35
43	A	410	BCR	C16-C17-C18-C36
43	C	615	BCR	C11-C10-C9-C34
43	C	615	BCR	C16-C17-C18-C36
43	D	405	BCR	C11-C10-C9-C34
43	a	410	BCR	C20-C21-C22-C37
43	c	615	BCR	C16-C17-C18-C36
43	d	406	BCR	C11-C10-C9-C34
43	t	101	BCR	C16-C17-C18-C36
34	C	619	LMG	C39-C40-C41-C42
31	R	316	CLA	C8-C10-C11-C12
31	c	610	CLA	C5-C6-C7-C8
33	z	102	LHG	C11-C10-C9-C8
33	d	408	LHG	O9-C7-O7-C5
30	4	607	CHL	C11-C10-C8-C9
34	w	201	LMG	C12-C13-C14-C15
38	m	101	SQD	C25-C26-C27-C28
31	5	611	CLA	CBD-CGD-O2D-CED
30	S	309	CHL	C2-C1-O2A-CGA
31	N	314	CLA	C2-C1-O2A-CGA
31	R	304	CLA	C2-C1-O2A-CGA
31	R	311	CLA	C2-C1-O2A-CGA
32	1	616	LUT	C29-C30-C31-C32
36	6	319	NEX	C13-C14-C15-C35
36	0	618	NEX	C13-C14-C15-C35
36	p	618	NEX	C29-C30-C31-C32
43	B	617	BCR	C15-C16-C17-C18
31	6	314	CLA	C8-C10-C11-C12
31	N	305	CLA	C13-C15-C16-C17
32	7	317	LUT	C27-C28-C29-C39
32	y	616	LUT	C7-C8-C9-C19
33	1	617	LHG	C5-C4-O6-P

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Mol	Chain	Res	Type	Atoms
30	3	307	CHL	CAA-CBA-CGA-O1A
30	5	605	CHL	CAA-CBA-CGA-O1A
33	d	408	LHG	C10-C11-C12-C13
45	c	617	DGD	CAB-CBB-CCB-CDB
34	7	322	LMG	C30-C31-C32-C33
33	1	617	LHG	C24-C25-C26-C27
34	S	321	LMG	C18-C19-C20-C21
34	k	102	LMG	C11-C12-C13-C14
45	c	617	DGD	C7B-C8B-C9B-CAB
30	7	321	CHL	C10-C11-C12-C13
43	V	101	BCR	C7-C8-C9-C10
47	E	101	HEM	C4D-C3D-CAD-CBD
31	s	312	CLA	C4-C3-C5-C6
31	1	613	CLA	C2-C3-C5-C6
44	D	406	PL9	C13-C14-C16-C17
30	4	609	CHL	C5-C6-C7-C8
30	n	308	CHL	C10-C11-C12-C13
31	S	312	CLA	C8-C10-C11-C12
34	5	620	LMG	C33-C34-C35-C36
34	d	410	LMG	C21-C22-C23-C24
30	7	310	CHL	C2A-CAA-CBA-CGA
31	6	304	CLA	C2A-CAA-CBA-CGA
31	B	616	CLA	C2A-CAA-CBA-CGA
44	d	407	PL9	C2-C3-C7-C8
30	9	307	CHL	CAA-CBA-CGA-O1A
33	C	623	LHG	C34-C35-C36-C37
31	q	313	CLA	C2C-C3C-CAC-CBC
33	Y	318	LHG	C4-C5-C6-O8
34	A	412	LMG	O1-C7-C8-C9
34	7	301	LMG	C7-C8-C9-O8
34	y	620	LMG	O1-C7-C8-C9
33	y	619	LHG	C25-C26-C27-C28
34	D	411	LMG	C21-C22-C23-C24
48	R	302	LMU	C2B-C1B-O1B-C4'
31	6	303	CLA	C3-C5-C6-C7
33	M	101	LHG	C32-C33-C34-C35
30	1	605	CHL	C14-C13-C15-C16
30	6	308	CHL	C11-C12-C13-C14
30	7	302	CHL	C14-C13-C15-C16
31	1	613	CLA	C11-C12-C13-C14
31	6	314	CLA	C14-C13-C15-C16
31	B	605	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	B	606	CLA	C11-C12-C13-C14
31	B	611	CLA	C11-C12-C13-C14
31	C	603	CLA	C14-C13-C15-C16
31	G	610	CLA	C6-C7-C8-C9
31	0	610	CLA	C6-C7-C8-C9
31	7	312	CLA	C11-C10-C8-C9
31	8	609	CLA	C11-C12-C13-C14
31	p	611	CLA	C11-C10-C8-C9
31	b	608	CLA	C6-C7-C8-C9
31	b	608	CLA	C11-C10-C8-C9
31	r	312	CLA	C6-C7-C8-C9
34	s	321	LMG	C11-C12-C13-C14
31	s	312	CLA	C16-C17-C18-C19
33	L	101	LHG	C16-C17-C18-C19
30	6	310	CHL	CBD-CGD-O2D-CED
34	W	201	LMG	C42-C43-C44-C45
30	r	308	CHL	O1A-CGA-O2A-C1
34	C	621	LMG	C12-C13-C14-C15
30	2	605	CHL	CAA-CBA-CGA-O1A
31	2	609	CLA	CAA-CBA-CGA-O2A
31	D	403	CLA	CAA-CBA-CGA-O2A
34	R	321	LMG	O7-C10-C11-C12
34	2	620	LMG	C7-C8-O7-C10
34	2	620	LMG	C9-C8-O7-C10
34	J	101	LMG	C9-C8-O7-C10
34	W	201	LMG	C9-C8-O7-C10
34	W	203	LMG	C7-C8-O7-C10
34	W	203	LMG	C9-C8-O7-C10
34	0	622	LMG	C7-C8-O7-C10
34	0	622	LMG	C9-C8-O7-C10
34	9	302	LMG	C9-C8-O7-C10
34	p	620	LMG	C7-C8-O7-C10
34	w	205	LMG	C7-C8-O7-C10
34	w	205	LMG	C9-C8-O7-C10
38	r	322	SQD	C44-C45-O47-C7
45	C	617	DGD	C3G-C2G-O2G-C1B
45	C	618	DGD	C1G-C2G-O2G-C1B
45	c	617	DGD	C1G-C2G-O2G-C1B
30	7	310	CHL	C8-C10-C11-C12
31	7	314	CLA	C8-C10-C11-C12
34	7	320	LMG	C29-C30-C31-C32
30	1	601	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	2	607	CHL	C1A-C2A-CAA-CBA
30	G	608	CHL	C1A-C2A-CAA-CBA
30	Y	308	CHL	C1A-C2A-CAA-CBA
30	8	608	CHL	C1A-C2A-CAA-CBA
30	s	309	CHL	C1A-C2A-CAA-CBA
30	y	608	CHL	C1A-C2A-CAA-CBA
45	C	618	DGD	O6D-C5D-C6D-O5D
45	c	616	DGD	O6D-C5D-C6D-O5D
31	B	608	CLA	C16-C17-C18-C19
34	C	624	LMG	C16-C17-C18-C19
31	0	614	CLA	CAA-CBA-CGA-O2A
30	1	606	CHL	C2-C3-C5-C6
42	D	401	PHO	C2-C3-C5-C6
33	8	618	LHG	C35-C36-C37-C38
33	n	320	LHG	C35-C36-C37-C38
33	s	320	LHG	O1-C1-C2-O2
30	q	309	CHL	O1A-CGA-O2A-C1
31	r	304	CLA	O1A-CGA-O2A-C1
33	A	415	LHG	C35-C36-C37-C38
30	3	308	CHL	C2A-CAA-CBA-CGA
31	N	303	CLA	C2A-CAA-CBA-CGA
31	0	604	CLA	C2A-CAA-CBA-CGA
31	g	310	CLA	C2A-CAA-CBA-CGA
31	3	306	CLA	C4C-C3C-CAC-CBC
34	c	620	LMG	O9-C10-C11-C12
34	g	320	LMG	O9-C10-C11-C12
31	3	301	CLA	C1A-C2A-CAA-CBA
31	G	613	CLA	C1A-C2A-CAA-CBA
31	R	304	CLA	C1A-C2A-CAA-CBA
31	R	313	CLA	C1A-C2A-CAA-CBA
31	a	406	CLA	C1A-C2A-CAA-CBA
32	2	615	LUT	C28-C29-C30-C31
32	R	317	LUT	C28-C29-C30-C31
32	9	318	LUT	C32-C33-C34-C35
32	p	616	LUT	C28-C29-C30-C31
32	p	617	LUT	C28-C29-C30-C31
35	2	614	RRX	C16-C17-C18-C19
35	4	615	RRX	C16-C17-C18-C19
35	G	614	RRX	C16-C17-C18-C19
35	9	317	RRX	C16-C17-C18-C19
35	q	317	RRX	C16-C17-C18-C19
35	g	315	RRX	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
36	5	618	NEX	C28-C29-C30-C31
36	8	617	NEX	C28-C29-C30-C31
36	s	319	NEX	C28-C29-C30-C31
43	A	410	BCR	C16-C17-C18-C19
43	C	615	BCR	C11-C10-C9-C8
43	C	615	BCR	C16-C17-C18-C19
43	D	405	BCR	C11-C10-C9-C8
43	a	410	BCR	C20-C21-C22-C23
43	c	615	BCR	C16-C17-C18-C19
43	d	406	BCR	C11-C10-C9-C8
43	t	101	BCR	C16-C17-C18-C19
34	d	411	LMG	C33-C34-C35-C36
34	w	202	LMG	C14-C15-C16-C17
31	5	615	CLA	C4C-C3C-CAC-CBC
38	B	620	SQD	C9-C10-C11-C12
45	c	616	DGD	C7A-C8A-C9A-CAA
31	3	312	CLA	C2B-C3B-CAB-CBB
31	C	601	CLA	C2B-C3B-CAB-CBB
31	G	613	CLA	C2B-C3B-CAB-CBB
31	N	321	CLA	C2B-C3B-CAB-CBB
31	R	307	CLA	C2B-C3B-CAB-CBB
31	R	313	CLA	C2B-C3B-CAB-CBB
31	Y	311	CLA	C2B-C3B-CAB-CBB
31	0	611	CLA	C2B-C3B-CAB-CBB
31	9	313	CLA	C2B-C3B-CAB-CBB
31	q	316	CLA	C2B-C3B-CAB-CBB
31	b	603	CLA	C2B-C3B-CAB-CBB
31	b	607	CLA	C2B-C3B-CAB-CBB
31	b	616	CLA	C2B-C3B-CAB-CBB
31	c	601	CLA	C2B-C3B-CAB-CBB
31	c	604	CLA	C2B-C3B-CAB-CBB
31	g	311	CLA	C2B-C3B-CAB-CBB
32	5	616	LUT	C1-C6-C7-C8
43	B	619	BCR	C23-C24-C25-C30
43	C	614	BCR	C1-C6-C7-C8
43	D	405	BCR	C23-C24-C25-C26
43	V	101	BCR	C5-C6-C7-C8
43	V	101	BCR	C23-C24-C25-C26
43	a	410	BCR	C23-C24-C25-C26
43	b	618	BCR	C23-C24-C25-C30
43	b	619	BCR	C23-C24-C25-C26
43	b	620	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
43	v	101	BCR	C5-C6-C7-C8
38	6	301	SQD	C8-C7-O47-C45
31	r	304	CLA	CBA-CGA-O2A-C1
33	D	407	LHG	C28-C29-C30-C31
33	e	101	LHG	C34-C35-C36-C37
31	R	305	CLA	O1A-CGA-O2A-C1
33	5	619	LHG	C5-C4-O6-P
33	a	415	LHG	C2-C3-O3-P
33	s	322	LHG	C2-C3-O3-P
45	c	618	DGD	O6D-C5D-C6D-O5D
33	G	618	LHG	C25-C26-C27-C28
31	p	610	CLA	C11-C10-C8-C9
31	N	303	CLA	C16-C17-C18-C19
31	D	404	CLA	C3-C5-C6-C7
31	7	303	CLA	C3-C5-C6-C7
30	5	607	CHL	CBD-CGD-O2D-CED
30	G	608	CHL	C4-C3-C5-C6
30	8	605	CHL	C4-C3-C5-C6
31	2	609	CLA	C4-C3-C5-C6
31	c	602	CLA	C4-C3-C5-C6
33	0	619	LHG	C28-C29-C30-C31
33	j	102	LHG	C10-C11-C12-C13
34	k	102	LMG	C30-C31-C32-C33
30	R	310	CHL	C2-C3-C5-C6
31	1	610	CLA	C2-C3-C5-C6
31	s	312	CLA	C2-C3-C5-C6
45	C	620	DGD	C9B-CAB-CBB-CCB
30	4	608	CHL	O2A-C1-C2-C3
34	c	624	LMG	C15-C16-C17-C18
30	3	310	CHL	C10-C11-C12-C13
30	1	605	CHL	C6-C7-C8-C10
31	1	610	CLA	C12-C13-C15-C16
31	2	612	CLA	C11-C12-C13-C15
31	3	316	CLA	C6-C7-C8-C10
31	6	303	CLA	C11-C10-C8-C7
31	B	603	CLA	C11-C10-C8-C7
31	B	612	CLA	C11-C10-C8-C7
31	C	607	CLA	C11-C10-C8-C7
31	C	607	CLA	C11-C12-C13-C15
31	C	607	CLA	C12-C13-C15-C16
31	G	602	CLA	C11-C10-C8-C7
31	G	610	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	R	316	CLA	C11-C10-C8-C7
31	7	313	CLA	C6-C7-C8-C10
31	q	304	CLA	C6-C7-C8-C10
31	b	609	CLA	C12-C13-C15-C16
31	b	612	CLA	C11-C10-C8-C7
31	b	613	CLA	C12-C13-C15-C16
31	b	614	CLA	C6-C7-C8-C10
31	b	616	CLA	C11-C10-C8-C7
31	c	602	CLA	C6-C7-C8-C10
31	c	606	CLA	C6-C7-C8-C10
31	s	310	CLA	C6-C7-C8-C10
34	G	619	LMG	O9-C10-C11-C12
33	2	617	LHG	C31-C32-C33-C34
38	A	411	SQD	C26-C27-C28-C29
31	B	607	CLA	C16-C17-C18-C20
31	S	312	CLA	C16-C17-C18-C19
31	A	406	CLA	C2A-CAA-CBA-CGA
31	G	604	CLA	C2A-CAA-CBA-CGA
31	7	303	CLA	C2A-CAA-CBA-CGA
31	b	607	CLA	C2A-CAA-CBA-CGA
33	d	408	LHG	C25-C26-C27-C28
31	g	311	CLA	C5-C6-C7-C8
33	G	618	LHG	O7-C5-C6-O8
34	G	619	LMG	O1-C7-C8-O7
34	d	411	LMG	O7-C8-C9-O8
34	r	321	LMG	O7-C8-C9-O8
38	x	201	SQD	O47-C45-C46-O48
45	c	616	DGD	O2G-C2G-C3G-O3G
45	c	617	DGD	O1G-C1G-C2G-O2G
33	Y	318	LHG	C26-C27-C28-C29
34	9	301	LMG	C15-C16-C17-C18
33	p	619	LHG	C9-C10-C11-C12
31	y	610	CLA	C3-C5-C6-C7
31	2	611	CLA	CAA-CBA-CGA-O2A
38	6	301	SQD	O47-C7-C8-C9
30	1	606	CHL	C8-C10-C11-C12
31	2	612	CLA	C8-C10-C11-C12
31	c	605	CLA	C10-C11-C12-C13
30	6	310	CHL	C11-C12-C13-C15
34	s	321	LMG	C13-C14-C15-C16
38	6	301	SQD	O49-C7-O47-C45
33	D	408	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
33	C	623	LHG	C29-C30-C31-C32
33	y	619	LHG	C31-C32-C33-C34
30	4	607	CHL	C11-C10-C8-C7
30	4	609	CHL	C11-C10-C8-C7
31	6	304	CLA	C11-C10-C8-C7
31	0	603	CLA	C11-C10-C8-C7
31	p	610	CLA	C11-C10-C8-C7
32	8	616	LUT	C11-C12-C13-C20
32	n	318	LUT	C11-C12-C13-C20
32	r	317	LUT	C7-C8-C9-C19
30	1	606	CHL	C4-C3-C5-C6
30	6	310	CHL	C4-C3-C5-C6
30	Y	309	CHL	C4-C3-C5-C6
30	p	609	CHL	C4-C3-C5-C6
30	n	306	CHL	C4-C3-C5-C6
31	S	312	CLA	C4-C3-C5-C6
45	c	618	DGD	C6A-C7A-C8A-C9A
38	x	201	SQD	O47-C7-C8-C9
30	2	601	CHL	C2-C3-C5-C6
30	4	607	CHL	C2-C3-C5-C6
31	C	611	CLA	C2-C3-C5-C6
31	q	305	CLA	C2-C3-C5-C6
31	b	604	CLA	C2-C3-C5-C6
34	a	413	LMG	C29-C30-C31-C32
33	j	102	LHG	C29-C30-C31-C32
34	q	301	LMG	C37-C38-C39-C40
31	C	605	CLA	C2-C1-O2A-CGA
31	Y	311	CLA	C2-C1-O2A-CGA
31	Y	313	CLA	C2-C1-O2A-CGA
33	0	619	LHG	C10-C11-C12-C13
31	b	605	CLA	C13-C15-C16-C17
31	c	602	CLA	C13-C15-C16-C17
47	e	102	HEM	C2D-C3D-CAD-CBD
31	5	602	CLA	C11-C12-C13-C15
33	d	408	LHG	C33-C34-C35-C36
31	S	313	CLA	CBA-CGA-O2A-C1
31	R	311	CLA	C4C-C3C-CAC-CBC
34	w	201	LMG	C16-C17-C18-C19
31	1	612	CLA	C6-C7-C8-C9
31	C	603	CLA	C6-C7-C8-C9
31	N	303	CLA	C6-C7-C8-C9
31	R	305	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	c	601	CLA	C11-C10-C8-C9
31	g	311	CLA	C6-C7-C8-C9
38	Y	320	SQD	C13-C14-C15-C16
34	a	413	LMG	C34-C35-C36-C37
33	c	622	LHG	C31-C32-C33-C34
38	S	301	SQD	C31-C32-C33-C34
30	n	306	CHL	O1D-CGD-O2D-CED
33	a	415	LHG	C11-C10-C9-C8
38	m	101	SQD	C13-C14-C15-C16
33	Y	318	LHG	C27-C28-C29-C30
34	5	620	LMG	C30-C31-C32-C33
38	A	413	SQD	C27-C28-C29-C30
30	4	607	CHL	C4-C3-C5-C6
30	y	607	CHL	C4-C3-C5-C6
30	y	609	CHL	C4-C3-C5-C6
31	B	606	CLA	C4-C3-C5-C6
31	C	611	CLA	C4-C3-C5-C6
31	y	612	CLA	C4-C3-C5-C6
31	a	407	CLA	C8-C10-C11-C12
33	5	619	LHG	C2-C3-O3-P
33	D	407	LHG	C2-C3-O3-P
31	4	614	CLA	C2-C3-C5-C6
31	B	606	CLA	C2-C3-C5-C6
31	C	613	CLA	C2-C3-C5-C6
31	S	312	CLA	C2-C3-C5-C6
31	9	304	CLA	C2-C3-C5-C6
44	a	414	PL9	C38-C39-C41-C42
31	y	614	CLA	CBD-CGD-O2D-CED
33	2	617	LHG	C25-C26-C27-C28
31	D	404	CLA	C10-C11-C12-C13
31	q	313	CLA	CAA-CBA-CGA-O2A
31	3	305	CLA	C5-C6-C7-C8
31	4	613	CLA	C5-C6-C7-C8
31	B	610	CLA	C15-C16-C17-C18
31	B	607	CLA	O1A-CGA-O2A-C1
33	l	101	LHG	C28-C29-C30-C31
34	J	101	LMG	C18-C19-C20-C21
30	6	310	CHL	O1D-CGD-O2D-CED
33	N	319	LHG	C4-C5-C6-O8
34	3	321	LMG	C7-C8-C9-O8
34	W	203	LMG	C7-C8-C9-O8
34	b	623	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
34	c	620	LMG	O1-C7-C8-C9
34	r	321	LMG	C7-C8-C9-O8
34	w	204	LMG	O1-C7-C8-C9
45	C	617	DGD	C1G-C2G-C3G-O3G
45	c	617	DGD	O1G-C1G-C2G-C3G
31	0	614	CLA	C6-C7-C8-C9
31	N	312	CLA	CAA-CBA-CGA-O2A
33	r	320	LHG	C24-C25-C26-C27
34	5	620	LMG	C11-C12-C13-C14
30	5	601	CHL	CAA-CBA-CGA-O1A
33	q	320	LHG	C35-C36-C37-C38
31	1	613	CLA	C2A-CAA-CBA-CGA
31	4	602	CLA	C2A-CAA-CBA-CGA
31	8	602	CLA	C2A-CAA-CBA-CGA
31	y	612	CLA	C16-C17-C18-C20
33	d	408	LHG	C35-C36-C37-C38
33	n	320	LHG	C16-C17-C18-C19
31	C	610	CLA	CAA-CBA-CGA-O2A
30	5	607	CHL	O1D-CGD-O2D-CED
33	8	618	LHG	C16-C17-C18-C19
31	p	602	CLA	C8-C10-C11-C12
30	7	321	CHL	C4-C3-C5-C6
30	n	308	CHL	C4-C3-C5-C6
31	C	609	CLA	C4-C3-C5-C6
31	c	612	CLA	C4-C3-C5-C6
33	D	407	LHG	C27-C28-C29-C30
33	K	102	LHG	C9-C10-C11-C12
33	F1	301	LHG	O7-C7-C8-C9
34	S	321	LMG	C10-C11-C12-C13
30	0	607	CHL	C13-C15-C16-C17
31	b	608	CLA	C5-C6-C7-C8
34	G	621	LMG	C11-C12-C13-C14
33	b	625	LHG	C34-C35-C36-C37
34	b	629	LMG	C29-C30-C31-C32
31	N	321	CLA	C4B-C3B-CAB-CBB
31	q	316	CLA	C4B-C3B-CAB-CBB
31	c	605	CLA	C4B-C3B-CAB-CBB
31	s	315	CLA	C4B-C3B-CAB-CBB
30	8	605	CHL	O1D-CGD-O2D-CED
33	j	102	LHG	C35-C36-C37-C38
33	8	618	LHG	C14-C15-C16-C17
33	n	320	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
34	9	321	LMG	C13-C14-C15-C16
34	d	410	LMG	C33-C34-C35-C36
31	1	612	CLA	CAA-CBA-CGA-O2A
30	7	321	CHL	C5-C6-C7-C8
30	n	308	CHL	C5-C6-C7-C8
34	D	411	LMG	C33-C34-C35-C36
34	a	416	LMG	C8-C9-O8-C28
30	Y	302	CHL	C16-C17-C18-C20
31	B	605	CLA	C8-C10-C11-C12
30	5	606	CHL	CHA-CBD-CGD-O1D
30	6	307	CHL	CHA-CBD-CGD-O1D
30	R	309	CHL	CHA-CBD-CGD-O1D
30	S	307	CHL	CHA-CBD-CGD-O1D
30	7	306	CHL	CHA-CBD-CGD-O2D
30	7	321	CHL	CHA-CBD-CGD-O1D
30	q	309	CHL	CHA-CBD-CGD-O2D
30	n	308	CHL	CHA-CBD-CGD-O1D
30	n	310	CHL	CHA-CBD-CGD-O1D
30	y	605	CHL	CHA-CBD-CGD-O1D
30	y	605	CHL	CHA-CBD-CGD-O2D
36	G	616	NEX	C39-C29-C30-C31
36	S	319	NEX	C39-C29-C30-C31
36	Y	317	NEX	C39-C29-C30-C31
36	8	617	NEX	C39-C29-C30-C31
36	9	319	NEX	C20-C13-C14-C15
36	9	319	NEX	C39-C29-C30-C31
37	2	619	XAT	C40-C33-C34-C35
37	G	620	XAT	C40-C33-C34-C35
37	9	322	XAT	C40-C33-C34-C35
37	q	321	XAT	C40-C33-C34-C35
31	4	610	CLA	C5-C6-C7-C8
34	n	321	LMG	O7-C10-C11-C12
38	a	411	SQD	C7-C8-C9-C10
33	G	618	LHG	C35-C36-C37-C38
33	R	320	LHG	O10-C23-C24-C25
34	W	201	LMG	C40-C41-C42-C43
33	c	622	LHG	O10-C23-O8-C6
34	0	622	LMG	C32-C33-C34-C35
38	X	201	SQD	O47-C45-C46-O48
38	g	301	SQD	O47-C45-C46-O48
38	m	101	SQD	C7-C8-C9-C10
34	1	618	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
30	6	310	CHL	C2-C3-C5-C6
30	Y	309	CHL	C2-C3-C5-C6
30	p	609	CHL	C2-C3-C5-C6
30	y	609	CHL	C2-C3-C5-C6
33	N	319	LHG	C35-C36-C37-C38
34	A	418	LMG	O6-C1-O1-C7
30	Y	301	CHL	C8-C10-C11-C12
31	R	305	CLA	C5-C6-C7-C8
31	d	404	CLA	C13-C15-C16-C17
33	B	624	LHG	C2-C3-O3-P
33	C	623	LHG	C25-C26-C27-C28
33	c	622	LHG	C16-C17-C18-C19
31	C	603	CLA	C6-C7-C8-C10
31	b	613	CLA	C11-C10-C8-C7
33	D	408	LHG	C14-C15-C16-C17
33	q	320	LHG	C9-C10-C11-C12
30	5	608	CHL	O2A-C1-C2-C3
30	7	309	CHL	O2A-C1-C2-C3
30	9	310	CHL	O2A-C1-C2-C3
36	3	319	NEX	C9-C10-C11-C12
33	N	319	LHG	C10-C11-C12-C13
33	l	101	LHG	C33-C34-C35-C36
30	4	601	CHL	C10-C11-C12-C13
34	s	321	LMG	C21-C22-C23-C24
30	1	607	CHL	C11-C12-C13-C14
30	N	307	CHL	C11-C10-C8-C9
30	0	607	CHL	C6-C7-C8-C9
30	7	306	CHL	C14-C13-C15-C16
30	g	309	CHL	C11-C10-C8-C9
31	1	610	CLA	C6-C7-C8-C9
31	C	606	CLA	C6-C7-C8-C9
31	Y	312	CLA	C11-C10-C8-C9
31	7	311	CLA	C6-C7-C8-C9
31	9	304	CLA	C6-C7-C8-C9
31	b	617	CLA	C6-C7-C8-C9
31	y	611	CLA	C11-C12-C13-C14
34	q	301	LMG	C8-C7-O1-C1
34	q1	101	LMG	C8-C7-O1-C1
38	a	411	SQD	C5-C6-S-O8
31	9	312	CLA	CAA-CBA-CGA-O2A
33	R	320	LHG	C10-C11-C12-C13
34	c	620	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
38	S	301	SQD	C12-C13-C14-C15
45	c	618	DGD	C9A-CAA-CBA-CCA
31	6	304	CLA	CAA-CBA-CGA-O1A
30	9	311	CHL	C2A-CAA-CBA-CGA
31	C	605	CLA	C2A-CAA-CBA-CGA
31	C	606	CLA	C2A-CAA-CBA-CGA
31	0	613	CLA	C2A-CAA-CBA-CGA
31	q	304	CLA	C2A-CAA-CBA-CGA
31	b	604	CLA	C2A-CAA-CBA-CGA
31	2	603	CLA	C2-C1-O2A-CGA
31	2	610	CLA	C2-C1-O2A-CGA
31	4	602	CLA	C2-C1-O2A-CGA
31	S	310	CLA	C2-C1-O2A-CGA
31	c	606	CLA	C2-C1-O2A-CGA
31	c	613	CLA	C2-C1-O2A-CGA
31	n	305	CLA	C2-C1-O2A-CGA
31	r	311	CLA	C2-C1-O2A-CGA
31	y	603	CLA	C2-C1-O2A-CGA
31	y	611	CLA	C2-C1-O2A-CGA
45	c	616	DGD	C4A-C5A-C6A-C7A
31	B	603	CLA	C5-C6-C7-C8
30	9	308	CHL	O1D-CGD-O2D-CED
33	a	415	LHG	C24-C23-O8-C6
33	e	101	LHG	C30-C31-C32-C33
33	s	322	LHG	C32-C33-C34-C35
30	0	601	CHL	C3A-C2A-CAA-CBA
31	4	614	CLA	C3A-C2A-CAA-CBA
31	5	612	CLA	C3A-C2A-CAA-CBA
31	N	305	CLA	C3A-C2A-CAA-CBA
31	8	612	CLA	C3A-C2A-CAA-CBA
31	a	406	CLA	C3A-C2A-CAA-CBA
31	n	305	CLA	C3A-C2A-CAA-CBA
31	n	314	CLA	C3A-C2A-CAA-CBA
34	5	620	LMG	O9-C10-C11-C12
34	A	414	LMG	C11-C12-C13-C14
48	R	302	LMU	C4-C5-C6-C7
33	R	320	LHG	C12-C13-C14-C15
38	B	623	SQD	C13-C14-C15-C16
38	a	412	SQD	C24-C25-C26-C27
33	7	319	LHG	C11-C10-C9-C8
34	w	201	LMG	C36-C37-C38-C39
31	2	613	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
31	3	313	CLA	CAA-CBA-CGA-O1A
34	k	102	LMG	C12-C13-C14-C15
31	6	316	CLA	C2C-C3C-CAC-CBC
34	D	410	LMG	C8-C9-O8-C28
34	B	625	LMG	C10-C11-C12-C13
34	g	322	LMG	C9-C8-O7-C10
48	K	101	LMU	C9-C10-C11-C12
38	s	301	SQD	C14-C15-C16-C17
47	E	101	HEM	C2D-C3D-CAD-CBD
31	b	609	CLA	C8-C10-C11-C12
31	c	605	CLA	C13-C15-C16-C17
42	D	401	PHO	C8-C10-C11-C12
31	q	313	CLA	CAA-CBA-CGA-O1A
30	2	601	CHL	C5-C6-C7-C8
30	q	311	CHL	C2A-CAA-CBA-CGA
31	R	311	CLA	C4-C3-C5-C6
34	j	101	LMG	C29-C30-C31-C32
31	N	312	CLA	CAA-CBA-CGA-O1A
30	4	609	CHL	C2-C3-C5-C6
30	9	309	CHL	C2-C3-C5-C6
31	R	311	CLA	C2-C3-C5-C6
44	a	414	PL9	C17-C18-C19-C21
34	d	409	LMG	C16-C17-C18-C19
31	1	612	CLA	C10-C11-C12-C13
31	a	407	CLA	C5-C6-C7-C8
31	g	310	CLA	C15-C16-C17-C18
34	w	202	LMG	C21-C22-C23-C24
36	5	618	NEX	O24-C26-C27-C28
36	G	616	NEX	C28-C29-C30-C31
36	S	319	NEX	C28-C29-C30-C31
36	Y	317	NEX	C28-C29-C30-C31
36	9	319	NEX	C28-C29-C30-C31
36	q	319	NEX	O24-C26-C27-C28
33	e	101	LHG	O9-C7-O7-C5
33	l	101	LHG	C5-C4-O6-P
30	1	608	CHL	O2A-C1-C2-C3
30	N	308	CHL	O2A-C1-C2-C3
31	b	602	CLA	O2A-C1-C2-C3
33	c	622	LHG	C25-C26-C27-C28
33	b	625	LHG	C35-C36-C37-C38
31	1	602	CLA	C10-C11-C12-C13
31	6	312	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
34	J	101	LMG	C30-C31-C32-C33
31	R	305	CLA	CBA-CGA-O2A-C1
31	8	611	CLA	CAA-CBA-CGA-O2A
31	n	313	CLA	CAA-CBA-CGA-O2A
34	b	626	LMG	C30-C31-C32-C33
34	6	323	LMG	O1-C7-C8-C9
34	C	622	LMG	O1-C7-C8-C9
34	W	201	LMG	C7-C8-C9-O8
38	G	617	SQD	O6-C44-C45-C46
45	c	618	DGD	C1G-C2G-C3G-O3G
30	9	308	CHL	CBD-CGD-O2D-CED
38	B	623	SQD	C31-C32-C33-C34
30	1	605	CHL	C5-C6-C7-C8
31	N	303	CLA	C8-C10-C11-C12
31	b	603	CLA	C10-C11-C12-C13
31	4	610	CLA	C11-C12-C13-C15
33	b	628	LHG	C14-C15-C16-C17
34	C	621	LMG	C32-C33-C34-C35
38	B	620	SQD	C27-C28-C29-C30
31	r	312	CLA	C3-C5-C6-C7
33	0	619	LHG	C25-C26-C27-C28
34	g	322	LMG	C34-C35-C36-C37
34	D	409	LMG	C10-C11-C12-C13
34	b	622	LMG	C39-C40-C41-C42
38	M	102	SQD	C16-C17-C18-C19
31	B	614	CLA	C2-C3-C5-C6
32	p	617	LUT	C13-C14-C15-C35
37	R	318	XAT	C29-C30-C31-C32
43	b	619	BCR	C13-C14-C15-C16
34	j	101	LMG	C18-C19-C20-C21
31	S	314	CLA	C15-C16-C17-C18
31	b	608	CLA	C8-C10-C11-C12
33	B	624	LHG	C11-C10-C9-C8
34	6	321	LMG	C14-C15-C16-C17
33	a	415	LHG	O10-C23-O8-C6
34	7	322	LMG	O7-C10-C11-C12
30	7	308	CHL	CBD-CGD-O2D-CED
33	d	408	LHG	C8-C7-O7-C5
33	e	101	LHG	C8-C7-O7-C5
45	c	619	DGD	O1A-C1A-C2A-C3A
34	2	621	LMG	O7-C8-C9-O8
34	3	321	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
30	9	311	CHL	C8-C10-C11-C12
31	4	613	CLA	C6-C7-C8-C9
31	5	610	CLA	C11-C10-C8-C9
31	6	313	CLA	C11-C10-C8-C9
31	B	606	CLA	C6-C7-C8-C9
31	C	605	CLA	C6-C7-C8-C9
31	C	605	CLA	C14-C13-C15-C16
31	G	602	CLA	C11-C12-C13-C14
31	S	311	CLA	C11-C10-C8-C9
31	b	614	CLA	C11-C12-C13-C14
31	c	603	CLA	C6-C7-C8-C9
31	c	607	CLA	C11-C10-C8-C9
31	c	611	CLA	C14-C13-C15-C16
31	d	404	CLA	C11-C10-C8-C9
31	s	303	CLA	C11-C10-C8-C9
42	A	408	PHO	C6-C7-C8-C9
42	a	408	PHO	C14-C13-C15-C16
38	M	102	SQD	C17-C18-C19-C20
45	C	618	DGD	C2B-C3B-C4B-C5B
30	2	601	CHL	O1A-CGA-O2A-C1
33	Y	318	LHG	O6-C4-C5-C6
34	B	621	LMG	C10-C11-C12-C13
43	a	410	BCR	C17-C18-C19-C20
38	A	411	SQD	C33-C34-C35-C36
31	1	614	CLA	C4-C3-C5-C6
30	7	308	CHL	O1D-CGD-O2D-CED
34	W	202	LMG	O9-C10-C11-C12
33	8	618	LHG	C19-C20-C21-C22
33	n	320	LHG	C19-C20-C21-C22
34	6	323	LMG	C34-C35-C36-C37
38	X	201	SQD	C10-C11-C12-C13
30	0	607	CHL	C6-C7-C8-C10
30	9	311	CHL	C6-C7-C8-C10
30	y	601	CHL	C11-C12-C13-C15
31	1	604	CLA	C11-C10-C8-C7
31	1	610	CLA	C6-C7-C8-C10
31	1	611	CLA	C11-C12-C13-C15
31	6	312	CLA	C11-C10-C8-C7
31	N	303	CLA	C6-C7-C8-C10
31	N	303	CLA	C11-C12-C13-C15
31	N	305	CLA	C11-C10-C8-C7
31	R	316	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
31	Y	312	CLA	C11-C10-C8-C7
31	Y	312	CLA	C11-C12-C13-C15
31	7	311	CLA	C6-C7-C8-C10
31	7	311	CLA	C11-C10-C8-C7
31	8	609	CLA	C6-C7-C8-C10
31	p	602	CLA	C6-C7-C8-C10
31	b	605	CLA	C6-C7-C8-C10
31	b	607	CLA	C6-C7-C8-C10
31	b	611	CLA	C6-C7-C8-C10
31	b	611	CLA	C11-C12-C13-C15
31	b	617	CLA	C6-C7-C8-C10
31	c	601	CLA	C11-C10-C8-C7
31	c	609	CLA	C11-C10-C8-C7
31	s	312	CLA	C11-C10-C8-C7
42	A	408	PHO	C11-C10-C8-C7
31	6	305	CLA	C2B-C3B-CAB-CBB
31	B	611	CLA	C2B-C3B-CAB-CBB
31	B	615	CLA	C2B-C3B-CAB-CBB
31	S	310	CLA	C2B-C3B-CAB-CBB
31	0	615	CLA	C2B-C3B-CAB-CBB
31	b	613	CLA	C2B-C3B-CAB-CBB
31	d	401	CLA	C2B-C3B-CAB-CBB
31	r	316	CLA	C2B-C3B-CAB-CBB
32	2	615	LUT	C5-C6-C7-C8
32	S	318	LUT	C5-C6-C7-C8
32	p	617	LUT	C5-C6-C7-C8
32	s	318	LUT	C5-C6-C7-C8
43	B	617	BCR	C23-C24-C25-C26
43	B	619	BCR	C5-C6-C7-C8
43	b	619	BCR	C5-C6-C7-C8
43	v	101	BCR	C23-C24-C25-C26
34	g	322	LMG	C30-C31-C32-C33
30	7	302	CHL	C10-C11-C12-C13
33	Y	318	LHG	C8-C7-O7-C5
33	d	408	LHG	O7-C7-C8-C9
34	x	202	LMG	O8-C28-C29-C30
34	4	621	LMG	C13-C14-C15-C16
30	R	310	CHL	C2-C1-O2A-CGA
31	3	301	CLA	C2-C1-O2A-CGA
31	3	306	CLA	C2-C1-O2A-CGA
31	A	409	CLA	C2-C1-O2A-CGA
31	S	313	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
31	S	314	CLA	C2-C1-O2A-CGA
31	0	615	CLA	C2-C1-O2A-CGA
31	a	409	CLA	C2-C1-O2A-CGA
31	b	604	CLA	C2-C1-O2A-CGA
31	b	608	CLA	C2-C1-O2A-CGA
31	c	605	CLA	C2-C1-O2A-CGA
31	s	305	CLA	C2-C1-O2A-CGA
31	7	311	CLA	O1A-CGA-O2A-C1
33	b	625	LHG	C33-C34-C35-C36
30	p	608	CHL	O2A-C1-C2-C3
31	7	311	CLA	CBA-CGA-O2A-C1
31	g	310	CLA	C16-C17-C18-C20
31	s	313	CLA	C4C-C3C-CAC-CBC
31	6	311	CLA	C15-C16-C17-C18
33	S	320	LHG	O7-C7-C8-C9
34	9	321	LMG	O8-C28-C29-C30
38	6	301	SQD	O48-C23-C24-C25
33	j	102	LHG	C33-C34-C35-C36
34	6	321	LMG	O6-C5-C6-O5
38	R	322	SQD	C29-C30-C31-C32
34	Y	319	LMG	C30-C31-C32-C33
31	G	612	CLA	CAA-CBA-CGA-O2A
34	7	301	LMG	O7-C10-C11-C12
38	M	102	SQD	O47-C7-C8-C9
38	x	201	SQD	O48-C23-C24-C25
31	1	614	CLA	C2-C3-C5-C6
31	6	315	CLA	C2-C3-C5-C6
31	B	612	CLA	C10-C11-C12-C13
31	S	311	CLA	C5-C6-C7-C8
34	7	301	LMG	C13-C14-C15-C16
31	c	612	CLA	C2A-CAA-CBA-CGA
31	n	303	CLA	C2A-CAA-CBA-CGA
31	B	604	CLA	C13-C15-C16-C17
31	C	608	CLA	C13-C15-C16-C17
31	7	311	CLA	C13-C15-C16-C17
34	A	418	LMG	C29-C30-C31-C32
31	C	603	CLA	CAA-CBA-CGA-O2A
33	p	619	LHG	O8-C23-C24-C25
34	D	410	LMG	O8-C28-C29-C30
34	N	320	LMG	O7-C10-C11-C12
34	r	321	LMG	O7-C10-C11-C12
31	y	612	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
34	d	410	LMG	C31-C32-C33-C34
31	8	612	CLA	C10-C11-C12-C13
31	b	615	CLA	C10-C11-C12-C13
31	n	314	CLA	C10-C11-C12-C13
34	D	411	LMG	C31-C32-C33-C34
31	C	605	CLA	CAA-CBA-CGA-O2A
31	S	314	CLA	CAA-CBA-CGA-O2A
31	a	406	CLA	CAA-CBA-CGA-O2A
33	2	617	LHG	O8-C23-C24-C25
33	3	320	LHG	O8-C23-C24-C25
33	4	618	LHG	O8-C23-C24-C25
34	C	622	LMG	O7-C10-C11-C12
33	B	624	LHG	O9-C7-C8-C9
33	Y	318	LHG	O9-C7-O7-C5
32	4	616	LUT	C13-C14-C15-C35
32	7	318	LUT	C13-C14-C15-C35
38	G	617	SQD	C4-C5-C6-S
38	a	412	SQD	C4-C5-C6-S
38	g	301	SQD	C4-C5-C6-S
38	s	301	SQD	C4-C5-C6-S
38	x	201	SQD	C4-C5-C6-S
31	1	602	CLA	C4-C3-C5-C6
34	9	302	LMG	C13-C14-C15-C16
31	7	314	CLA	CAA-CBA-CGA-O2A
33	S	320	LHG	O8-C23-C24-C25
30	2	601	CHL	CBA-CGA-O2A-C1
34	6	321	LMG	C10-C11-C12-C13
33	N	319	LHG	C27-C28-C29-C30
31	S	311	CLA	C2A-CAA-CBA-CGA
33	B	624	LHG	C18-C19-C20-C21
33	c	622	LHG	C26-C27-C28-C29
31	3	315	CLA	CAA-CBA-CGA-O2A
31	Y	313	CLA	CAA-CBA-CGA-O2A
31	0	613	CLA	CAA-CBA-CGA-O2A
33	L	101	LHG	C27-C28-C29-C30
34	w	204	LMG	C33-C34-C35-C36
33	S	322	LHG	O9-C7-O7-C5
31	C	609	CLA	C8-C10-C11-C12
30	s	302	CHL	CAA-CBA-CGA-O2A
31	4	611	CLA	CAA-CBA-CGA-O2A
31	5	602	CLA	C11-C10-C8-C9
31	A	409	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
31	B	612	CLA	C11-C10-C8-C9
31	C	607	CLA	C11-C10-C8-C9
31	G	602	CLA	C11-C10-C8-C9
31	G	602	CLA	C14-C13-C15-C16
31	a	409	CLA	C11-C10-C8-C9
31	n	311	CLA	C11-C12-C13-C14
31	y	602	CLA	C11-C10-C8-C9
42	A	408	PHO	C14-C13-C15-C16
38	b	627	SQD	C27-C28-C29-C30
36	2	616	NEX	C11-C12-C13-C20
30	p	607	CHL	CAA-CBA-CGA-O2A
31	1	613	CLA	CAA-CBA-CGA-O2A
31	4	613	CLA	CAA-CBA-CGA-O2A
31	S	303	CLA	CAA-CBA-CGA-O2A
31	0	615	CLA	CAA-CBA-CGA-O2A
31	7	312	CLA	CAA-CBA-CGA-O2A
33	3	320	LHG	O7-C7-C8-C9
33	L	101	LHG	O7-C7-C8-C9
33	0	619	LHG	O8-C23-C24-C25
33	l	101	LHG	O8-C23-C24-C25
33	F1	301	LHG	O8-C23-C24-C25
34	I	101	LMG	O8-C28-C29-C30
34	0	622	LMG	O7-C10-C11-C12
34	b	601	LMG	O7-C10-C11-C12
33	p	619	LHG	C4-C5-C6-O8
38	s	301	SQD	O6-C44-C45-C46
31	5	602	CLA	C11-C12-C13-C14
31	1	612	CLA	C1A-C2A-CAA-CBA
31	5	612	CLA	C1A-C2A-CAA-CBA
31	A	405	CLA	C1A-C2A-CAA-CBA
31	B	602	CLA	C4B-C3B-CAB-CBB
31	G	610	CLA	C4B-C3B-CAB-CBB
31	R	311	CLA	C1A-C2A-CAA-CBA
31	R	314	CLA	C4B-C3B-CAB-CBB
31	R	316	CLA	C4B-C3B-CAB-CBB
31	S	312	CLA	C4B-C3B-CAB-CBB
31	9	316	CLA	C1A-C2A-CAA-CBA
31	d	401	CLA	C4B-C3B-CAB-CBB
31	r	314	CLA	C4B-C3B-CAB-CBB
31	s	310	CLA	C4B-C3B-CAB-CBB
31	8	611	CLA	CAA-CBA-CGA-O1A
34	G	621	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
38	b	627	SQD	C28-C29-C30-C31
30	Y	308	CHL	CBA-CGA-O2A-C1
34	A	414	LMG	C34-C35-C36-C37
34	s	321	LMG	C15-C16-C17-C18
31	B	607	CLA	C5-C6-C7-C8
31	B	615	CLA	C13-C15-C16-C17
30	8	605	CHL	CAA-CBA-CGA-O2A
30	n	306	CHL	CAA-CBA-CGA-O2A
31	5	613	CLA	CAA-CBA-CGA-O2A
31	B	604	CLA	CAA-CBA-CGA-O2A
31	S	316	CLA	CAA-CBA-CGA-O2A
31	p	614	CLA	CAA-CBA-CGA-O2A
31	b	609	CLA	CAA-CBA-CGA-O2A
31	y	613	CLA	CAA-CBA-CGA-O2A
33	A	415	LHG	O7-C7-C8-C9
33	a	415	LHG	O8-C23-C24-C25
34	I	101	LMG	O7-C10-C11-C12
34	j	101	LMG	O7-C10-C11-C12
34	k	101	LMG	O7-C10-C11-C12
38	S	301	SQD	O47-C7-C8-C9
30	8	605	CHL	C2-C3-C5-C6
30	n	306	CHL	C2-C3-C5-C6
31	N	315	CLA	C2-C3-C5-C6
34	2	618	LMG	O7-C8-C9-O8
45	C	618	DGD	O2G-C2G-C3G-O3G
44	D	406	PL9	C21-C22-C23-C24
34	n	322	LMG	C11-C12-C13-C14
32	7	317	LUT	C27-C28-C29-C30
32	8	616	LUT	C11-C12-C13-C14
32	n	318	LUT	C11-C12-C13-C14
32	r	317	LUT	C7-C8-C9-C10
32	y	616	LUT	C7-C8-C9-C10
36	2	616	NEX	C11-C12-C13-C14
43	H	101	BCR	C17-C18-C19-C20
43	h	101	BCR	C17-C18-C19-C20
36	N	318	NEX	C9-C10-C11-C12
30	Y	308	CHL	O1A-CGA-O2A-C1
31	B	615	CLA	C16-C17-C18-C19
31	y	613	CLA	C16-C17-C18-C20
42	A	408	PHO	C16-C17-C18-C19
30	q	309	CHL	CBA-CGA-O2A-C1
34	W	201	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
31	n	313	CLA	CAA-CBA-CGA-O1A
30	N	306	CHL	CAA-CBA-CGA-O2A
30	p	608	CHL	CAA-CBA-CGA-O2A
30	q	308	CHL	CAA-CBA-CGA-O2A
30	n	301	CHL	CAA-CBA-CGA-O2A
31	6	316	CLA	CAA-CBA-CGA-O2A
31	9	306	CLA	CAA-CBA-CGA-O2A
33	6	320	LHG	O7-C7-C8-C9
33	y	619	LHG	O8-C23-C24-C25
34	9	302	LMG	O7-C10-C11-C12
38	G	624	SQD	O47-C7-C8-C9
38	m	101	SQD	O47-C7-C8-C9
33	L	101	LHG	C17-C18-C19-C20
45	c	617	DGD	C4B-C5B-C6B-C7B
31	b	607	CLA	C5-C6-C7-C8
33	0	619	LHG	C24-C25-C26-C27
31	R	304	CLA	C8-C10-C11-C12
31	8	604	CLA	C8-C10-C11-C12
38	a	411	SQD	C29-C30-C31-C32
31	c	610	CLA	C16-C17-C18-C20
30	r	308	CHL	CAA-CBA-CGA-O2A
31	2	612	CLA	CAA-CBA-CGA-O2A
31	6	315	CLA	CAA-CBA-CGA-O2A
31	B	614	CLA	CAA-CBA-CGA-O2A
31	B	616	CLA	CAA-CBA-CGA-O2A
33	1	617	LHG	O7-C7-C8-C9
33	R	320	LHG	O7-C7-C8-C9
33	t	102	LHG	O8-C23-C24-C25
34	x	202	LMG	O7-C10-C11-C12
34	k	101	LMG	C37-C38-C39-C40
33	F1	301	LHG	C25-C26-C27-C28
34	r	321	LMG	O6-C5-C6-O5
38	A	411	SQD	C5-C6-S-O9
38	a	411	SQD	C5-C6-S-O9
44	d	407	PL9	C11-C12-C13-C14
31	6	303	CLA	C10-C11-C12-C13
31	b	611	CLA	C15-C16-C17-C18
31	G	604	CLA	C4-C3-C5-C6
31	q	315	CLA	C4-C3-C5-C6
31	c	611	CLA	C4-C3-C5-C6
31	d	405	CLA	C4-C3-C5-C6
34	m	102	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
31	G	612	CLA	C2-C1-O2A-CGA
31	p	603	CLA	C2-C1-O2A-CGA
31	p	610	CLA	C2-C1-O2A-CGA
31	b	615	CLA	C2-C1-O2A-CGA
31	b	617	CLA	C2-C1-O2A-CGA
31	s	303	CLA	C2-C1-O2A-CGA
30	6	308	CHL	CAA-CBA-CGA-O2A
30	Y	307	CHL	CAA-CBA-CGA-O2A
33	r	320	LHG	O7-C7-C8-C9
30	1	601	CHL	C11-C12-C13-C15
30	g	309	CHL	C6-C7-C8-C10
31	1	610	CLA	C11-C12-C13-C15
31	5	611	CLA	C6-C7-C8-C10
31	B	609	CLA	C12-C13-C15-C16
31	B	613	CLA	C11-C10-C8-C7
31	C	605	CLA	C12-C13-C15-C16
31	C	609	CLA	C11-C12-C13-C15
31	S	305	CLA	C12-C13-C15-C16
31	7	312	CLA	C11-C12-C13-C15
31	9	304	CLA	C6-C7-C8-C10
31	q	315	CLA	C12-C13-C15-C16
31	b	604	CLA	C6-C7-C8-C10
31	d	404	CLA	C11-C12-C13-C15
31	n	311	CLA	C6-C7-C8-C10
31	r	305	CLA	C11-C10-C8-C7
31	6	305	CLA	C5-C6-C7-C8
33	2	617	LHG	C19-C20-C21-C22
34	I	101	LMG	C11-C12-C13-C14
34	c	620	LMG	C29-C30-C31-C32
34	n	321	LMG	C34-C35-C36-C37
34	2	621	LMG	C7-C8-O7-C10
34	A	414	LMG	C7-C8-O7-C10
34	p	620	LMG	C9-C8-O7-C10
34	g	322	LMG	C7-C8-O7-C10
42	d	402	PHO	O2A-C1-C2-C3
45	c	617	DGD	C3G-C2G-O2G-C1B
33	c	622	LHG	C28-C29-C30-C31
30	N	308	CHL	O1A-CGA-O2A-C1
30	N	301	CHL	CAA-CBA-CGA-O2A
31	R	316	CLA	CAA-CBA-CGA-O2A
31	b	607	CLA	CAA-CBA-CGA-O2A
34	b	626	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
31	r	311	CLA	C5-C6-C7-C8
31	y	612	CLA	C10-C11-C12-C13
33	l	101	LHG	C10-C11-C12-C13
38	G	617	SQD	C24-C25-C26-C27
38	a	411	SQD	C25-C26-C27-C28
31	2	602	CLA	C2A-CAA-CBA-CGA
31	5	615	CLA	C2A-CAA-CBA-CGA
31	s	305	CLA	C2A-CAA-CBA-CGA
31	s	311	CLA	C2A-CAA-CBA-CGA
31	g	311	CLA	C11-C12-C13-C14
33	l	101	LHG	C17-C18-C19-C20
34	J	102	LMG	C31-C32-C33-C34
30	6	306	CHL	CAA-CBA-CGA-O1A
34	4	621	LMG	C14-C15-C16-C17
38	M	102	SQD	C13-C14-C15-C16
30	q	309	CHL	C5-C6-C7-C8
30	5	608	CHL	CAA-CBA-CGA-O2A
33	t	102	LHG	C10-C11-C12-C13
31	3	316	CLA	C5-C6-C7-C8
31	B	605	CLA	C10-C11-C12-C13
30	G	605	CHL	C3A-C2A-CAA-CBA
30	0	607	CHL	C3A-C2A-CAA-CBA
30	g	306	CHL	C3A-C2A-CAA-CBA
31	5	614	CLA	C3A-C2A-CAA-CBA
31	8	604	CLA	C3A-C2A-CAA-CBA
31	9	304	CLA	C3A-C2A-CAA-CBA
31	s	316	CLA	C3A-C2A-CAA-CBA
42	D	401	PHO	C3A-C2A-CAA-CBA
33	S	320	LHG	O9-C7-C8-C9
31	0	614	CLA	O1A-CGA-O2A-C1
30	0	607	CHL	C5-C6-C7-C8
31	B	612	CLA	C16-C17-C18-C19
31	b	606	CLA	C16-C17-C18-C20
38	6	301	SQD	C26-C27-C28-C29
30	y	606	CHL	CAA-CBA-CGA-O2A
31	R	312	CLA	CAA-CBA-CGA-O2A
31	s	314	CLA	CAA-CBA-CGA-O2A
31	r	311	CLA	C2-C3-C5-C6
31	1	610	CLA	C13-C15-C16-C17
31	N	303	CLA	C15-C16-C17-C18
33	t	102	LHG	C33-C34-C35-C36
31	C	603	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
31	G	612	CLA	CAA-CBA-CGA-O1A
38	6	301	SQD	O10-C23-C24-C25
30	8	608	CHL	CAA-CBA-CGA-O2A
34	9	302	LMG	O8-C28-C29-C30
34	4	621	LMG	C12-C13-C14-C15
31	0	615	CLA	CAA-CBA-CGA-O1A
33	d	408	LHG	O9-C7-C8-C9
34	r	321	LMG	O9-C10-C11-C12
31	r	311	CLA	C4C-C3C-CAC-CBC
45	c	616	DGD	C4D-C5D-C6D-O5D
31	0	611	CLA	C8-C10-C11-C12
31	b	606	CLA	C10-C11-C12-C13
38	A	413	SQD	C13-C14-C15-C16
30	1	619	CHL	C11-C10-C8-C9
31	1	610	CLA	C11-C12-C13-C14
31	1	610	CLA	C14-C13-C15-C16
31	6	303	CLA	C11-C12-C13-C14
31	B	603	CLA	C11-C10-C8-C9
31	B	604	CLA	C14-C13-C15-C16
31	R	316	CLA	C11-C10-C8-C9
31	7	312	CLA	C11-C12-C13-C14
31	b	604	CLA	C6-C7-C8-C9
31	b	607	CLA	C6-C7-C8-C9
34	2	620	LMG	C11-C12-C13-C14
31	3	306	CLA	CAA-CBA-CGA-O2A
34	b	624	LMG	O7-C10-C11-C12
31	C	605	CLA	CAA-CBA-CGA-O1A
31	S	316	CLA	CAA-CBA-CGA-O1A
31	a	406	CLA	CAA-CBA-CGA-O1A
33	4	618	LHG	O10-C23-C24-C25
33	p	619	LHG	O10-C23-C24-C25
34	0	622	LMG	O9-C10-C11-C12
34	7	322	LMG	O9-C10-C11-C12
38	M	102	SQD	O49-C7-C8-C9
31	6	315	CLA	C5-C6-C7-C8
33	C	623	LHG	C30-C31-C32-C33
34	S	321	LMG	C19-C20-C21-C22
31	r	311	CLA	C2C-C3C-CAC-CBC
31	Y	312	CLA	C8-C10-C11-C12
31	c	601	CLA	C10-C11-C12-C13
37	r	318	XAT	C29-C30-C31-C32
43	C	615	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
31	4	611	CLA	CAA-CBA-CGA-O1A
34	x	202	LMG	C29-C30-C31-C32
31	y	614	CLA	O1D-CGD-O2D-CED
30	0	607	CHL	C10-C11-C12-C13
31	5	611	CLA	C8-C10-C11-C12
31	S	310	CLA	C8-C10-C11-C12
31	s	314	CLA	C10-C11-C12-C13
31	S	314	CLA	CAA-CBA-CGA-O1A
34	k	101	LMG	O9-C10-C11-C12
38	y	621	SQD	C24-C23-O48-C46
31	b	605	CLA	CAA-CBA-CGA-O2A
31	g	313	CLA	CAA-CBA-CGA-O2A
33	s	320	LHG	O8-C23-C24-C25
30	y	607	CHL	C2-C3-C5-C6
38	G	624	SQD	O5-C5-C6-S
30	s	302	CHL	CAA-CBA-CGA-O1A
31	1	613	CLA	CAA-CBA-CGA-O1A
31	3	315	CLA	CAA-CBA-CGA-O1A
31	7	314	CLA	CAA-CBA-CGA-O1A
33	r	320	LHG	O9-C7-C8-C9
34	N	320	LMG	O9-C10-C11-C12
34	x	202	LMG	O10-C28-C29-C30
33	A	417	LHG	C10-C11-C12-C13
34	3	321	LMG	C11-C12-C13-C14
45	C	620	DGD	C6B-C7B-C8B-C9B
31	6	316	CLA	C3-C5-C6-C7
33	D	408	LHG	C19-C20-C21-C22
34	y	620	LMG	C31-C32-C33-C34
30	n	310	CHL	CAA-CBA-CGA-O2A
33	8	618	LHG	O8-C23-C24-C25
32	7	318	LUT	C31-C32-C33-C34
30	N	308	CHL	CBA-CGA-O2A-C1
30	p	601	CHL	CAA-CBA-CGA-O1A
31	2	612	CLA	CAA-CBA-CGA-O1A
31	4	613	CLA	CAA-CBA-CGA-O1A
31	B	604	CLA	CAA-CBA-CGA-O1A
31	B	616	CLA	CAA-CBA-CGA-O1A
31	N	314	CLA	CAA-CBA-CGA-O1A
33	F1	301	LHG	O10-C23-C24-C25
34	9	321	LMG	O10-C28-C29-C30
33	q	320	LHG	C12-C13-C14-C15
34	d	409	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
45	C	616	DGD	C5D-C6D-O5D-C1E
45	C	617	DGD	C2G-C3G-O3G-C1D
33	p	619	LHG	O7-C5-C6-O8
34	D	410	LMG	O7-C8-C9-O8
34	B	625	LMG	C32-C33-C34-C35
33	A	417	LHG	C34-C35-C36-C37
38	B	623	SQD	C24-C25-C26-C27
31	S	303	CLA	CAA-CBA-CGA-O1A
31	p	614	CLA	CAA-CBA-CGA-O1A
33	S	320	LHG	O10-C23-C24-C25
34	C	622	LMG	O9-C10-C11-C12
34	D	410	LMG	O10-C28-C29-C30
34	7	301	LMG	O9-C10-C11-C12
34	9	302	LMG	O9-C10-C11-C12
38	m	101	SQD	O49-C7-C8-C9
30	2	606	CHL	CAA-CBA-CGA-O2A
30	4	606	CHL	CAA-CBA-CGA-O2A
30	R	308	CHL	CAA-CBA-CGA-O2A
30	0	605	CHL	CAA-CBA-CGA-O2A
31	G	613	CLA	CAA-CBA-CGA-O2A
31	q	315	CLA	CAA-CBA-CGA-O2A
33	n	320	LHG	O8-C23-C24-C25
38	a	411	SQD	C11-C10-C9-C8
31	4	613	CLA	C14-C13-C15-C16
34	3	321	LMG	C29-C30-C31-C32
33	5	619	LHG	C24-C25-C26-C27
38	b	627	SQD	C17-C18-C19-C20
45	c	617	DGD	C4A-C5A-C6A-C7A
30	p	608	CHL	CAA-CBA-CGA-O1A
33	2	617	LHG	O10-C23-C24-C25
33	3	320	LHG	O9-C7-C8-C9
33	0	619	LHG	O10-C23-C24-C25
33	a	415	LHG	O10-C23-C24-C25
33	l	101	LHG	O10-C23-C24-C25
34	j	101	LMG	O9-C10-C11-C12
38	G	624	SQD	O49-C7-C8-C9
44	D	406	PL9	C11-C12-C13-C14
44	d	407	PL9	C31-C32-C33-C34
45	c	617	DGD	C2B-C3B-C4B-C5B
31	c	609	CLA	C8-C10-C11-C12
30	1	619	CHL	CAA-CBA-CGA-O2A
31	Y	311	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	0	604	CLA	CAA-CBA-CGA-O2A
33	9	320	LHG	O7-C7-C8-C9
34	1	618	LMG	O7-C10-C11-C12
31	9	306	CLA	C2-C3-C5-C6
31	q	315	CLA	C2-C3-C5-C6
30	N	306	CHL	CAA-CBA-CGA-O1A
30	p	607	CHL	CAA-CBA-CGA-O1A
30	q	308	CHL	CAA-CBA-CGA-O1A
31	b	609	CLA	CAA-CBA-CGA-O1A
31	y	613	CLA	CAA-CBA-CGA-O1A
33	1	617	LHG	O9-C7-C8-C9
33	3	320	LHG	O10-C23-C24-C25
34	b	626	LMG	O10-C28-C29-C30
34	a	413	LMG	C28-C29-C30-C31
30	5	607	CHL	CAD-CBD-CGD-O2D
30	0	605	CHL	CAD-CBD-CGD-O2D
31	G	604	CLA	CAD-CBD-CGD-O2D
31	y	612	CLA	CAD-CBD-CGD-O2D
31	r	303	CLA	C2C-C3C-CAC-CBC
30	8	608	CHL	C10-C11-C12-C13
30	1	605	CHL	CAA-CBA-CGA-O2A
30	7	309	CHL	CAA-CBA-CGA-O2A
31	b	617	CLA	CAA-CBA-CGA-O2A
33	9	320	LHG	O8-C23-C24-C25
33	s	322	LHG	O7-C7-C8-C9
34	b	622	LMG	O7-C10-C11-C12
34	w	204	LMG	O7-C10-C11-C12
38	M	102	SQD	O48-C23-C24-C25
44	A	416	PL9	C7-C8-C9-C10
34	d	409	LMG	C15-C16-C17-C18
31	0	613	CLA	CAA-CBA-CGA-O1A
31	7	312	CLA	CAA-CBA-CGA-O1A
33	t	102	LHG	O10-C23-C24-C25
33	y	619	LHG	O10-C23-C24-C25
45	c	617	DGD	O1A-C1A-C2A-C3A
31	6	316	CLA	C4C-C3C-CAC-CBC
31	Y	305	CLA	C2-C1-O2A-CGA
31	Y	312	CLA	C2-C1-O2A-CGA
34	d	411	LMG	C11-C12-C13-C14
31	6	316	CLA	CAA-CBA-CGA-O1A
34	I	101	LMG	O10-C28-C29-C30
38	x	201	SQD	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
30	R	309	CHL	CAA-CBA-CGA-O2A
31	B	608	CLA	CAA-CBA-CGA-O2A
31	s	303	CLA	CAA-CBA-CGA-O2A
31	y	615	CLA	CAA-CBA-CGA-O2A
34	B	621	LMG	O7-C10-C11-C12
30	0	601	CHL	C1A-C2A-CAA-CBA
30	0	607	CHL	C1A-C2A-CAA-CBA
31	1	612	CLA	C16-C17-C18-C20
34	A	412	LMG	C11-C12-C13-C14
34	2	620	LMG	C40-C41-C42-C43
34	2	620	LMG	C19-C20-C21-C22
34	6	322	LMG	C32-C33-C34-C35
30	5	608	CHL	CAA-CBA-CGA-O1A
30	N	301	CHL	CAA-CBA-CGA-O1A
31	6	315	CLA	CAA-CBA-CGA-O1A
31	Y	313	CLA	CAA-CBA-CGA-O1A
33	L	101	LHG	O9-C7-C8-C9
31	5	611	CLA	C5-C6-C7-C8
31	7	305	CLA	C13-C15-C16-C17
31	C	602	CLA	C4-C3-C5-C6
34	A	418	LMG	O6-C5-C6-O5
30	7	321	CHL	CAA-CBA-CGA-O2A
30	n	308	CHL	CAA-CBA-CGA-O2A
31	2	610	CLA	CAA-CBA-CGA-O2A
31	C	604	CLA	CAA-CBA-CGA-O2A
31	D	404	CLA	CAA-CBA-CGA-O2A
33	1	617	LHG	O8-C23-C24-C25
33	D	407	LHG	O8-C23-C24-C25
33	Y	318	LHG	O8-C23-C24-C25
33	e	101	LHG	O7-C7-C8-C9
33	j	102	LHG	O7-C7-C8-C9
34	4	620	LMG	O7-C10-C11-C12
34	C	624	LMG	O7-C10-C11-C12
34	d	409	LMG	O7-C10-C11-C12
38	A	413	SQD	O47-C7-C8-C9
38	a	411	SQD	O47-C7-C8-C9
38	a	412	SQD	O47-C7-C8-C9
34	C	624	LMG	C19-C20-C21-C22
42	a	408	PHO	C13-C15-C16-C17
33	S	322	LHG	C8-C7-O7-C5
30	Y	307	CHL	CAA-CBA-CGA-O1A
30	r	308	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
31	b	617	CLA	CAA-CBA-CGA-O1A
31	s	303	CLA	CAA-CBA-CGA-O1A
34	I	101	LMG	O9-C10-C11-C12
45	C	620	DGD	C7B-C8B-C9B-CAB
38	a	412	SQD	C25-C26-C27-C28
30	8	605	CHL	CBD-CGD-O2D-CED
30	4	607	CHL	CAA-CBA-CGA-O2A
31	2	602	CLA	CAA-CBA-CGA-O2A
31	N	305	CLA	CAA-CBA-CGA-O2A
31	p	613	CLA	CAA-CBA-CGA-O2A
34	c	621	LMG	O7-C10-C11-C12
38	X	201	SQD	O47-C7-C8-C9
34	B	621	LMG	C33-C34-C35-C36
34	G	622	LMG	C14-C15-C16-C17
31	n	305	CLA	C5-C6-C7-C8
30	6	306	CHL	CAA-CBA-CGA-O2A
30	6	308	CHL	CAA-CBA-CGA-O1A
30	7	309	CHL	CAA-CBA-CGA-O1A
30	8	605	CHL	CAA-CBA-CGA-O1A
30	n	301	CHL	CAA-CBA-CGA-O1A
31	5	613	CLA	CAA-CBA-CGA-O1A
31	B	614	CLA	CAA-CBA-CGA-O1A
31	b	605	CLA	CAA-CBA-CGA-O1A
33	1	617	LHG	O10-C23-C24-C25
34	9	302	LMG	O10-C28-C29-C30
34	b	601	LMG	O9-C10-C11-C12
33	t	102	LHG	C31-C32-C33-C34
34	C	624	LMG	C29-C30-C31-C32
45	c	619	DGD	C9A-CAA-CBA-CCA
33	e	101	LHG	C35-C36-C37-C38
30	3	309	CHL	O1D-CGD-O2D-CED
33	Y	318	LHG	C25-C26-C27-C28

There are no ring outliers.

654 monomers are involved in 3749 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	b	601	LMG	4	0
31	s	306	CLA	11	0
31	S	303	CLA	9	0
33	Y	318	LHG	4	0
32	1	615	LUT	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	5	620	LMG	11	0
30	5	605	CHL	11	0
31	q	312	CLA	22	0
31	9	312	CLA	15	0
31	4	604	CLA	16	0
43	b	619	BCR	4	0
30	9	309	CHL	13	0
33	8	618	LHG	4	0
31	3	311	CLA	8	0
31	7	315	CLA	3	0
31	B	609	CLA	7	0
30	S	309	CHL	3	0
34	D	412	LMG	2	0
30	q	311	CHL	6	0
31	N	303	CLA	2	0
31	7	303	CLA	3	0
31	r	312	CLA	5	0
33	b	628	LHG	13	0
42	D	401	PHO	9	0
31	n	311	CLA	14	0
34	Y	319	LMG	5	0
31	r	316	CLA	4	0
31	y	613	CLA	8	0
34	G	622	LMG	12	0
36	2	616	NEX	6	0
38	g	301	SQD	12	0
30	g	307	CHL	9	0
31	p	604	CLA	4	0
33	b	625	LHG	8	0
31	8	603	CLA	12	0
31	B	601	CLA	2	0
31	g	303	CLA	4	0
31	6	304	CLA	7	0
38	S	301	SQD	4	0
30	n	310	CHL	9	0
34	a	416	LMG	3	0
31	A	405	CLA	7	0
34	f	101	LMG	1	0
30	1	609	CHL	6	0
31	B	608	CLA	5	0
33	r	320	LHG	3	0
34	b	622	LMG	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	7	308	CHL	11	0
31	G	613	CLA	1	0
31	a	407	CLA	3	0
31	6	316	CLA	4	0
31	C	613	CLA	7	0
31	c	613	CLA	8	0
31	9	305	CLA	9	0
31	1	613	CLA	2	0
32	0	616	LUT	6	0
30	Y	302	CHL	10	0
33	C	623	LHG	7	0
31	9	316	CLA	1	0
36	0	618	NEX	10	0
31	C	606	CLA	8	0
30	G	606	CHL	10	0
31	c	606	CLA	14	0
32	9	318	LUT	15	0
34	0	622	LMG	5	0
34	J	102	LMG	1	0
30	6	306	CHL	6	0
30	n	306	CHL	10	0
32	7	317	LUT	11	0
30	p	606	CHL	8	0
30	3	307	CHL	16	0
48	c	623	LMU	3	0
31	D	403	CLA	8	0
30	4	609	CHL	9	0
30	q	307	CHL	9	0
32	2	615	LUT	8	0
33	1	617	LHG	5	0
30	2	601	CHL	5	0
31	R	315	CLA	2	0
34	k	101	LMG	3	0
32	R	317	LUT	3	0
31	C	608	CLA	9	0
31	c	604	CLA	2	0
31	c	608	CLA	9	0
31	b	613	CLA	9	0
31	C	605	CLA	6	0
30	G	605	CHL	7	0
32	S	318	LUT	8	0
31	1	611	CLA	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	3	321	LMG	13	0
31	3	301	CLA	10	0
30	n	302	CHL	8	0
31	b	606	CLA	5	0
30	y	606	CHL	10	0
42	d	402	PHO	5	0
33	S	322	LHG	5	0
30	0	608	CHL	7	0
32	3	317	LUT	11	0
31	r	305	CLA	8	0
31	r	303	CLA	3	0
33	z	102	LHG	3	0
31	Y	311	CLA	8	0
38	6	301	SQD	4	0
34	A	414	LMG	2	0
30	1	601	CHL	7	0
38	a	412	SQD	4	0
48	K	101	LMU	1	0
31	b	608	CLA	7	0
36	g	317	NEX	2	0
31	c	603	CLA	5	0
43	D	405	BCR	13	0
31	0	604	CLA	2	0
33	s	322	LHG	6	0
38	G	617	SQD	9	0
34	D	409	LMG	8	0
31	S	315	CLA	5	0
31	s	303	CLA	12	0
31	N	304	CLA	10	0
36	S	319	NEX	4	0
31	7	314	CLA	4	0
34	p	620	LMG	5	0
31	3	313	CLA	4	0
31	4	613	CLA	5	0
45	c	617	DGD	9	0
32	8	615	LUT	9	0
33	G	618	LHG	15	0
31	S	312	CLA	6	0
37	R	318	XAT	7	0
34	w	203	LMG	1	0
30	3	303	CHL	8	0
31	S	313	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	6	312	CLA	4	0
30	5	608	CHL	11	0
34	B	625	LMG	5	0
31	b	611	CLA	10	0
43	A	410	BCR	3	0
31	R	306	CLA	9	0
31	B	613	CLA	10	0
31	B	605	CLA	7	0
31	B	611	CLA	11	0
34	q1	101	LMG	11	0
31	9	304	CLA	9	0
34	S	321	LMG	2	0
30	3	310	CHL	7	0
30	g	309	CHL	5	0
38	X	201	SQD	1	0
38	y	621	SQD	3	0
33	l	101	LHG	11	0
34	2	621	LMG	5	0
34	0	620	LMG	8	0
32	N	316	LUT	14	0
43	t	101	BCR	13	0
34	9	301	LMG	14	0
30	R	309	CHL	9	0
31	Y	314	CLA	3	0
32	7	318	LUT	5	0
30	0	606	CHL	5	0
34	c	620	LMG	9	0
45	C	618	DGD	6	0
45	c	618	DGD	5	0
31	p	612	CLA	8	0
31	7	313	CLA	3	0
38	s	301	SQD	6	0
30	6	308	CHL	11	0
35	2	614	RRX	12	0
30	2	605	CHL	9	0
38	b	621	SQD	2	0
33	q	320	LHG	12	0
30	0	605	CHL	7	0
38	0	621	SQD	2	0
31	c	609	CLA	2	0
31	0	602	CLA	4	0
30	1	606	CHL	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	2	603	CLA	10	0
31	3	306	CLA	12	0
36	8	617	NEX	4	0
34	A	418	LMG	3	0
31	S	306	CLA	14	0
31	Y	310	CLA	13	0
30	G	608	CHL	8	0
35	G	614	RRX	28	0
30	p	609	CHL	7	0
30	9	308	CHL	9	0
31	1	602	CLA	5	0
30	0	609	CHL	7	0
33	n	320	LHG	3	0
31	p	615	CLA	9	0
30	8	607	CHL	3	0
31	A	406	CLA	8	0
34	C	624	LMG	6	0
34	c	624	LMG	7	0
33	7	319	LHG	3	0
30	g	306	CHL	7	0
31	0	615	CLA	5	0
31	n	314	CLA	14	0
30	0	601	CHL	4	0
34	4	620	LMG	13	0
30	p	601	CHL	2	0
30	3	309	CHL	13	0
34	7	322	LMG	4	0
34	q	301	LMG	4	0
48	r	302	LMU	11	0
31	n	305	CLA	14	0
34	A	412	LMG	4	0
31	N	305	CLA	13	0
36	R	319	NEX	8	0
43	B	617	BCR	7	0
31	7	316	CLA	11	0
33	6	320	LHG	2	0
31	Y	312	CLA	8	0
33	p	619	LHG	3	0
34	g	320	LMG	4	0
45	c	619	DGD	26	0
31	N	313	CLA	15	0
31	S	304	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	N	319	LHG	3	0
32	5	616	LUT	23	0
30	4	605	CHL	12	0
34	6	321	LMG	10	0
30	9	307	CHL	6	0
31	s	304	CLA	4	0
32	y	616	LUT	11	0
43	v	101	BCR	3	0
31	5	612	CLA	6	0
31	n	315	CLA	16	0
33	B	624	LHG	6	0
33	K	102	LHG	6	0
30	q	308	CHL	7	0
31	b	615	CLA	6	0
33	0	619	LHG	3	0
31	g	313	CLA	12	0
44	A	416	PL9	5	0
36	4	617	NEX	8	0
31	b	603	CLA	7	0
31	n	312	CLA	3	0
32	6	317	LUT	9	0
31	6	313	CLA	3	0
36	r	301	NEX	6	0
31	6	315	CLA	10	0
44	a	414	PL9	9	0
30	5	609	CHL	9	0
38	B	623	SQD	7	0
30	n	301	CHL	8	0
32	Y	315	LUT	9	0
33	D	408	LHG	8	0
43	b	620	BCR	1	0
34	j	101	LMG	4	0
48	R	302	LMU	8	0
33	4	618	LHG	5	0
43	a	410	BCR	4	0
31	N	311	CLA	4	0
34	7	320	LMG	2	0
31	b	609	CLA	7	0
30	N	301	CHL	10	0
30	7	310	CHL	6	0
35	q	317	RRX	20	0
31	q	313	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	a	413	LMG	4	0
39	A	401	OEX	1	0
30	n	309	CHL	3	0
43	h	101	BCR	4	0
31	r	313	CLA	4	0
31	d	404	CLA	6	0
30	n	308	CHL	15	0
38	r	322	SQD	4	0
42	a	408	PHO	3	0
30	S	307	CHL	6	0
33	s	320	LHG	5	0
34	X	203	LMG	1	0
34	m	102	LMG	5	0
30	2	608	CHL	10	0
30	s	307	CHL	9	0
31	r	304	CLA	3	0
44	d	407	PL9	9	0
31	8	610	CLA	3	0
32	S	317	LUT	9	0
31	7	305	CLA	13	0
30	y	608	CHL	4	0
36	Y	317	NEX	2	0
31	c	607	CLA	5	0
43	B	619	BCR	8	0
31	p	613	CLA	25	0
31	p	611	CLA	8	0
30	n	307	CHL	8	0
31	5	613	CLA	10	0
34	g	322	LMG	6	0
31	r	306	CLA	5	0
31	S	305	CLA	10	0
33	c	622	LHG	8	0
34	B	621	LMG	8	0
31	7	304	CLA	10	0
37	9	322	XAT	3	0
31	n	303	CLA	8	0
30	7	302	CHL	4	0
43	H	101	BCR	4	0
33	j	102	LHG	5	0
31	3	315	CLA	7	0
31	2	610	CLA	7	0
31	Y	304	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	R	313	CLA	2	0
31	y	603	CLA	9	0
31	R	311	CLA	5	0
31	3	314	CLA	13	0
31	9	313	CLA	4	0
36	r	319	NEX	3	0
31	C	604	CLA	6	0
30	r	309	CHL	9	0
47	e	102	HEM	11	0
32	N	317	LUT	8	0
30	S	308	CHL	5	0
31	B	615	CLA	6	0
34	w	202	LMG	20	0
43	T	101	BCR	6	0
30	6	309	CHL	8	0
31	B	610	CLA	11	0
30	6	310	CHL	7	0
31	0	611	CLA	5	0
31	N	321	CLA	14	0
34	C	621	LMG	9	0
34	c	621	LMG	1	0
30	p	605	CHL	7	0
30	6	302	CHL	6	0
31	2	604	CLA	6	0
30	2	606	CHL	11	0
31	s	305	CLA	9	0
31	R	304	CLA	7	0
31	8	612	CLA	13	0
34	w	201	LMG	7	0
45	C	620	DGD	21	0
31	b	605	CLA	6	0
31	g	305	CLA	7	0
30	R	308	CHL	5	0
31	D	404	CLA	8	0
31	R	316	CLA	6	0
31	8	604	CLA	9	0
30	y	607	CHL	12	0
30	8	606	CHL	9	0
38	x	201	SQD	3	0
44	D	406	PL9	7	0
30	6	307	CHL	12	0
32	y	617	LUT	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	A	413	SQD	3	0
43	B	618	BCR	5	0
31	1	610	CLA	15	0
31	d	405	CLA	6	0
31	8	602	CLA	8	0
31	y	604	CLA	8	0
31	y	612	CLA	9	0
31	B	607	CLA	5	0
30	Y	307	CHL	8	0
30	8	608	CHL	8	0
31	5	610	CLA	27	0
30	4	601	CHL	6	0
31	B	616	CLA	9	0
32	p	617	LUT	9	0
31	B	612	CLA	9	0
30	3	308	CHL	11	0
34	6	322	LMG	11	0
32	6	318	LUT	10	0
30	N	308	CHL	4	0
34	w	205	LMG	6	0
31	B	602	CLA	4	0
35	4	615	RRX	17	0
34	a	401	LMG	5	0
43	C	614	BCR	3	0
43	c	614	BCR	6	0
31	y	615	CLA	11	0
31	Y	305	CLA	5	0
34	9	321	LMG	7	0
30	q	303	CHL	8	0
36	N	318	NEX	7	0
30	g	308	CHL	6	0
34	7	301	LMG	6	0
34	I	101	LMG	5	0
34	b	626	LMG	2	0
30	s	302	CHL	1	0
31	0	612	CLA	3	0
30	R	310	CHL	2	0
31	Y	303	CLA	5	0
30	1	607	CHL	12	0
31	8	614	CLA	12	0
30	p	607	CHL	13	0
42	A	408	PHO	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	g	314	CLA	4	0
31	s	314	CLA	4	0
31	B	603	CLA	3	0
32	s	317	LUT	12	0
37	G	620	XAT	22	0
31	N	315	CLA	9	0
31	9	306	CLA	10	0
33	A	417	LHG	4	0
43	d	406	BCR	5	0
31	S	316	CLA	4	0
30	y	609	CHL	11	0
32	n	317	LUT	10	0
30	9	303	CHL	8	0
34	X	202	LMG	5	0
36	3	319	NEX	10	0
43	V	101	BCR	1	0
31	3	312	CLA	4	0
31	y	614	CLA	5	0
31	b	616	CLA	4	0
34	d	411	LMG	2	0
31	q	314	CLA	8	0
33	F1	301	LHG	1	0
30	N	309	CHL	14	0
31	4	612	CLA	5	0
31	g	304	CLA	4	0
30	2	607	CHL	10	0
30	0	607	CHL	15	0
34	d	410	LMG	5	0
31	g	310	CLA	5	0
31	s	312	CLA	6	0
31	9	315	CLA	8	0
30	4	606	CHL	17	0
31	5	604	CLA	4	0
31	0	610	CLA	15	0
36	n	319	NEX	2	0
31	G	610	CLA	8	0
34	d	409	LMG	4	0
31	4	602	CLA	10	0
31	C	612	CLA	5	0
31	s	315	CLA	3	0
31	r	315	CLA	7	0
31	N	310	CLA	16	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	p	610	CLA	19	0
34	G	621	LMG	10	0
34	x	202	LMG	5	0
31	r	311	CLA	5	0
31	5	615	CLA	10	0
33	L	101	LHG	4	0
31	q	305	CLA	7	0
34	2	618	LMG	7	0
30	s	308	CHL	8	0
32	q	318	LUT	12	0
31	q	315	CLA	7	0
33	y	619	LHG	11	0
31	C	607	CLA	5	0
31	s	310	CLA	3	0
36	q	319	NEX	4	0
32	8	616	LUT	9	0
31	0	613	CLA	2	0
36	9	319	NEX	9	0
31	n	313	CLA	4	0
38	B	620	SQD	7	0
32	3	318	LUT	13	0
33	2	617	LHG	4	0
31	s	316	CLA	5	0
38	m	101	SQD	2	0
38	a	411	SQD	4	0
31	8	611	CLA	4	0
33	g	319	LHG	12	0
32	1	616	LUT	3	0
30	S	302	CHL	3	0
33	a	415	LHG	4	0
33	e	101	LHG	7	0
37	g	321	XAT	20	0
31	q	306	CLA	8	0
33	9	320	LHG	9	0
31	R	303	CLA	1	0
31	n	316	CLA	11	0
31	6	311	CLA	15	0
34	G	619	LMG	3	0
30	5	607	CHL	11	0
31	C	610	CLA	5	0
31	c	610	CLA	6	0
31	r	307	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	S	311	CLA	6	0
31	G	602	CLA	5	0
36	5	618	NEX	16	0
30	8	601	CHL	10	0
31	5	614	CLA	6	0
36	6	319	NEX	11	0
36	p	618	NEX	2	0
30	N	307	CHL	13	0
33	t	102	LHG	1	0
34	b	629	LMG	5	0
32	n	318	LUT	8	0
30	y	605	CHL	2	0
31	3	305	CLA	14	0
31	p	602	CLA	9	0
30	N	302	CHL	3	0
31	B	614	CLA	6	0
34	1	618	LMG	2	0
30	q	310	CHL	14	0
38	M	102	SQD	3	0
30	9	310	CHL	11	0
30	q	309	CHL	19	0
36	s	319	NEX	4	0
34	q	302	LMG	6	0
30	s	309	CHL	3	0
31	0	603	CLA	5	0
32	4	616	LUT	11	0
31	b	617	CLA	7	0
30	5	601	CHL	7	0
38	G	624	SQD	4	0
31	y	602	CLA	1	0
32	s	318	LUT	12	0
30	r	308	CHL	6	0
34	4	621	LMG	12	0
38	b	627	SQD	9	0
31	2	613	CLA	7	0
30	Y	301	CHL	18	0
30	r	310	CHL	3	0
31	G	611	CLA	3	0
31	c	605	CLA	6	0
33	5	619	LHG	9	0
34	n	322	LMG	14	0
34	D	411	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	p	603	CLA	5	0
43	z	101	BCR	4	0
32	5	617	LUT	15	0
30	G	623	CHL	14	0
35	9	317	RRX	13	0
31	G	612	CLA	12	0
33	M	101	LHG	1	0
34	W	202	LMG	1	0
36	R	301	NEX	7	0
34	k	102	LMG	2	0
31	c	611	CLA	5	0
31	8	613	CLA	15	0
30	Y	308	CHL	5	0
31	b	610	CLA	10	0
31	5	611	CLA	8	0
31	q	304	CLA	7	0
34	W	201	LMG	13	0
30	1	619	CHL	8	0
31	C	602	CLA	4	0
31	c	602	CLA	6	0
33	A	415	LHG	4	0
31	y	611	CLA	7	0
34	B	622	LMG	3	0
37	r	318	XAT	4	0
34	2	620	LMG	2	0
38	A	411	SQD	1	0
30	7	306	CHL	5	0
31	A	409	CLA	7	0
33	S	320	LHG	6	0
30	1	608	CHL	3	0
31	6	303	CLA	4	0
31	G	603	CLA	10	0
31	S	314	CLA	4	0
30	p	608	CHL	10	0
30	G	601	CHL	11	0
31	1	603	CLA	9	0
30	3	302	CHL	15	0
31	2	602	CLA	8	0
31	R	312	CLA	5	0
38	R	322	SQD	6	0
30	G	607	CHL	3	0
31	7	311	CLA	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	606	CLA	6	0
31	b	602	CLA	3	0
33	D	407	LHG	4	0
30	g	302	CHL	7	0
34	b	624	LMG	2	0
31	5	603	CLA	12	0
31	6	305	CLA	12	0
31	y	610	CLA	14	0
31	C	611	CLA	5	0
32	0	617	LUT	6	0
34	C	622	LMG	2	0
30	8	605	CHL	5	0
34	w	204	LMG	1	0
31	R	307	CLA	2	0
31	b	607	CLA	3	0
31	1	604	CLA	8	0
34	s	321	LMG	4	0
43	b	618	BCR	11	0
34	W	203	LMG	1	0
45	C	617	DGD	9	0
30	5	606	CHL	12	0
30	N	306	CHL	10	0
31	p	614	CLA	11	0
31	3	304	CLA	5	0
34	9	302	LMG	11	0
31	b	612	CLA	14	0
30	Y	306	CHL	2	0
31	4	610	CLA	18	0
31	5	602	CLA	9	0
32	Y	316	LUT	3	0
31	4	611	CLA	4	0
30	7	309	CHL	3	0
31	3	316	CLA	10	0
31	7	312	CLA	7	0
34	J	101	LMG	4	0
31	2	609	CLA	16	0
31	C	603	CLA	3	0
31	2	611	CLA	9	0
31	b	614	CLA	13	0
47	E	101	HEM	10	0
32	g	316	LUT	8	0
30	7	321	CHL	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	C	615	BCR	3	0
34	n	321	LMG	6	0
43	c	615	BCR	9	0
31	G	604	CLA	7	0
34	6	323	LMG	2	0
34	y	620	LMG	4	0
31	C	609	CLA	2	0
31	N	314	CLA	17	0
32	p	616	LUT	15	0
38	Y	320	SQD	5	0
31	0	614	CLA	7	0
35	g	315	RRX	3	0
31	a	406	CLA	3	0
36	G	616	NEX	1	0
33	3	320	LHG	7	0
36	y	618	NEX	5	0
31	G	609	CLA	10	0
30	7	307	CHL	10	0
31	1	612	CLA	12	0
31	4	603	CLA	10	0
33	R	320	LHG	1	0
30	1	605	CHL	6	0
34	D	410	LMG	5	0
37	q	321	XAT	16	0
31	R	305	CLA	7	0
34	Q1	101	LMG	14	0
31	b	604	CLA	3	0
38	g	318	SQD	9	0
33	d	408	LHG	13	0
30	4	607	CHL	18	0
30	Y	309	CHL	11	0
34	r	321	LMG	5	0
37	4	619	XAT	9	0
31	s	311	CLA	8	0
30	y	601	CHL	8	0
31	4	614	CLA	3	0
31	6	314	CLA	9	0
31	9	314	CLA	9	0
31	g	311	CLA	5	0
31	N	312	CLA	5	0
31	8	609	CLA	11	0
31	c	612	CLA	8	0

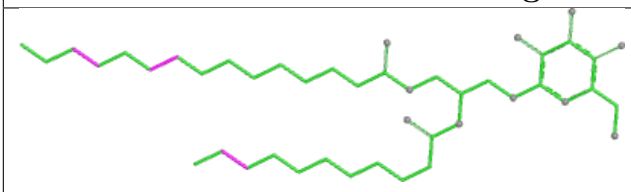
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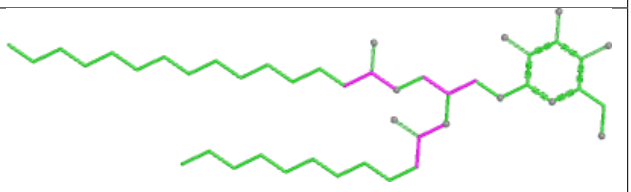
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	S	310	CLA	2	0
31	Y	313	CLA	2	0
31	s	313	CLA	9	0
37	2	619	XAT	11	0
31	a	409	CLA	14	0
43	Z	101	BCR	3	0
34	N	320	LMG	2	0
31	g	312	CLA	6	0
30	4	608	CHL	9	0
45	c	616	DGD	13	0
31	n	304	CLA	11	0
30	9	311	CHL	6	0
31	r	314	CLA	1	0
31	B	604	CLA	8	0
32	r	317	LUT	4	0
32	G	615	LUT	8	0
31	1	614	CLA	4	0
31	C	601	CLA	4	0
31	c	601	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.

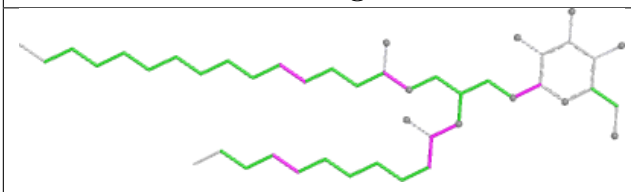
Ligand LMG b 601



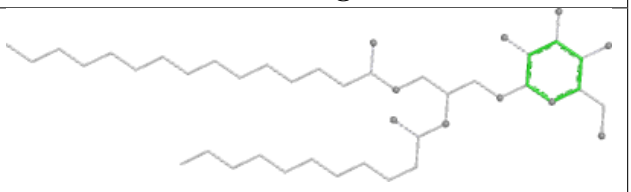
Bond lengths



Bond angles

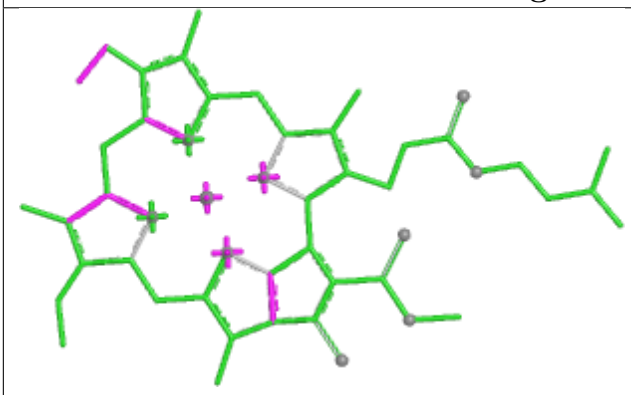


Torsions

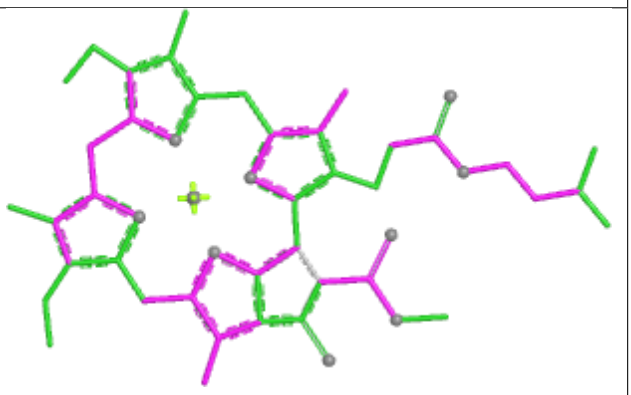


Rings

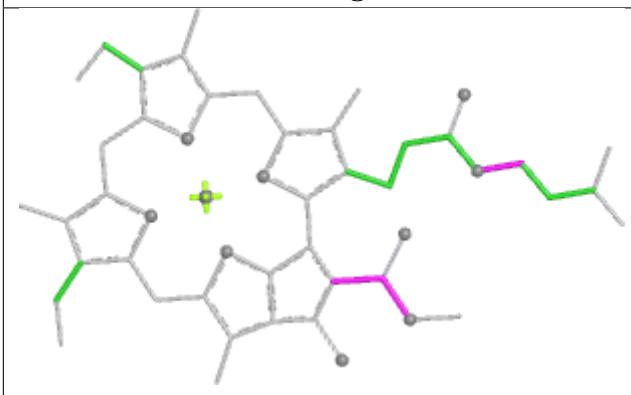
Ligand CLA s 306



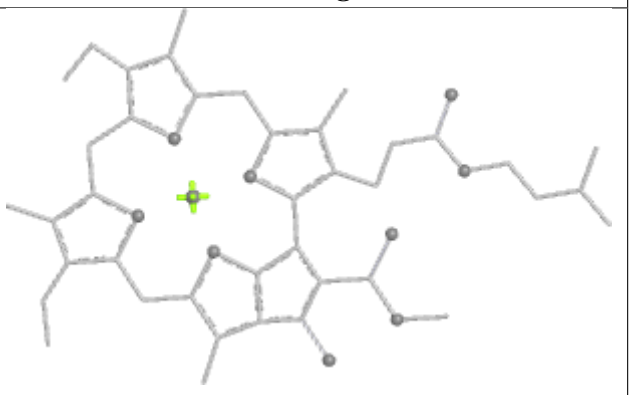
Bond lengths



Bond angles

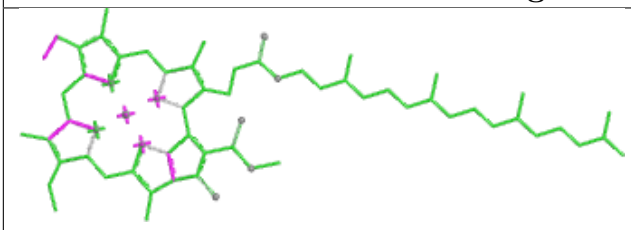


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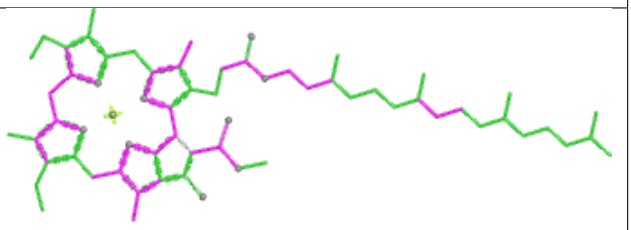


Rings

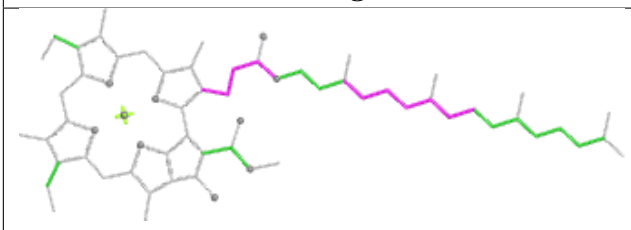
Ligand CLA S 303



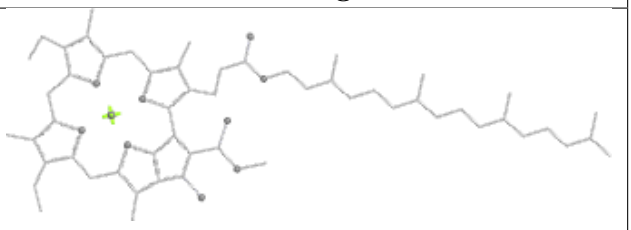
Bond lengths



Bond angles

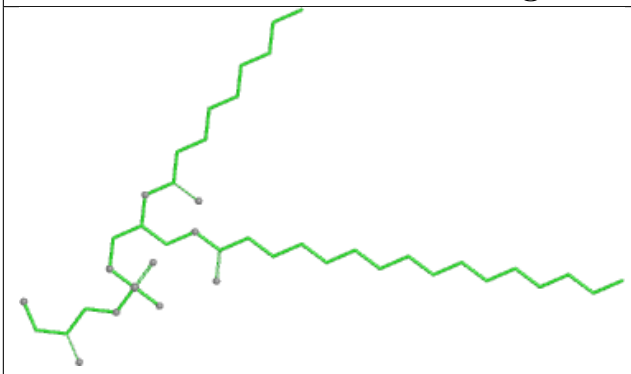


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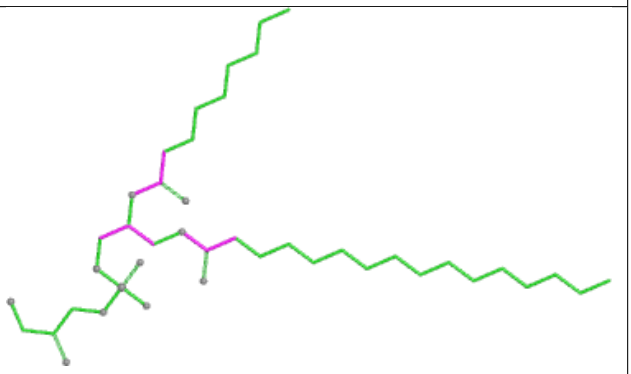


Rings

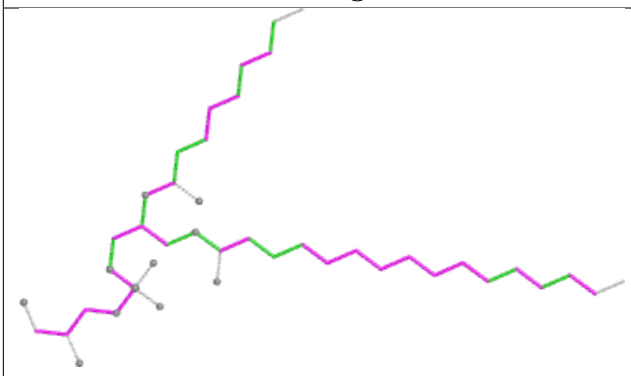
Ligand LHG Y 318



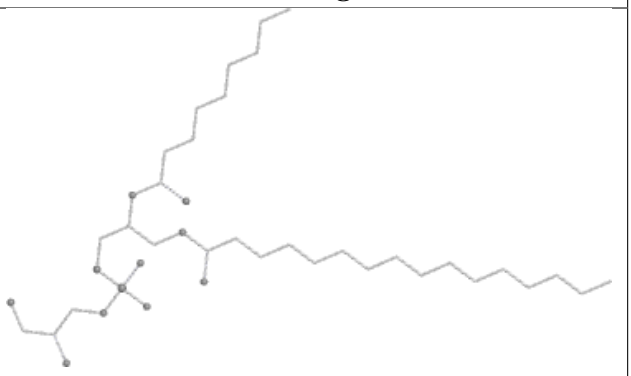
Bond lengths



Bond angles

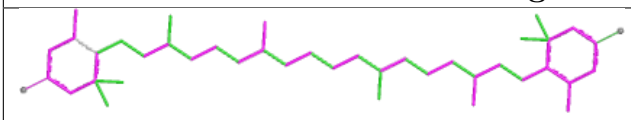


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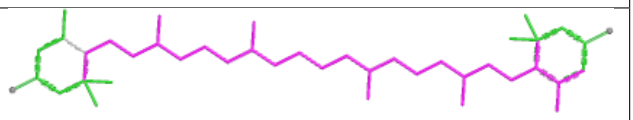


Rings

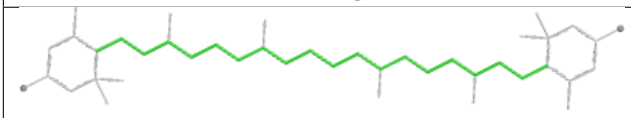
Ligand LUT 1 615



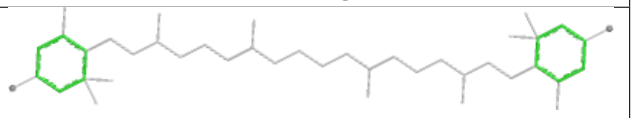
Bond lengths



Bond angles

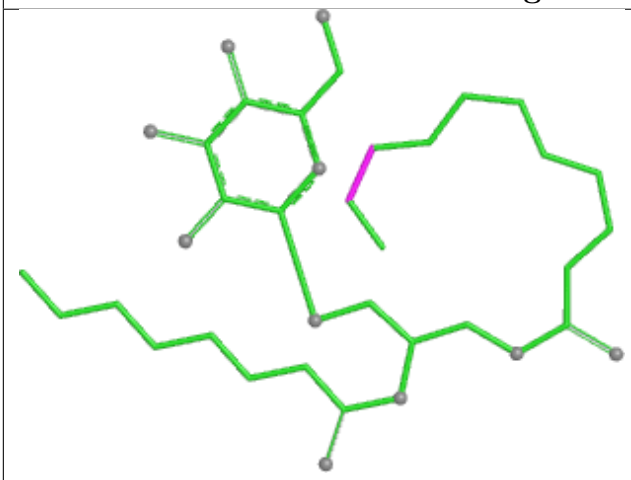


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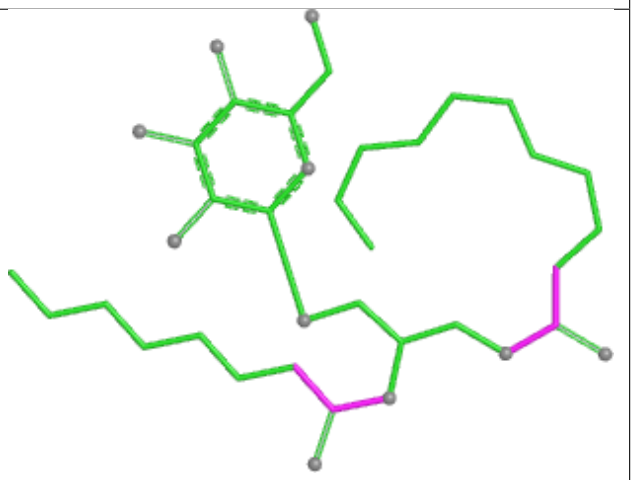


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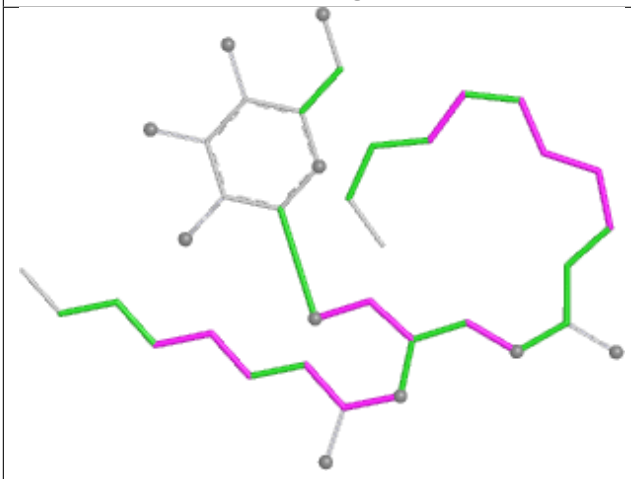
Ligand LMG 5 620



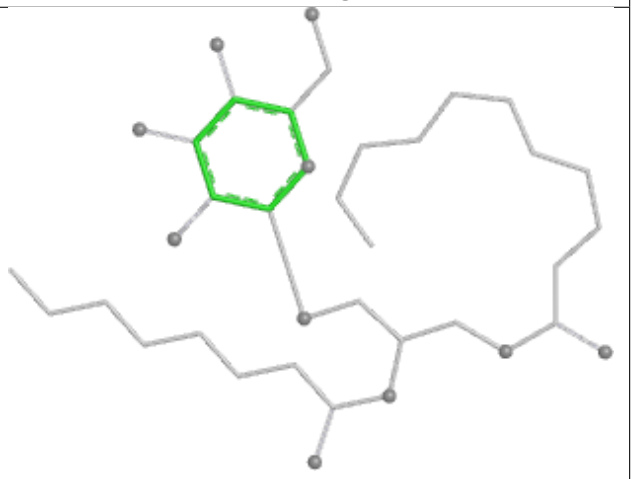
Bond lengths



Bond angles

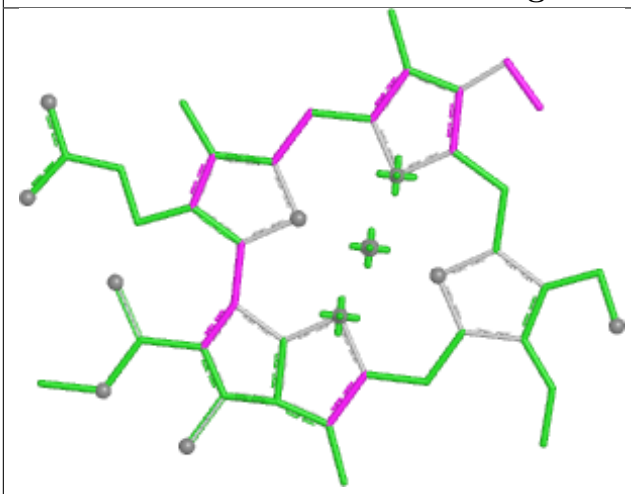


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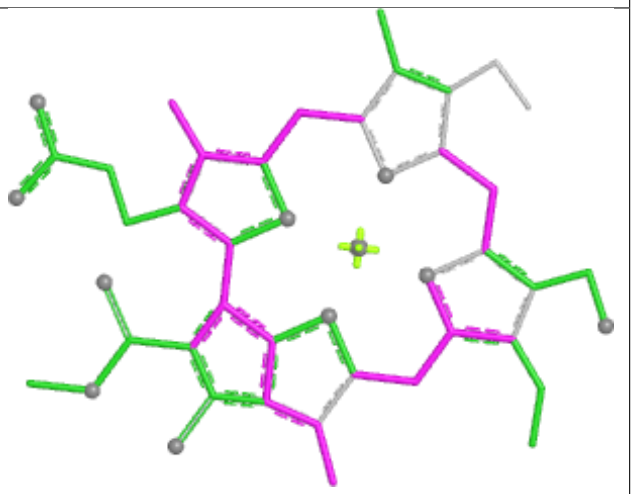


Rings

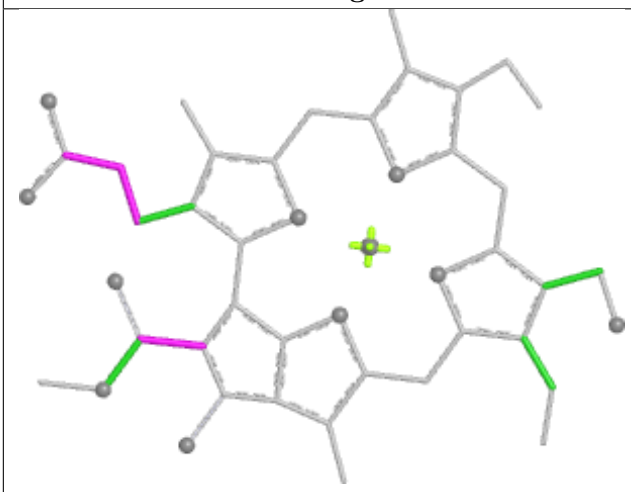
Ligand CHL 5 605



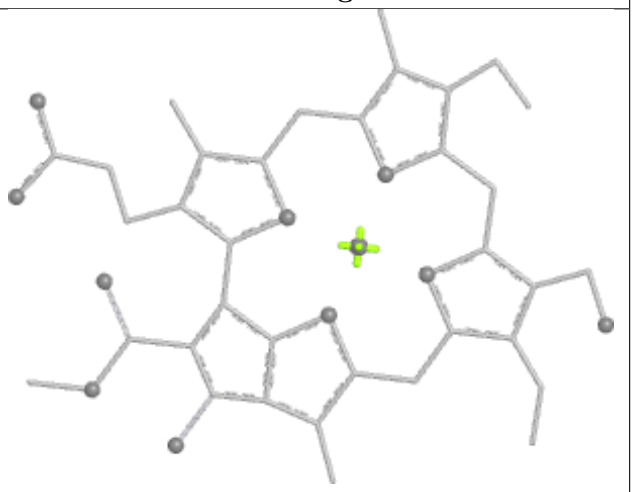
Bond lengths



Bond angles

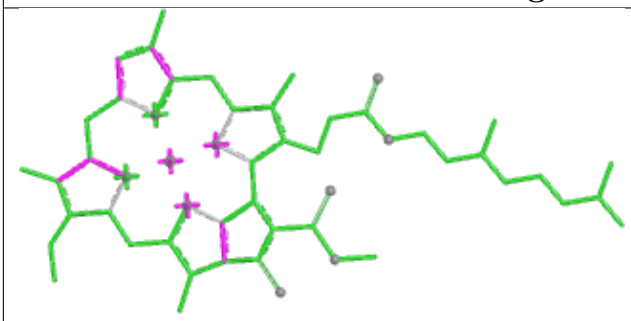


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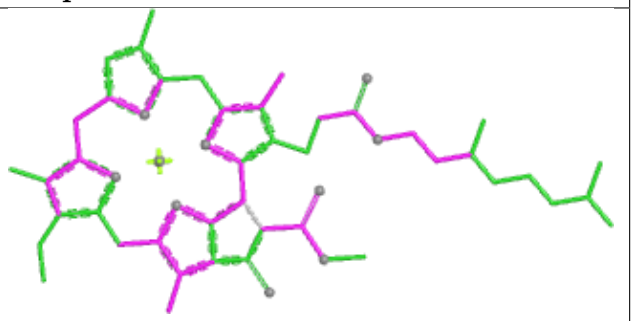


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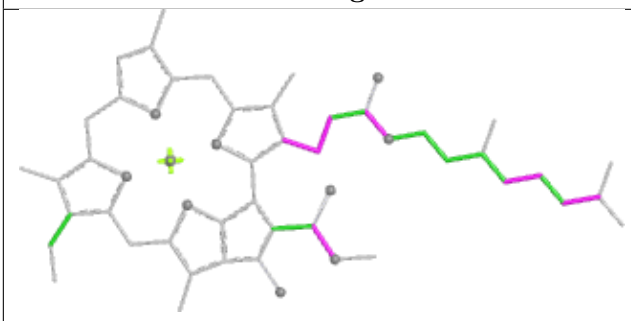
Ligand CLA q 312



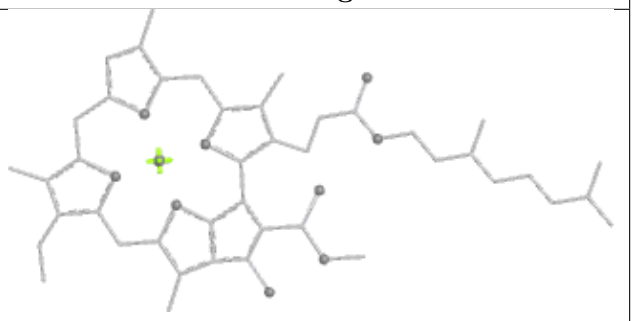
Bond lengths



Bond angles

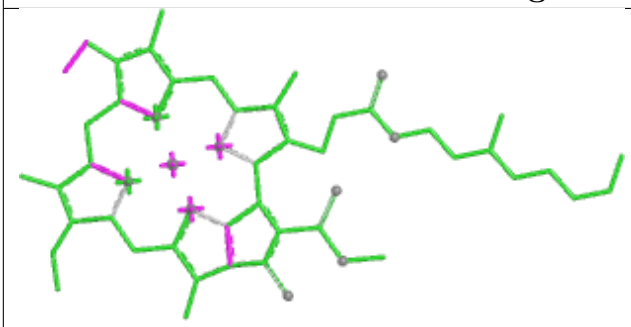


Torsions

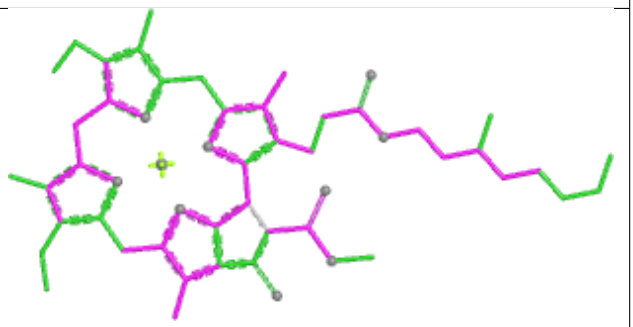


Rings

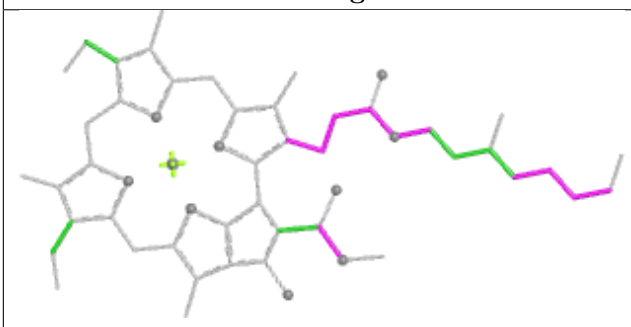
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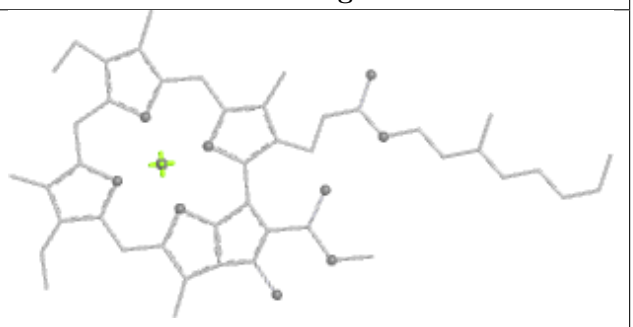
Bond lengths



Bond angles

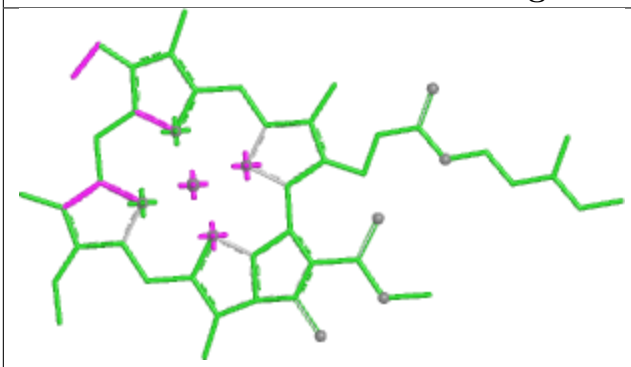


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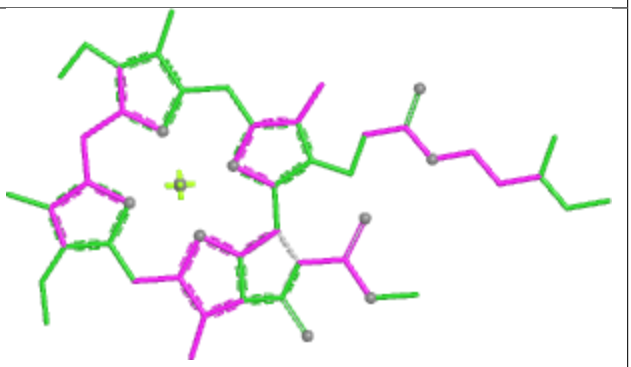


Rings

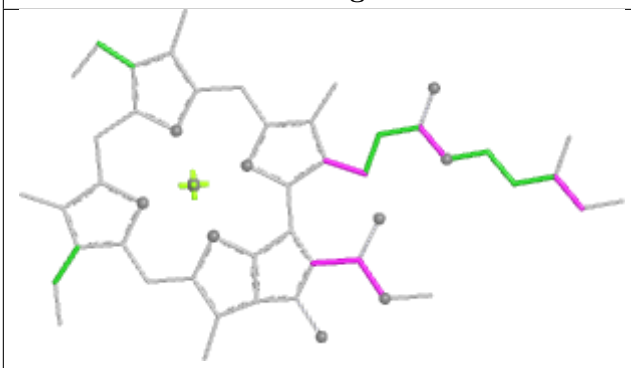
Ligand CLA 4 604



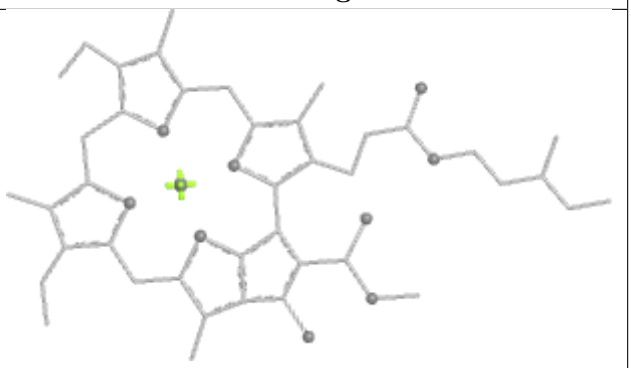
Bond lengths



Bond angles

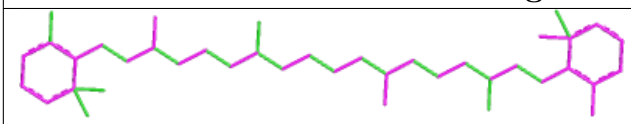


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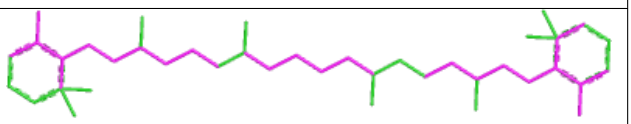


Rings

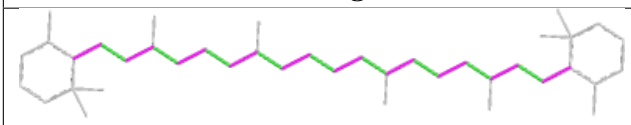
Ligand BCR b 619



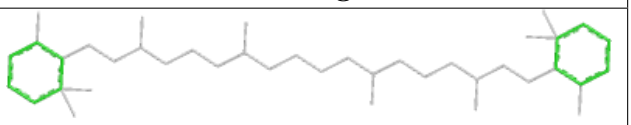
Bond lengths



Bond angles

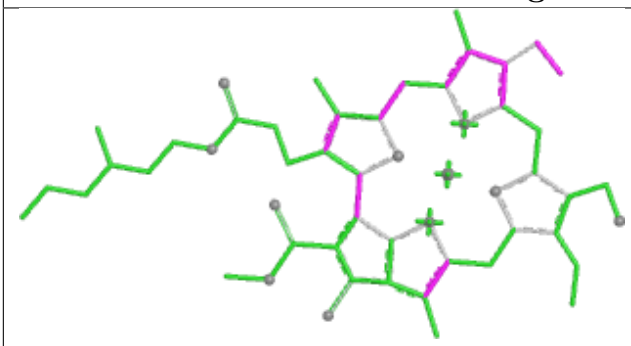


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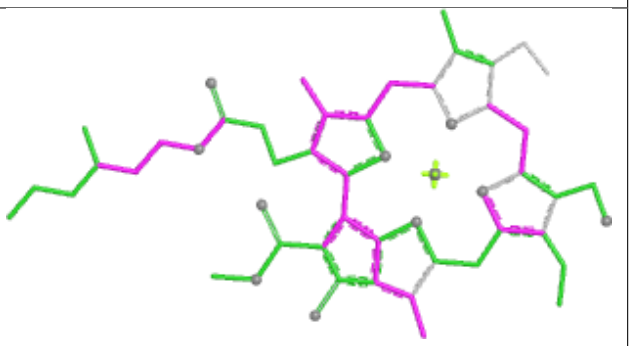


Rings

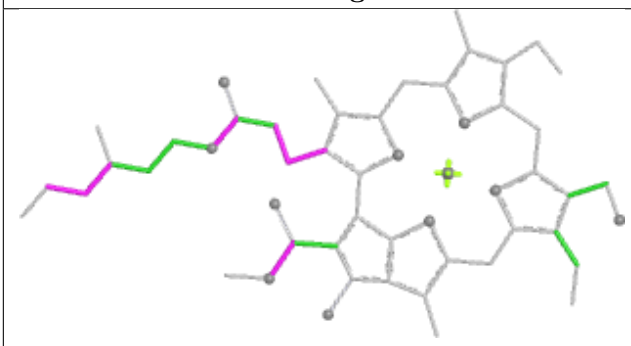
Ligand CHL 9 309



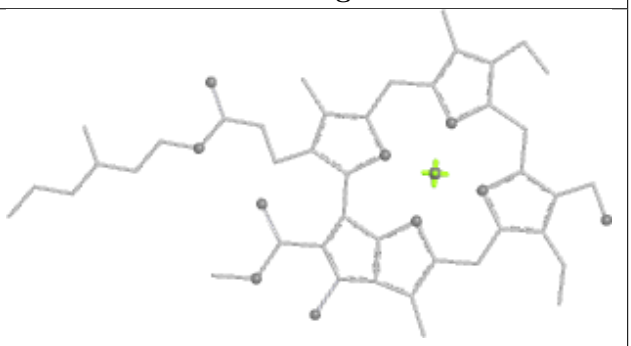
Bond lengths



Bond angles

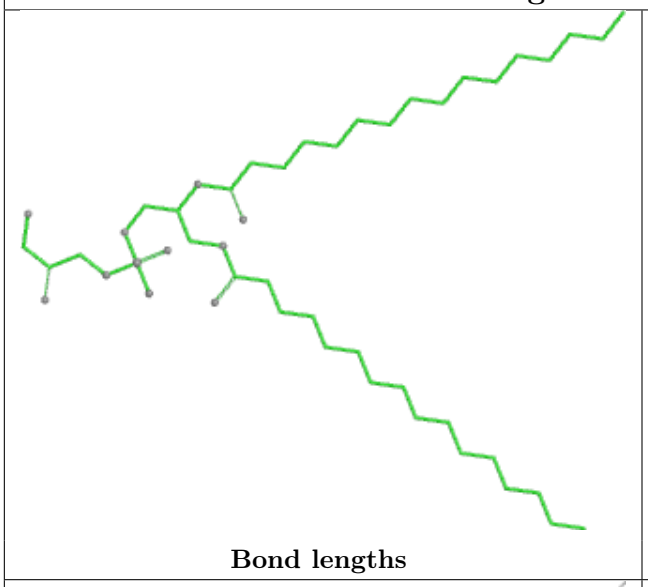


Torsions

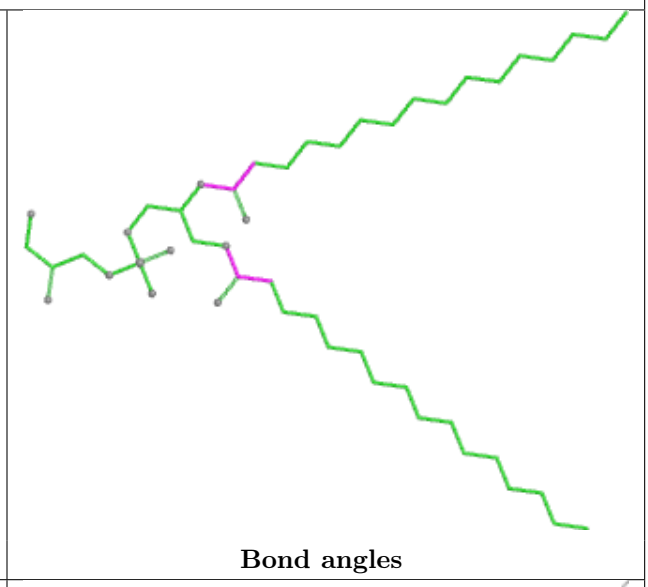


Rings

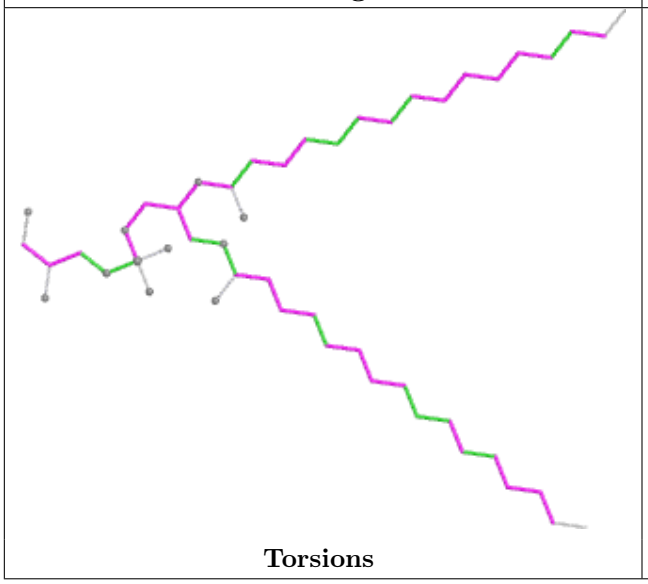
Ligand LHG 8 618



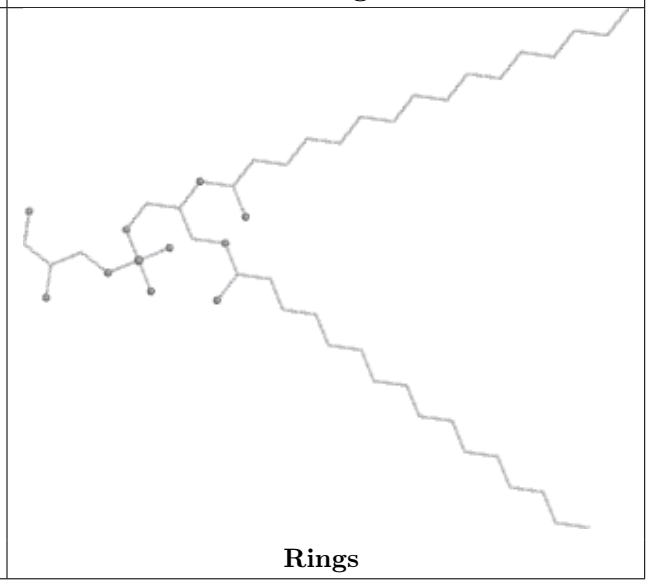
Bond lengths



Bond angles

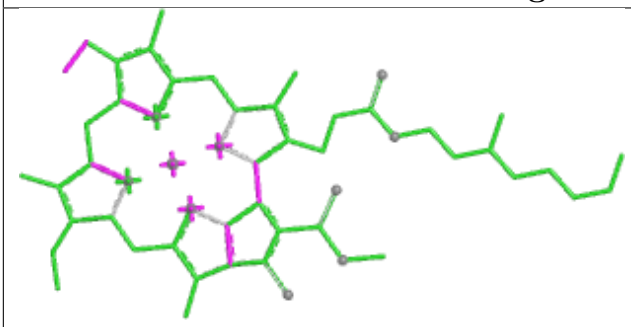


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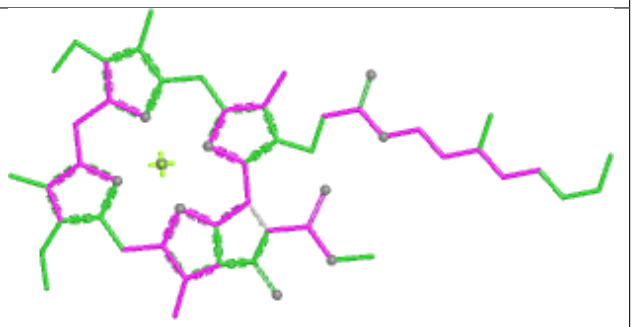


Rings

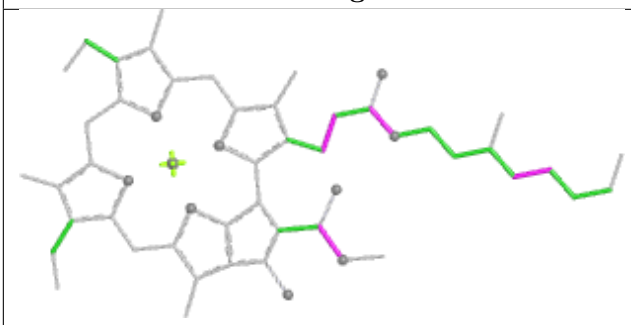
Ligand CLA 3 311



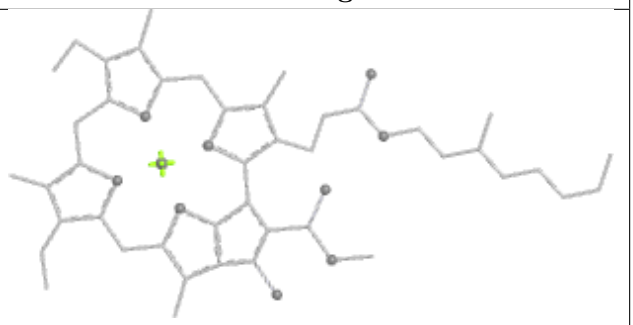
Bond lengths



Bond angles

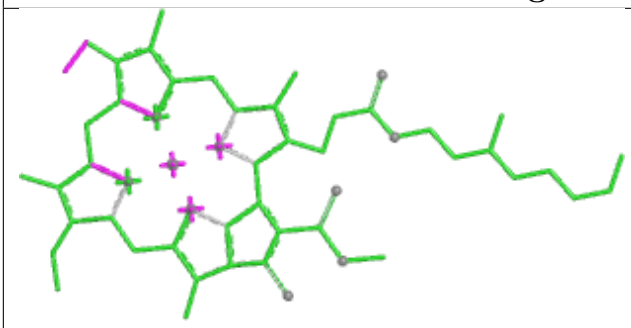


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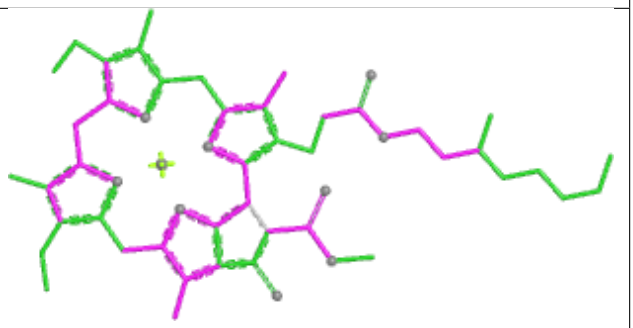


Rings

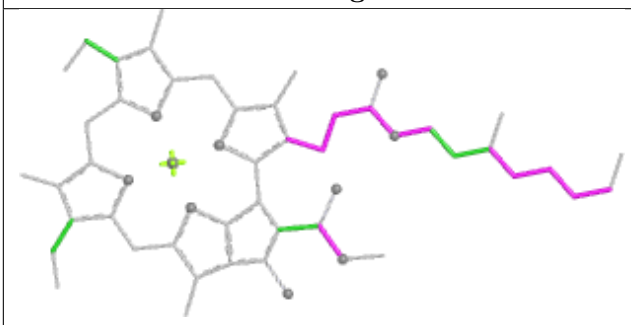
Ligand CLA 7 315



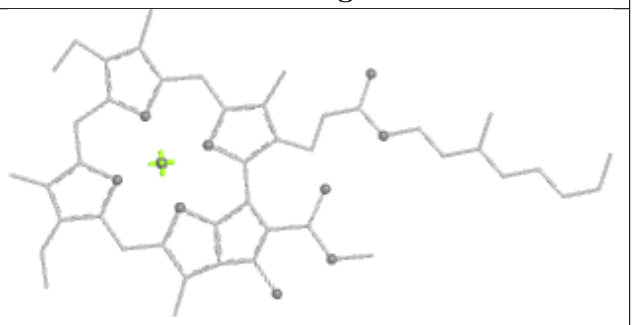
Bond lengths



Bond angles

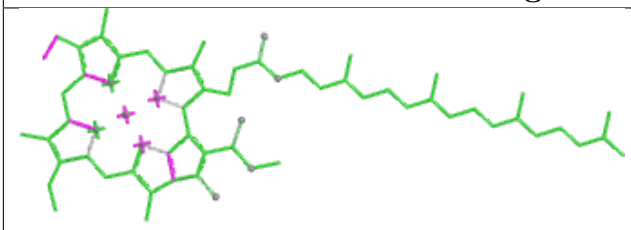


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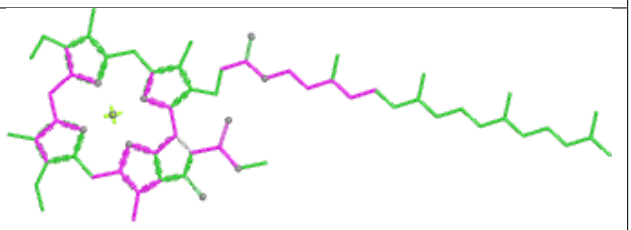


Rings

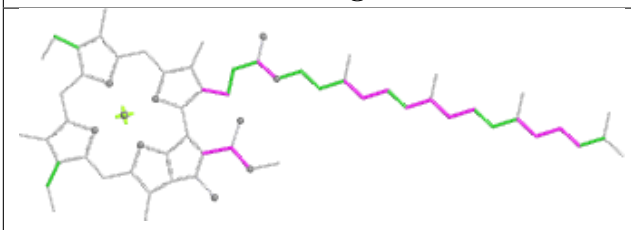
Ligand CLA B 609



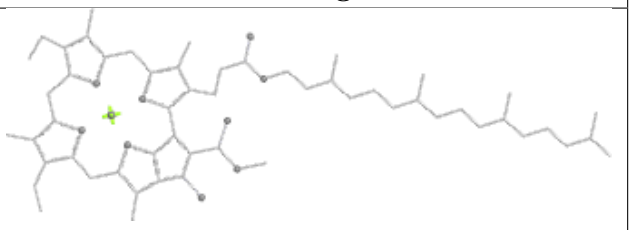
Bond lengths



Bond angles

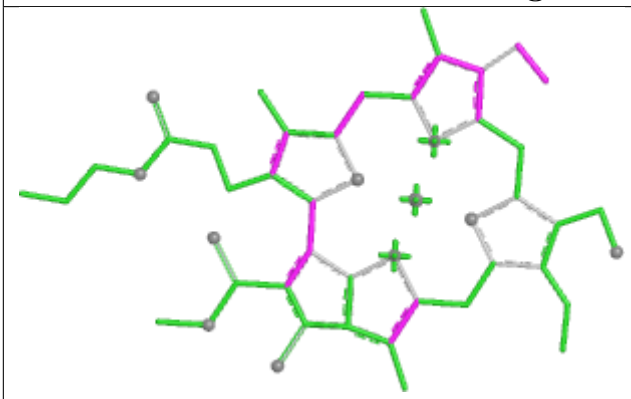


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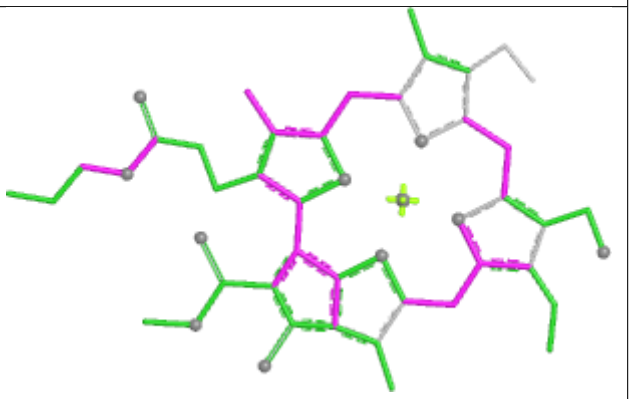


Rings

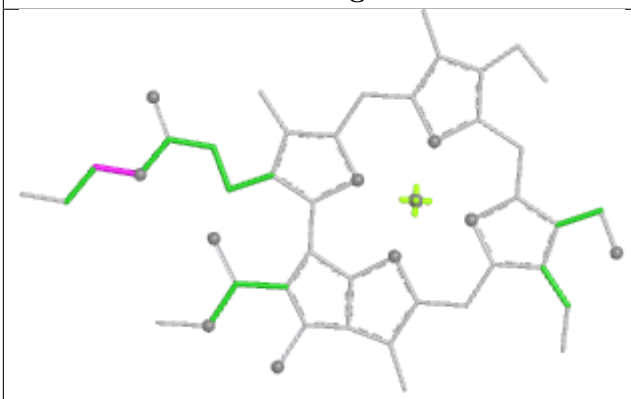
Ligand CHL S 309



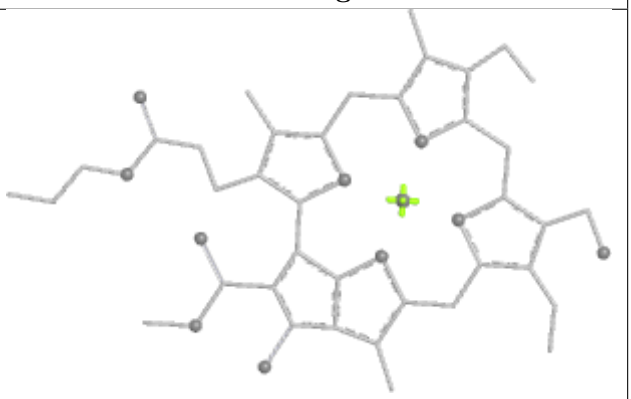
Bond lengths



Bond angles

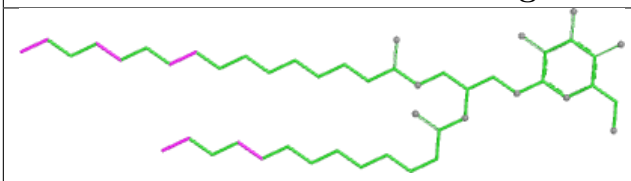


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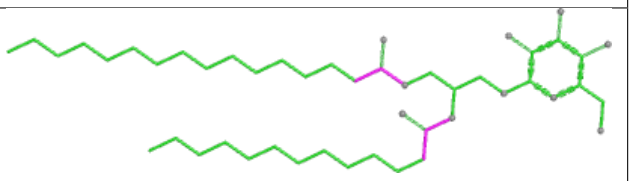


Rings

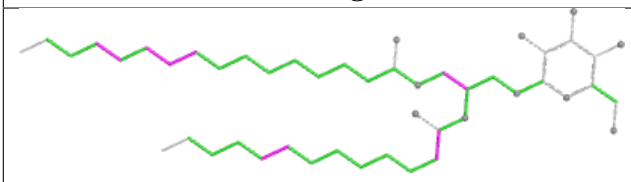
Ligand LMG D 412



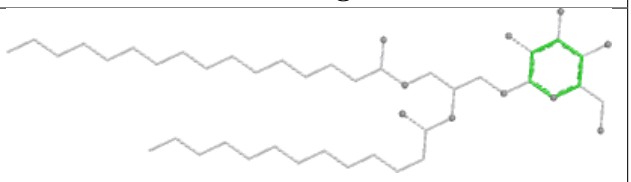
Bond lengths



Bond angles

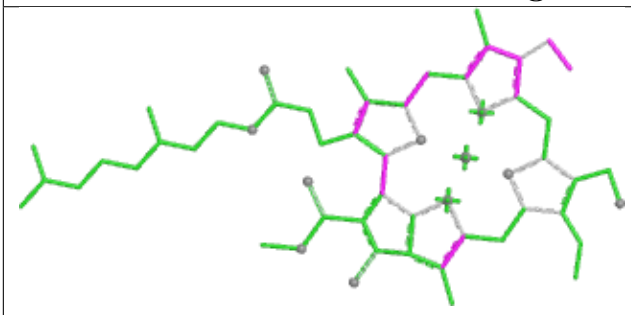


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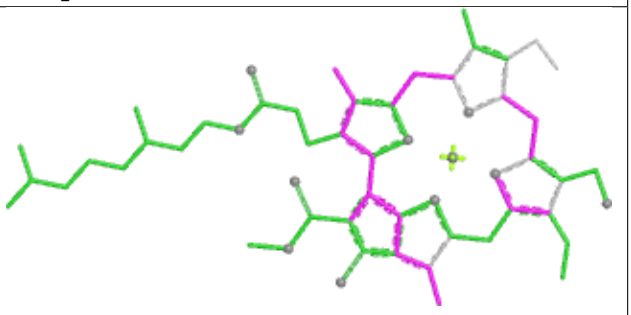


Rings

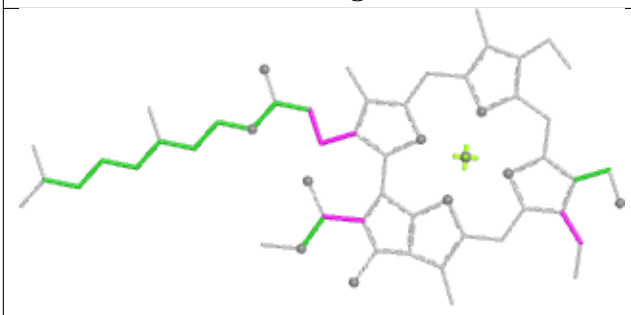
Ligand CHL q 311



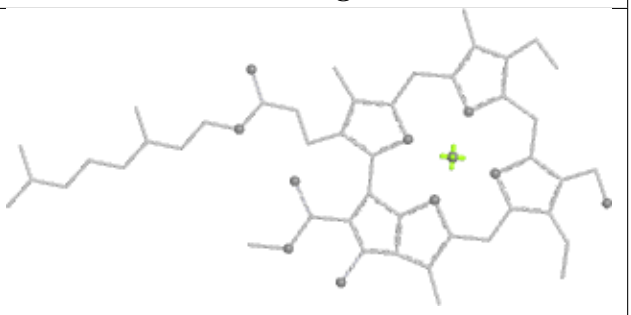
Bond lengths



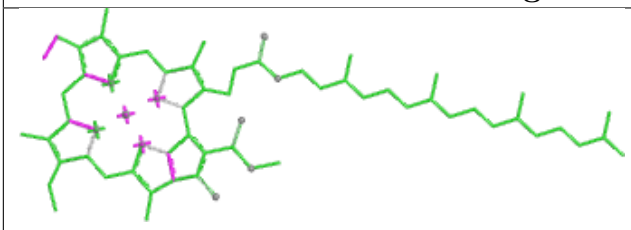
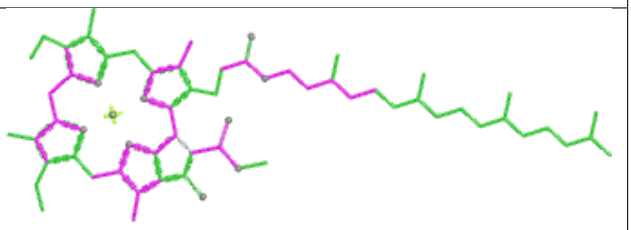
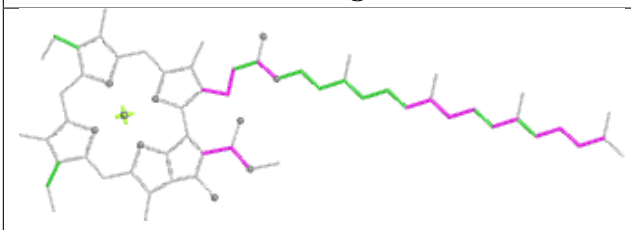
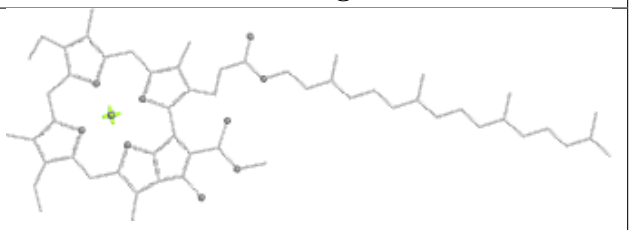
Bond angles

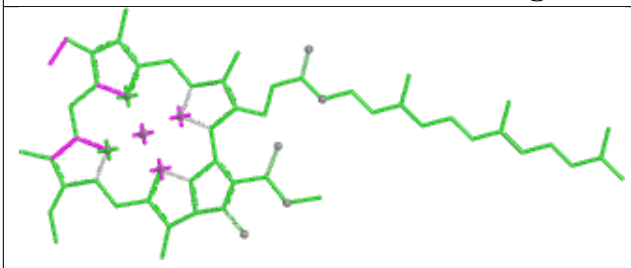
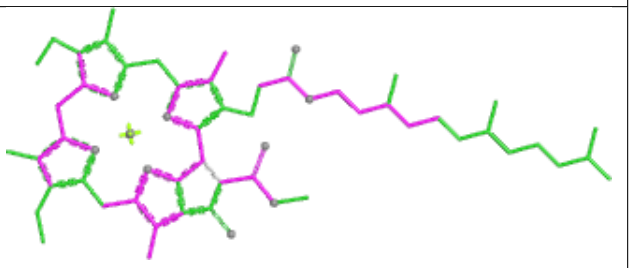
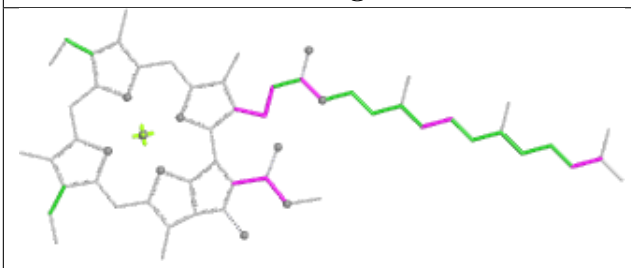
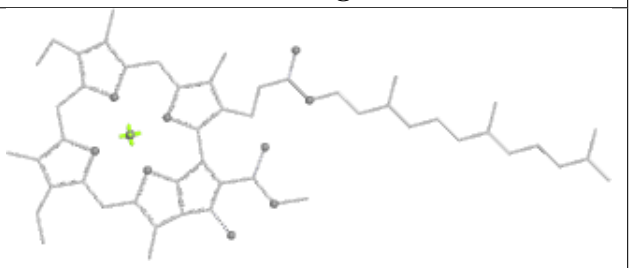


Torsions

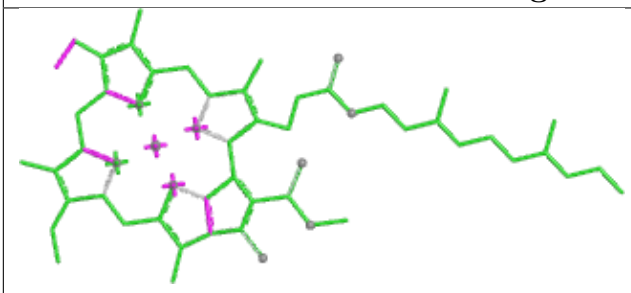


Rings

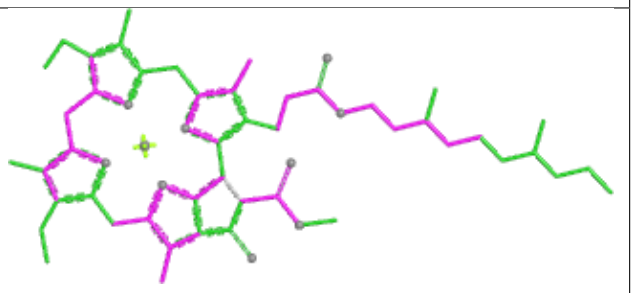
Ligand CLA N 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

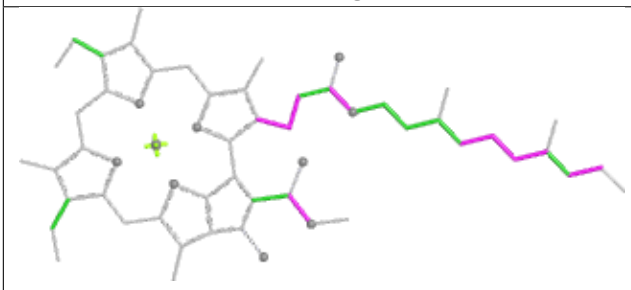
Ligand CLA r 312



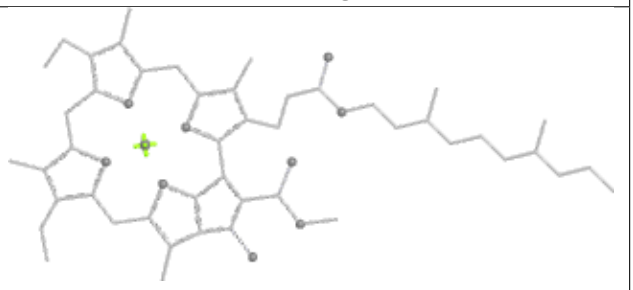
Bond lengths



Bond angles

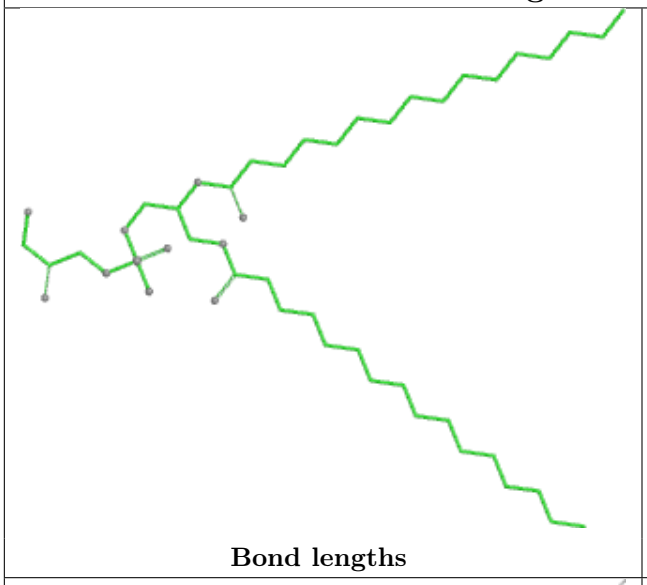


Torsions

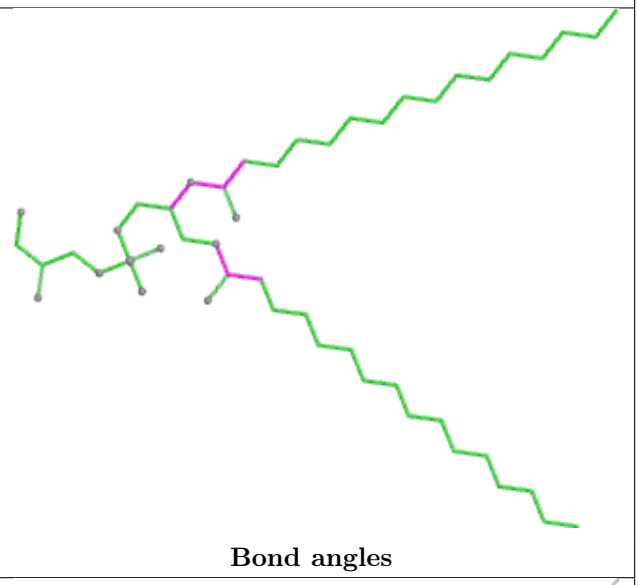


Rings

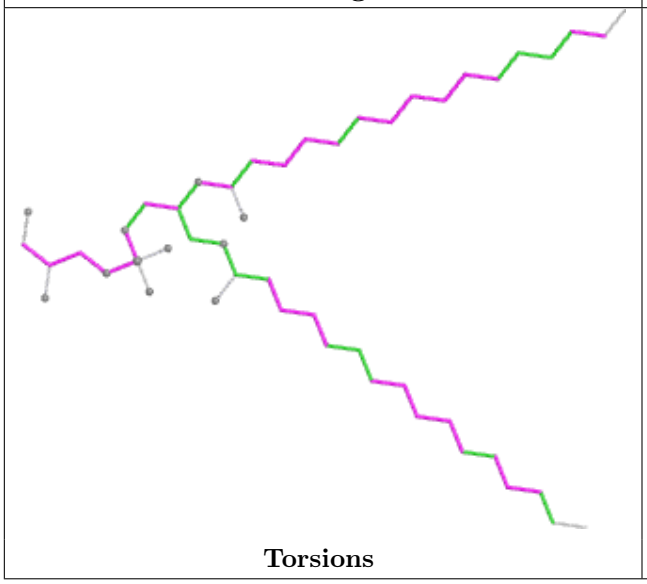
Ligand LHG b 628



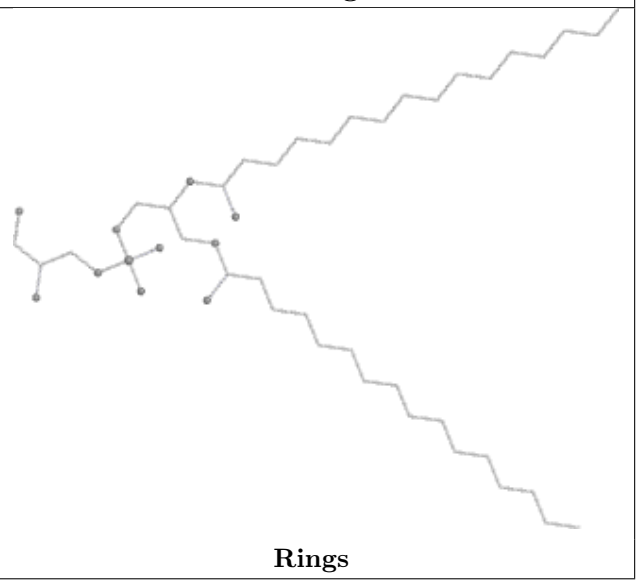
Bond lengths



Bond angles



Torsions

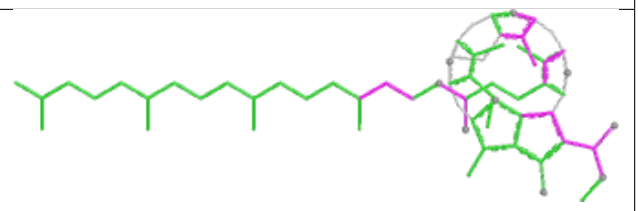


Rings

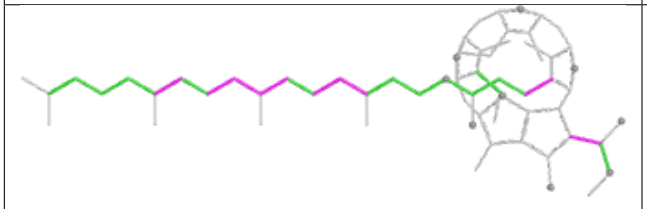
Ligand PHO D 401



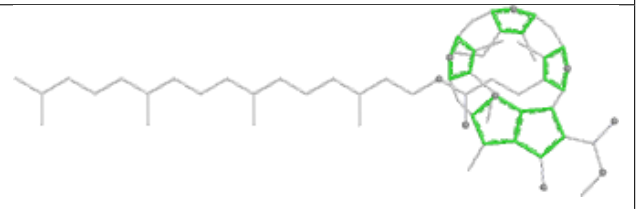
Bond lengths



Bond angles

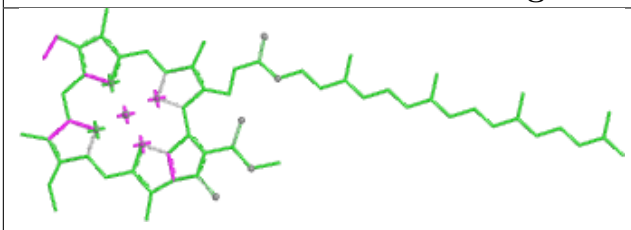


Torsions

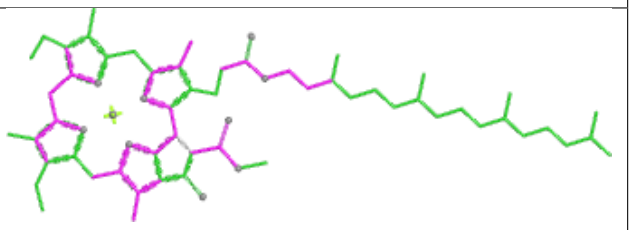


Rings

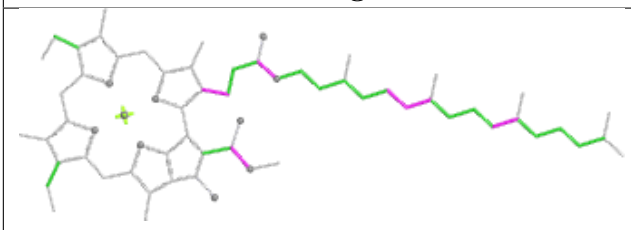
Ligand CLA n 311



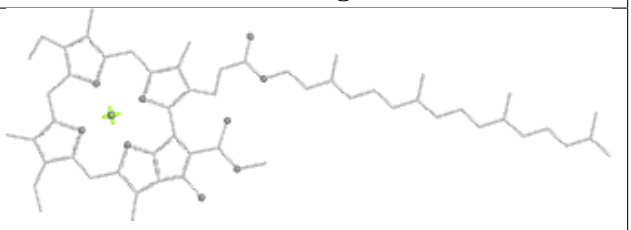
Bond lengths



Bond angles

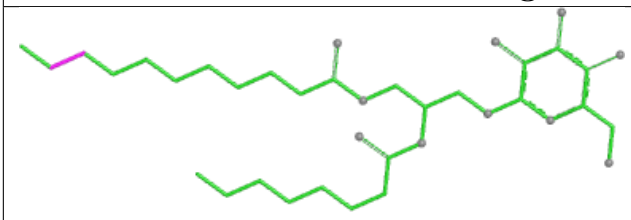


Torsions

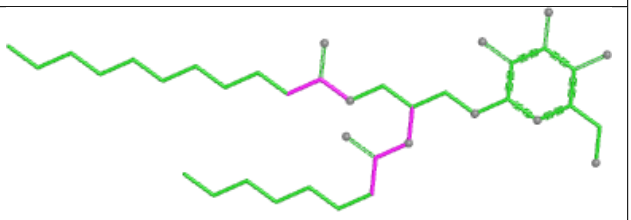


Rings

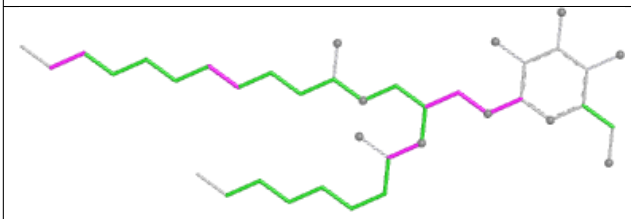
Ligand LMG Y 319



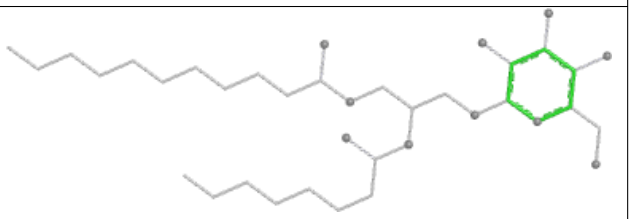
Bond lengths



Bond angles

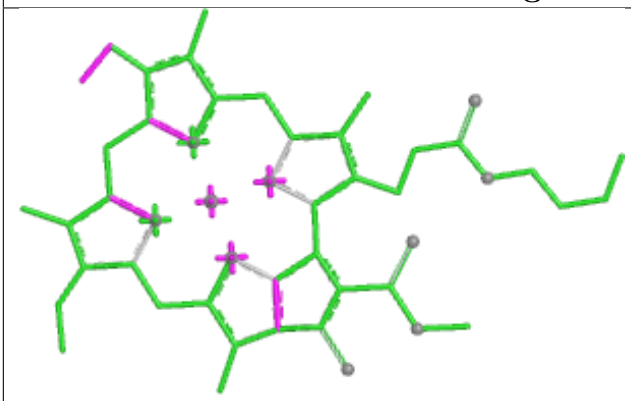


Torsions

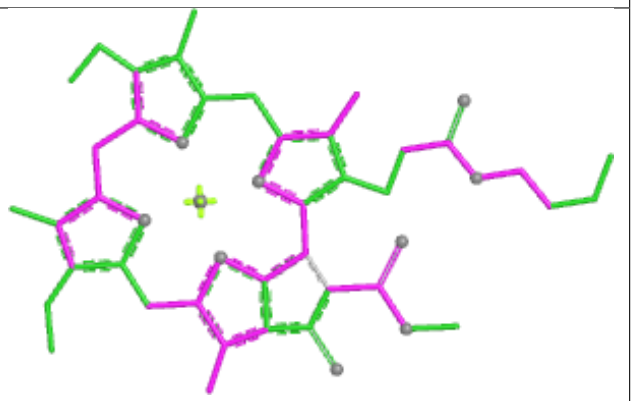


Rings

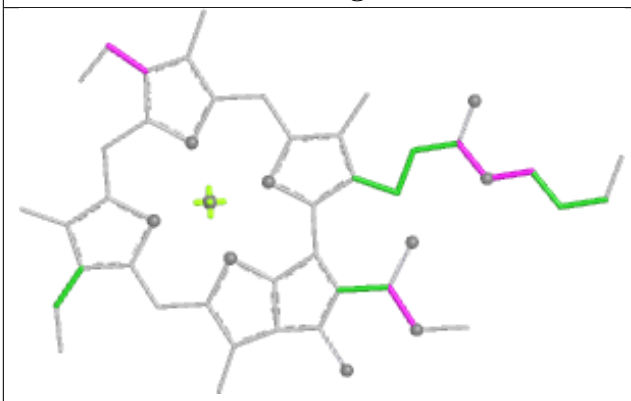
Ligand CLA R 314



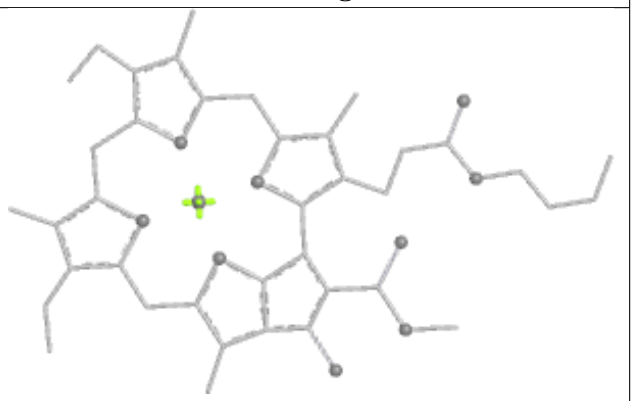
Bond lengths



Bond angles

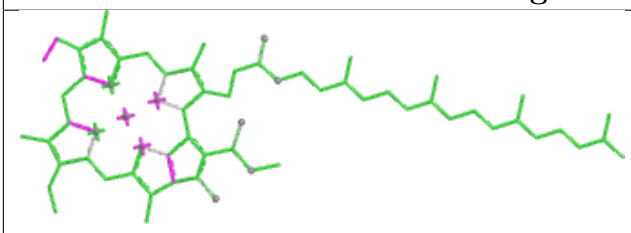


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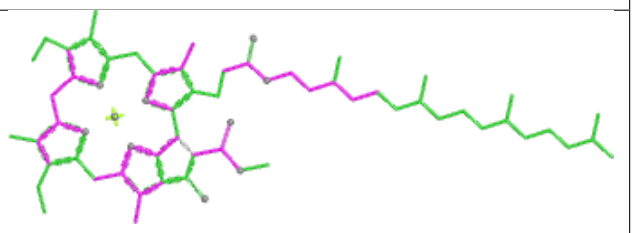


Rings

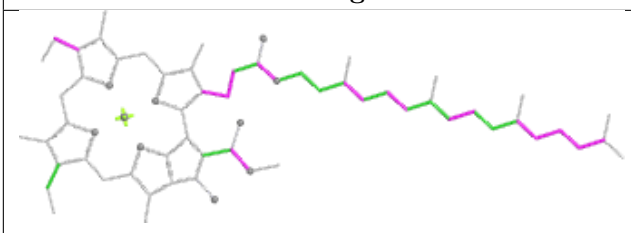
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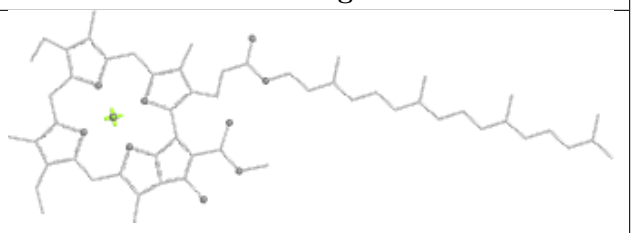
Bond lengths



Bond angles

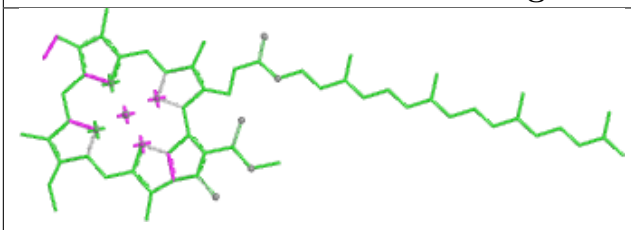


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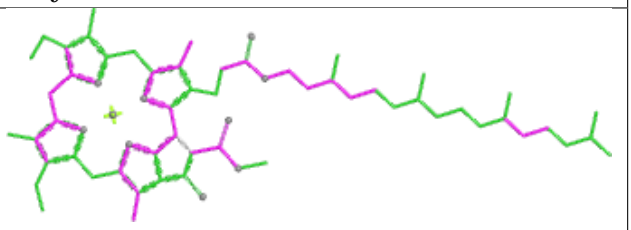


Rings

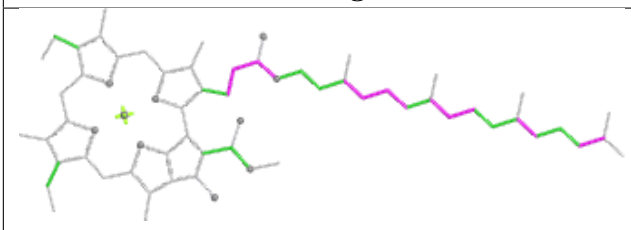
Ligand CLA y 613



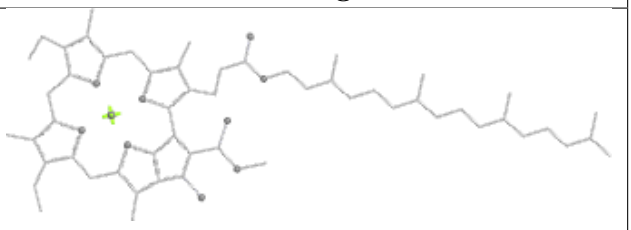
Bond lengths



Bond angles

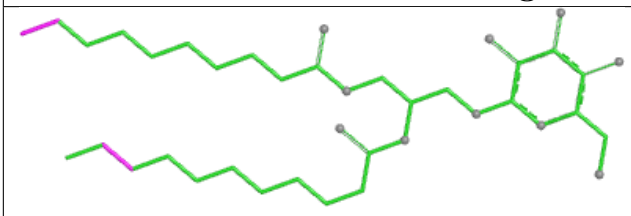


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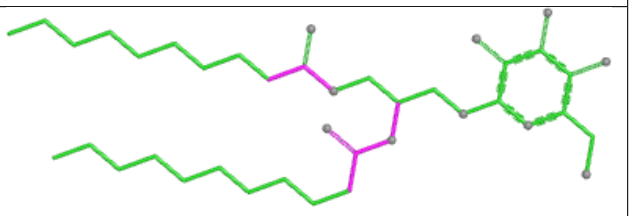


Rings

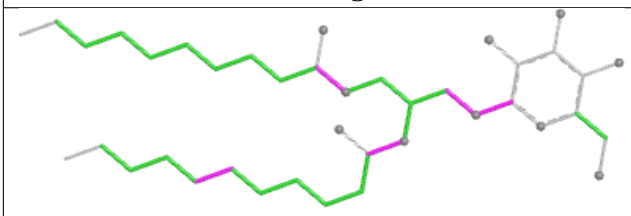
Ligand LMG G 622



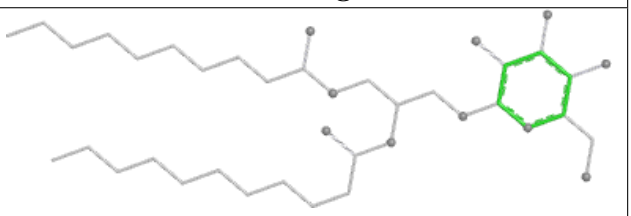
Bond lengths



Bond angles

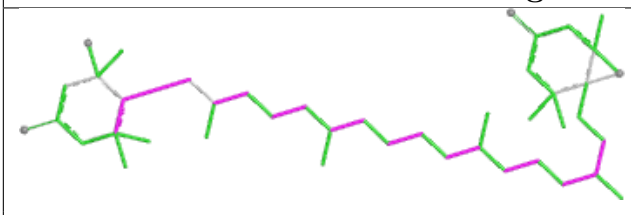


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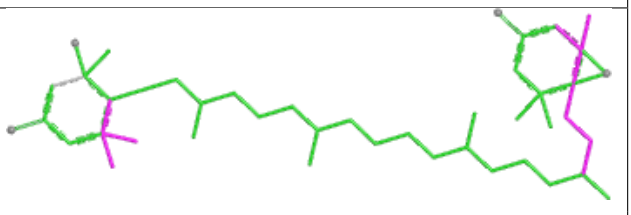


Rings

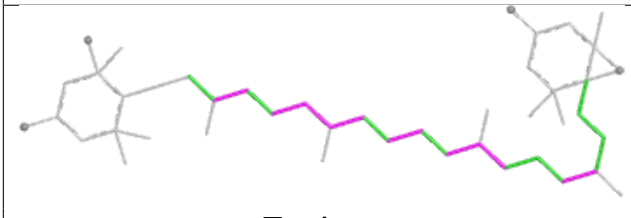
Ligand NEX 2 616



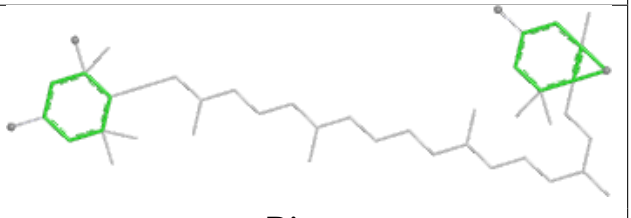
Bond lengths



Bond angles

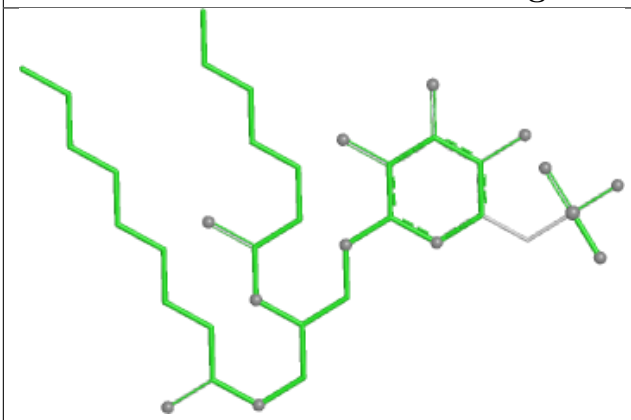


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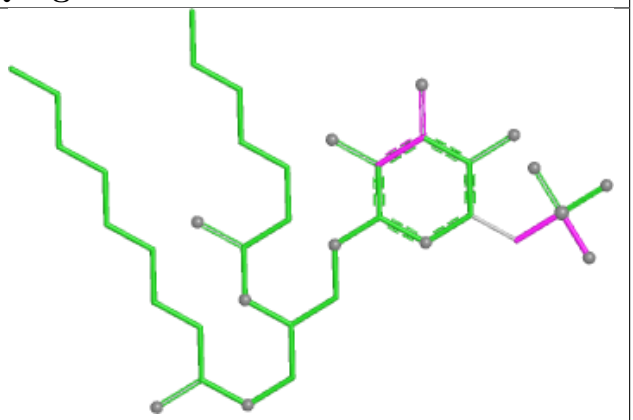


Rings

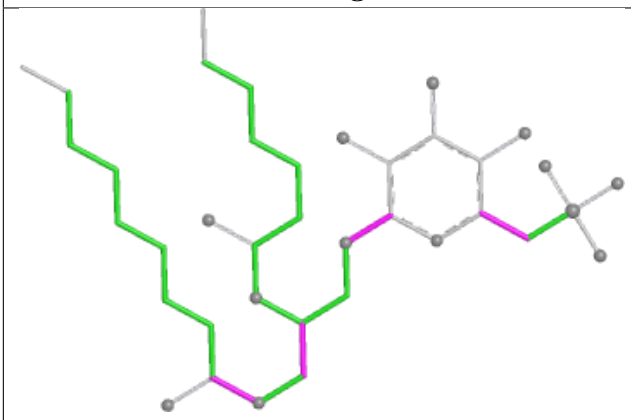
Ligand SQD g 301



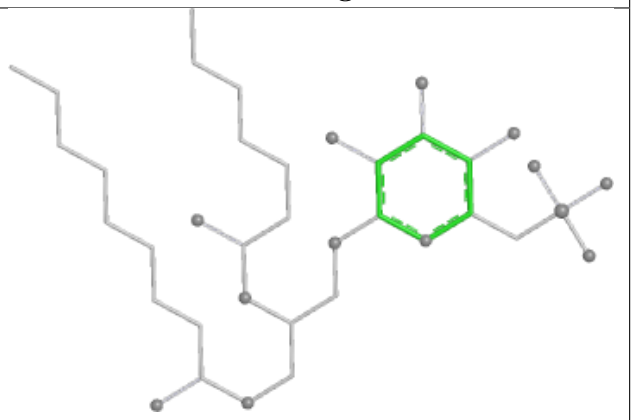
Bond lengths



Bond angles

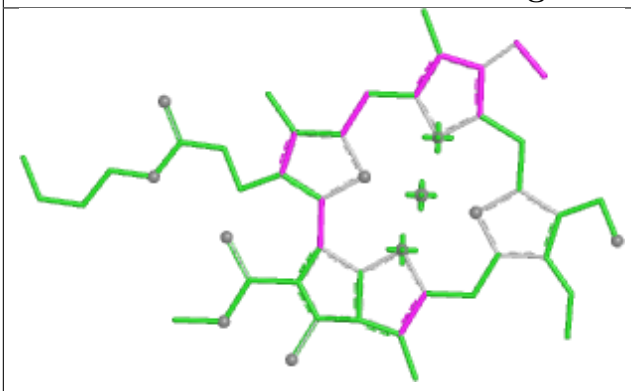


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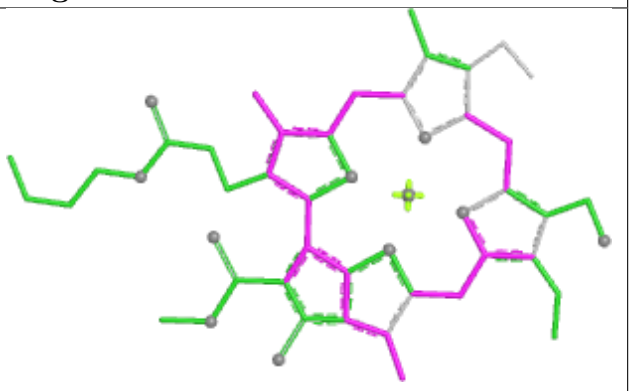


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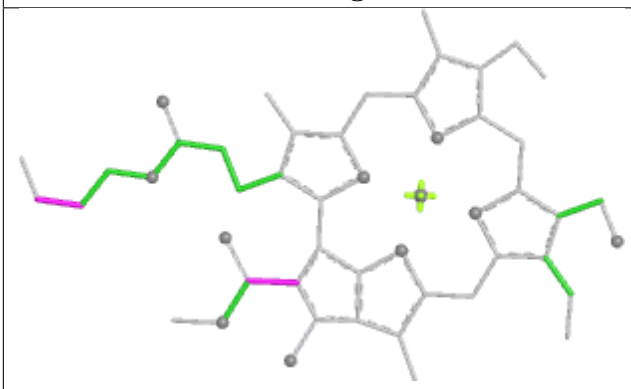
Ligand CHL g 307



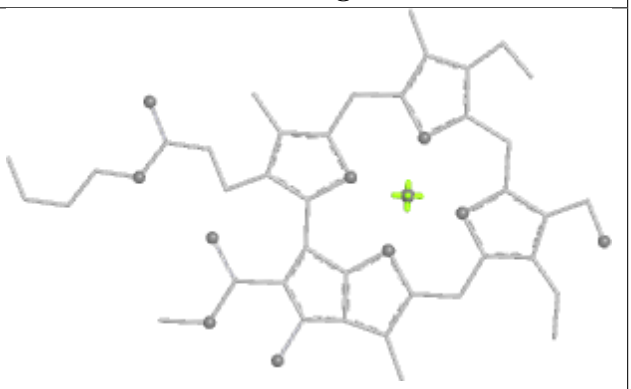
Bond lengths



Bond angles

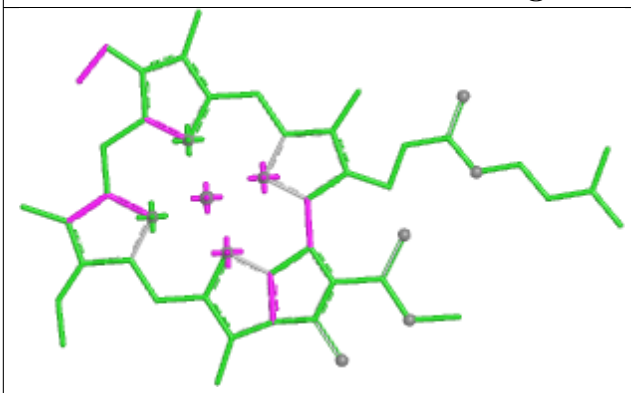


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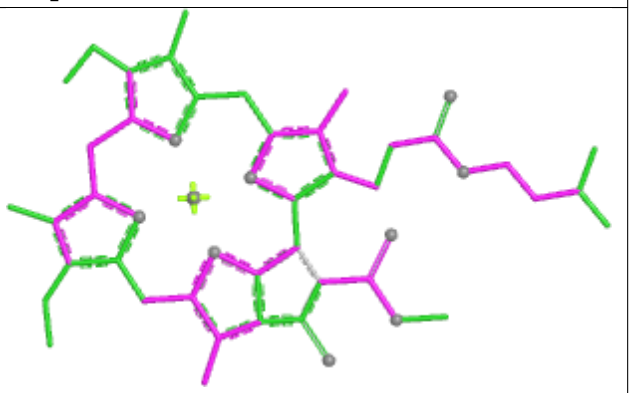


Rings

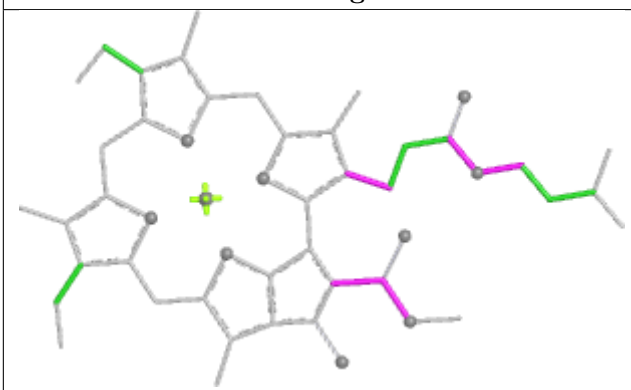
Ligand CLA p 604



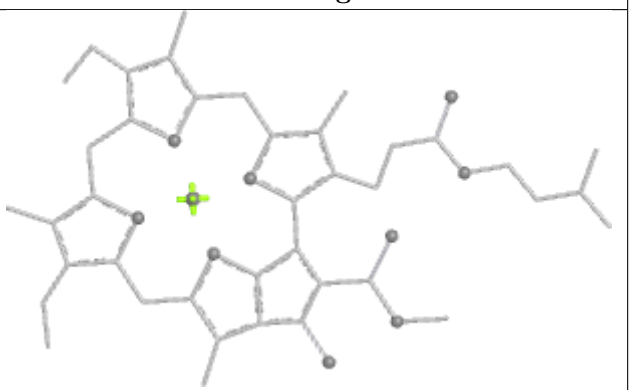
Bond lengths



Bond angles

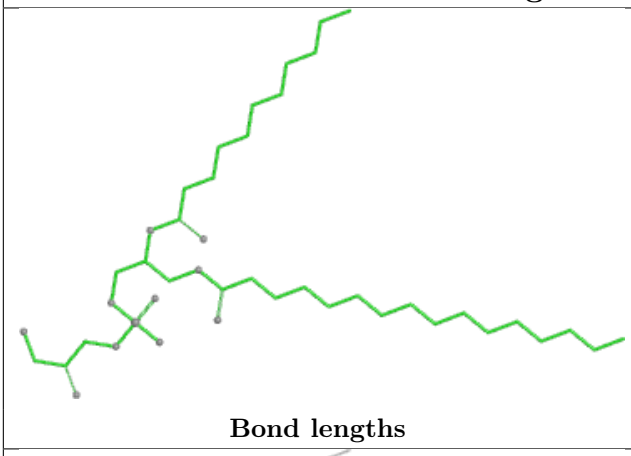


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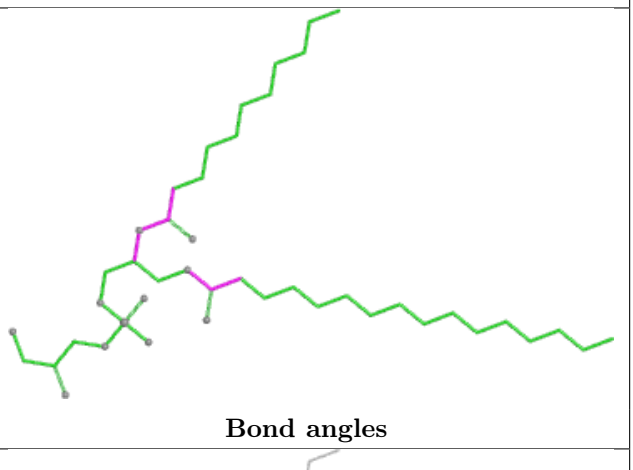


Rings

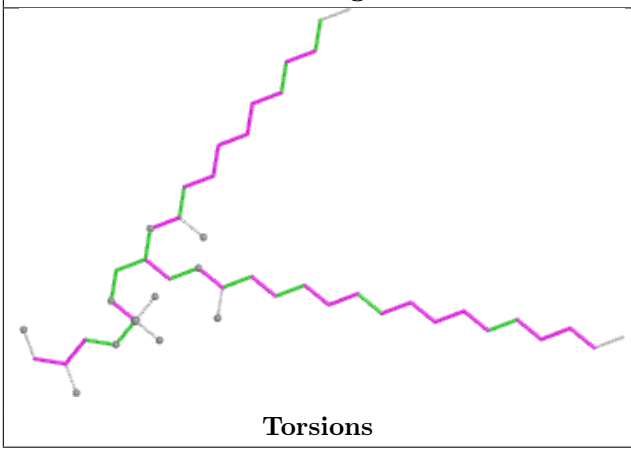
Ligand LHG b 625



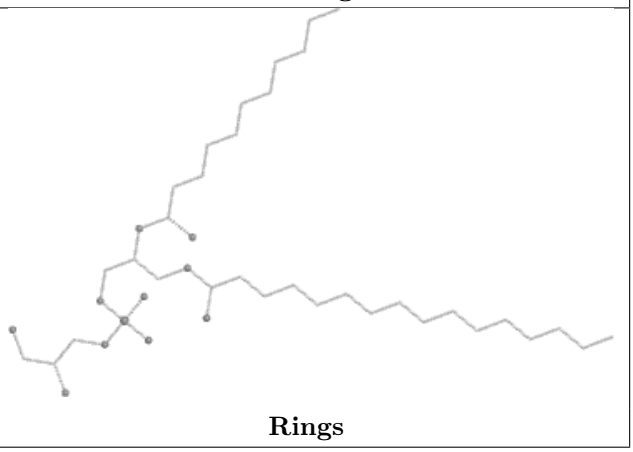
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Bond angles

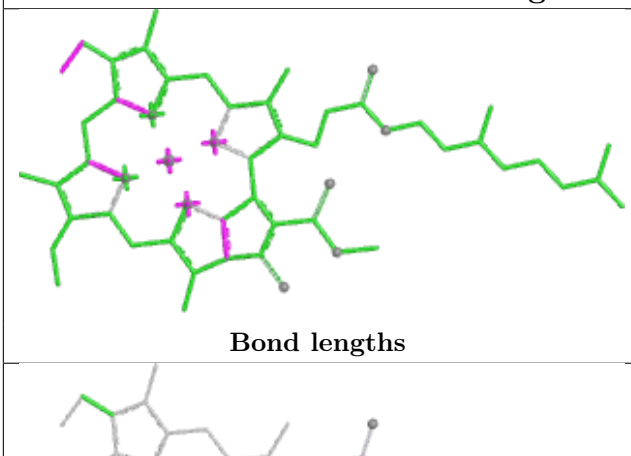


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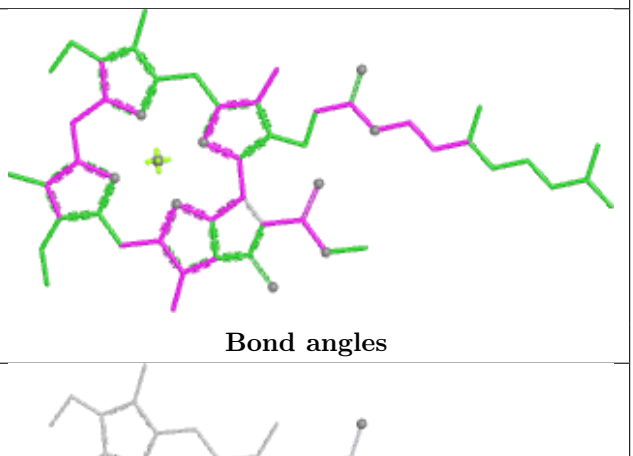


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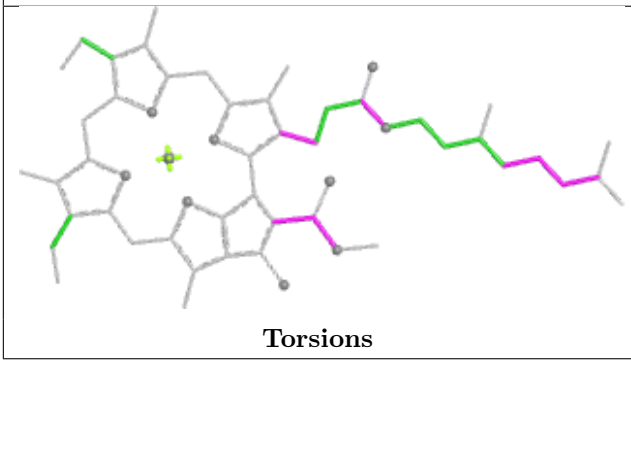
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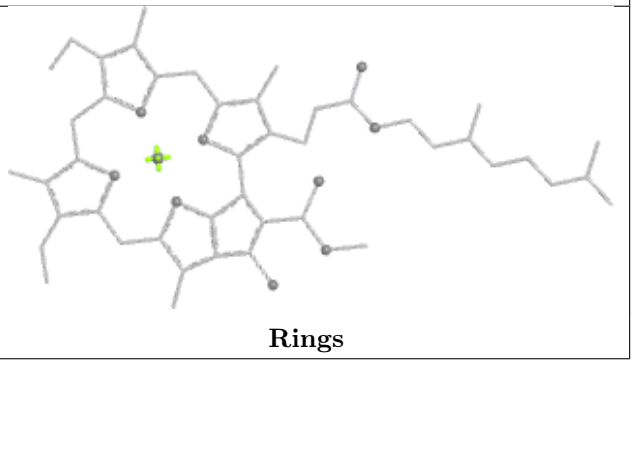
Bond lengths



Bond angles

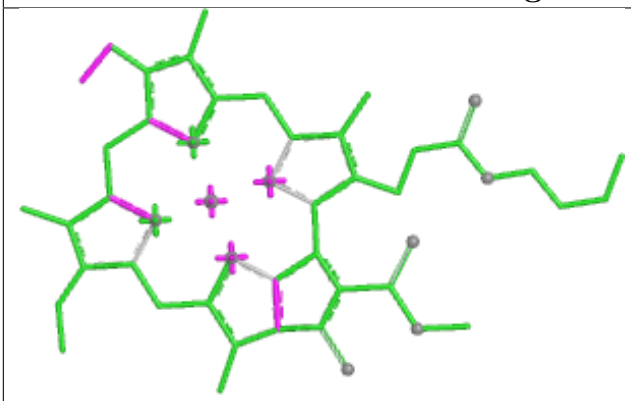


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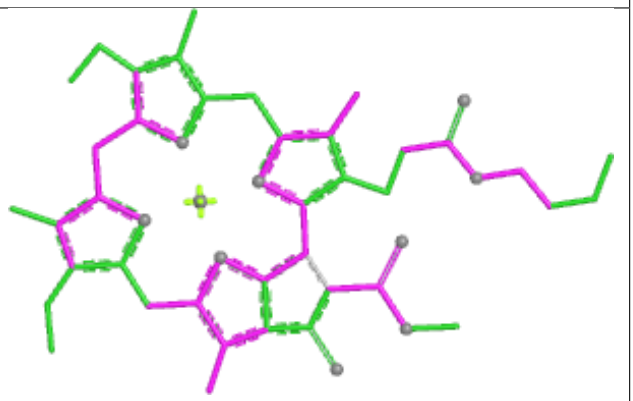


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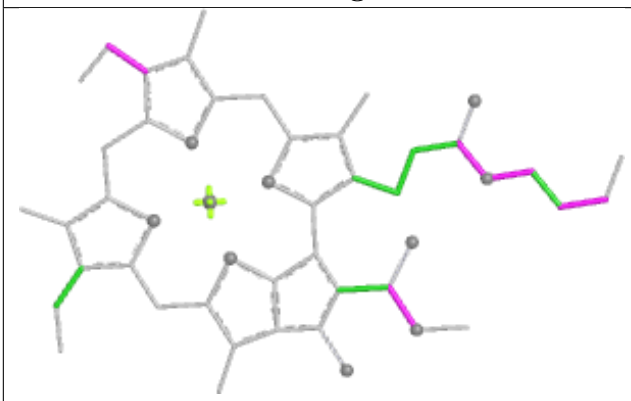
Ligand CLA B 601



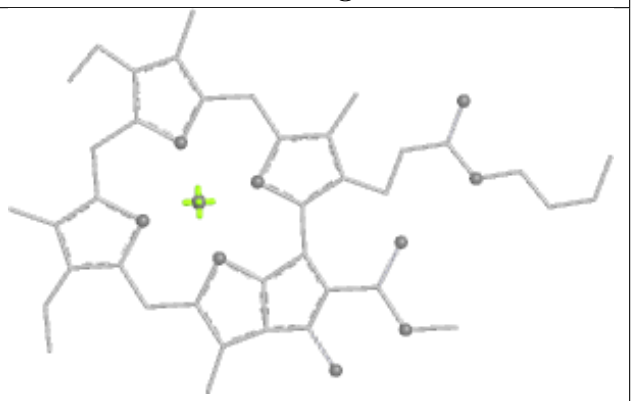
Bond lengths



Bond angles

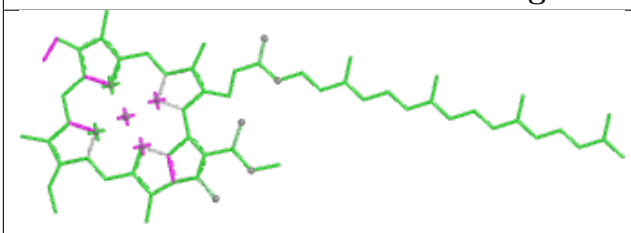


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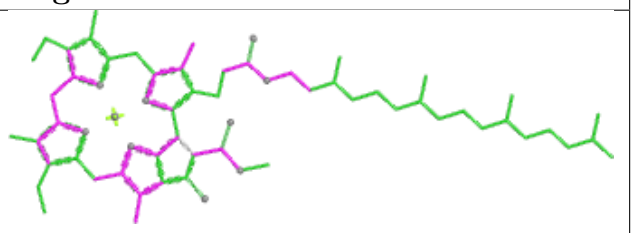


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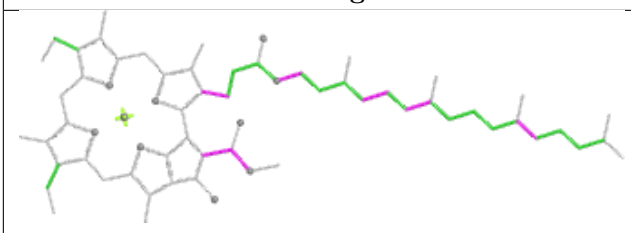
Ligand CLA g 303



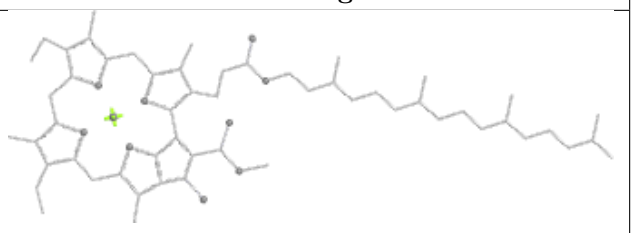
Bond lengths



Bond angles

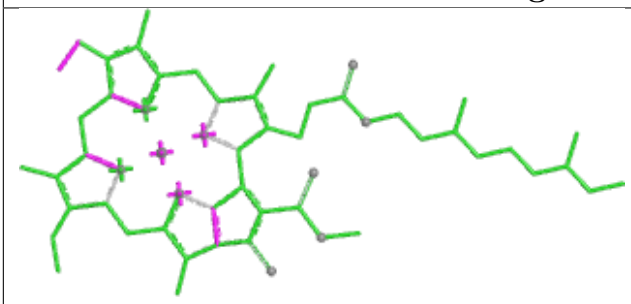


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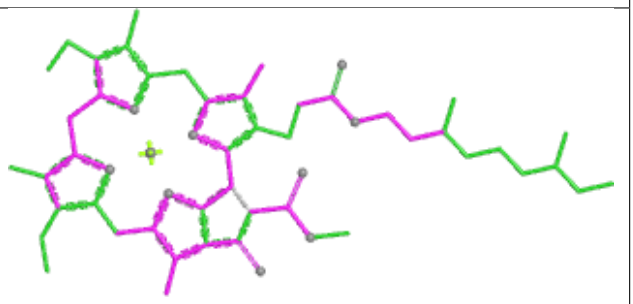


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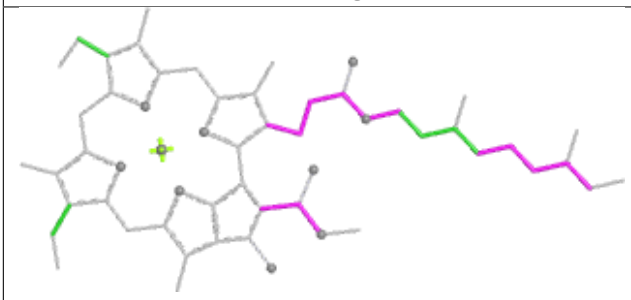
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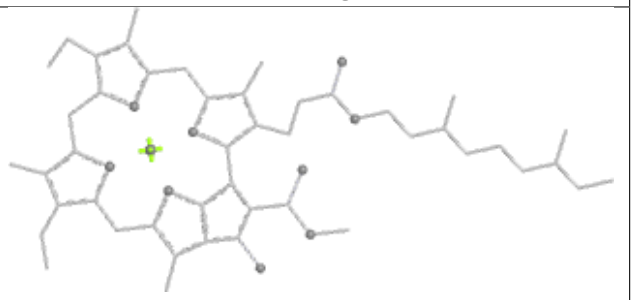
Bond lengths



Bond angles

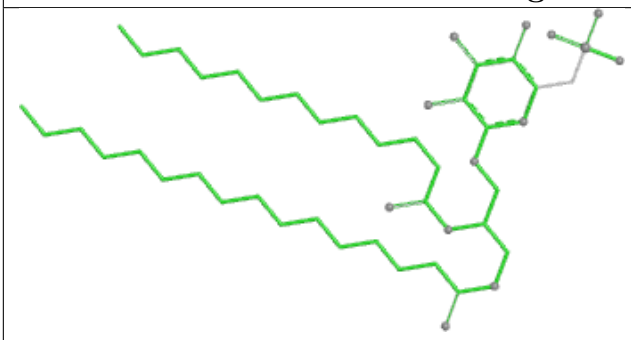


Torsions

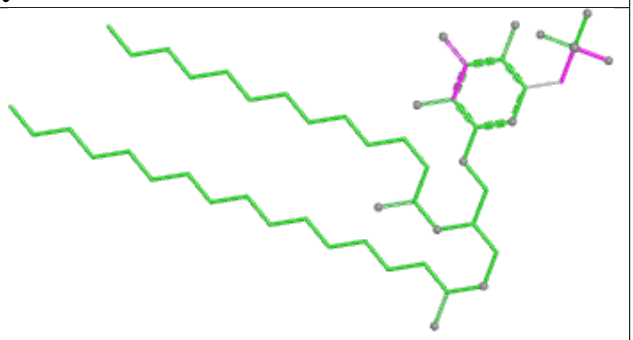


Rings

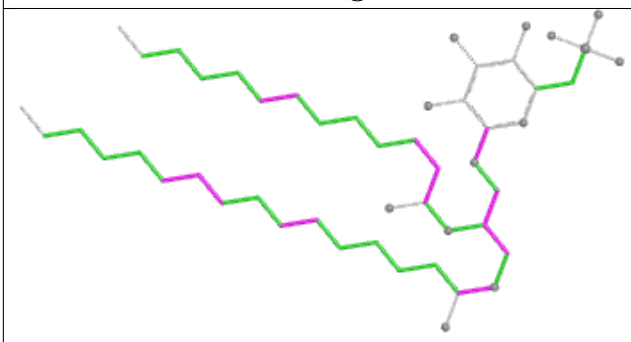
Ligand SQD S 301



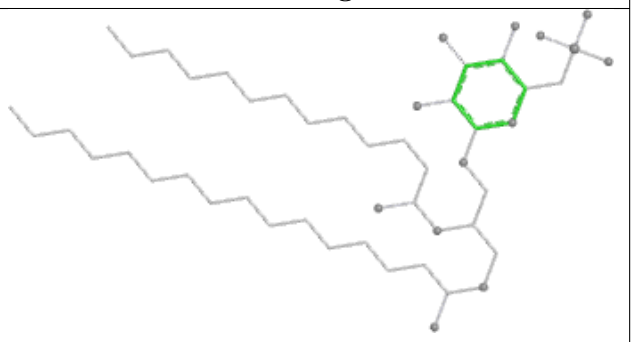
Bond lengths



Bond angles

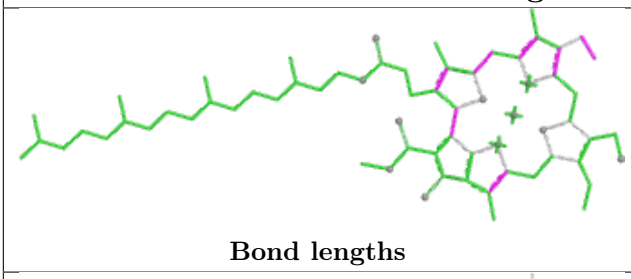


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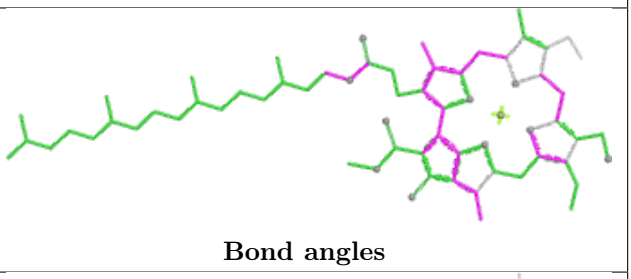


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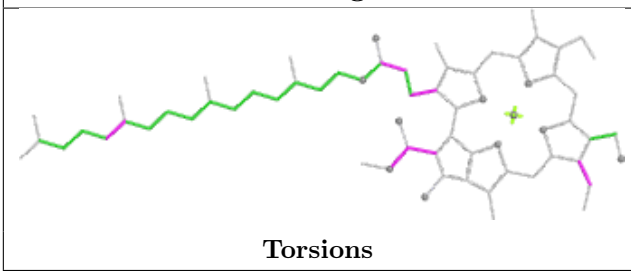
Ligand CHL n 310



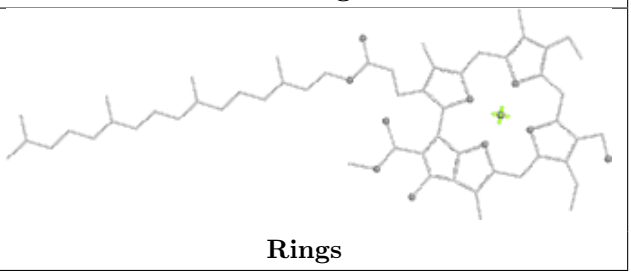
Bond lengths



Bond angles

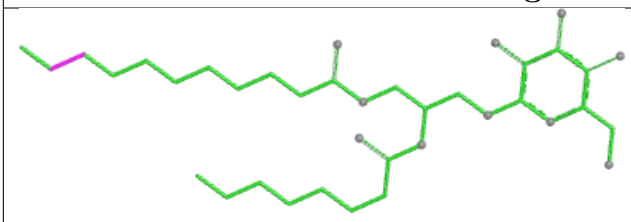


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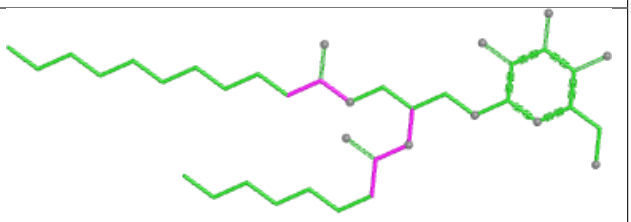


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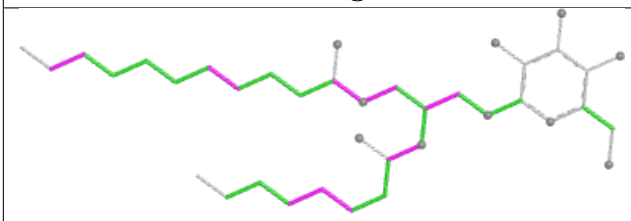
Ligand LMG a 416



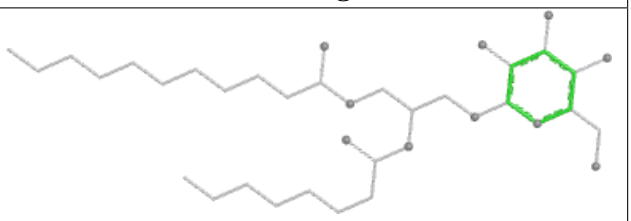
Bond lengths



Bond angles

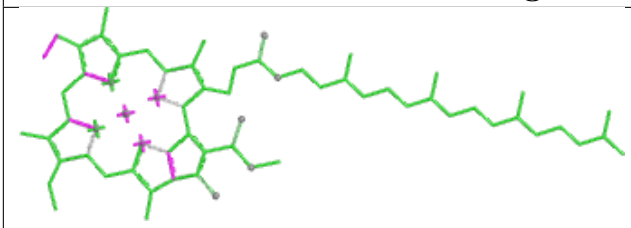


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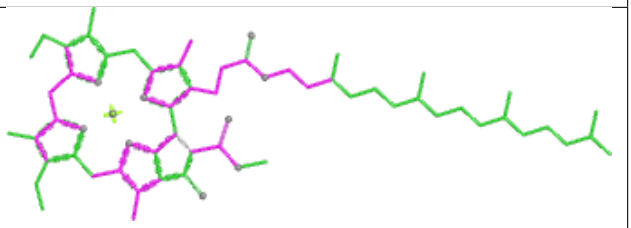


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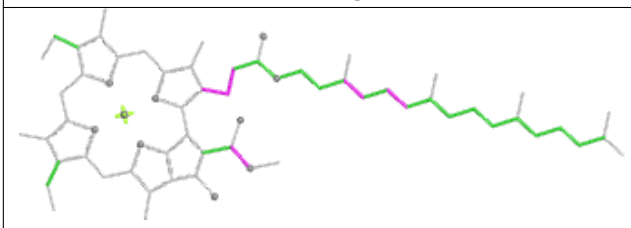
Ligand CLA A 405



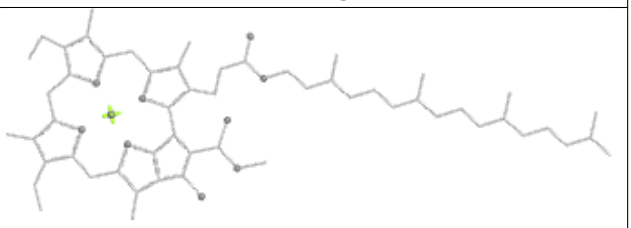
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Bond angles

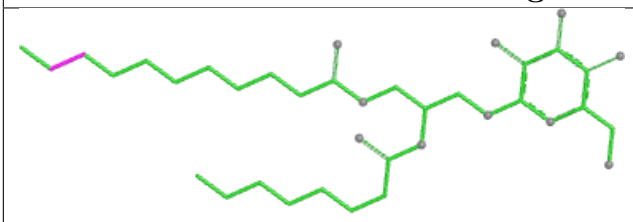


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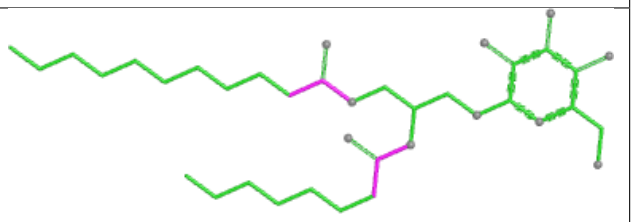


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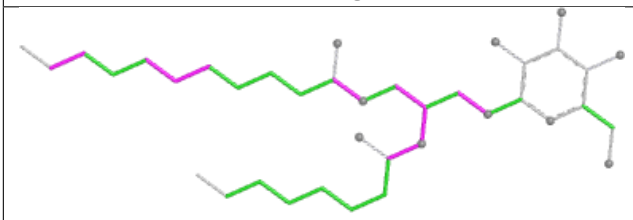
Ligand LMG f 101



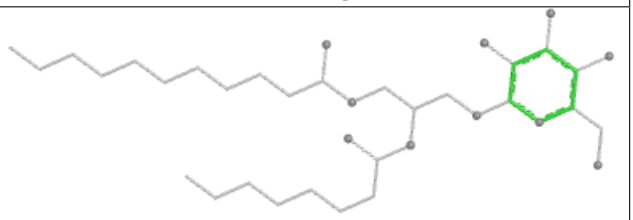
Bond lengths



Bond angles

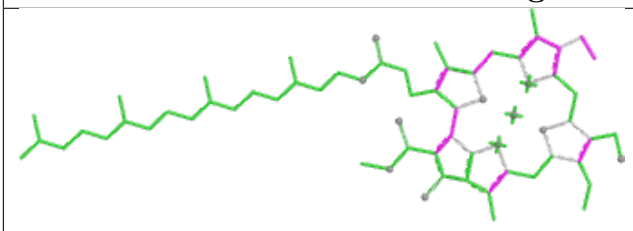


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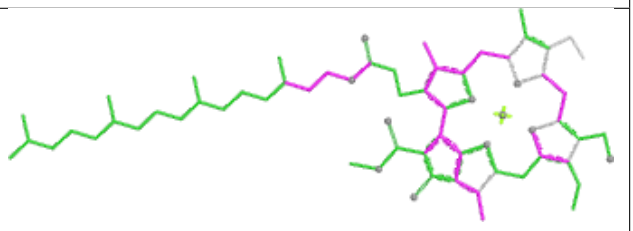


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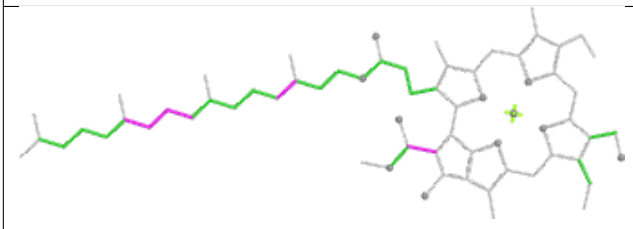
Ligand CHL 1 609



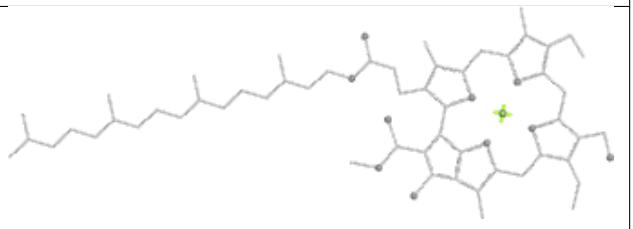
Bond lengths



Bond angles

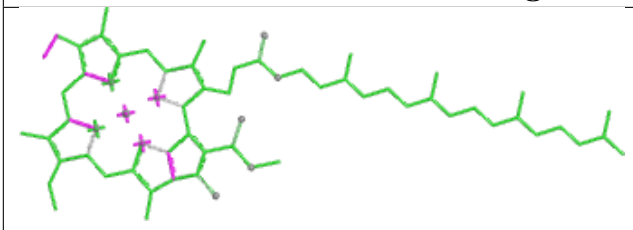


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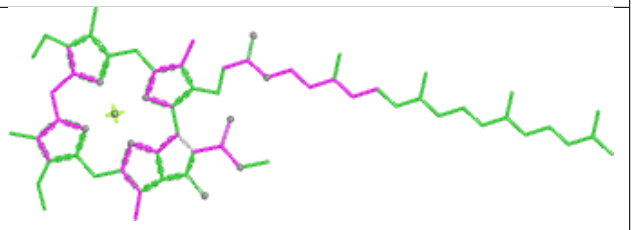


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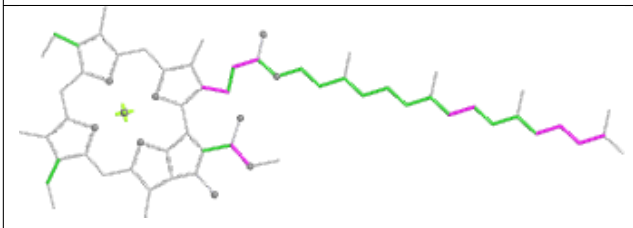
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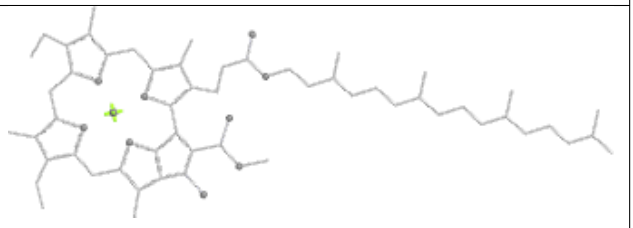
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Bond angles

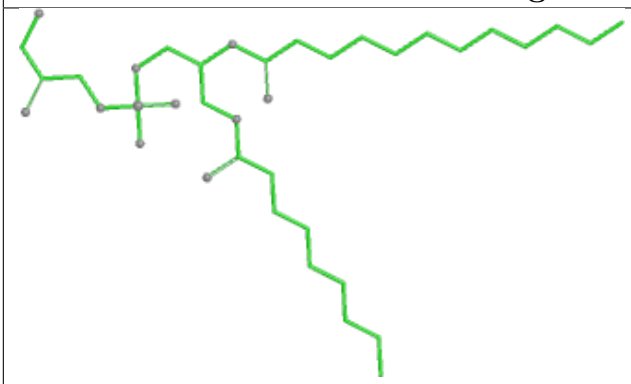


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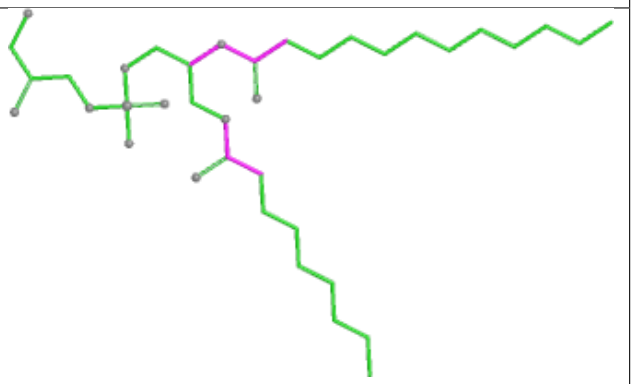


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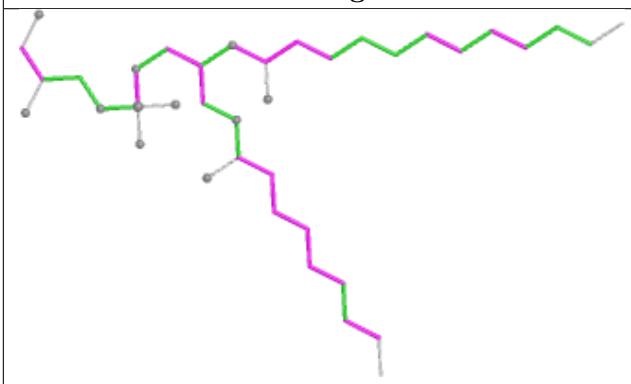
Ligand LHG r 320



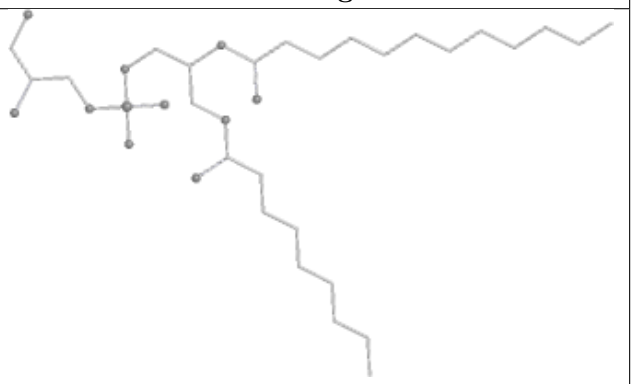
Bond lengths



Bond angles

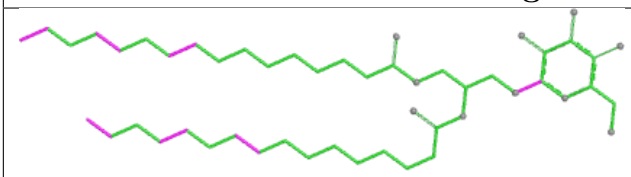


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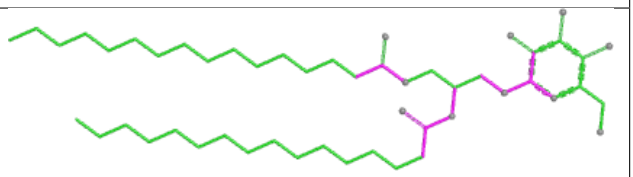


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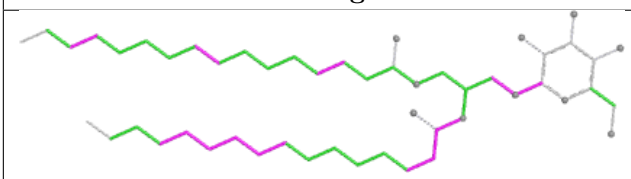
Ligand LMG b 622



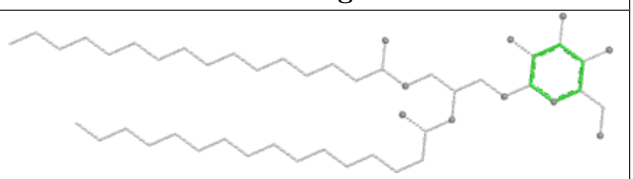
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Bond angles

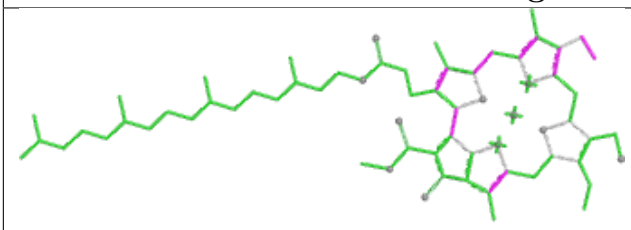


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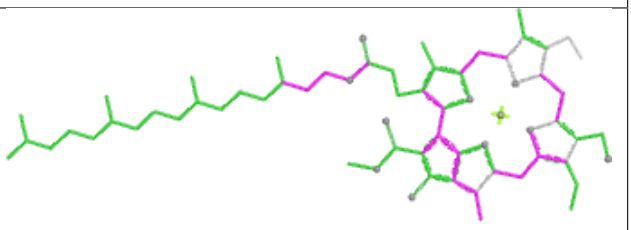


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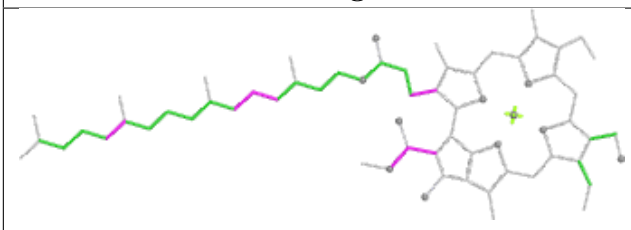
Ligand CHL 7 308



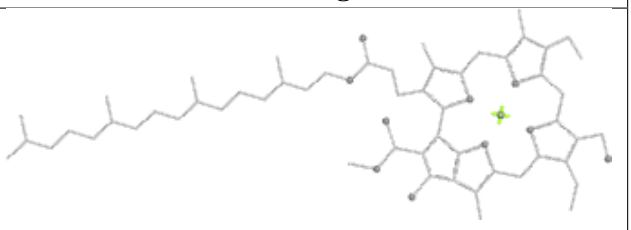
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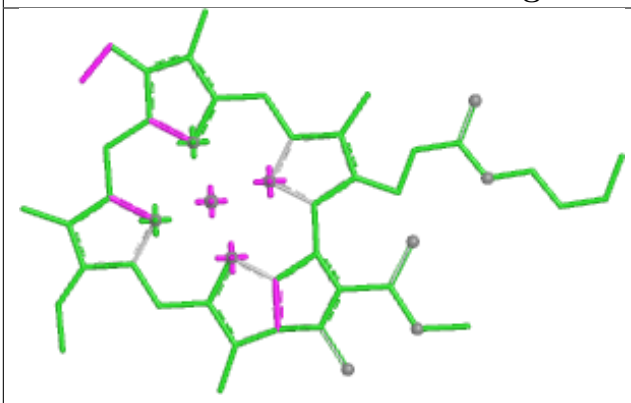


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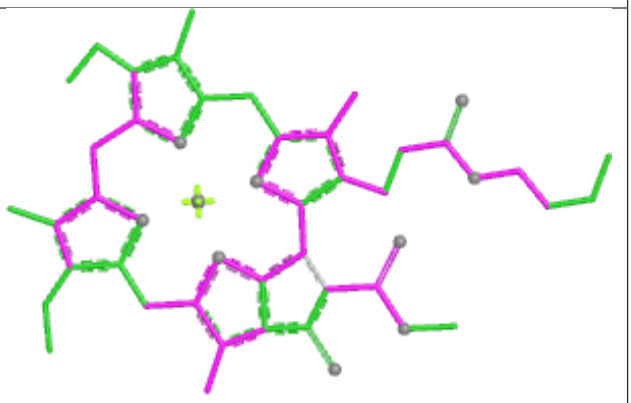


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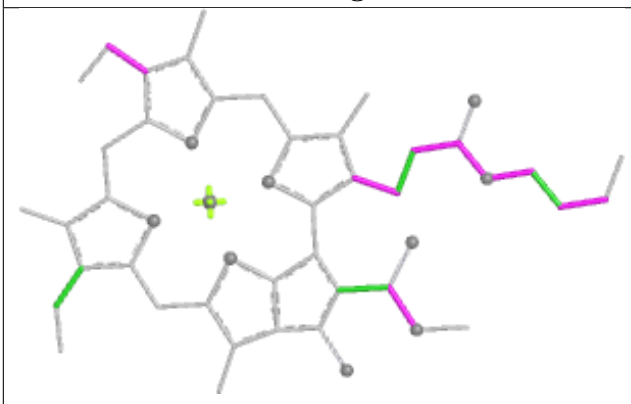
Ligand CLA G 613



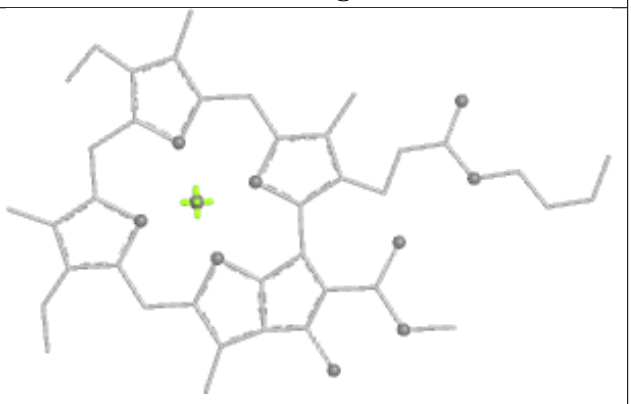
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Bond angles

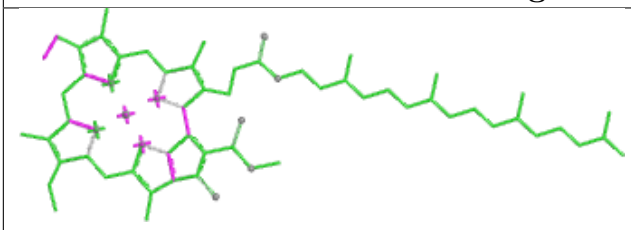


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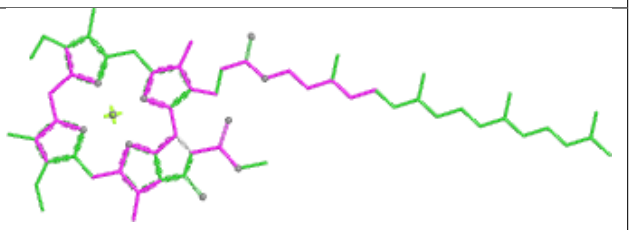


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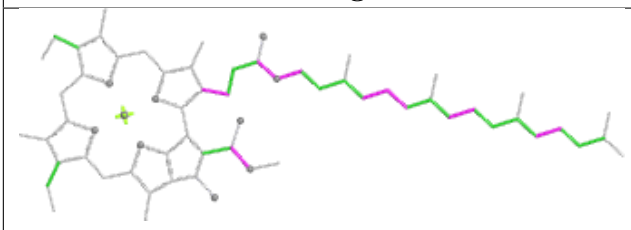
Ligand CLA a 407



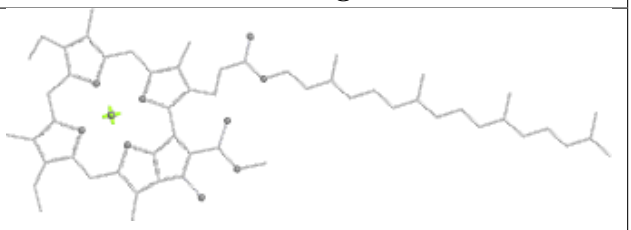
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Bond angles

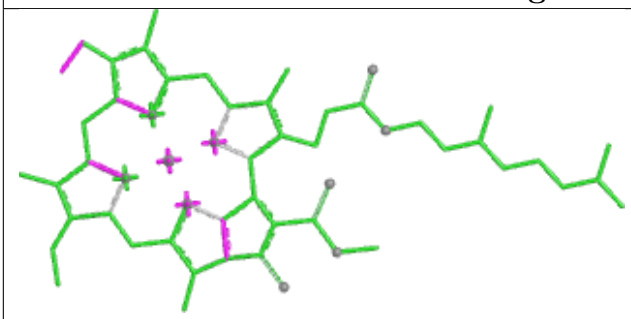


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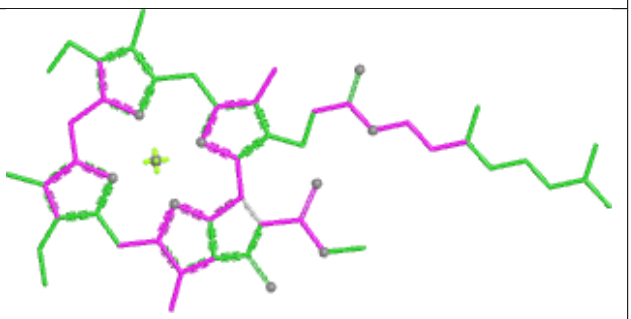


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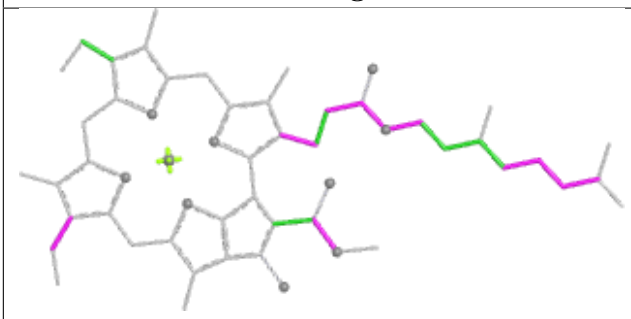
Ligand CLA 6 316



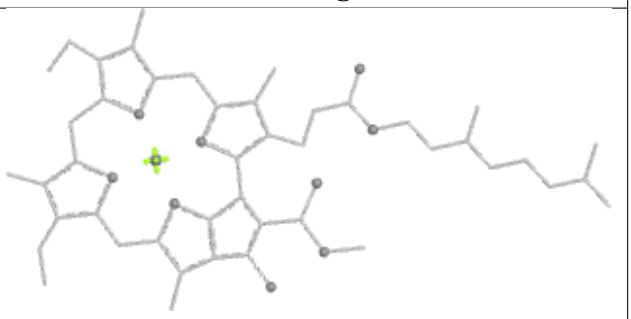
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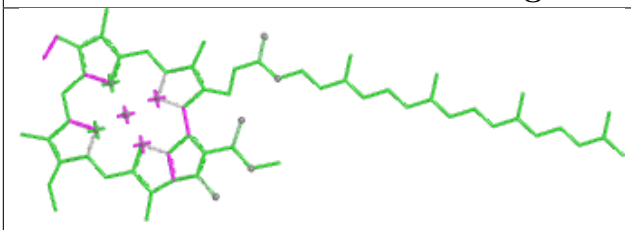
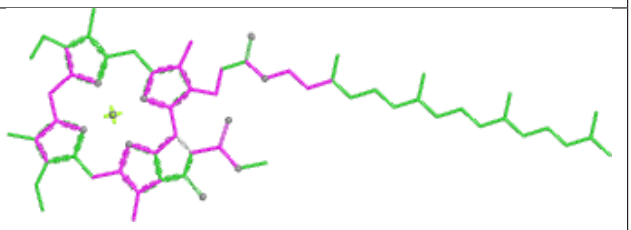
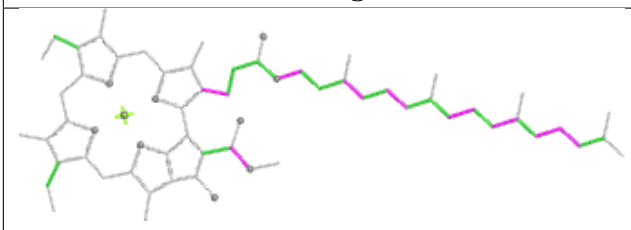
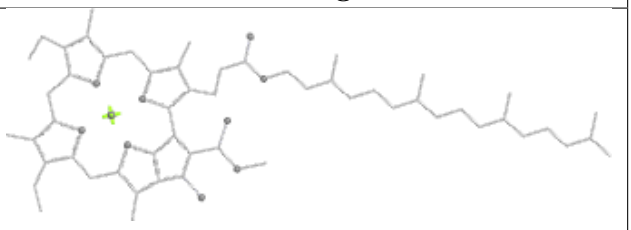
Bond angles

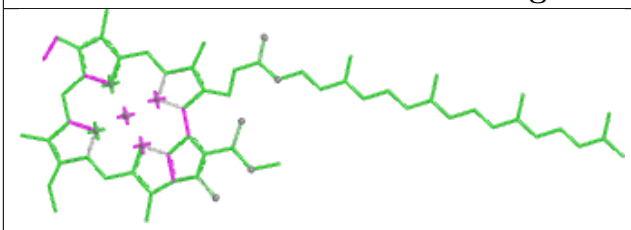
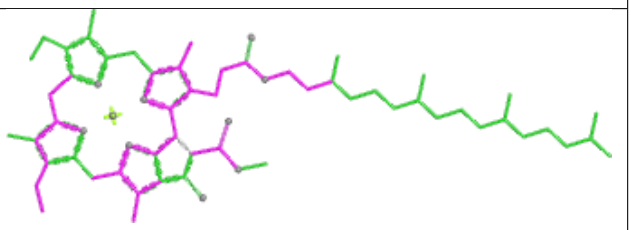
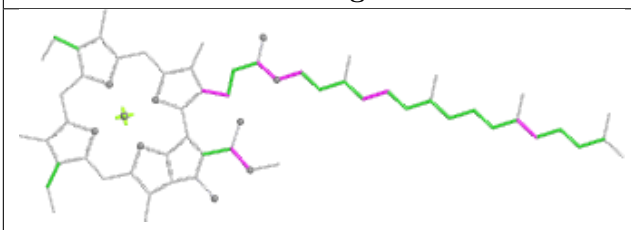
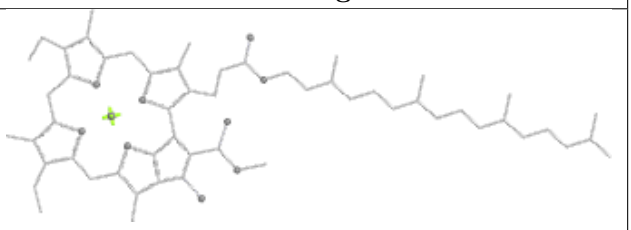


Torsions

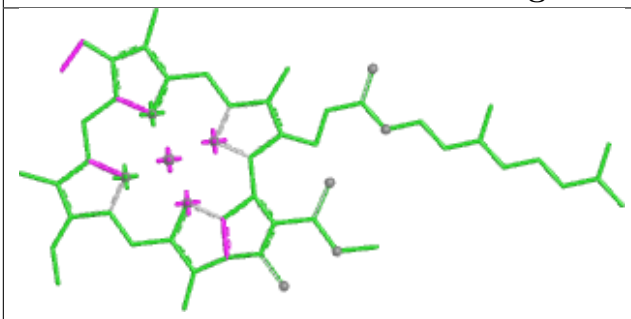


Rings

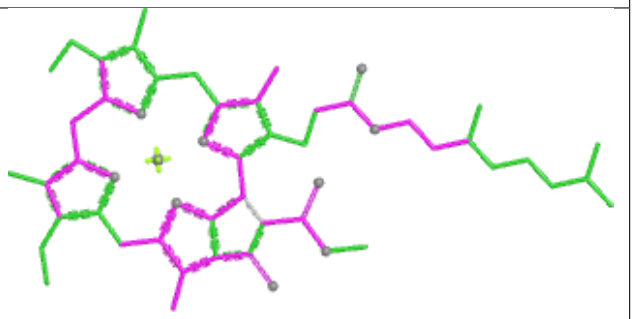
Ligand CLA C 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

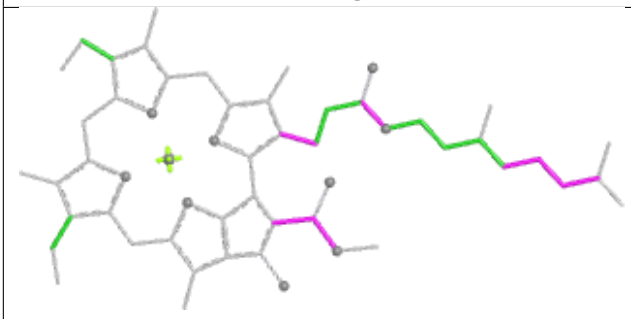
Ligand CLA 9 305



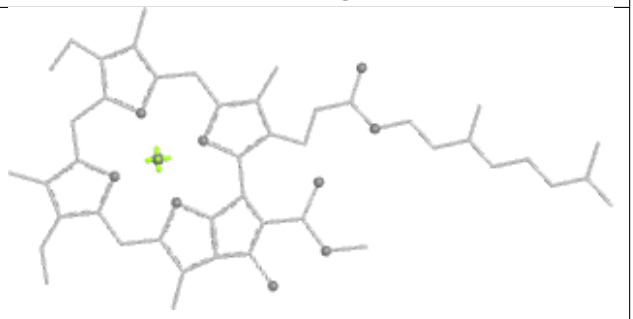
Bond lengths



Bond angles

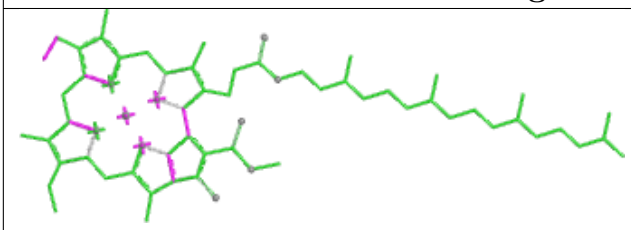


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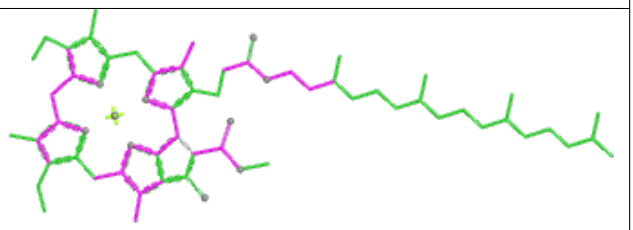


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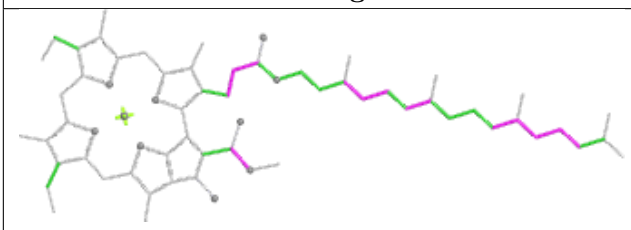
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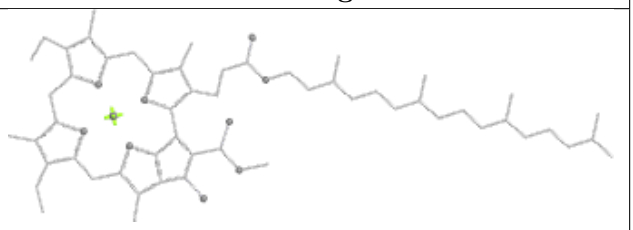
Bond lengths



Bond angles

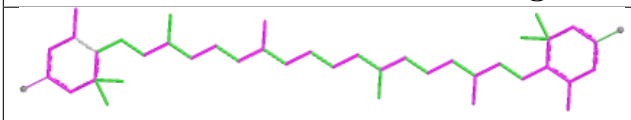


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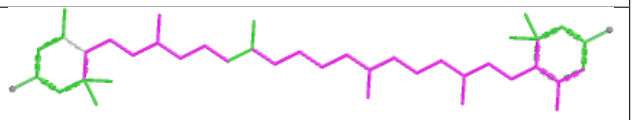


Rings

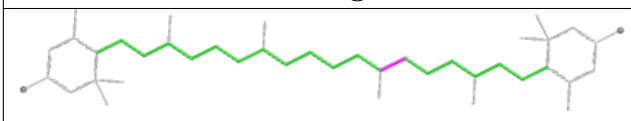
Ligand LUT 0 616



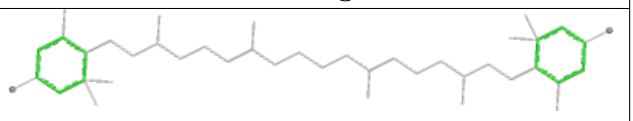
Bond lengths



Bond angles

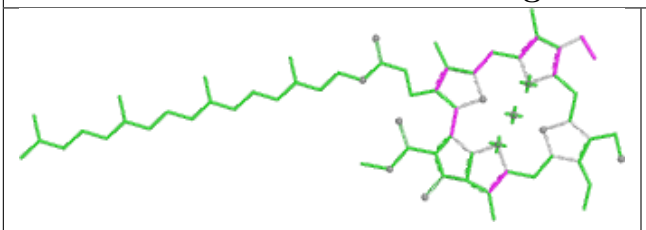


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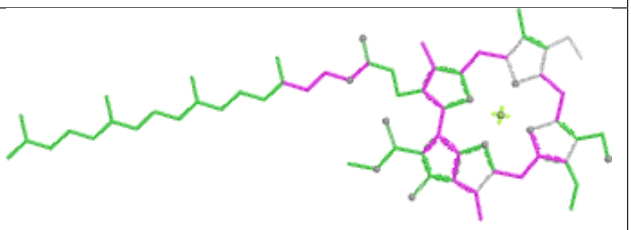


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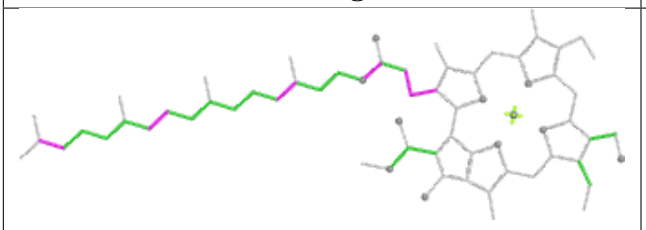
Ligand CHL Y 302



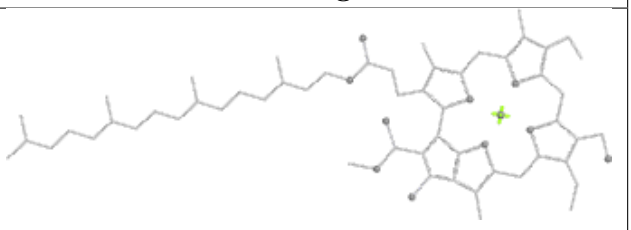
Bond lengths



Bond angles

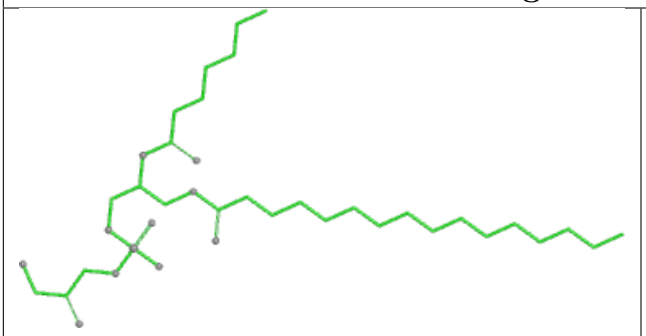


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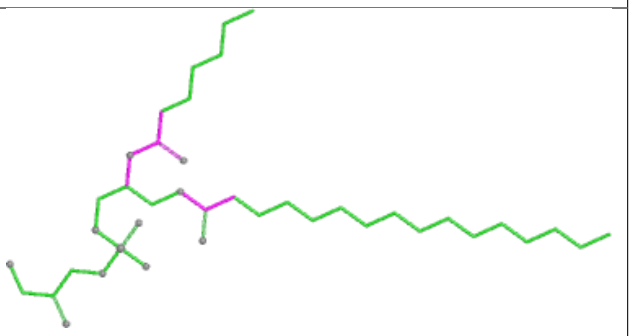


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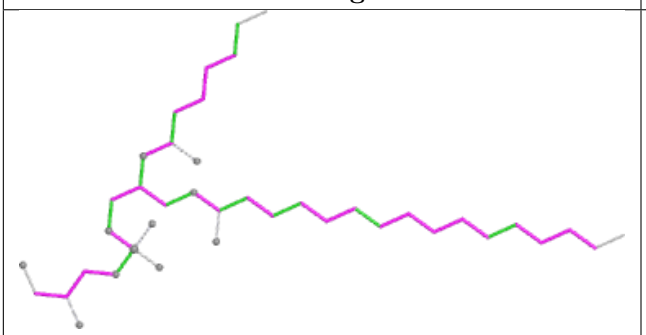
Ligand LHG C 623



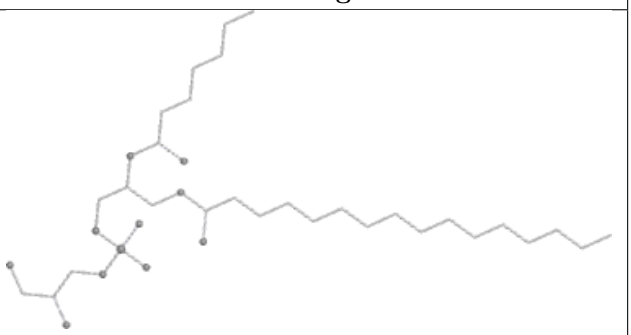
Bond lengths



Bond angles

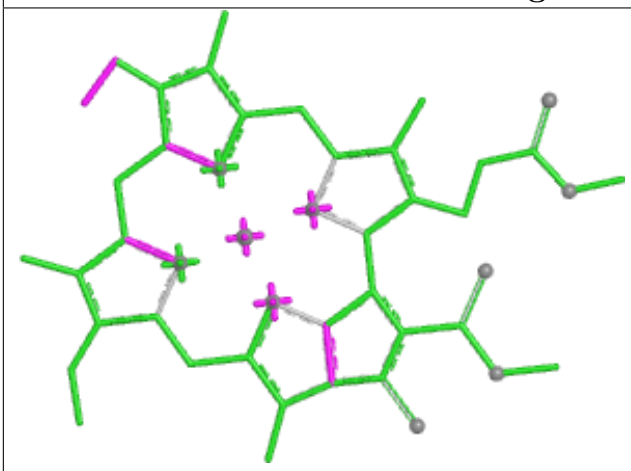


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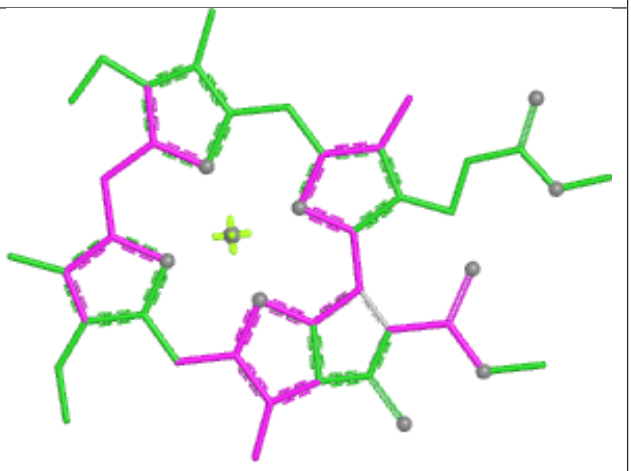


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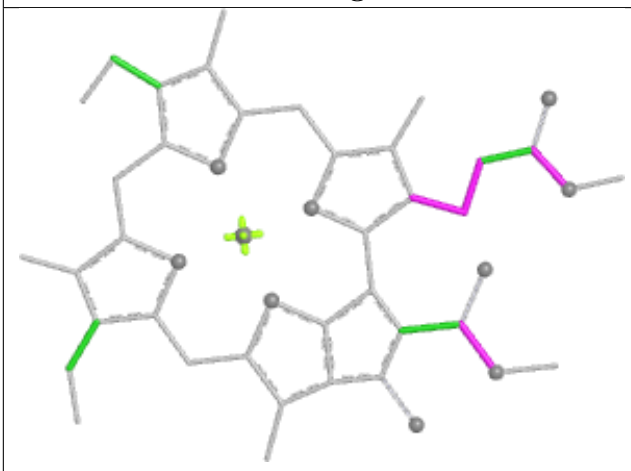
Ligand CLA 9 316



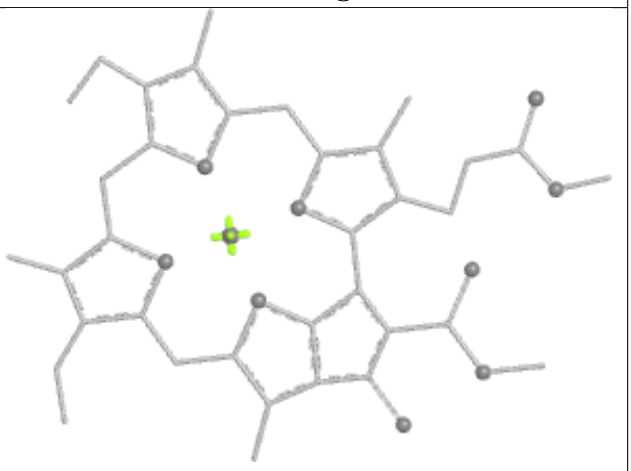
Bond lengths



Bond angles



Torsions

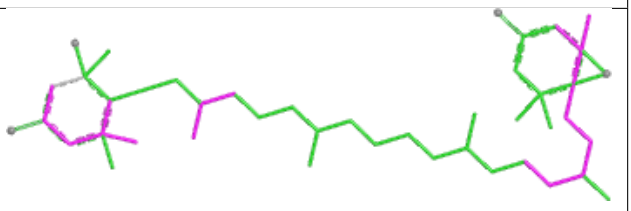


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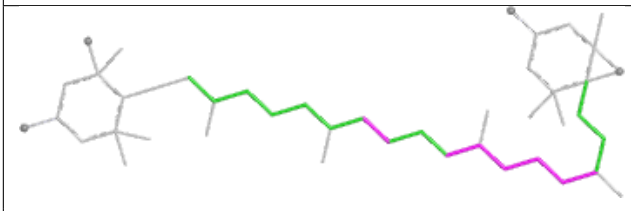
Ligand NEX 0 618



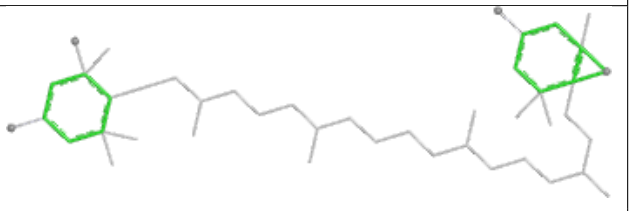
Bond lengths



Bond angles

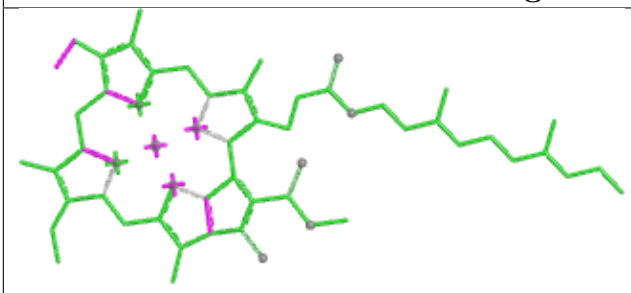


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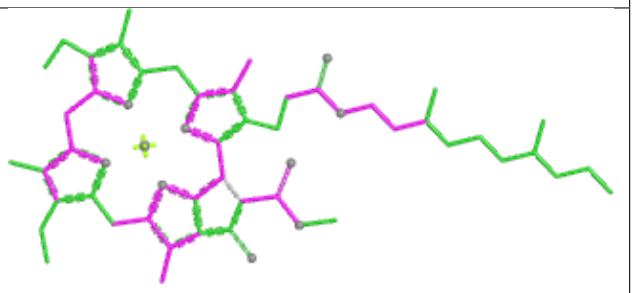


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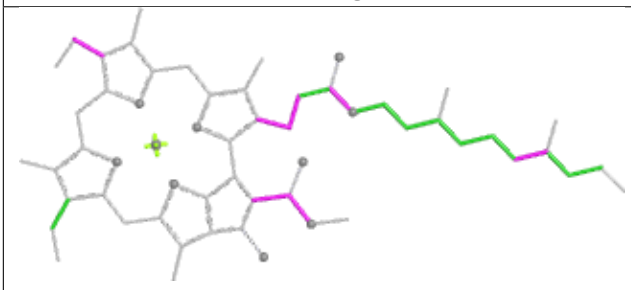
Ligand CLA C 606



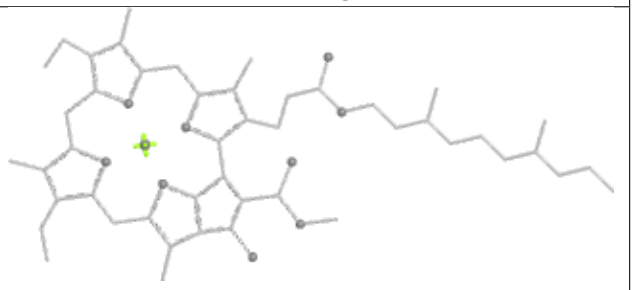
Bond lengths



Bond angles

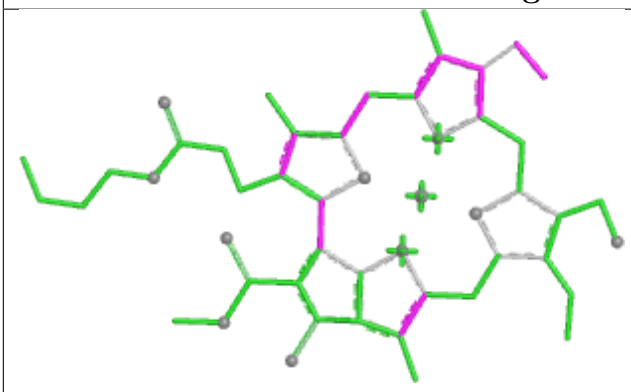


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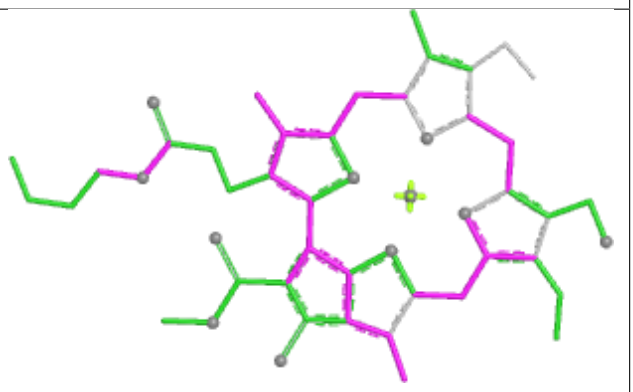


Rings

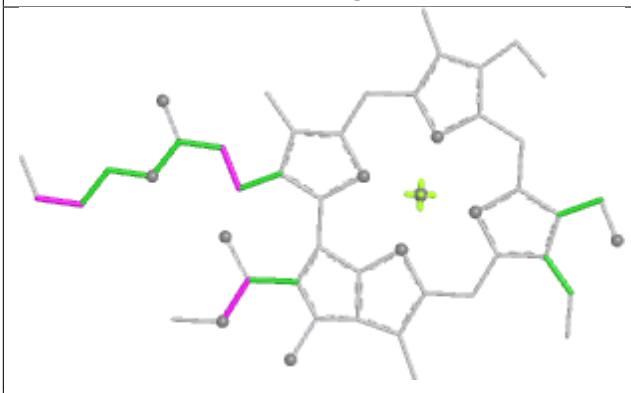
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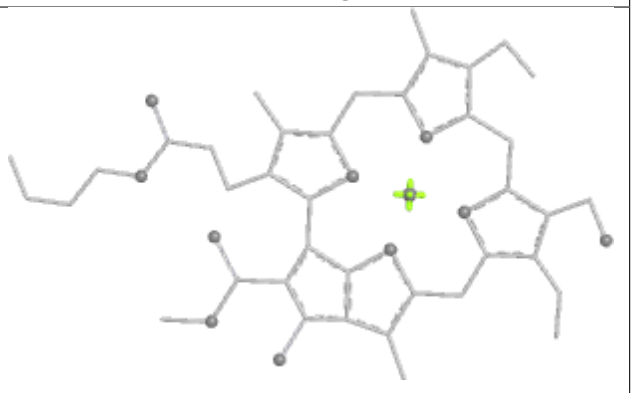
Bond lengths



Bond angles

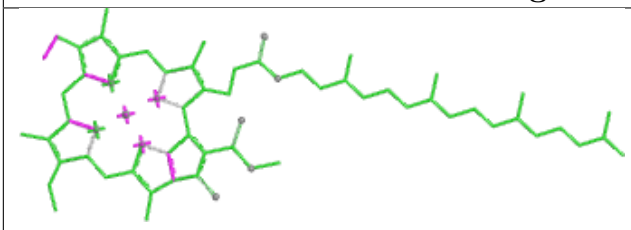


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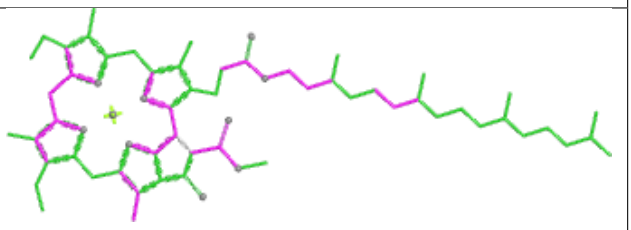


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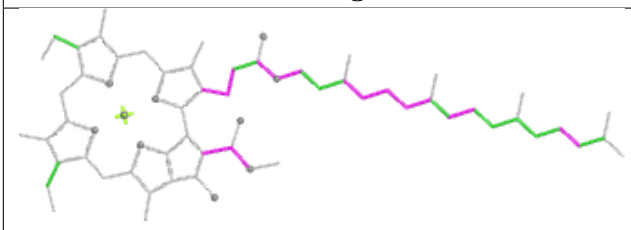
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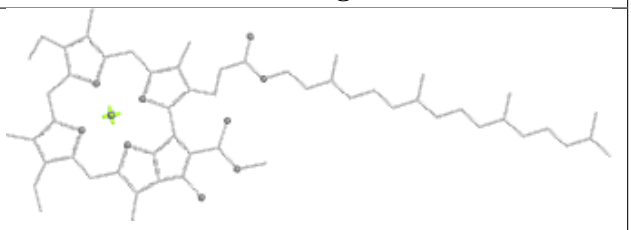
Bond lengths



Bond angles

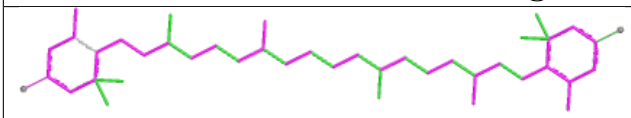


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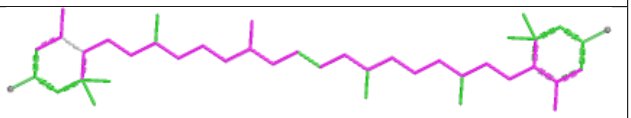


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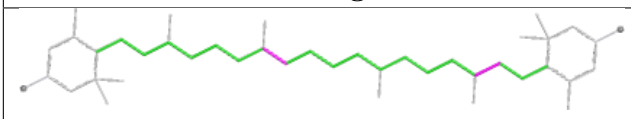
Ligand LUT 9 318



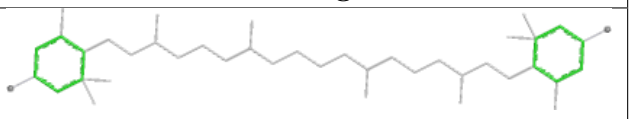
Bond lengths



Bond angles

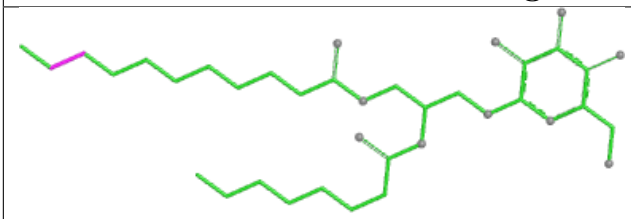


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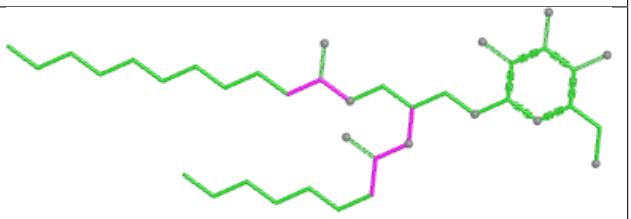


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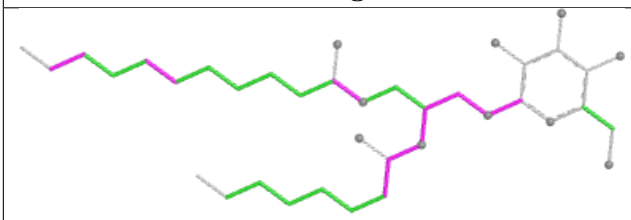
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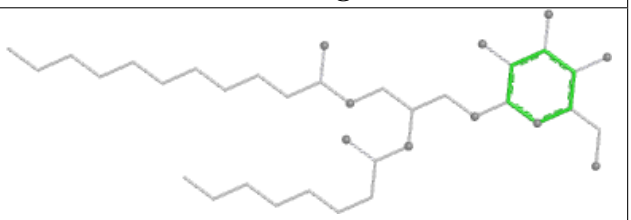
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Bond angles

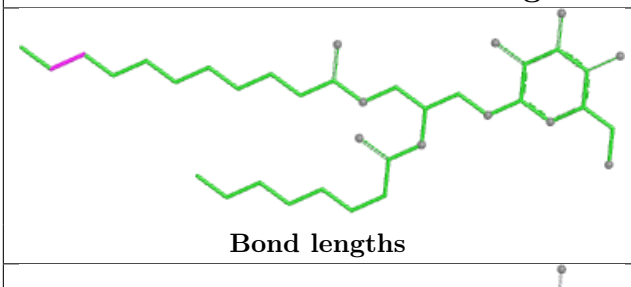


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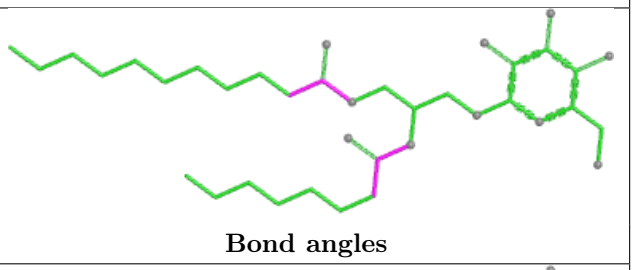


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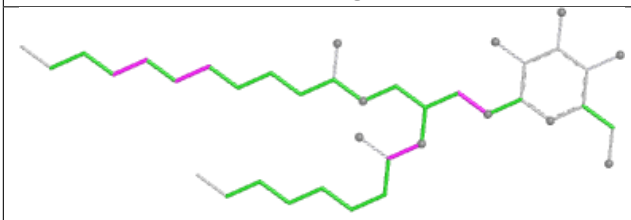
Ligand LMG J 102



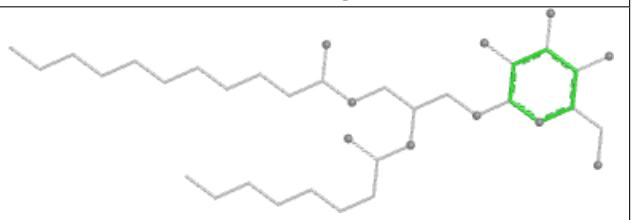
Bond lengths



Bond angles

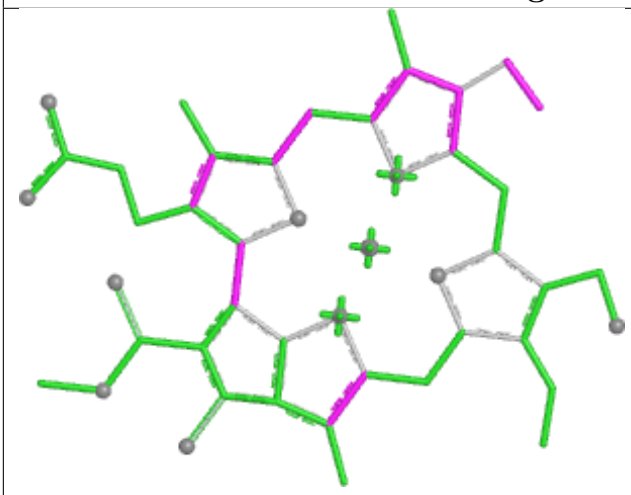


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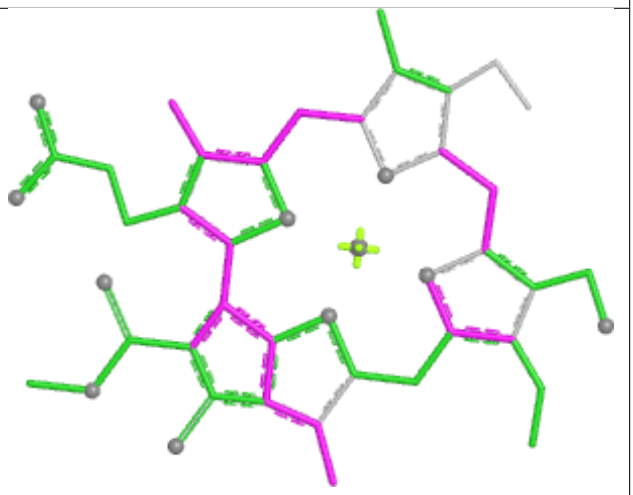


Rings

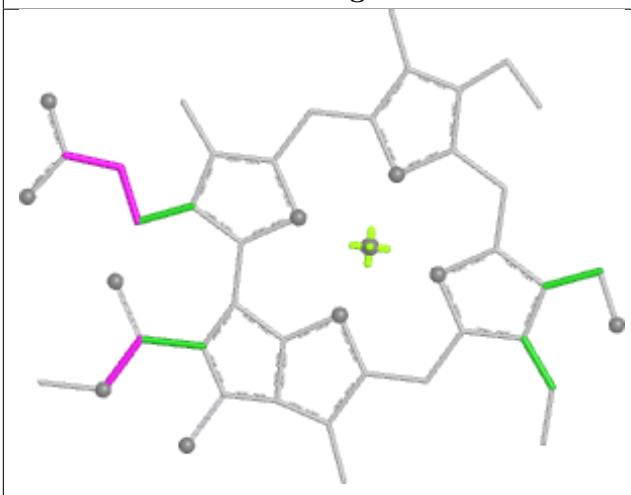
Ligand CHL 6 306



Bond lengths



Bond angles

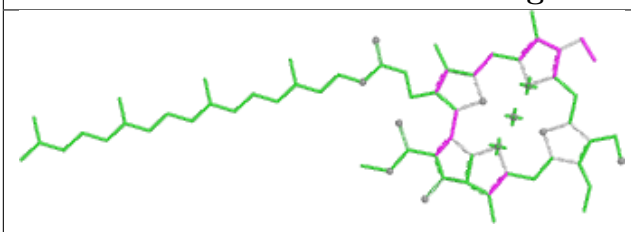


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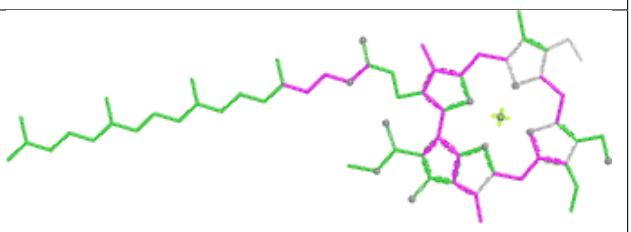


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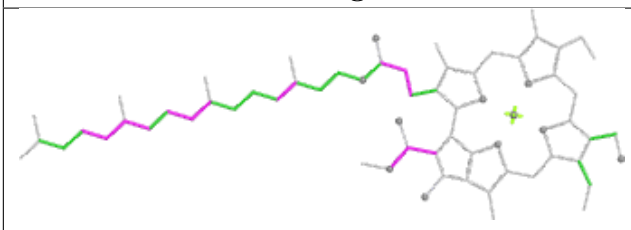
Ligand CHL n 306



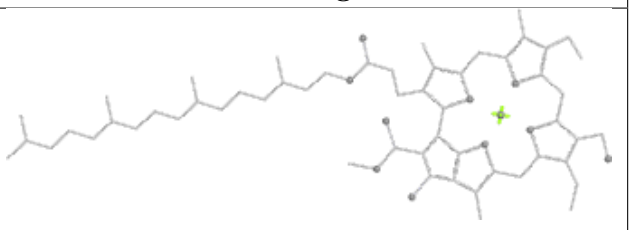
Bond lengths



Bond angles

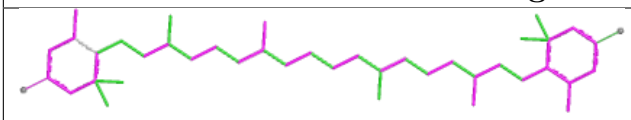


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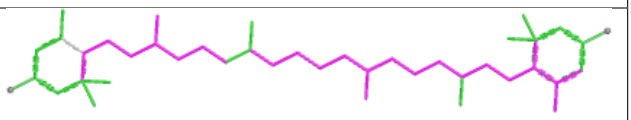


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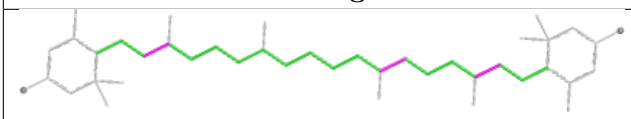
Ligand LUT 7 317



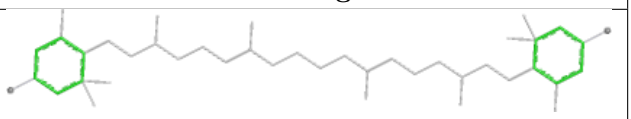
Bond lengths



Bond angles

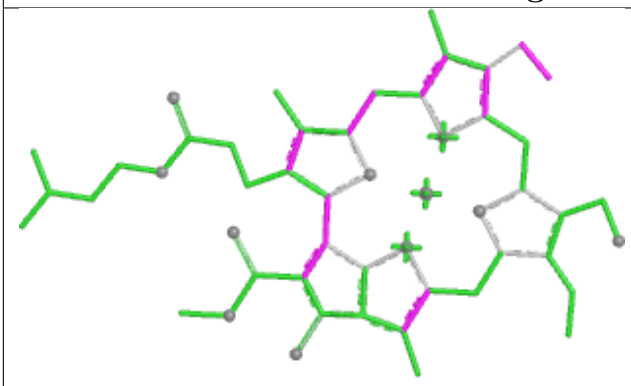


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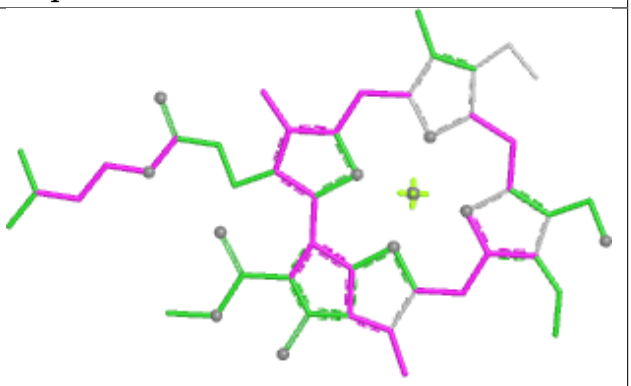


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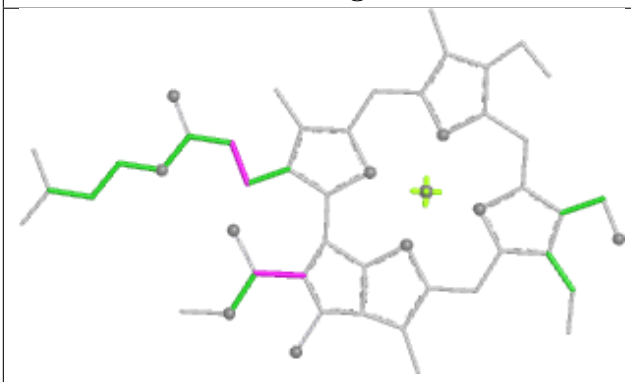
Ligand CHL p 606



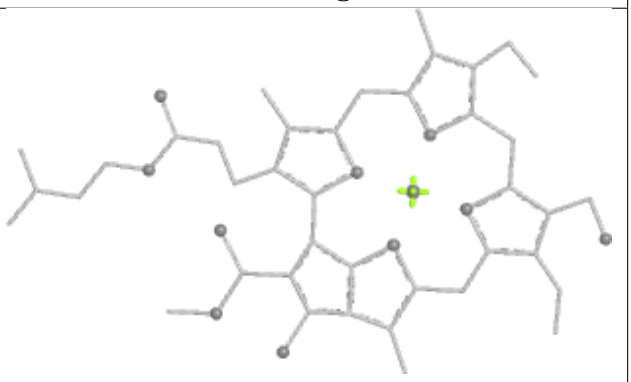
Bond lengths



Bond angles

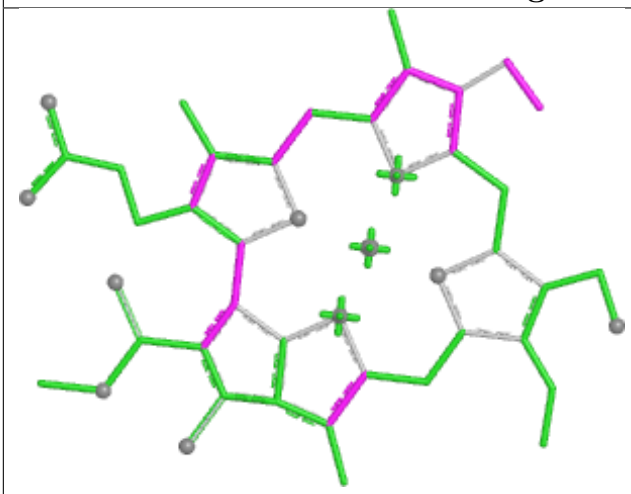


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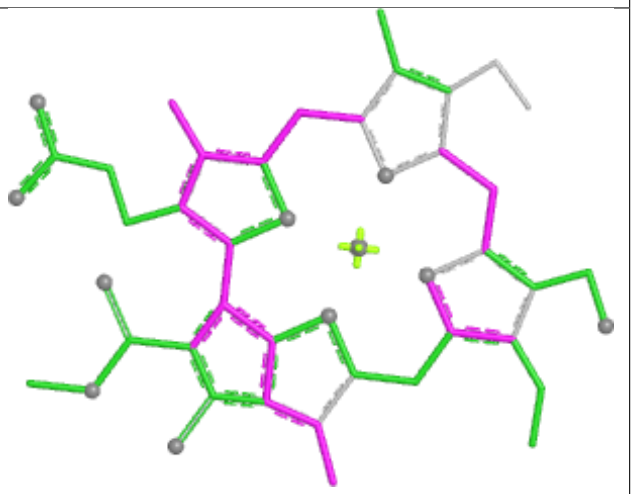


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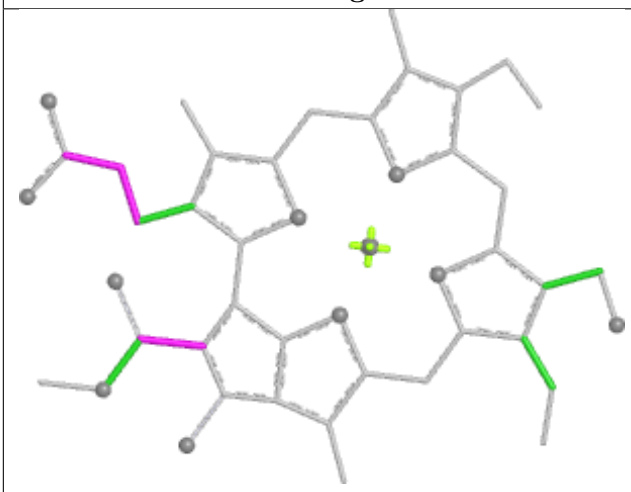
Ligand CHL 3 307



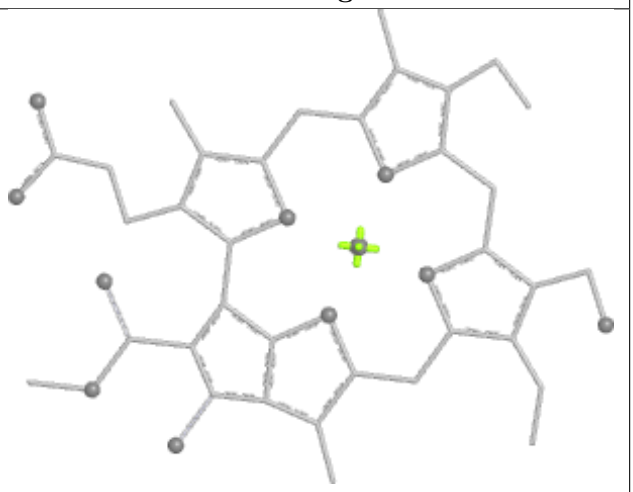
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Bond angles

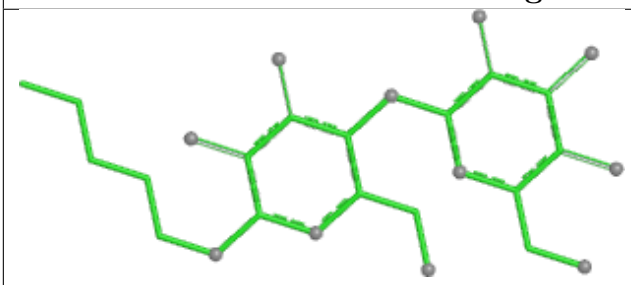


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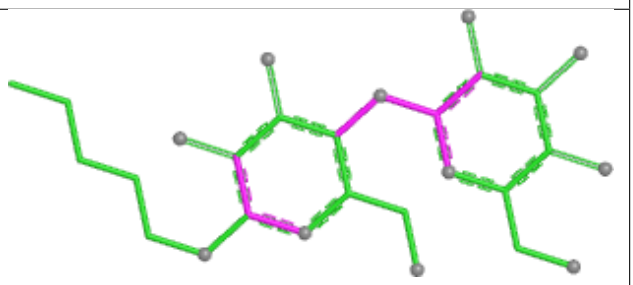


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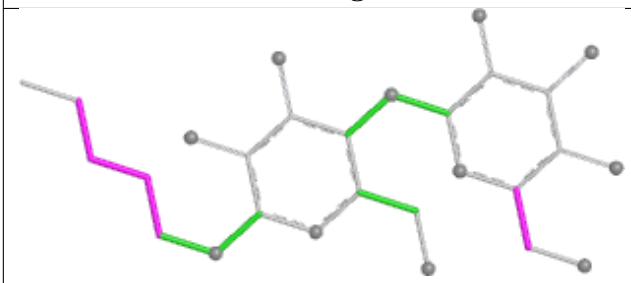
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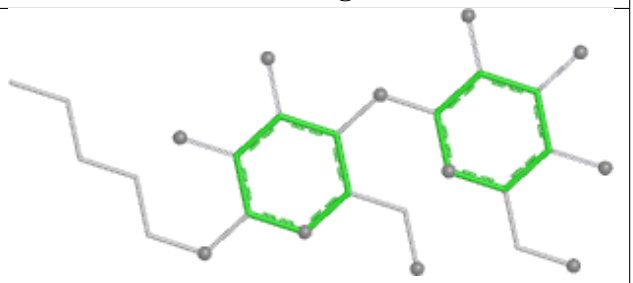
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Bond angles

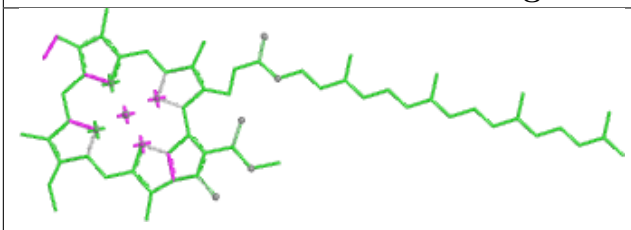


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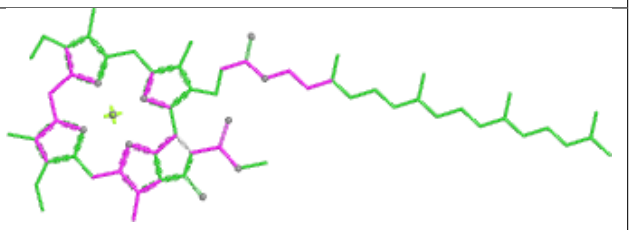


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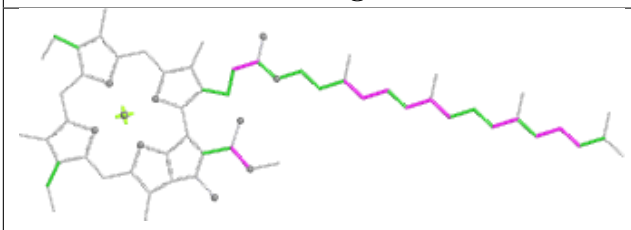
Ligand CLA D 403



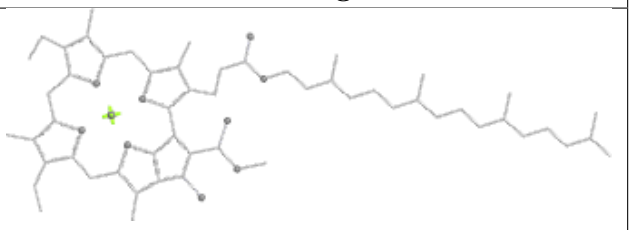
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Bond angles

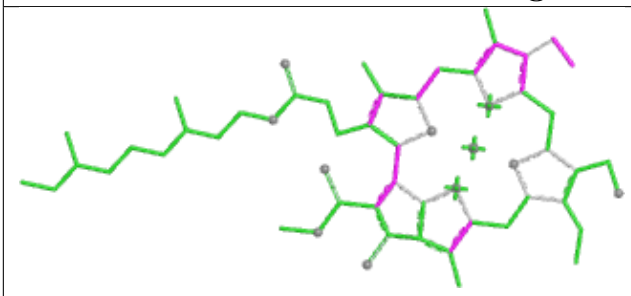


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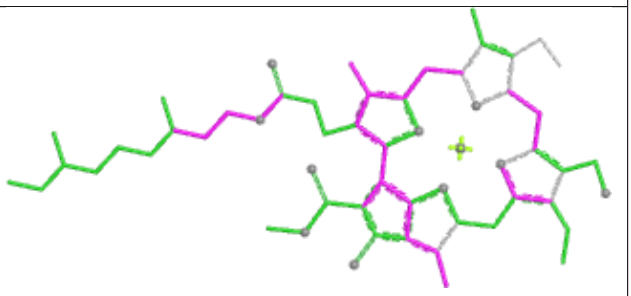


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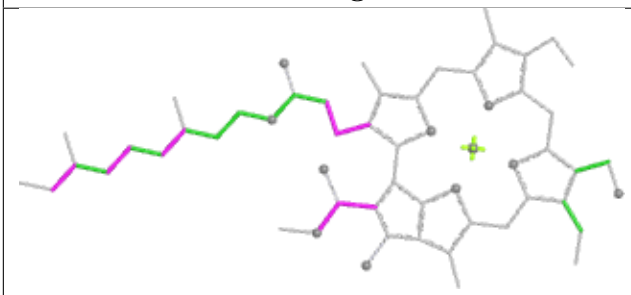
Ligand CHL 4 609



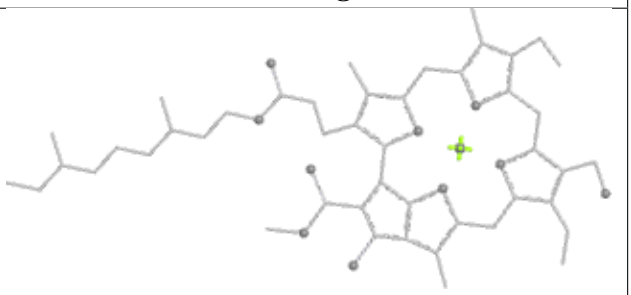
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Bond angles

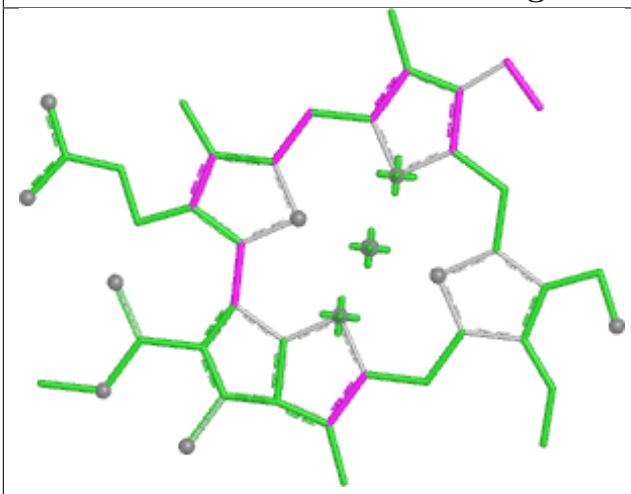


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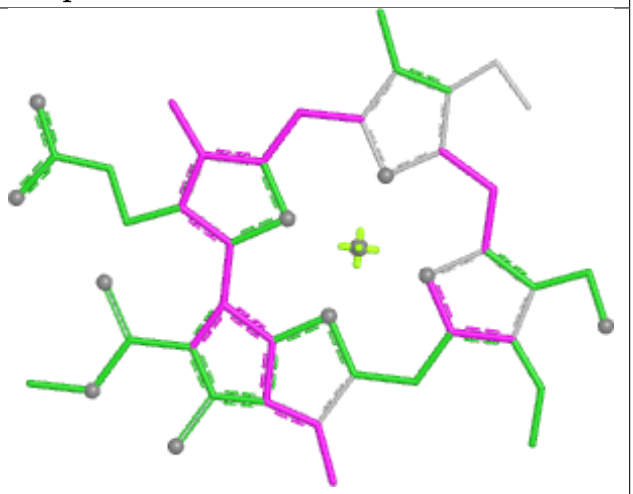


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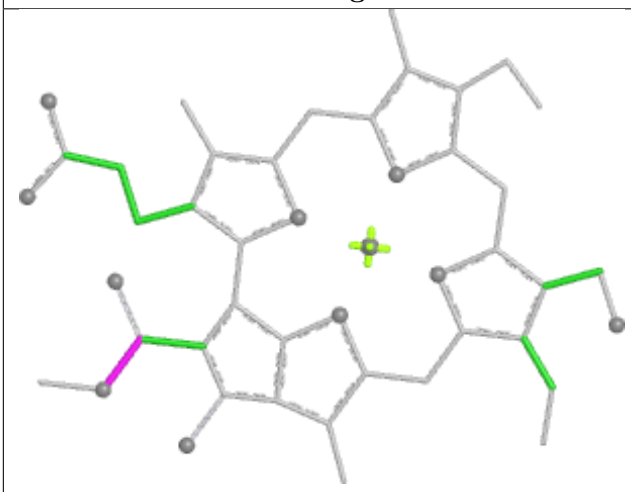
Ligand CHL q 307



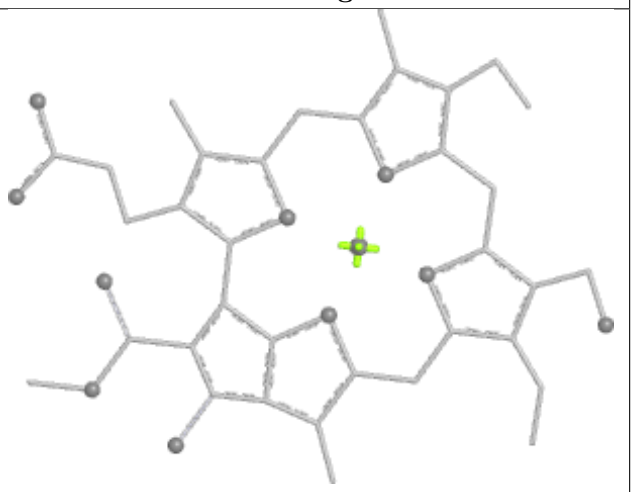
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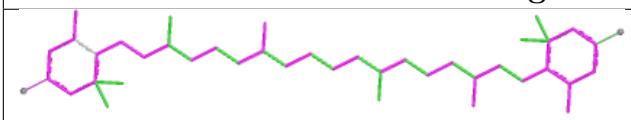


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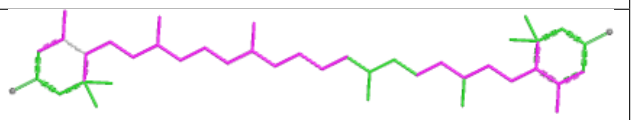


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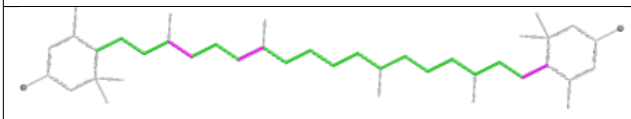
Ligand LUT 2 615



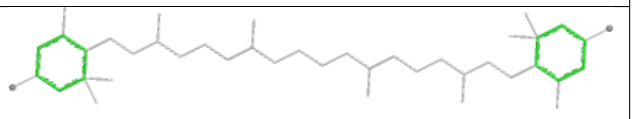
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Bond angles

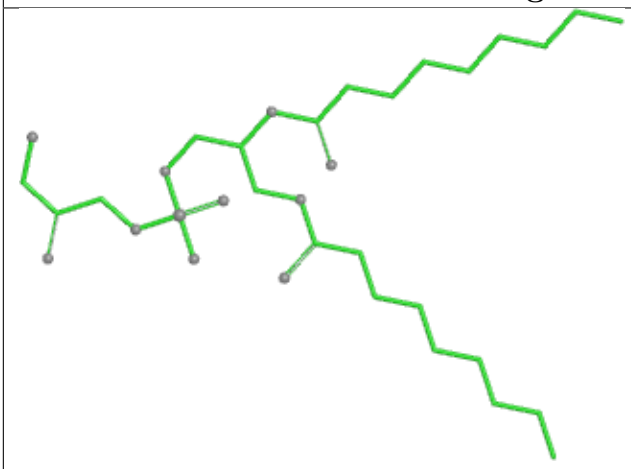


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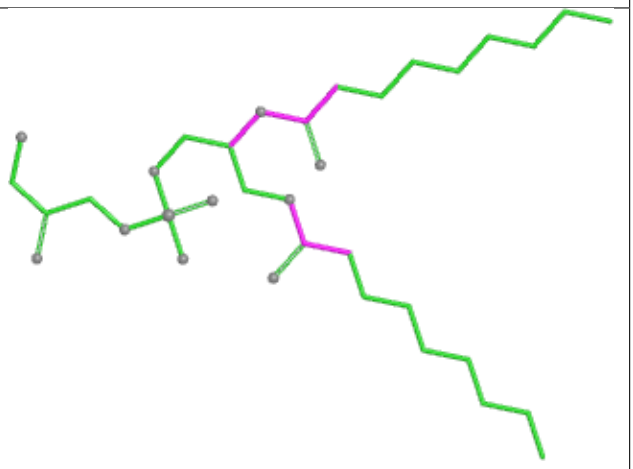


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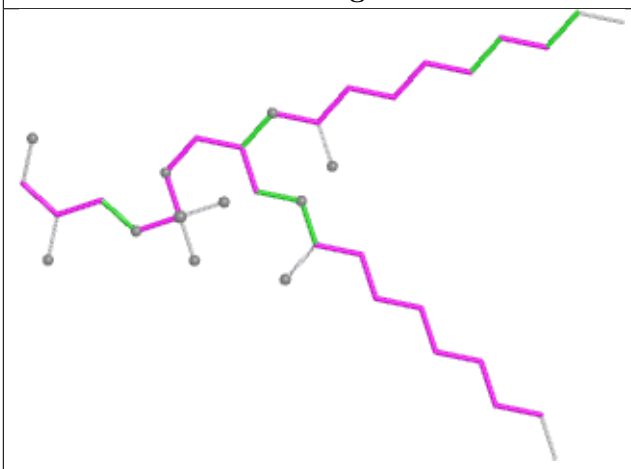
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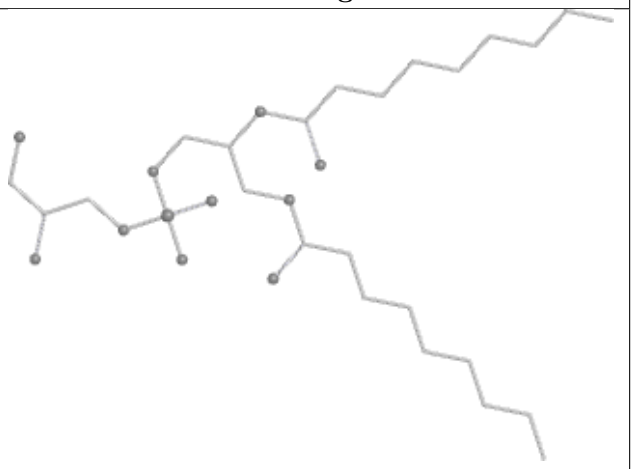
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Bond angles

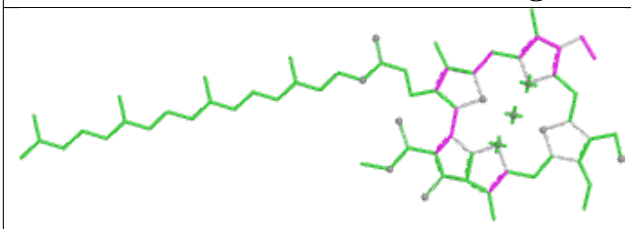


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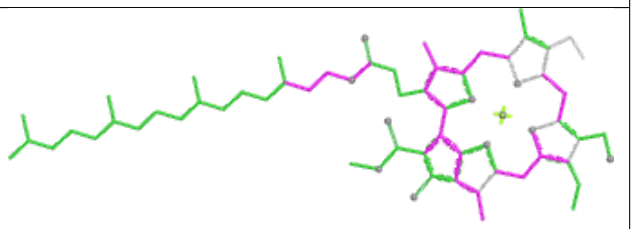


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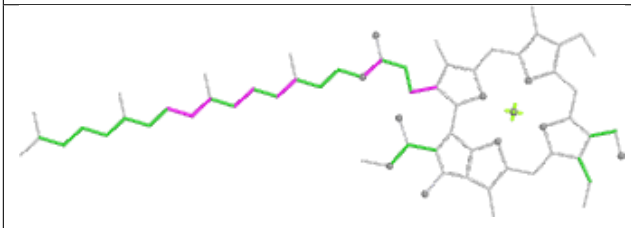
Ligand CHL 2 601



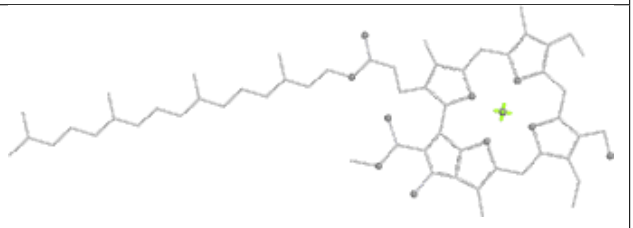
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Bond angles

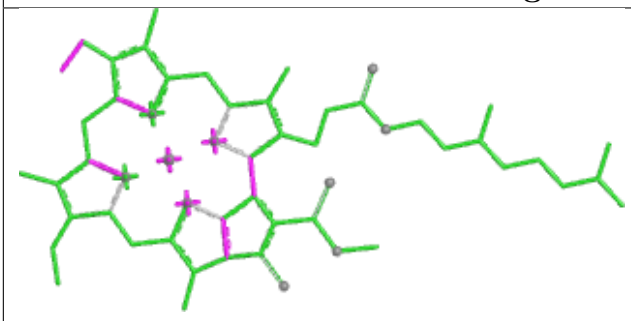


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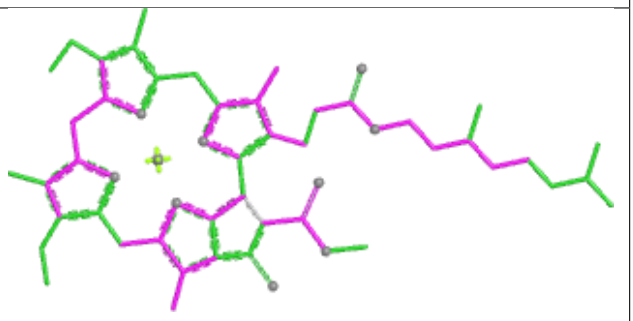


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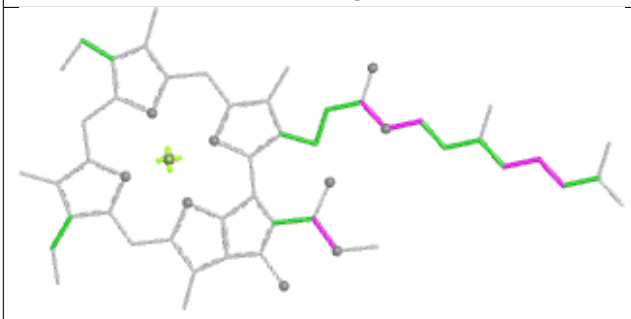
Ligand CLA R 315



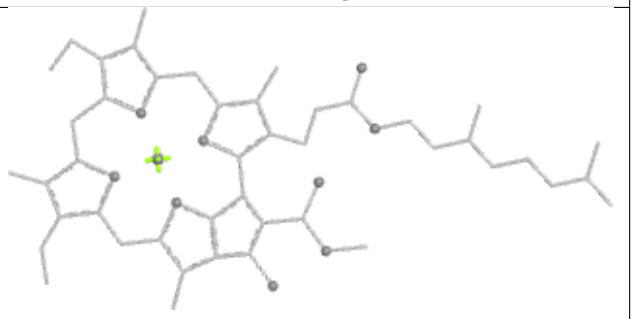
Bond lengths



Bond angles

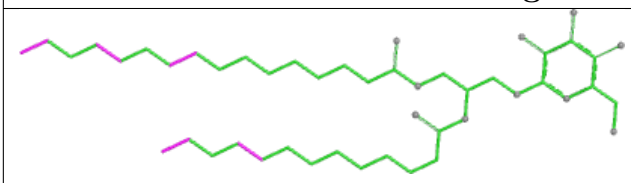


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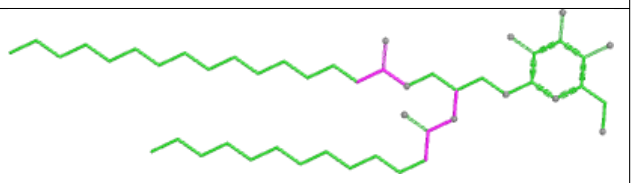


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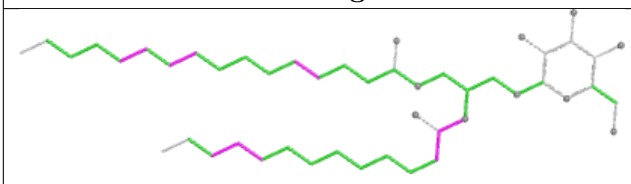
Ligand LMG k 101



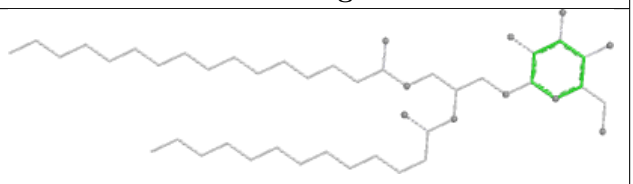
Bond lengths



Bond angles



Torsions

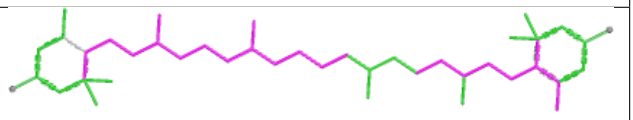


Rings

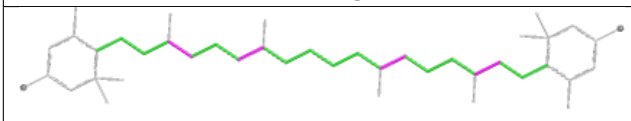
Ligand LUT R 317



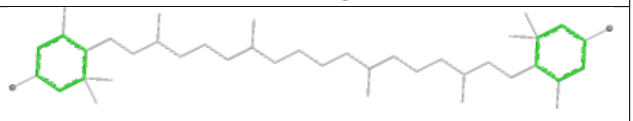
Bond lengths



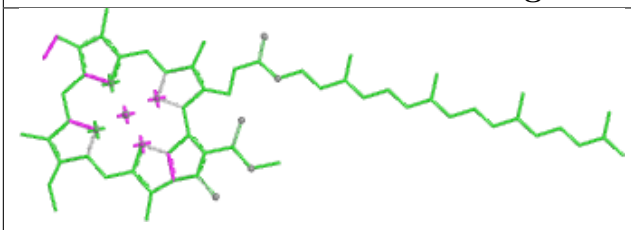
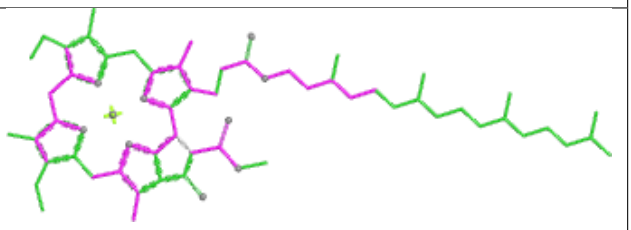
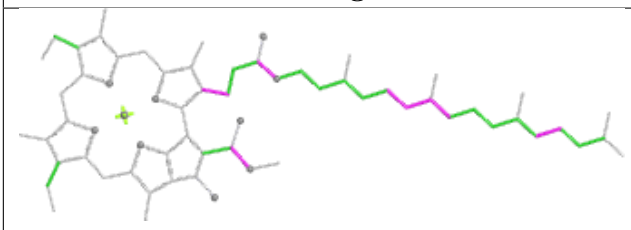
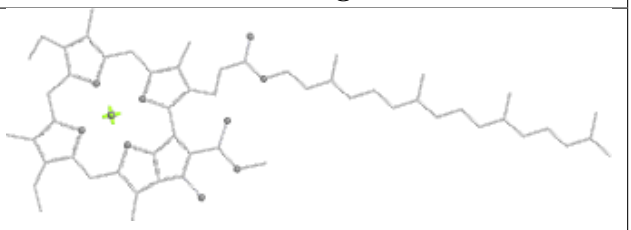
Bond angles

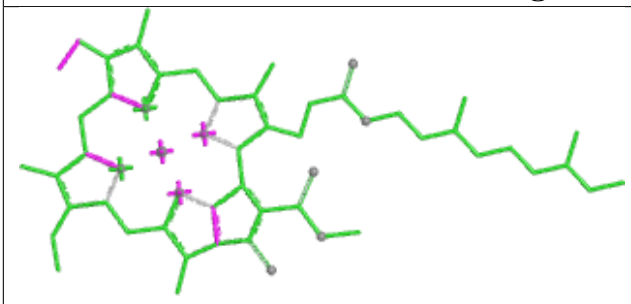
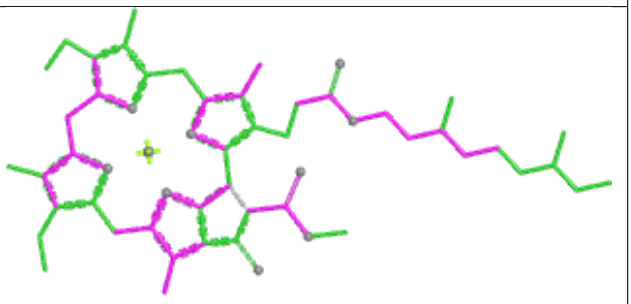
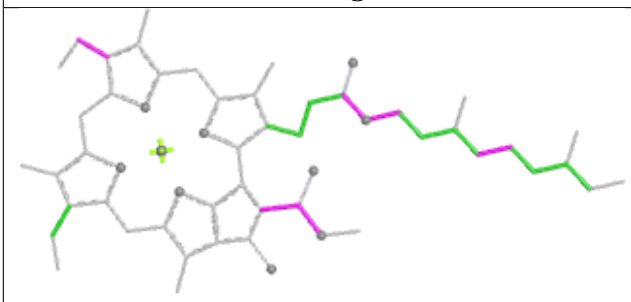
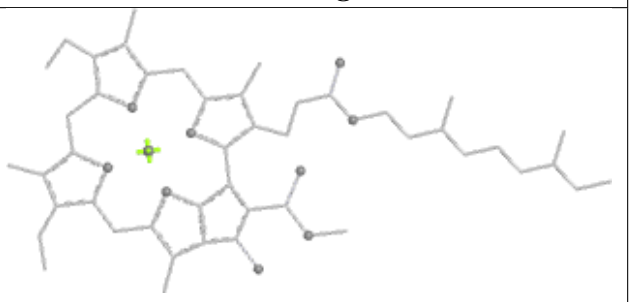


Torsions

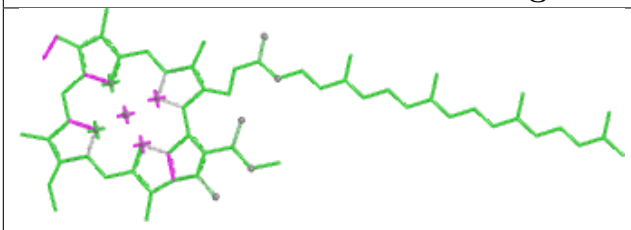


Rings

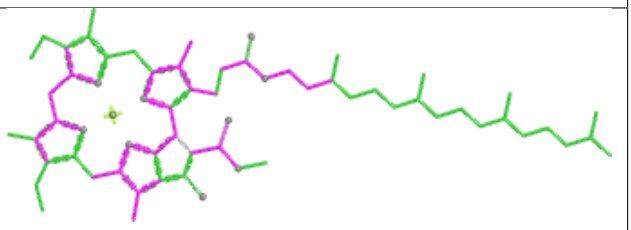
Ligand CLA C 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

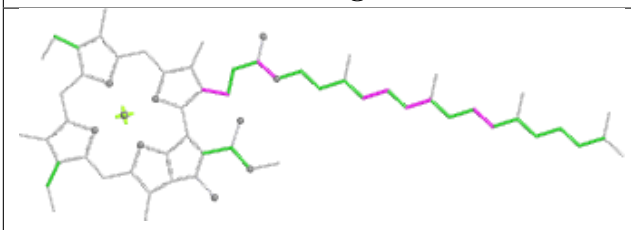
Ligand CLA c 608



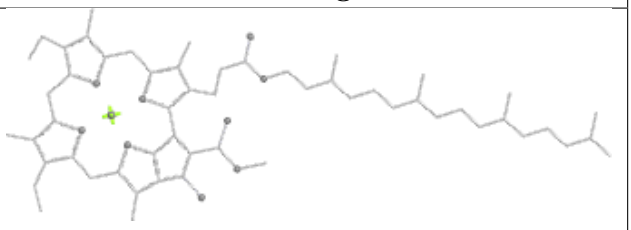
Bond lengths



Bond angles

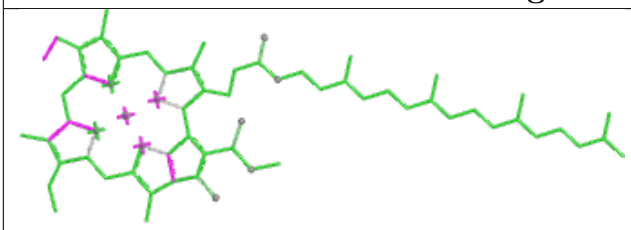


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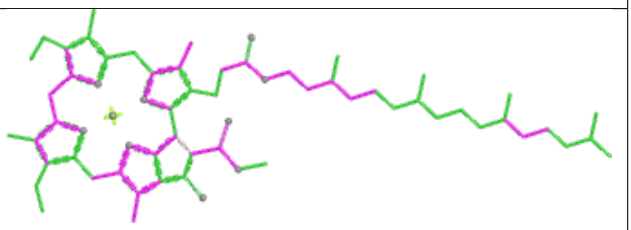


Rings

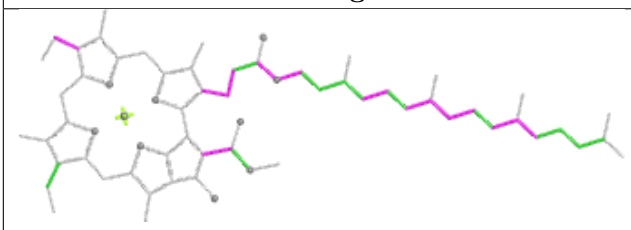
Ligand CLA b 613



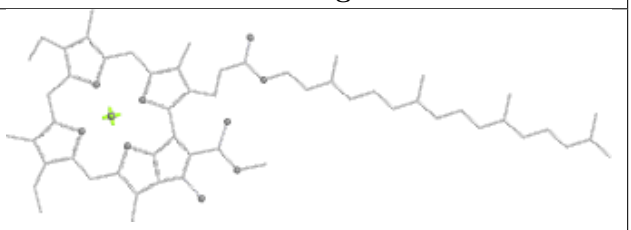
Bond lengths



Bond angles

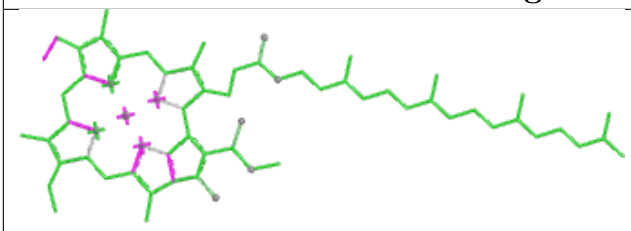


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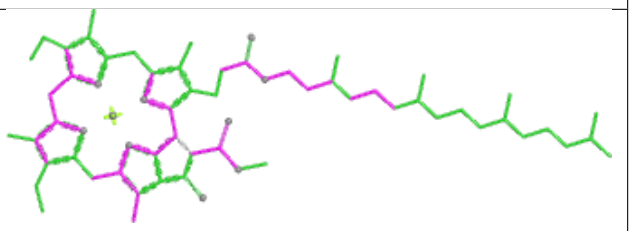


Rings

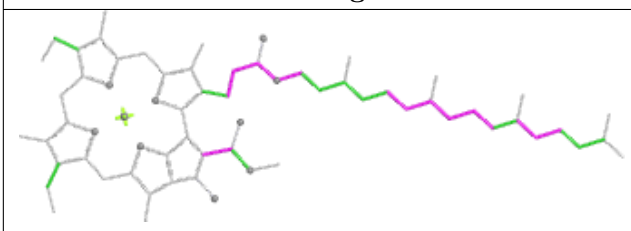
Ligand CLA C 605



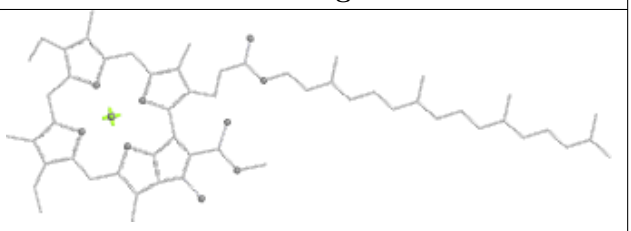
Bond lengths



Bond angles

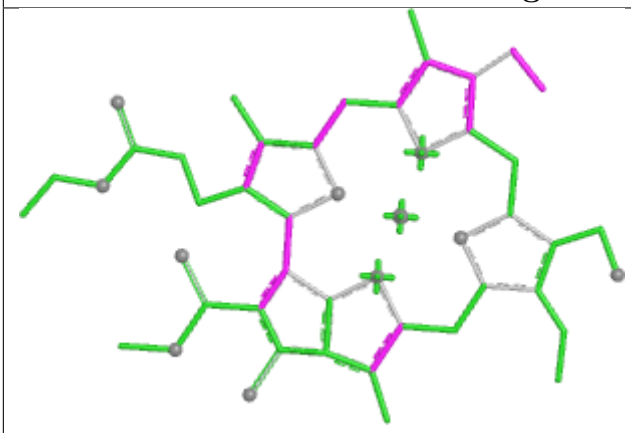


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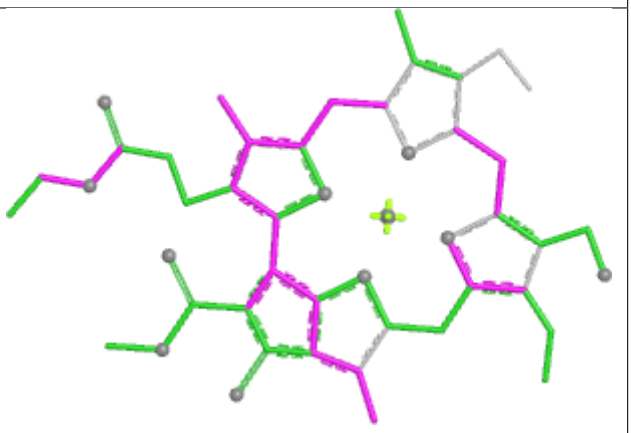


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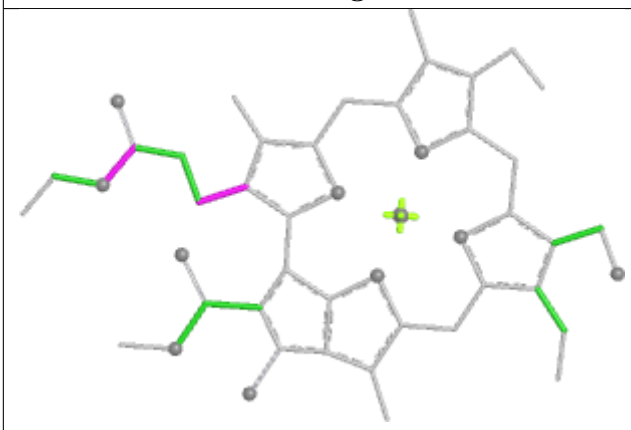
Ligand CHL G 605



Bond lengths



Bond angles

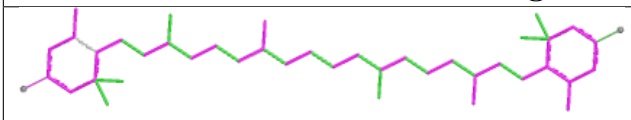


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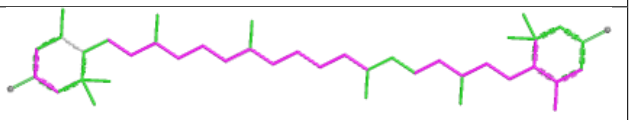


Rings

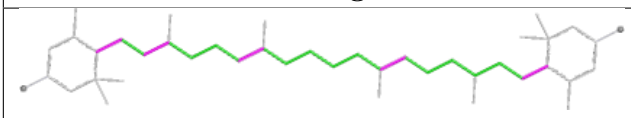
Ligand LUT S 318



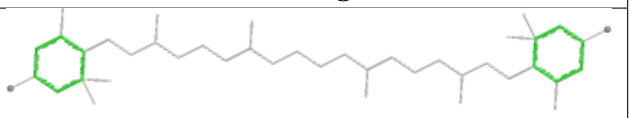
Bond lengths



Bond angles

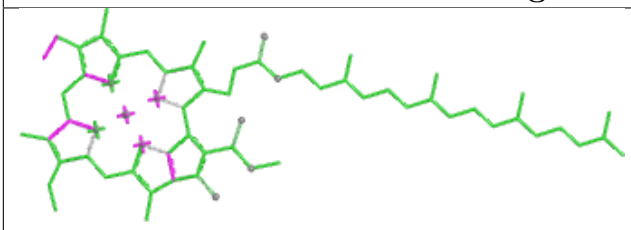


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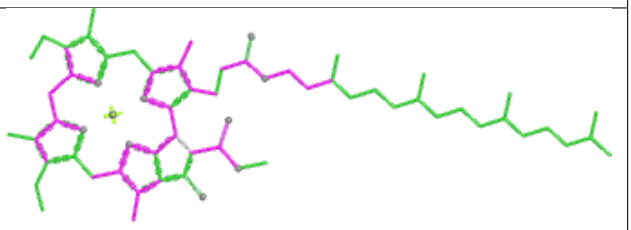


Rings

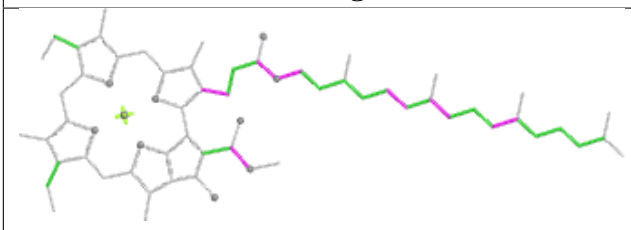
Ligand CLA 1 611



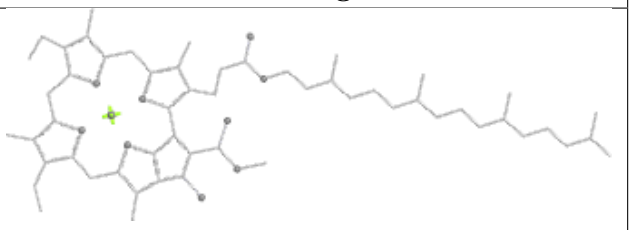
Bond lengths



Bond angles

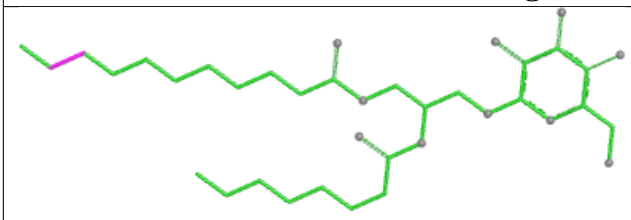


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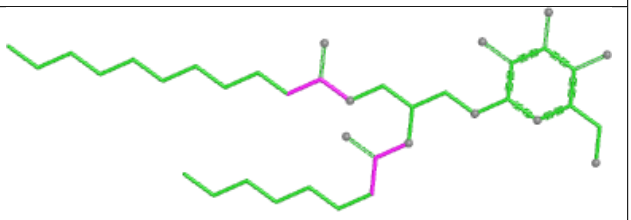


Rings

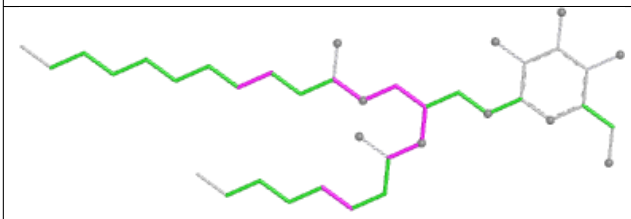
Ligand LMG 3 321



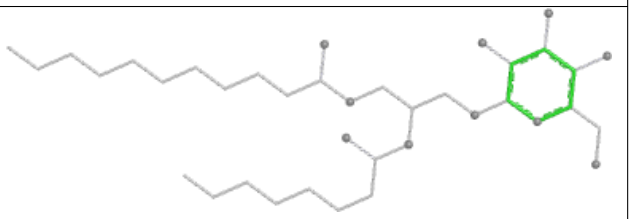
Bond lengths



Bond angles

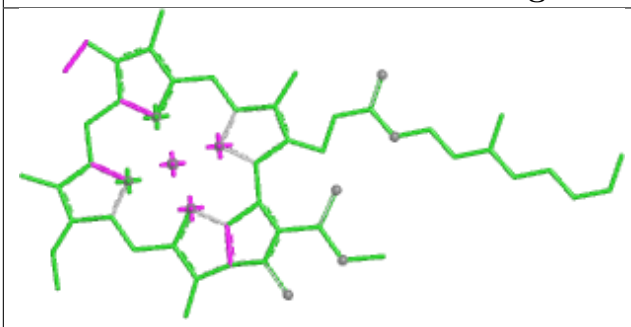


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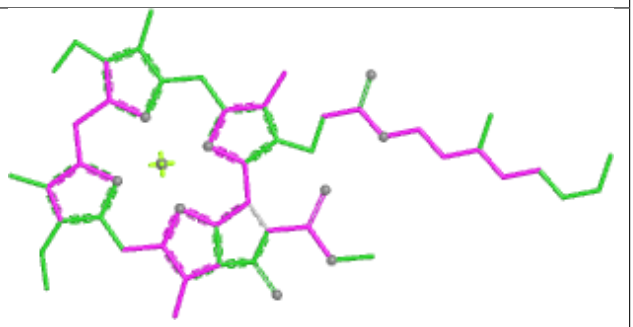


Rings

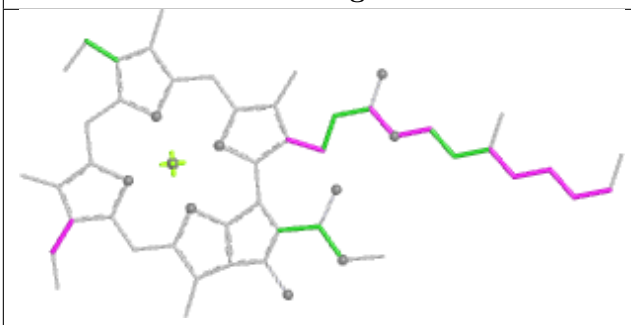
Ligand CLA 3 301



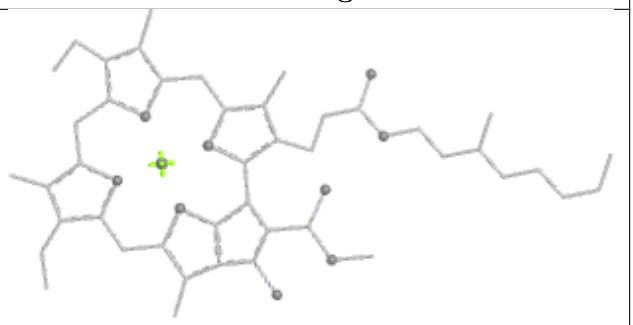
Bond lengths



Bond angles

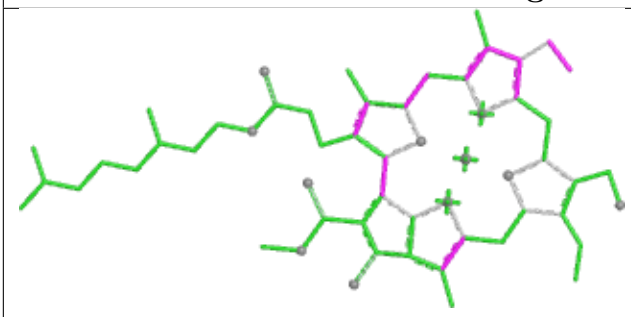


Torsions

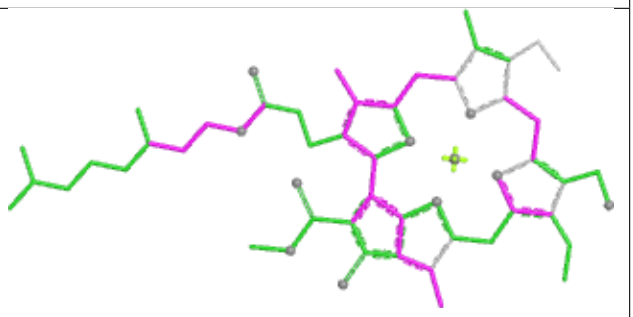


Rings

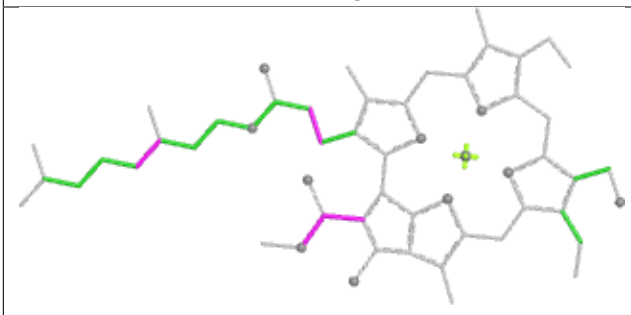
Ligand CHL n 302



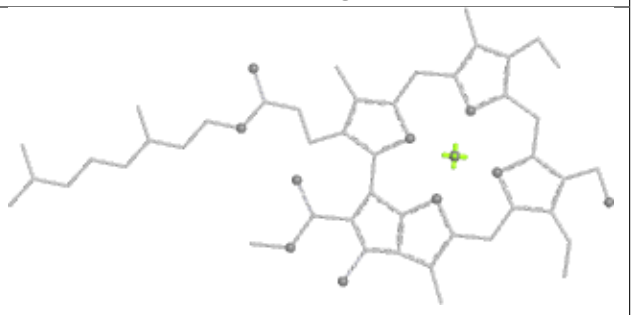
Bond lengths



Bond angles

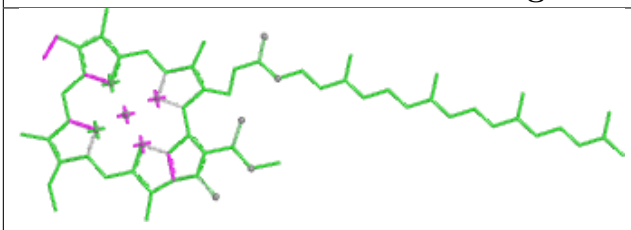


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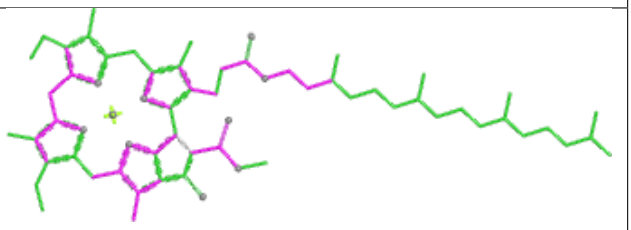


Rings

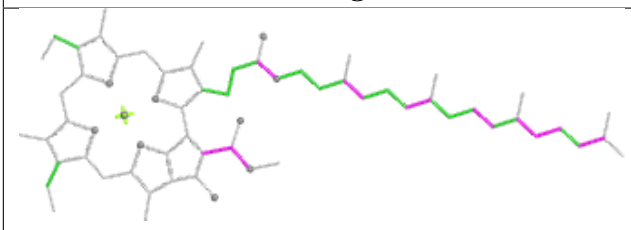
Ligand CLA b 606



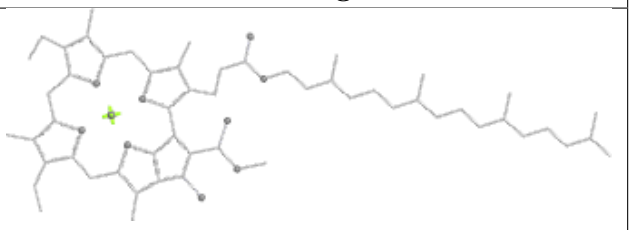
Bond lengths



Bond angles

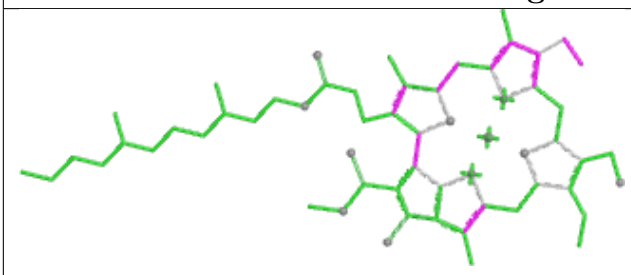


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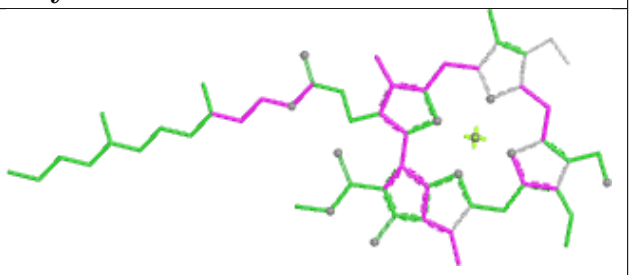


Rings

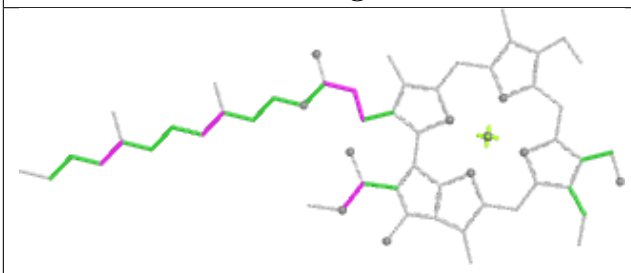
Ligand CHL y 606



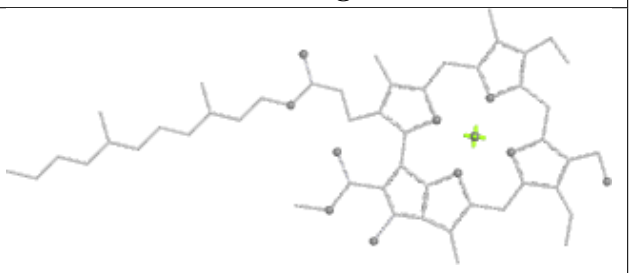
Bond lengths



Bond angles

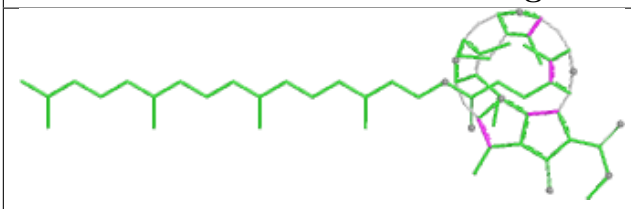


Torsions

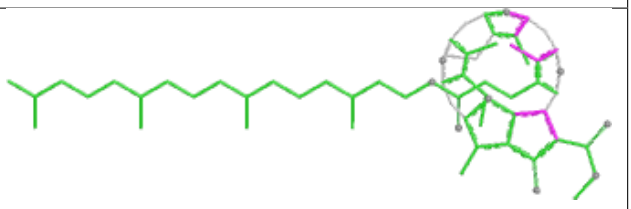


Rings

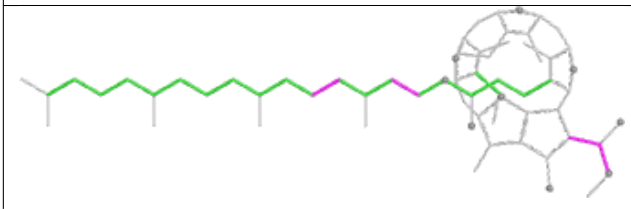
Ligand PHO d 402



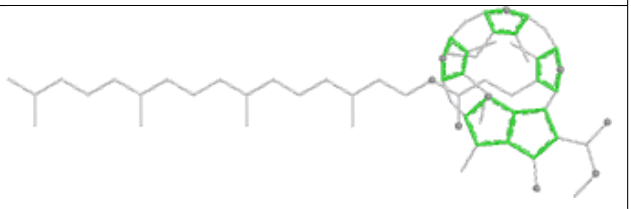
Bond lengths



Bond angles

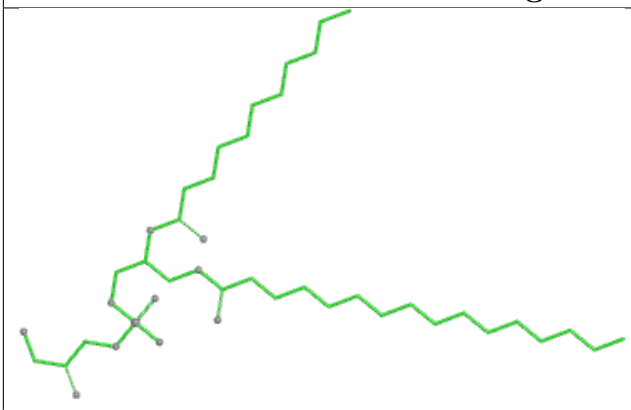


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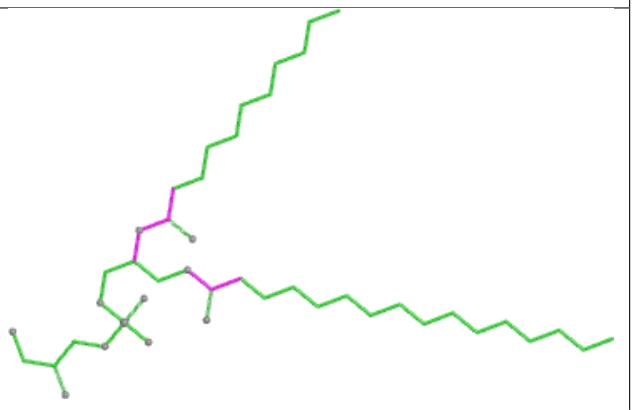


Rings

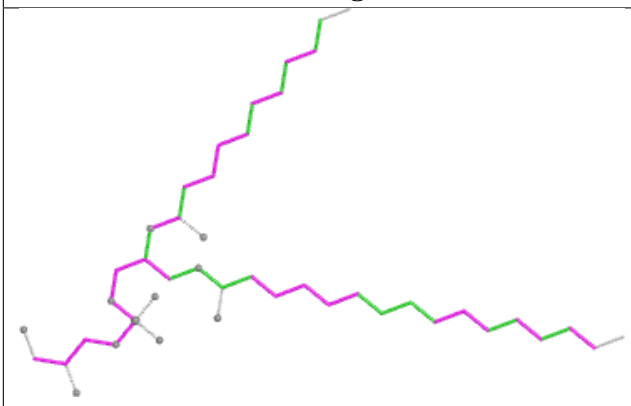
Ligand LHG S 322



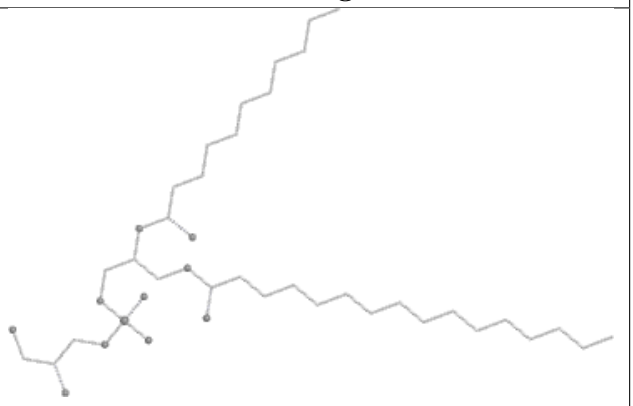
Bond lengths



Bond angles

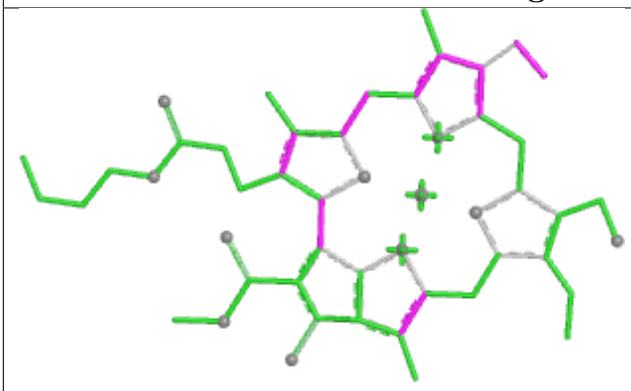


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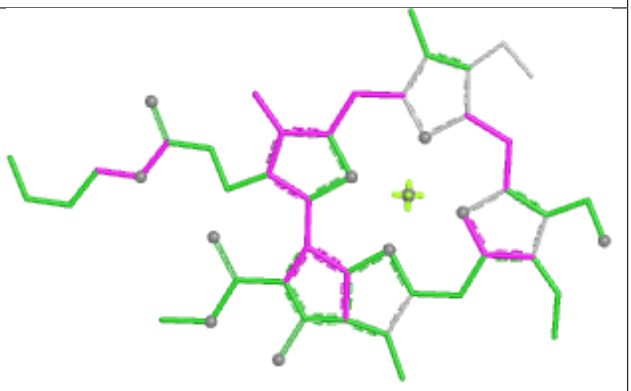


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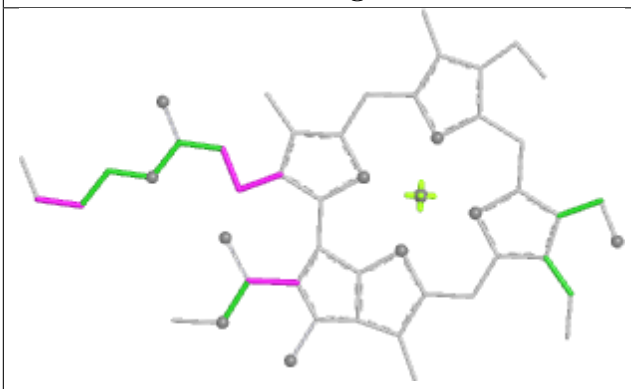
Ligand CHL 0 608



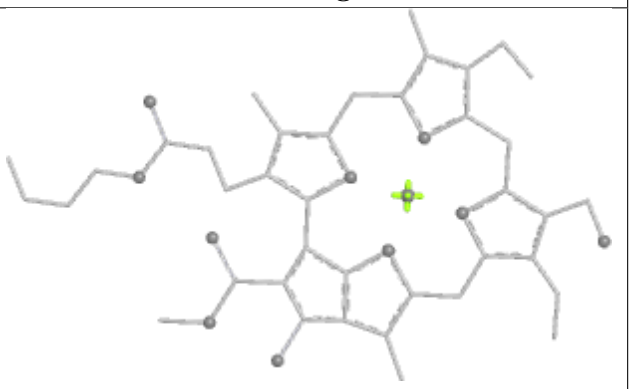
Bond lengths



Bond angles

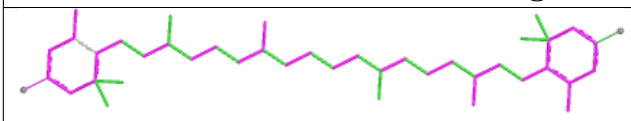


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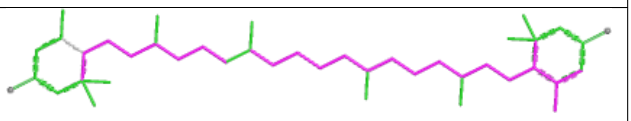


Rings

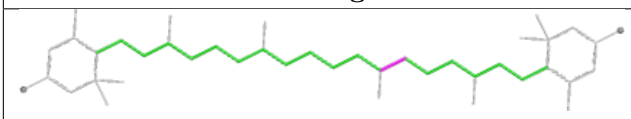
Ligand LUT 3 317



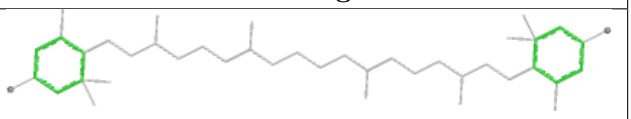
Bond lengths



Bond angles

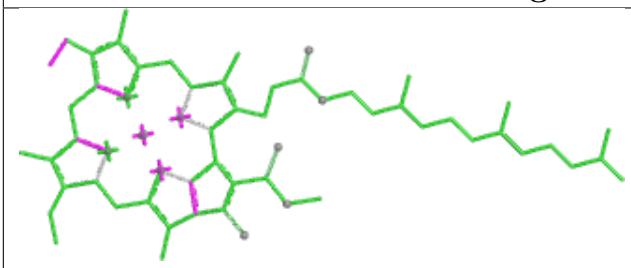


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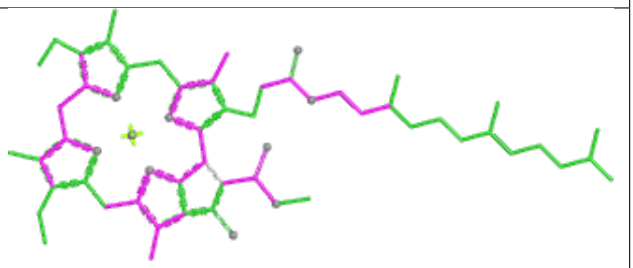


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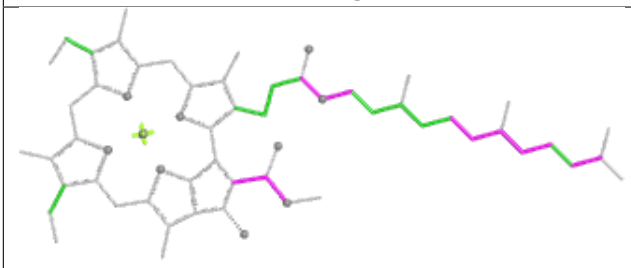
Ligand CLA r 305



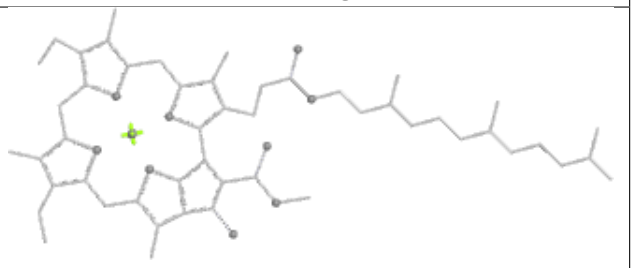
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Bond angles

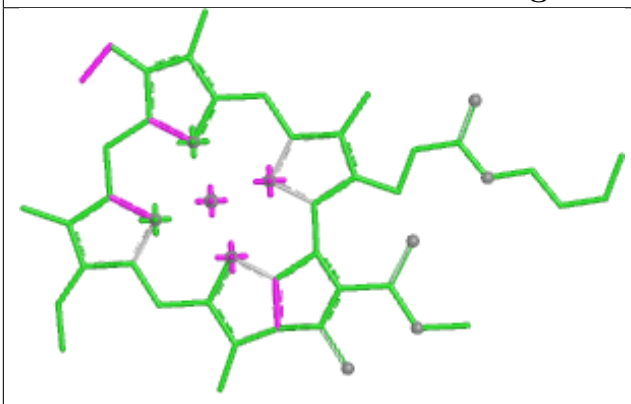


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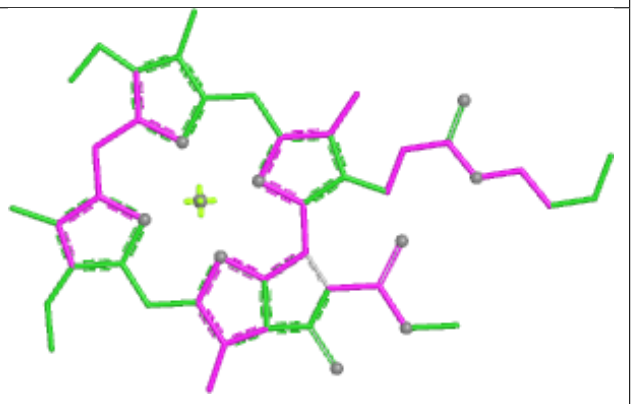


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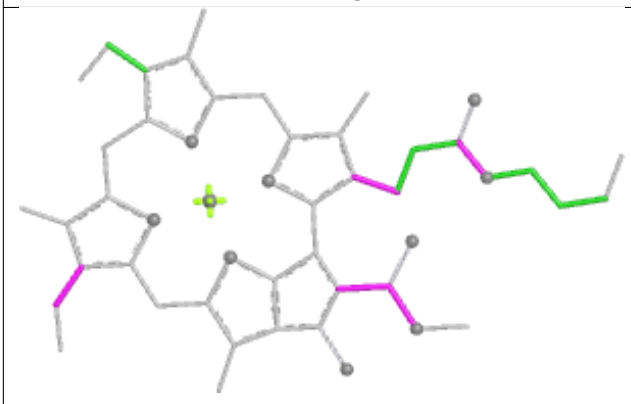
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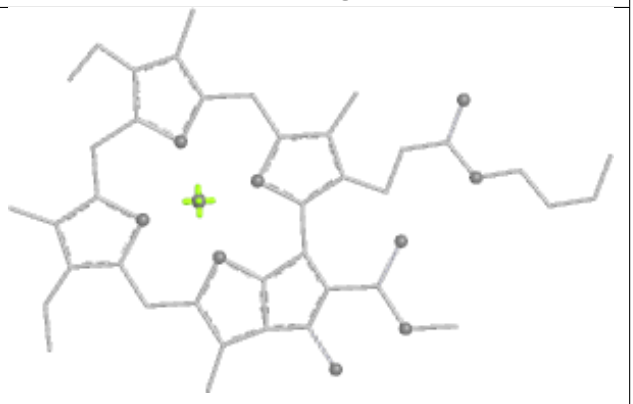
Bond lengths



Bond angles

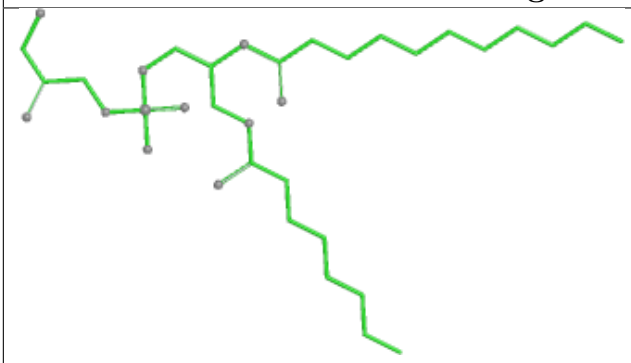


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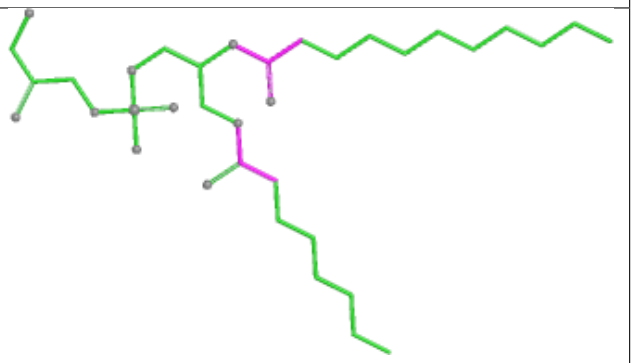


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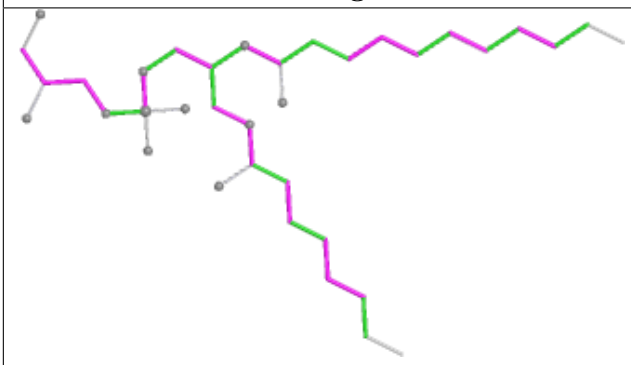
Ligand LHG z 102



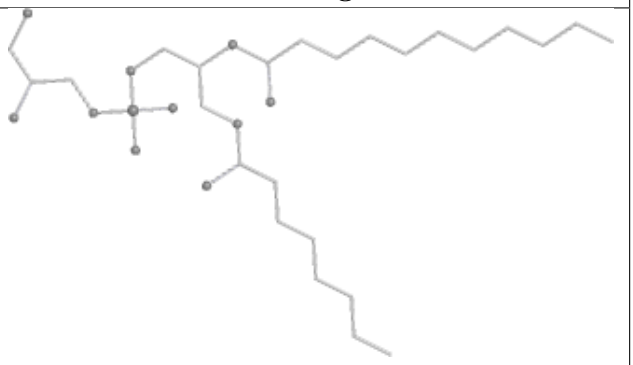
Bond lengths



Bond angles

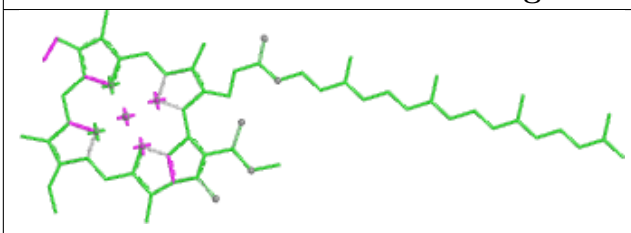


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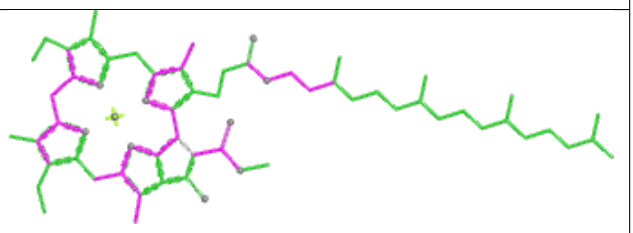


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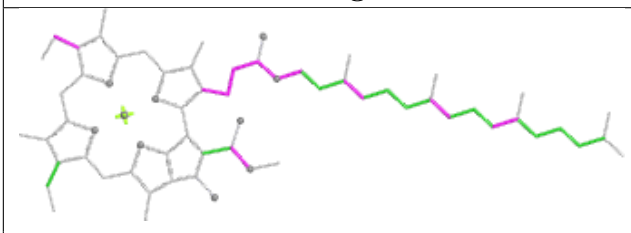
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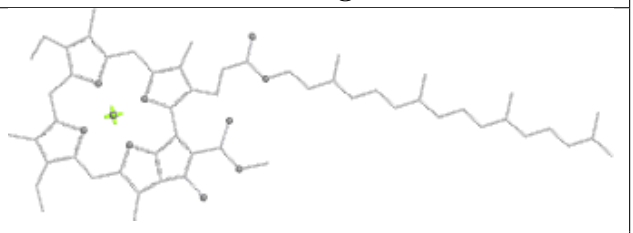
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Bond angles

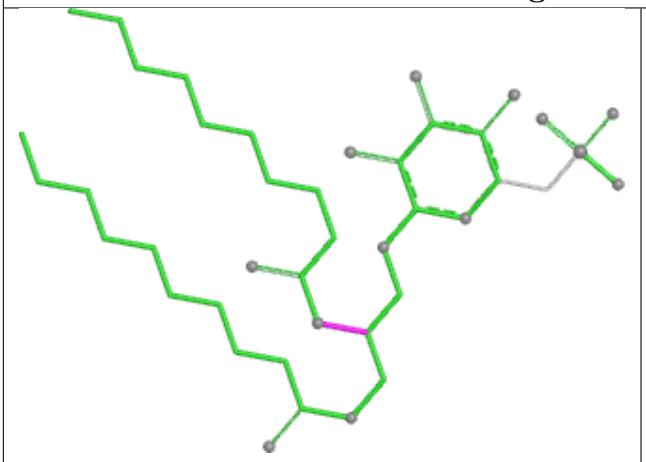


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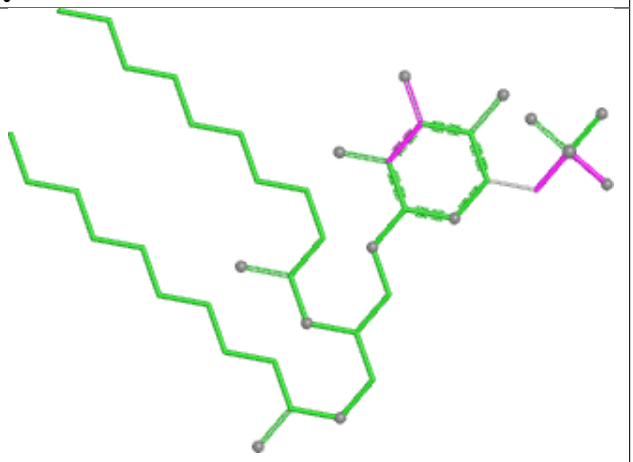


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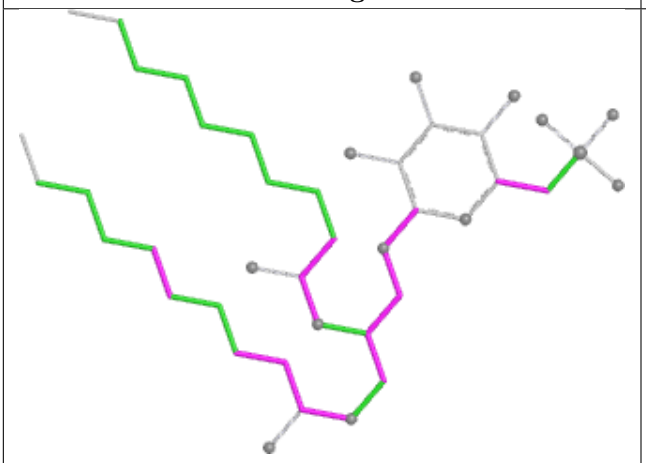
Ligand SQD 6 301



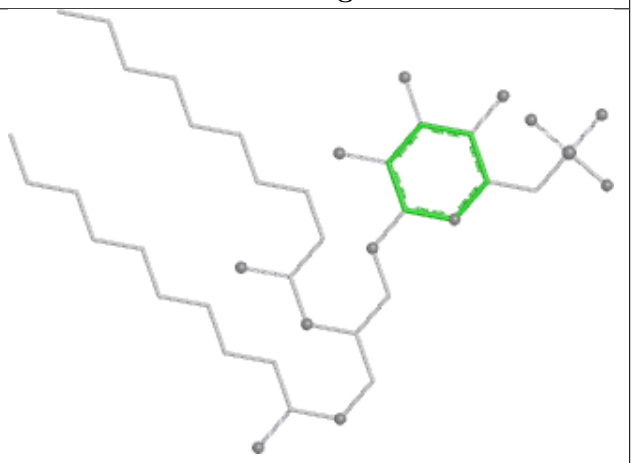
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Bond angles

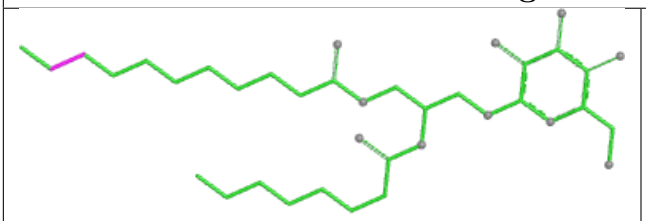


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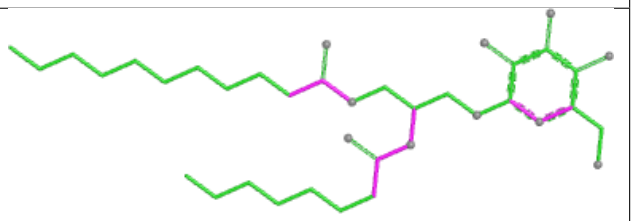


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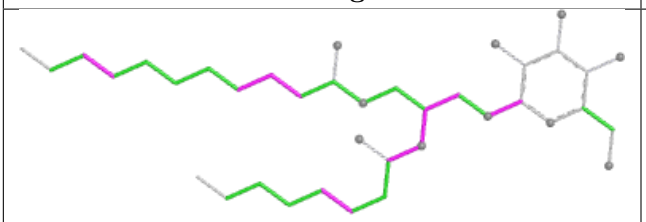
Ligand LMG A 414



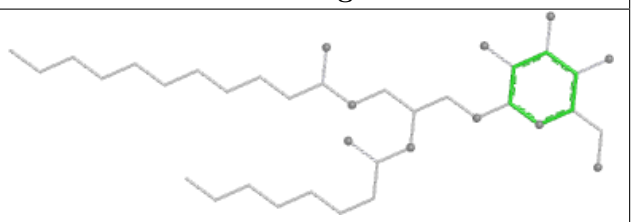
Bond lengths



Bond angles

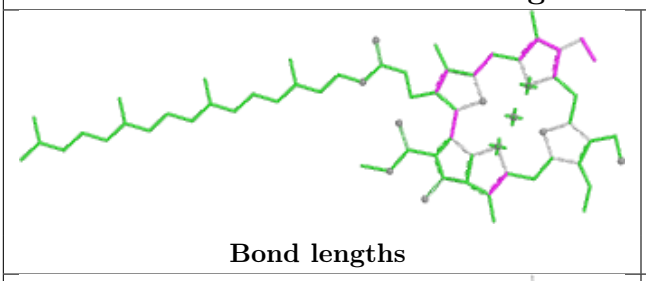


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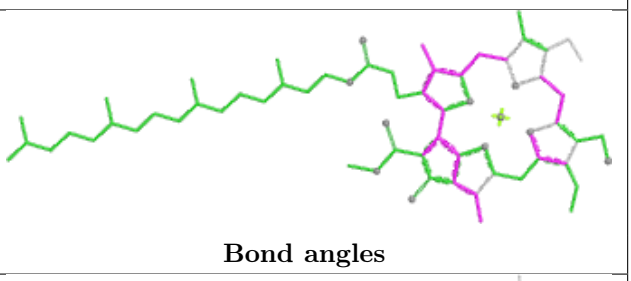


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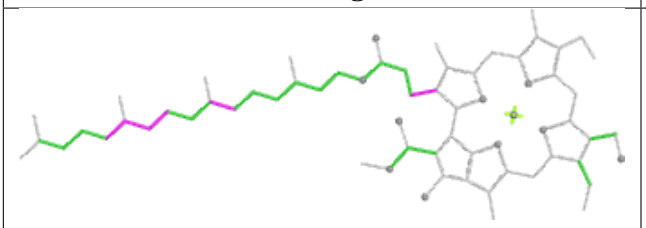
Ligand CHL 1 601



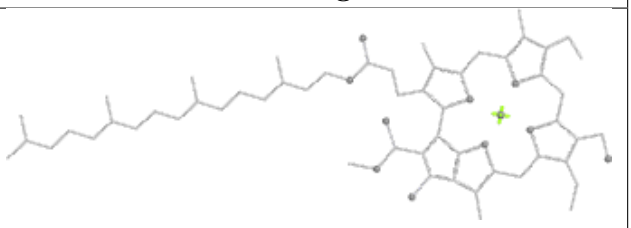
Bond lengths



Bond angles

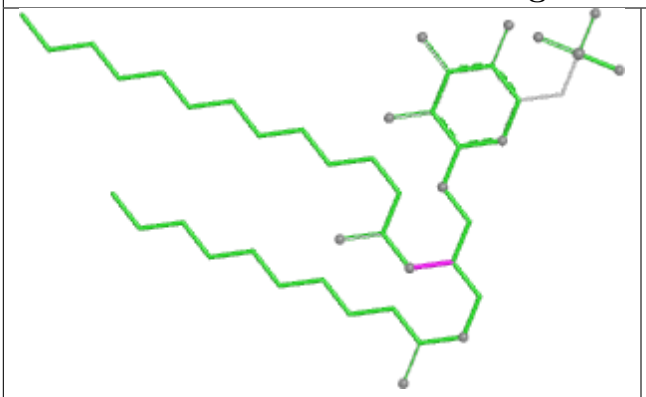


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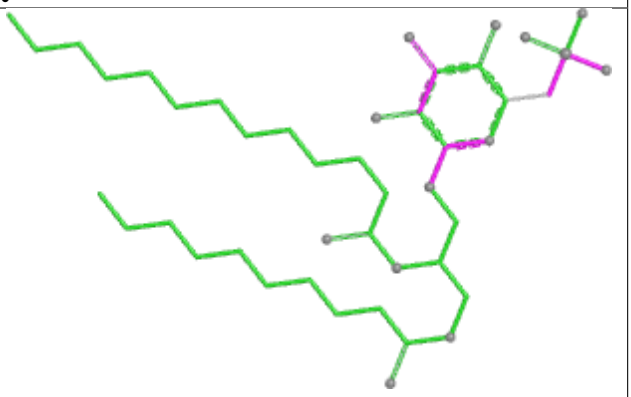


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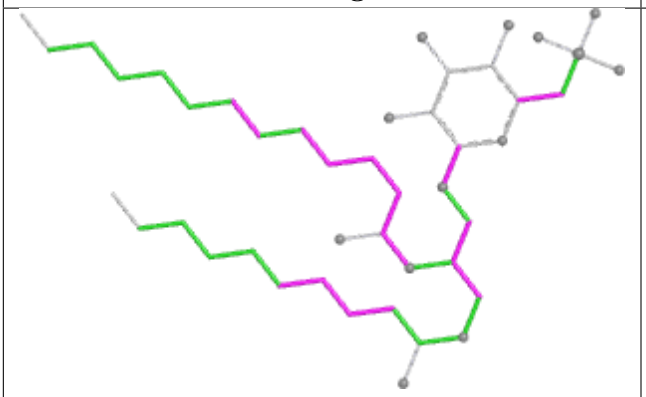
Ligand SQD a 412



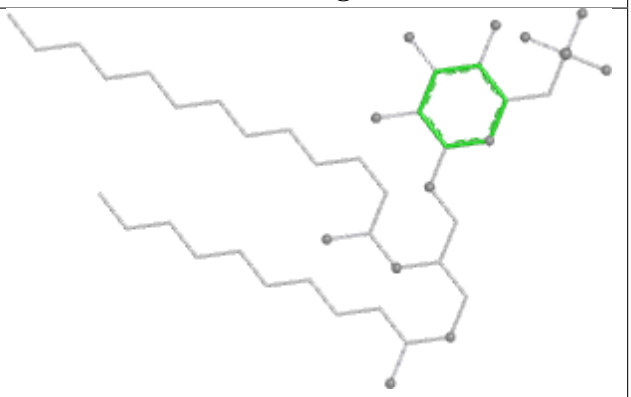
Bond lengths



Bond angles

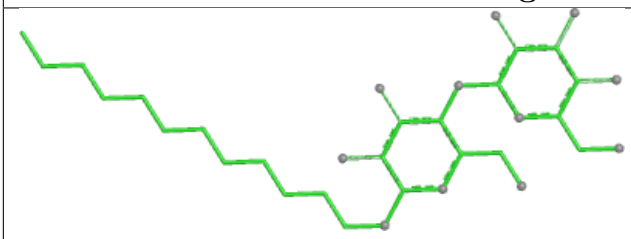


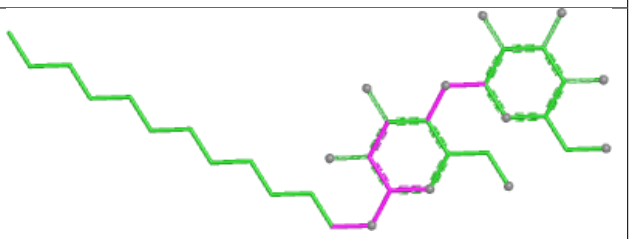
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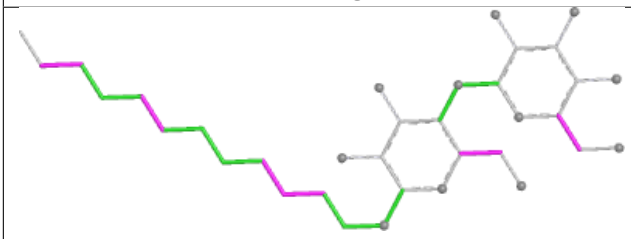


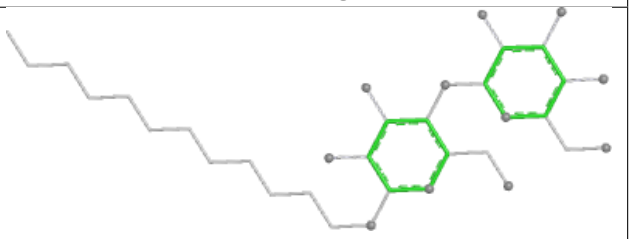
Rings

Ligand LMU K 101

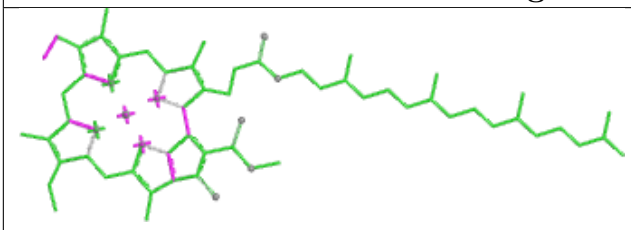

Bond lengths

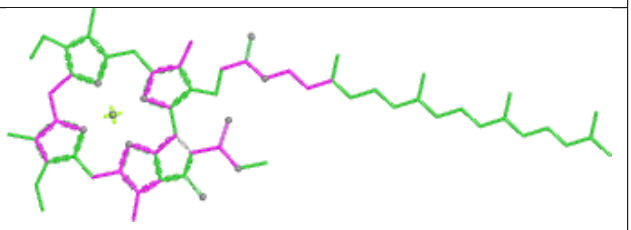

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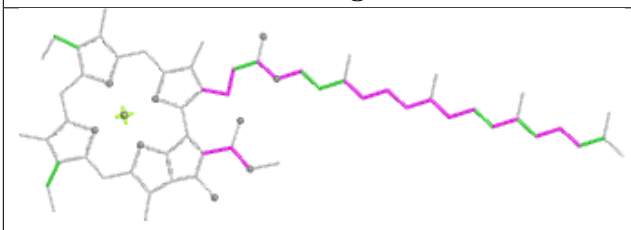

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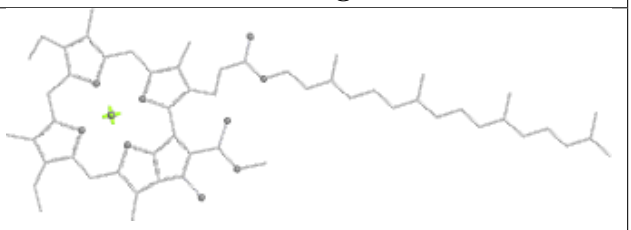

Rings

Ligand CLA b 608

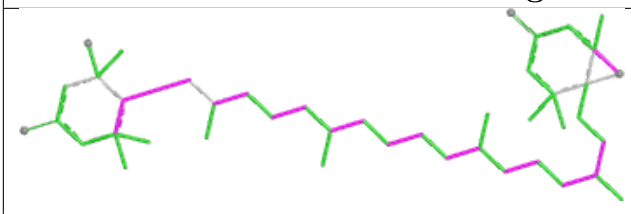

Bond lengths

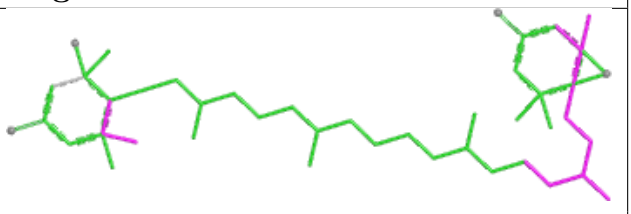

Bond angles

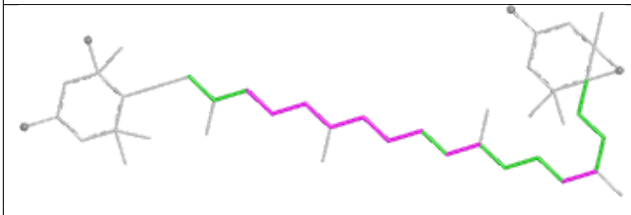

Torsions

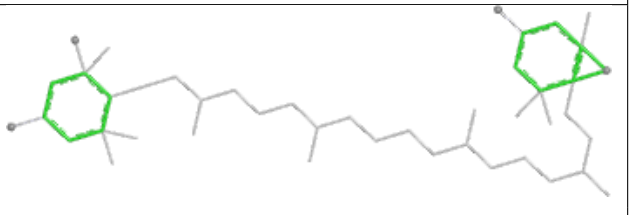

Rings

Ligand NEX g 317

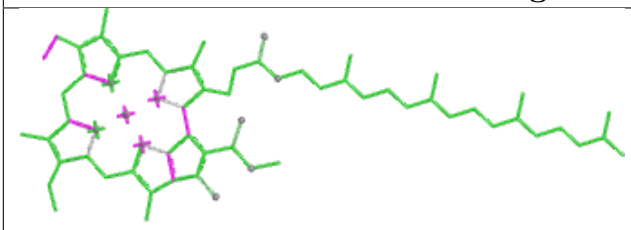

Bond lengths


Bond angles

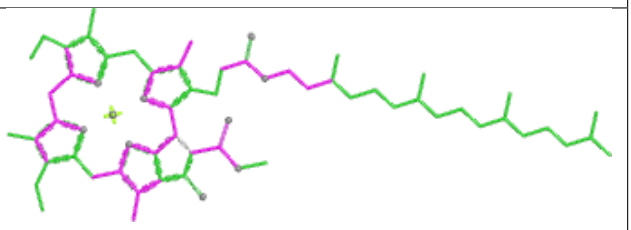

Torsions


Rings

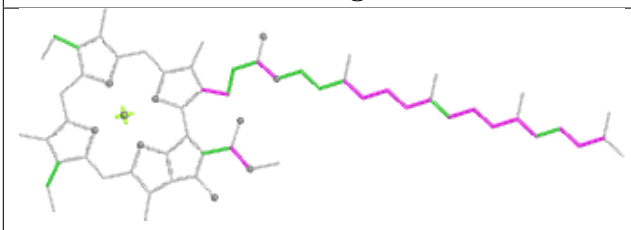
Ligand CLA c 603



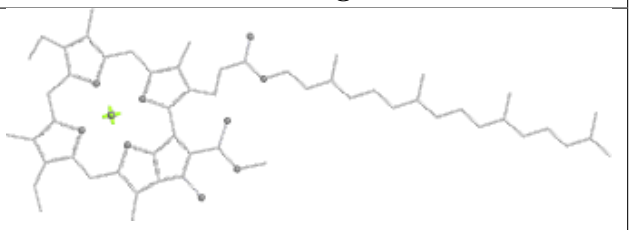
Bond lengths



Bond angles

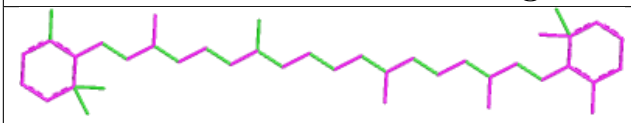


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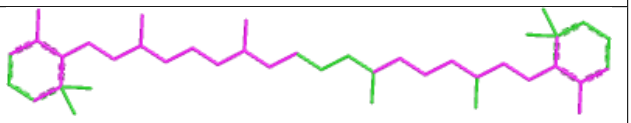


Rings

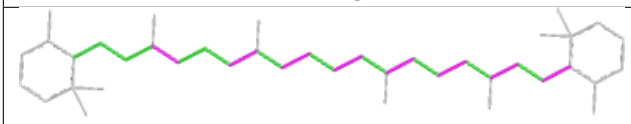
Ligand BCR D 405



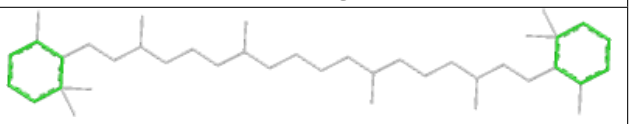
Bond lengths



Bond angles

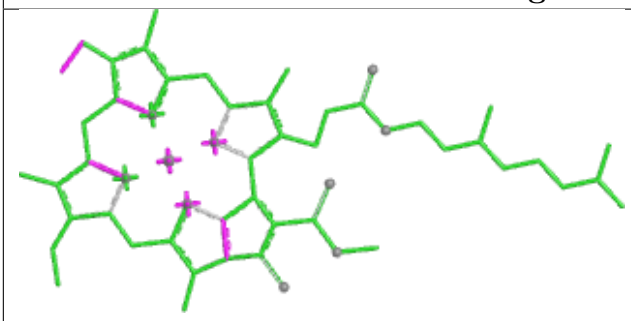


Torsions

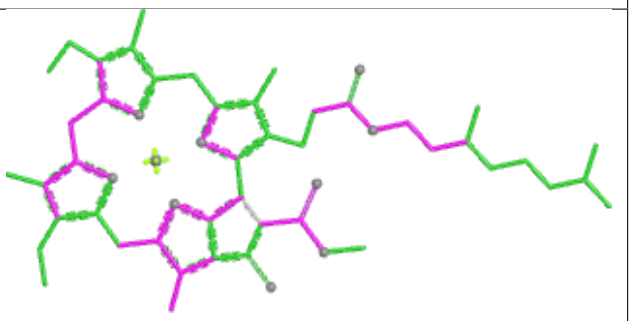


Rings

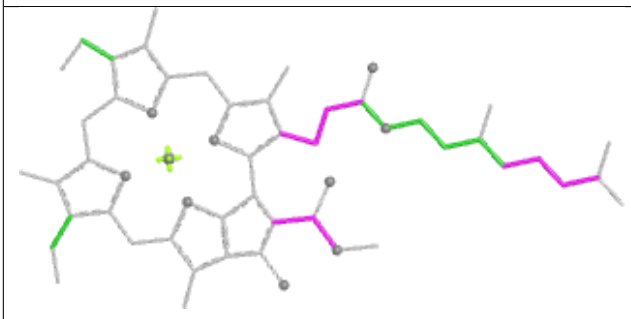
Ligand CLA 0 604



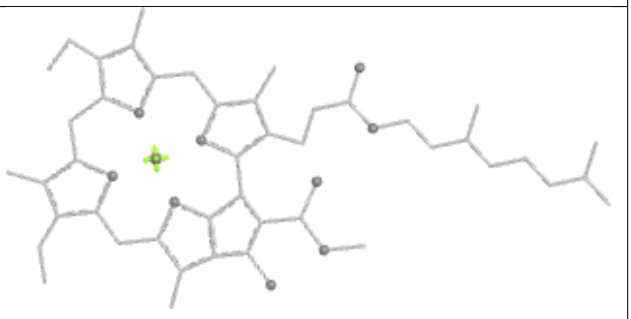
Bond lengths



Bond angles

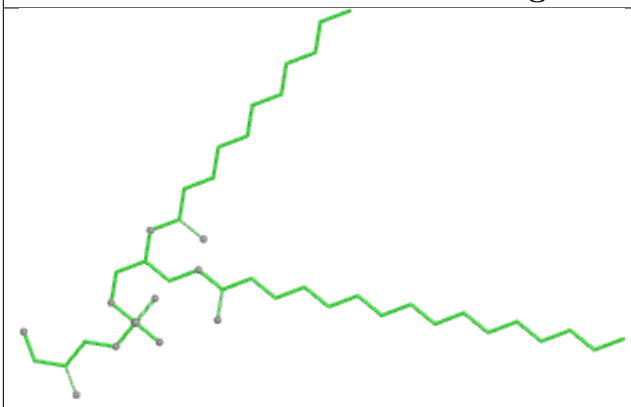


Torsions

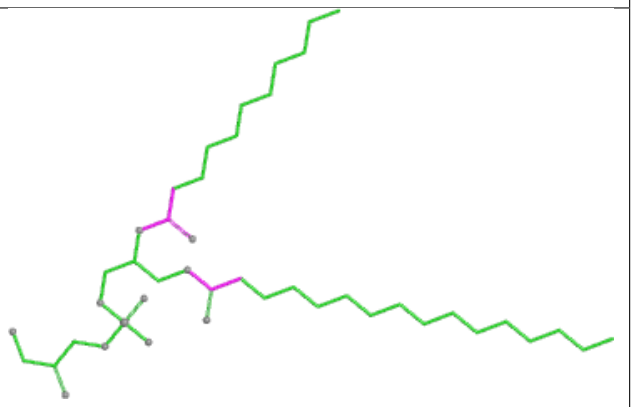


Rings

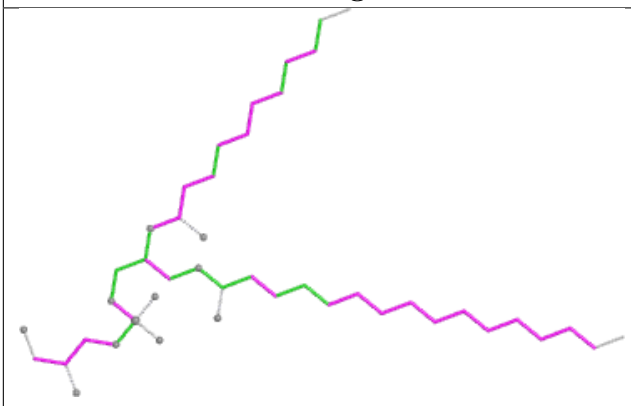
Ligand LHG s 322



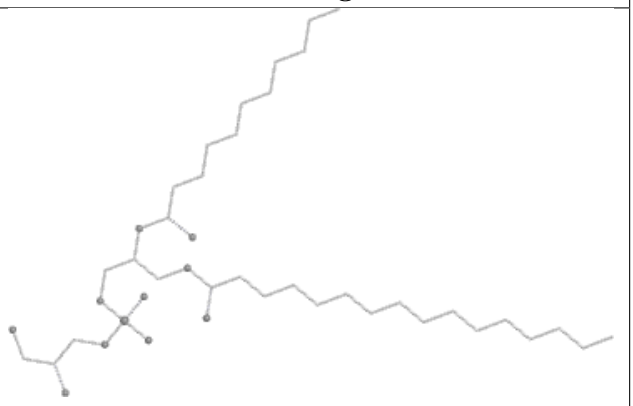
Bond lengths



Bond angles

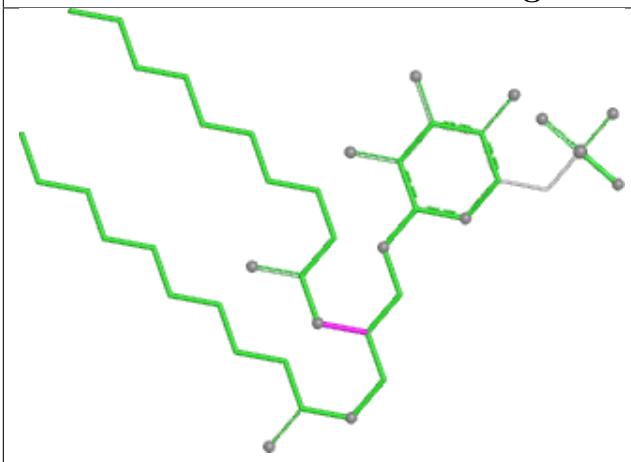


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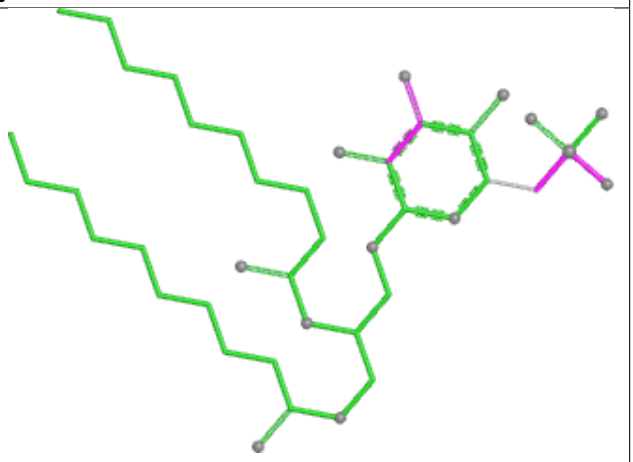


Rings

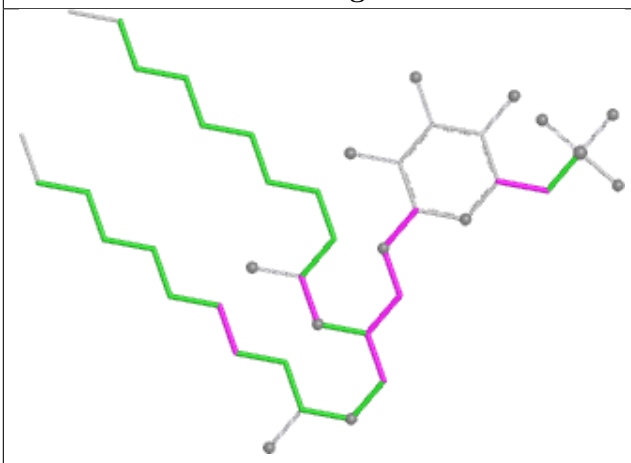
Ligand SQD G 617



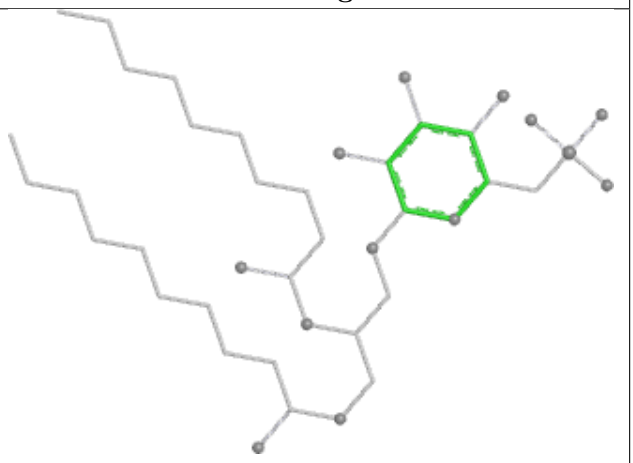
Bond lengths



Bond angles

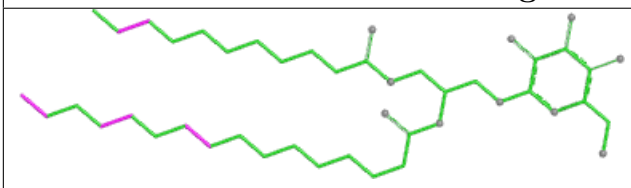


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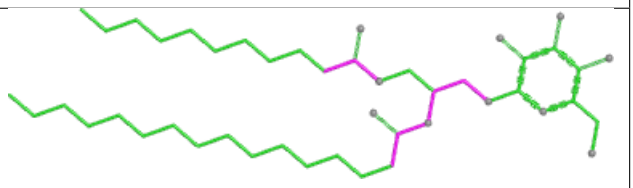


Rings

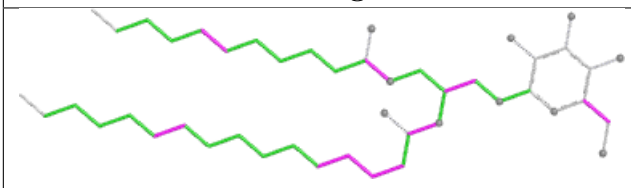
Ligand LMG D 409



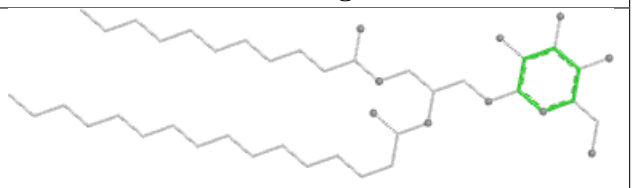
Bond lengths



Bond angles

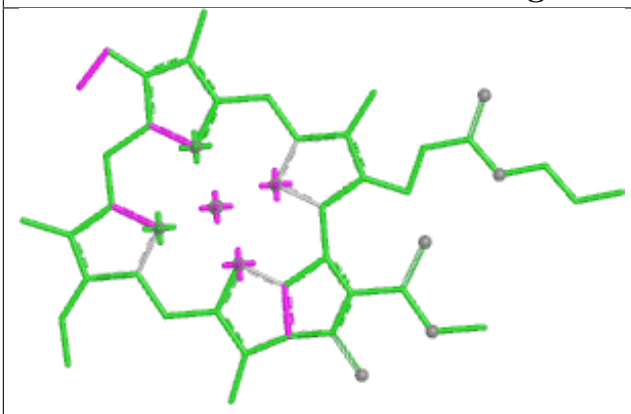


Torsions

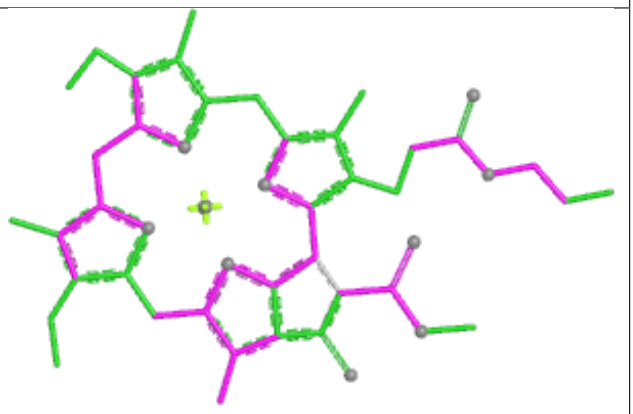


Rings

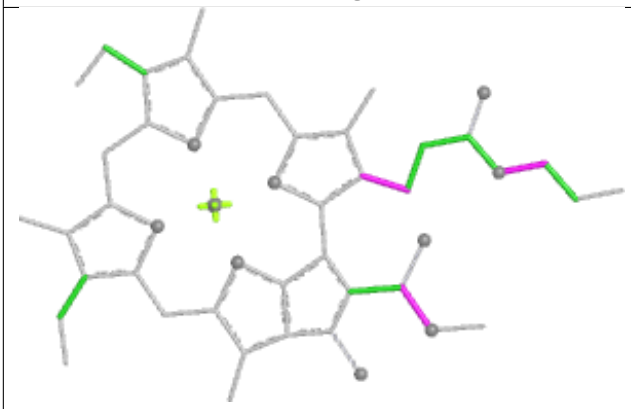
Ligand CLA S 315



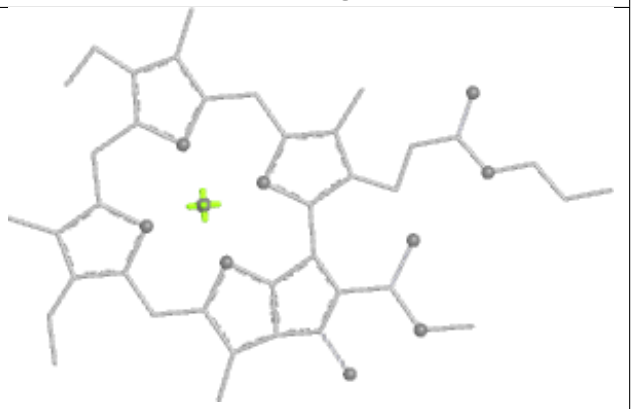
Bond lengths



Bond angles

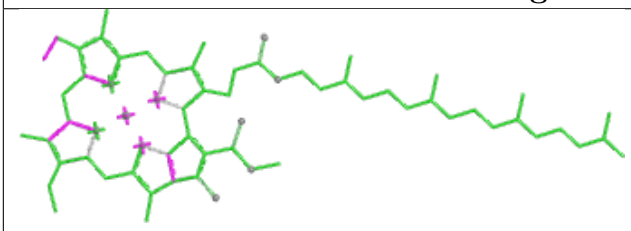


Torsions

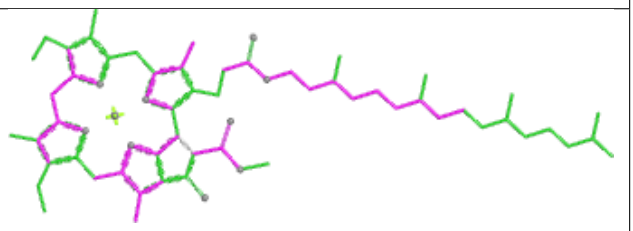


Rings

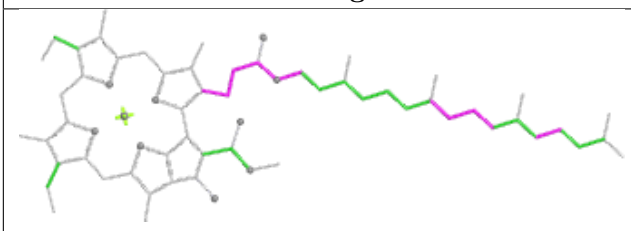
Ligand CLA s 303



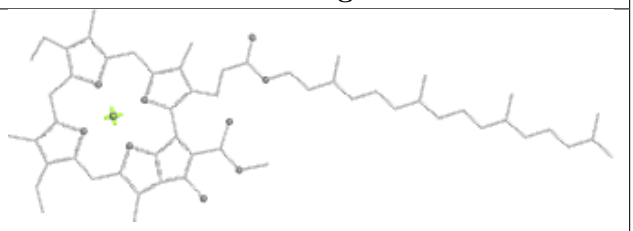
Bond lengths



Bond angles

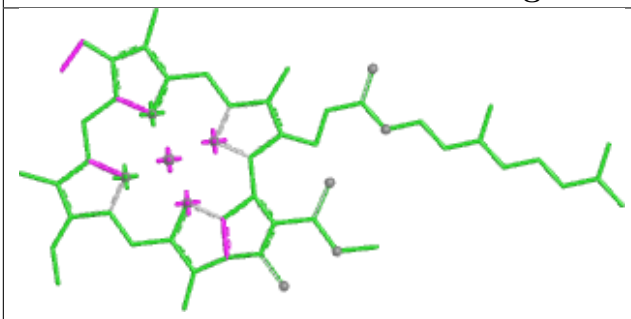


Torsions

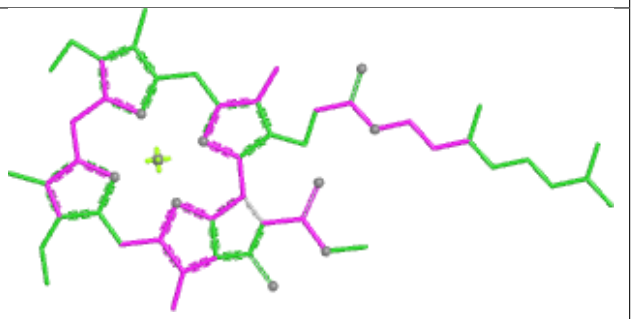


Rings

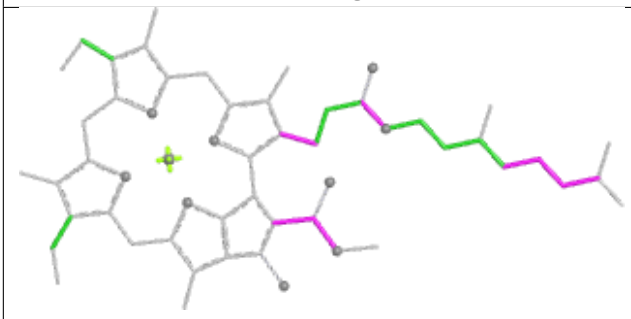
Ligand CLA N 304



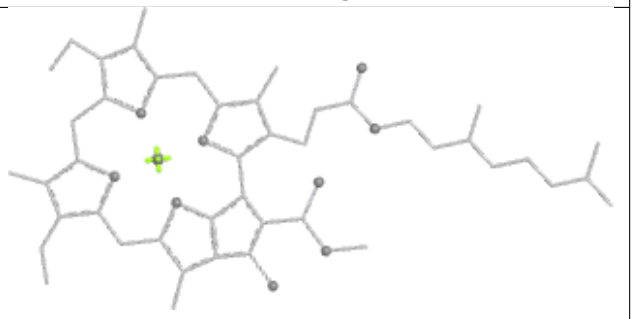
Bond lengths



Bond angles

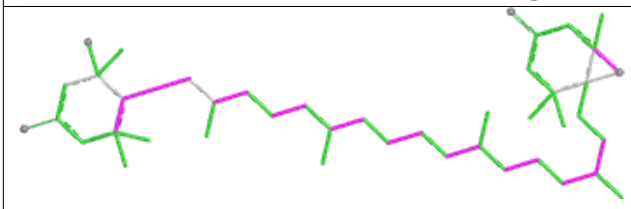


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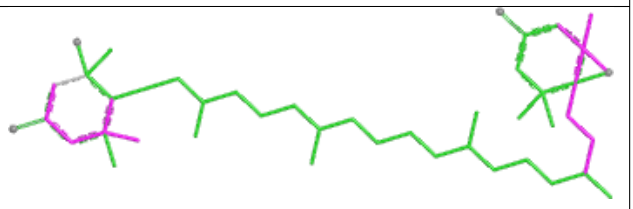


Rings

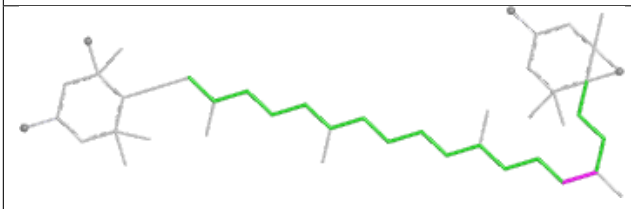
Ligand NEX S 319



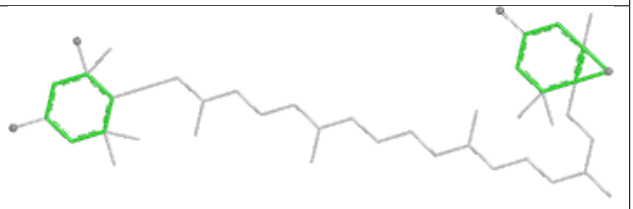
Bond lengths



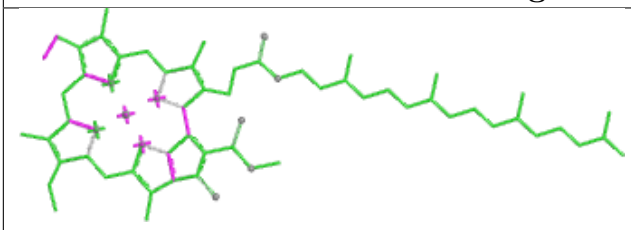
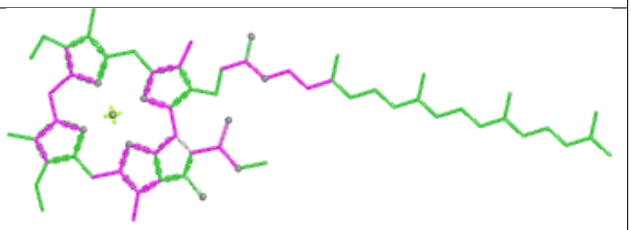
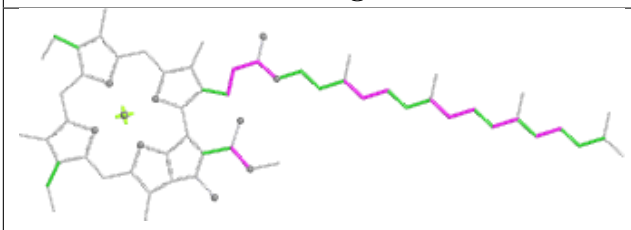
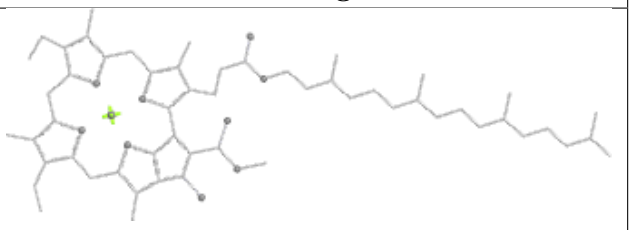
Bond angles

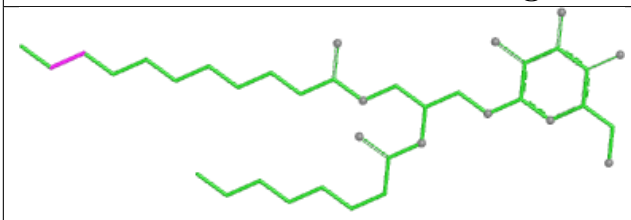
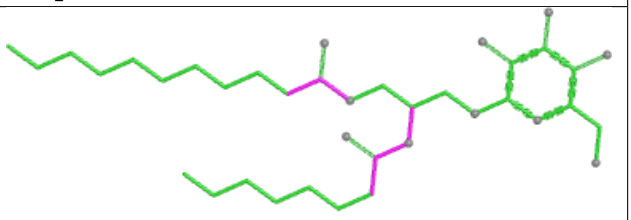
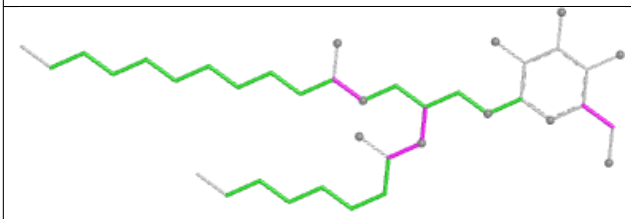
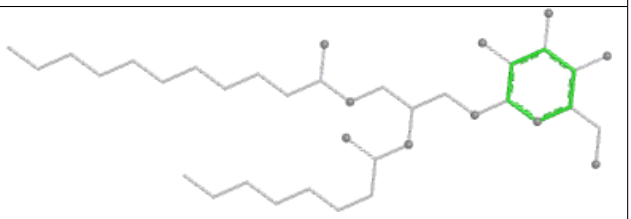


Torsions

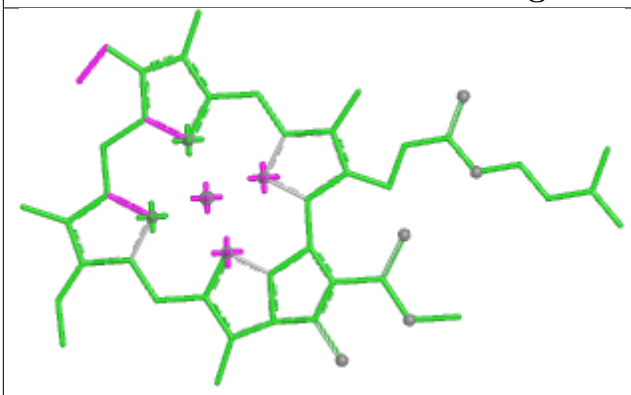


Rings

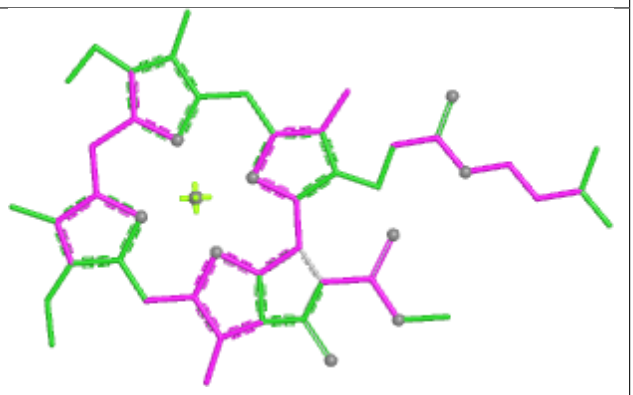
Ligand CLA 7 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG p 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

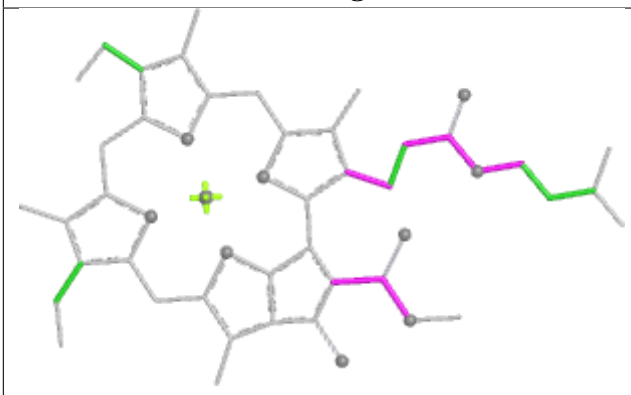
Ligand CLA 3 313



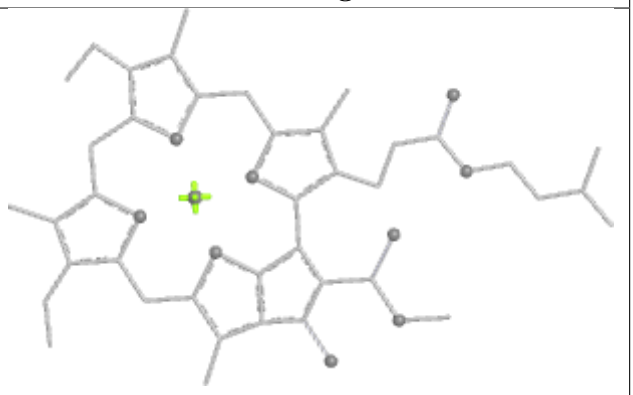
Bond lengths



Bond angles

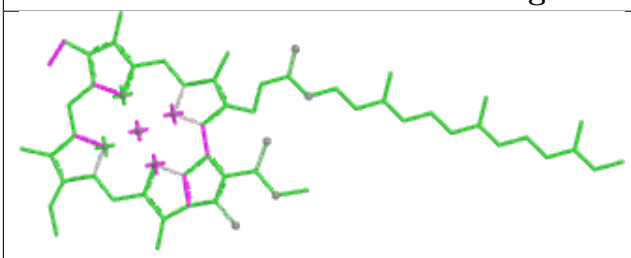


Torsions

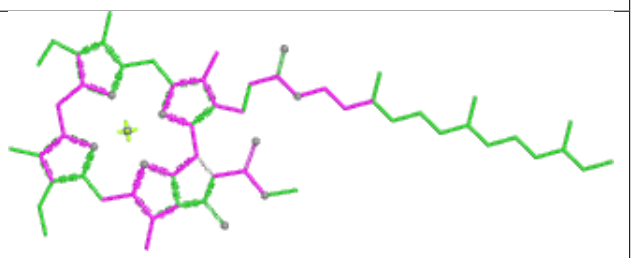


Rings

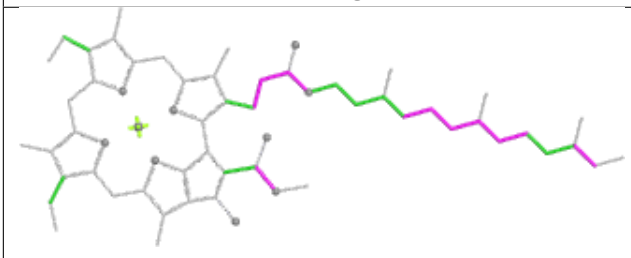
Ligand CLA 4 613



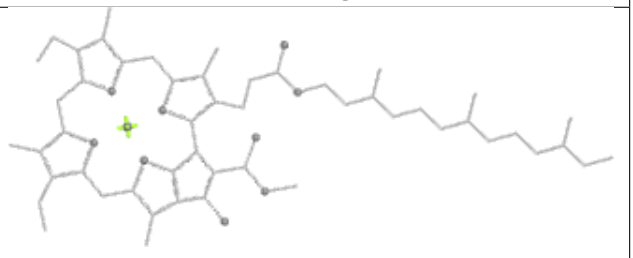
Bond lengths



Bond angles

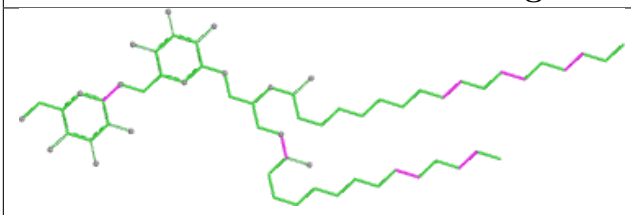


Torsions

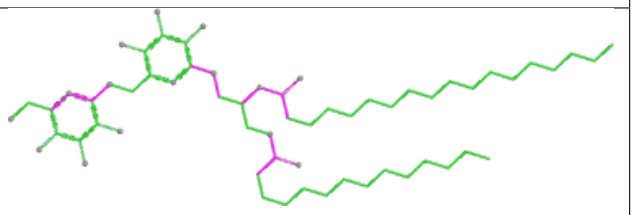


Rings

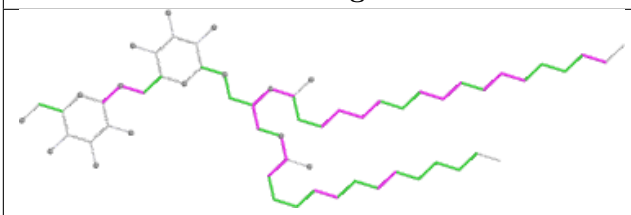
Ligand DGD c 617



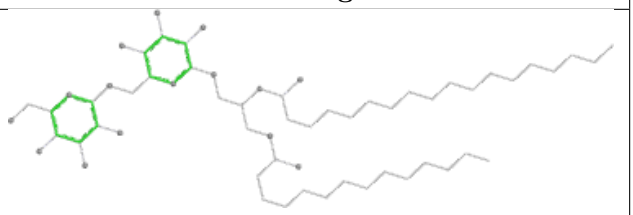
Bond lengths



Bond angles

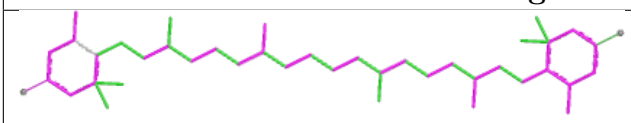


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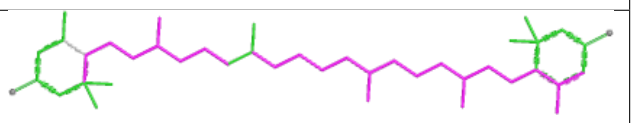


Rings

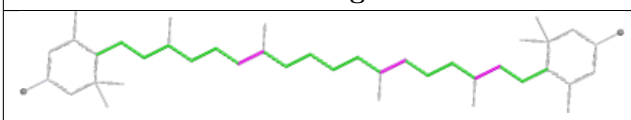
Ligand LUT 8 615



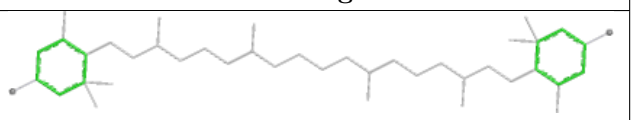
Bond lengths



Bond angles

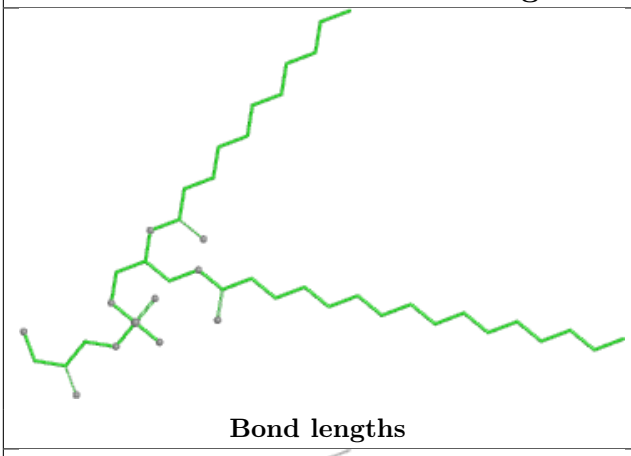


Torsions

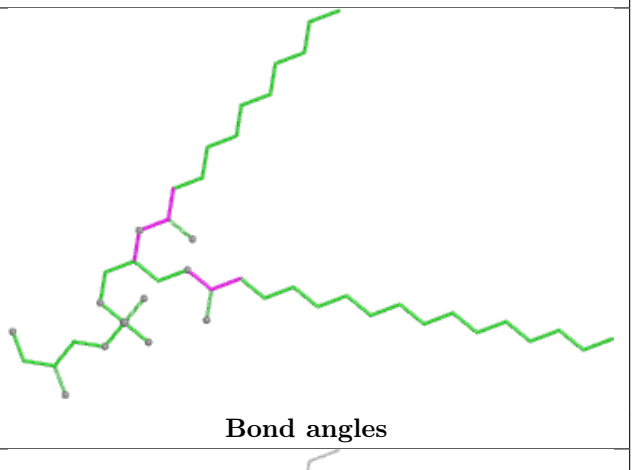


Rings

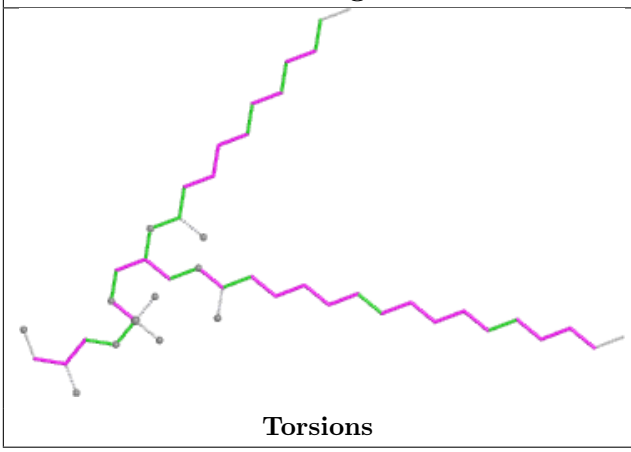
Ligand LHG G 618



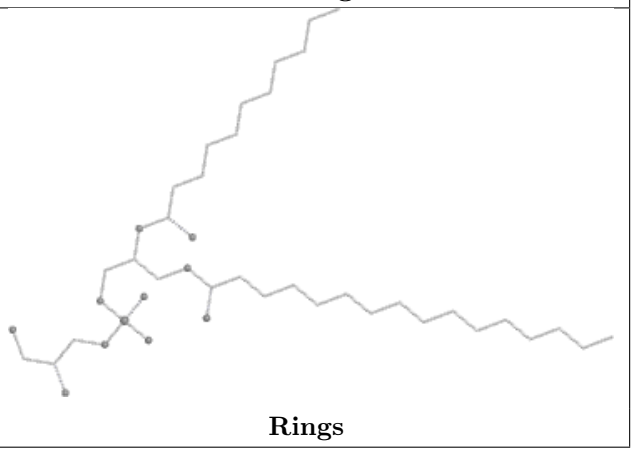
Bond lengths



Bond angles

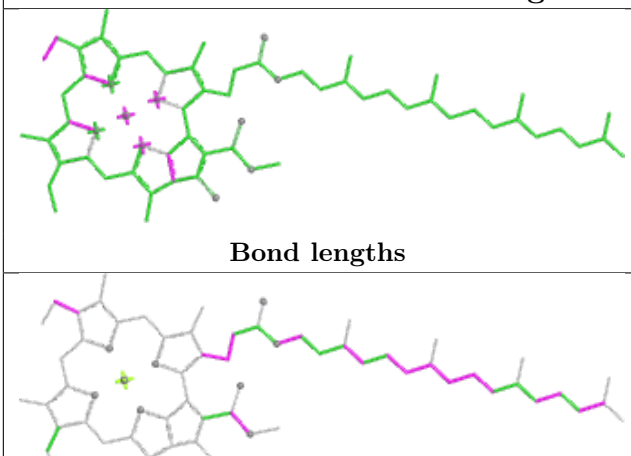


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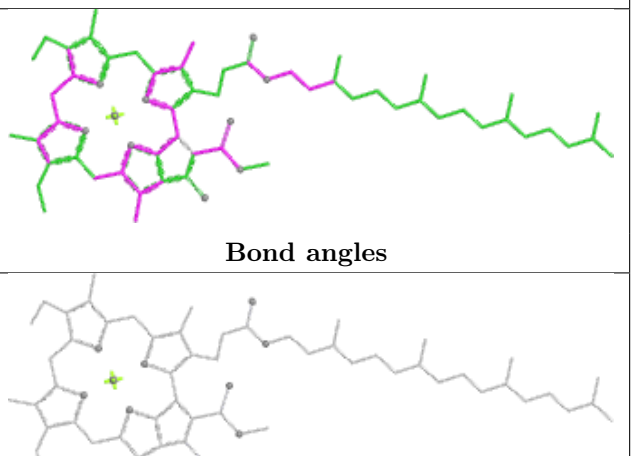


Rings

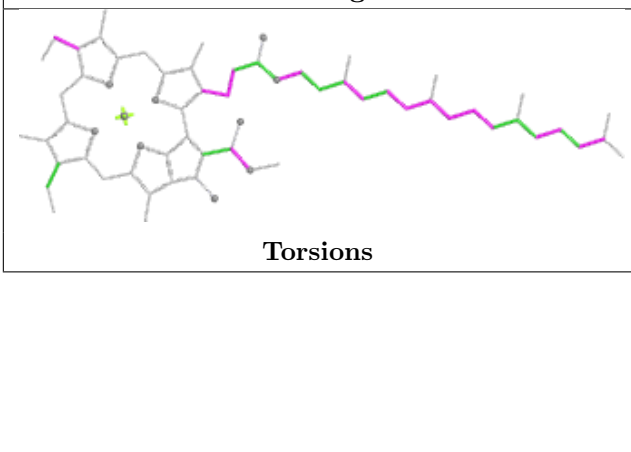
Ligand CLA S 312



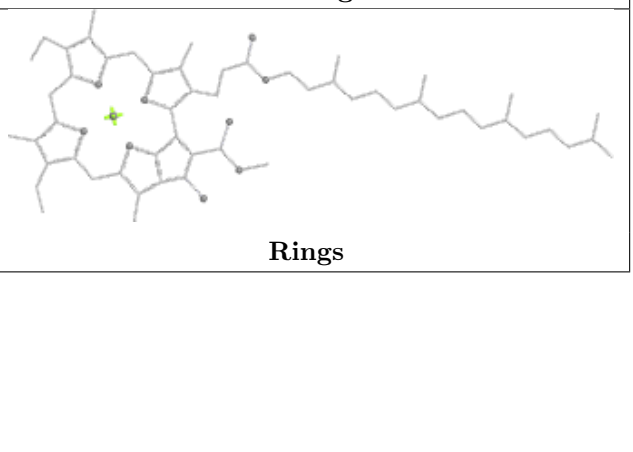
Bond lengths



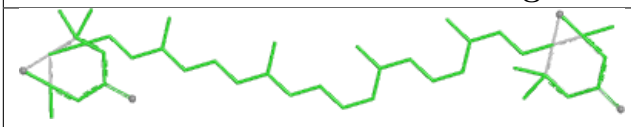
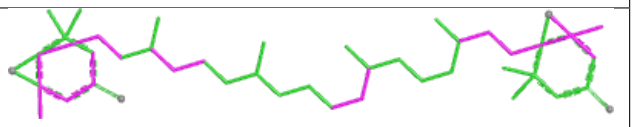
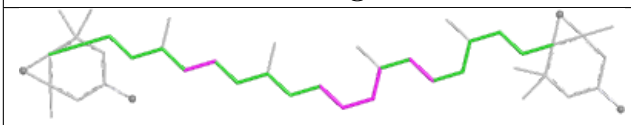
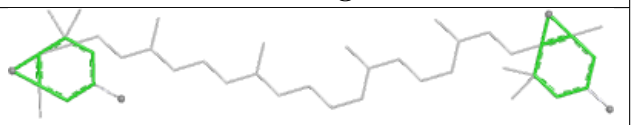
Bond angles

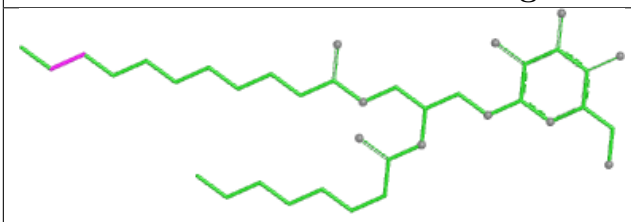
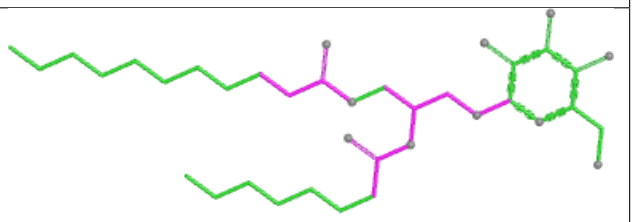
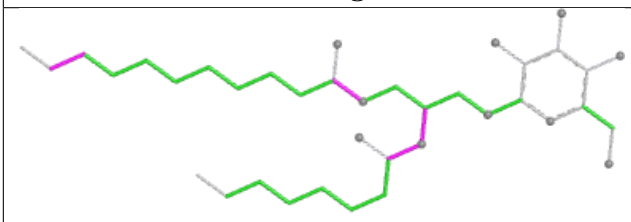
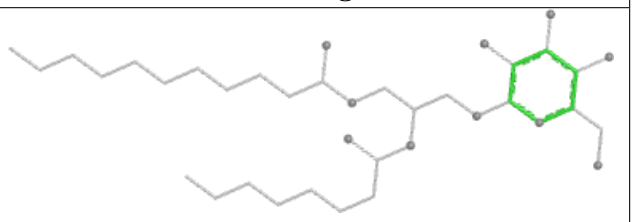


Torsions

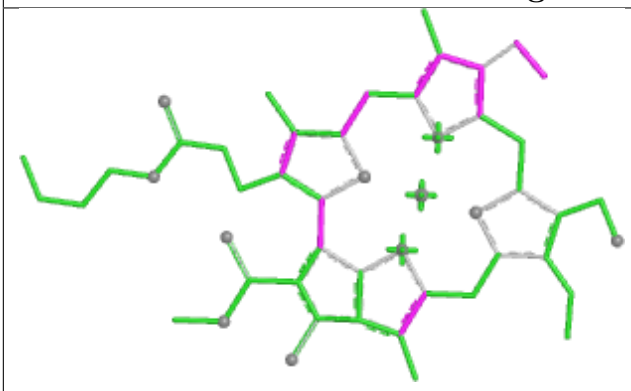


Rings

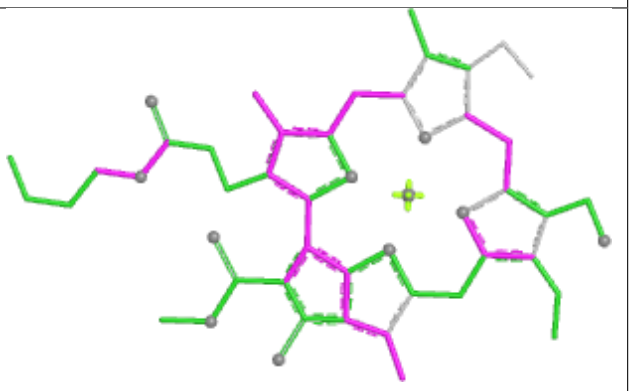
Ligand XAT R 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG w 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

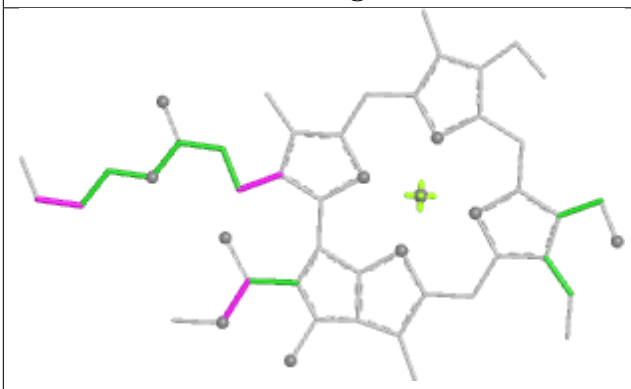
Ligand CHL 3 303



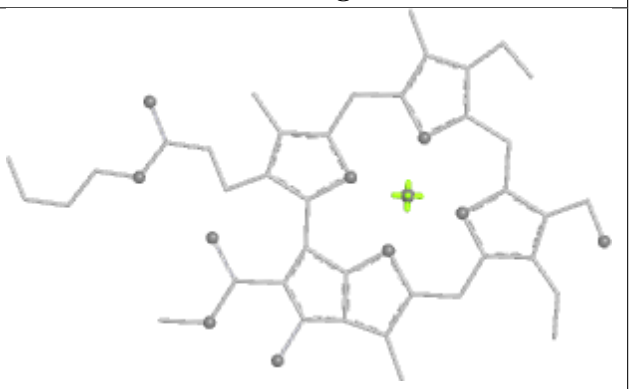
Bond lengths



Bond angles

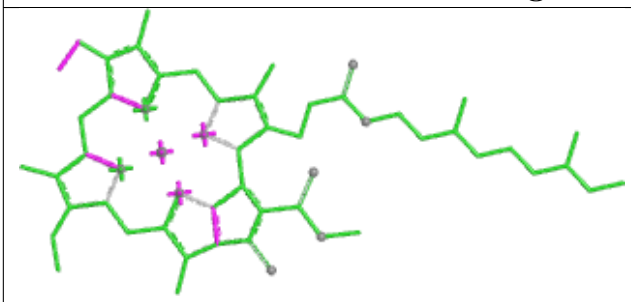


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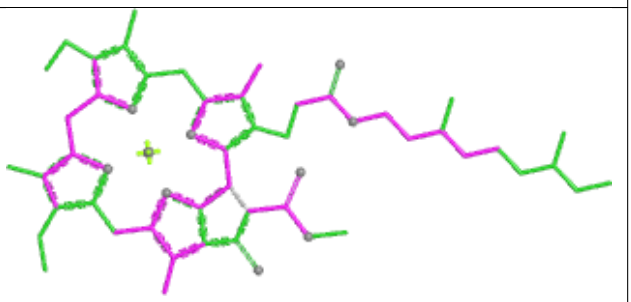


Rings

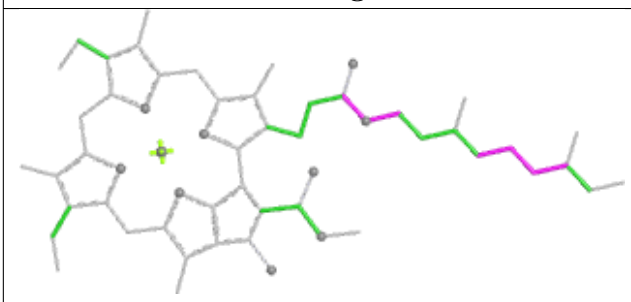
Ligand CLA S 313



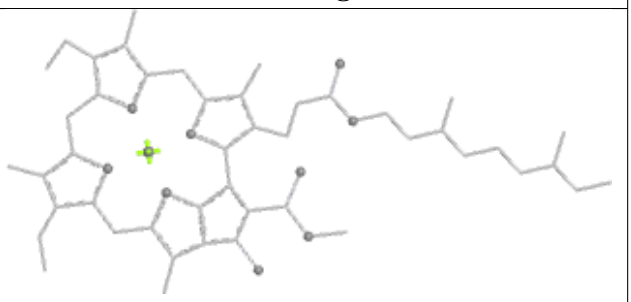
Bond lengths



Bond angles

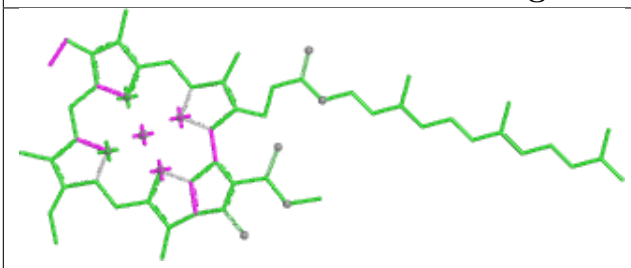


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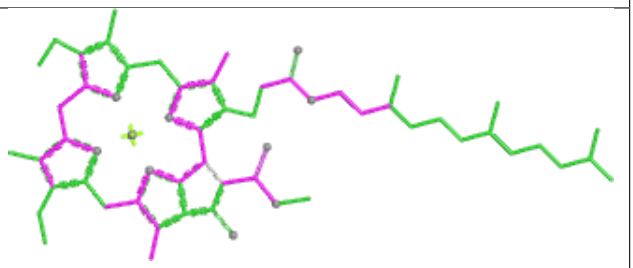


Rings

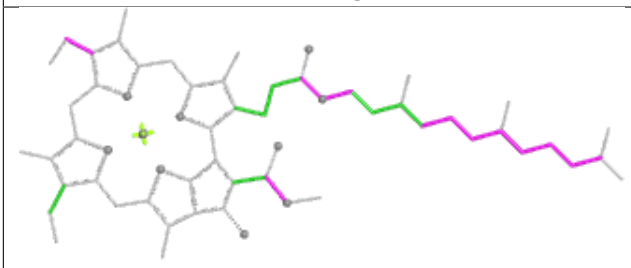
Ligand CLA 6 312



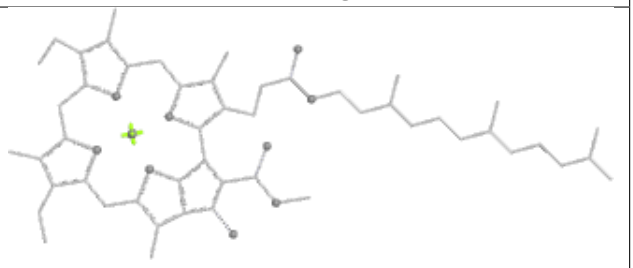
Bond lengths



Bond angles

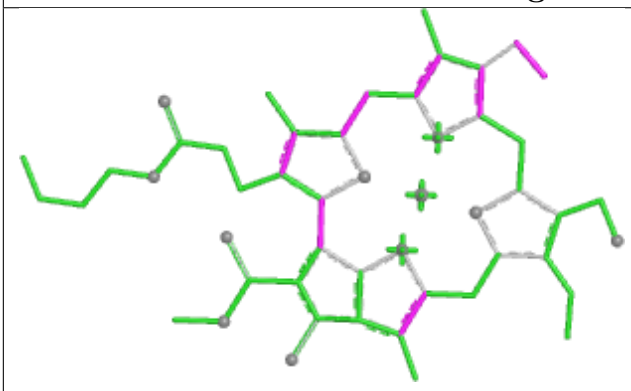


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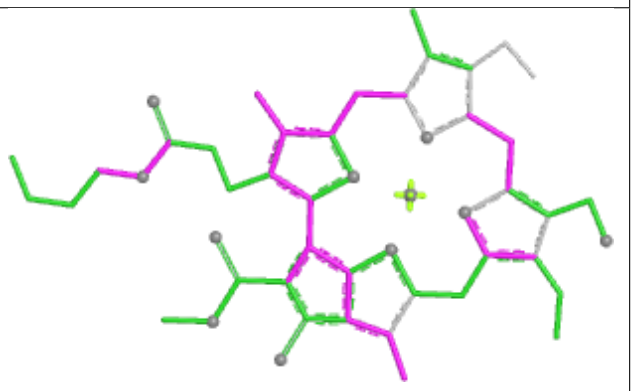


Rings

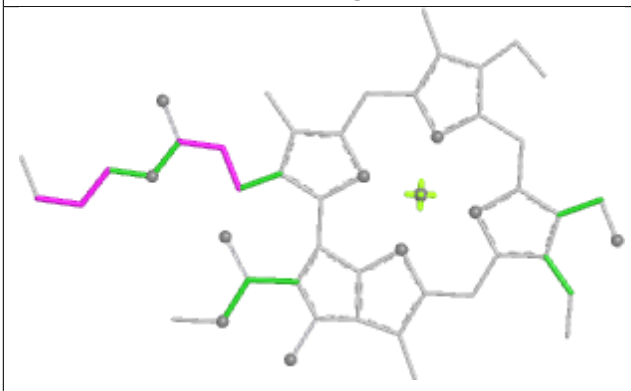
Ligand CHL 5 608



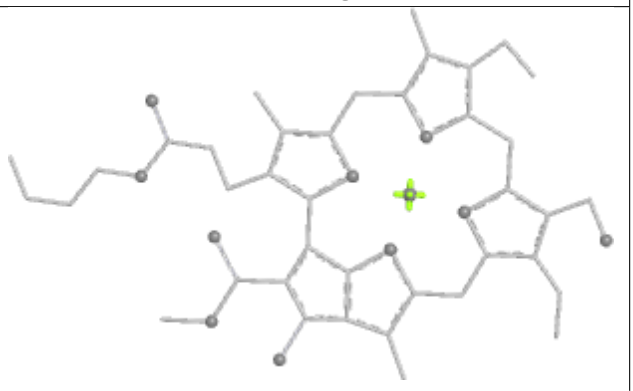
Bond lengths



Bond angles

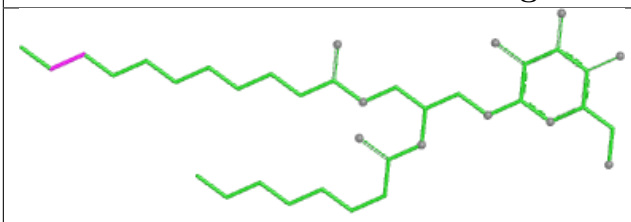


Torsions

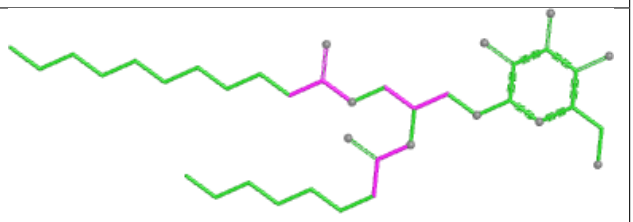


Rings

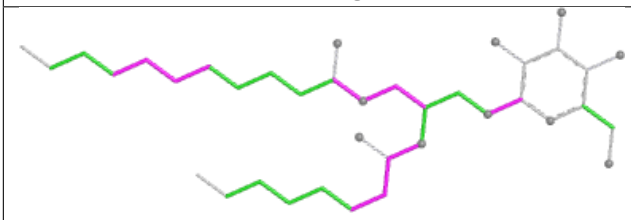
Ligand LMG B 625



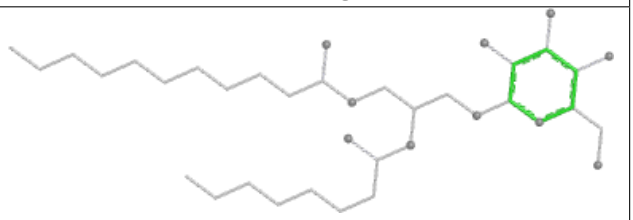
Bond lengths



Bond angles

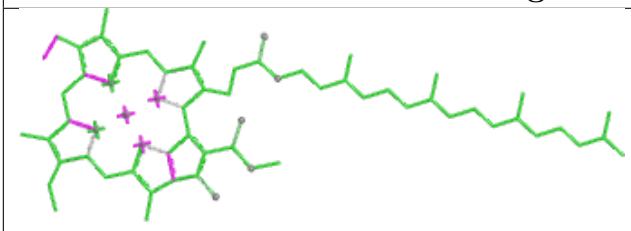


Torsions

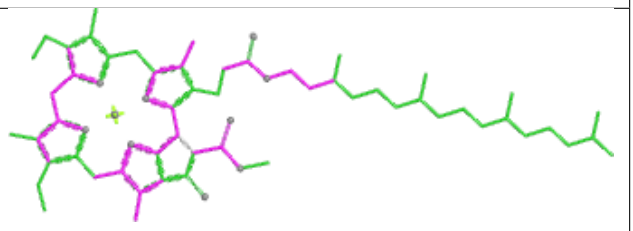


Rings

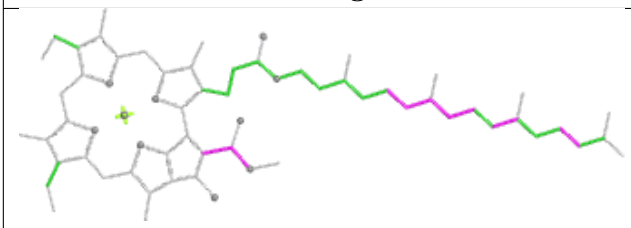
Ligand CLA b 611



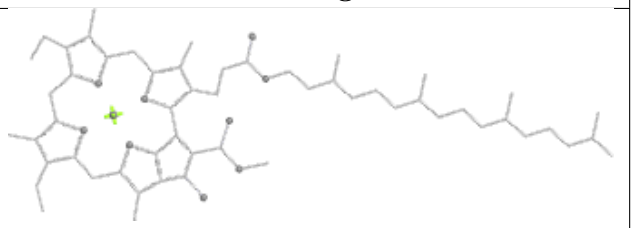
Bond lengths



Bond angles

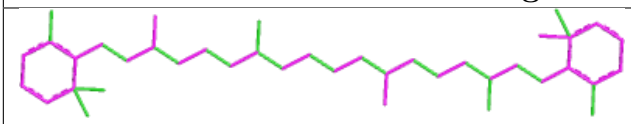


Torsions

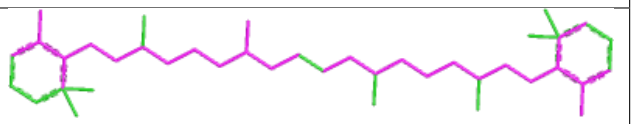


Rings

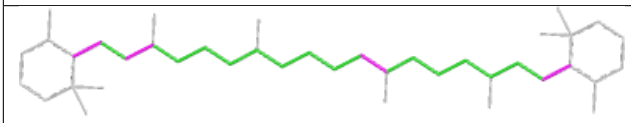
Ligand BCR A 410



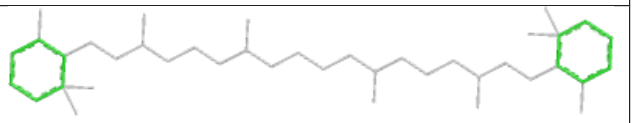
Bond lengths



Bond angles

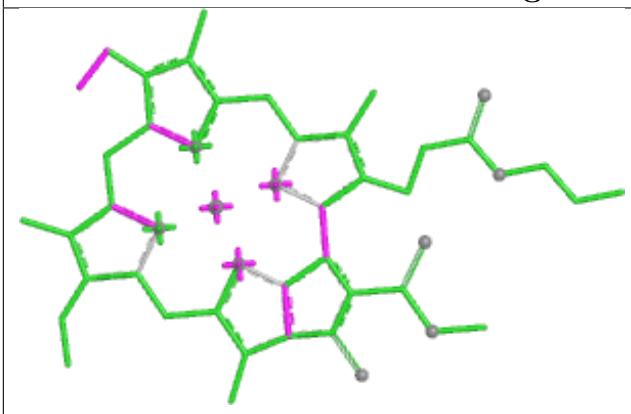


Torsions

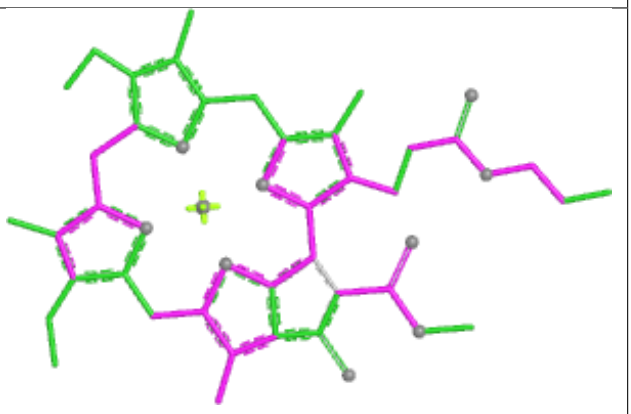


Rings

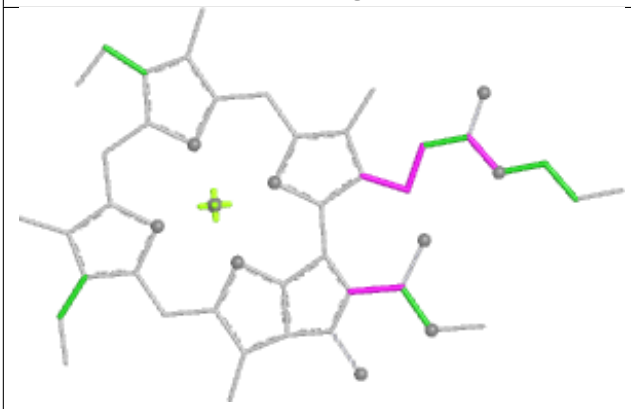
Ligand CLA R 306



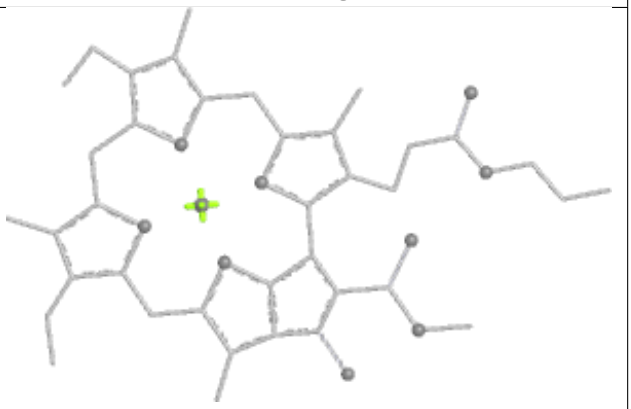
Bond lengths



Bond angles

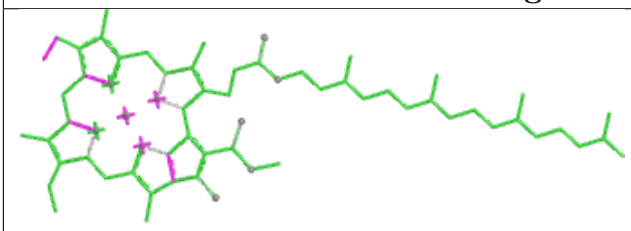


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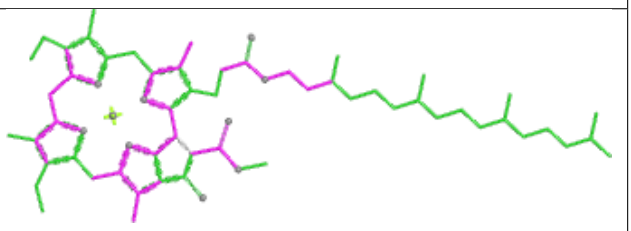


Rings

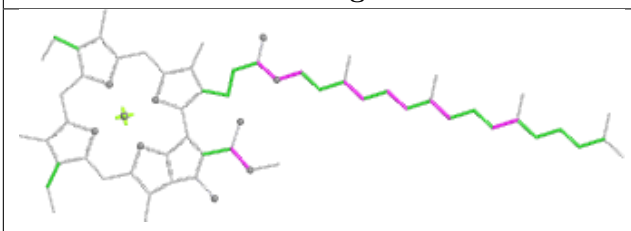
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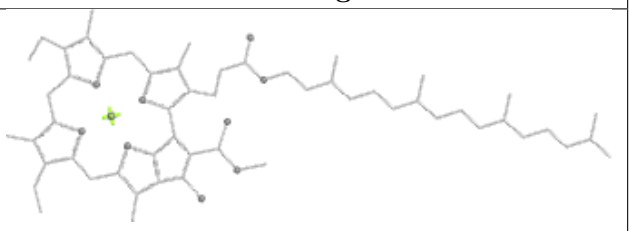
Bond lengths



Bond angles

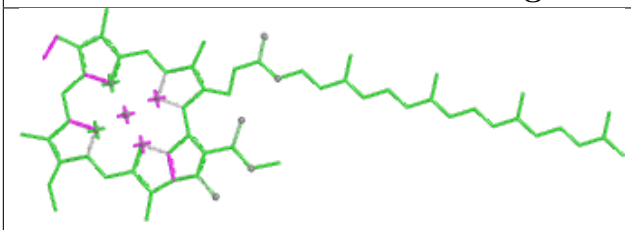


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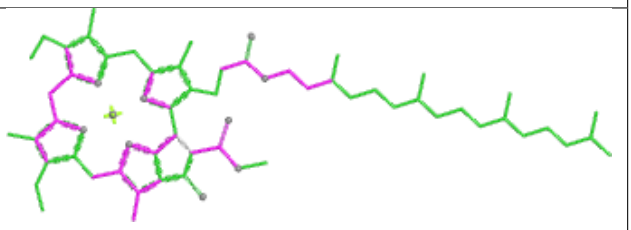


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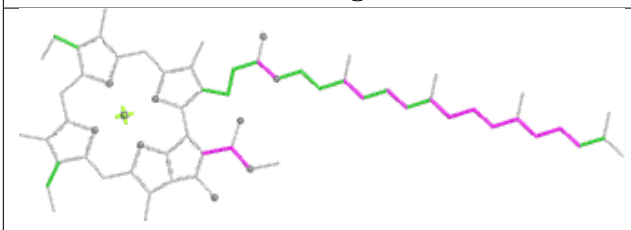
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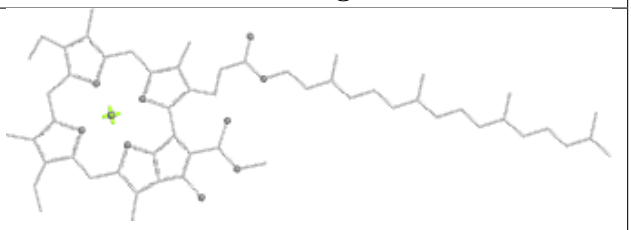
Bond lengths



Bond angles

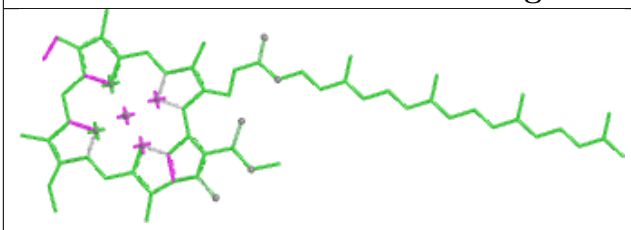


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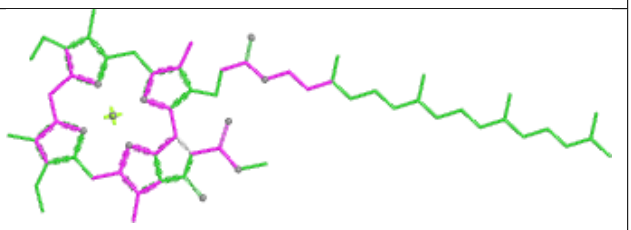


Rings

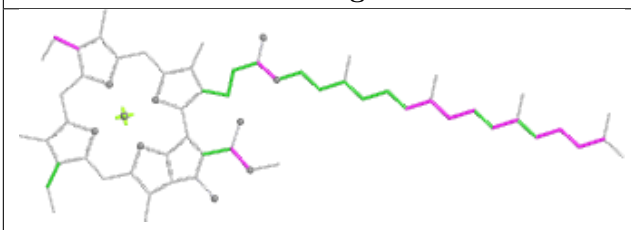
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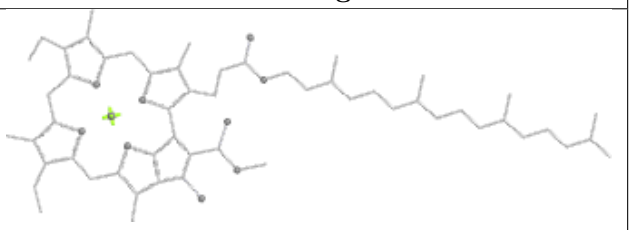
Bond lengths



Bond angles

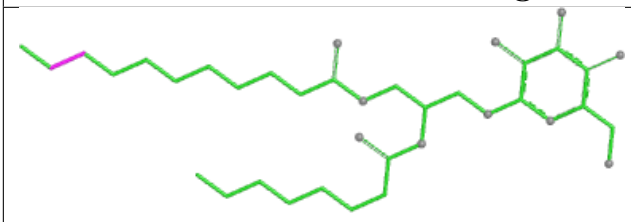


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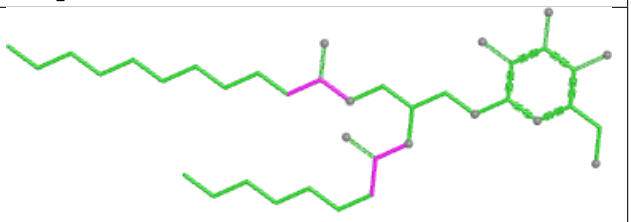


Rings

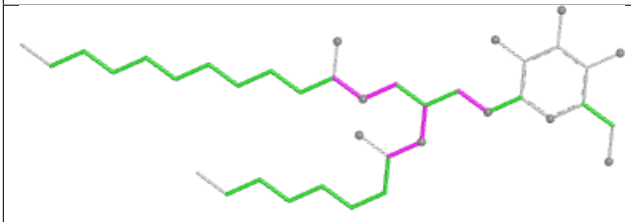
Ligand LMG q1 101



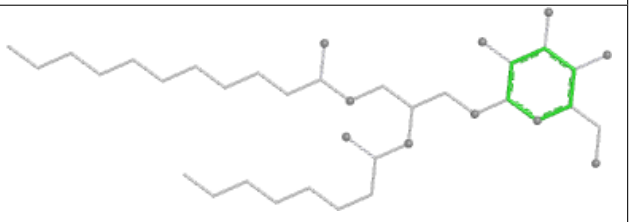
Bond lengths



Bond angles

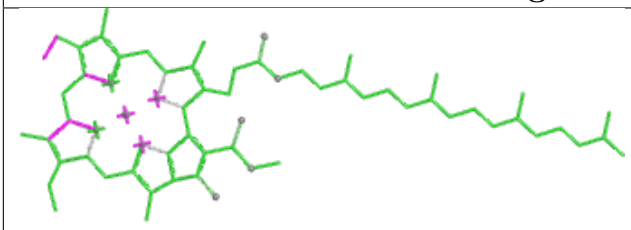


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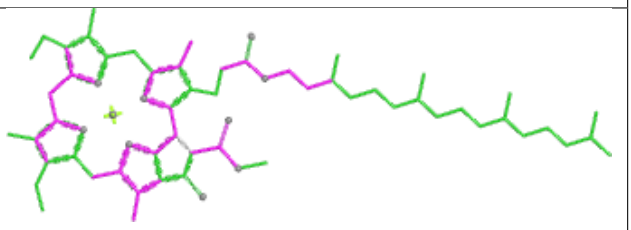


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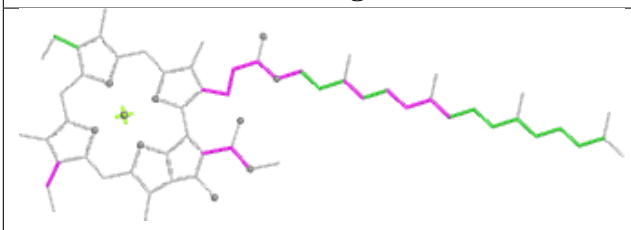
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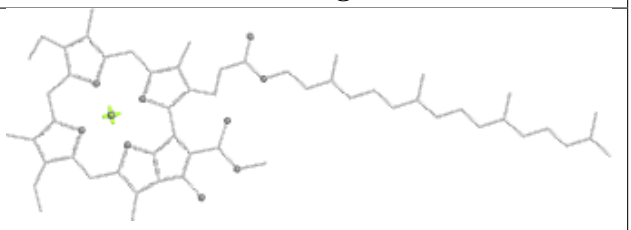
Bond lengths



Bond angles

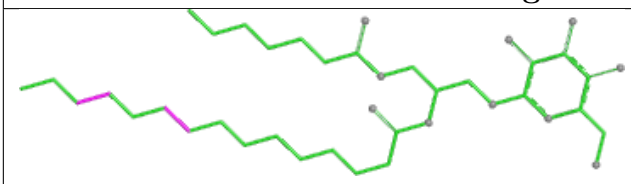


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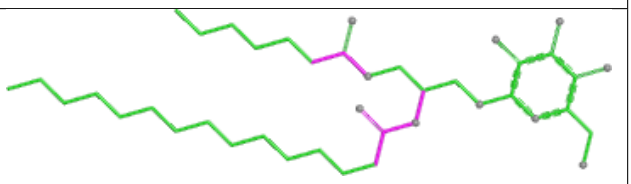


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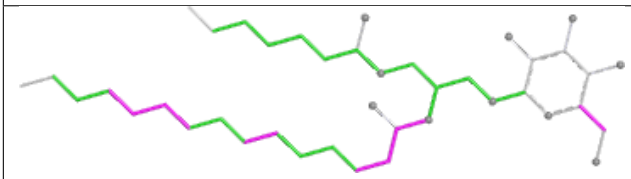
Ligand LMG S 321



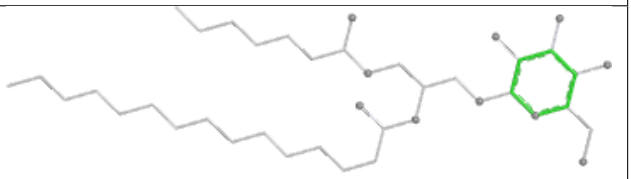
Bond lengths



Bond angles

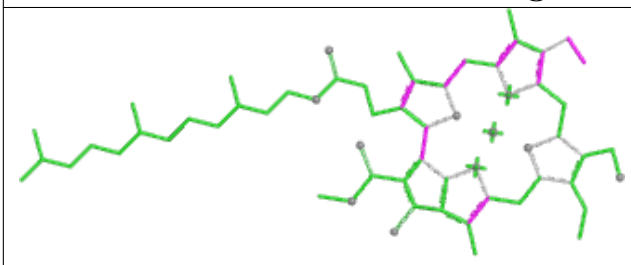


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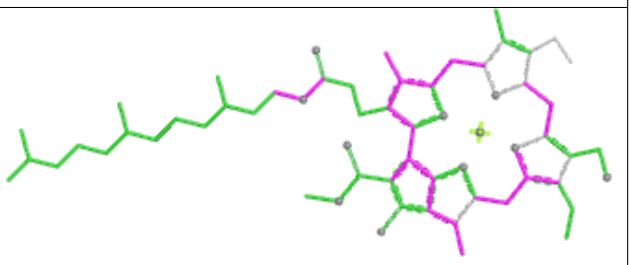


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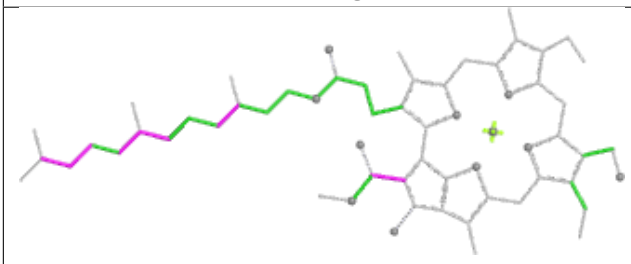
Ligand CHL 3 310



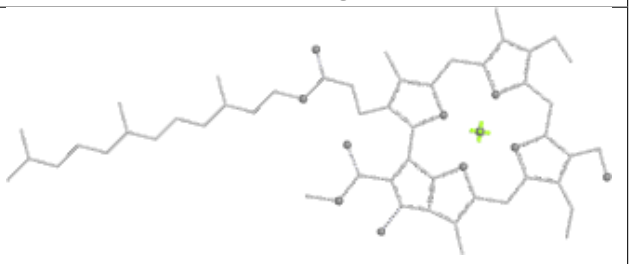
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Bond angles

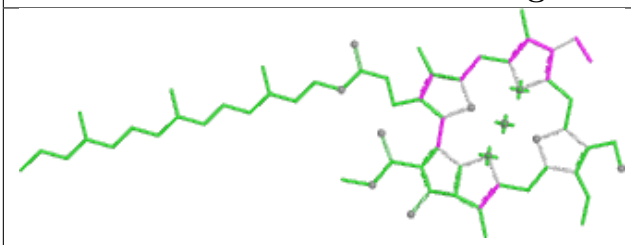


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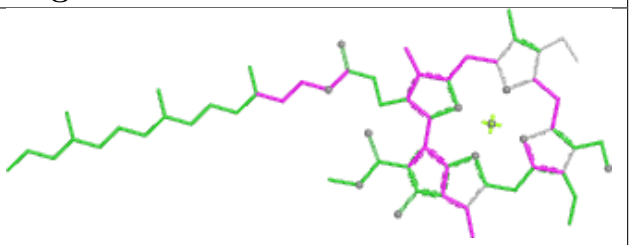


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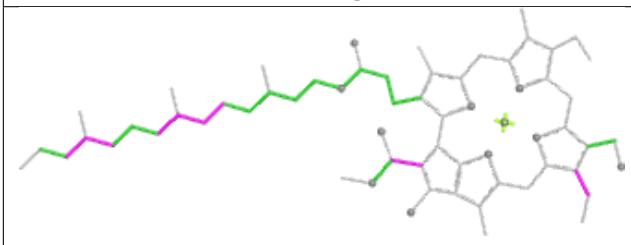
Ligand CHL g 309



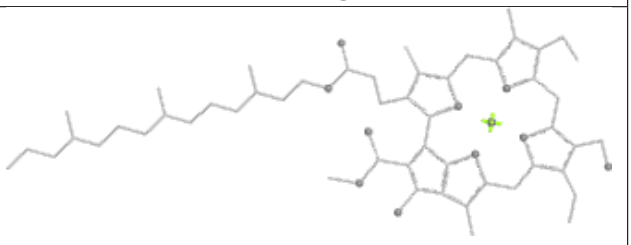
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Bond angles

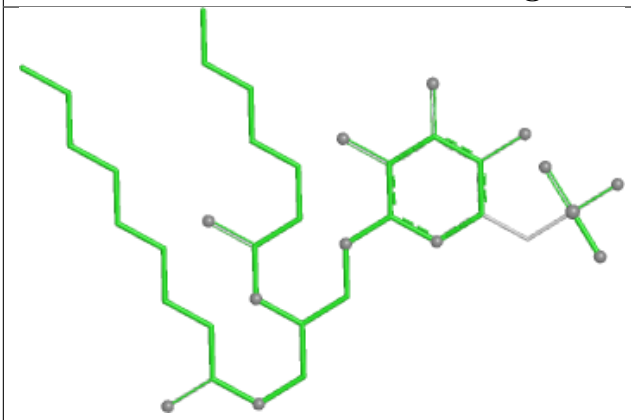


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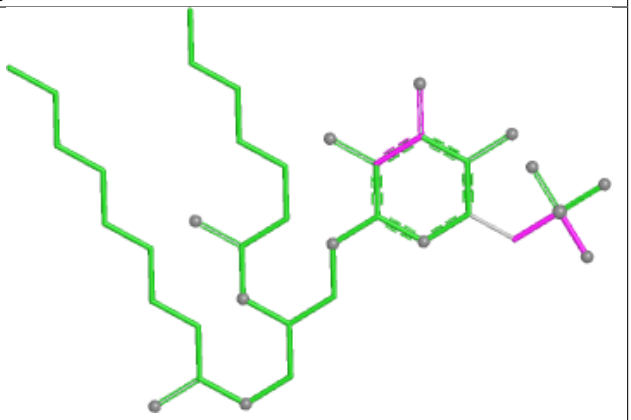


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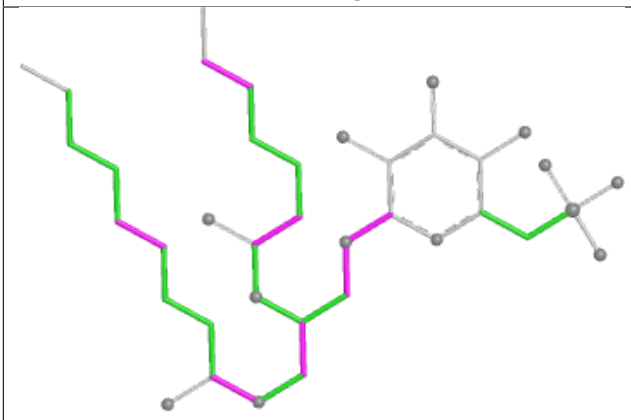
Ligand SQD X 201



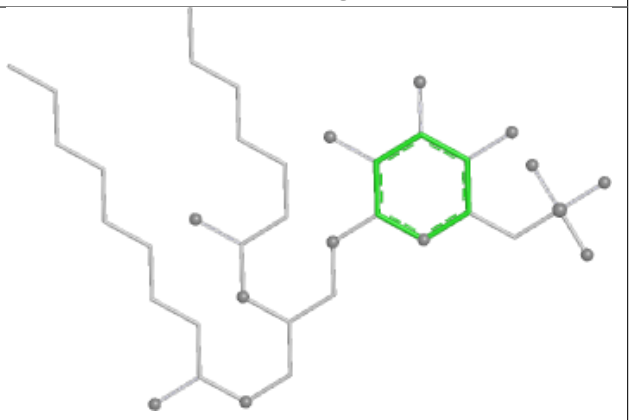
Bond lengths



Bond angles

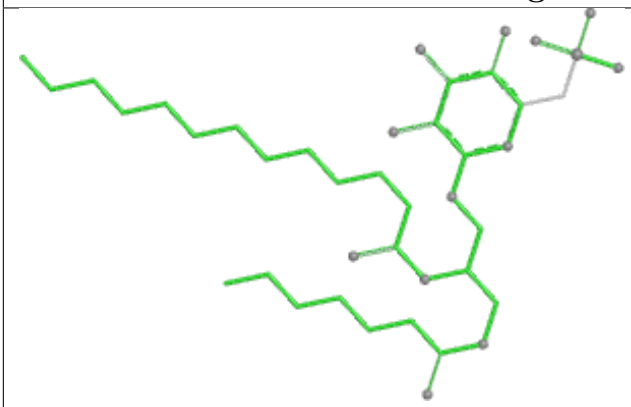


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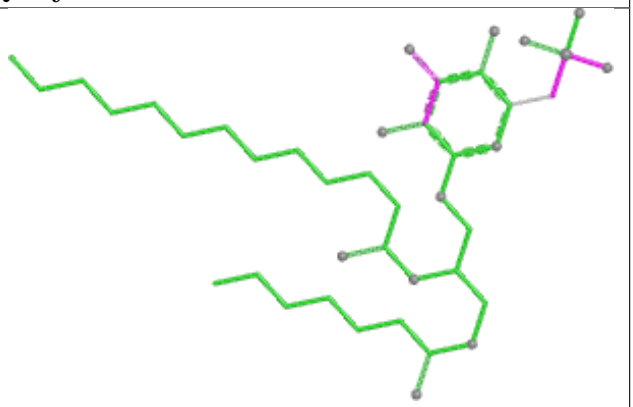


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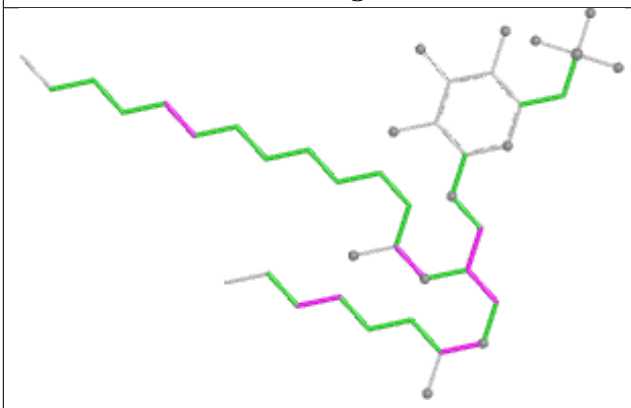
Ligand SQD y 621



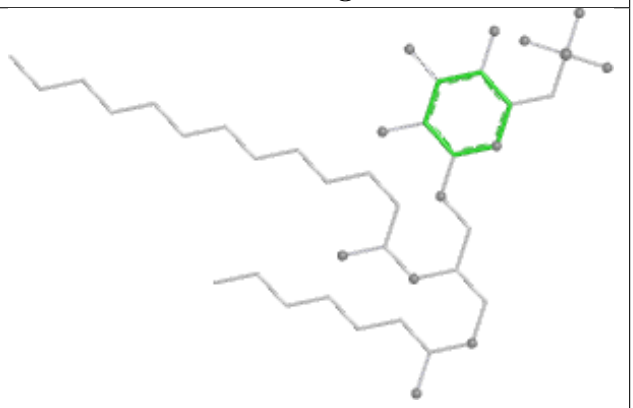
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Bond angles

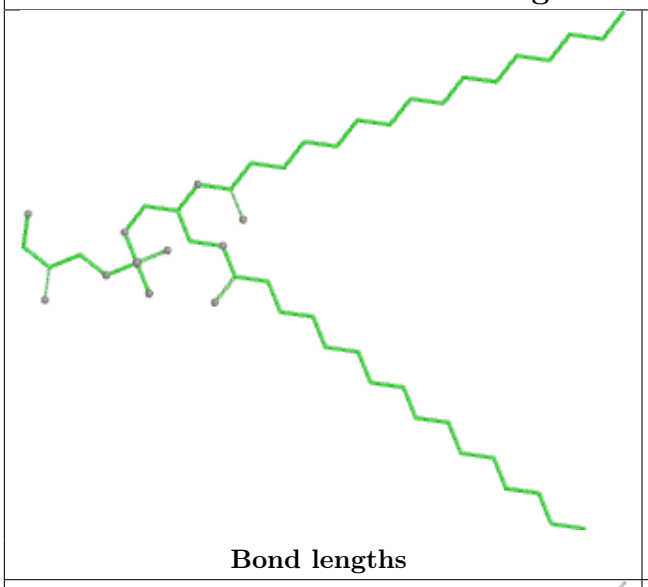


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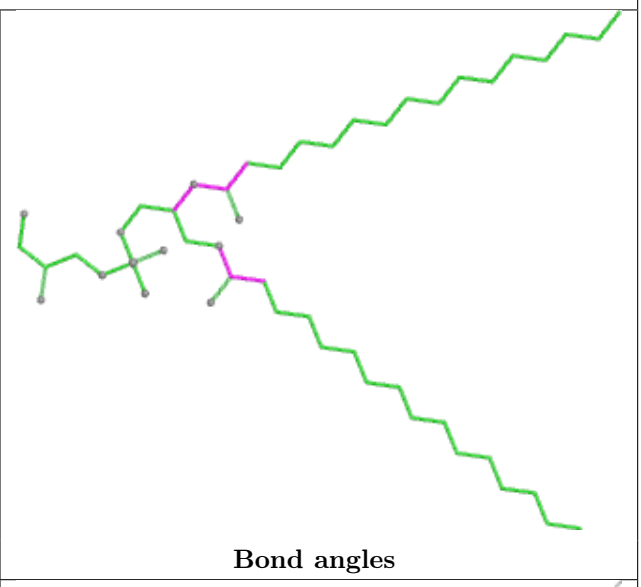


Rings

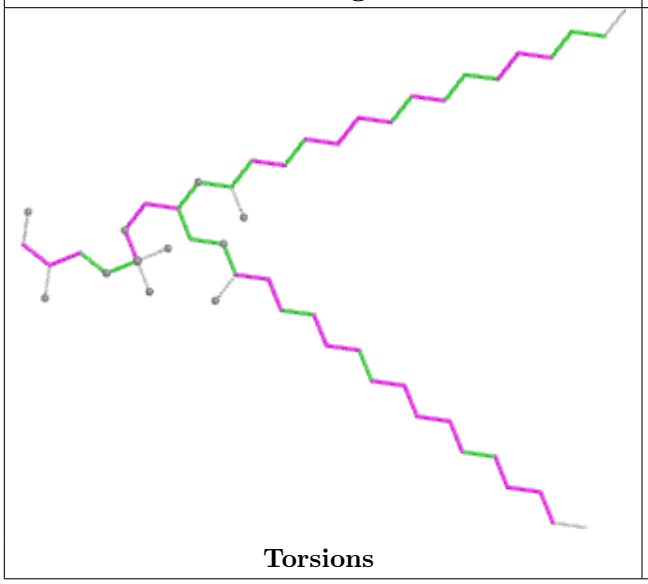
Ligand LHG l 101



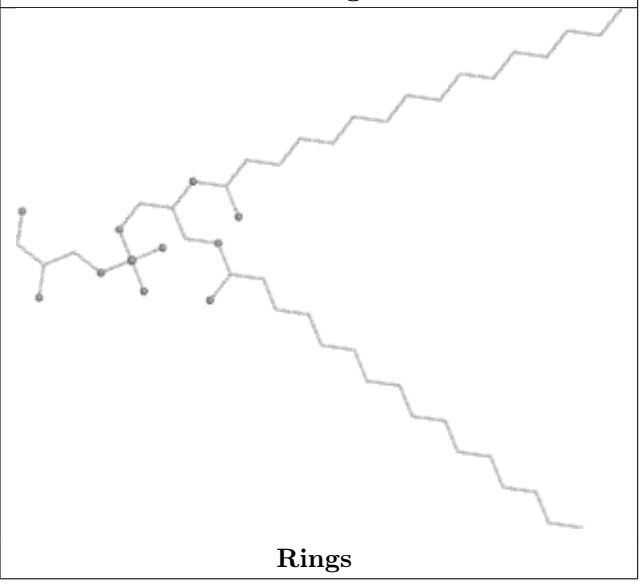
Bond lengths



Bond angles

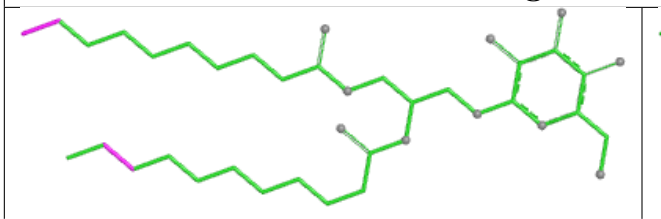


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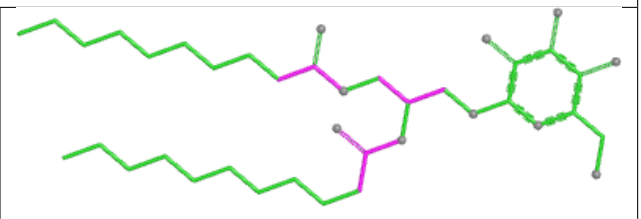


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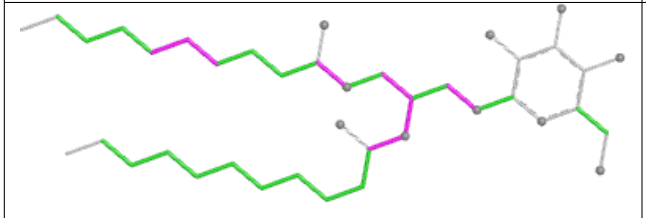
Ligand LMG 2 621



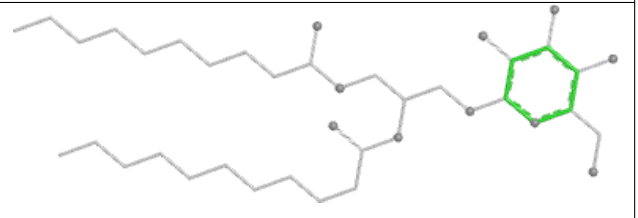
Bond lengths



Bond angles

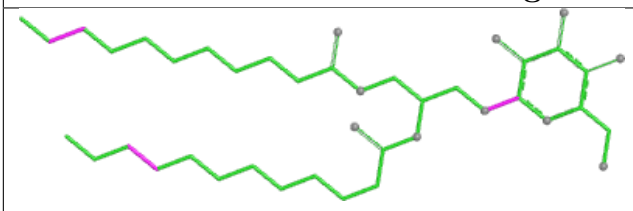


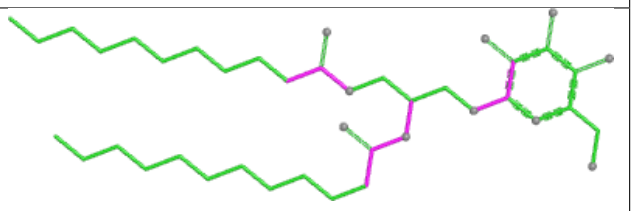
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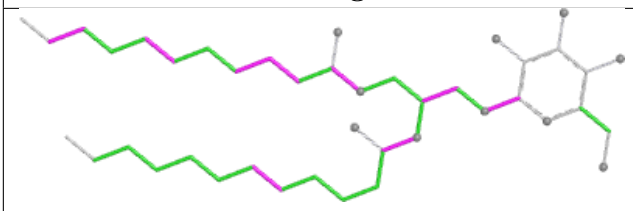


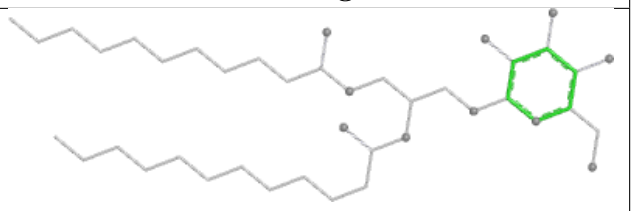
Rings

Ligand LMG 0 620

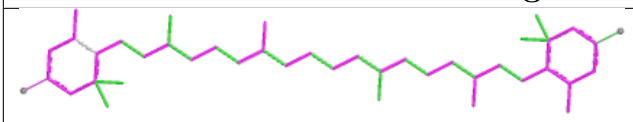

Bond lengths

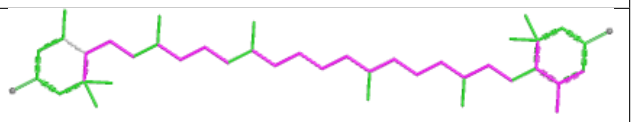

Bond angles

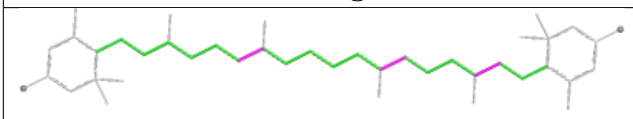

Torsions

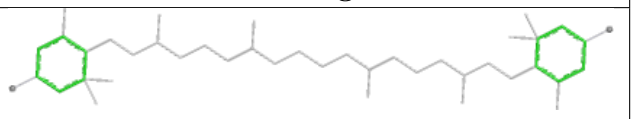

Rings

Ligand LUT N 316

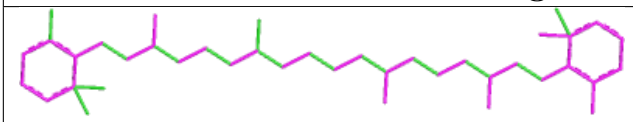

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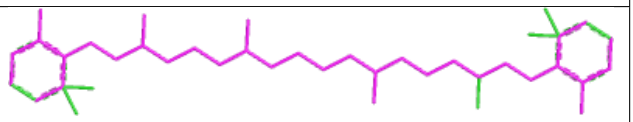

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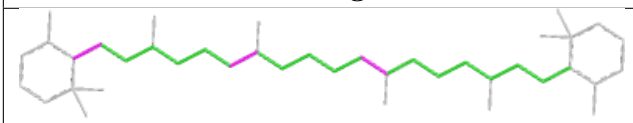

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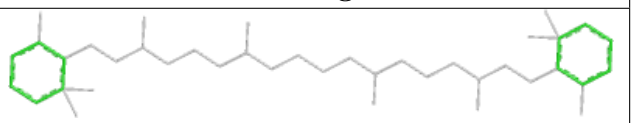

Rings

Ligand BCR t 101

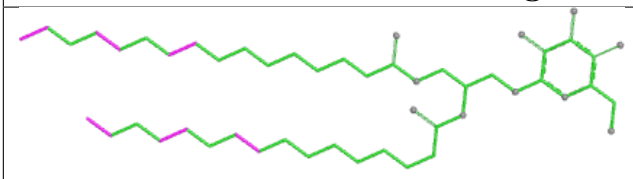

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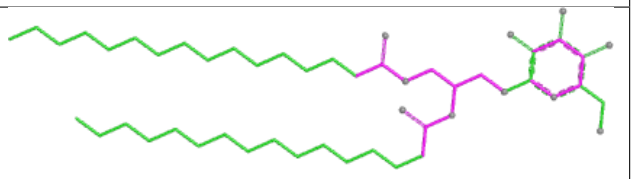

Bond angles

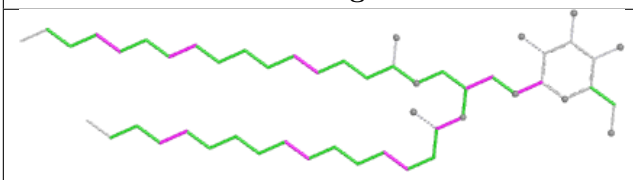

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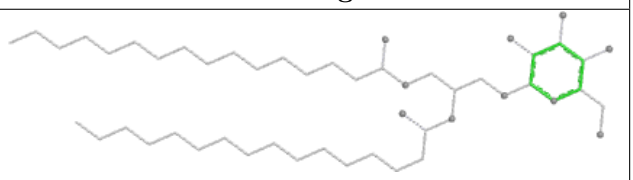

Rings

Ligand LMG 9 301

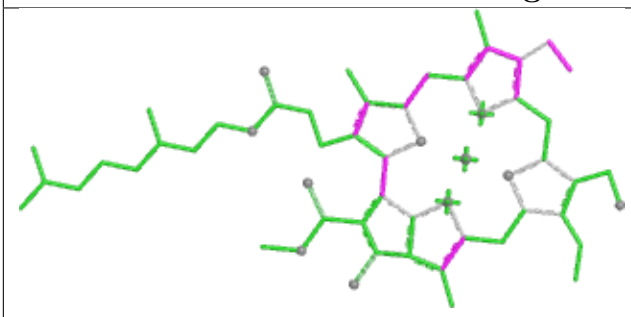

Bond lengths


Bond angles

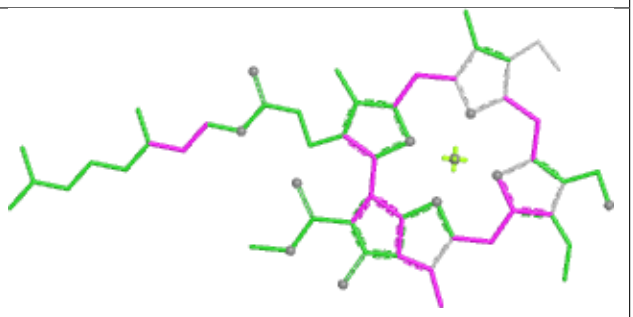

Torsions


Rings

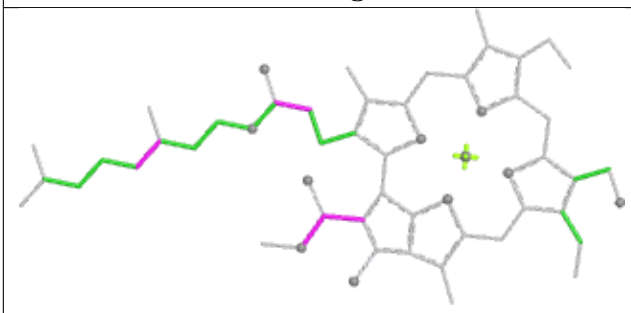
Ligand CHL R 309



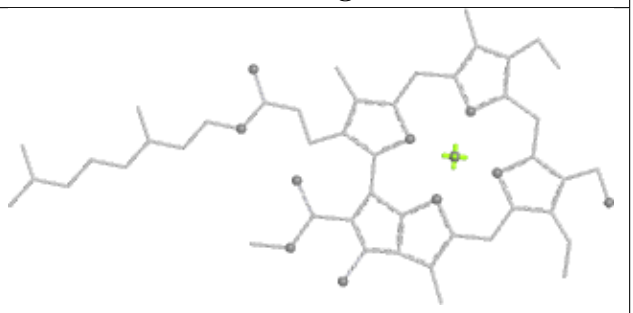
Bond lengths



Bond angles

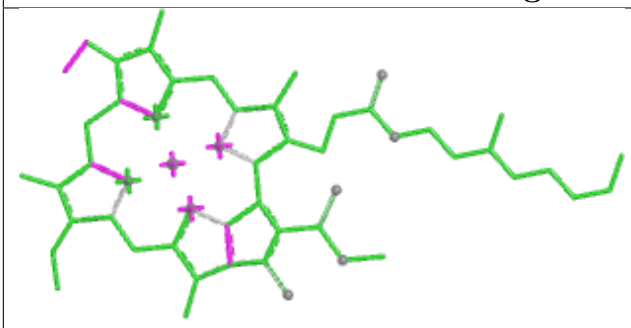


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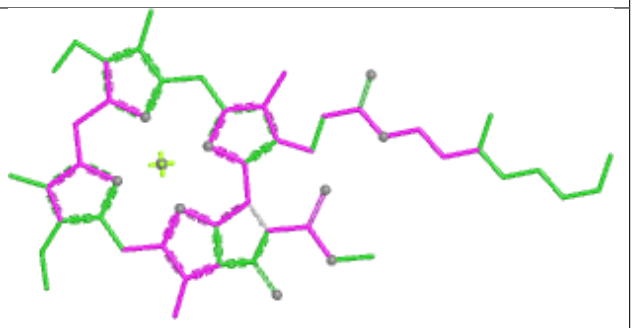


Rings

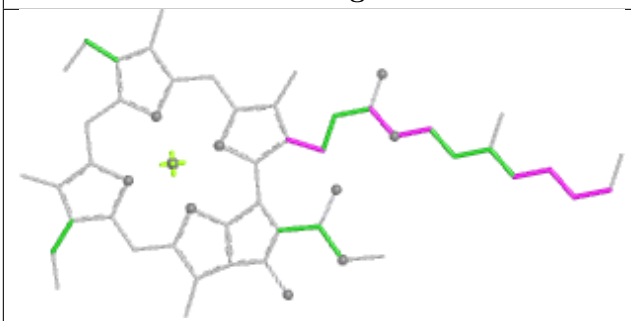
Ligand CLA Y 314



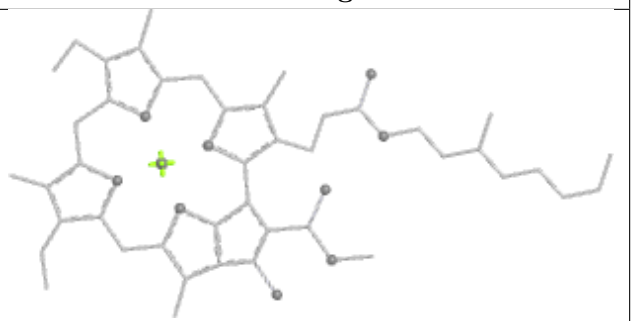
Bond lengths



Bond angles

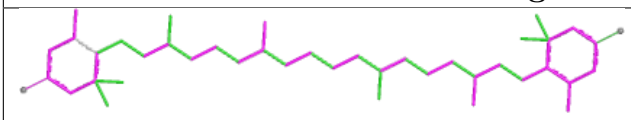


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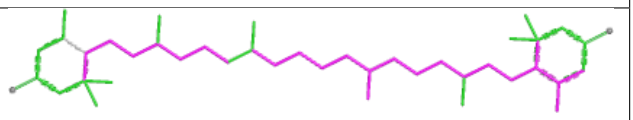


Rings

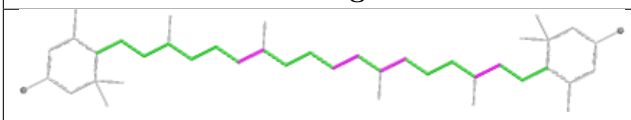
Ligand LUT 7 318



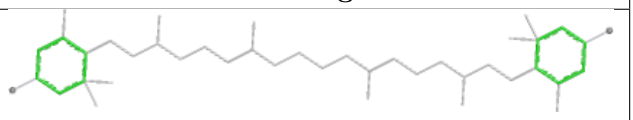
Bond lengths



Bond angles

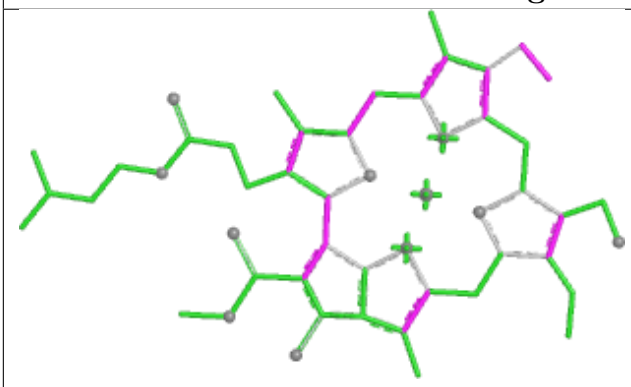


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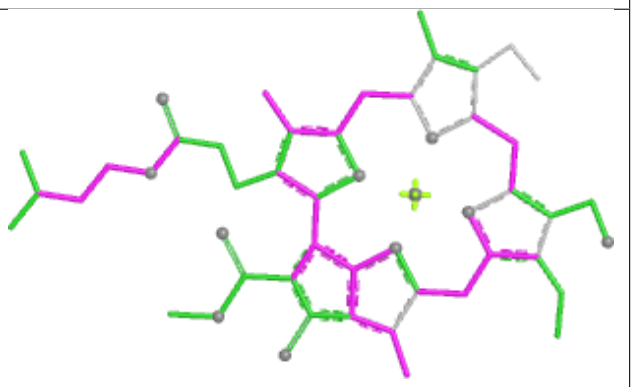


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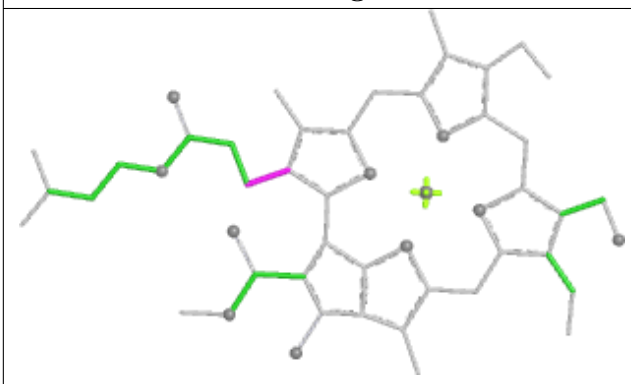
Ligand CHL 0 606



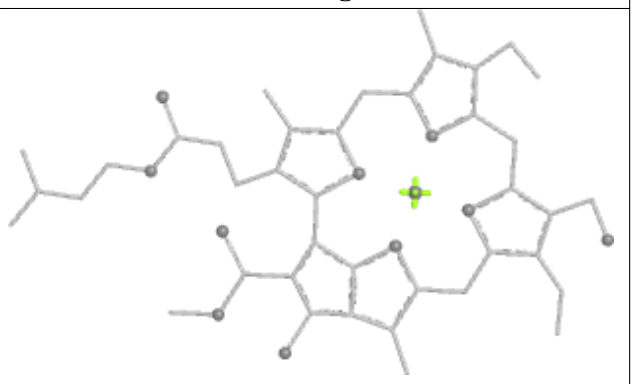
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Bond angles

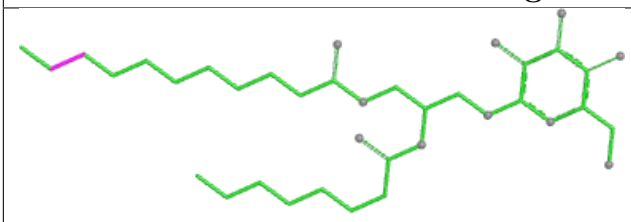


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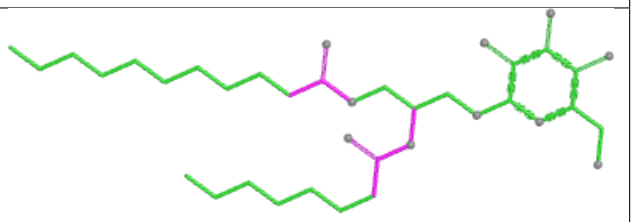


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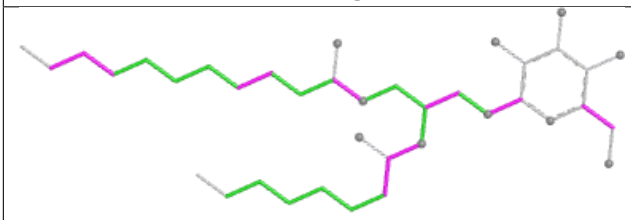
Ligand LMG c 620



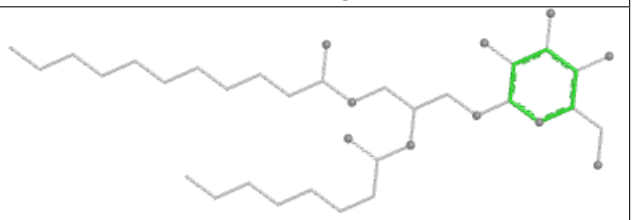
Bond lengths



Bond angles

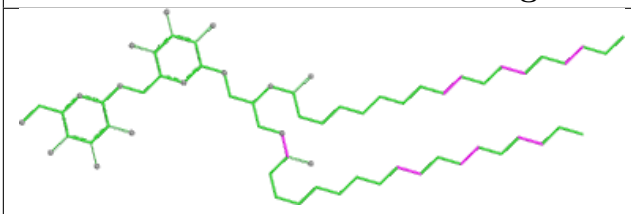


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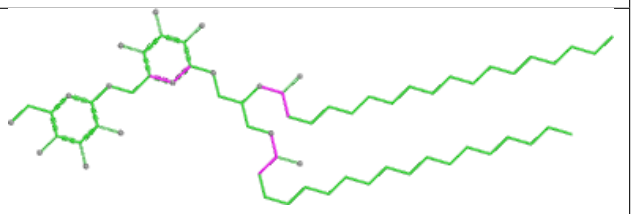


Rings

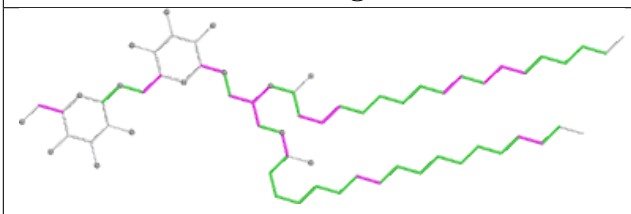
Ligand DGD C 618



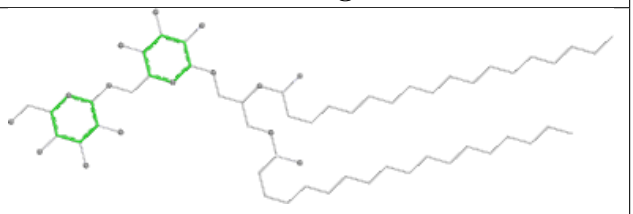
Bond lengths



Bond angles

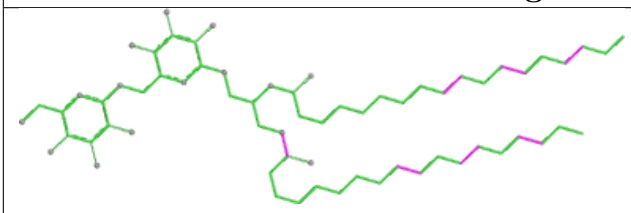


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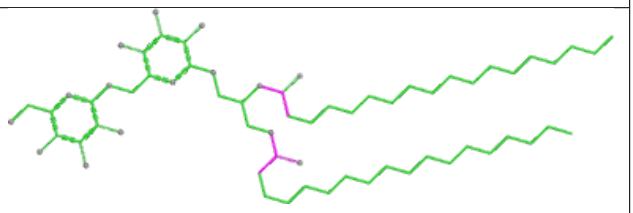


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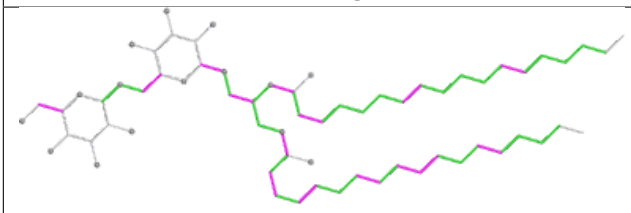
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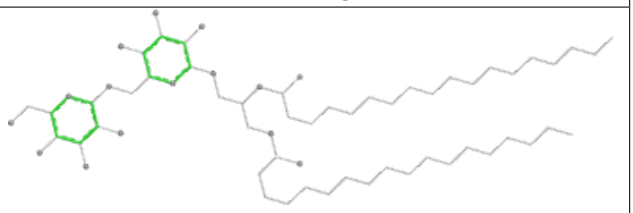
Bond lengths



Bond angles

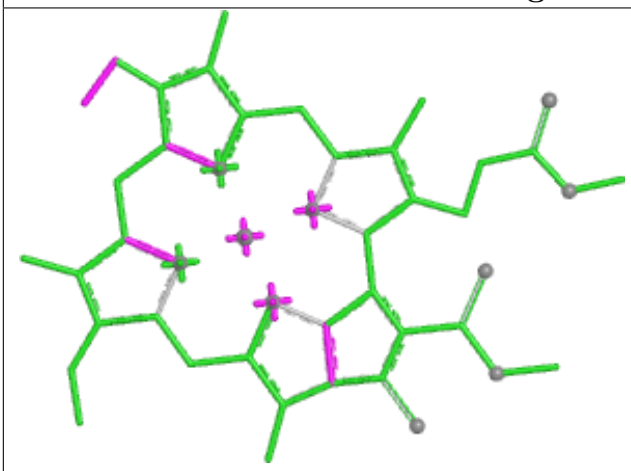


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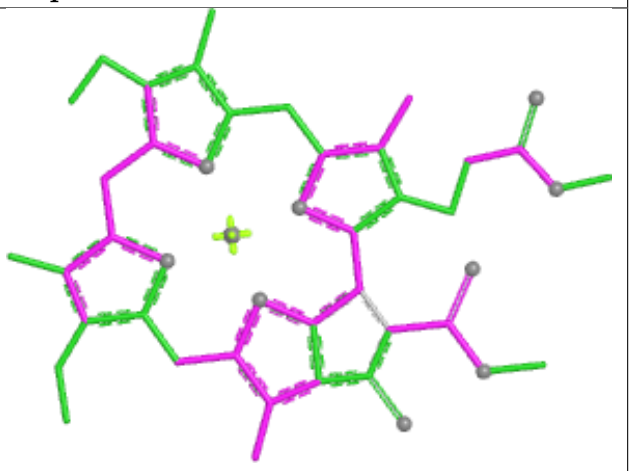


Rings

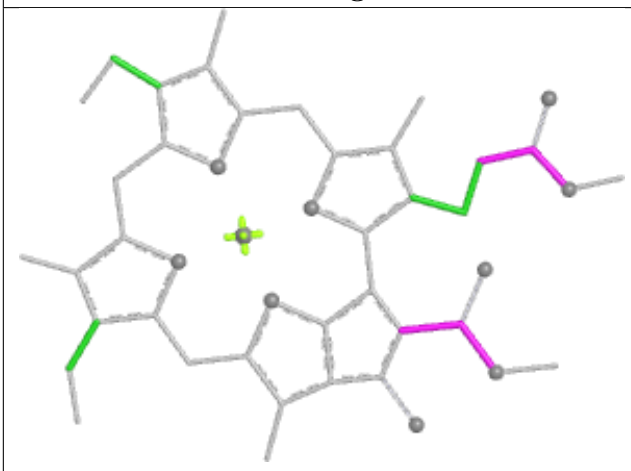
Ligand CLA p 612



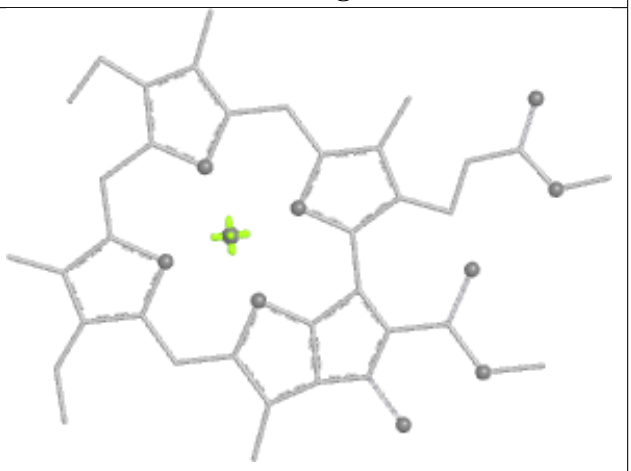
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Bond angles

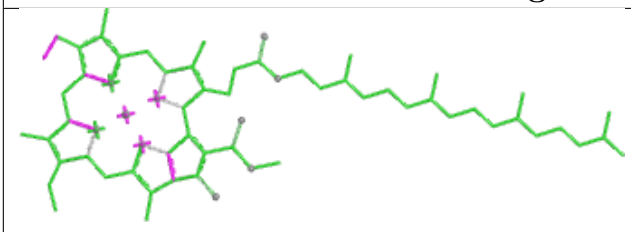


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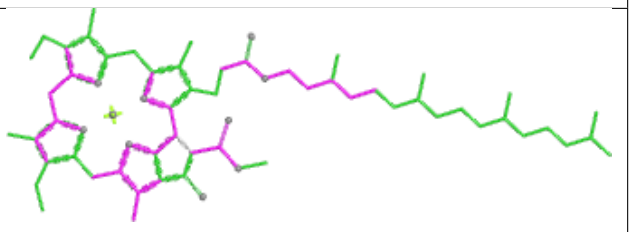


Rings

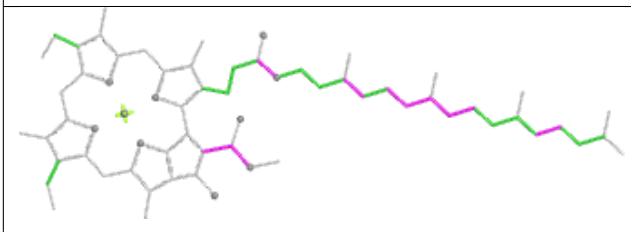
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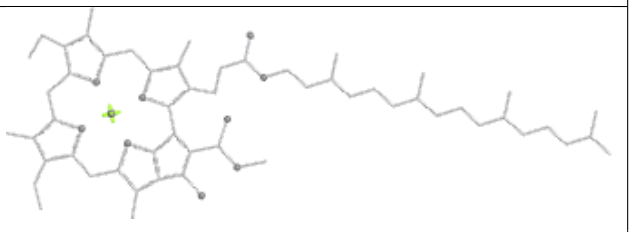
Bond lengths



Bond angles

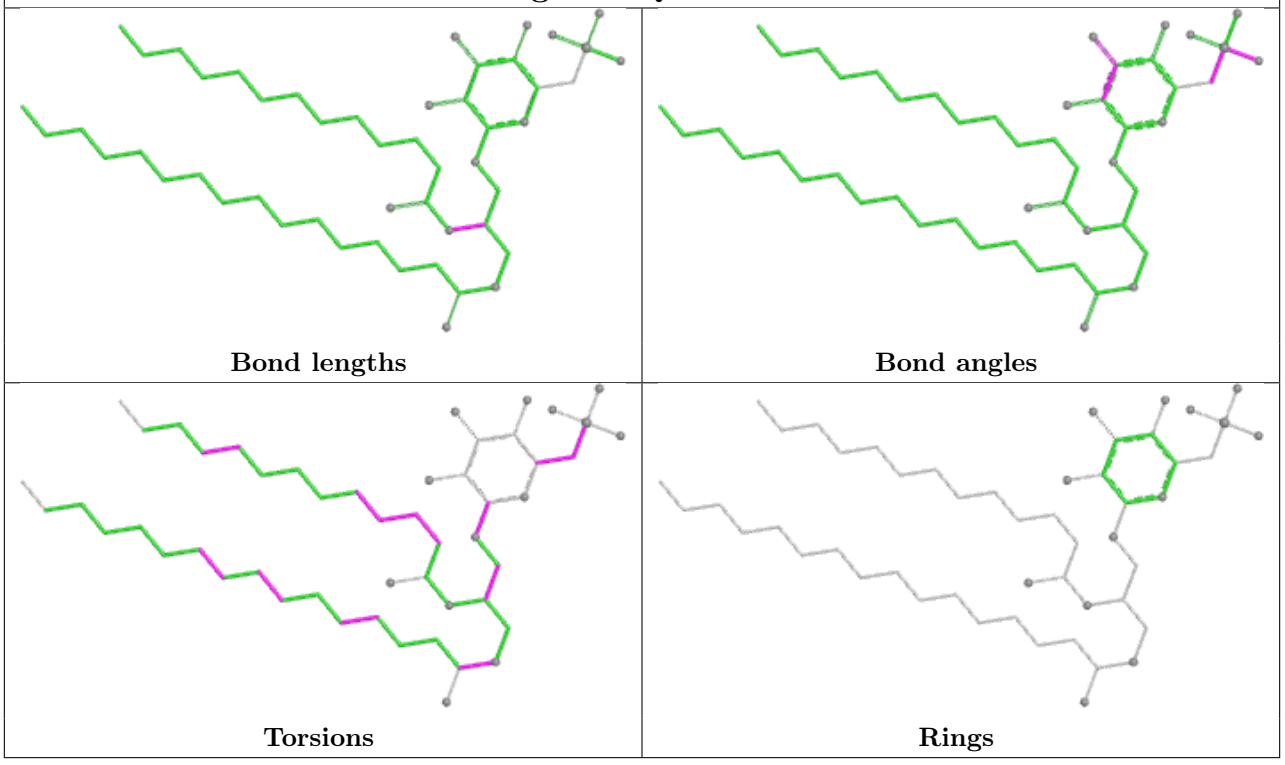


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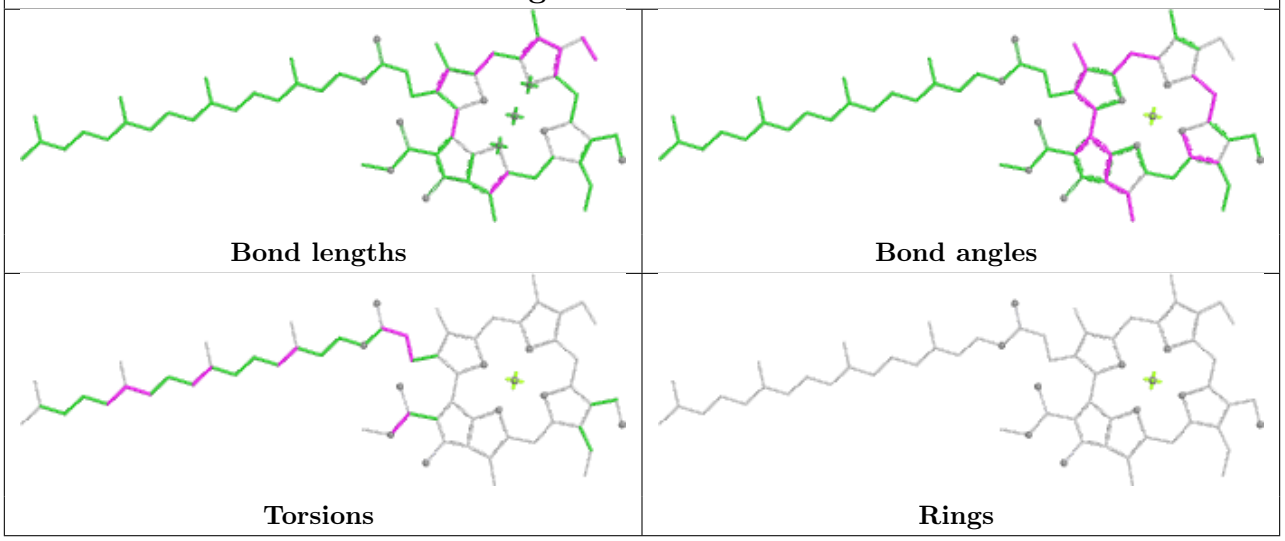


Rings

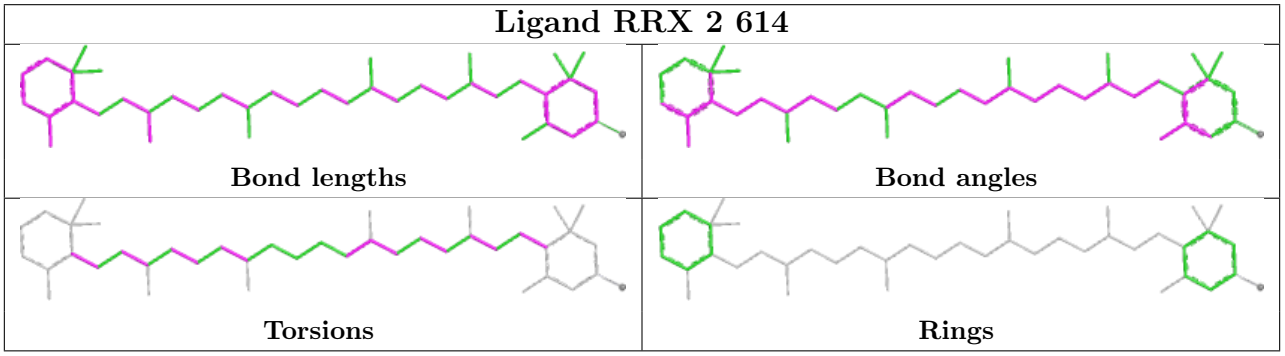
Ligand SQD s 301



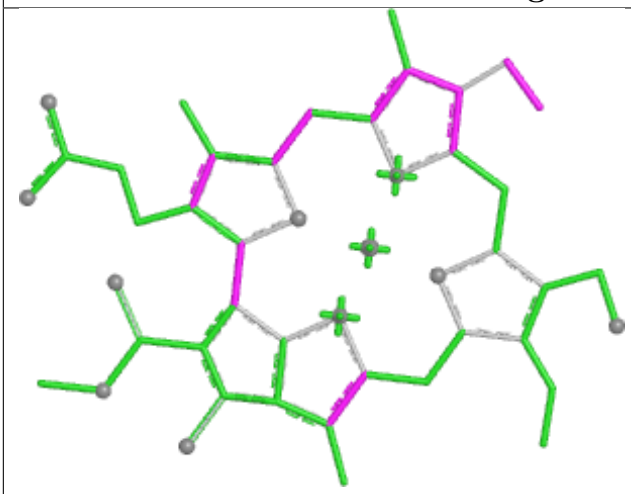
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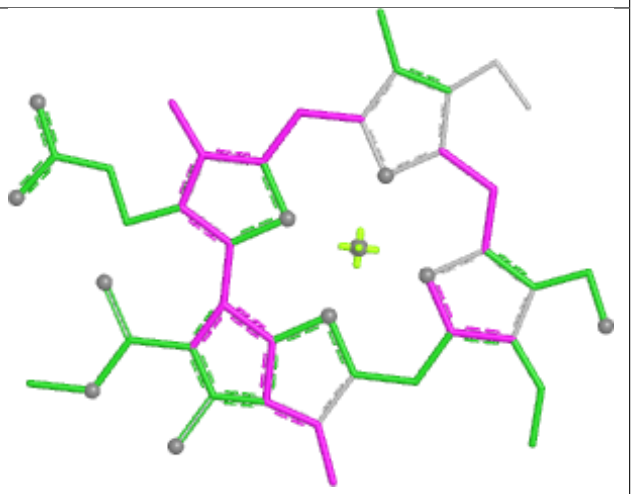
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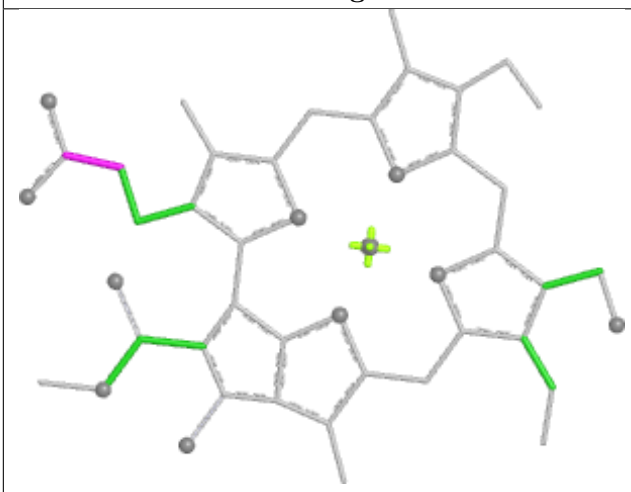
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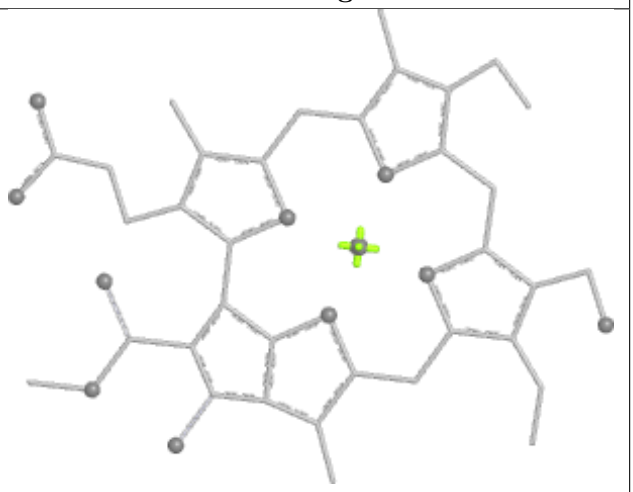
Bond lengths



Bond angles

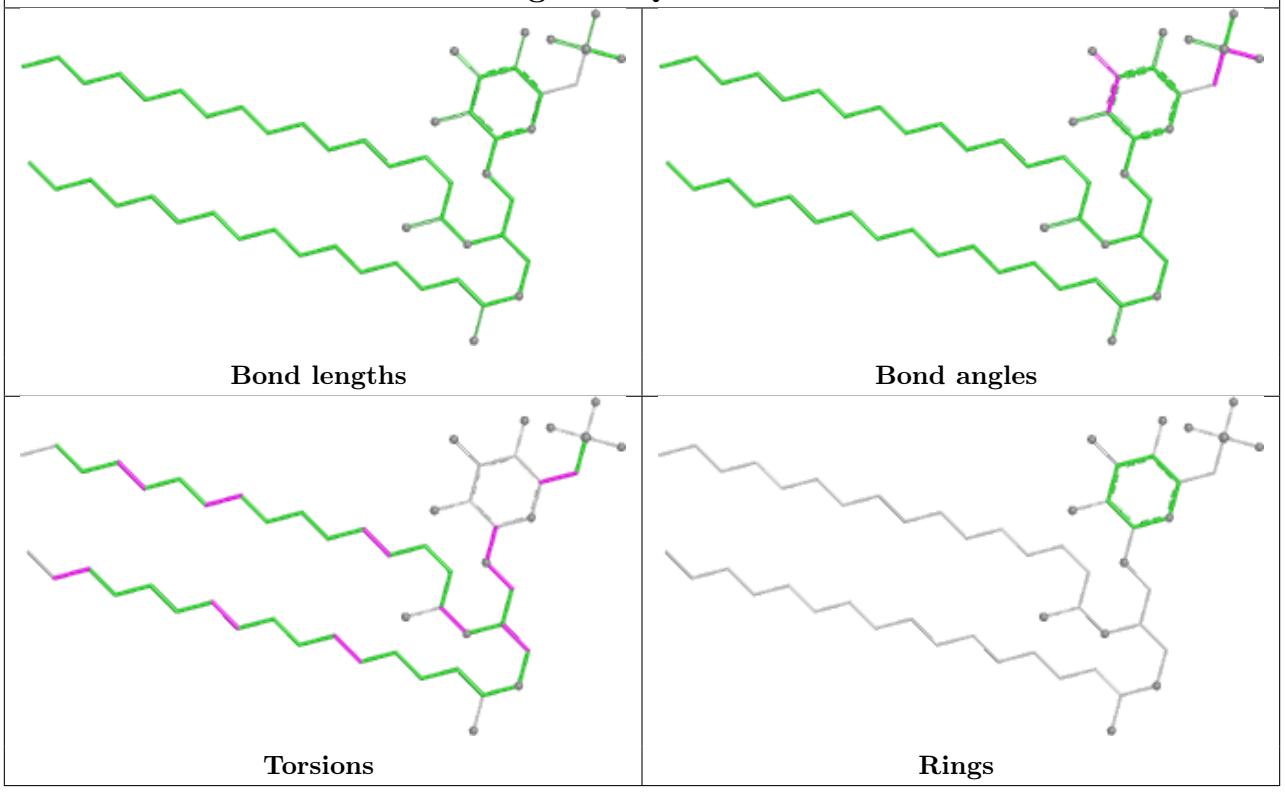


Torsions

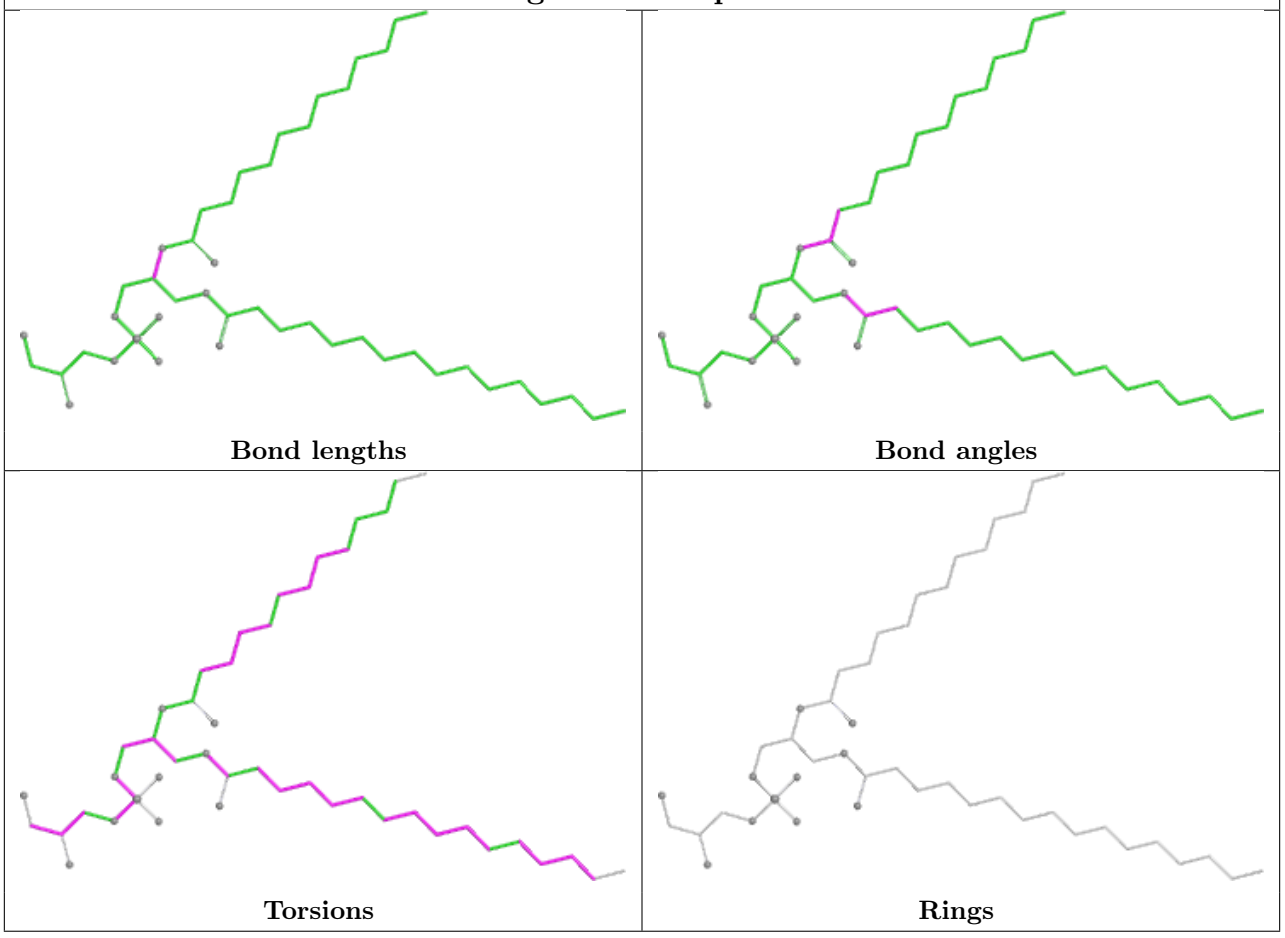


Rings

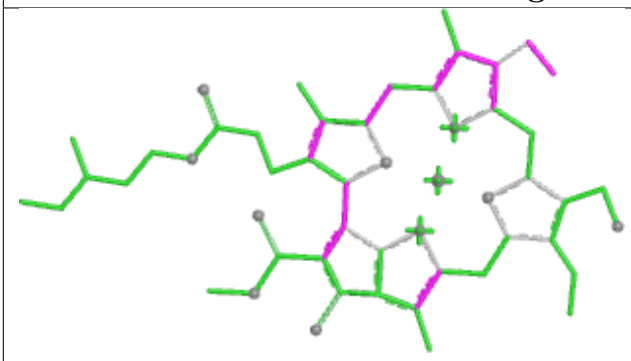
Ligand SQD b 621



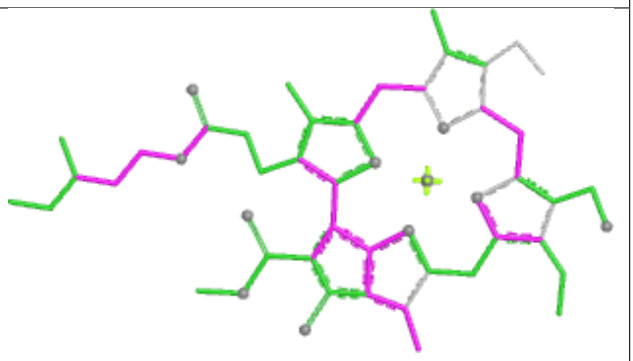
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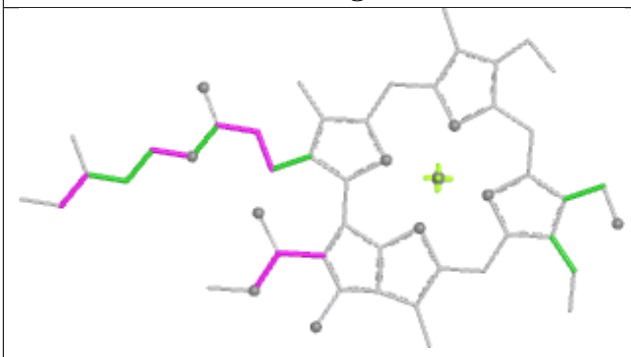
Ligand CHL 0 605



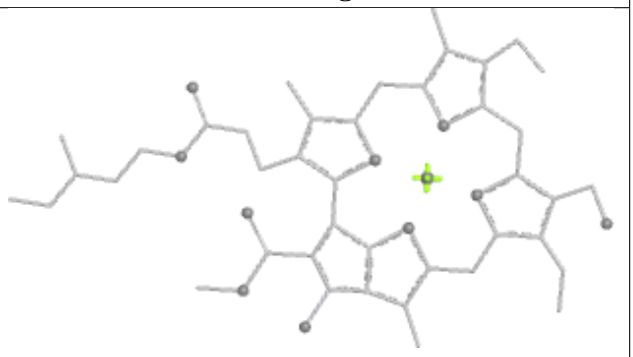
Bond lengths



Bond angles

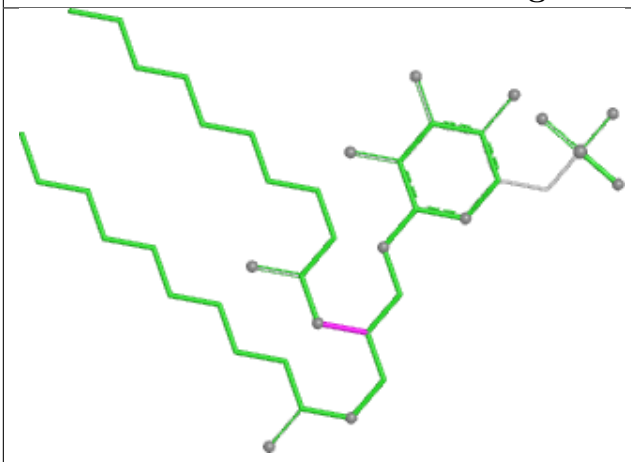


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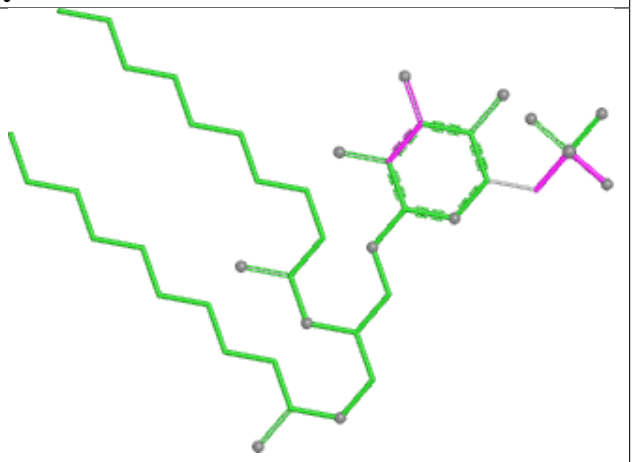


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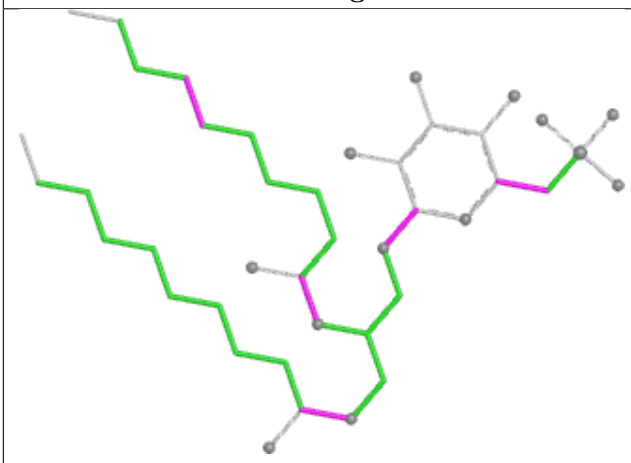
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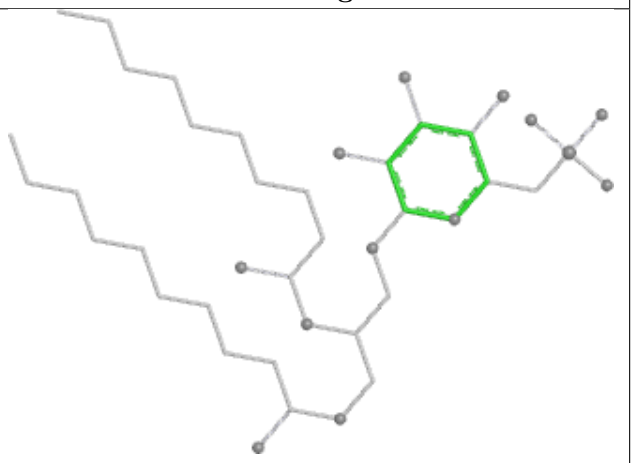
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Bond angles

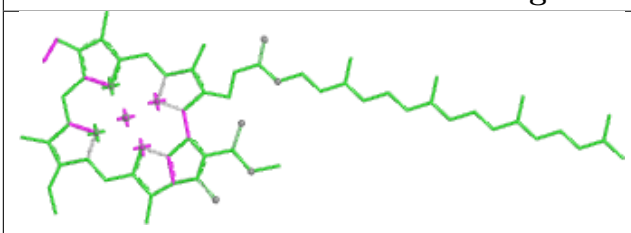


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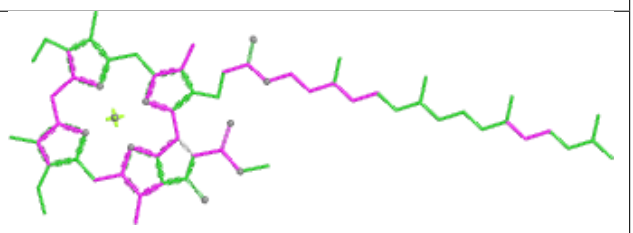


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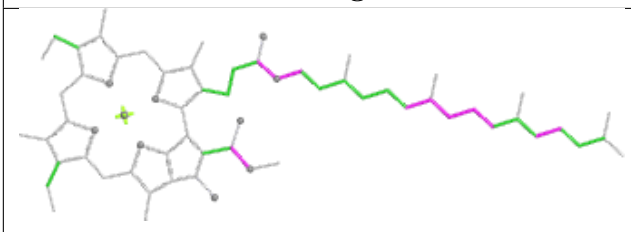
Ligand CLA c 609



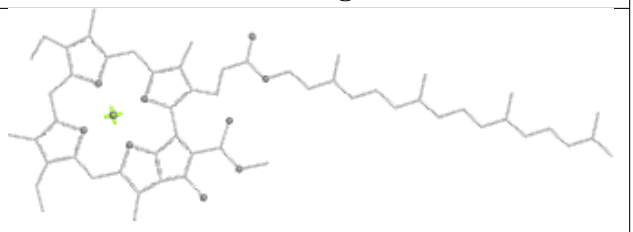
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Bond angles

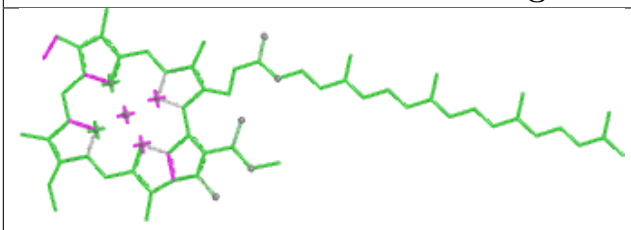


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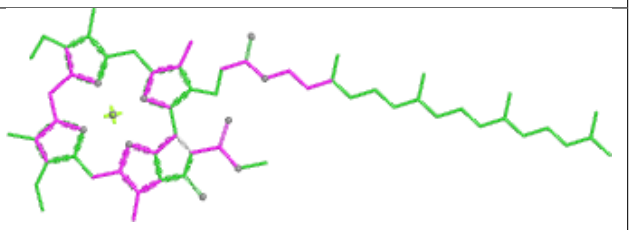


Rings

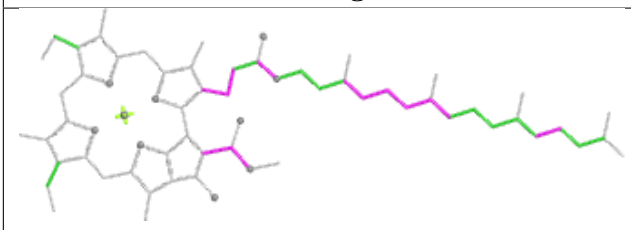
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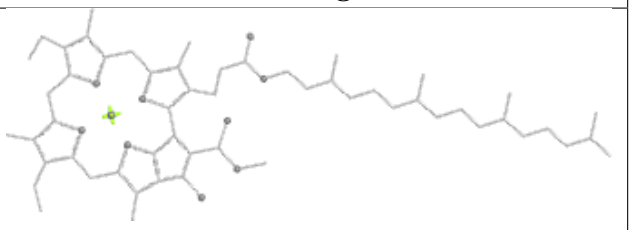
Bond lengths



Bond angles

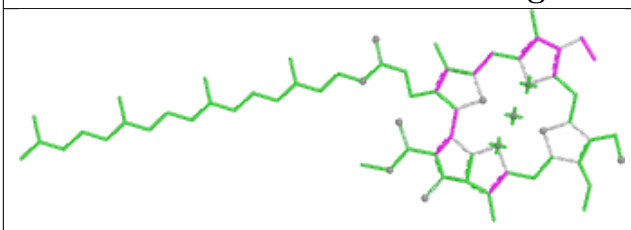


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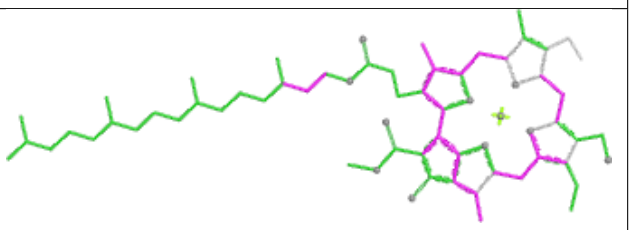


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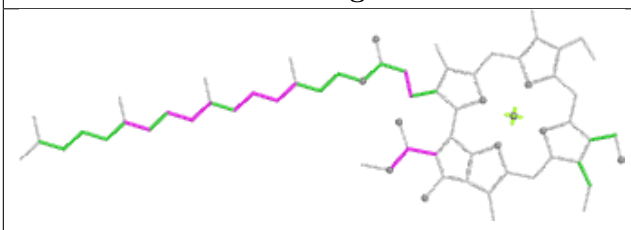
Ligand CHL 1 606



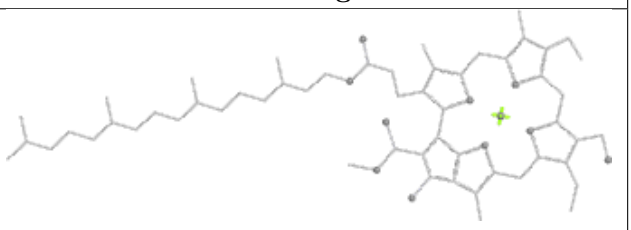
Bond lengths



Bond angles

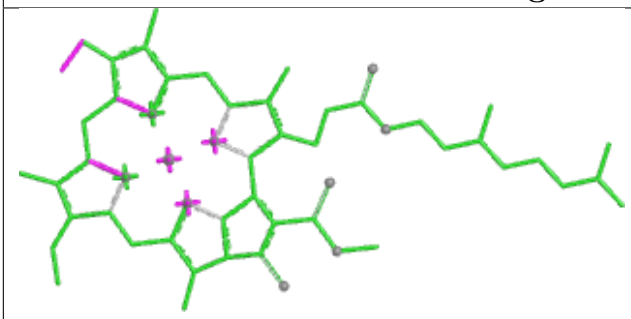


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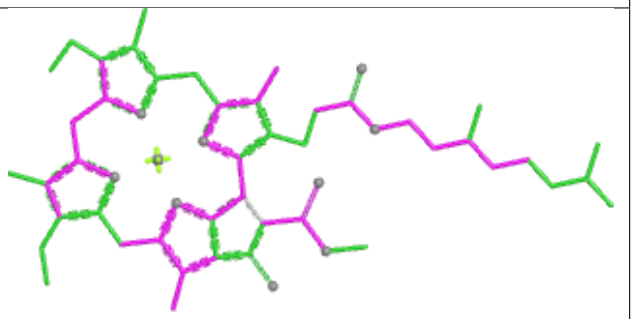


Rings

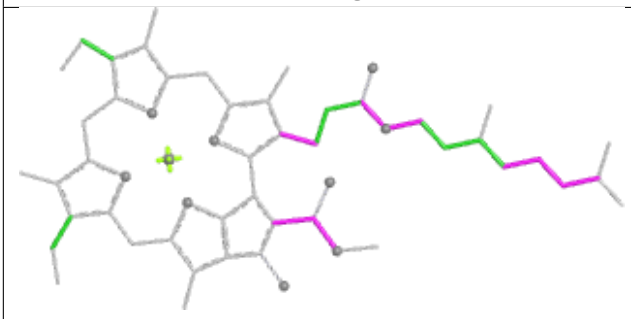
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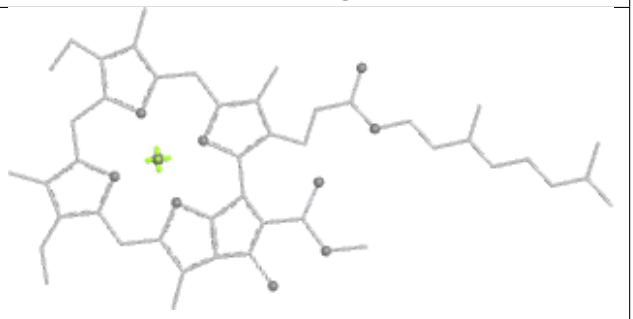
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Bond angles

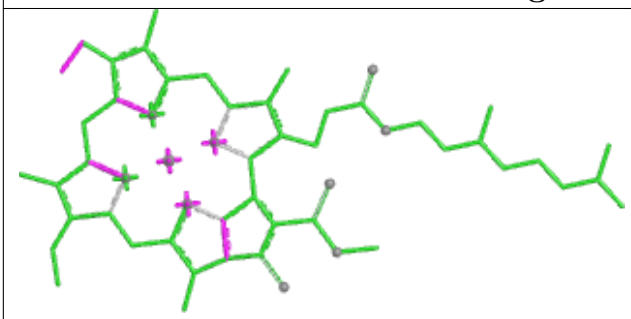


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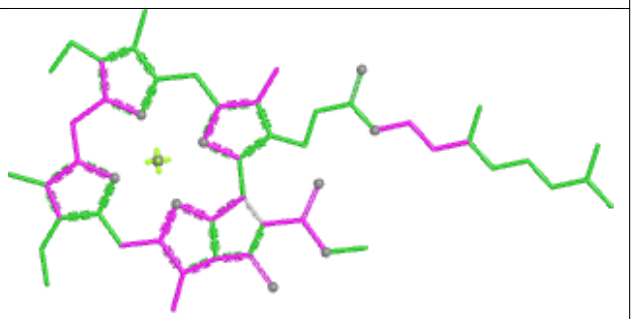


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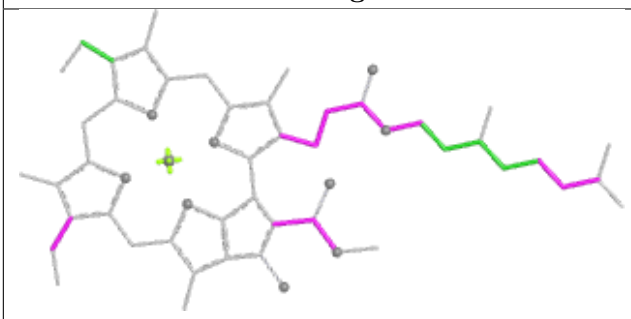
Ligand CLA 3 306



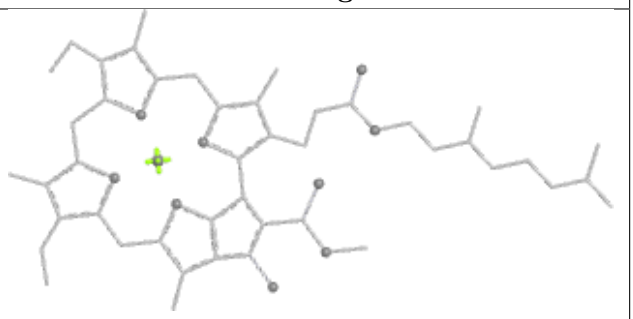
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Bond angles

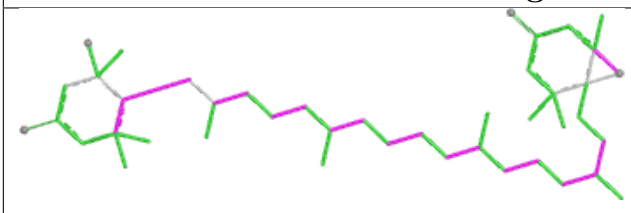


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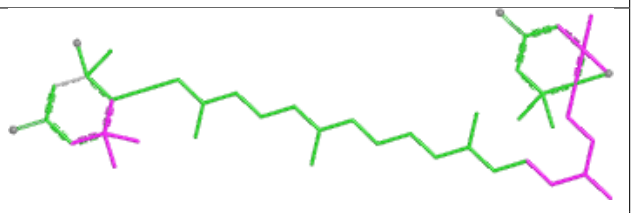


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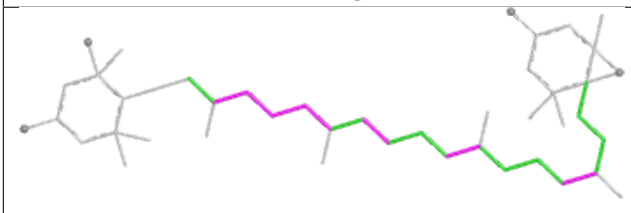
Ligand NEX 8 617



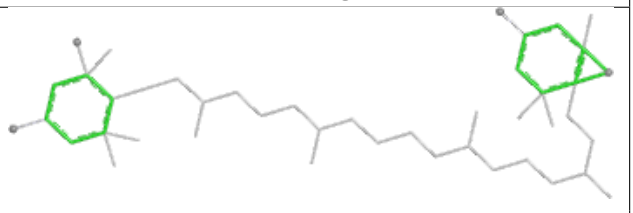
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Bond angles

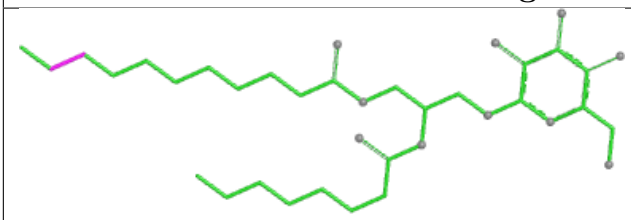


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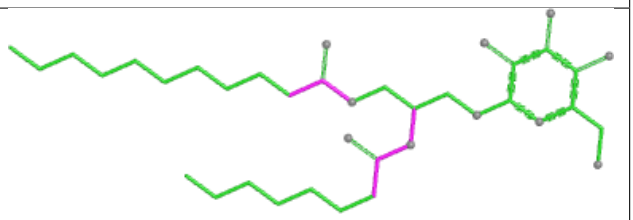


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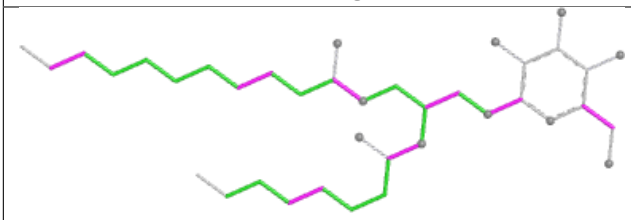
Ligand LMG A 418



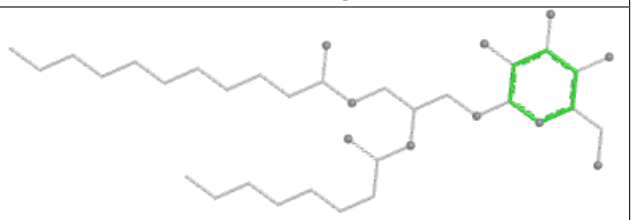
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Bond angles

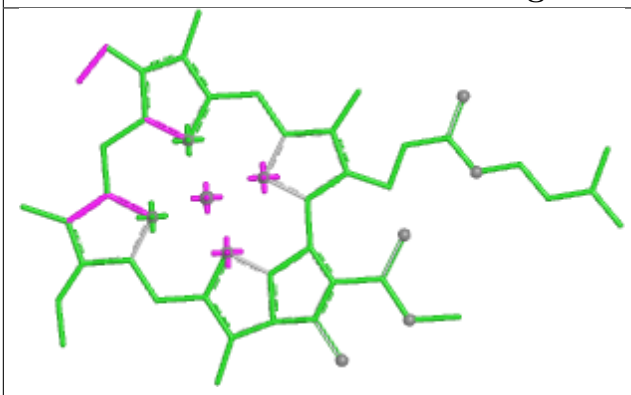


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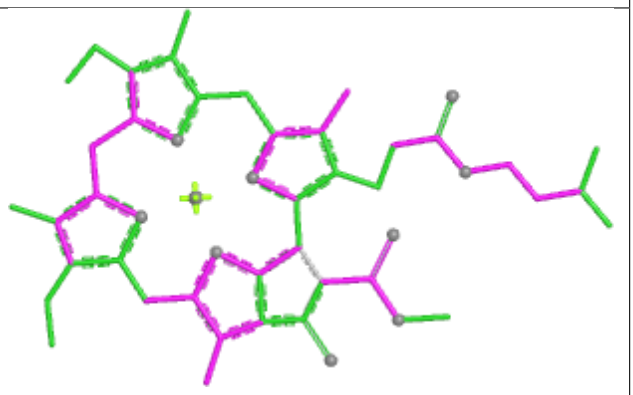


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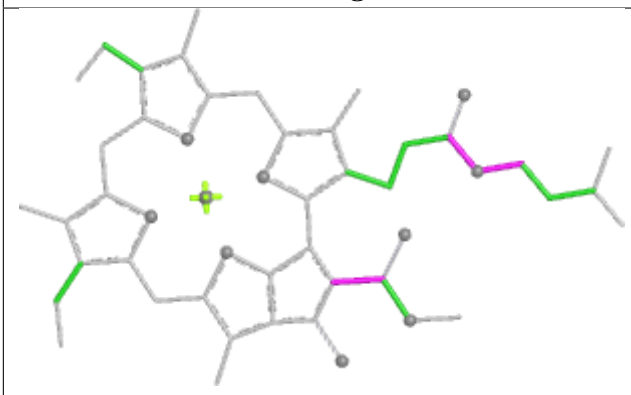
Ligand CLA S 306



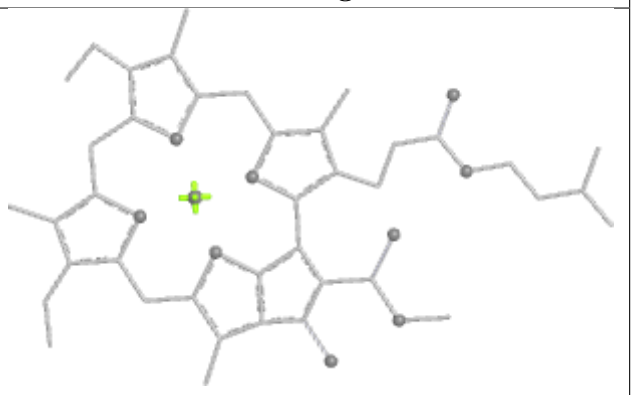
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Bond angles

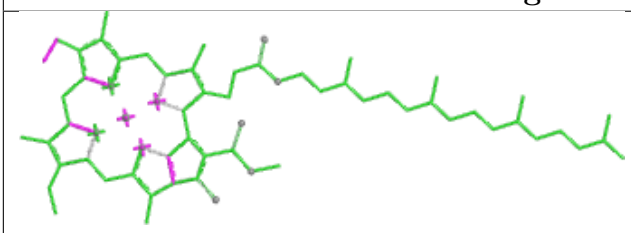


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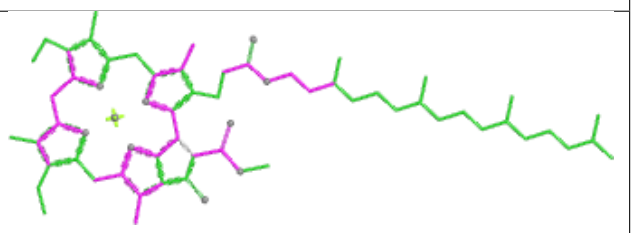


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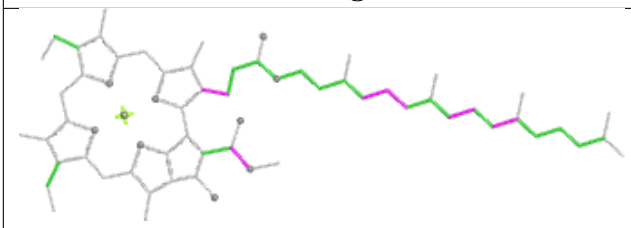
Ligand CLA Y 310



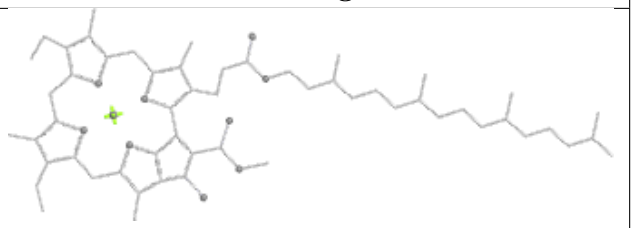
Bond lengths



Bond angles

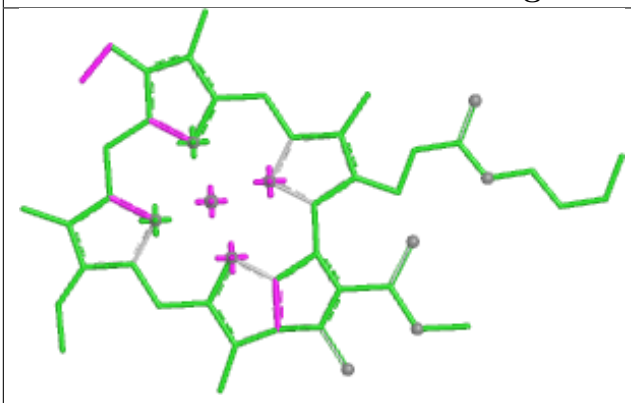


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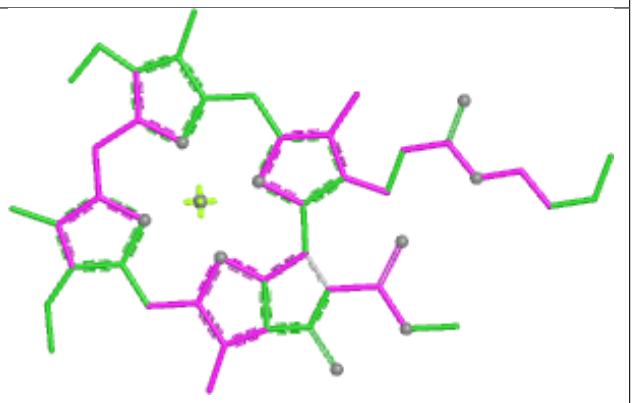


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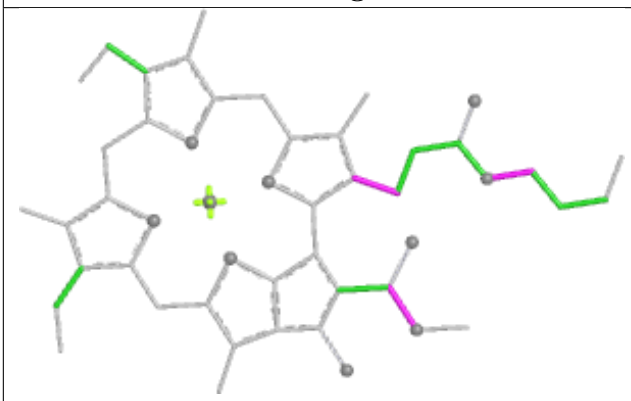
Ligand CLA A 407



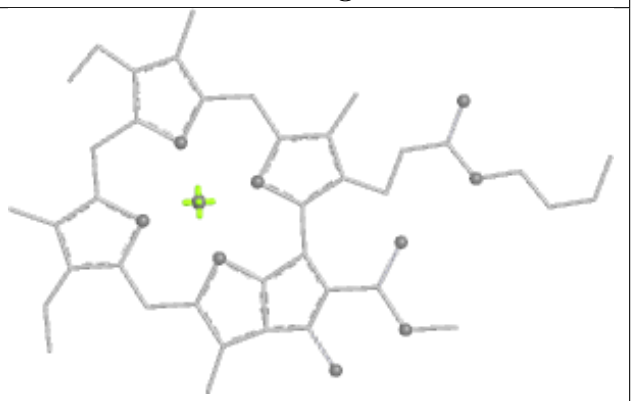
Bond lengths



Bond angles

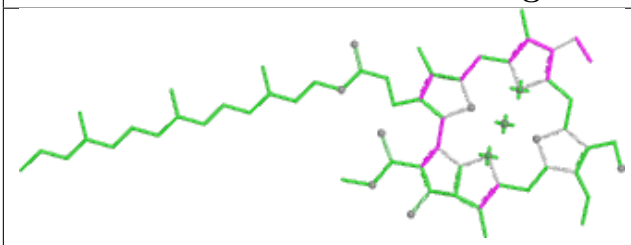


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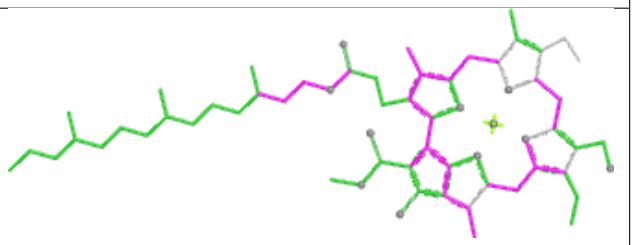


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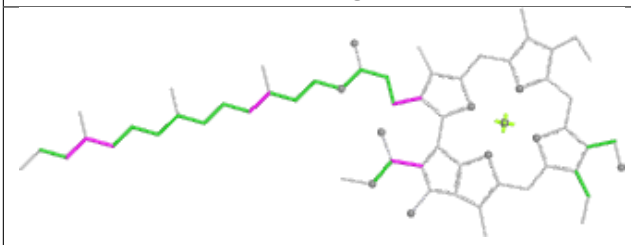
Ligand CHL G 608



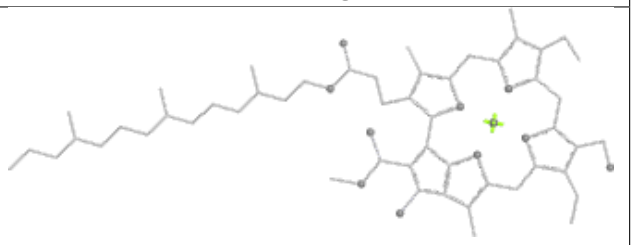
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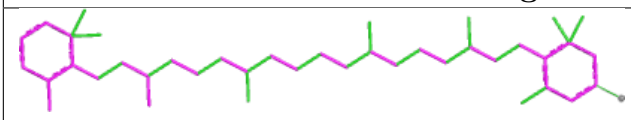
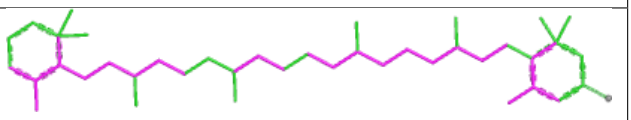
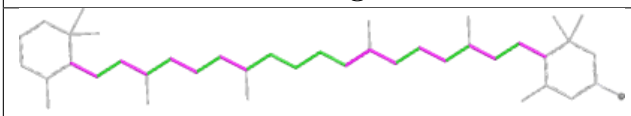
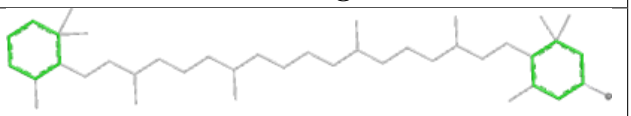
Bond angles

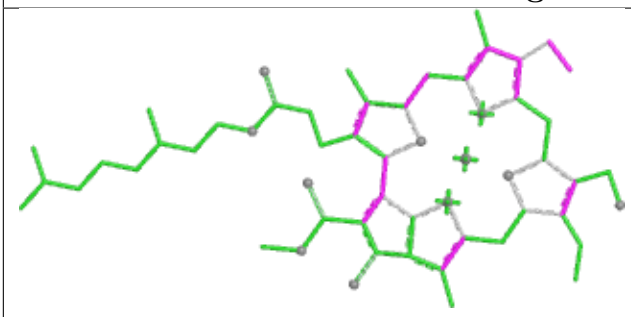
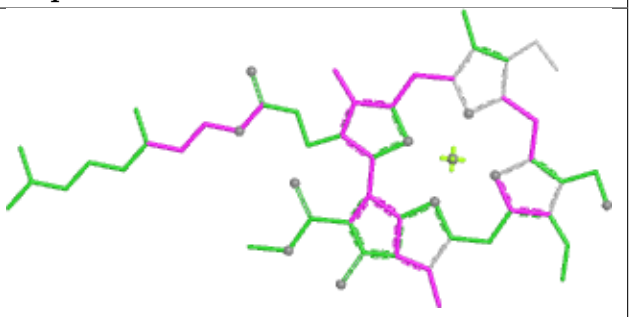
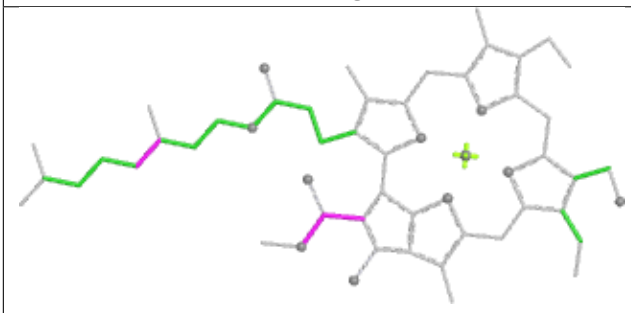
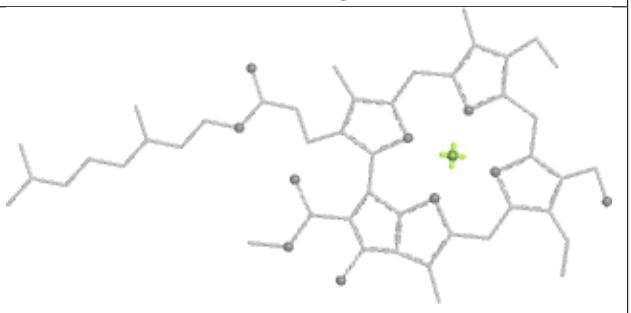


Torsions

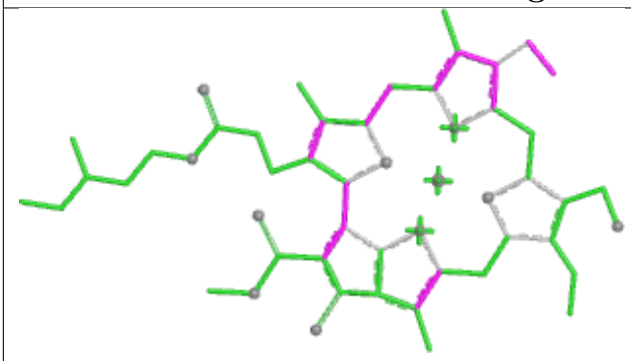


Rings

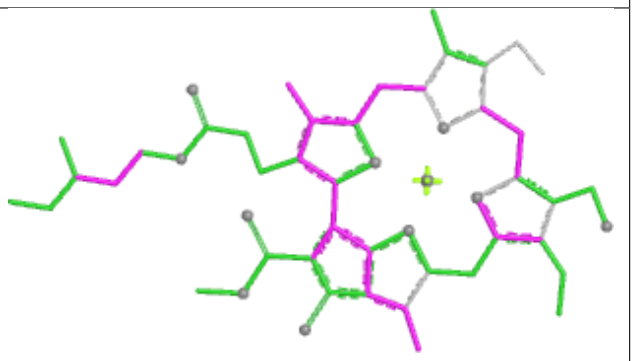
Ligand RRX G 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL p 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

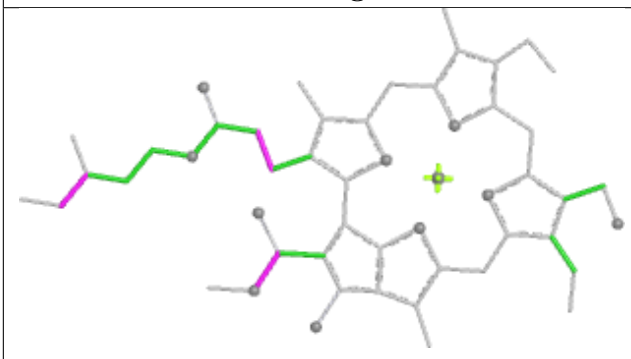
Ligand CHL 9 308



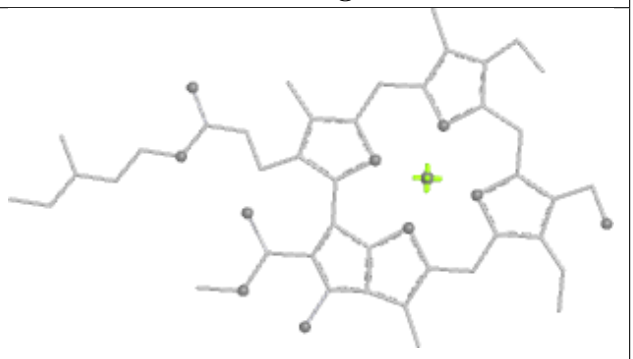
Bond lengths



Bond angles

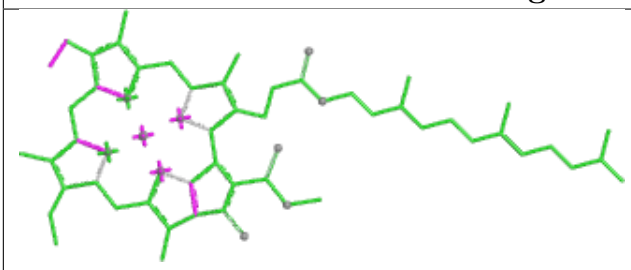


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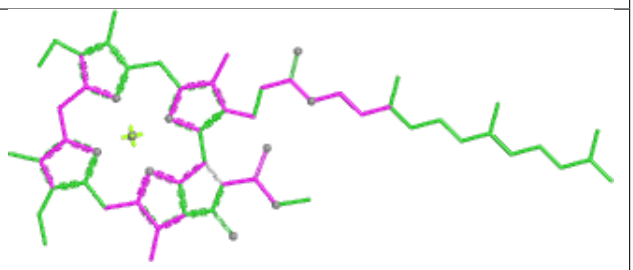


Rings

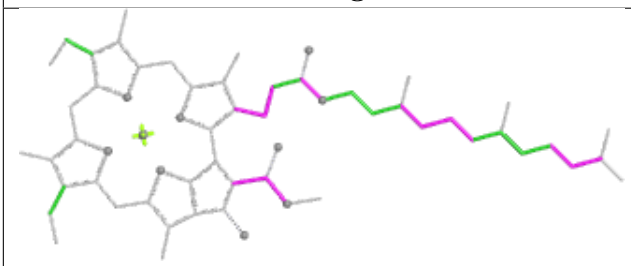
Ligand CLA 1 602



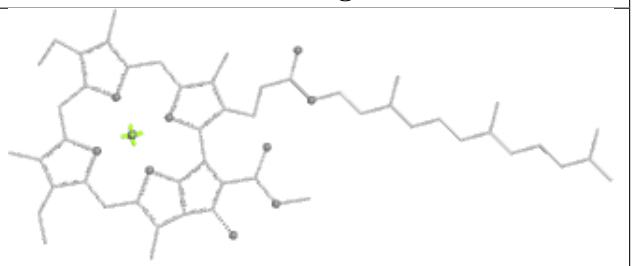
Bond lengths



Bond angles

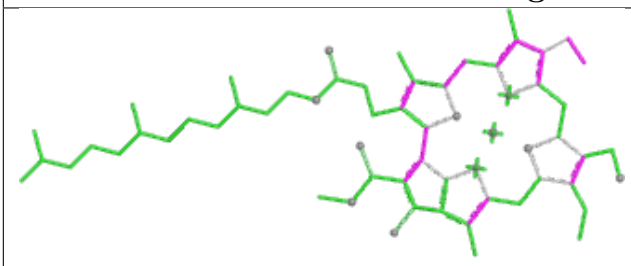


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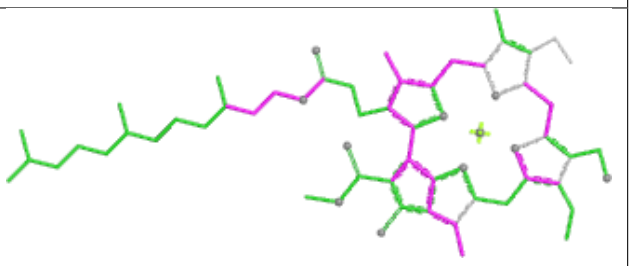


Rings

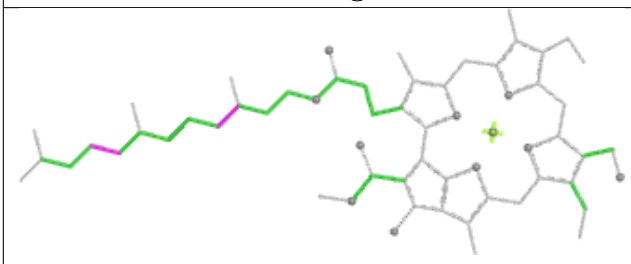
Ligand CHL 0 609



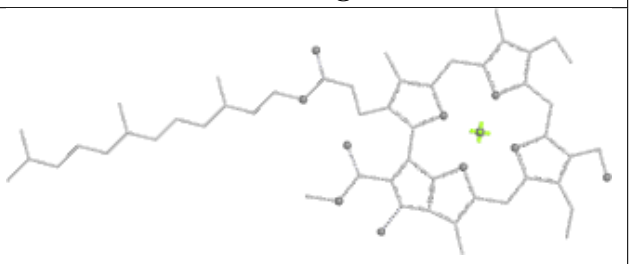
Bond lengths



Bond angles

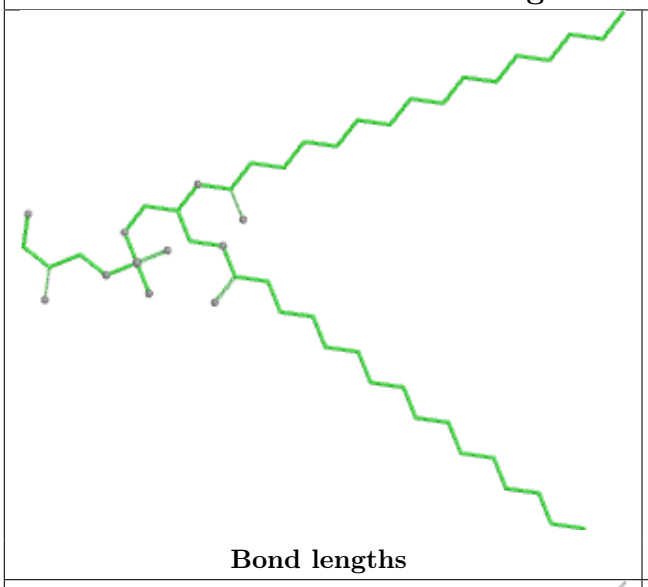


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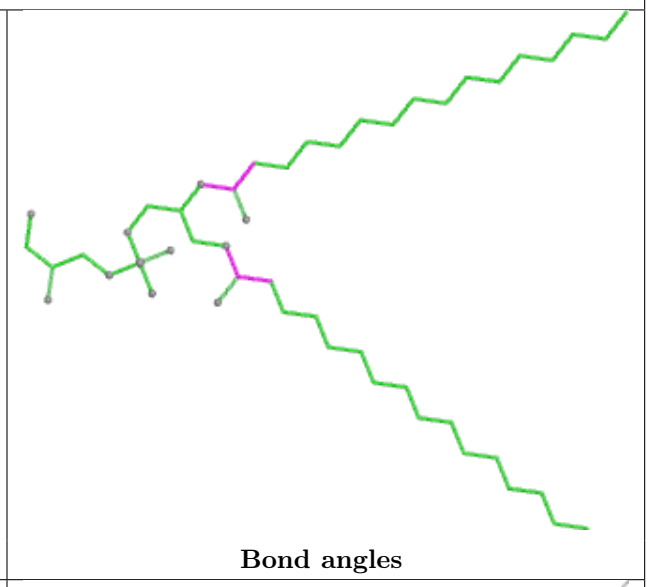


Rings

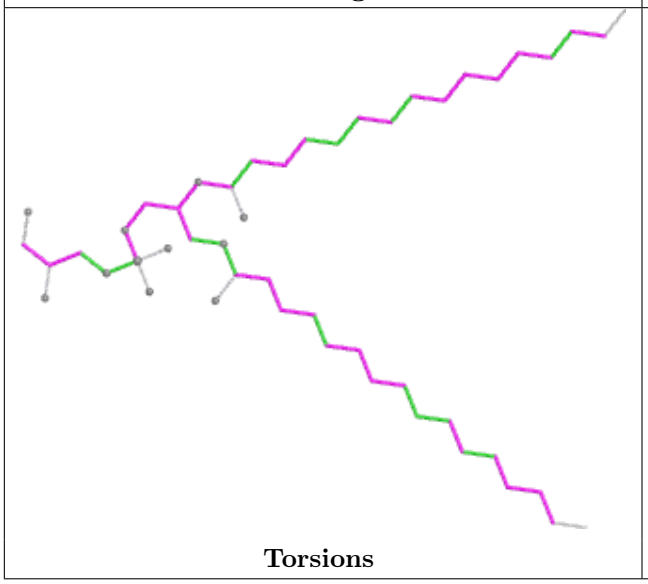
Ligand LHG n 320



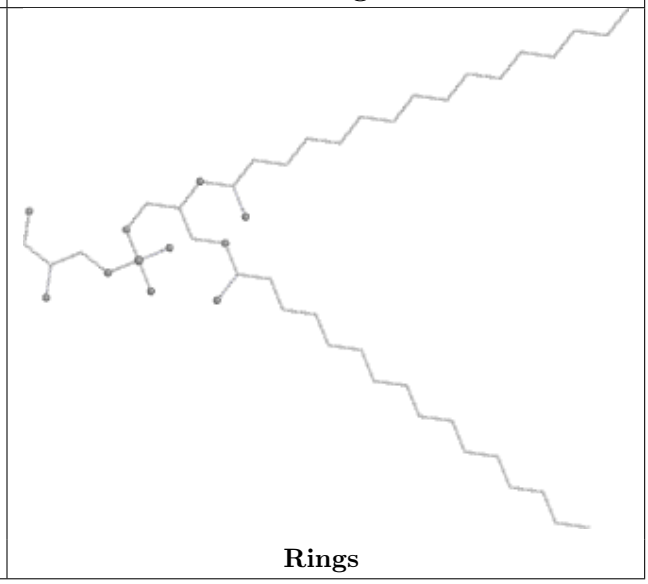
Bond lengths



Bond angles

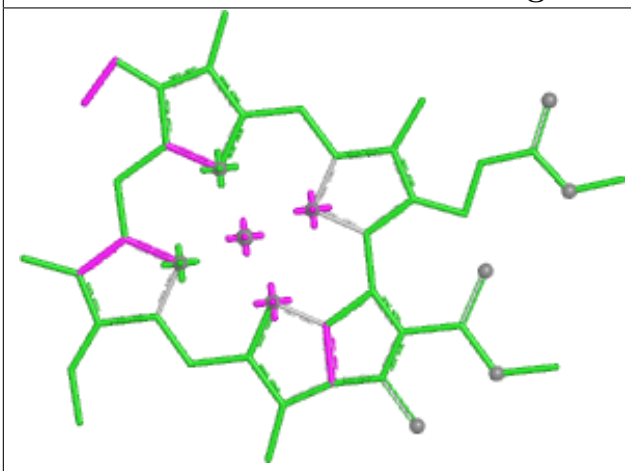


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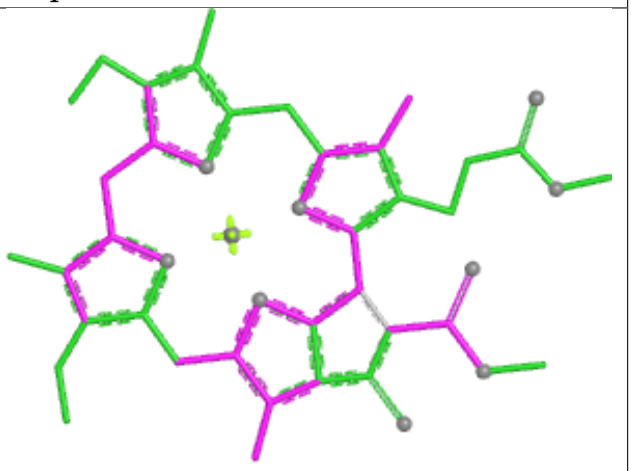


Rings

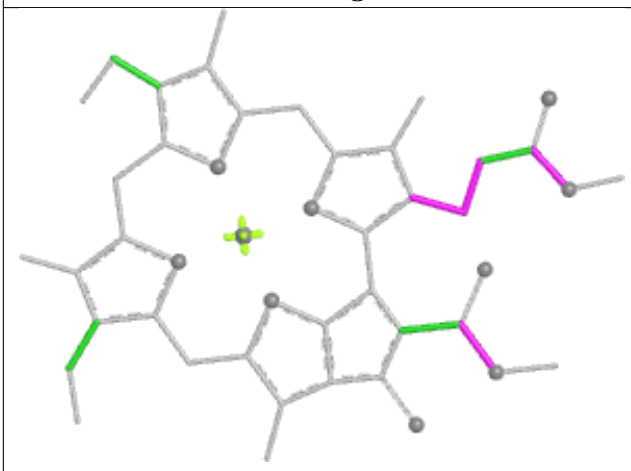
Ligand CLA p 615



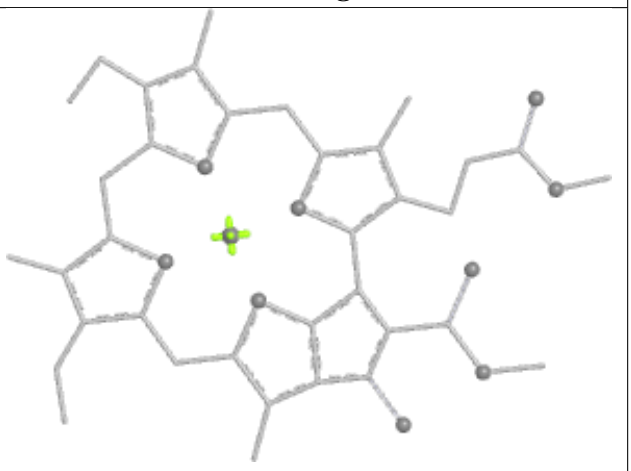
Bond lengths



Bond angles

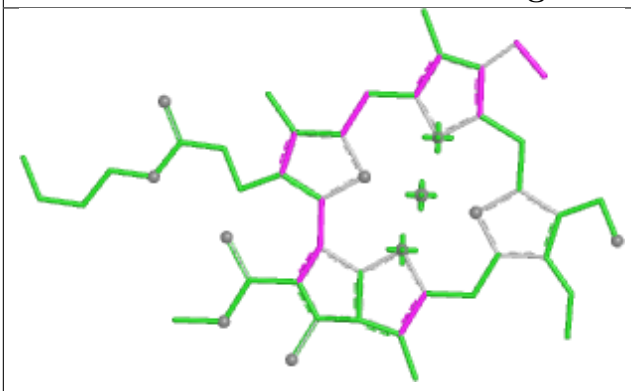


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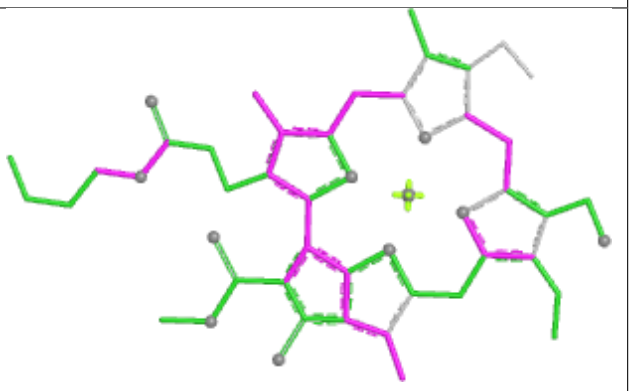


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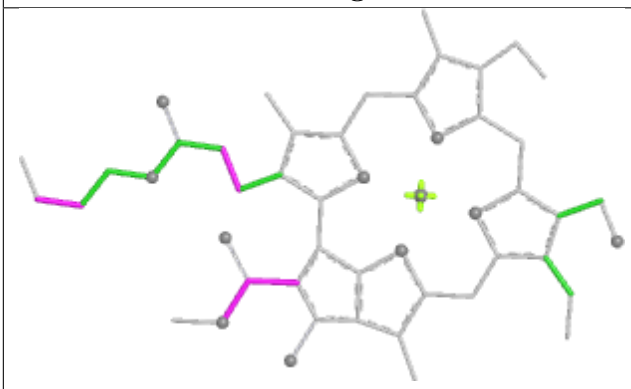
Ligand CHL 8 607



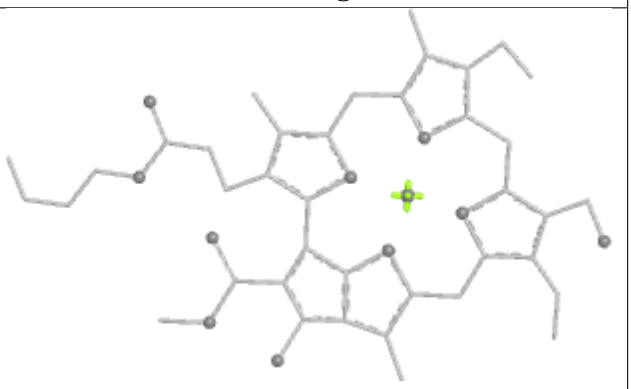
Bond lengths



Bond angles

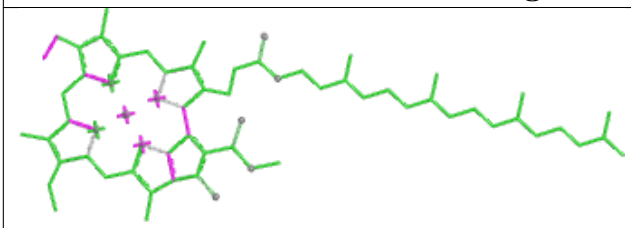


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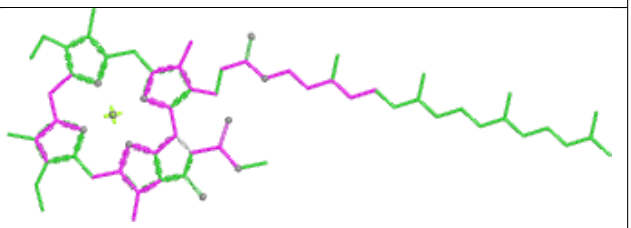


Rings

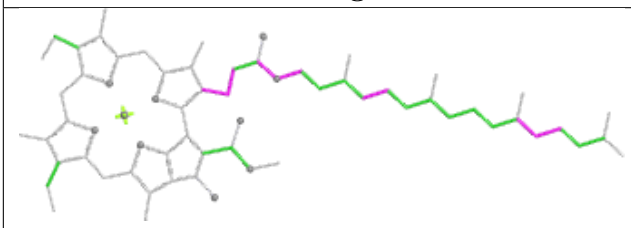
Ligand CLA A 406



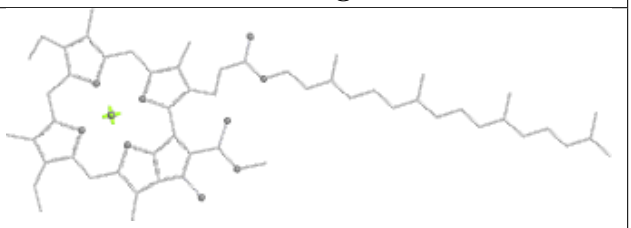
Bond lengths



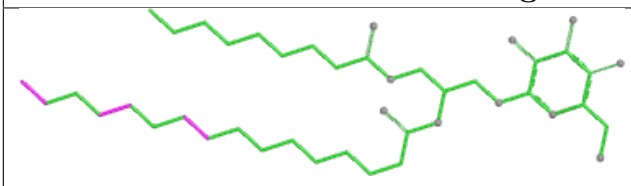
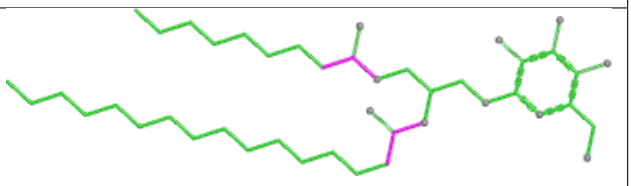
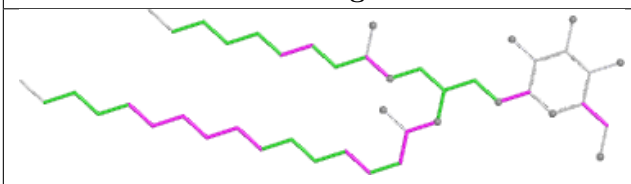
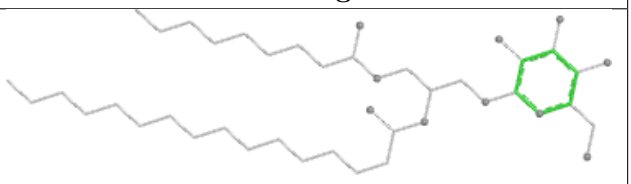
Bond angles

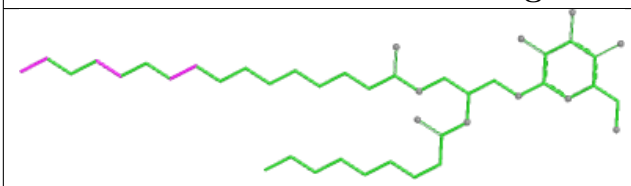
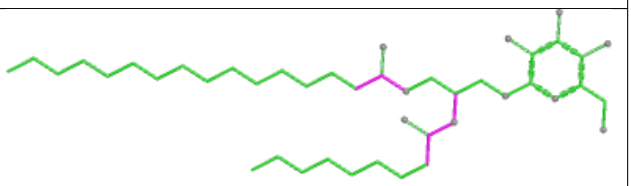
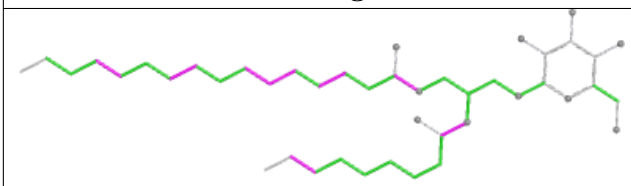
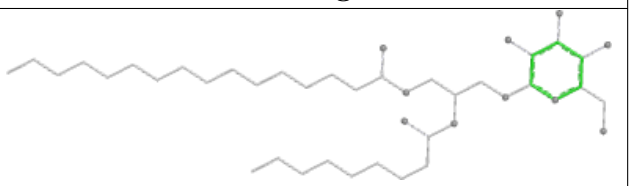


Torsions

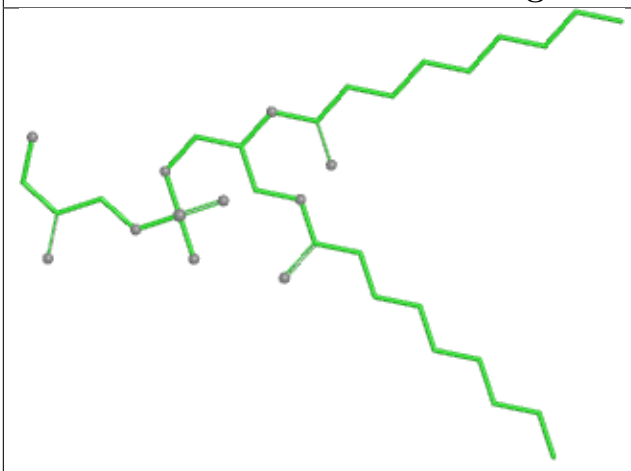


Rings

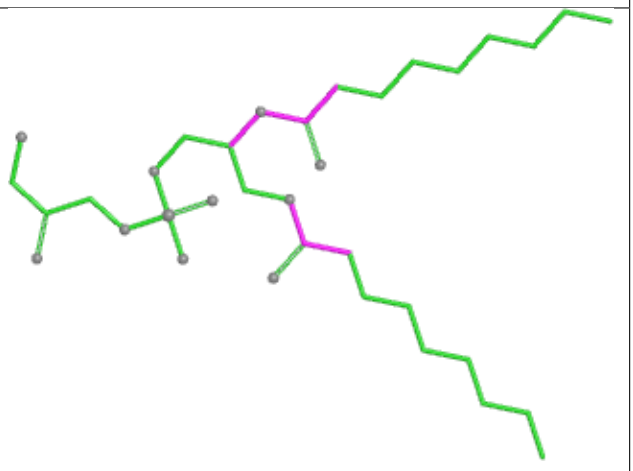
Ligand LMG C 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG c 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

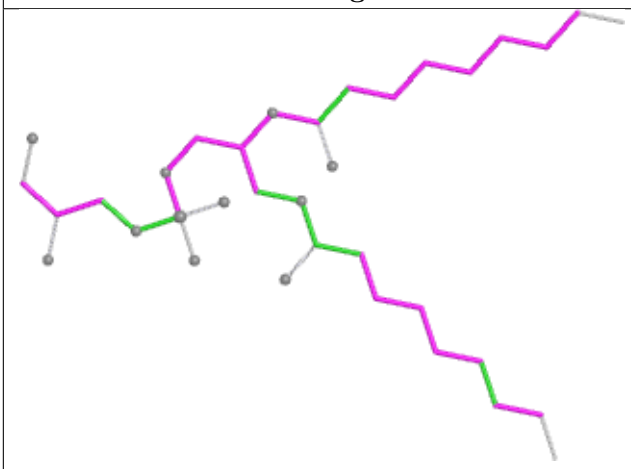
Ligand LHG 7 319



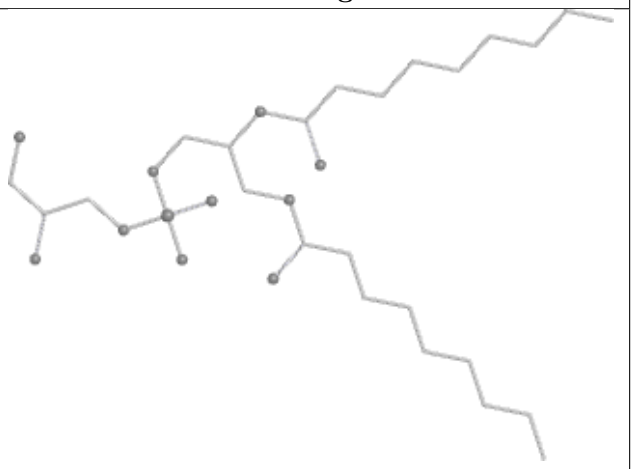
Bond lengths



Bond angles

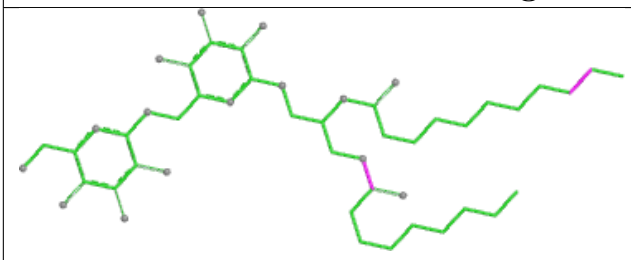


Torsions

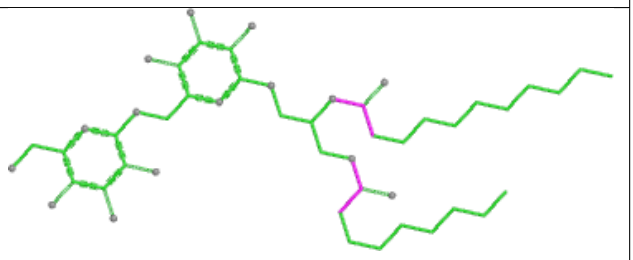


Rings

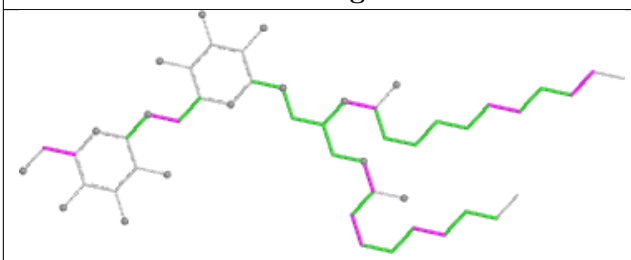
Ligand DGD C 616



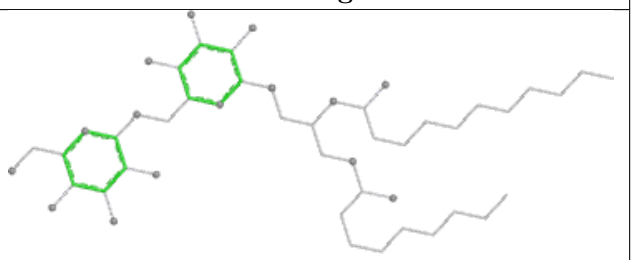
Bond lengths



Bond angles

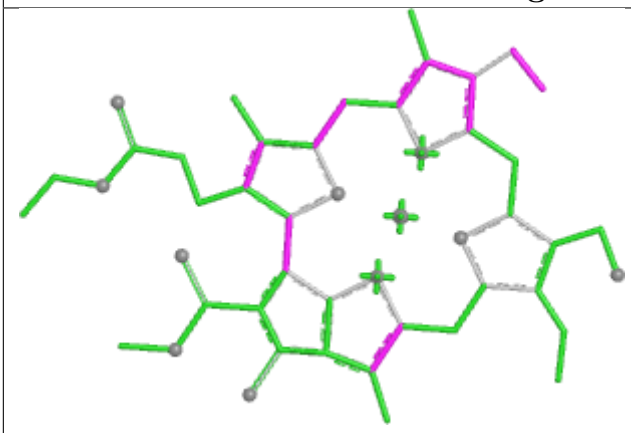


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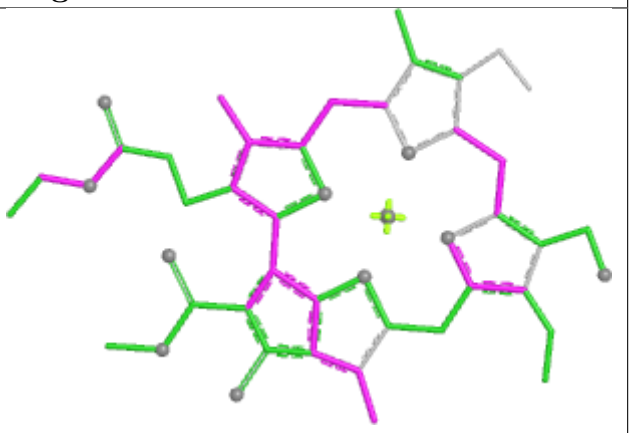


Rings

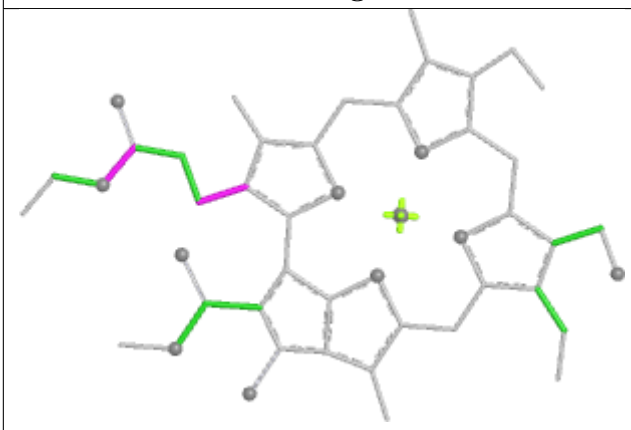
Ligand CHL g 306



Bond lengths



Bond angles

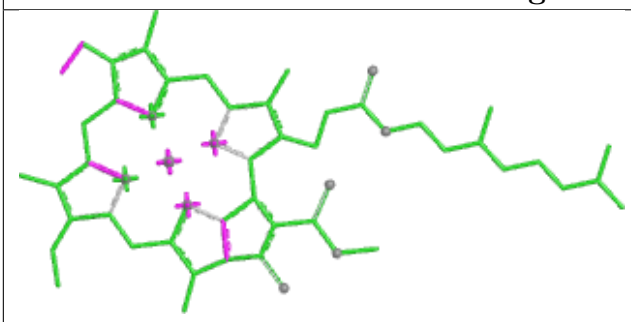


Torsions

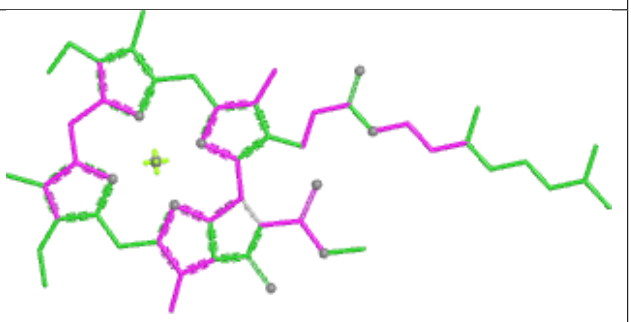


Rings

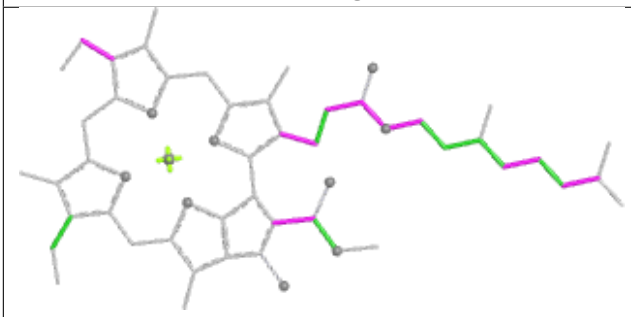
Ligand CLA 0 615



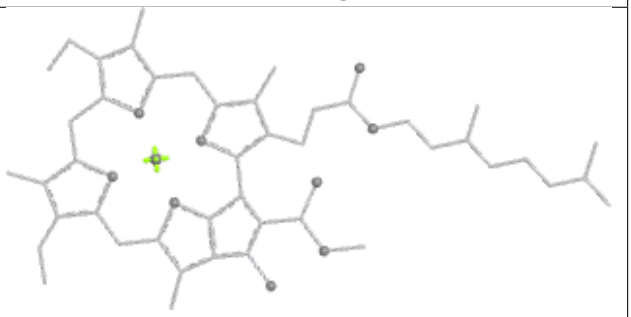
Bond lengths



Bond angles

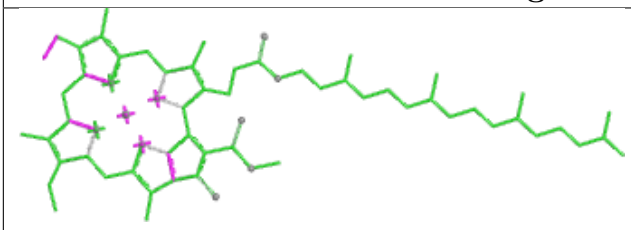


Torsions

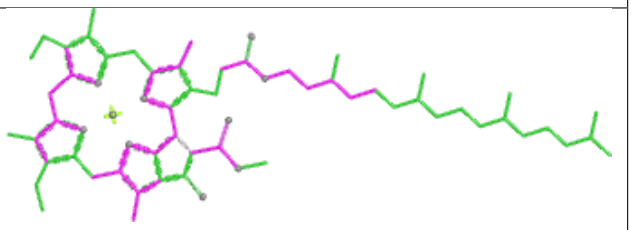


Rings

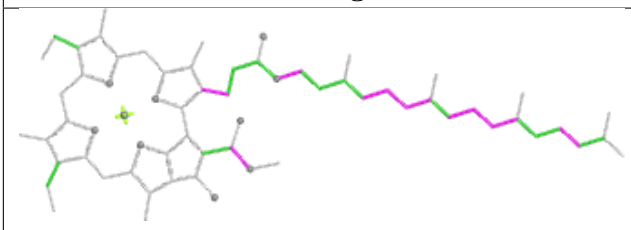
Ligand CLA n 314



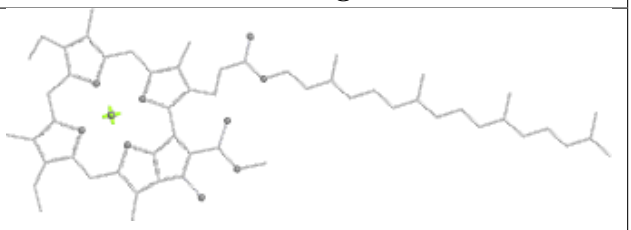
Bond lengths



Bond angles

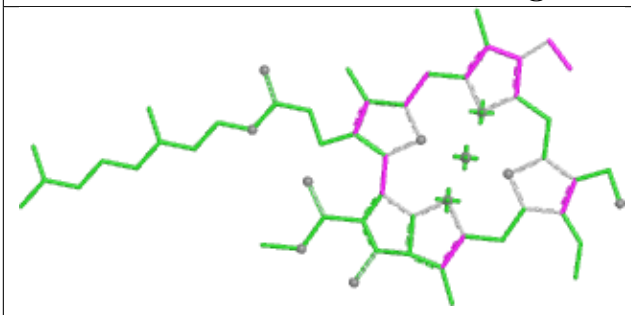


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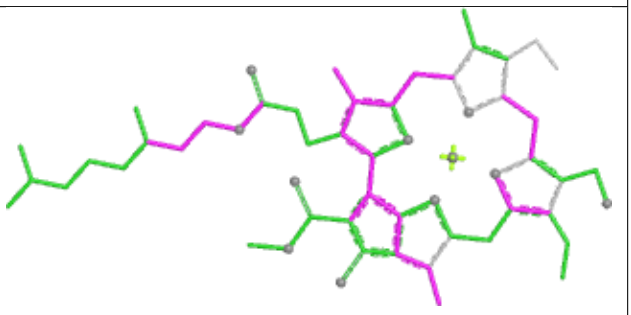


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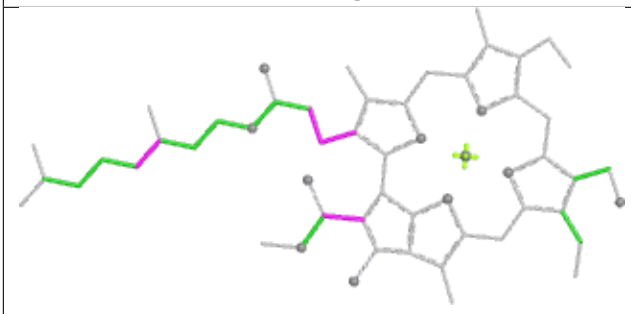
Ligand CHL 0 601



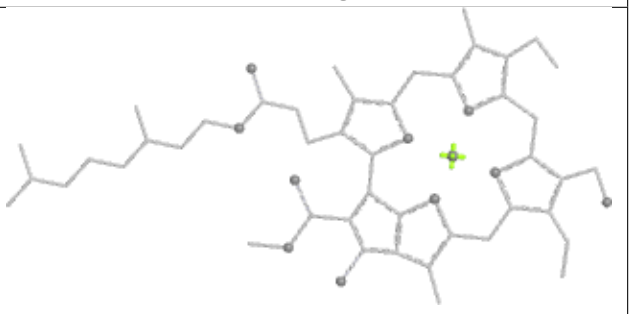
Bond lengths



Bond angles

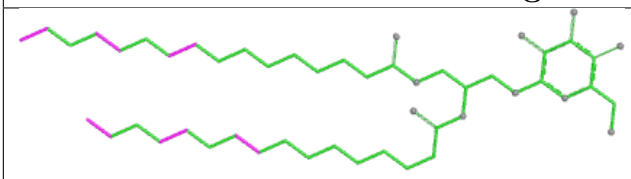


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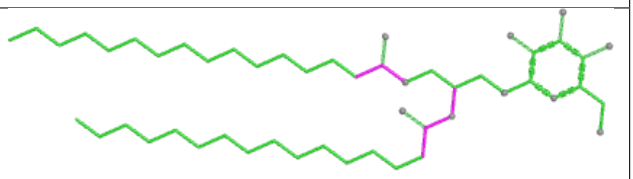


Rings

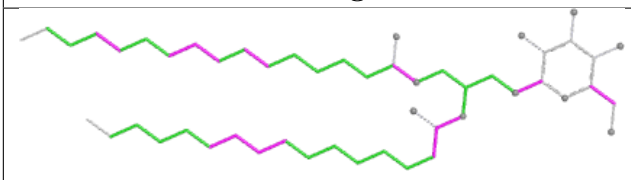
Ligand LMG 4 620



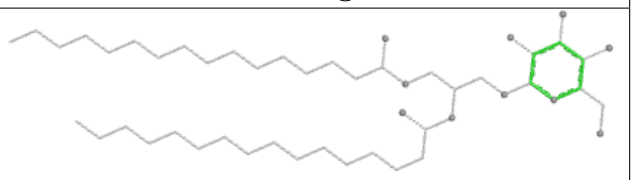
Bond lengths



Bond angles

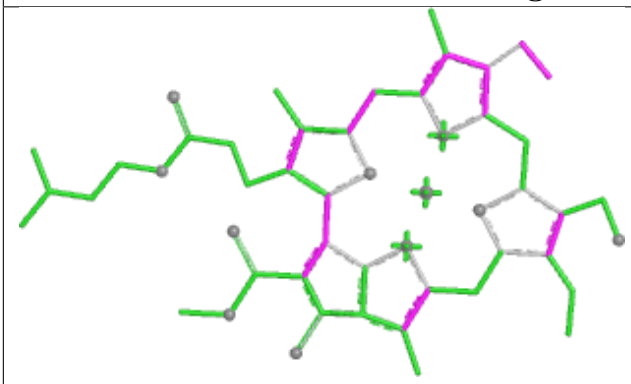


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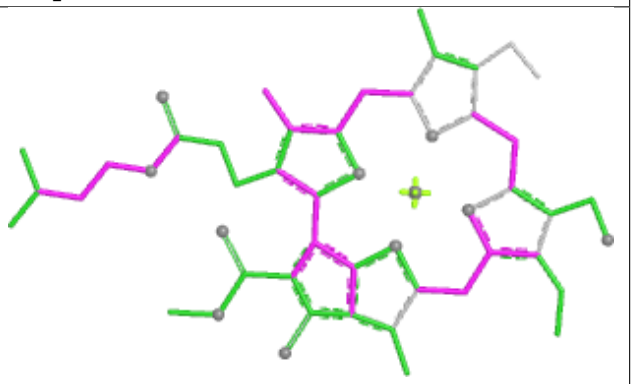


Rings

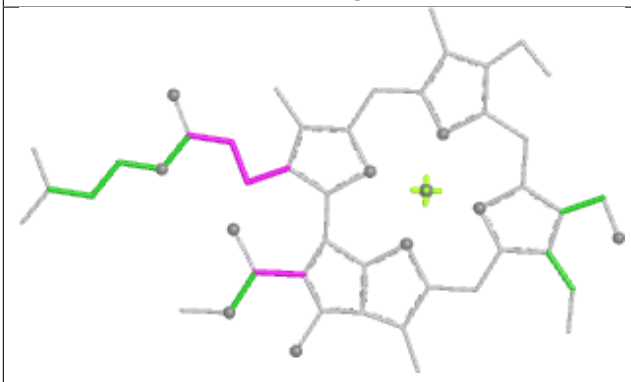
Ligand CHL p 601



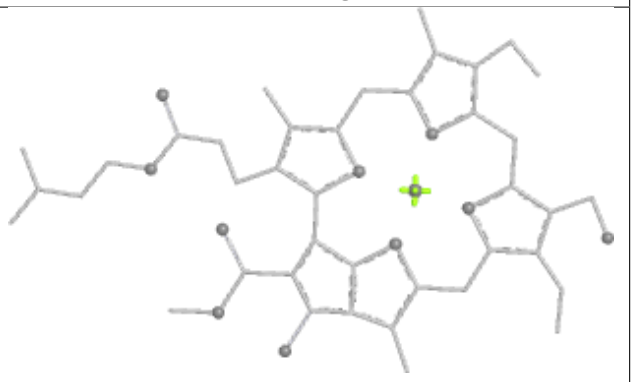
Bond lengths



Bond angles

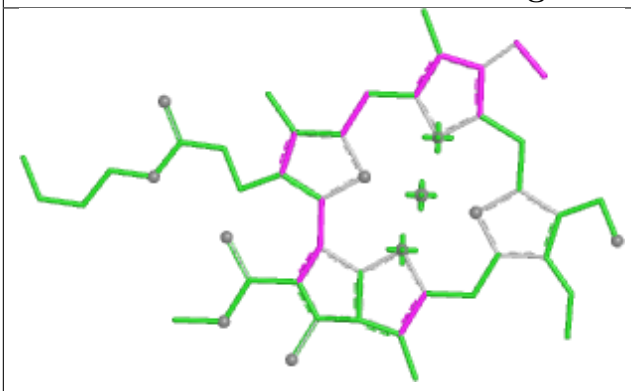


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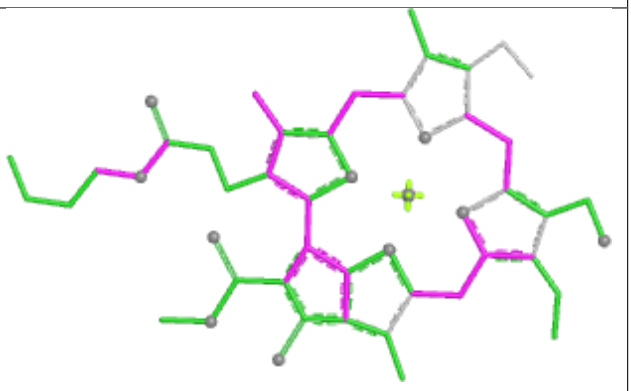


Rings

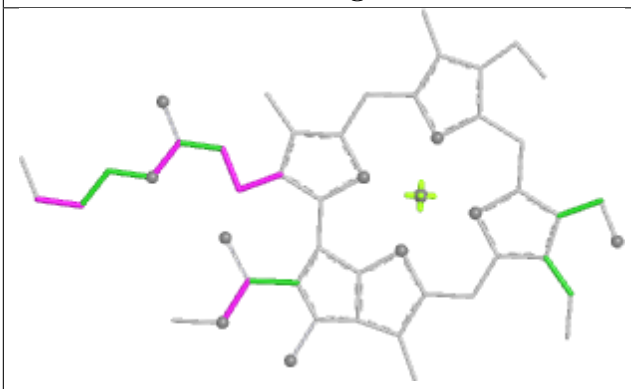
Ligand CHL 3 309



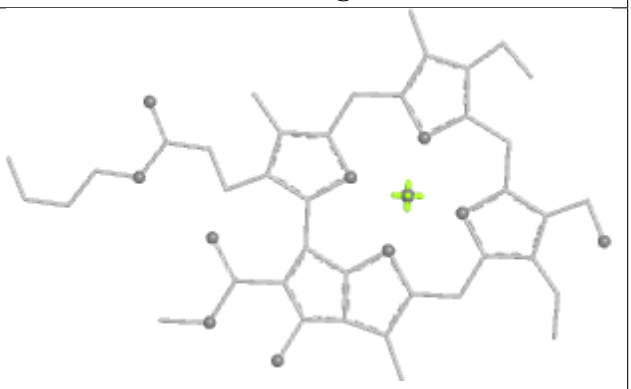
Bond lengths



Bond angles

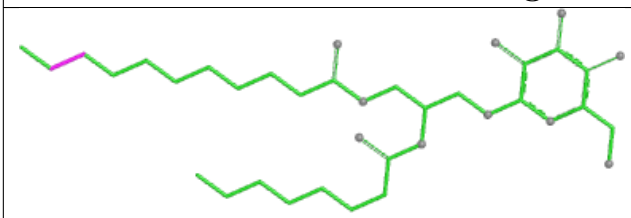


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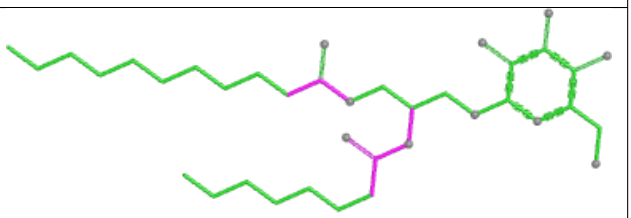


Rings

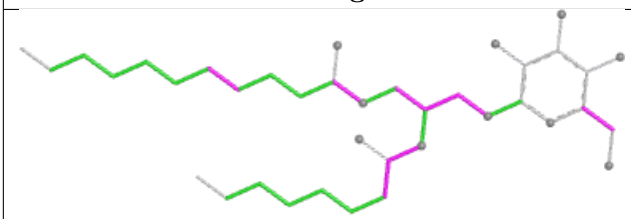
Ligand LMG 7 322



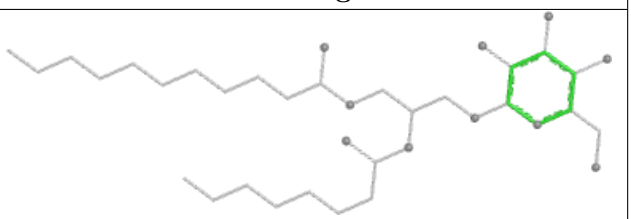
Bond lengths



Bond angles

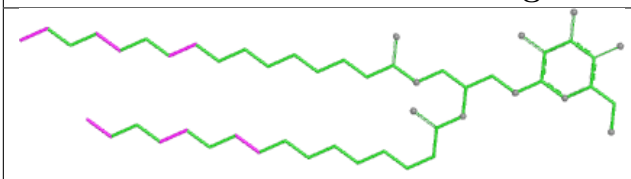


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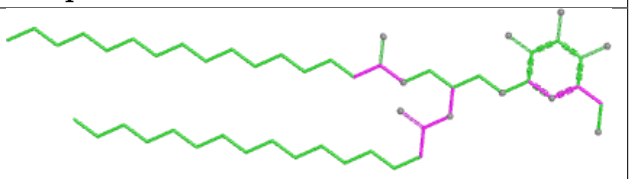


Rings

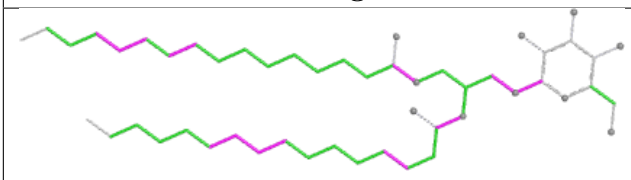
Ligand LMG q 301



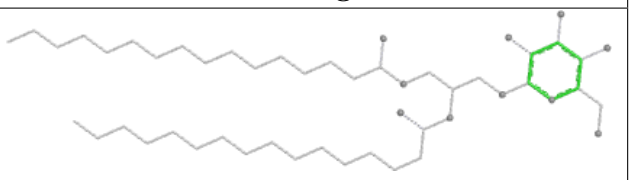
Bond lengths



Bond angles

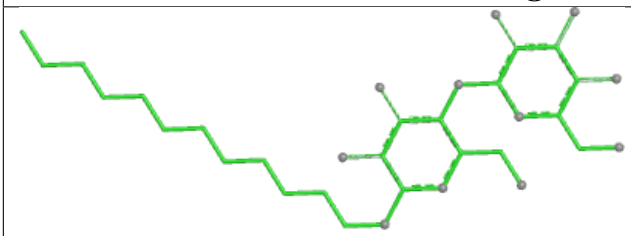


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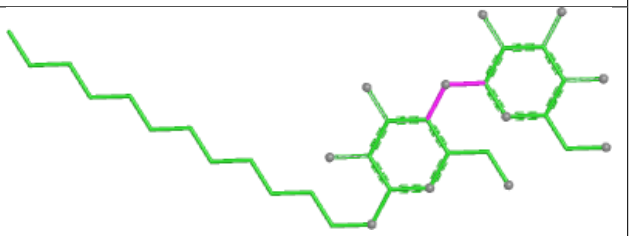


Rings

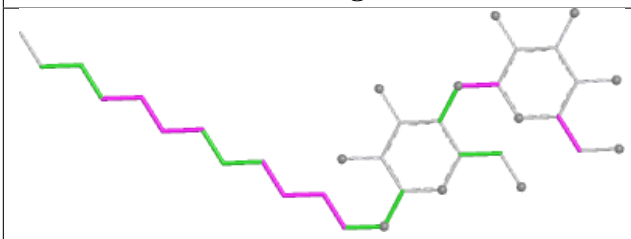
Ligand LMU r 302



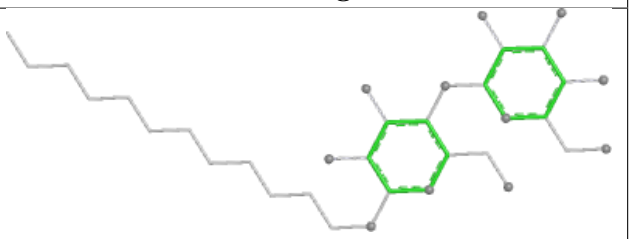
Bond lengths



Bond angles

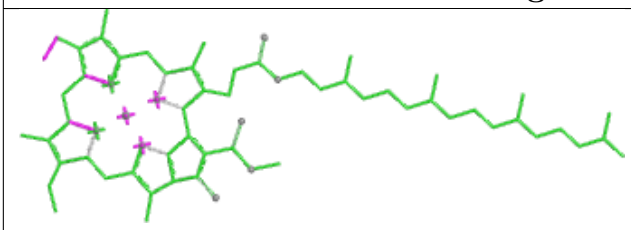


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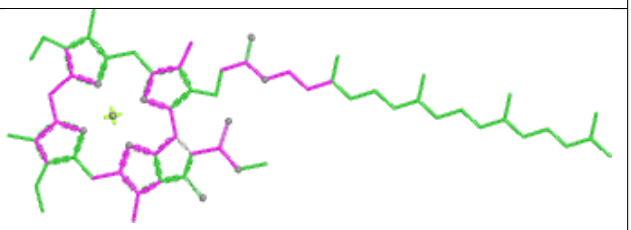


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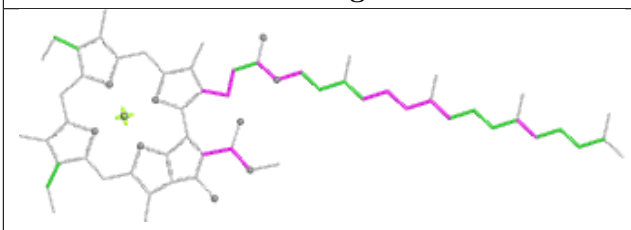
Ligand CLA n 305



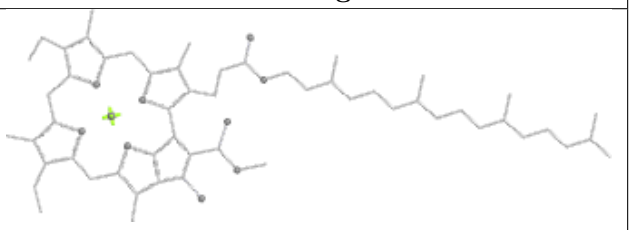
Bond lengths



Bond angles

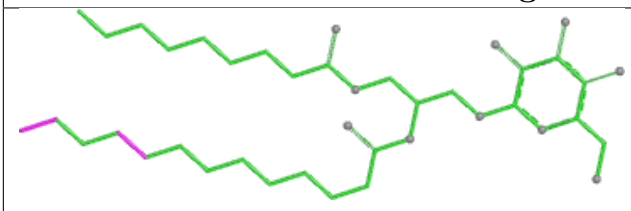


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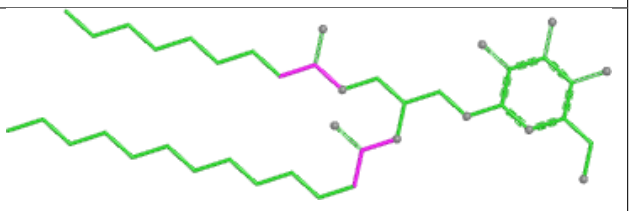


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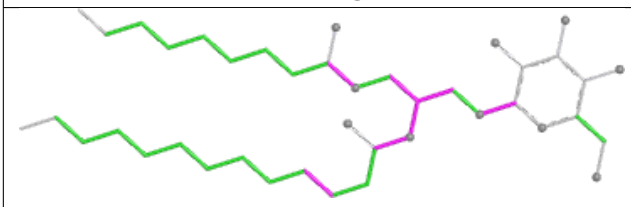
Ligand LMG A 412



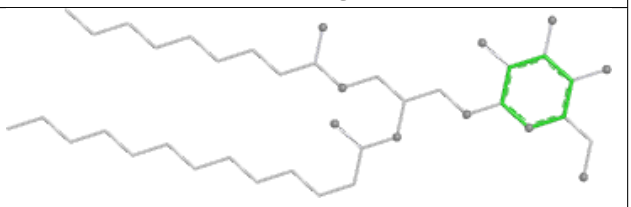
Bond lengths



Bond angles

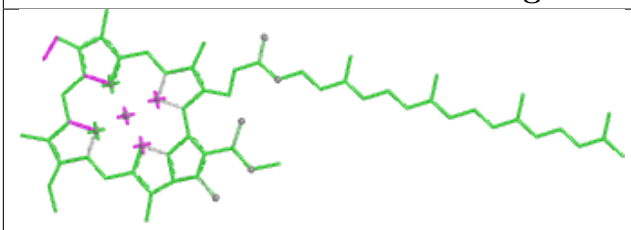


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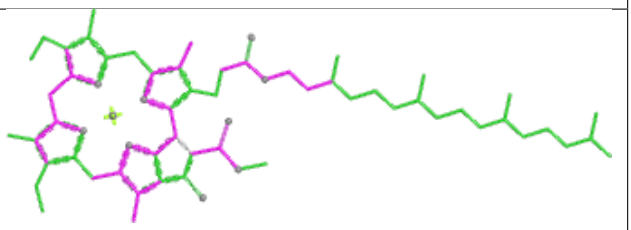


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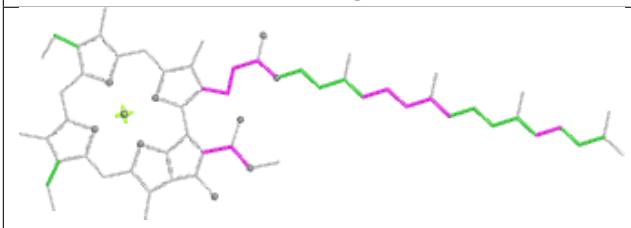
Ligand CLA N 305



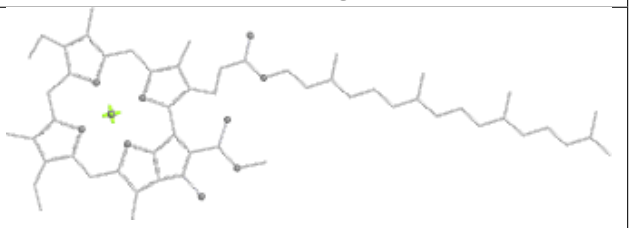
Bond lengths



Bond angles

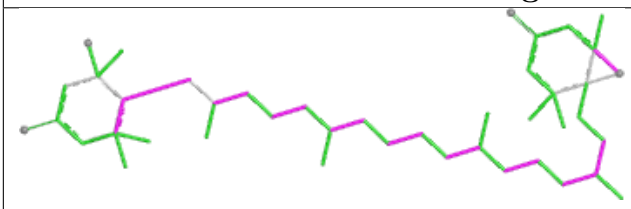


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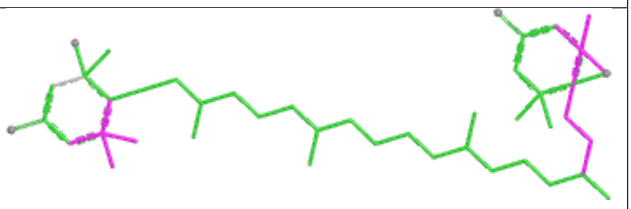


Rings

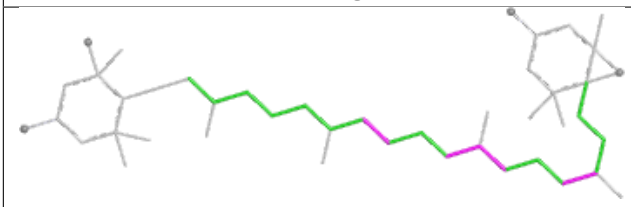
Ligand NEX R 319



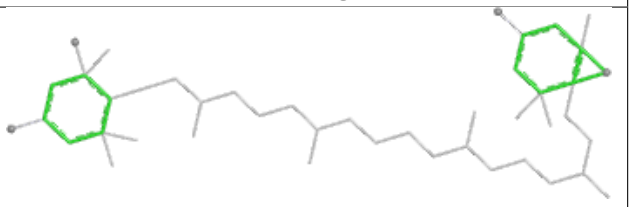
Bond lengths



Bond angles

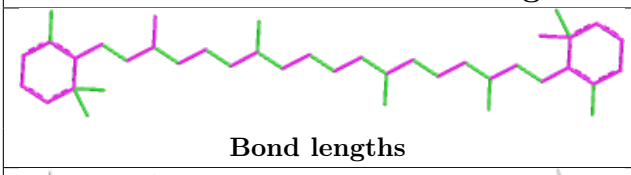


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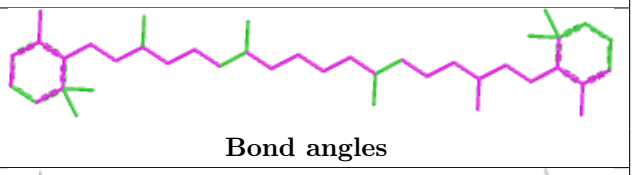


Rings

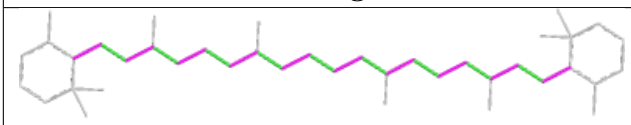
Ligand BCR B 617



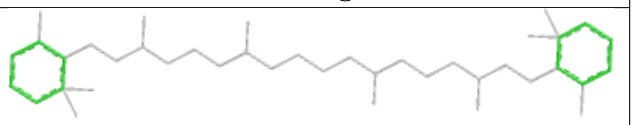
Bond lengths



Bond angles

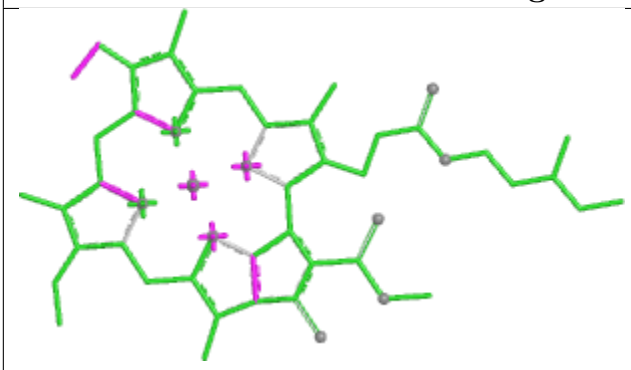


Torsions

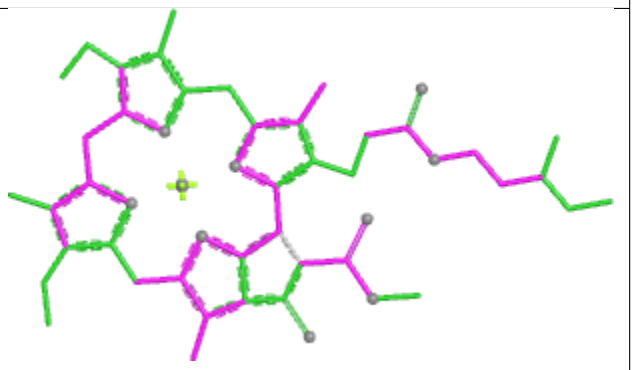


Rings

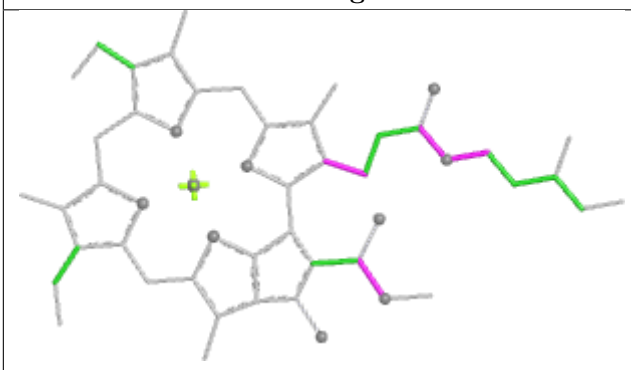
Ligand CLA 7 316



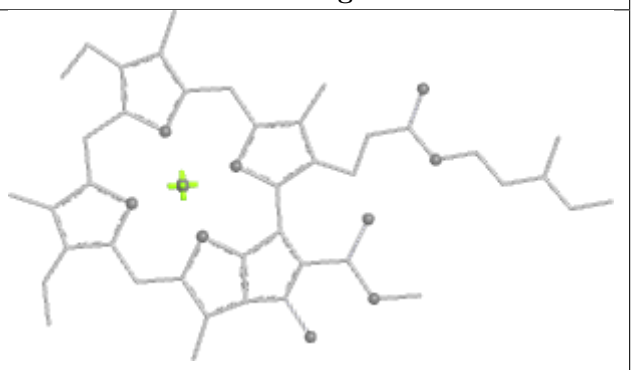
Bond lengths



Bond angles

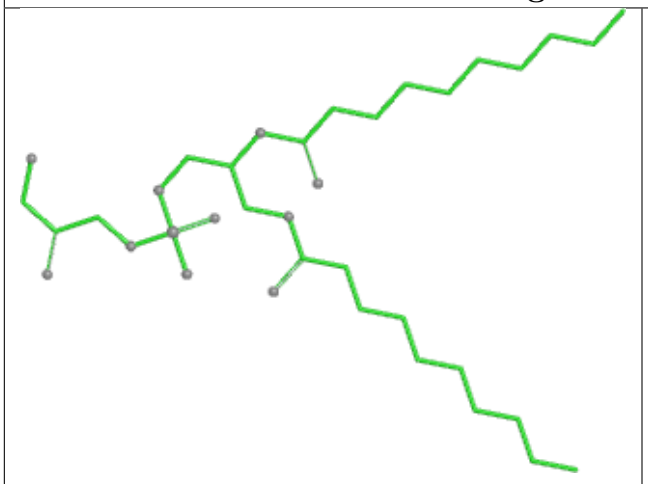


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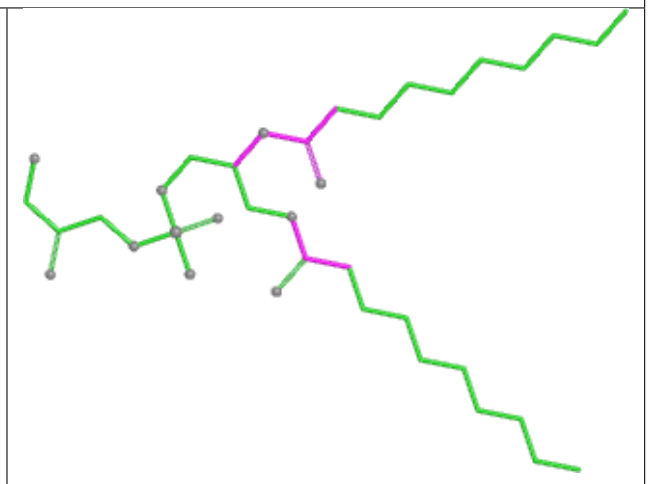


Rings

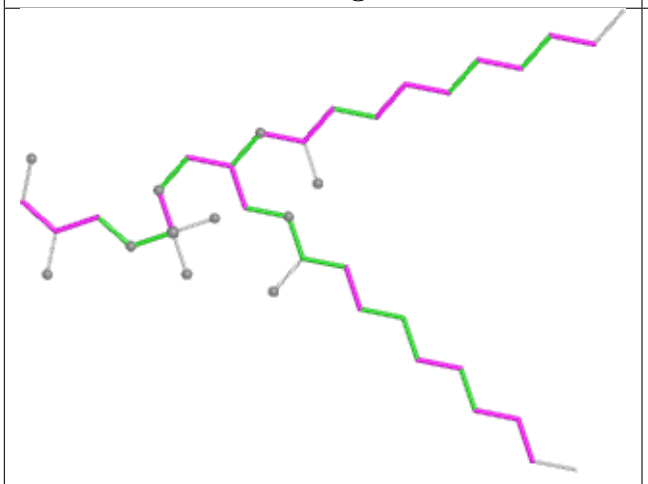
Ligand LHG 6 320



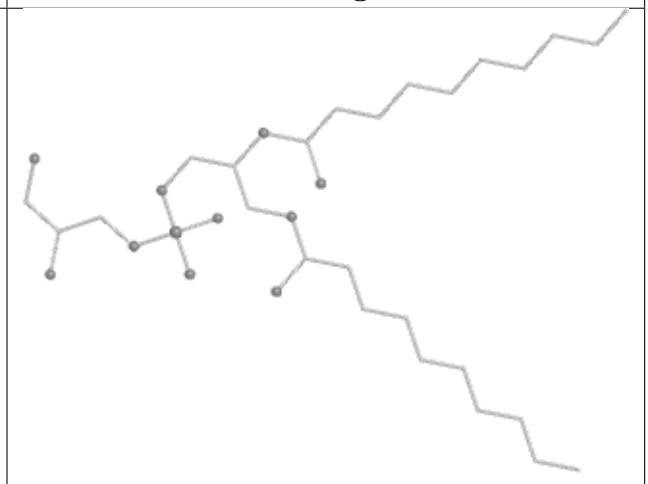
Bond lengths



Bond angles

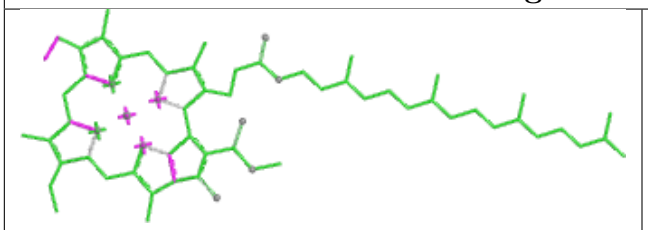


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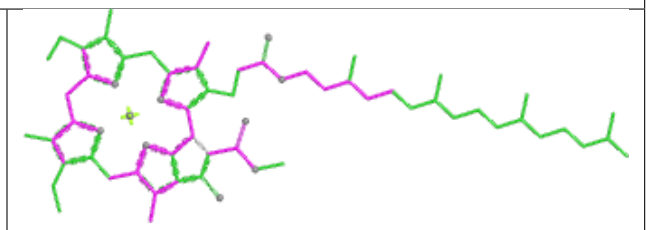


Rings

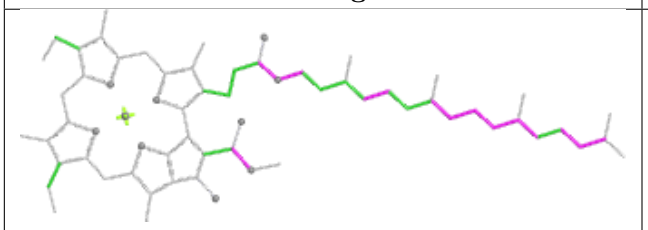
Ligand CLA Y 312



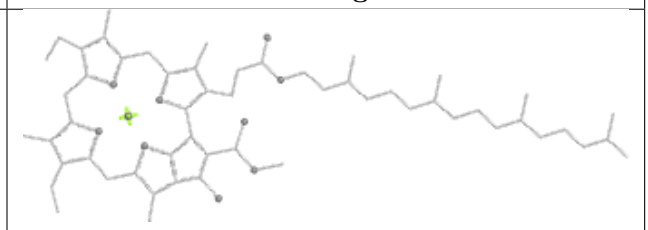
Bond lengths



Bond angles

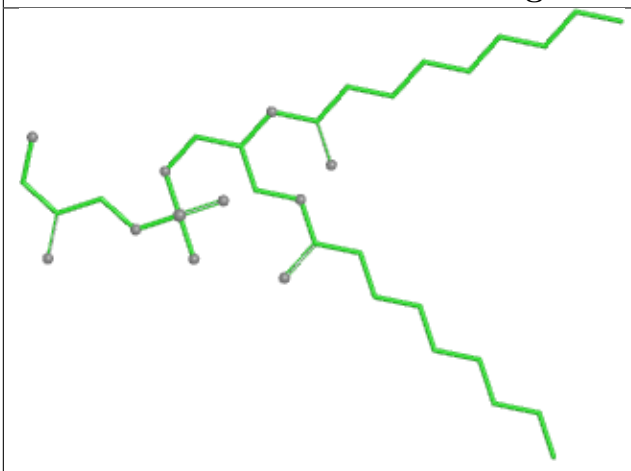


Torsions

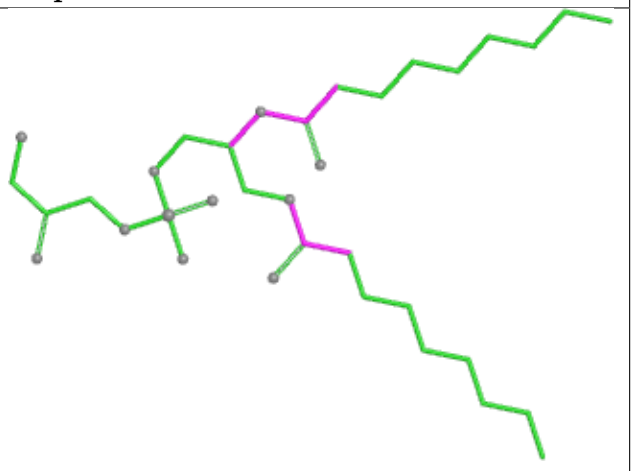


Rings

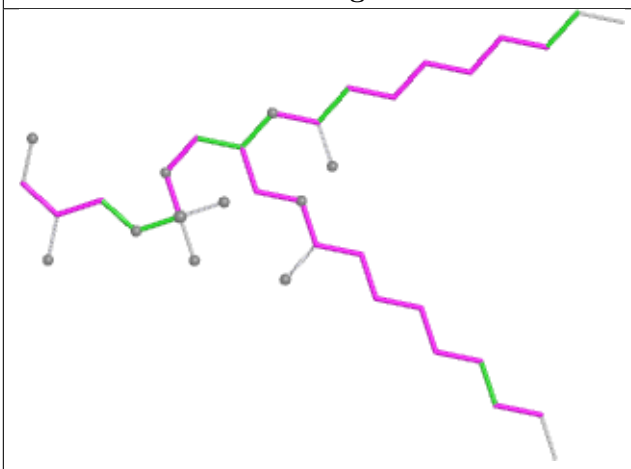
Ligand LHG p 619



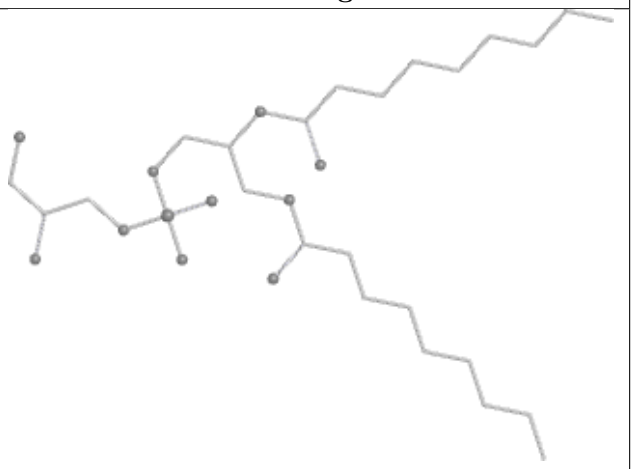
Bond lengths



Bond angles

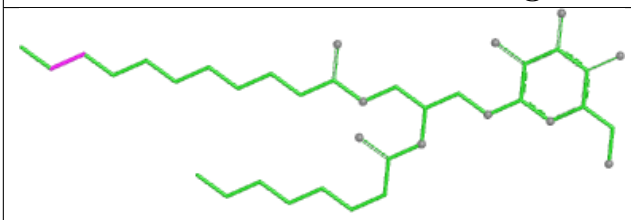


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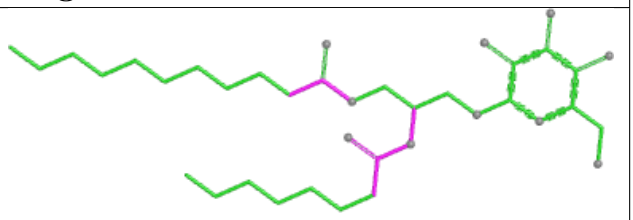


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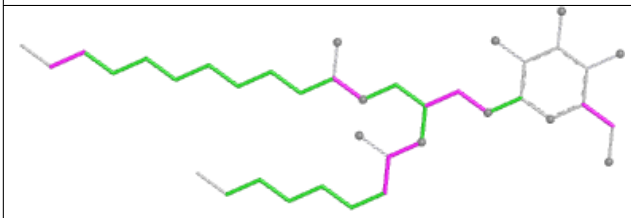
Ligand LMG g 320



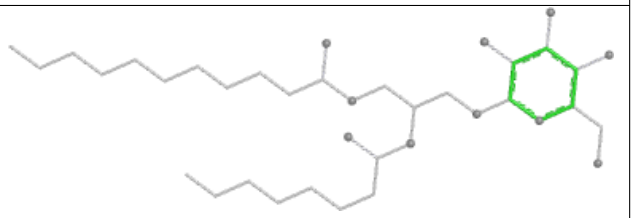
Bond lengths



Bond angles

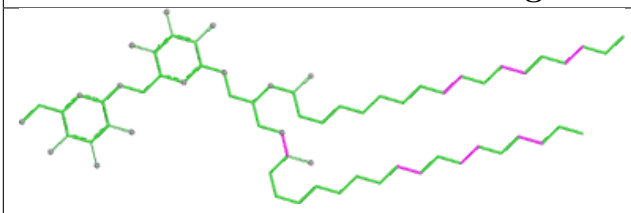


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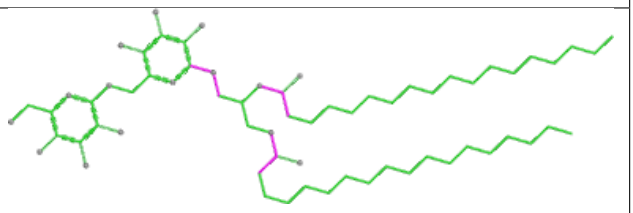


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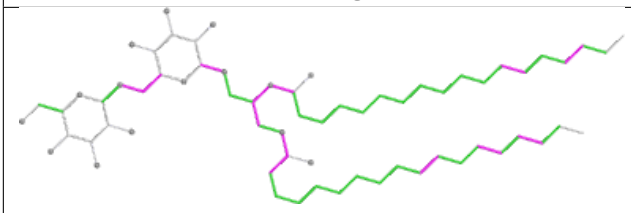
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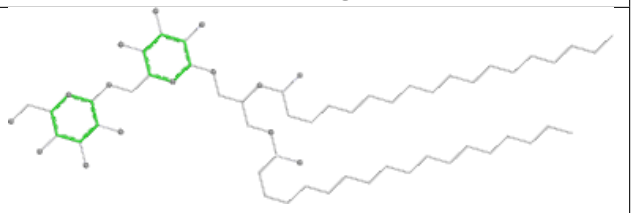
Bond lengths



Bond angles

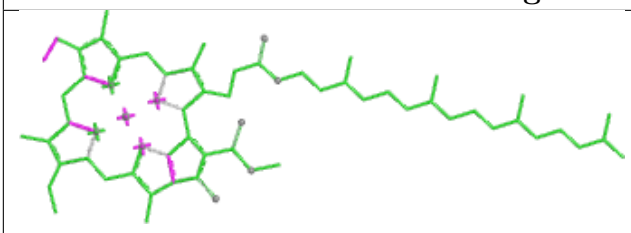


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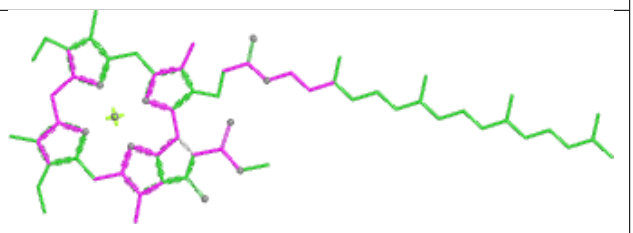


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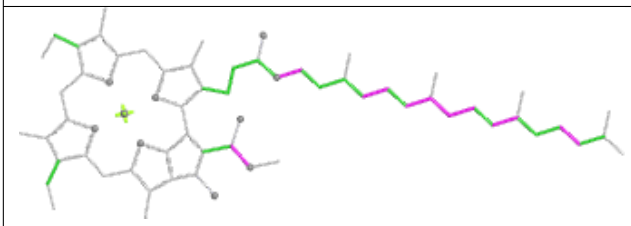
Ligand CLA N 313



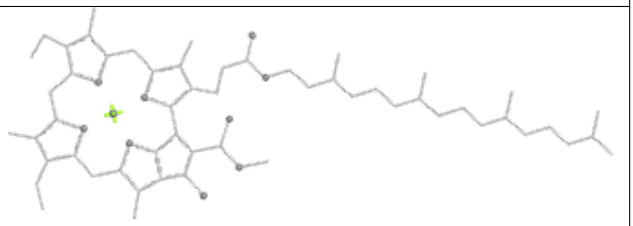
Bond lengths



Bond angles

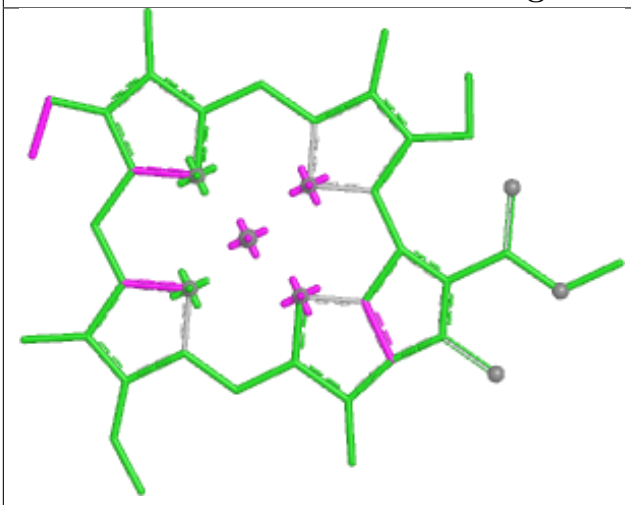


Torsions



Rings

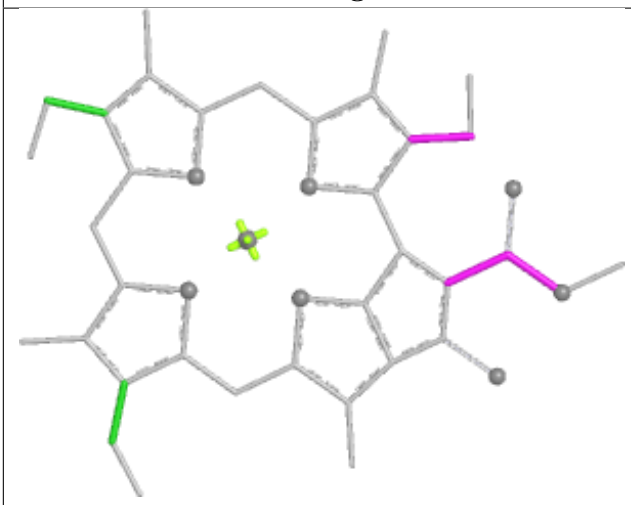
Ligand CLA S 304



Bond lengths



Bond angles

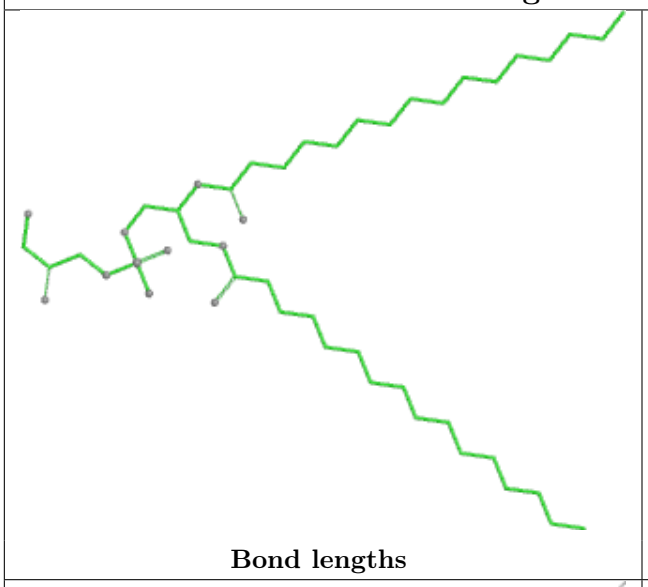


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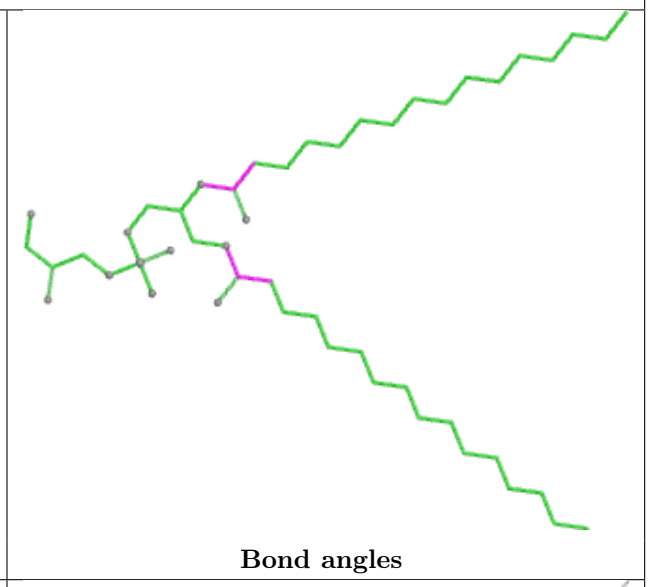


Rings

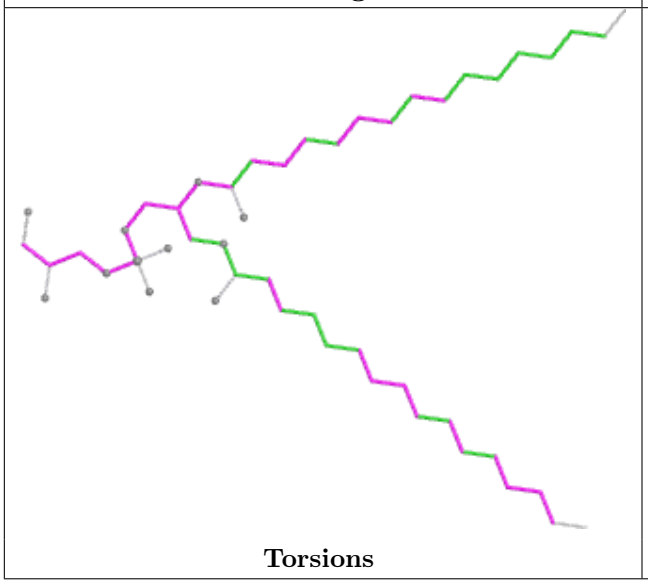
Ligand LHG N 319



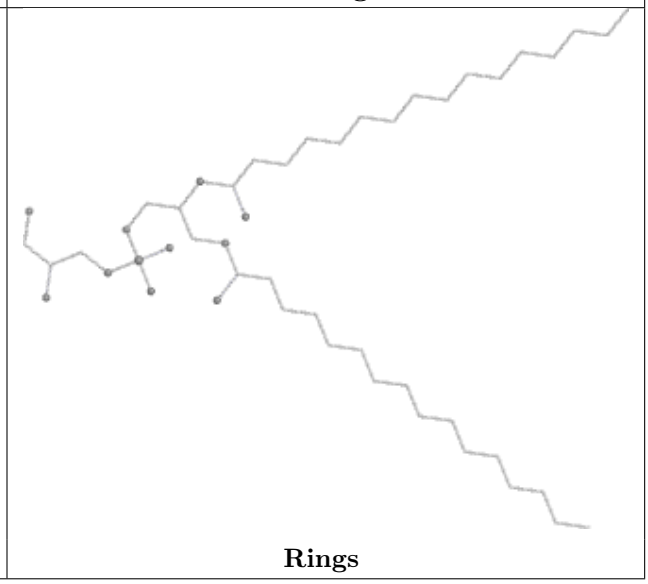
Bond lengths



Bond angles

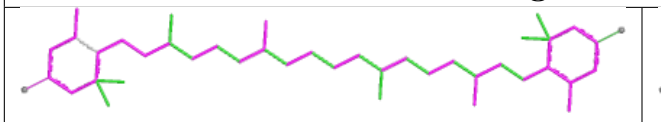


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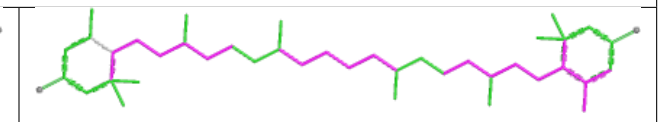


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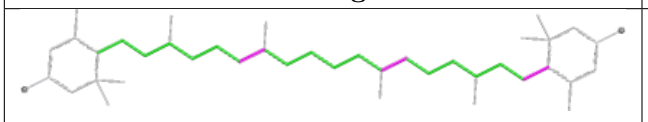
Ligand LUT 5 616



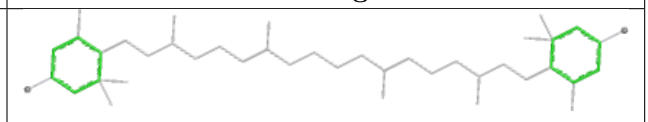
Bond lengths



Bond angles

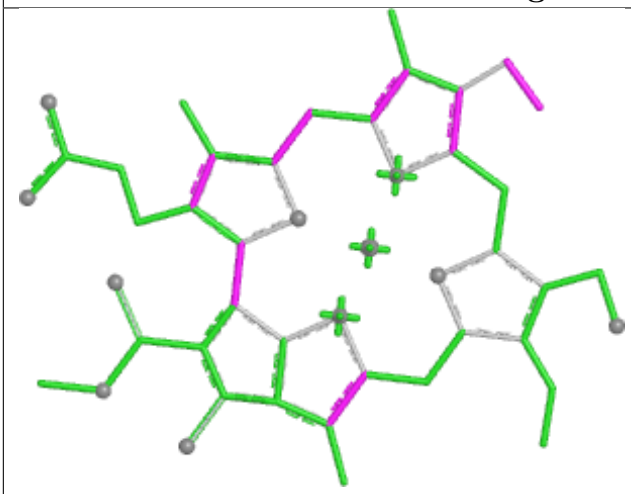


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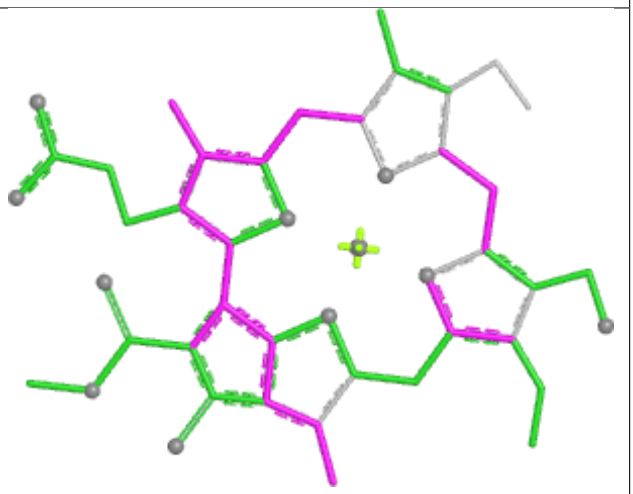


Rings

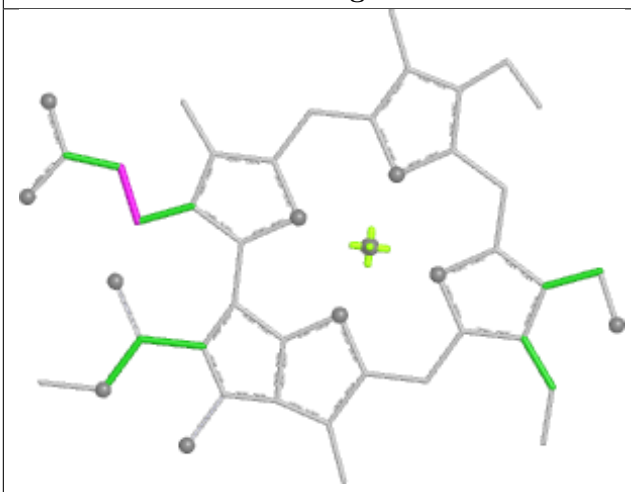
Ligand CHL 4 605



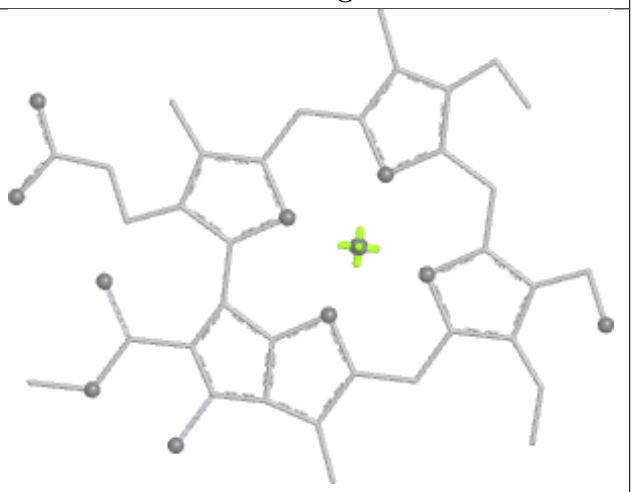
Bond lengths



Bond angles

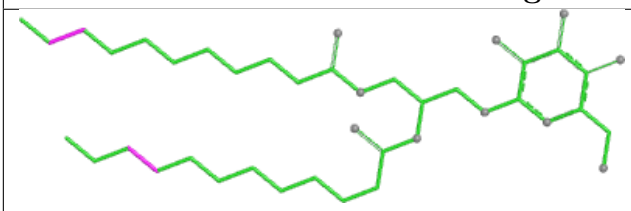


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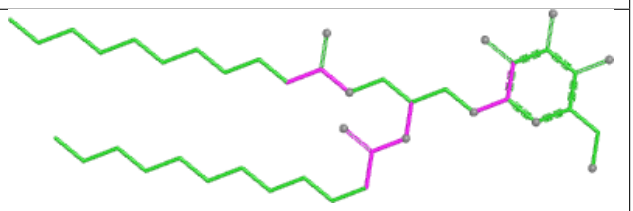


Rings

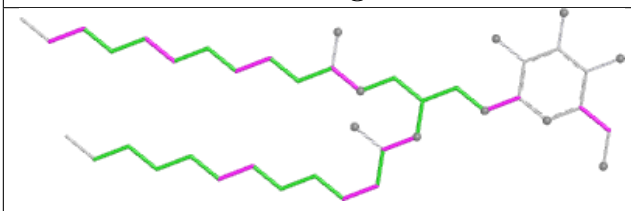
Ligand LMG 6 321



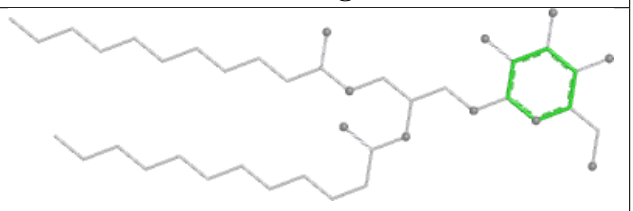
Bond lengths



Bond angles

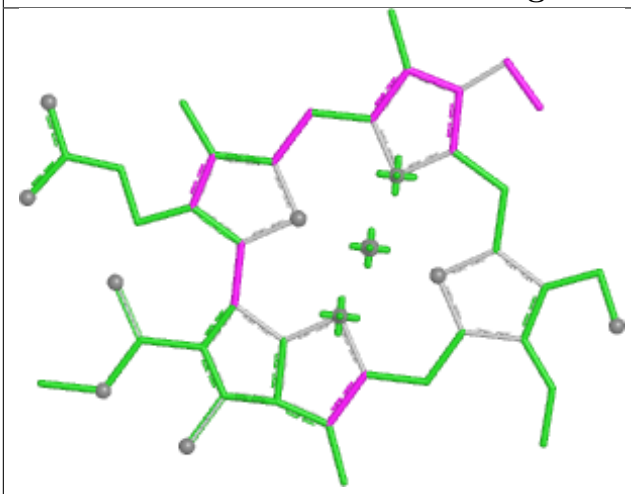


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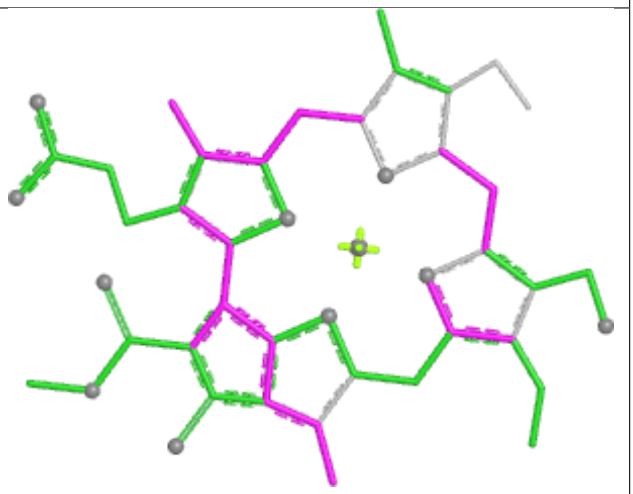


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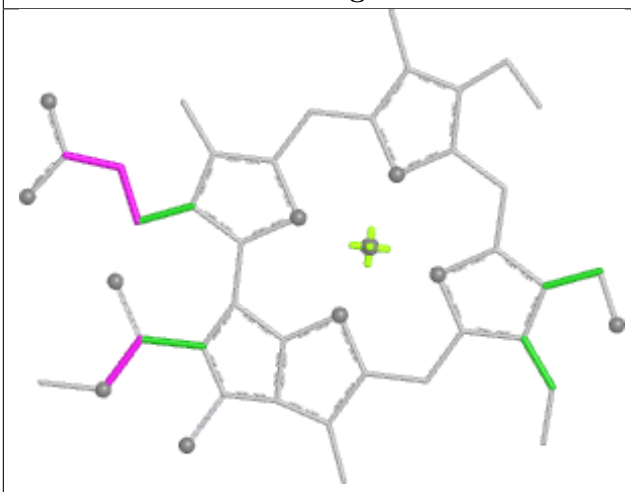
Ligand CHL 9 307



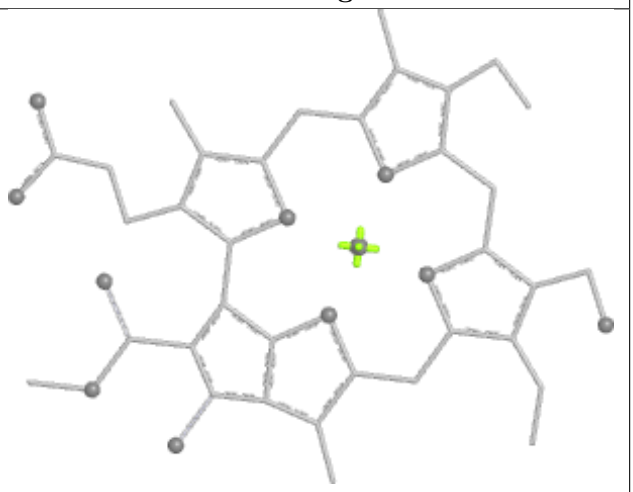
Bond lengths



Bond angles

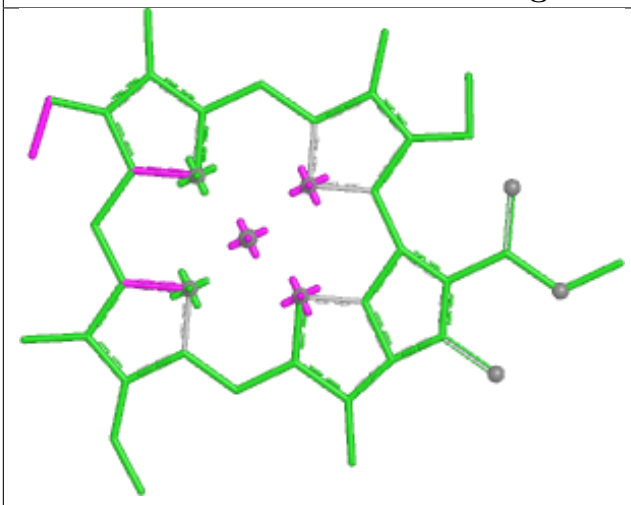


Torsions



Rings

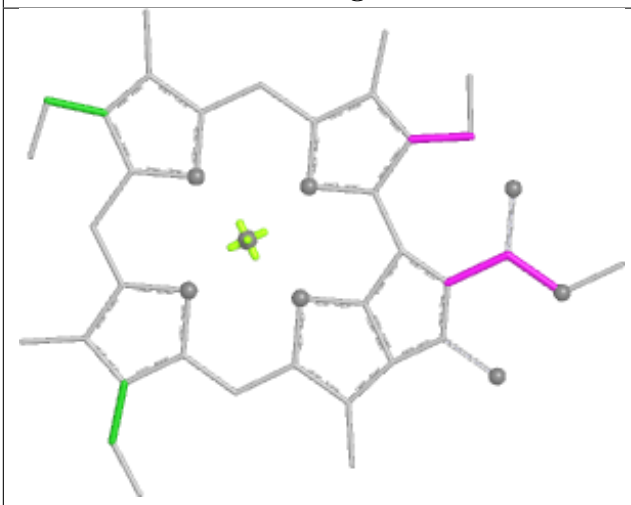
Ligand CLA s 304



Bond lengths



Bond angles

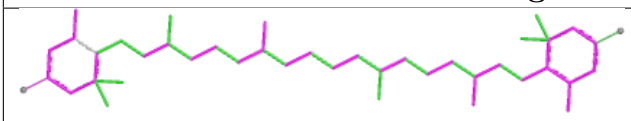


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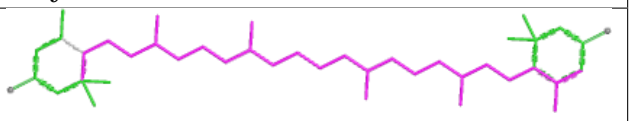


Rings

Ligand LUT y 616



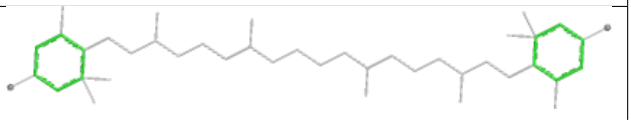
Bond lengths



Bond angles

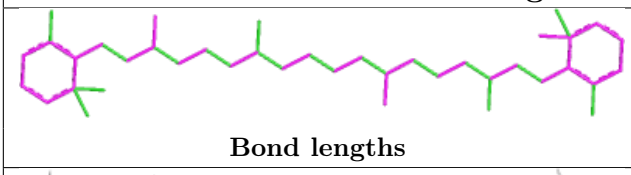


Torsions

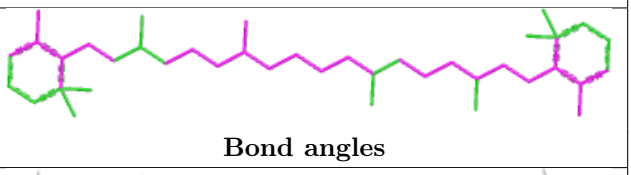


Rings

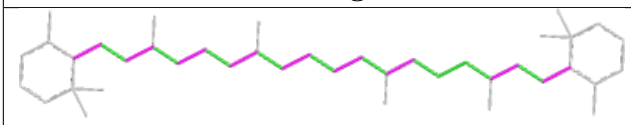
Ligand BCR v 101



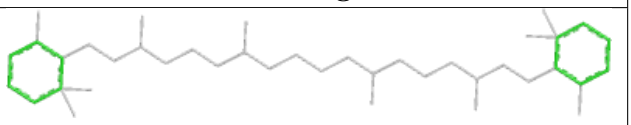
Bond lengths



Bond angles

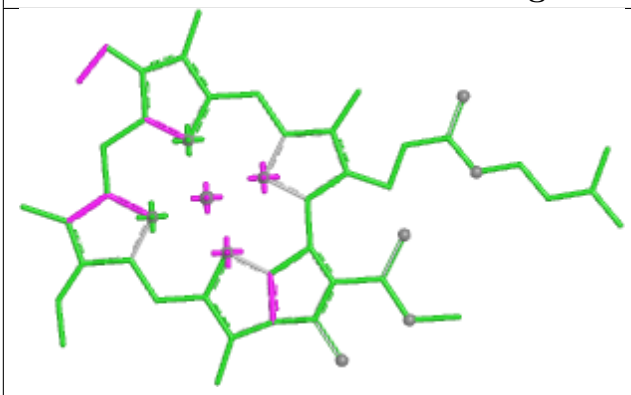


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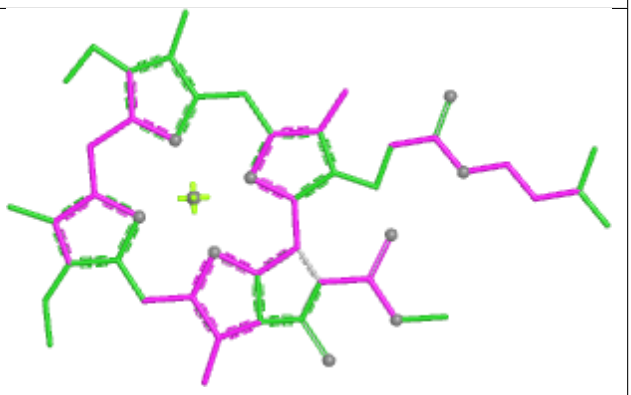


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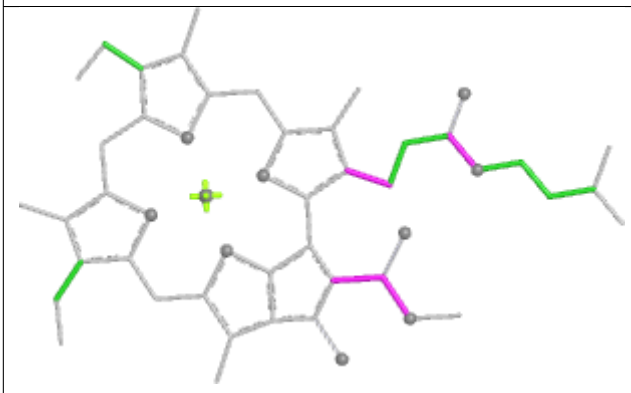
Ligand CLA 5 612



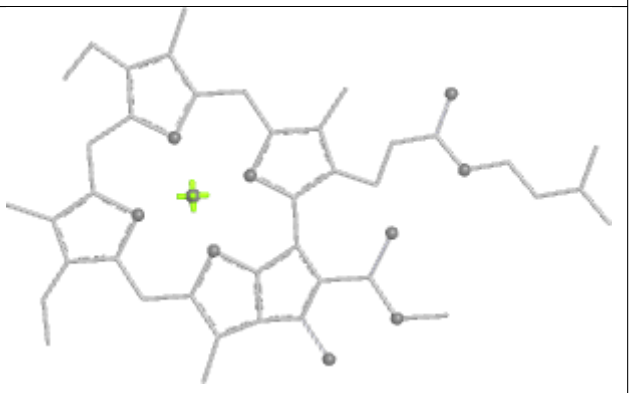
Bond lengths



Bond angles

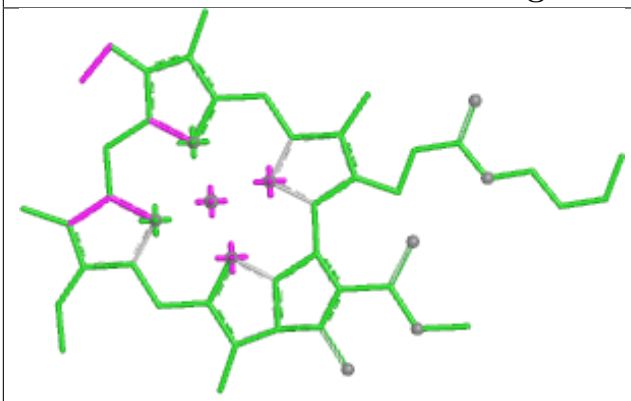


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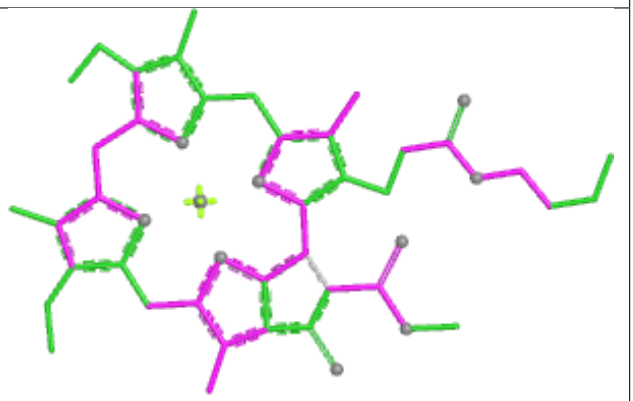


Rings

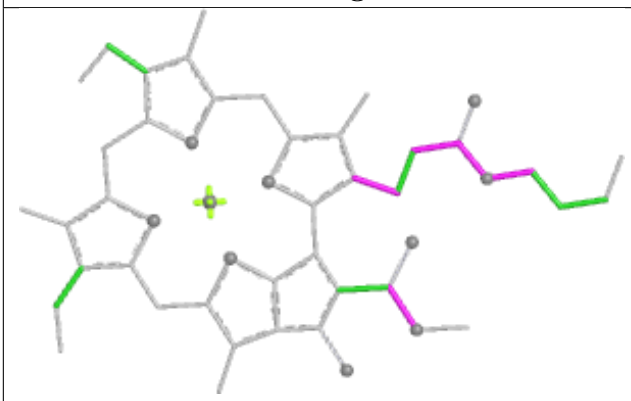
Ligand CLA n 315



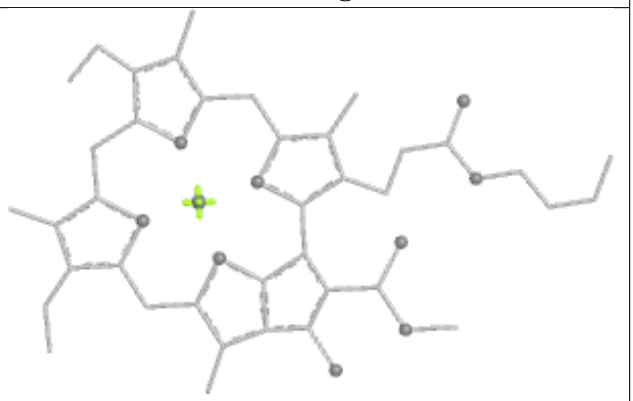
Bond lengths



Bond angles

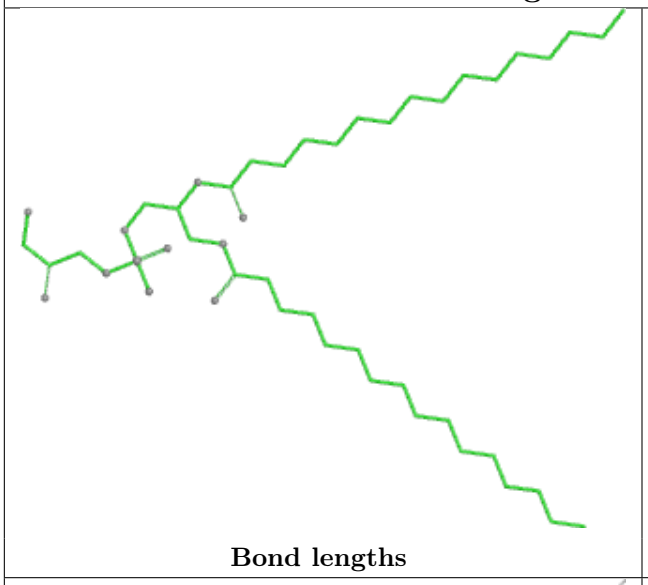


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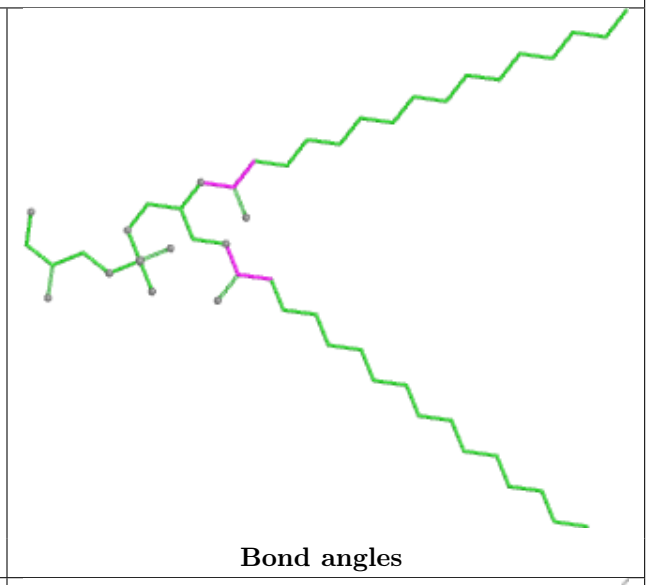


Rings

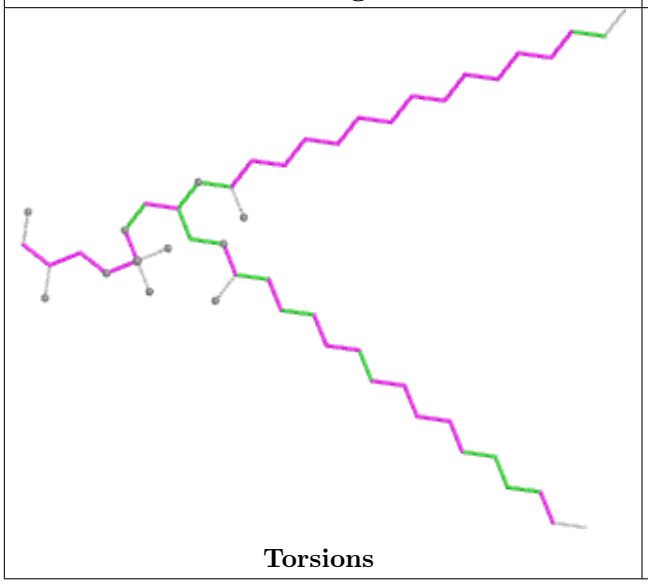
Ligand LHG B 624



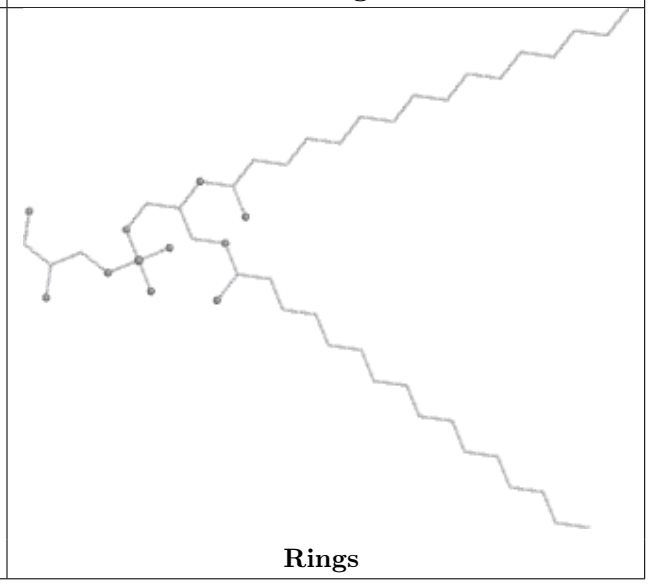
Bond lengths



Bond angles

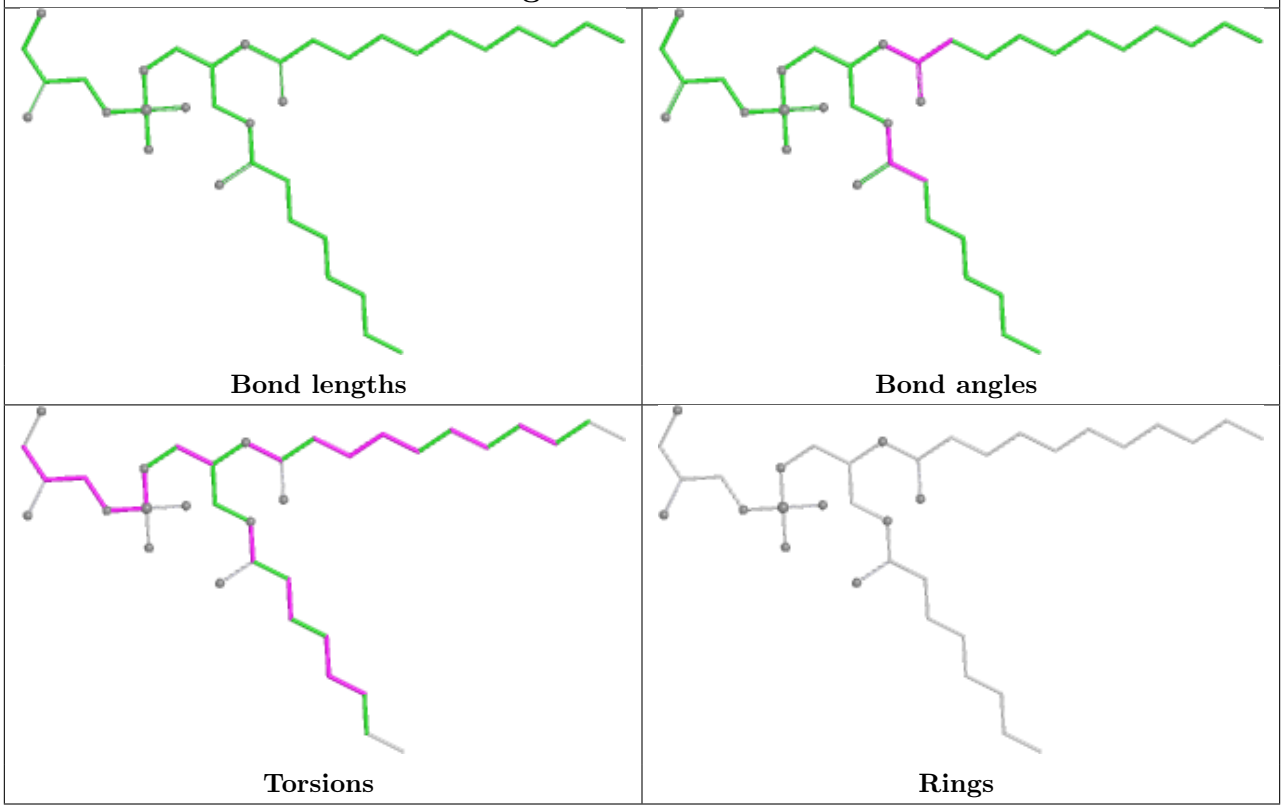


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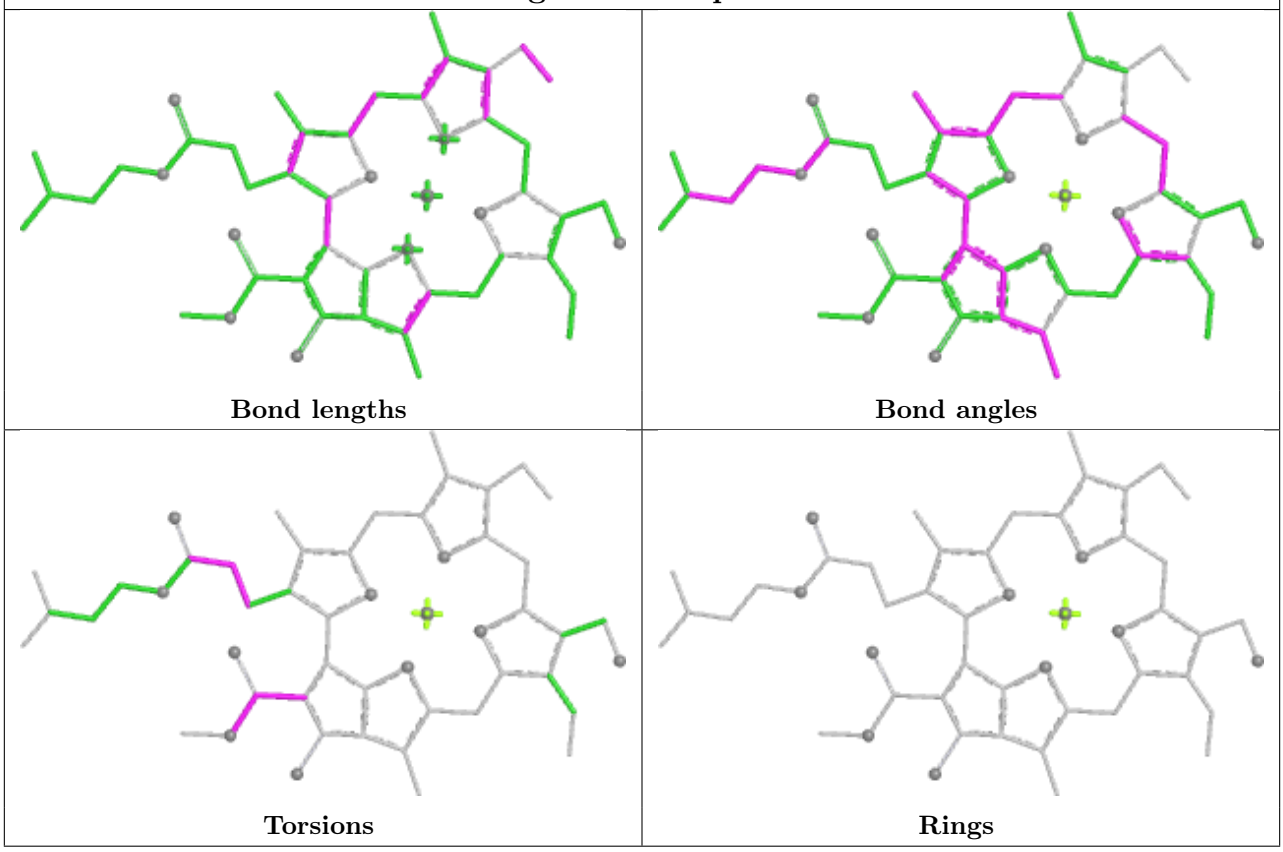


Rings

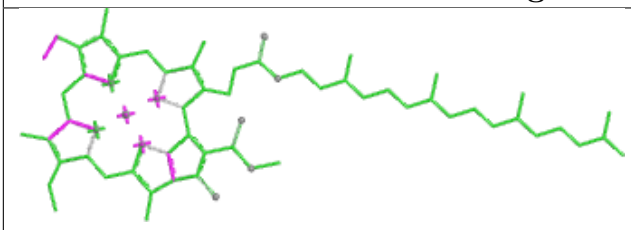
Ligand LHG K 102



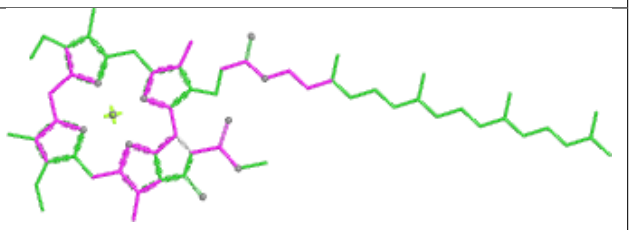
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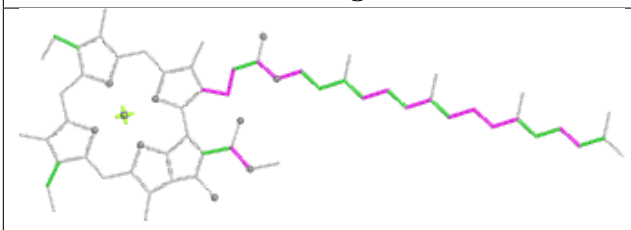
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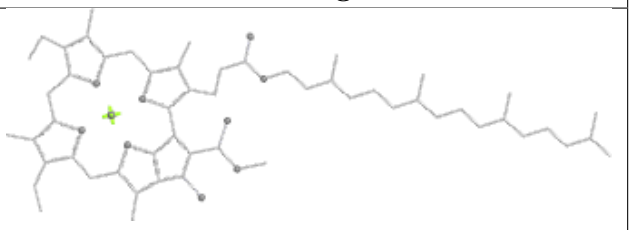
Bond lengths



Bond angles

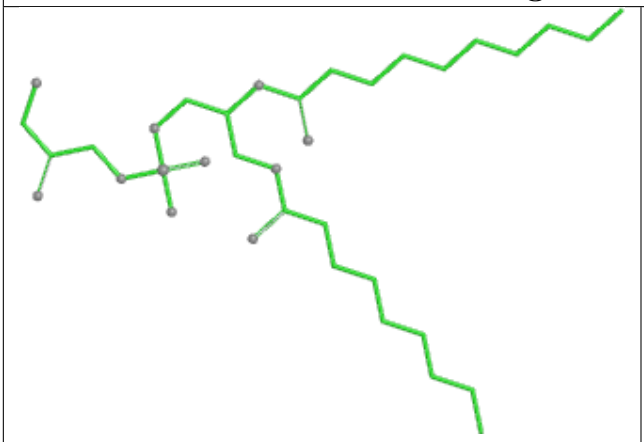


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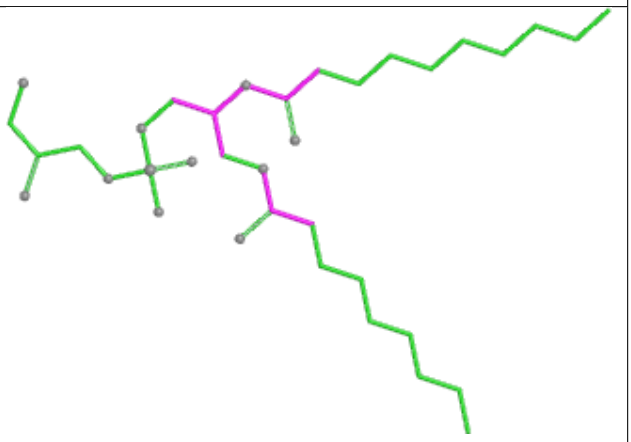


Rings

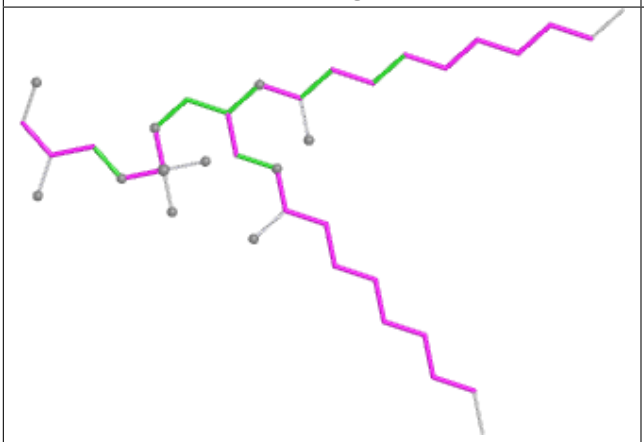
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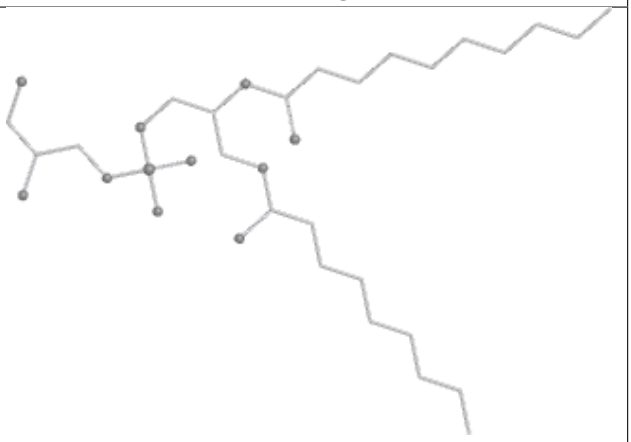
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Bond angles

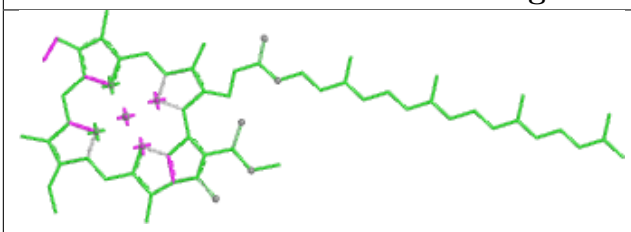


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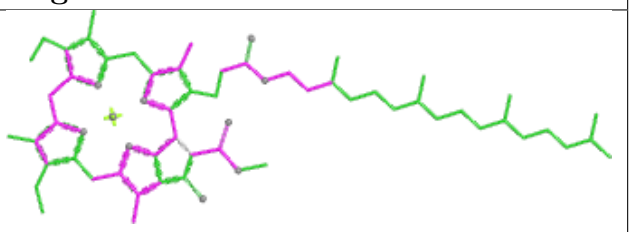


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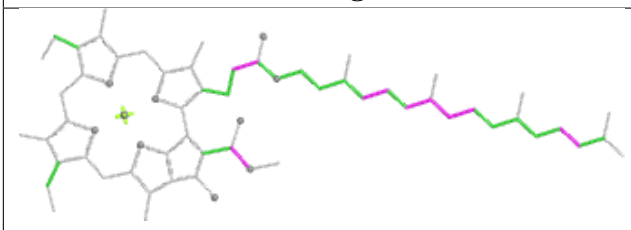
Ligand CLA g 313



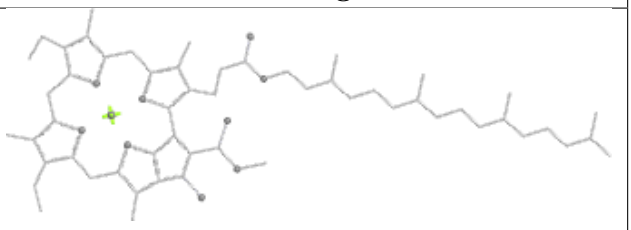
Bond lengths



Bond angles

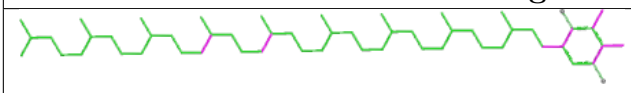


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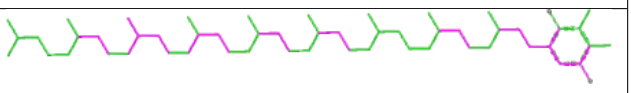


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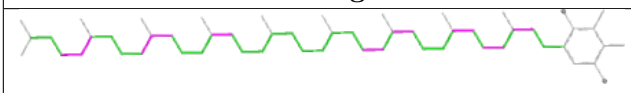
Ligand PL9 A 416



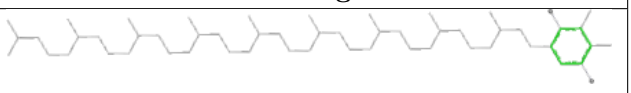
Bond lengths



Bond angles



Torsions



Rings

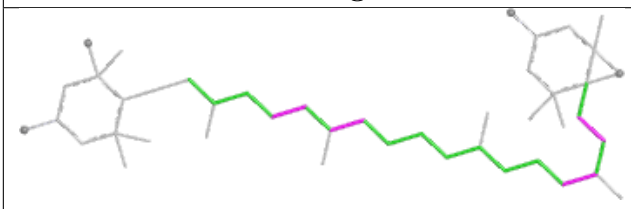
Ligand NEX 4 617



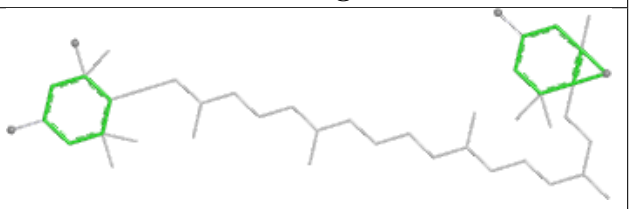
Bond lengths



Bond angles

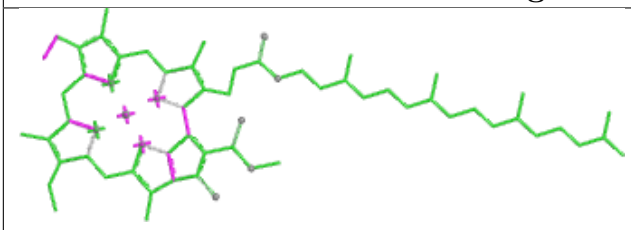


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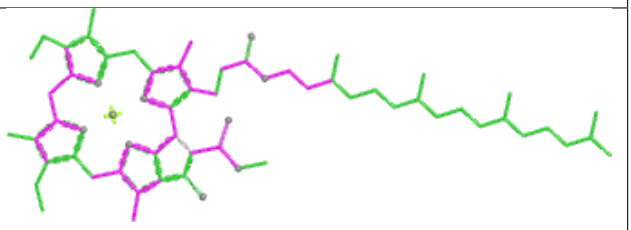


Rings

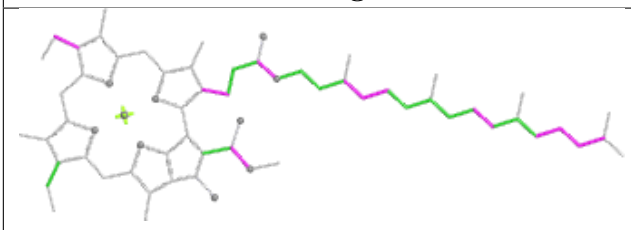
Ligand CLA b 603



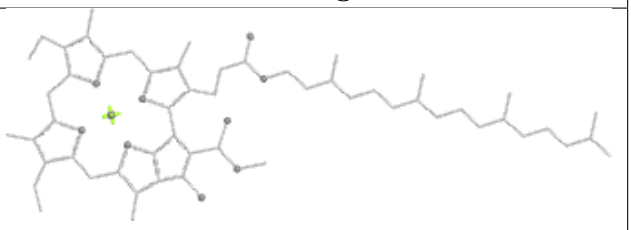
Bond lengths



Bond angles

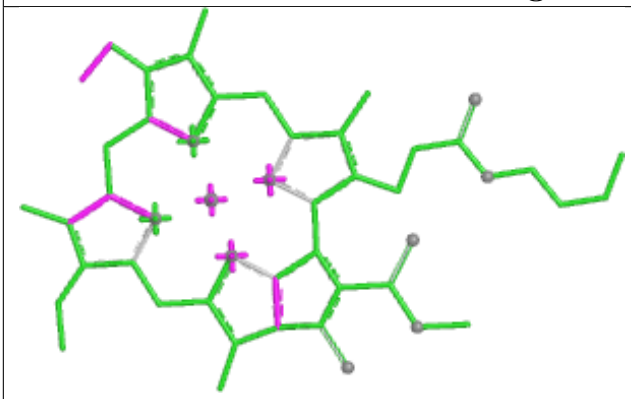


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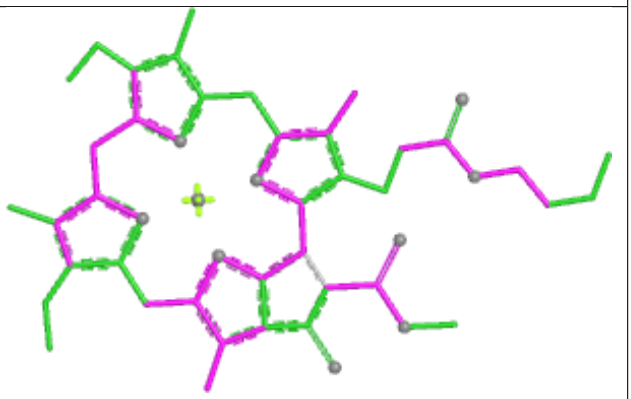


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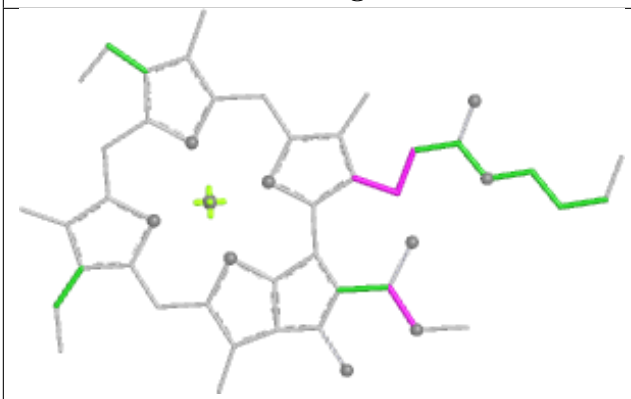
Ligand CLA n 312



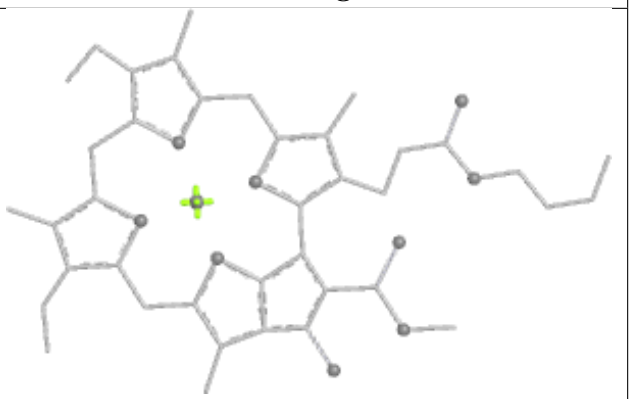
Bond lengths



Bond angles

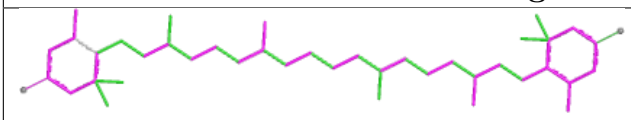


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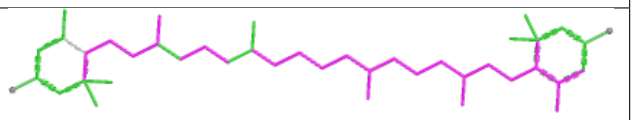


Rings

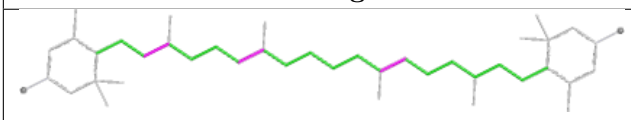
Ligand LUT 6 317



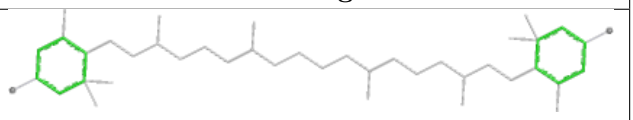
Bond lengths



Bond angles

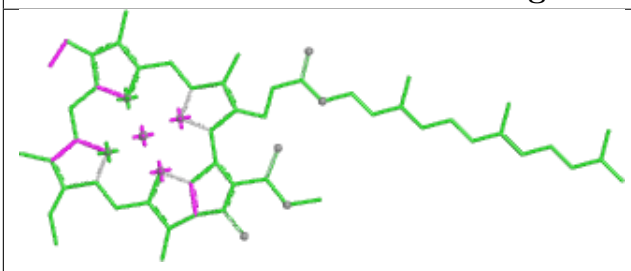


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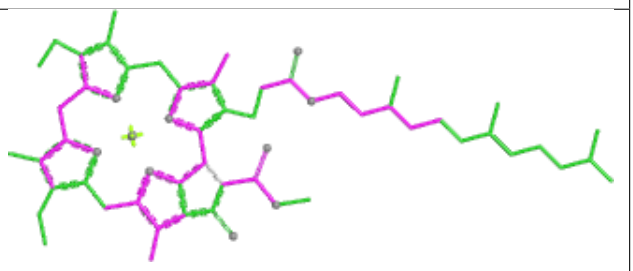


Rings

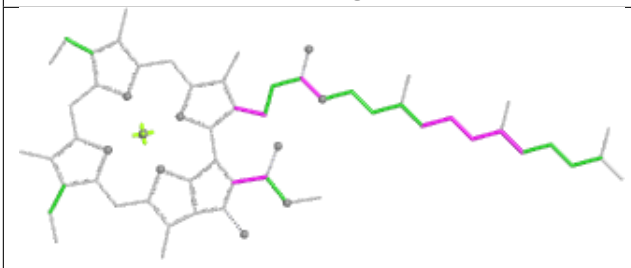
Ligand CLA 6 313



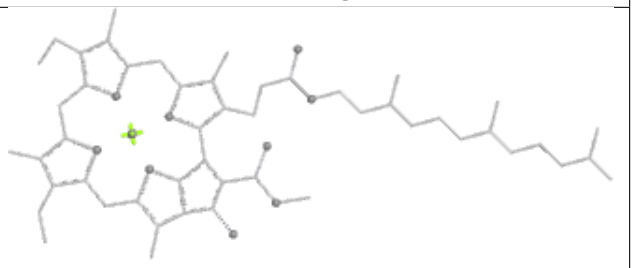
Bond lengths



Bond angles

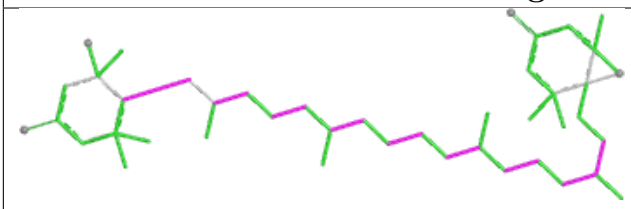


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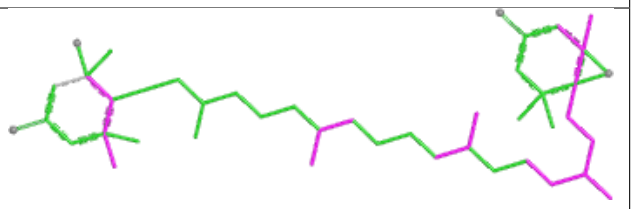


Rings

Ligand NEX r 301



Bond lengths



Bond angles

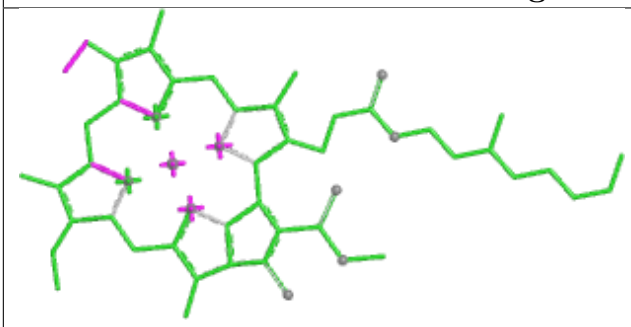


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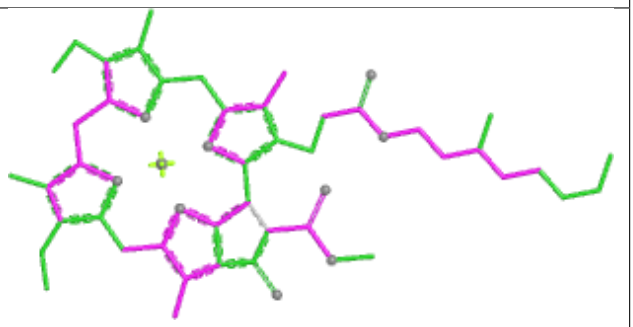


Rings

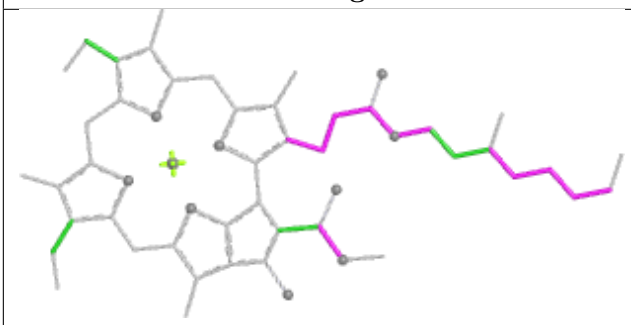
Ligand CLA 6 315



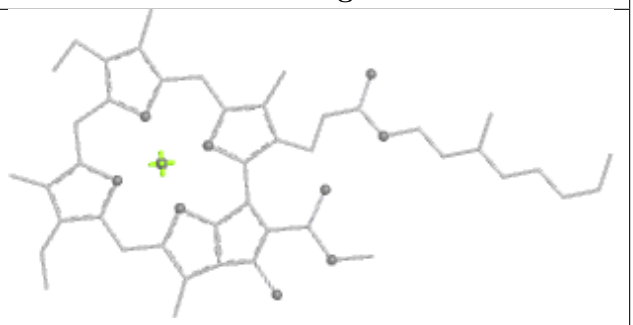
Bond lengths



Bond angles



Torsions



Rings

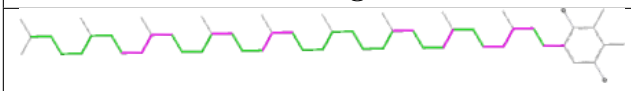
Ligand PL9 a 414



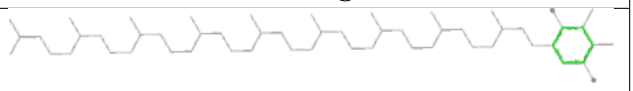
Bond lengths



Bond angles

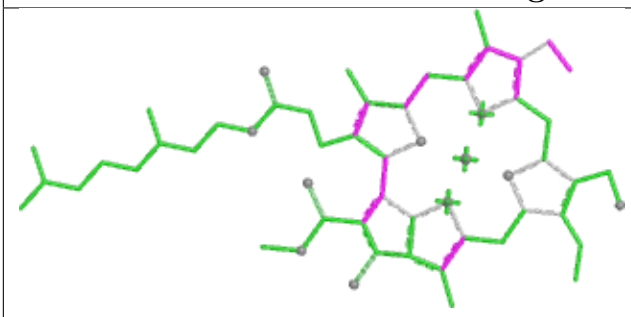


Torsions

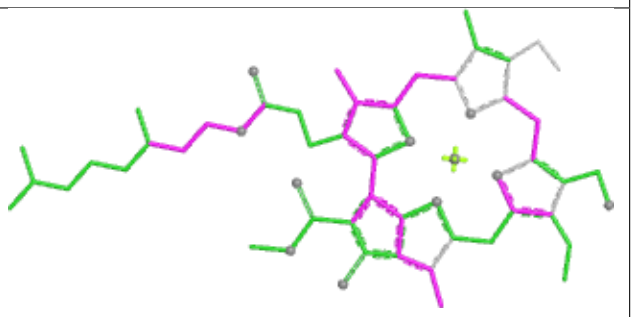


Rings

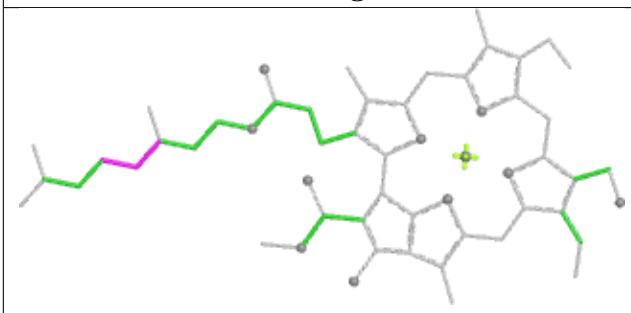
Ligand CHL 5 609



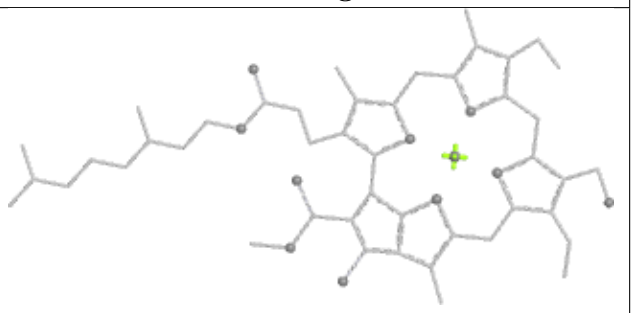
Bond lengths



Bond angles

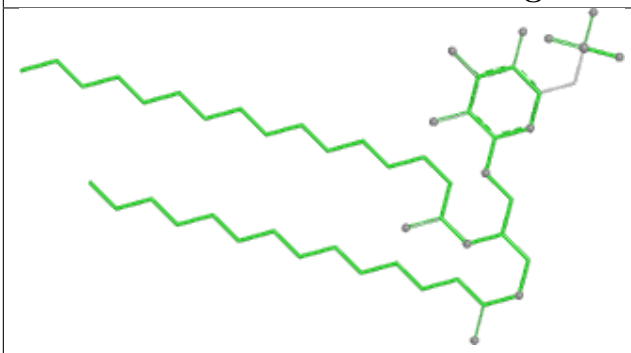


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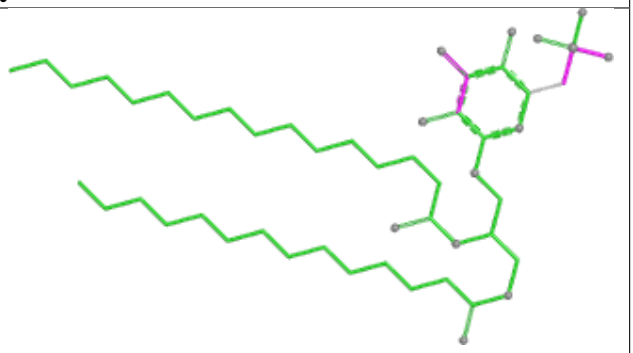


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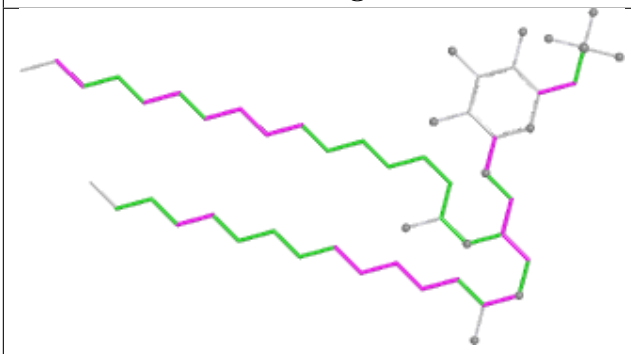
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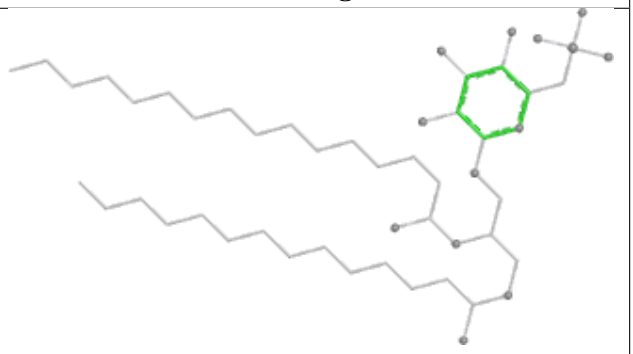
Bond lengths



Bond angles

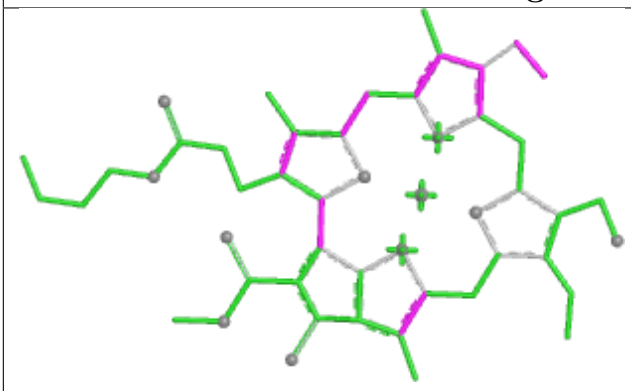


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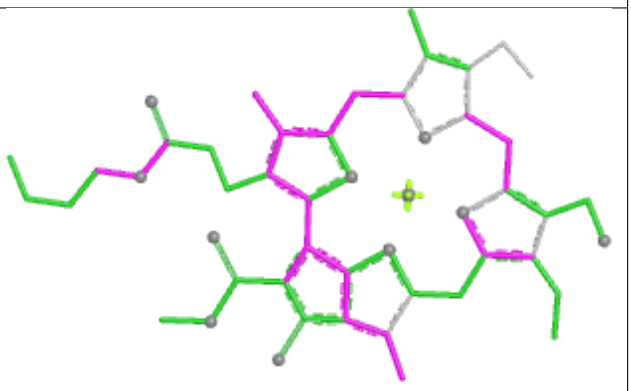


Rings

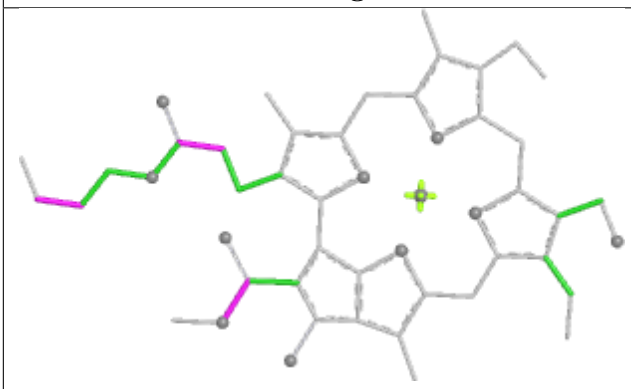
Ligand CHL n 301



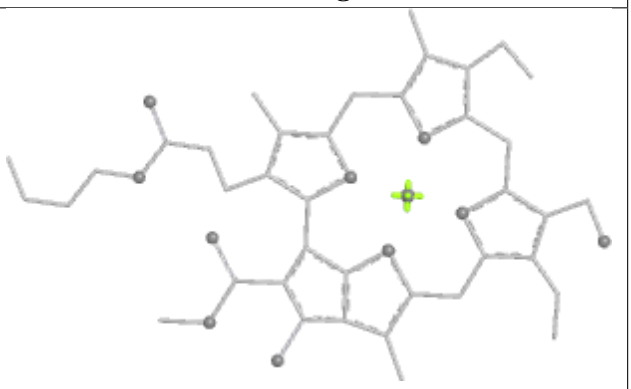
Bond lengths



Bond angles

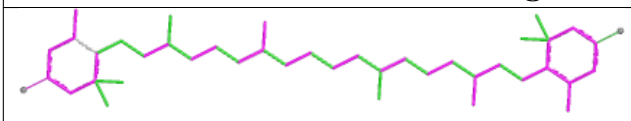


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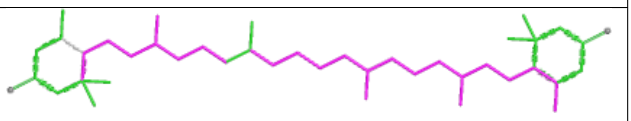


Rings

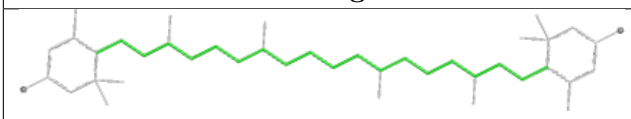
Ligand LUT Y 315



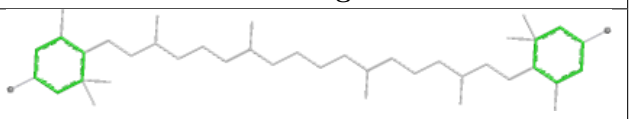
Bond lengths



Bond angles

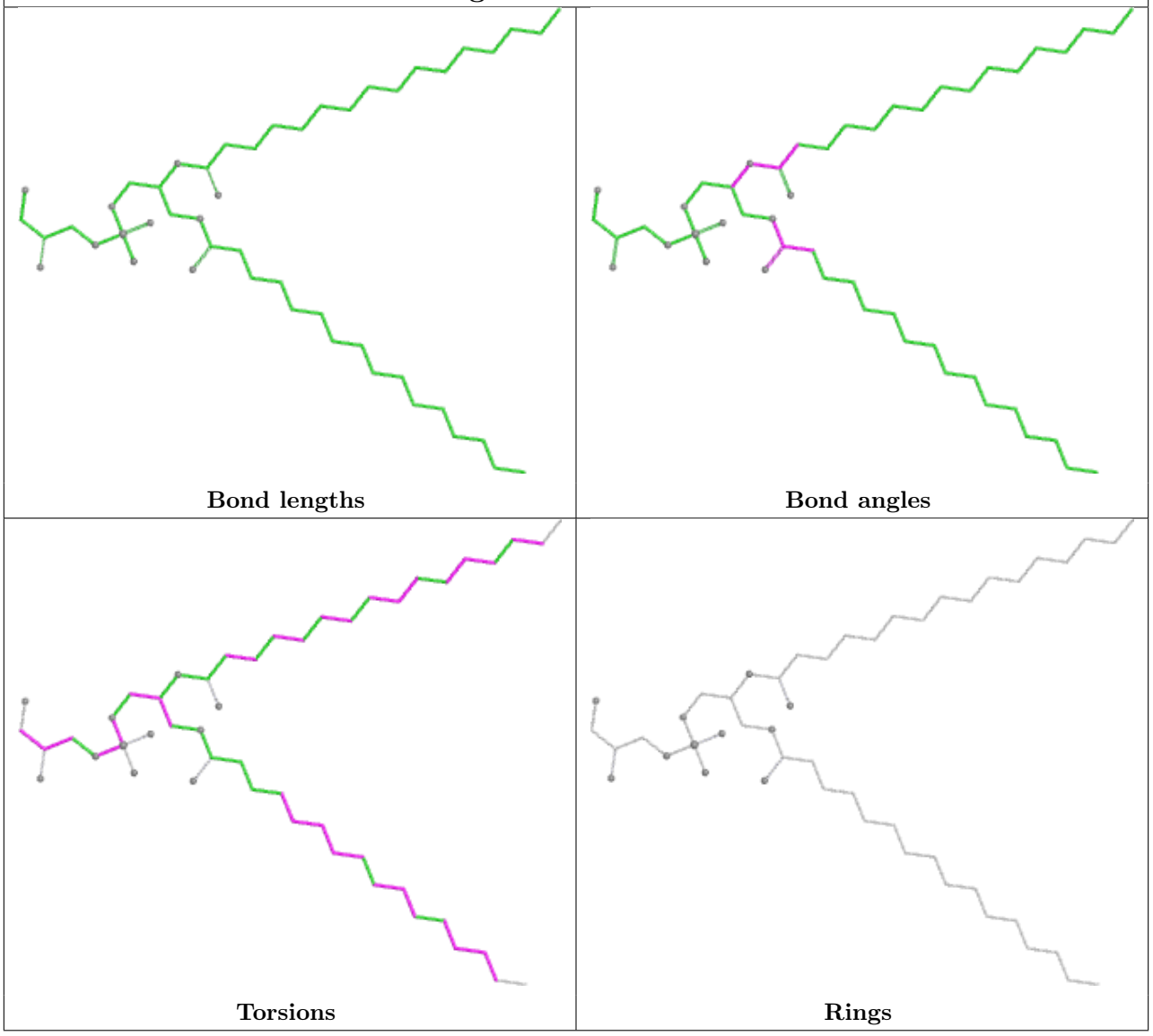


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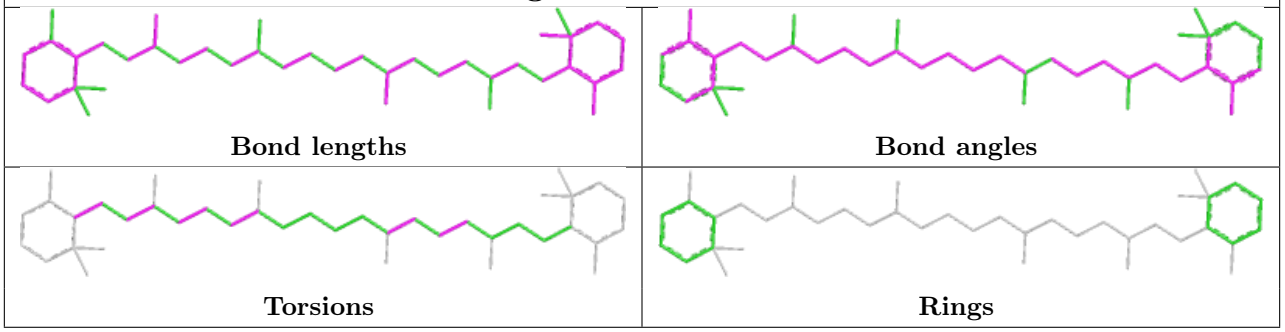


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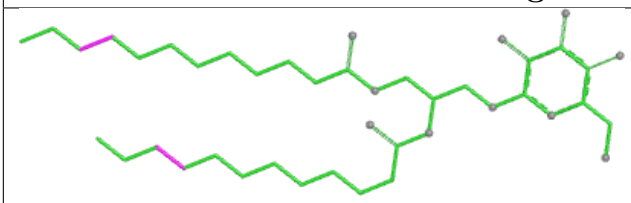
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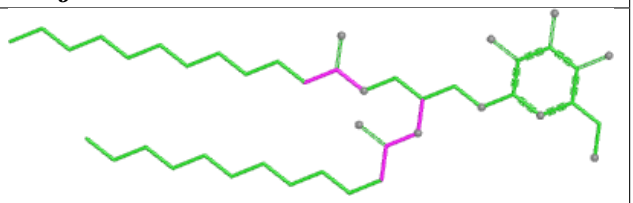
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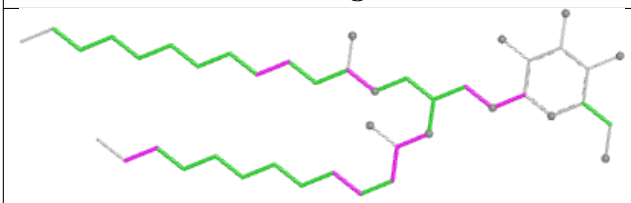
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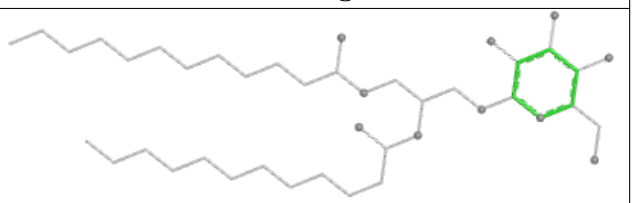
Bond lengths



Bond angles

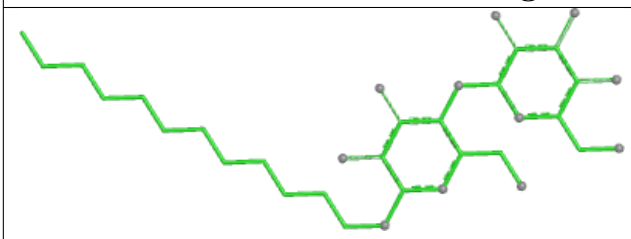


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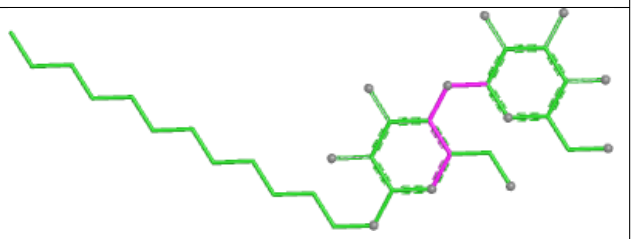


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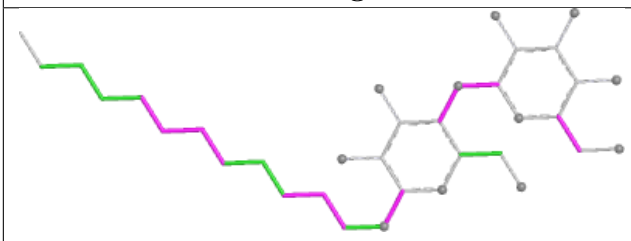
Ligand LMU R 302



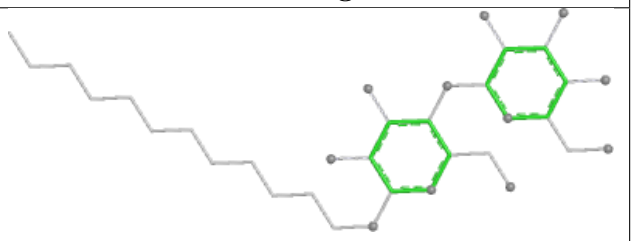
Bond lengths



Bond angles

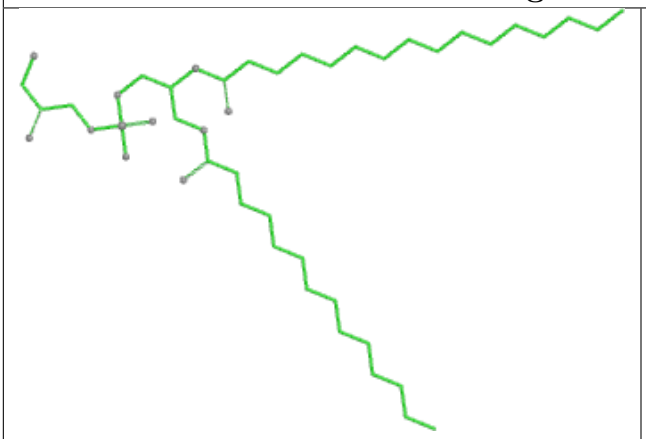


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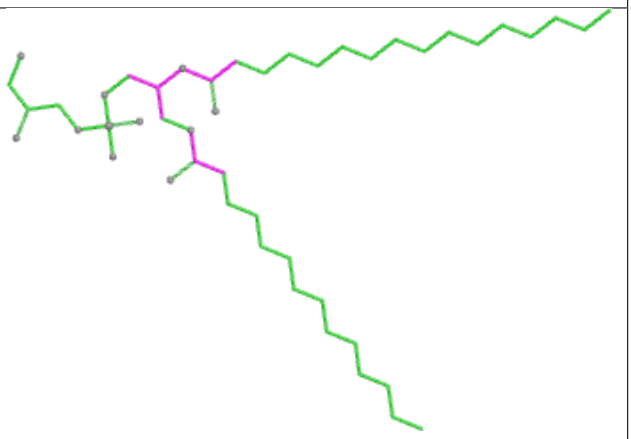


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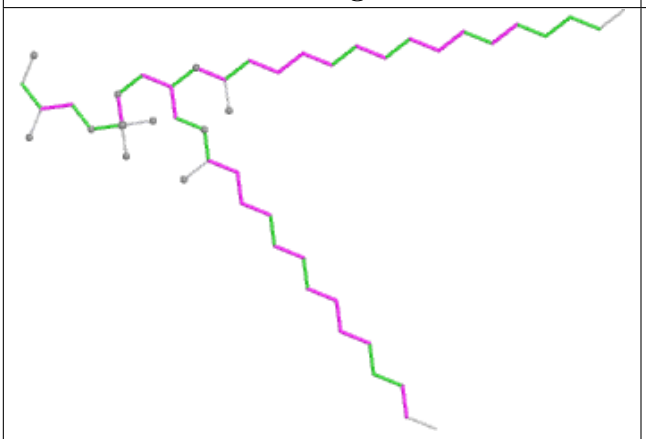
Ligand LHG 4 618



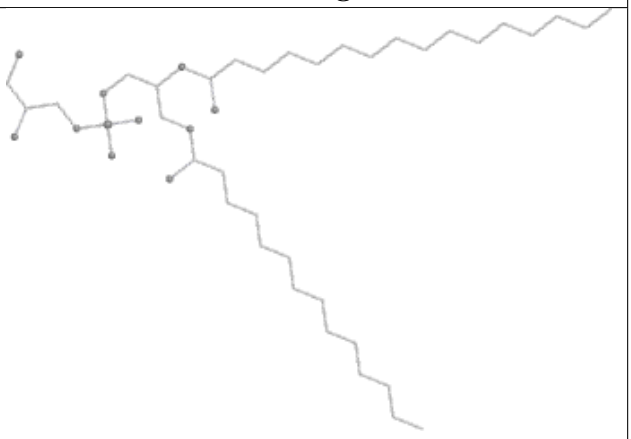
Bond lengths



Bond angles

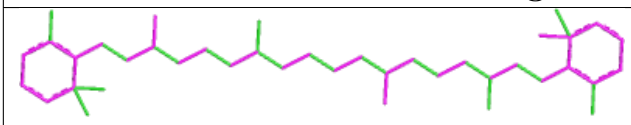


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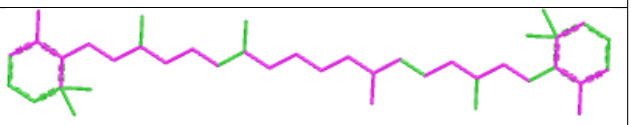


Rings

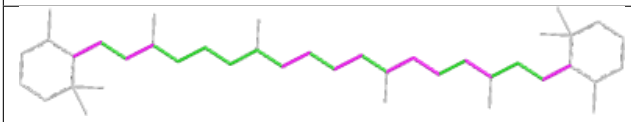
Ligand BCR a 410



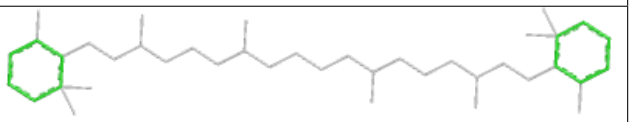
Bond lengths



Bond angles

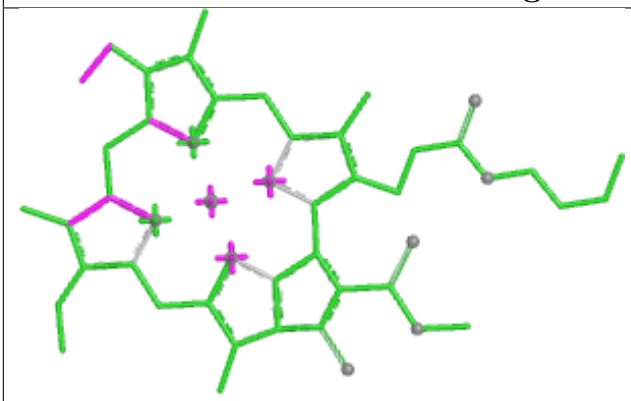


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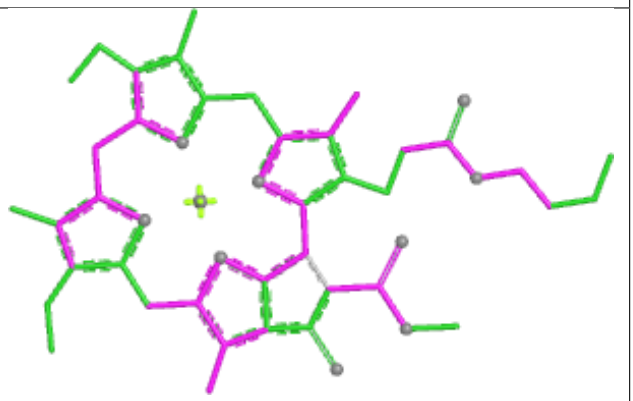


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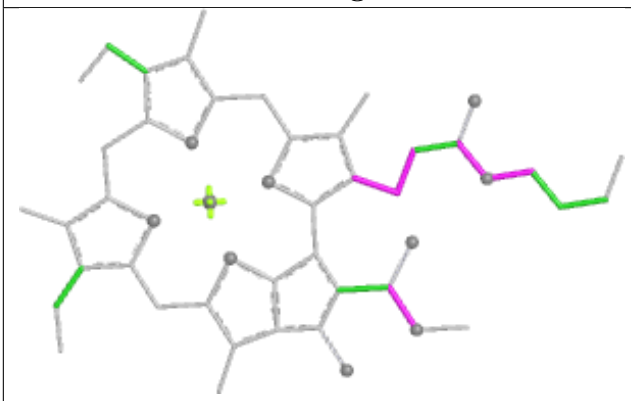
Ligand CLA N 311



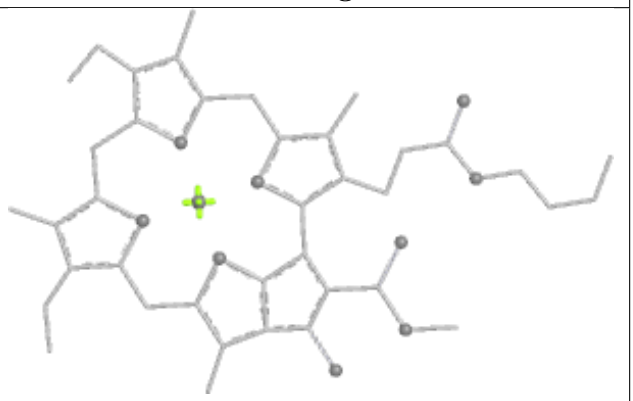
Bond lengths



Bond angles

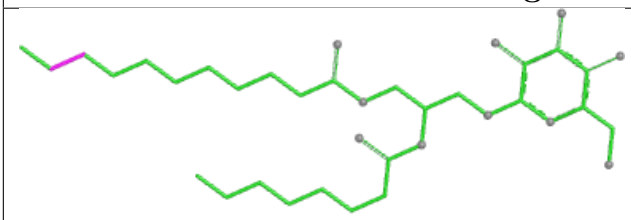


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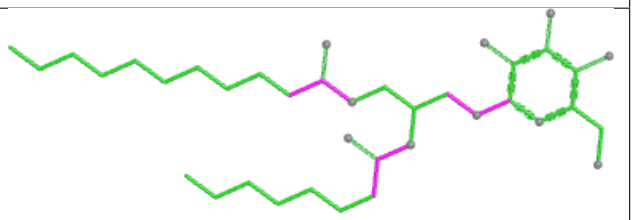


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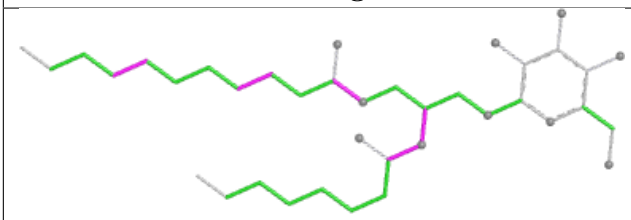
Ligand LMG 7 320



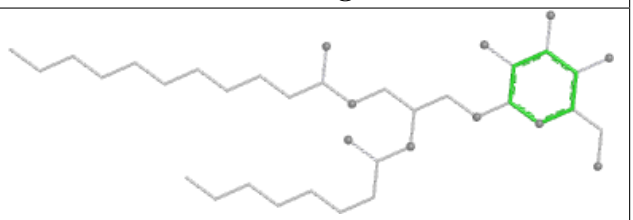
Bond lengths



Bond angles

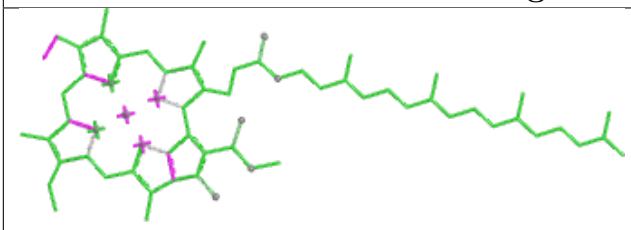


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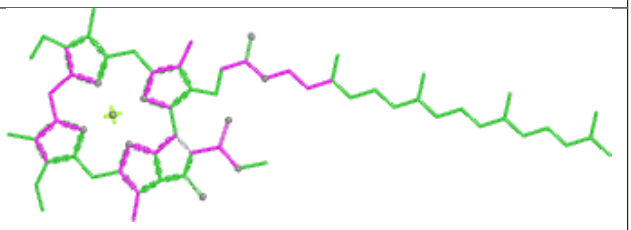


Rings

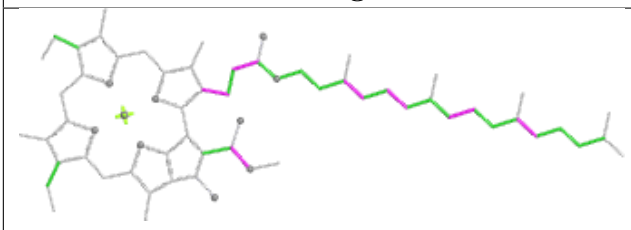
Ligand CLA b 609



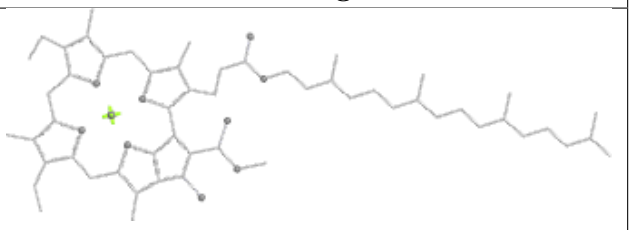
Bond lengths



Bond angles

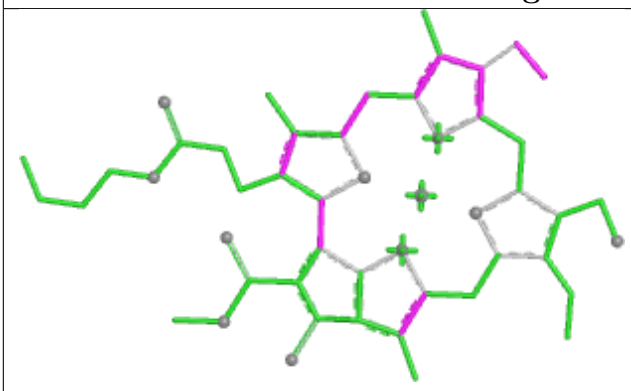


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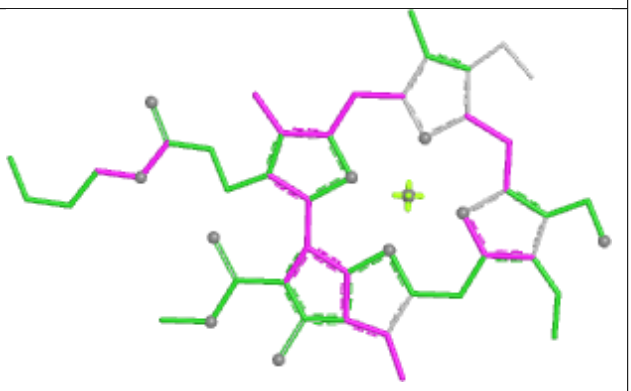


Rings

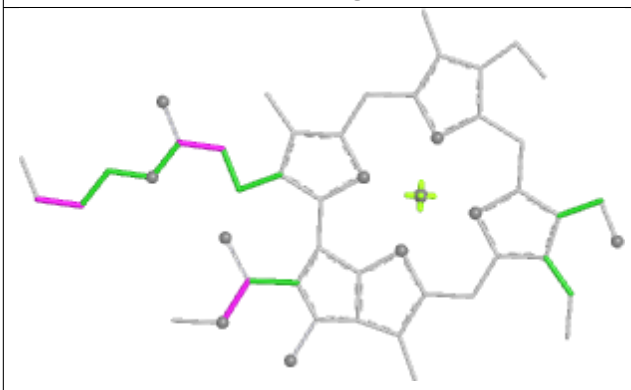
Ligand CHL N 301



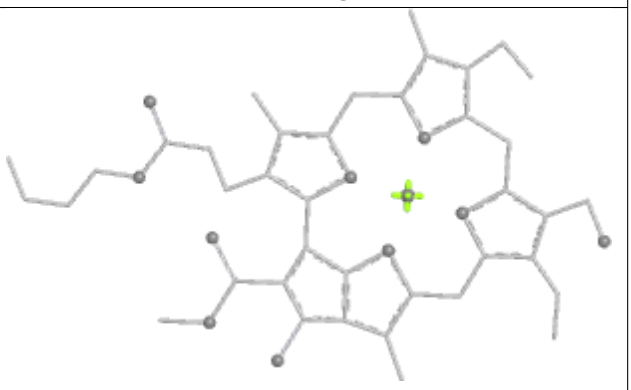
Bond lengths



Bond angles

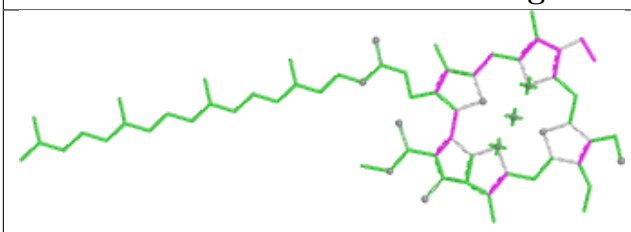


Torsions

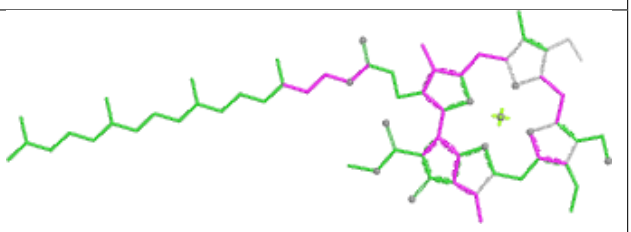


Rings

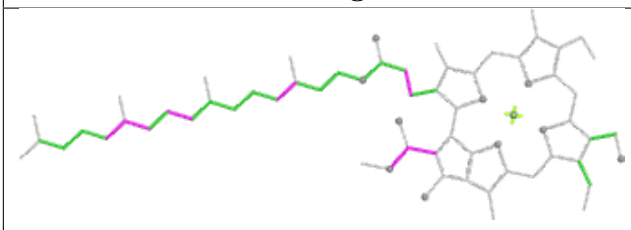
Ligand CHL 7 310



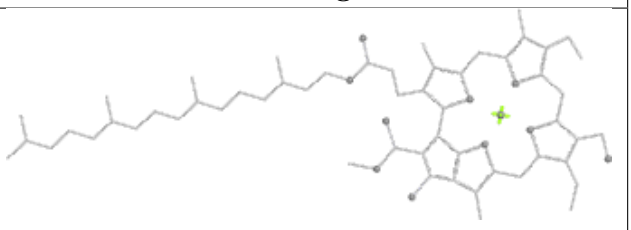
Bond lengths



Bond angles

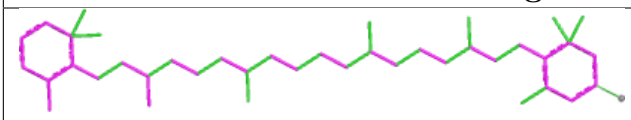


Torsions

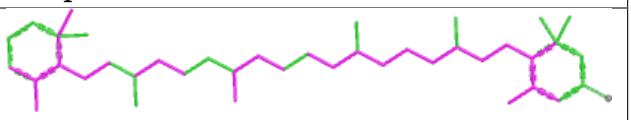


Rings

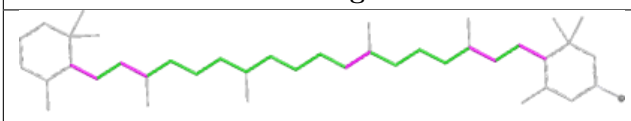
Ligand RRX q 317



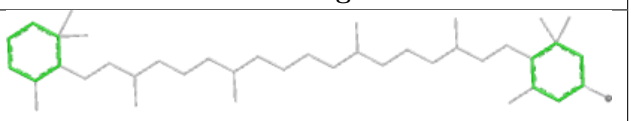
Bond lengths



Bond angles

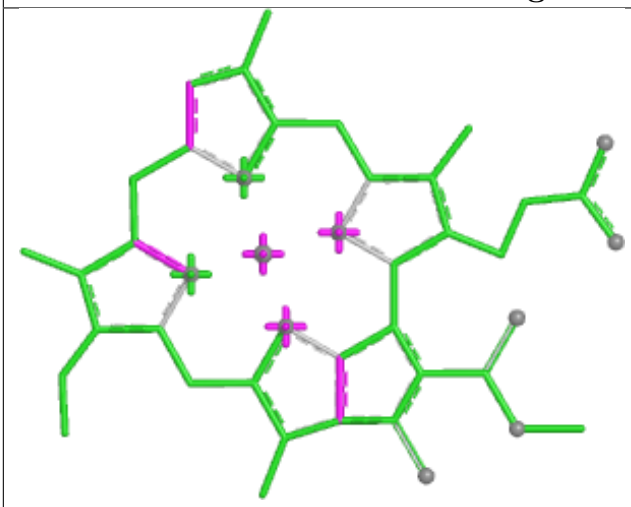


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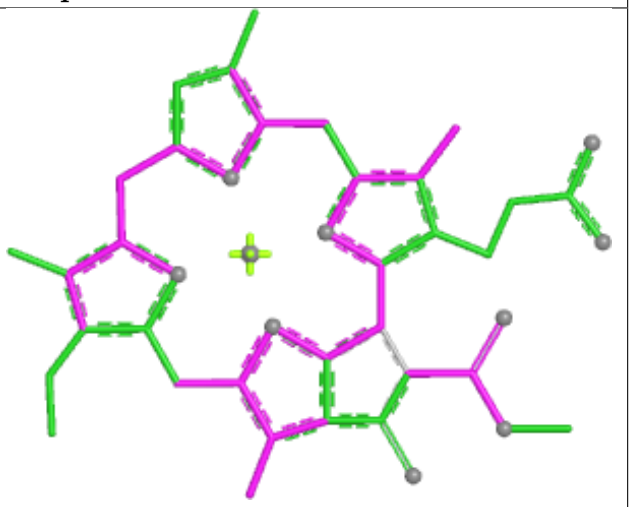


Rings

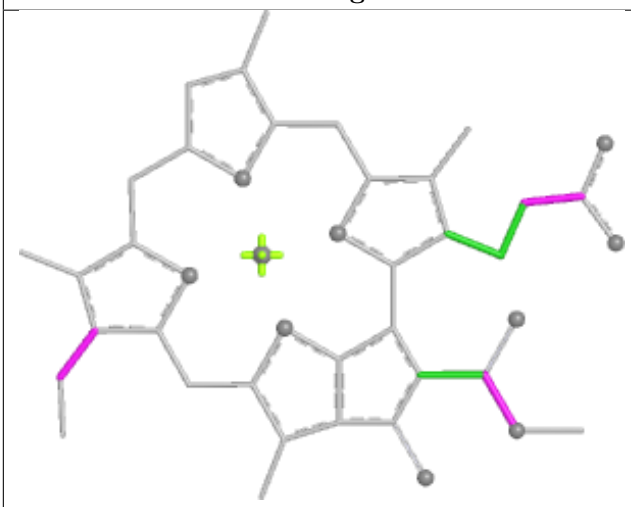
Ligand CLA q 313



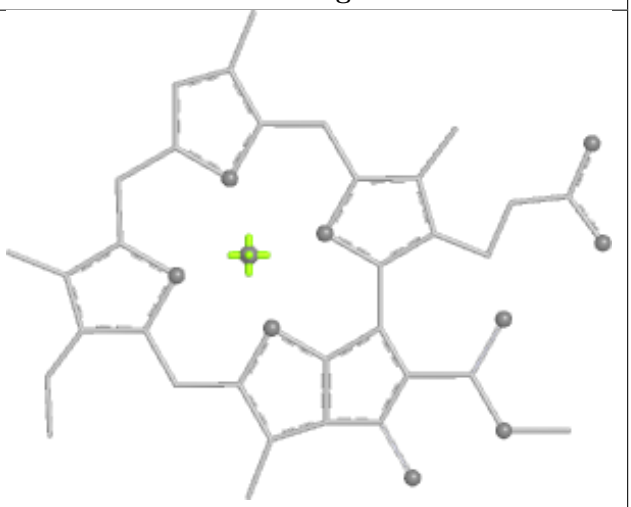
Bond lengths



Bond angles

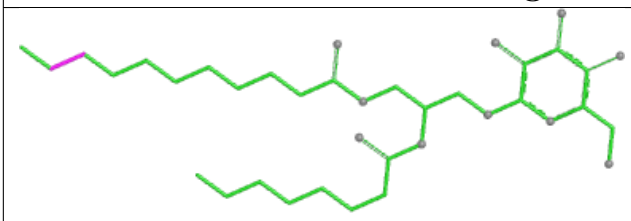


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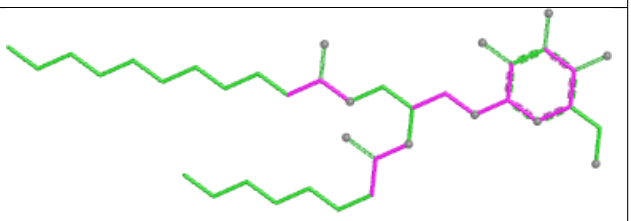


Rings

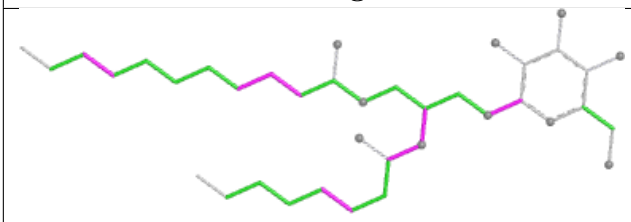
Ligand LMG a 413



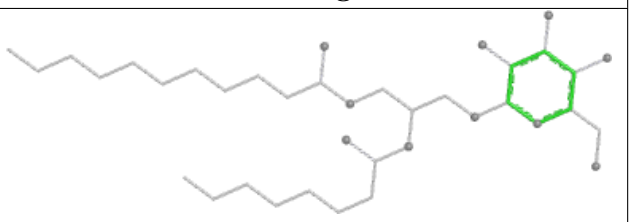
Bond lengths



Bond angles

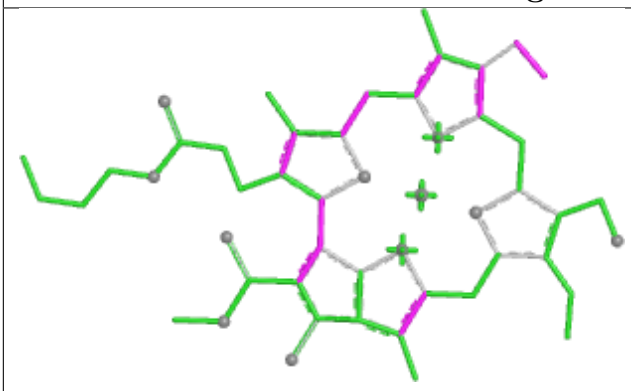


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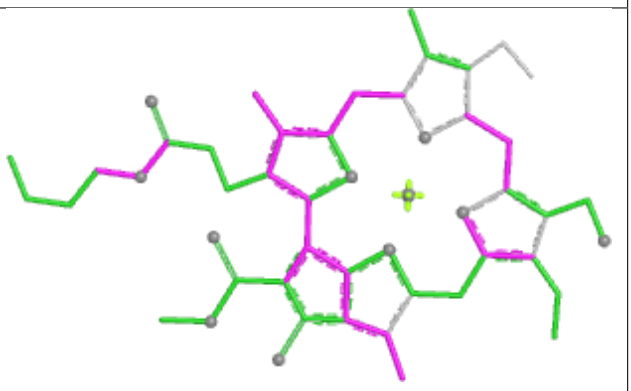


Rings

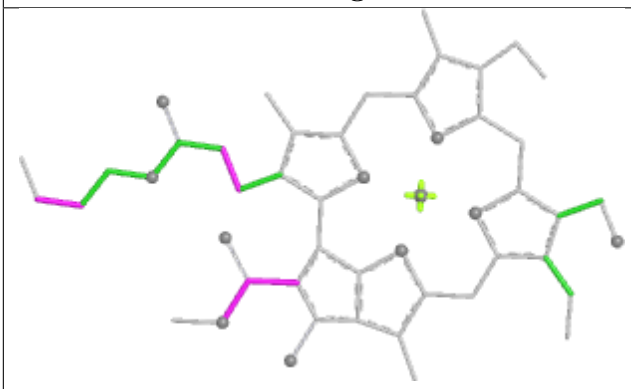
Ligand CHL n 309



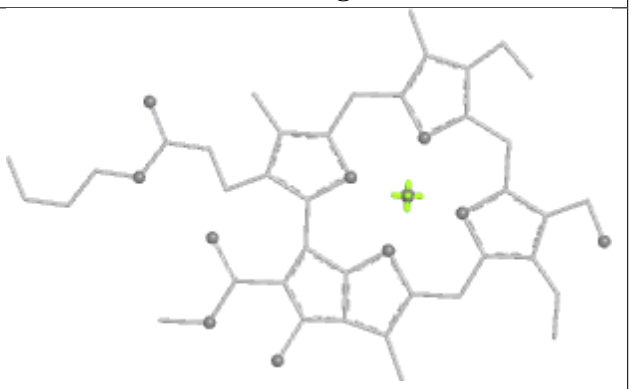
Bond lengths



Bond angles

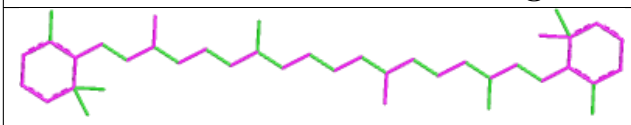


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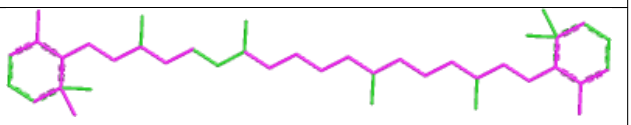


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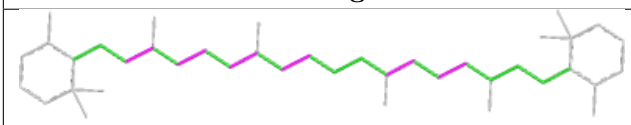
Ligand BCR h 101



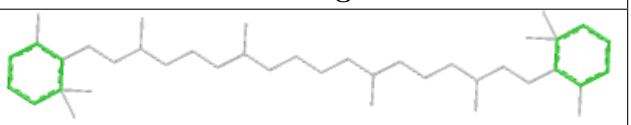
Bond lengths



Bond angles

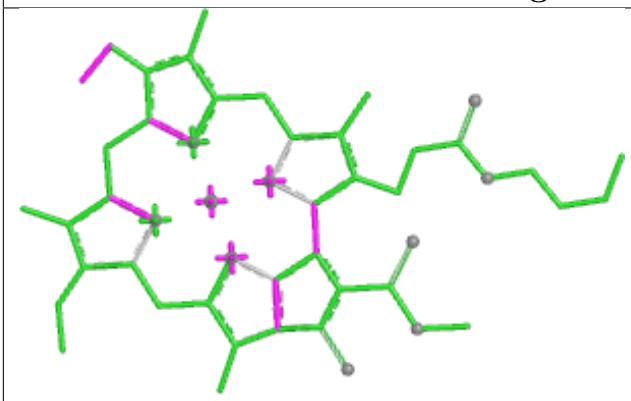


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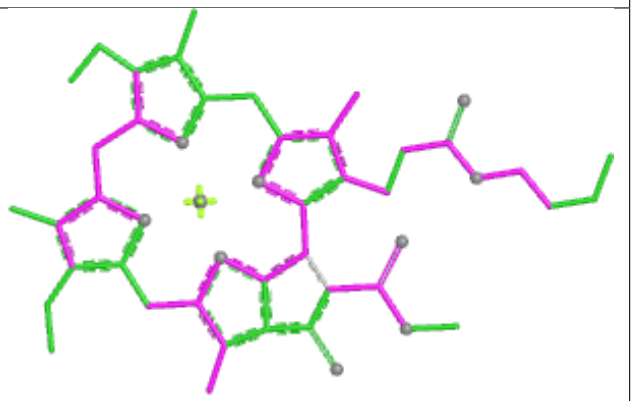


Rings

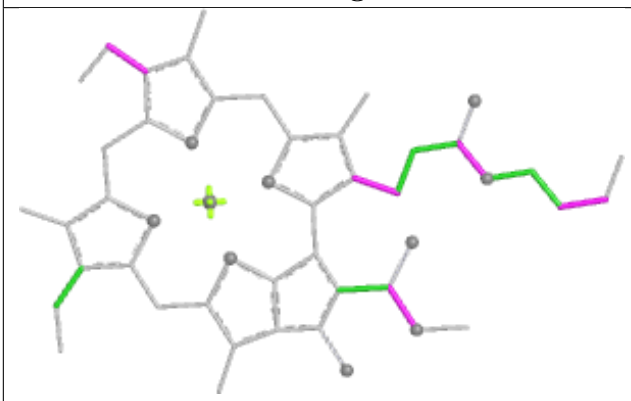
Ligand CLA r 313



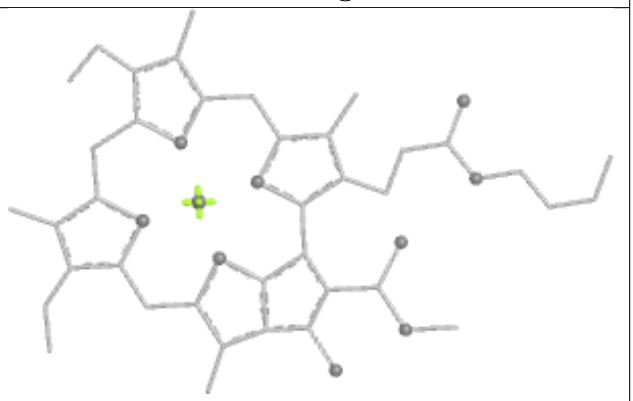
Bond lengths



Bond angles

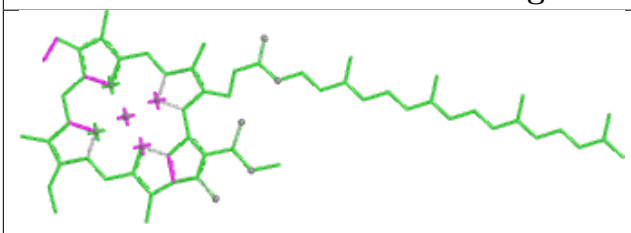


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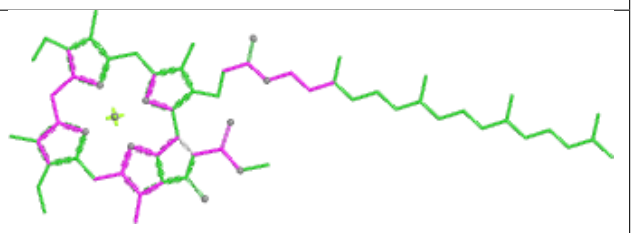


Rings

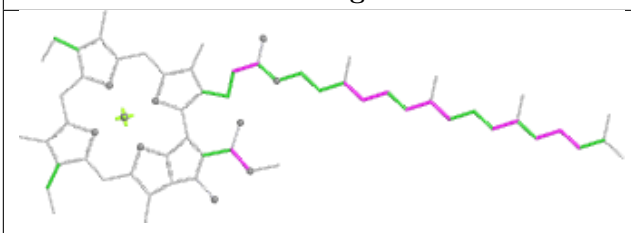
Ligand CLA d 404



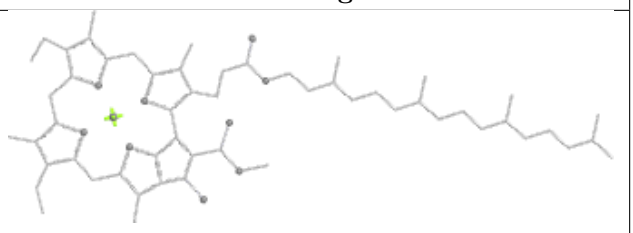
Bond lengths



Bond angles

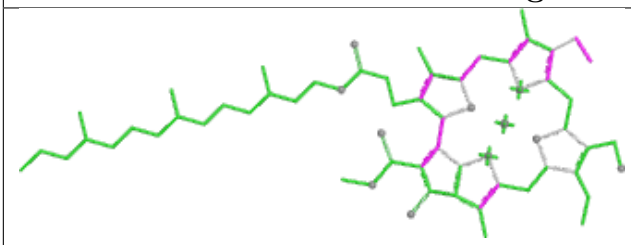


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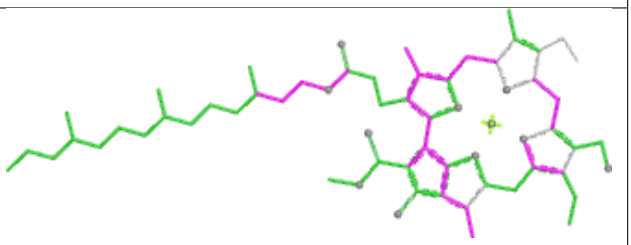


Rings

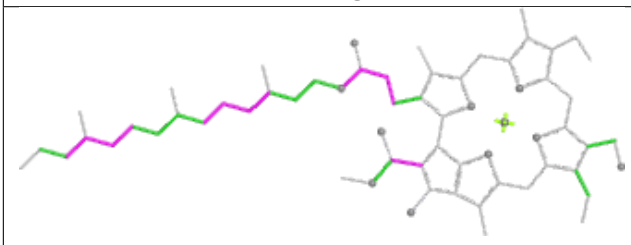
Ligand CHL n 308



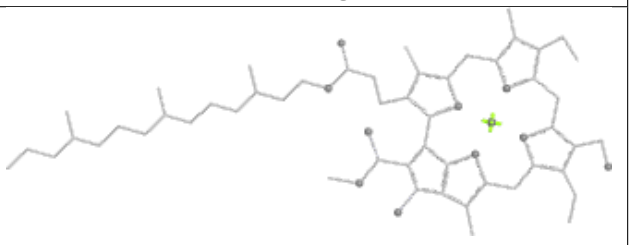
Bond lengths



Bond angles

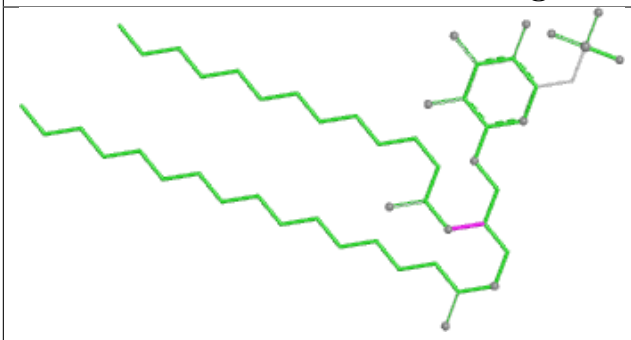


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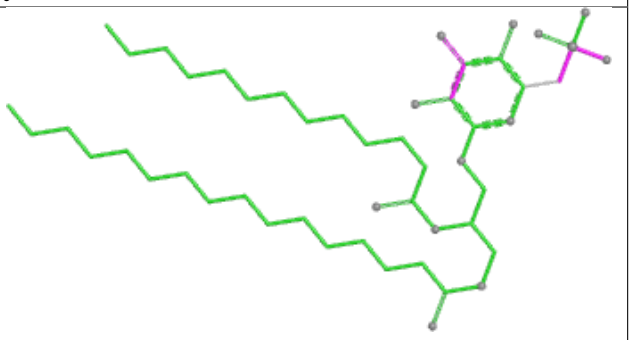


Rings

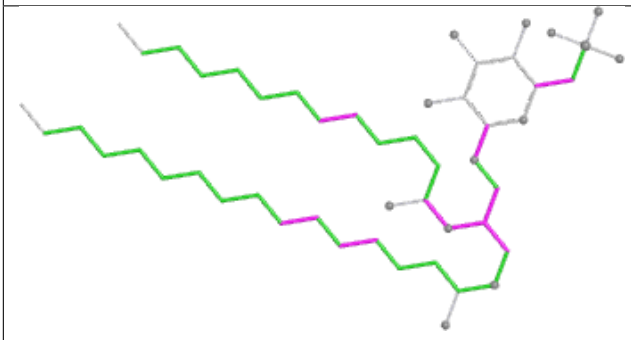
Ligand SQD r 322



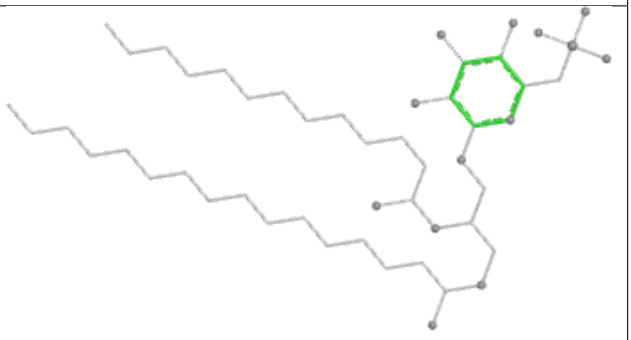
Bond lengths



Bond angles

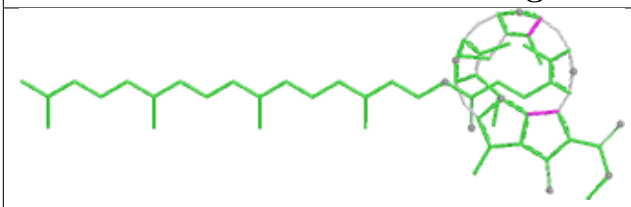


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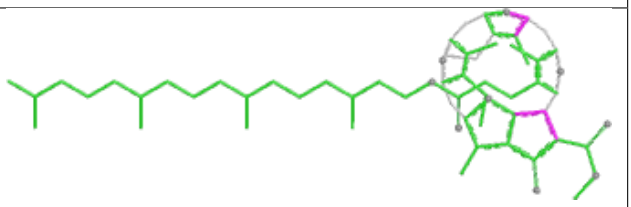


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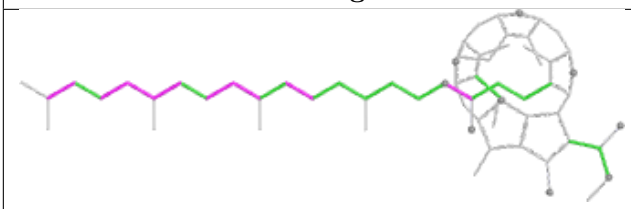
Ligand PHO a 408



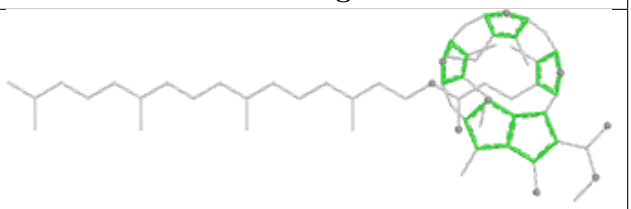
Bond lengths



Bond angles

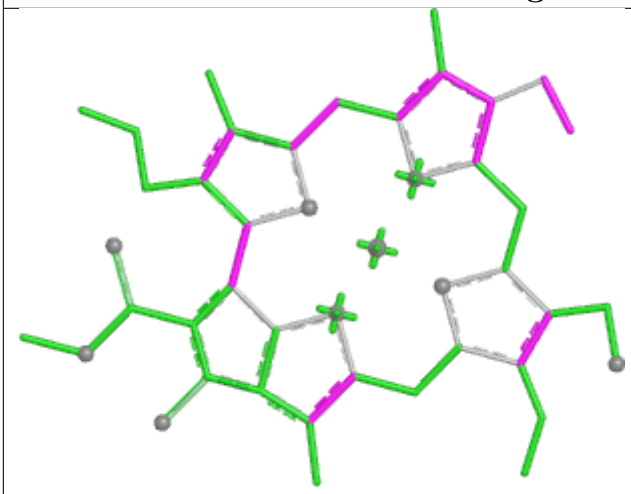


Torsions



Rings

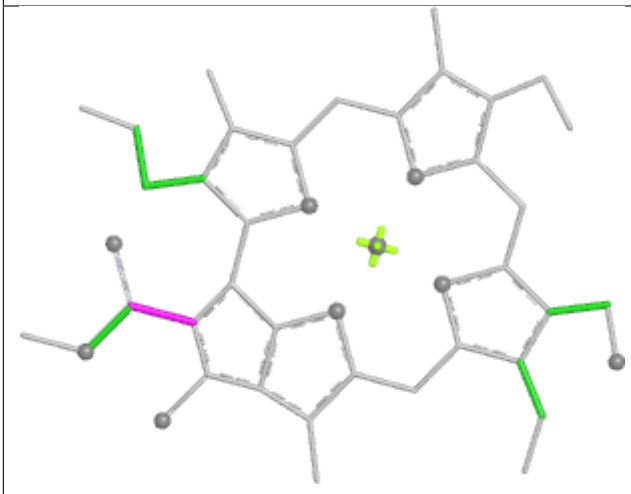
Ligand CHL S 307



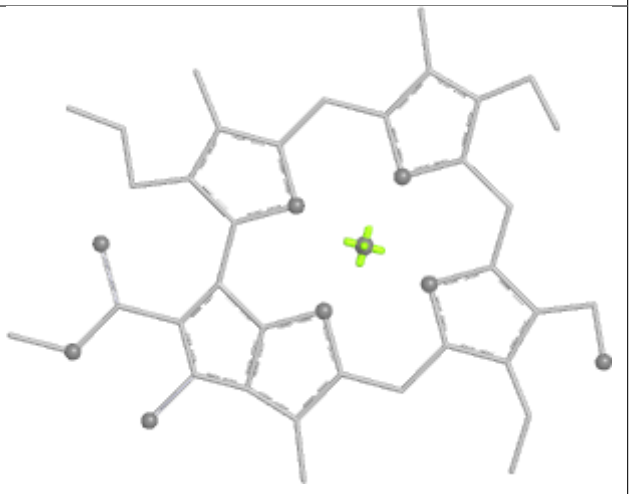
Bond lengths



Bond angles

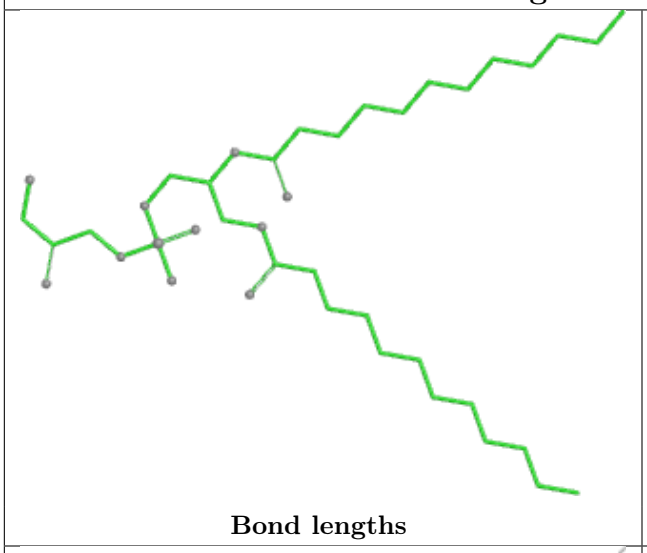


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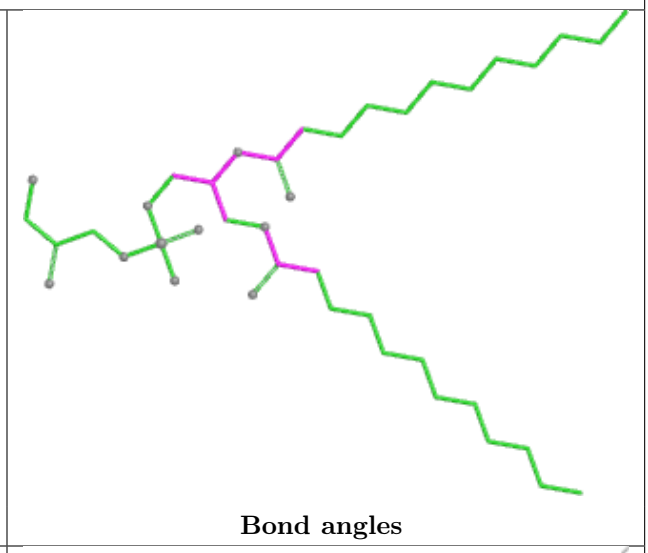


Rings

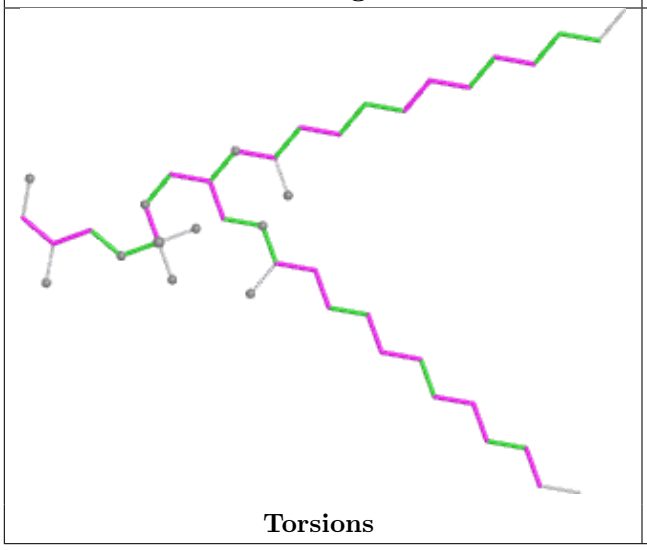
Ligand LHG s 320



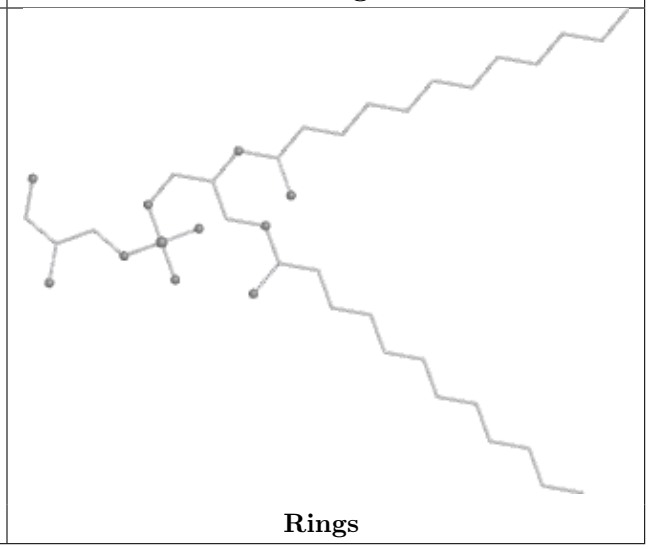
Bond lengths



Bond angles

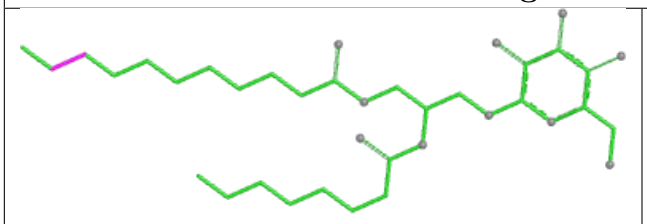


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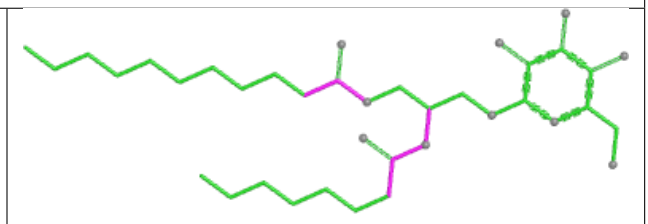


Rings

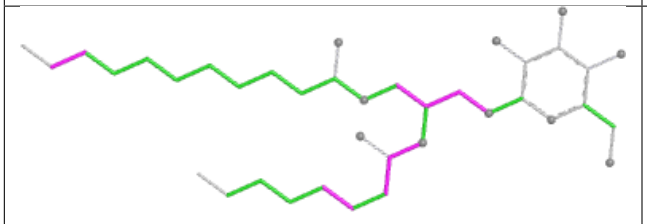
Ligand LMG X 203



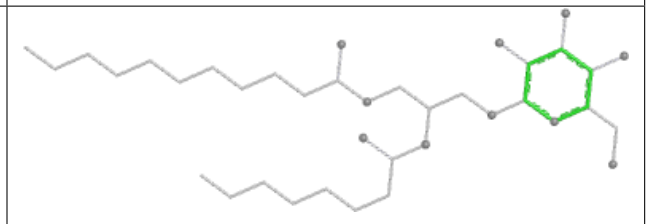
Bond lengths



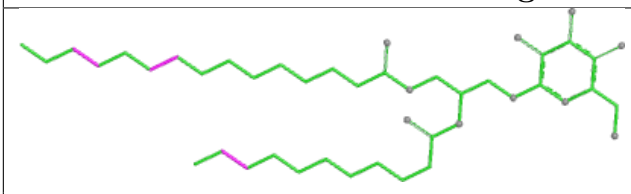
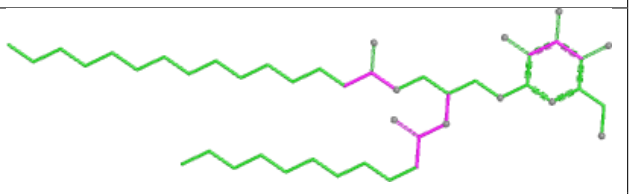
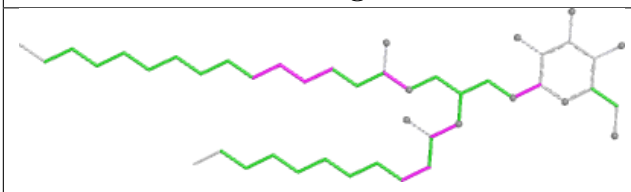
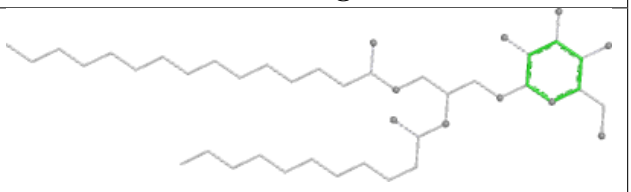
Bond angles

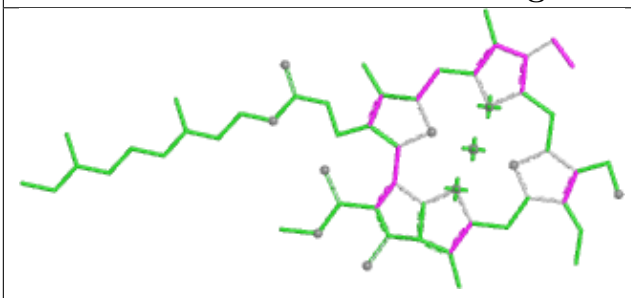
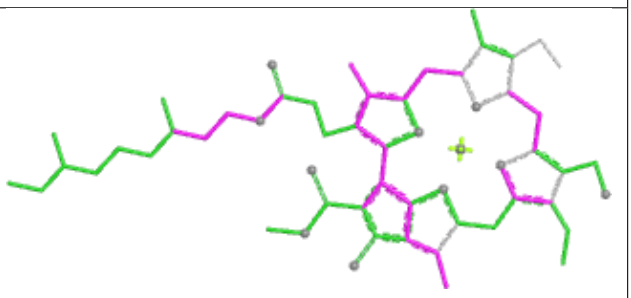
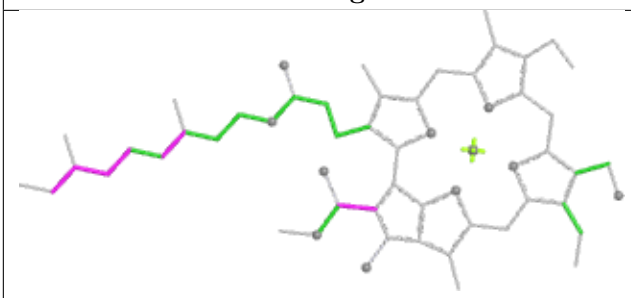
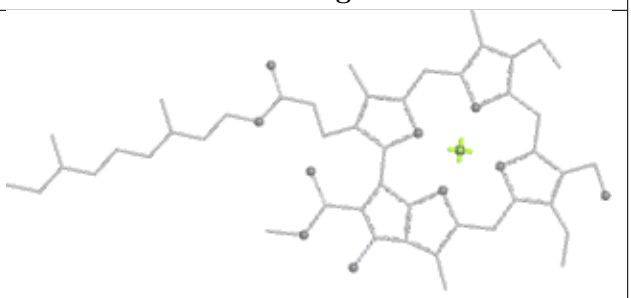


Torsions

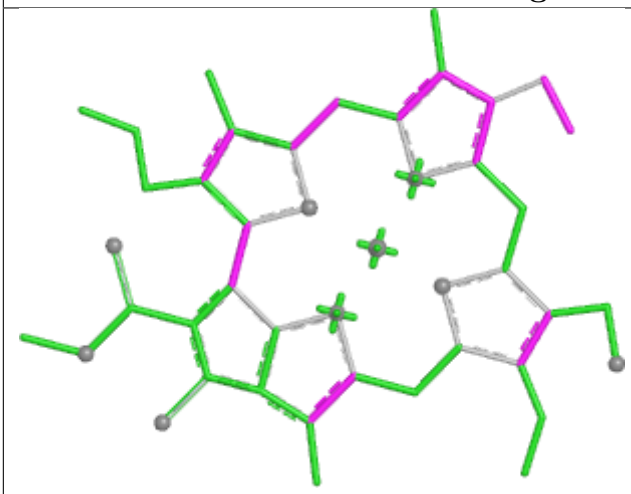


Rings

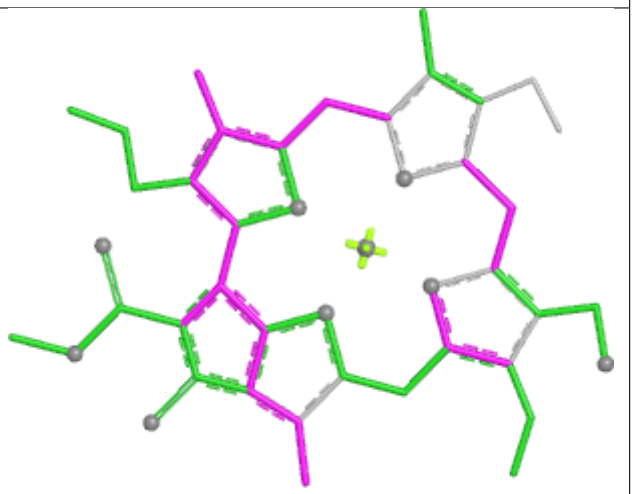
Ligand LMG m 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 2 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

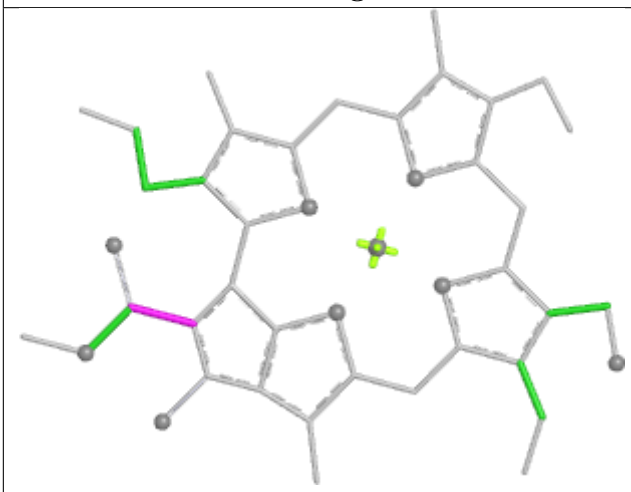
Ligand CHL s 307



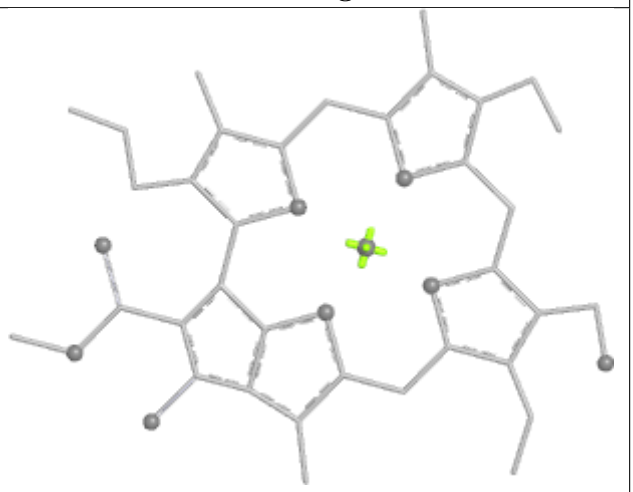
Bond lengths



Bond angles

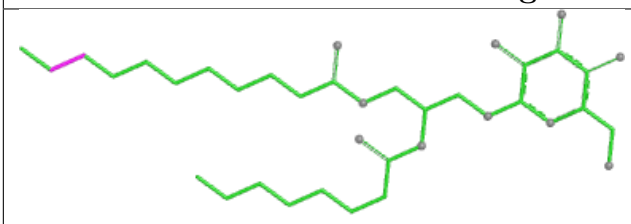


Torsions

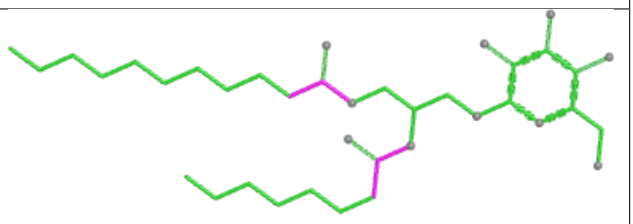


Rings

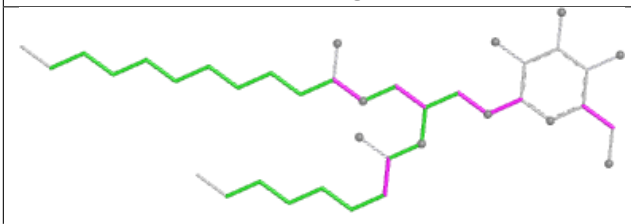
Ligand LMG R 321



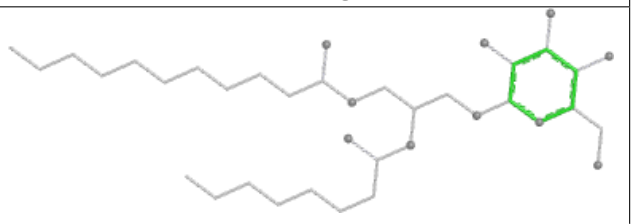
Bond lengths



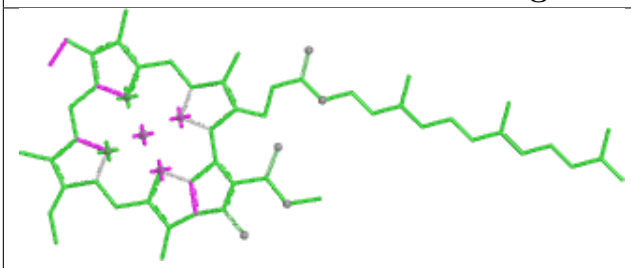
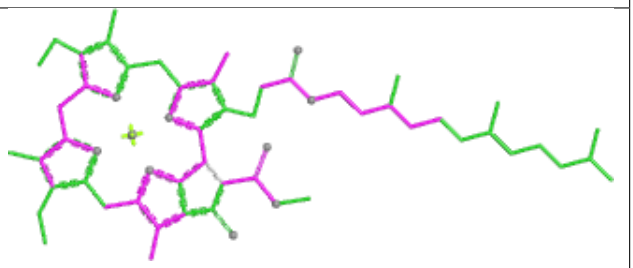
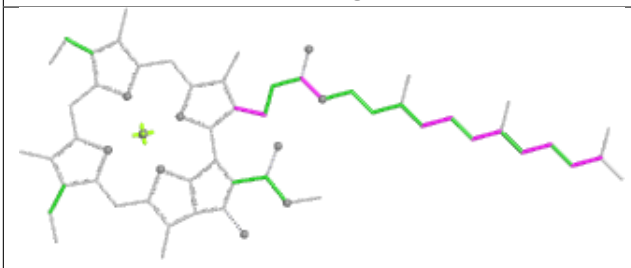
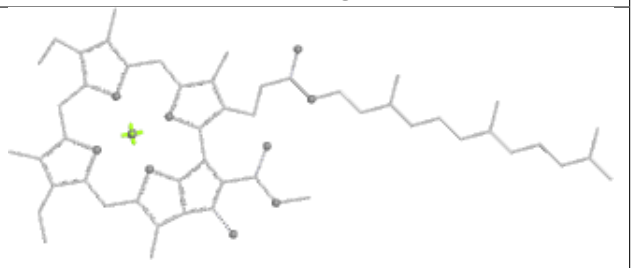
Bond angles

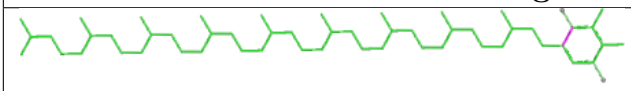
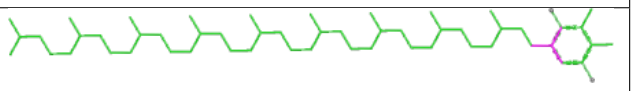
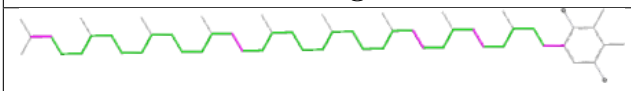
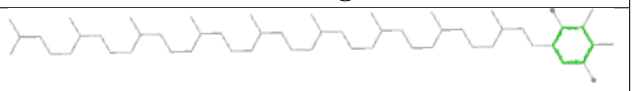


Torsions

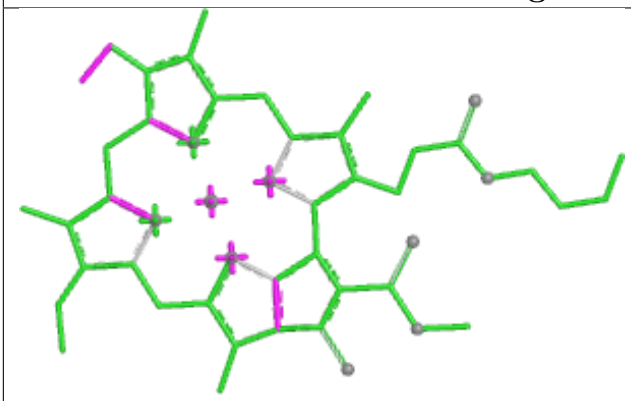


Rings

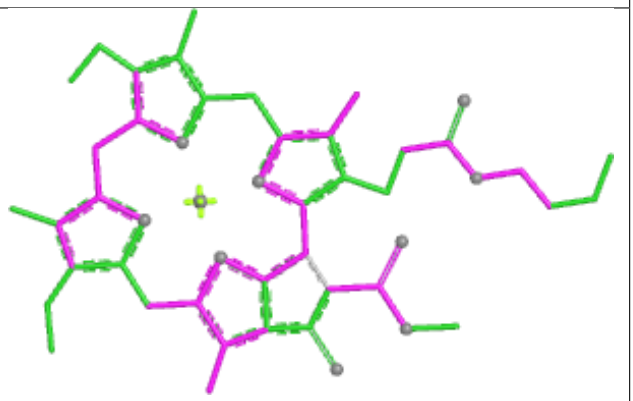
Ligand CLA r 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 d 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

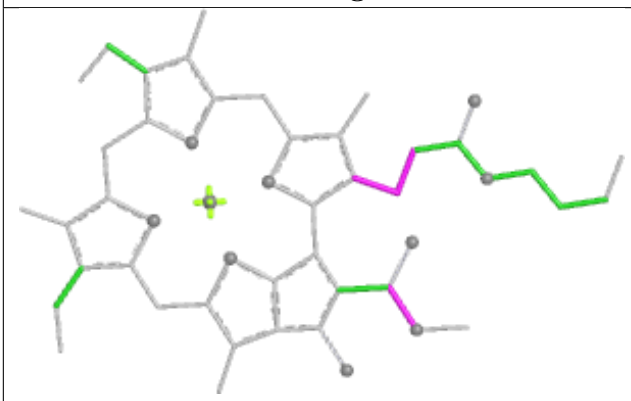
Ligand CLA 8 610



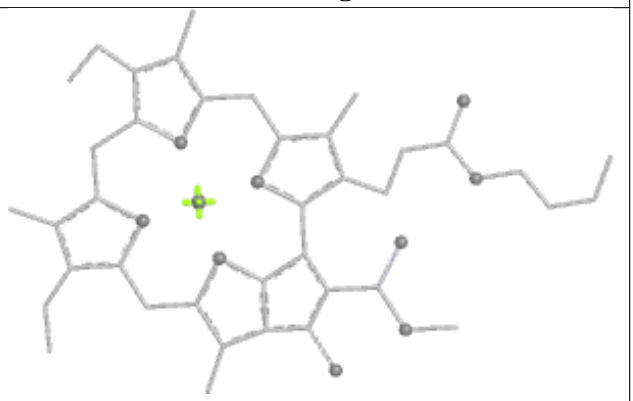
Bond lengths



Bond angles

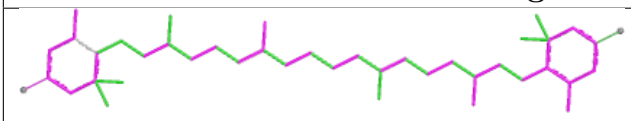


Torsions

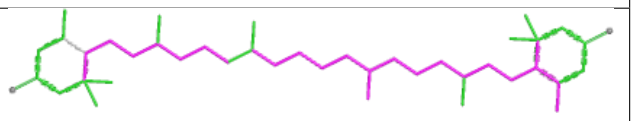


Rings

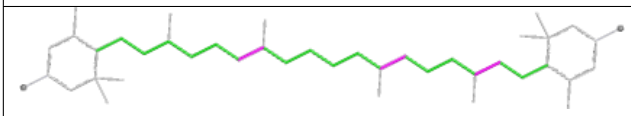
Ligand LUT S 317



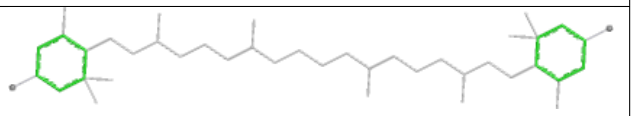
Bond lengths



Bond angles

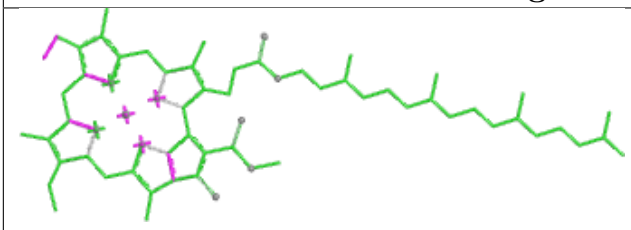


Torsions

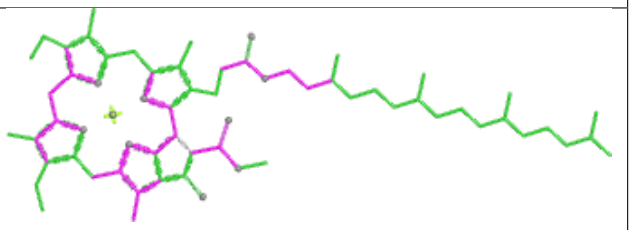


Rings

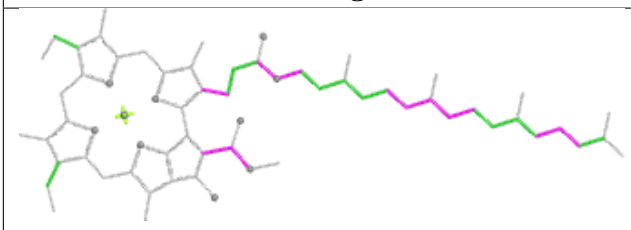
Ligand CLA 7 305



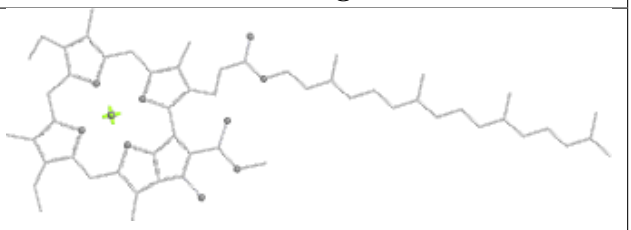
Bond lengths



Bond angles

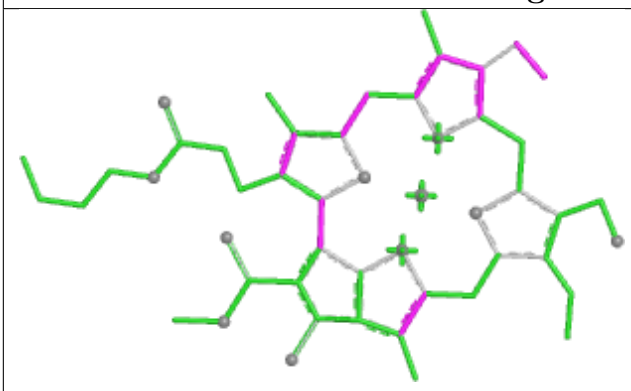


Torsions

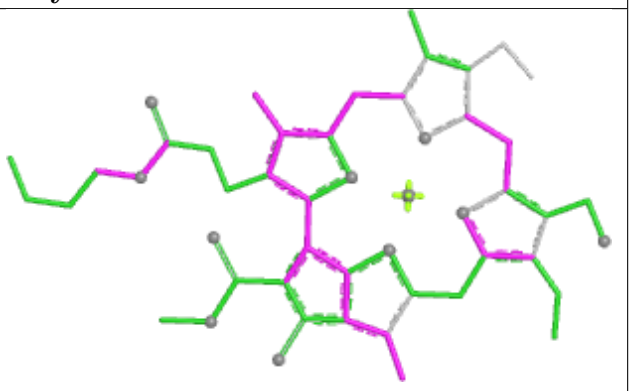


Rings

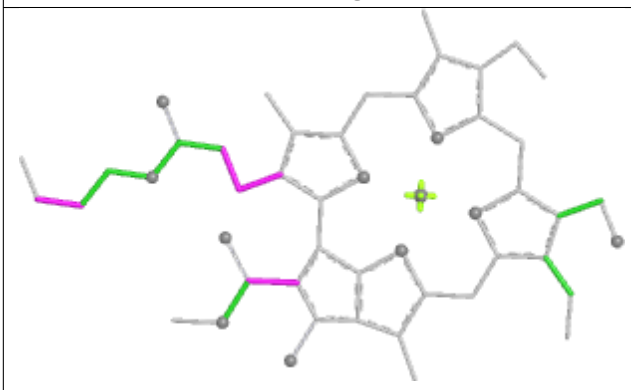
Ligand CHL y 608



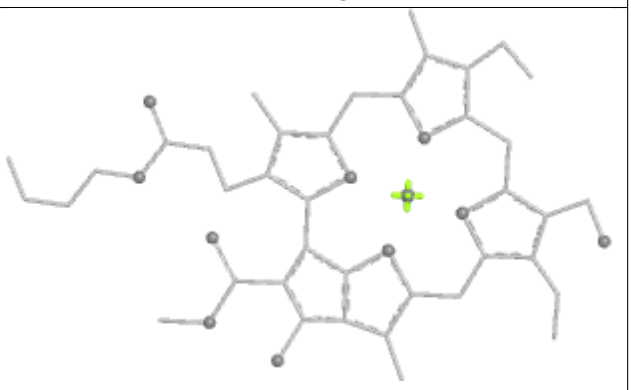
Bond lengths



Bond angles

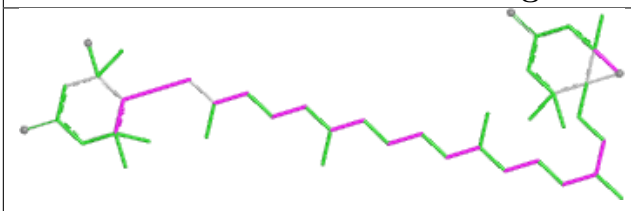


Torsions

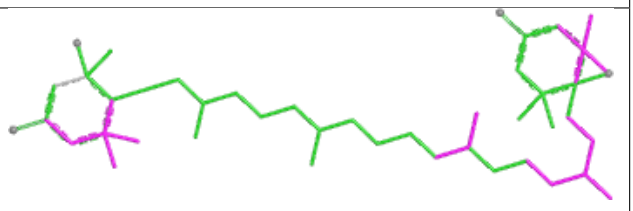


Rings

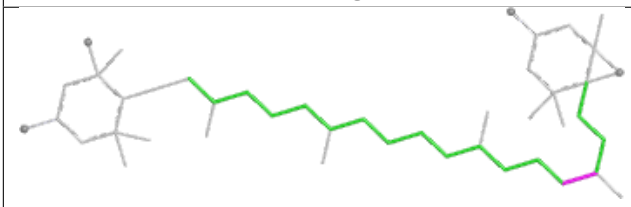
Ligand NEX Y 317



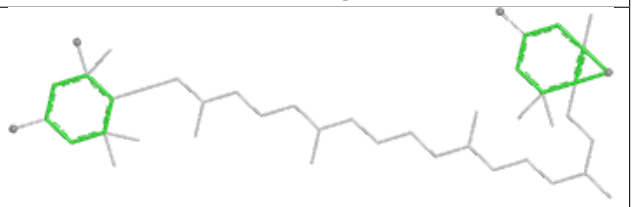
Bond lengths



Bond angles

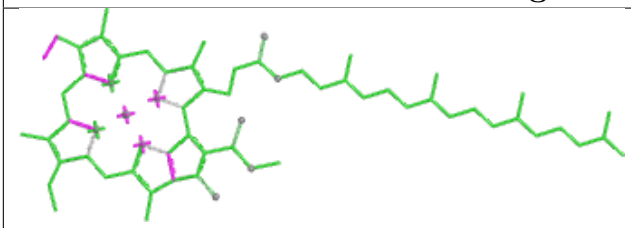


Torsions

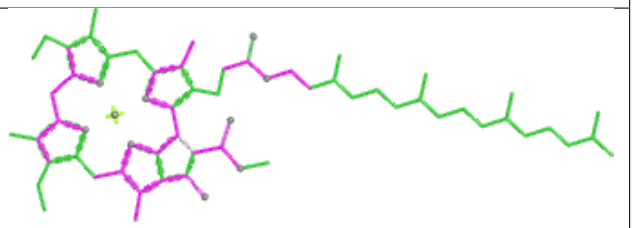


Rings

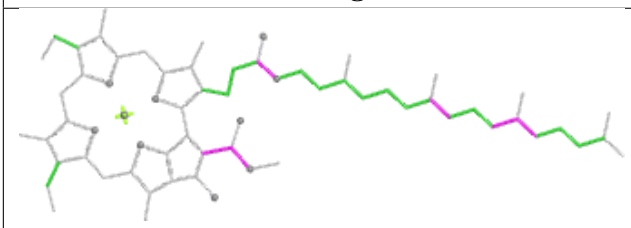
Ligand CLA c 607



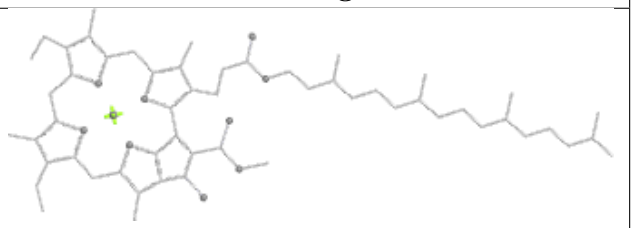
Bond lengths



Bond angles

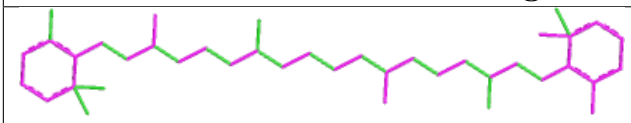


Torsions

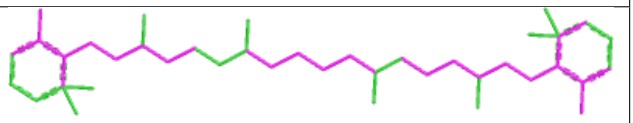


Rings

Ligand BCR B 619



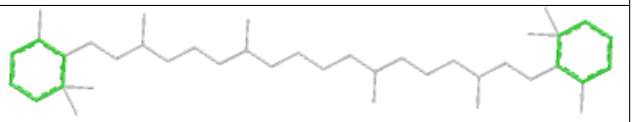
Bond lengths



Bond angles

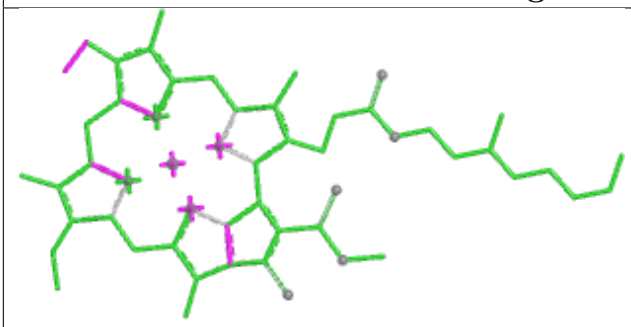


Torsions

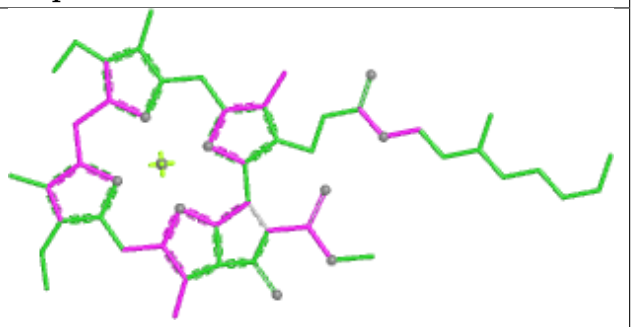


Rings

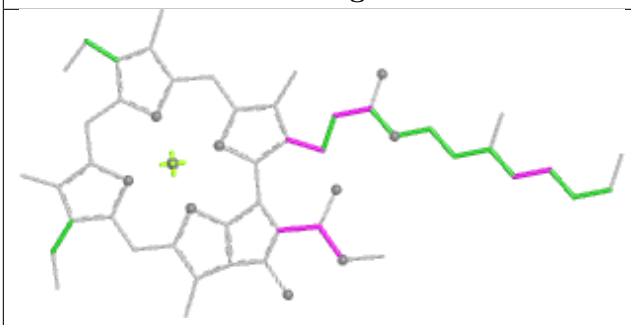
Ligand CLA p 613



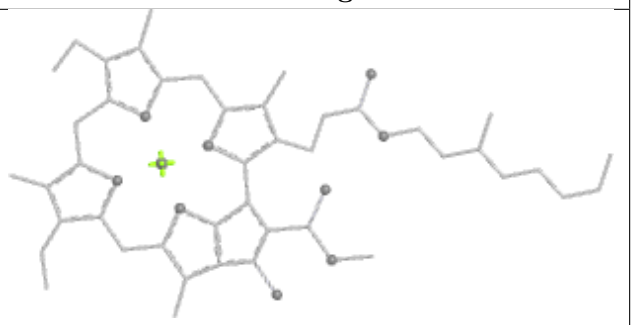
Bond lengths



Bond angles

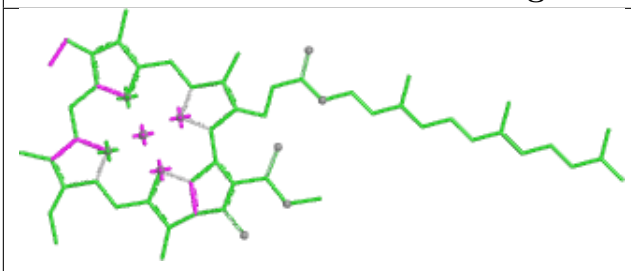


Torsions

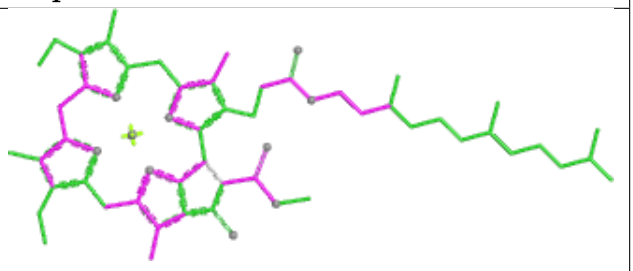


Rings

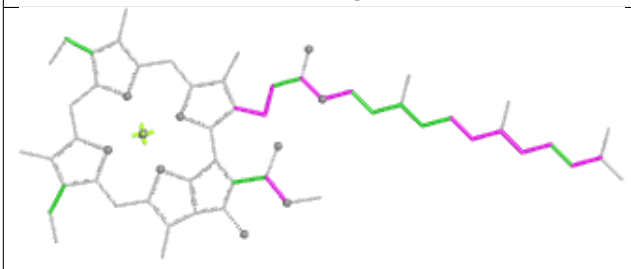
Ligand CLA p 611



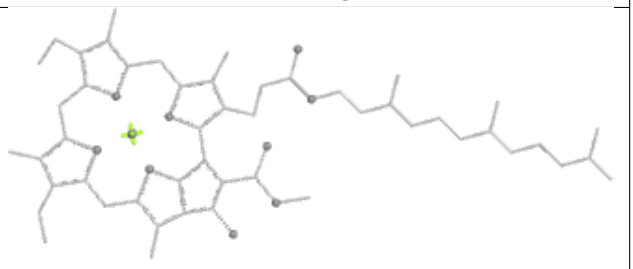
Bond lengths



Bond angles

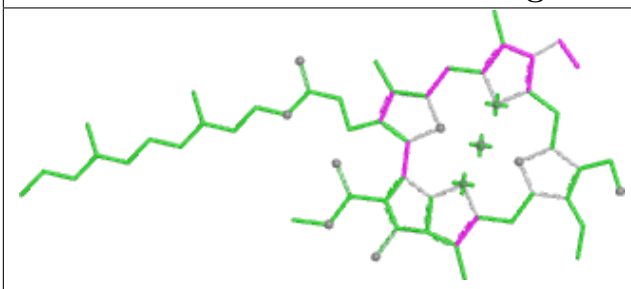


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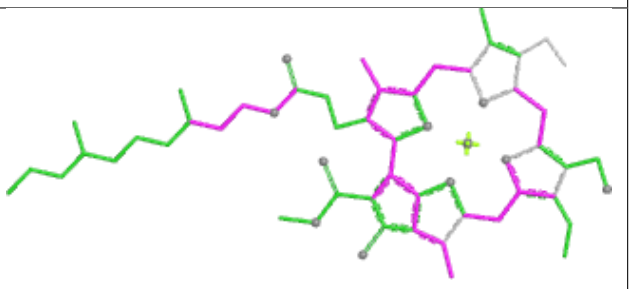


Rings

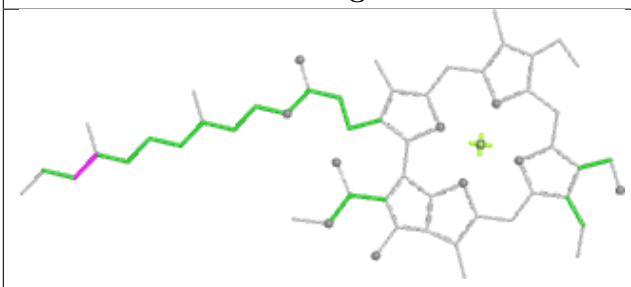
Ligand CHL n 307



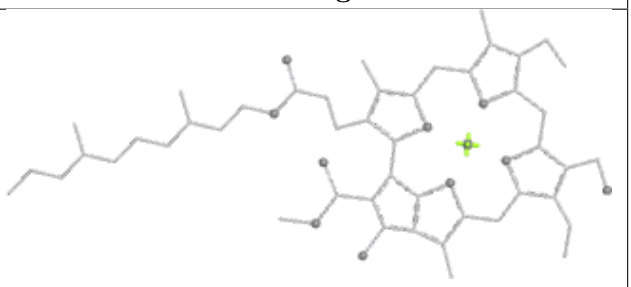
Bond lengths



Bond angles

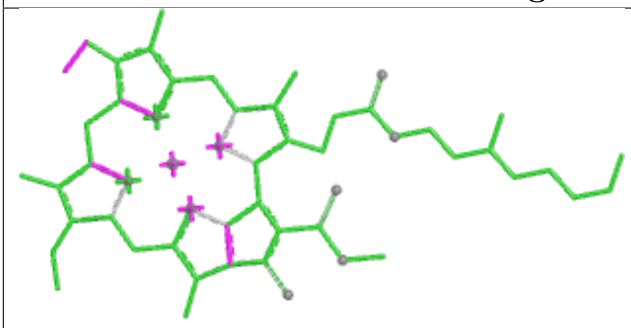


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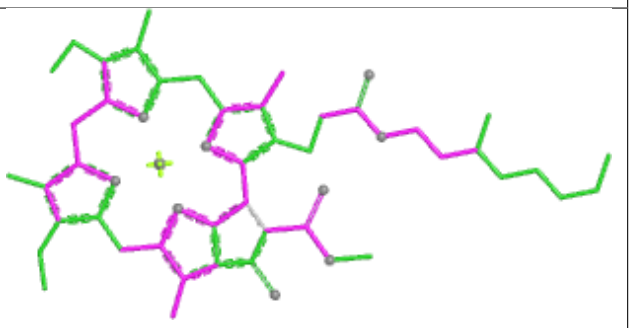


Rings

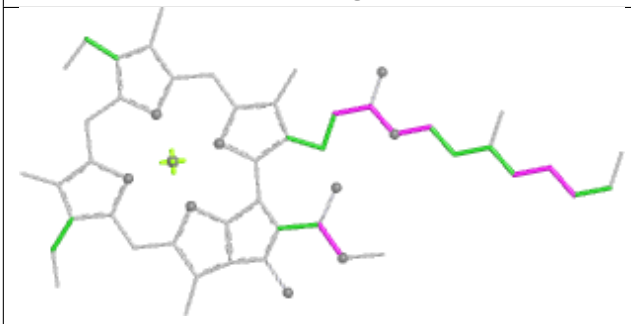
Ligand CLA 5 613



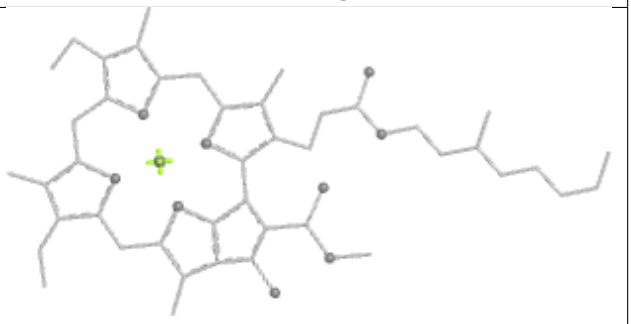
Bond lengths



Bond angles

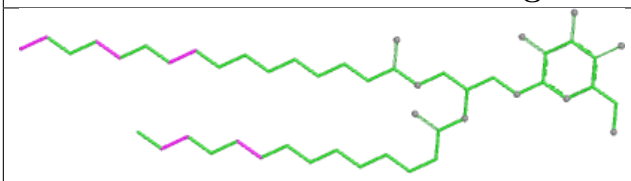


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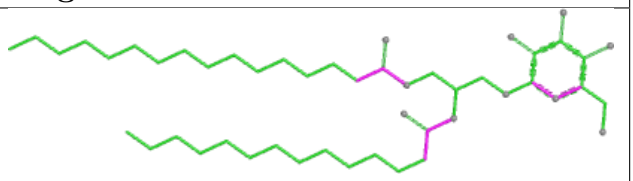


Rings

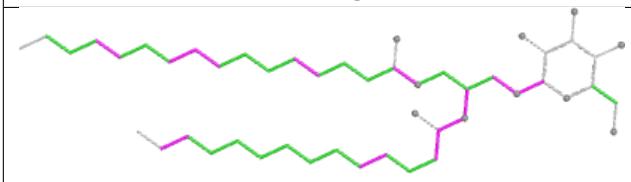
Ligand LMG g 322



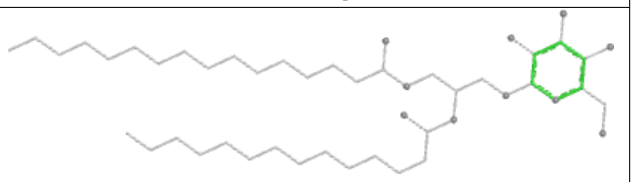
Bond lengths



Bond angles

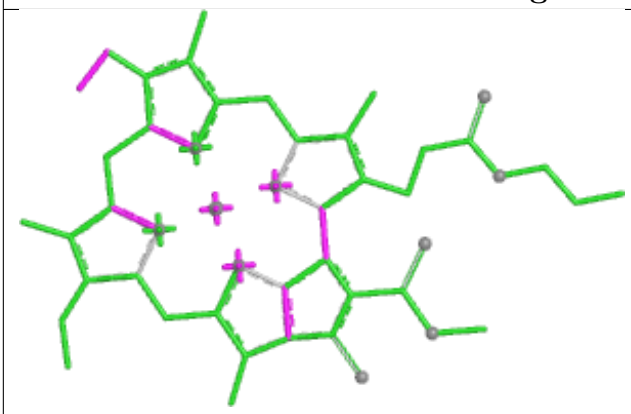


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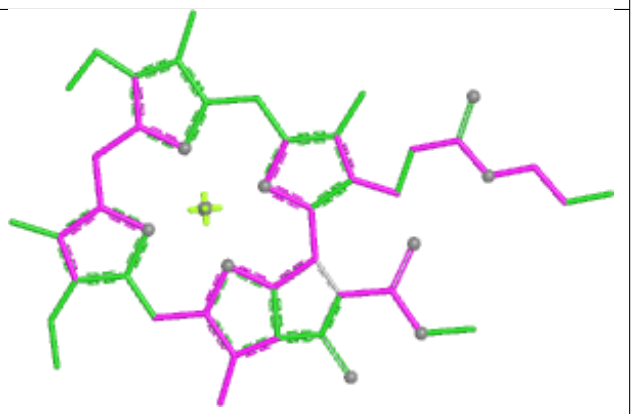


Rings

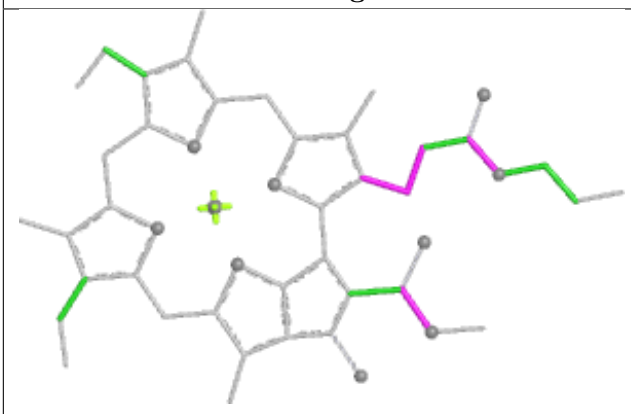
Ligand CLA r 306



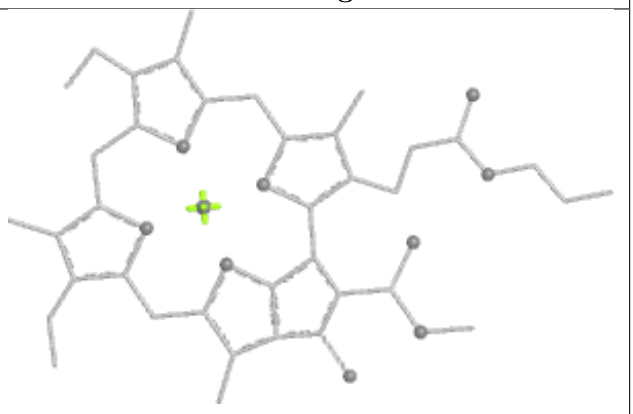
Bond lengths



Bond angles

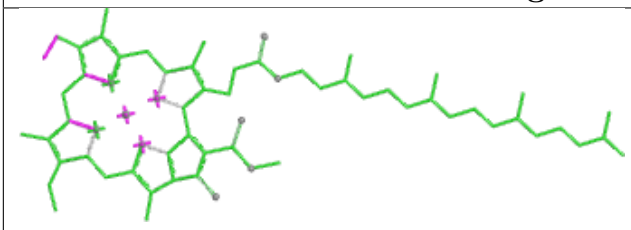


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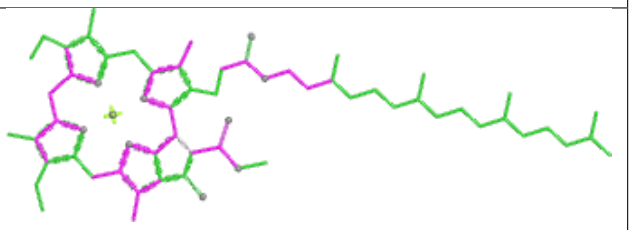


Rings

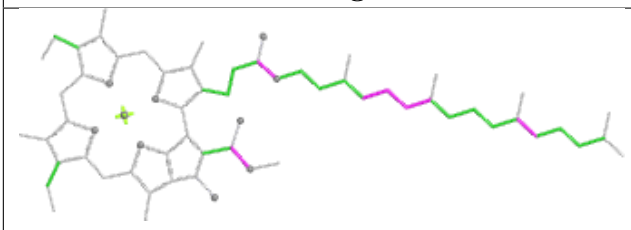
Ligand CLA S 305



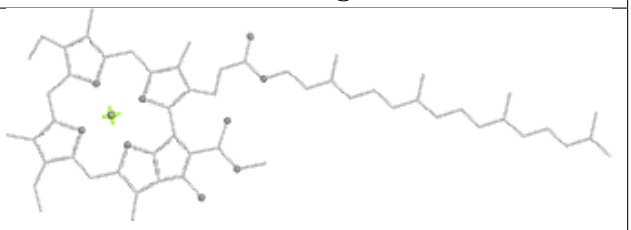
Bond lengths



Bond angles

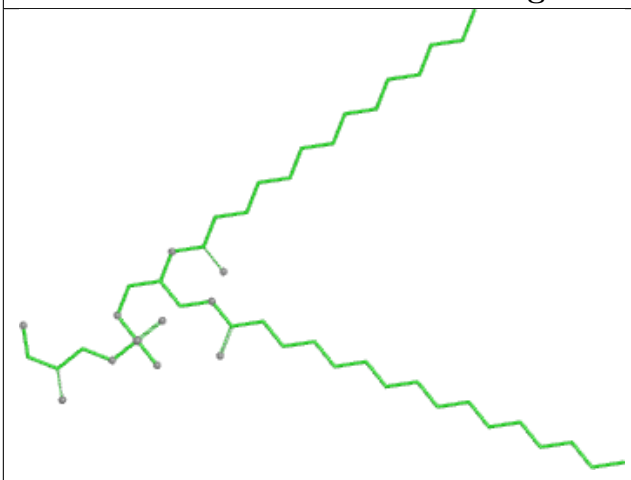


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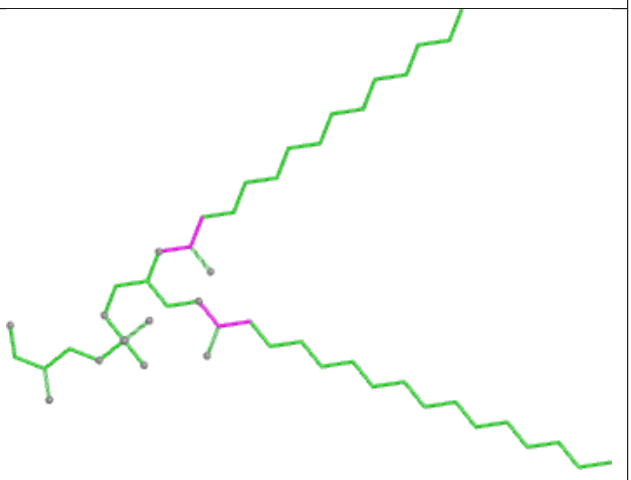


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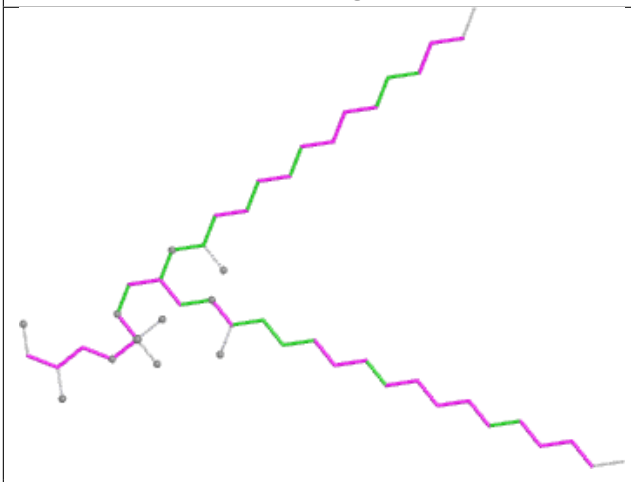
Ligand LHG c 622



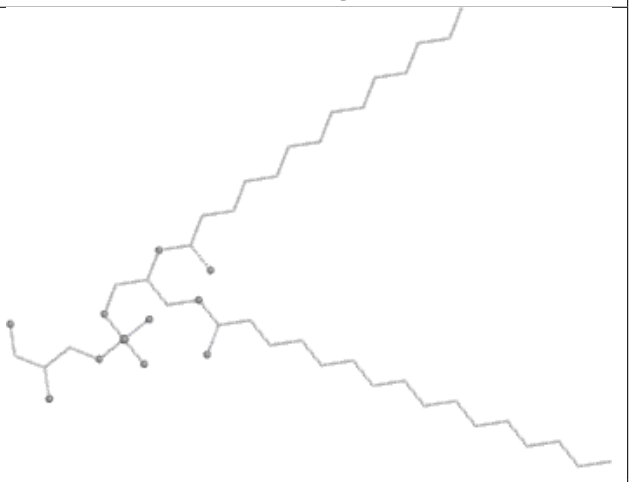
Bond lengths



Bond angles

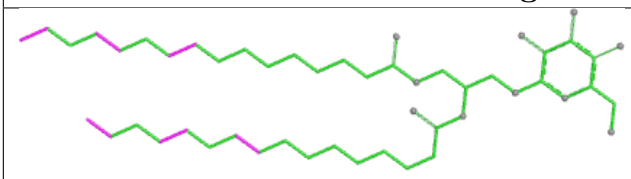


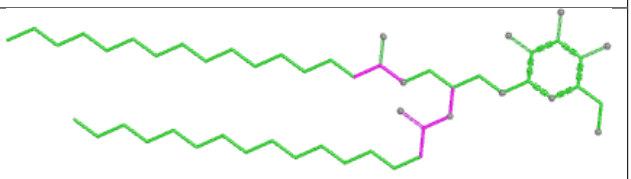
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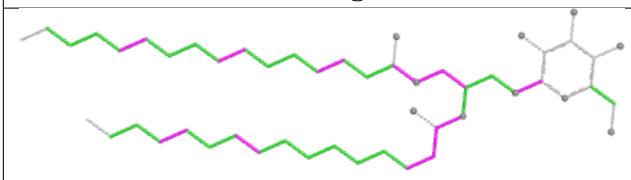


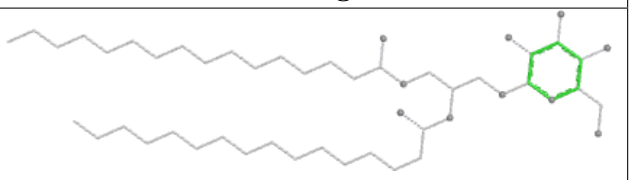
Rings

Ligand LMG B 621

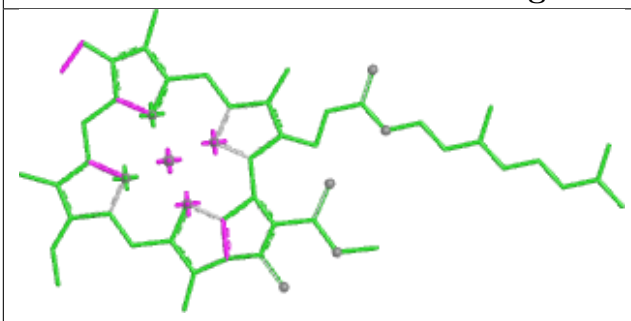

Bond lengths

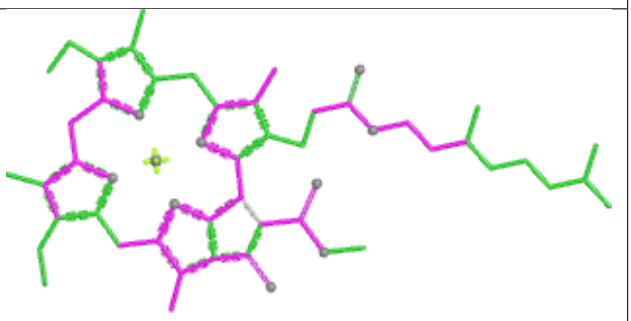

Bond angles

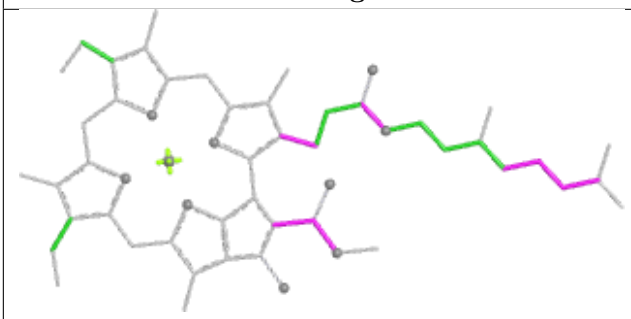

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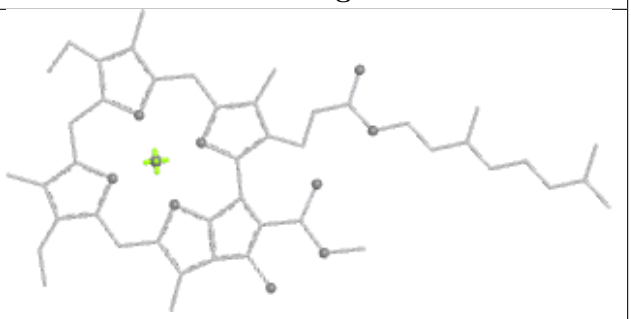

Rings

Ligand CLA 7 304


Bond lengths

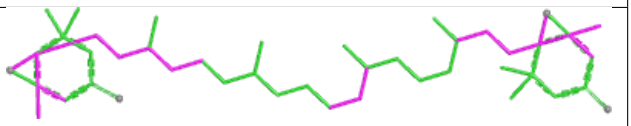

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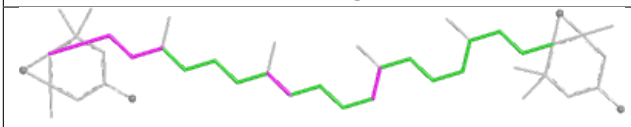

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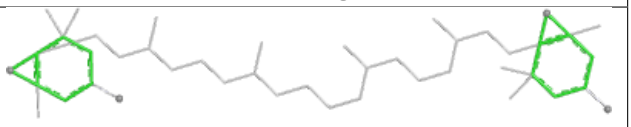

Rings

Ligand XAT 9 322

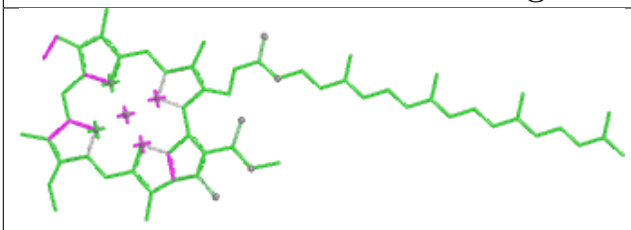

Bond lengths


Bond angles

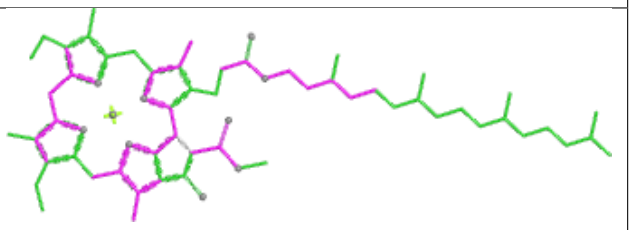

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Rings

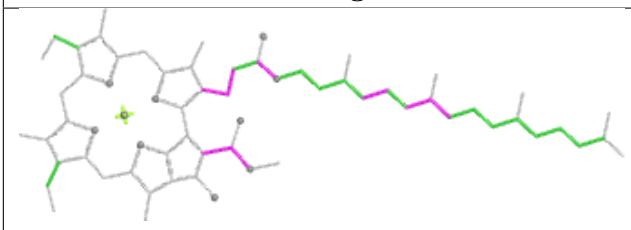
Ligand CLA n 303



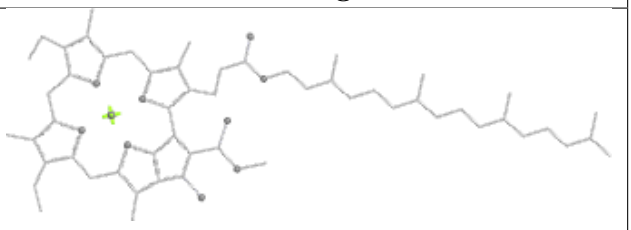
Bond lengths



Bond angles

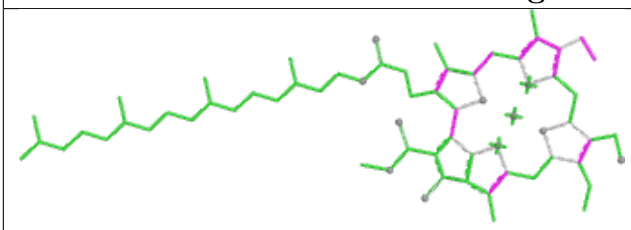


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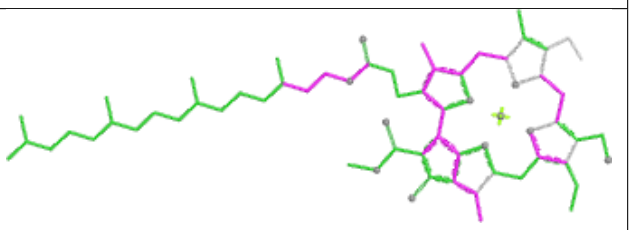


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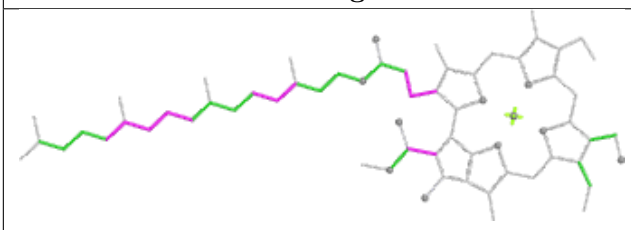
Ligand CHL 7 302



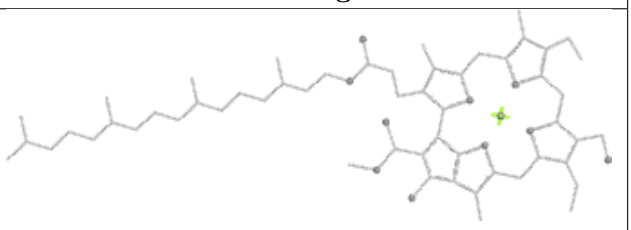
Bond lengths



Bond angles

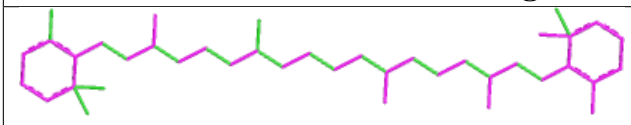


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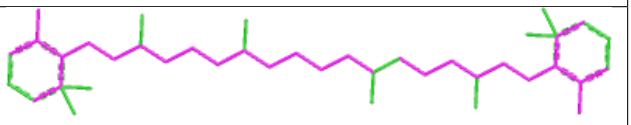


Rings

Ligand BCR H 101



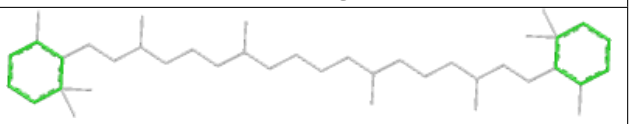
Bond lengths



Bond angles

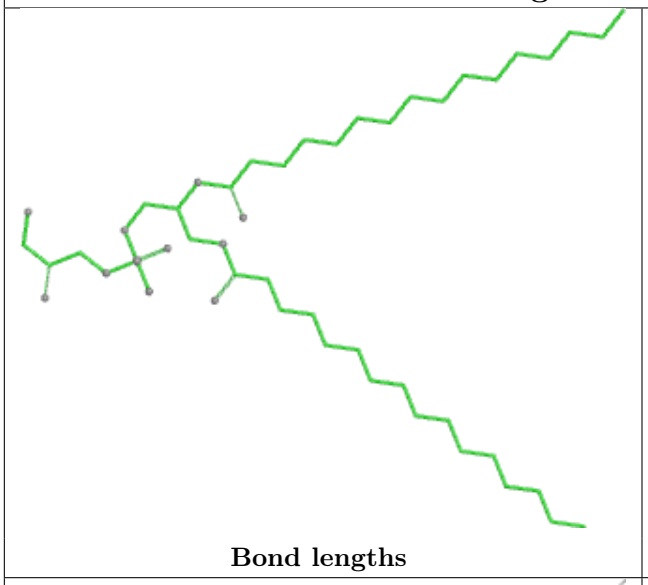


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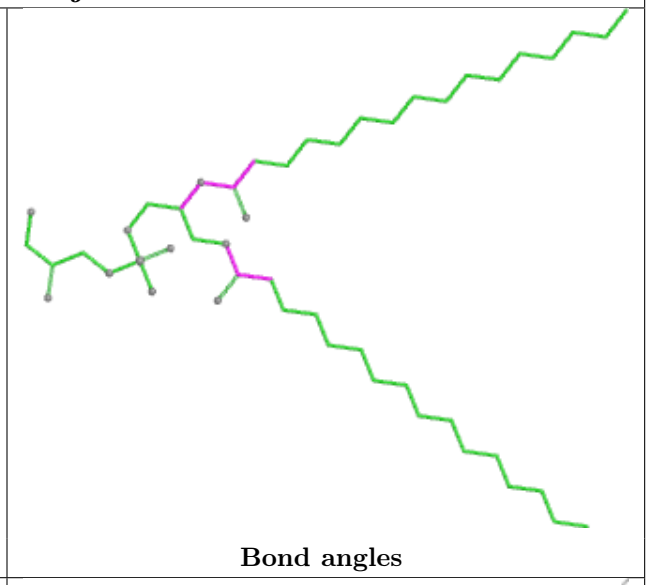


Rings

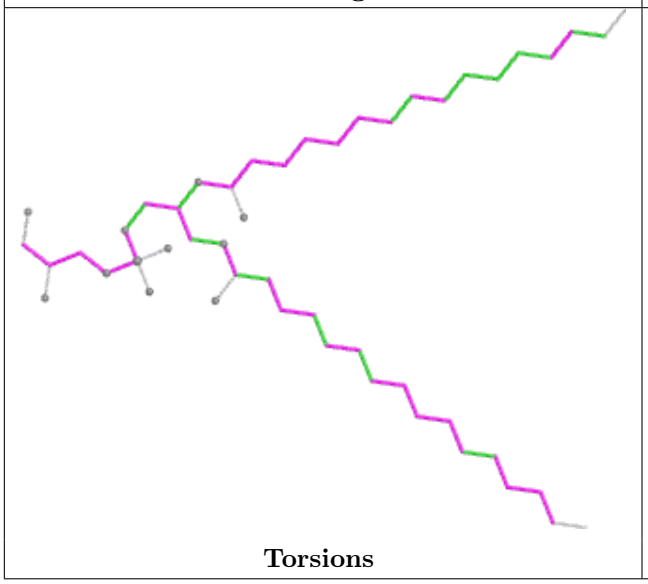
Ligand LHG j 102



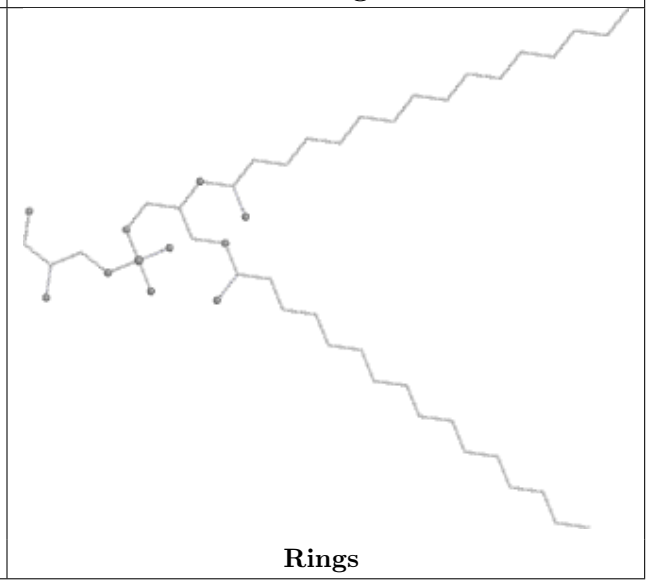
Bond lengths



Bond angles

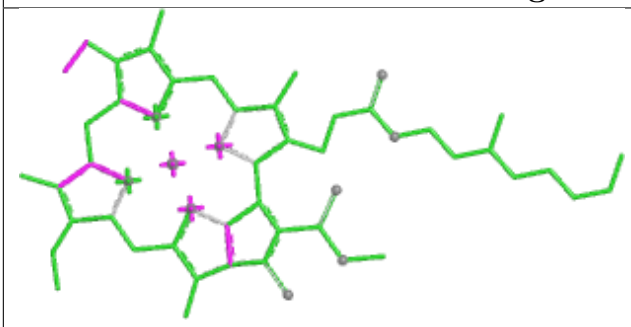


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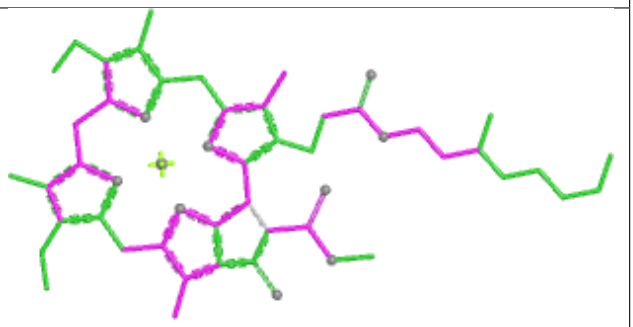


Rings

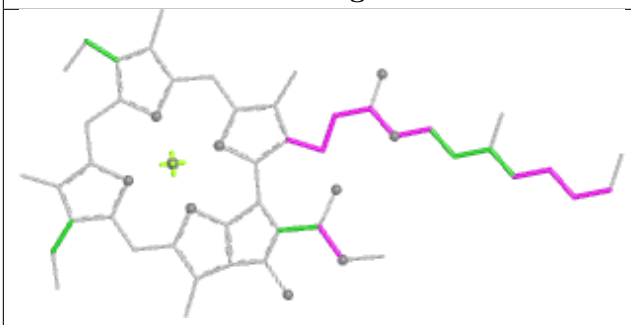
Ligand CLA 3 315



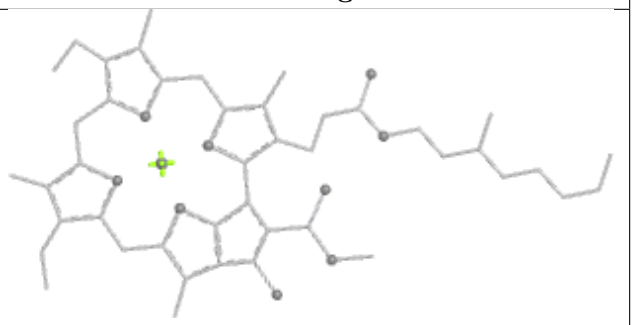
Bond lengths



Bond angles

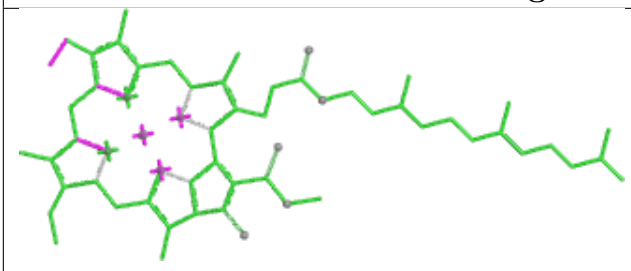


Torsions

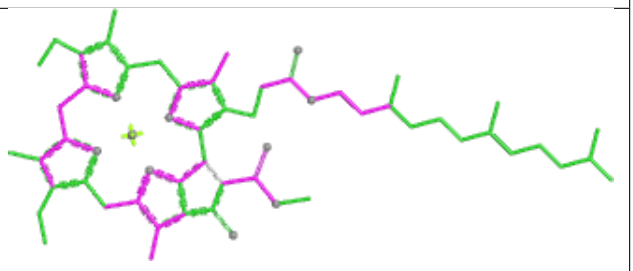


Rings

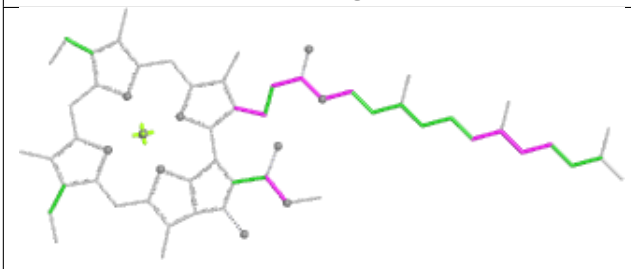
Ligand CLA 2 610



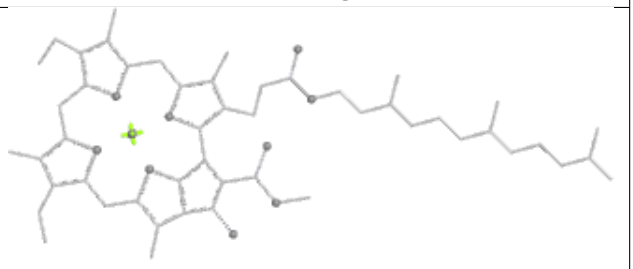
Bond lengths



Bond angles

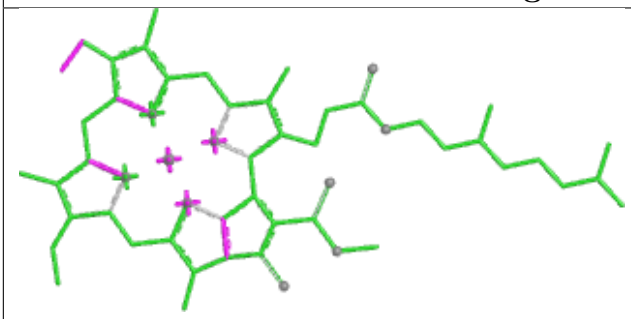


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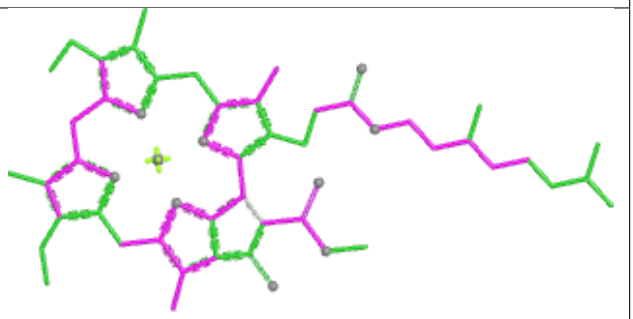


Rings

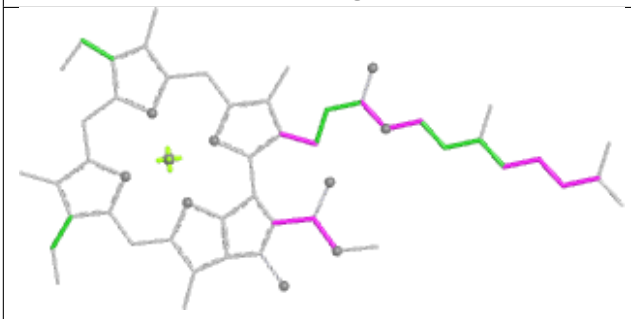
Ligand CLA Y 304



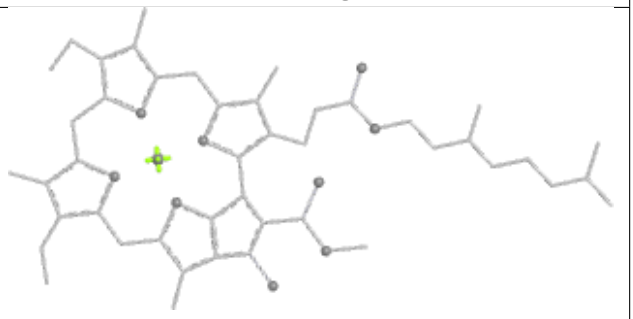
Bond lengths



Bond angles

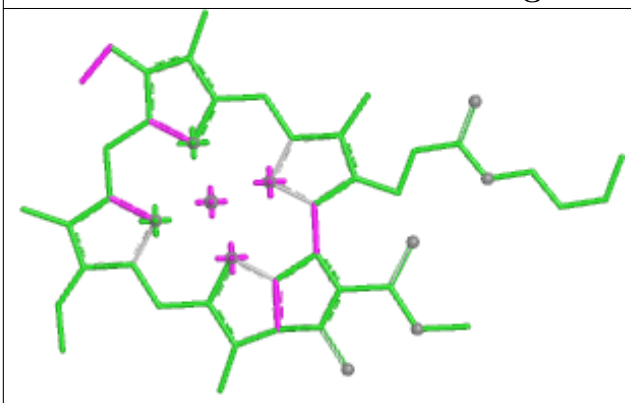


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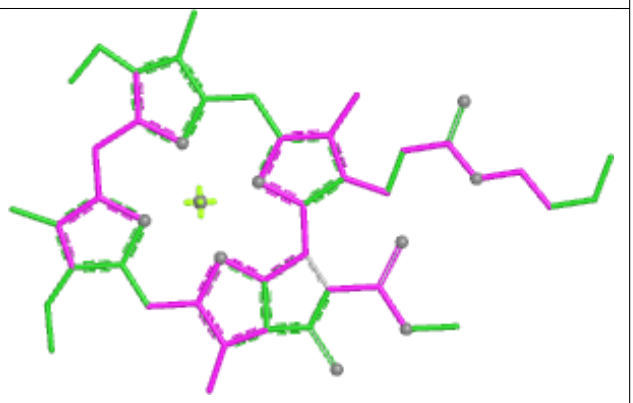


Rings

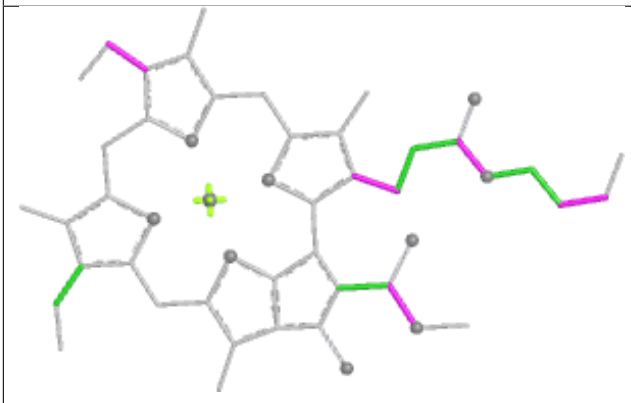
Ligand CLA R 313



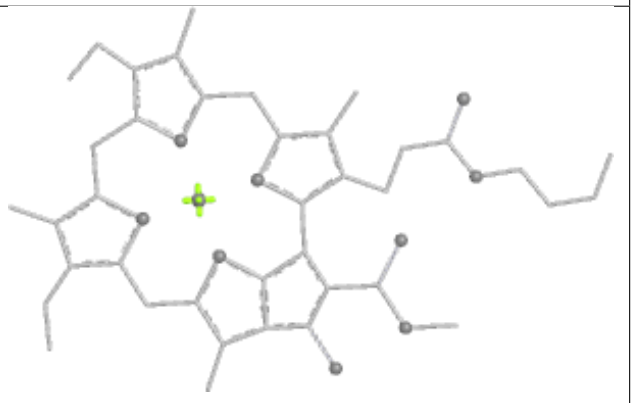
Bond lengths



Bond angles

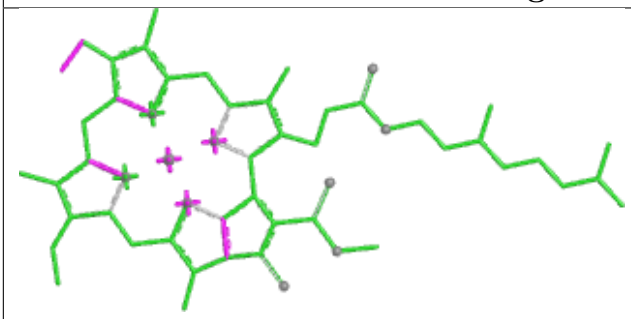


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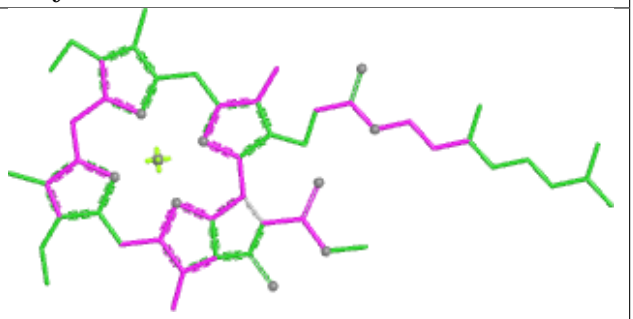


Rings

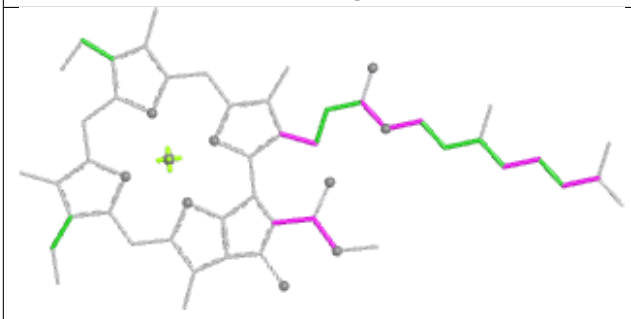
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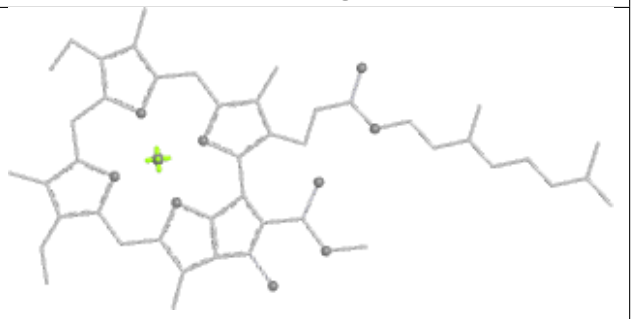
Bond lengths



Bond angles

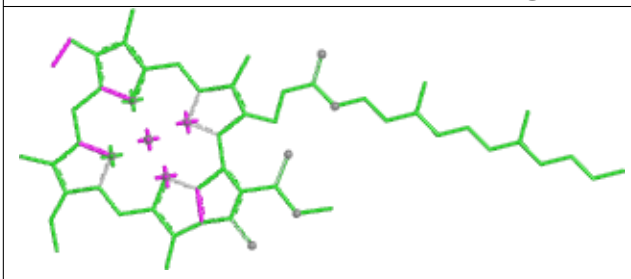


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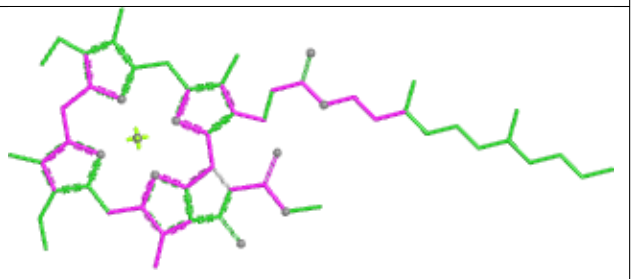


Rings

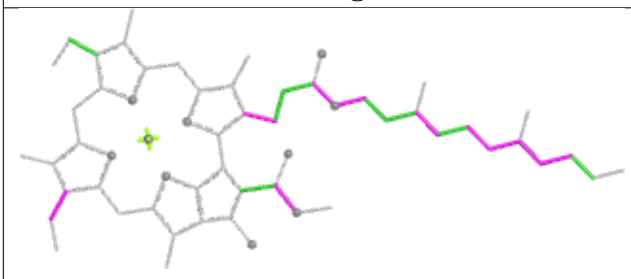
Ligand CLA R 311



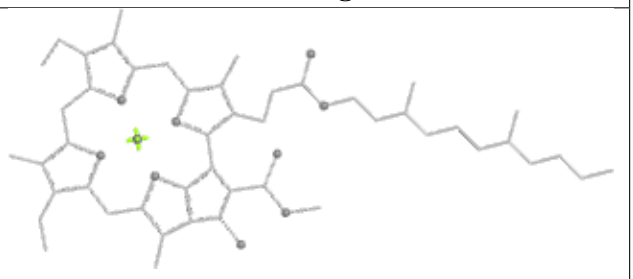
Bond lengths



Bond angles

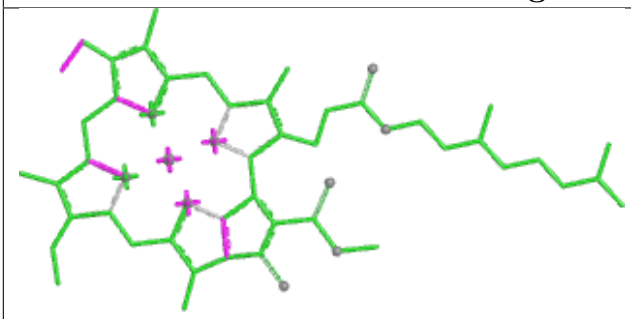


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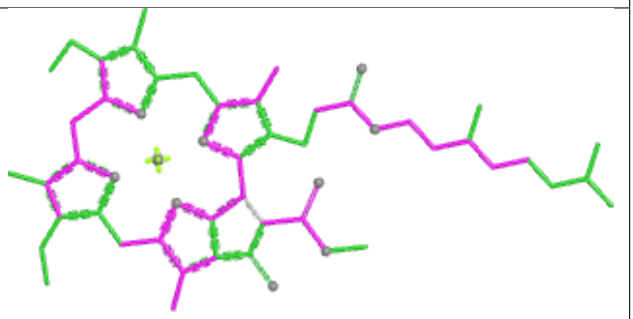


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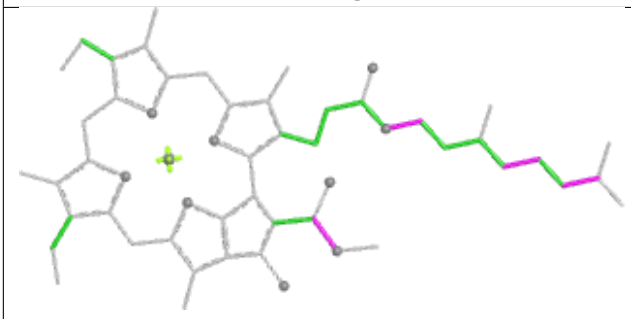
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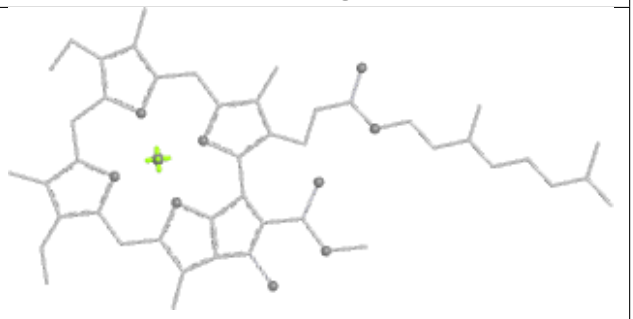
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Bond angles

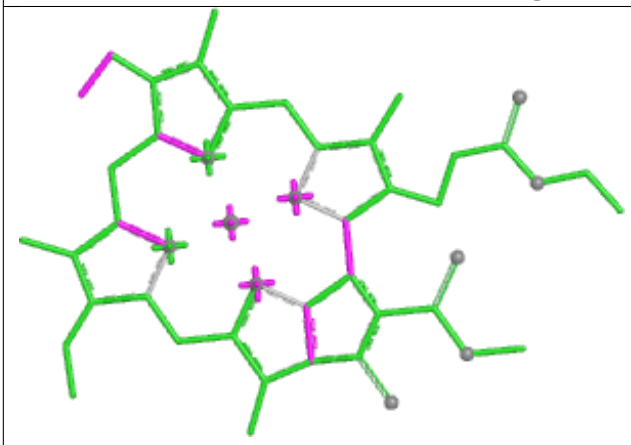


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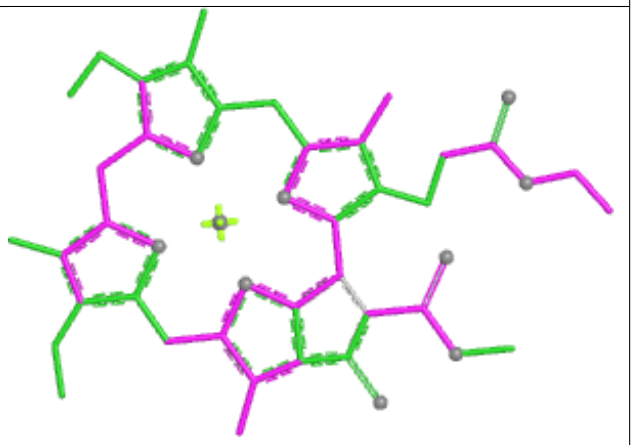


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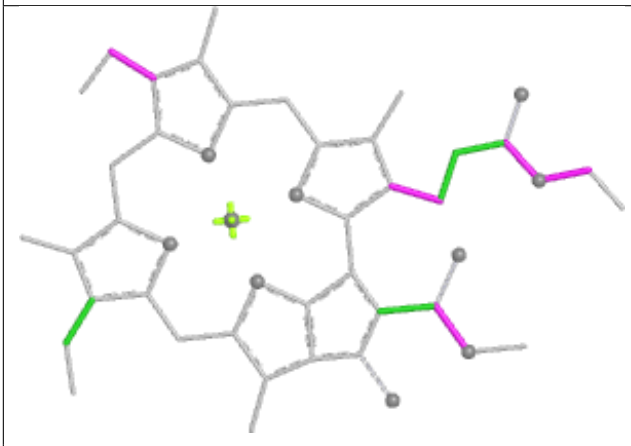
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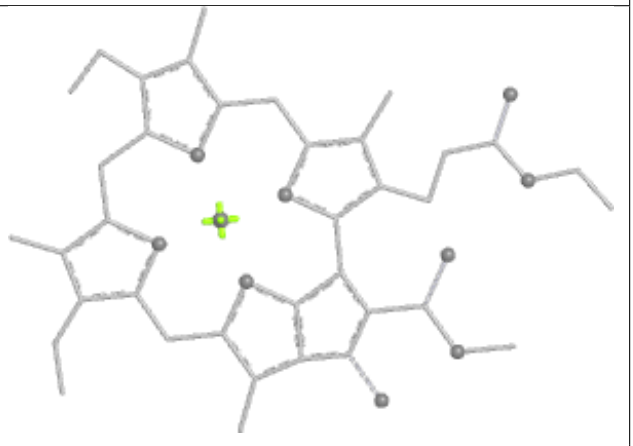
Bond lengths



Bond angles

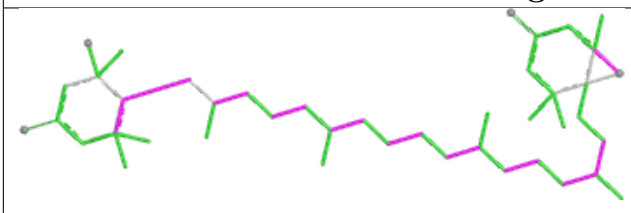


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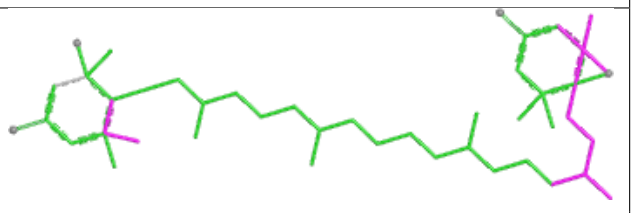


Rings

Ligand NEX r 319



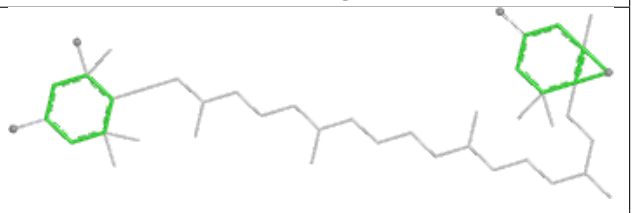
Bond lengths



Bond angles

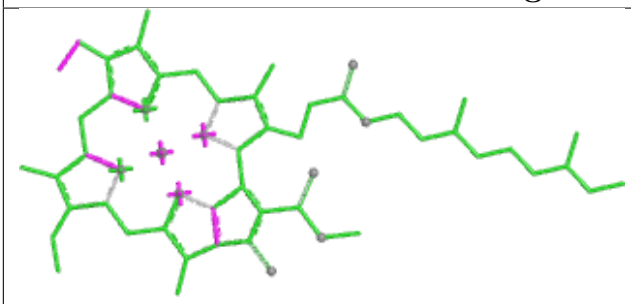


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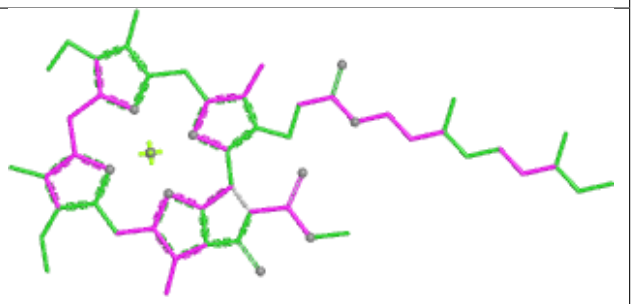


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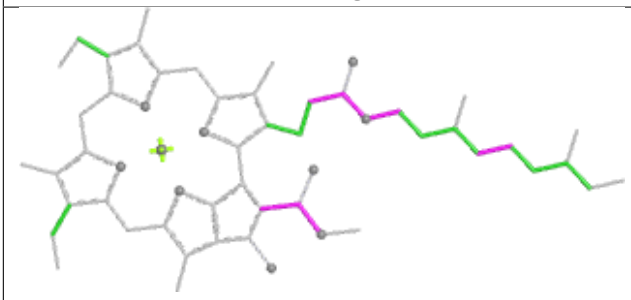
Ligand CLA C 604



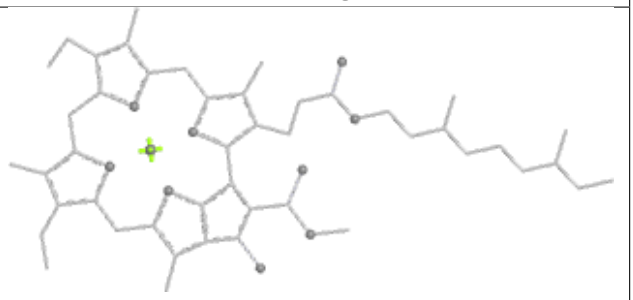
Bond lengths



Bond angles

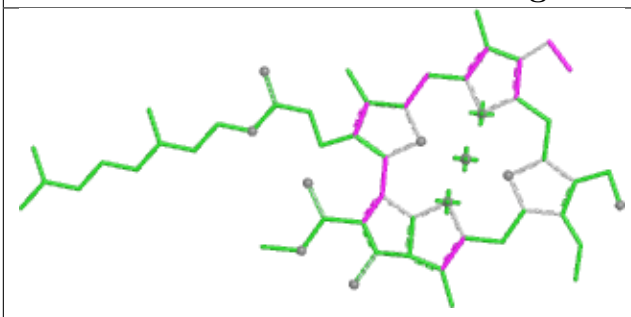


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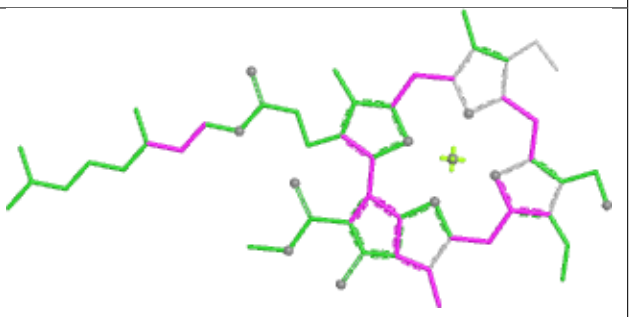


Rings

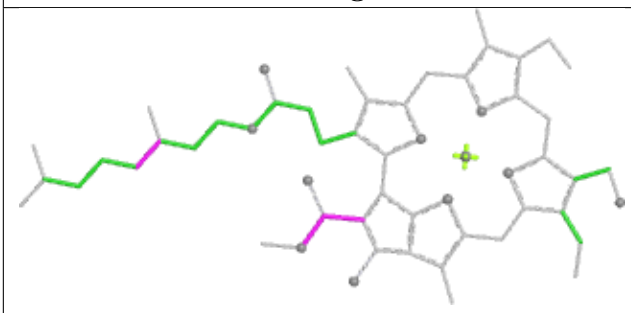
Ligand CHL r 309



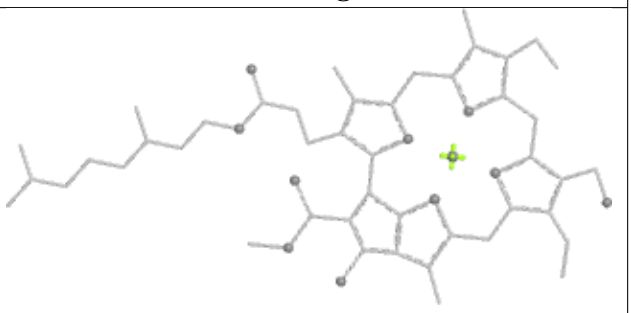
Bond lengths



Bond angles

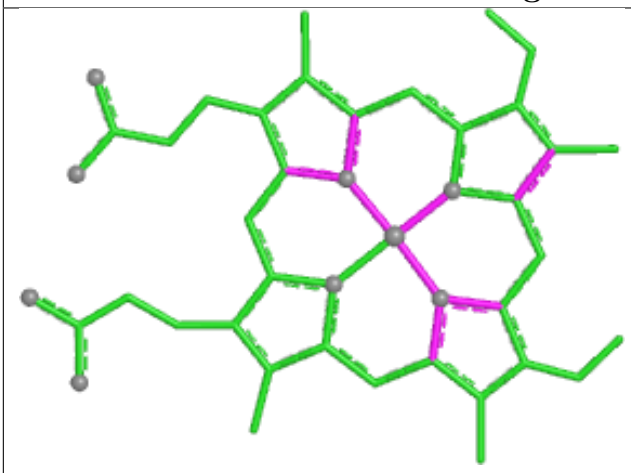


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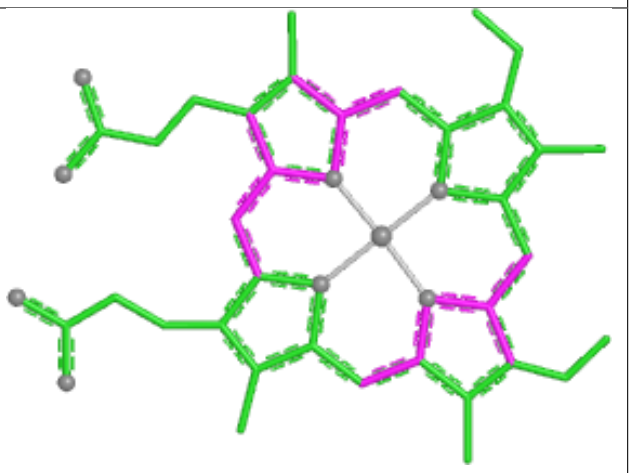


Rings

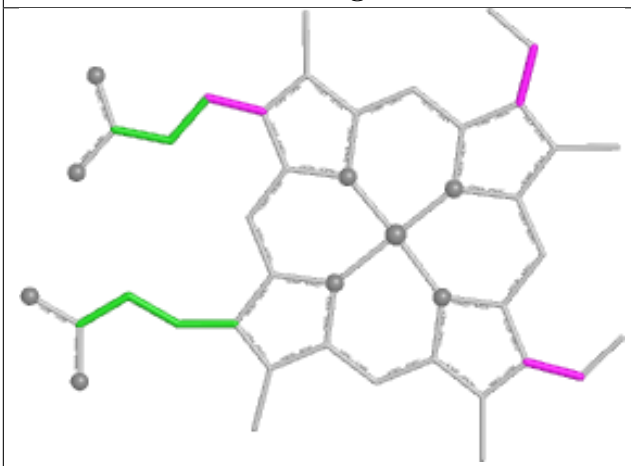
Ligand HEM e 102



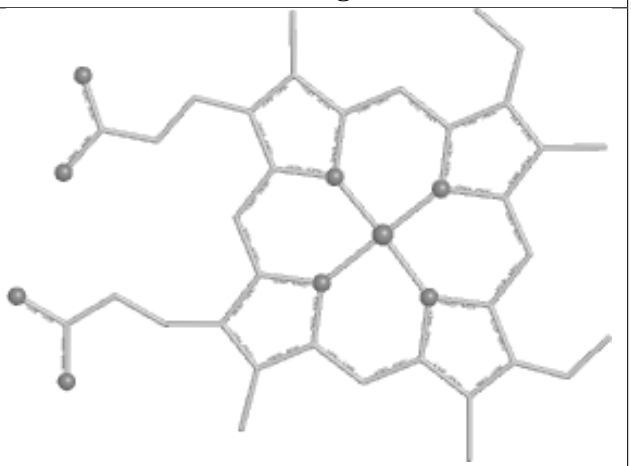
Bond lengths



Bond angles

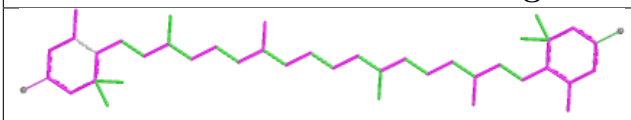


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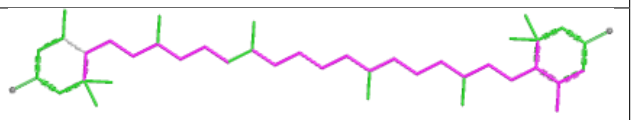


Rings

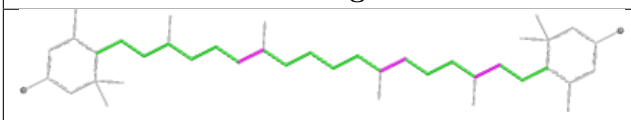
Ligand LUT N 317



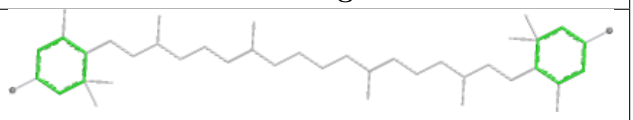
Bond lengths



Bond angles

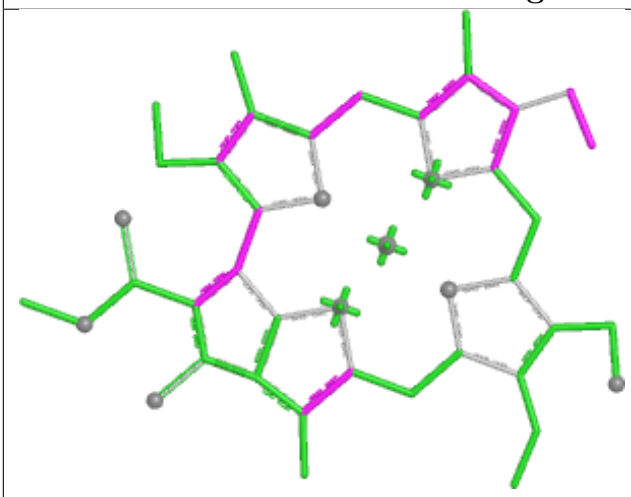


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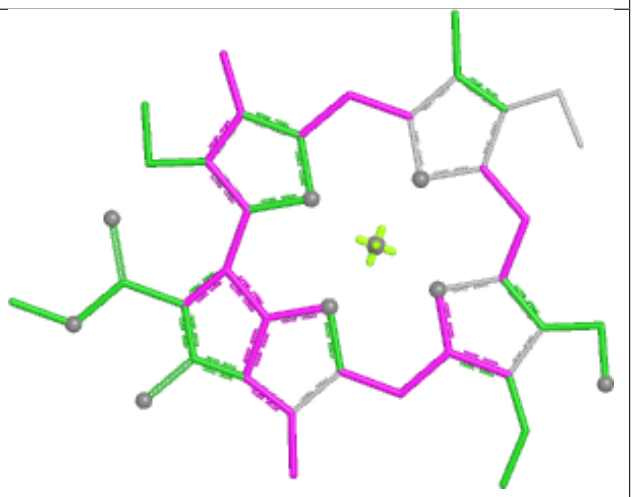


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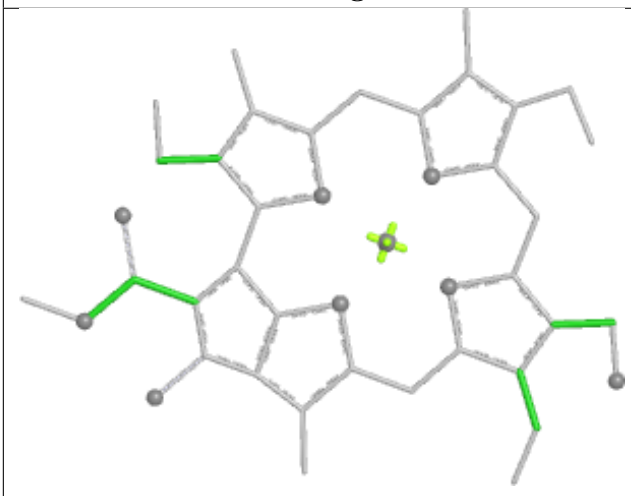
Ligand CHL S 308



Bond lengths



Bond angles

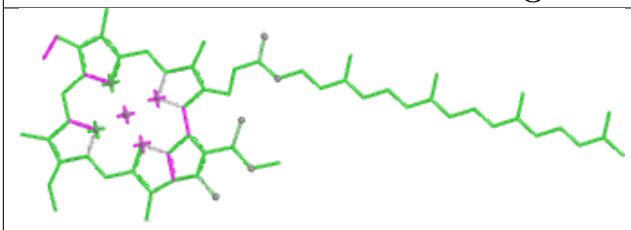


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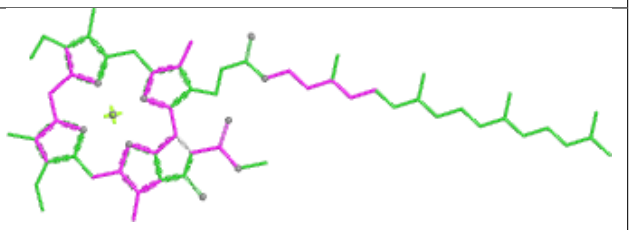


Rings

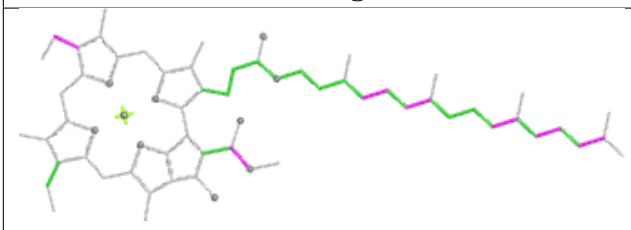
Ligand CLA B 615



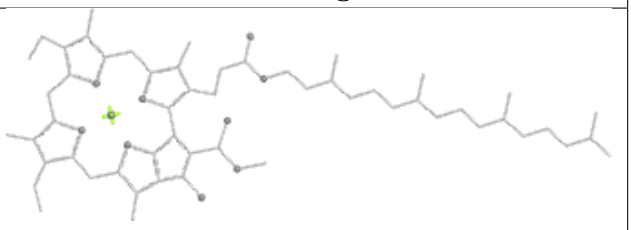
Bond lengths



Bond angles

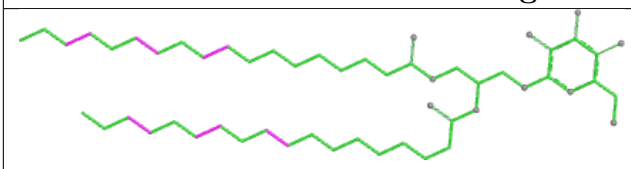


Torsions

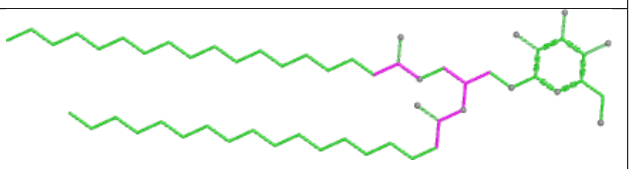


Rings

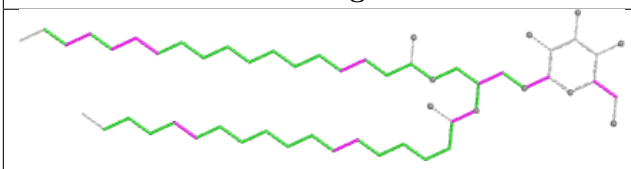
Ligand LMG w 202



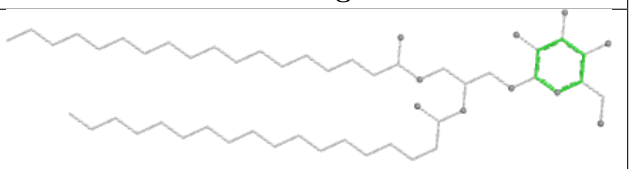
Bond lengths



Bond angles



Torsions

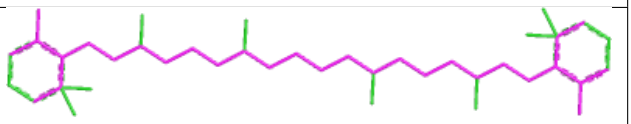


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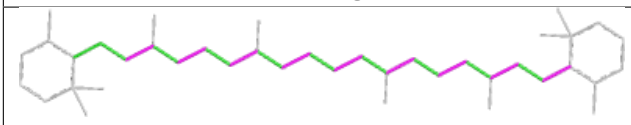
Ligand BCR T 101



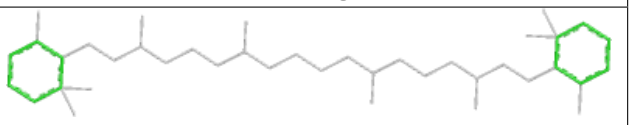
Bond lengths



Bond angles

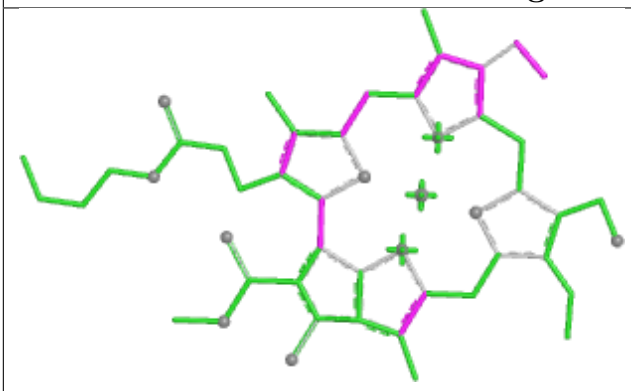


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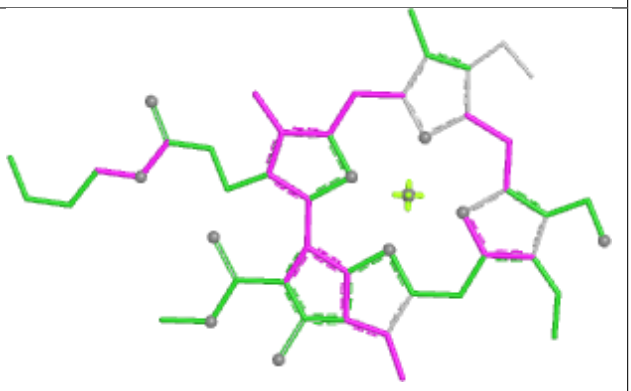


Rings

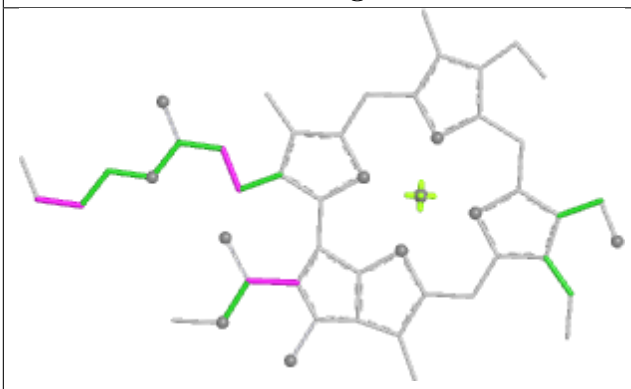
Ligand CHL 6 309



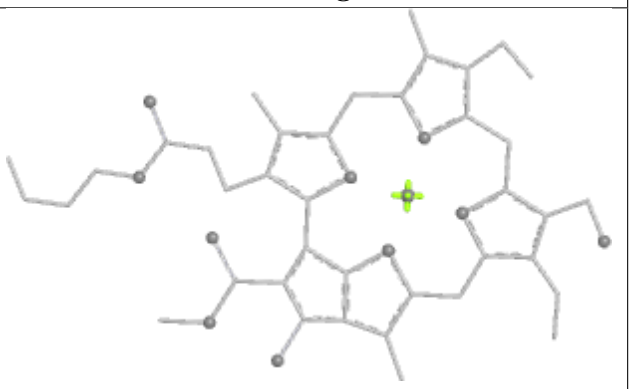
Bond lengths



Bond angles

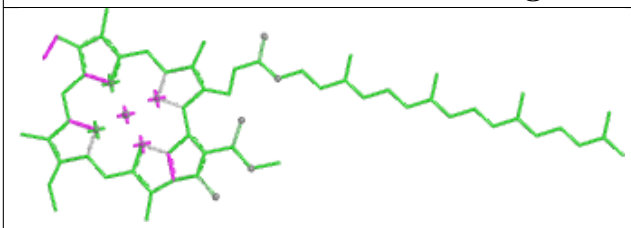


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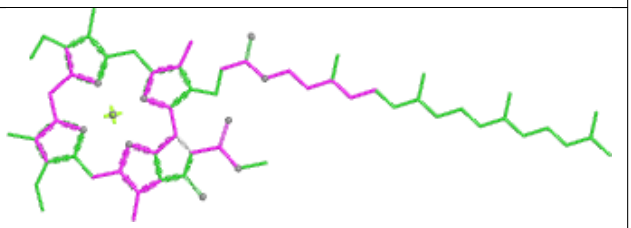


Rings

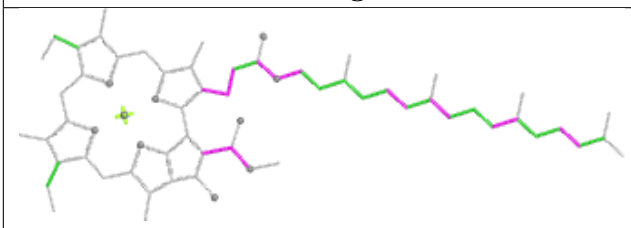
Ligand CLA B 610



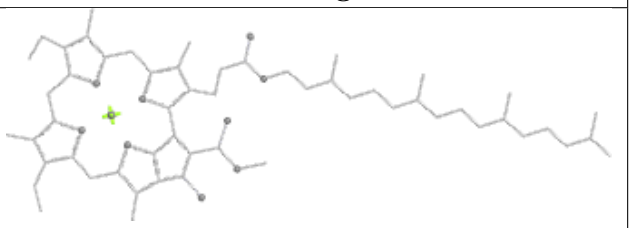
Bond lengths



Bond angles

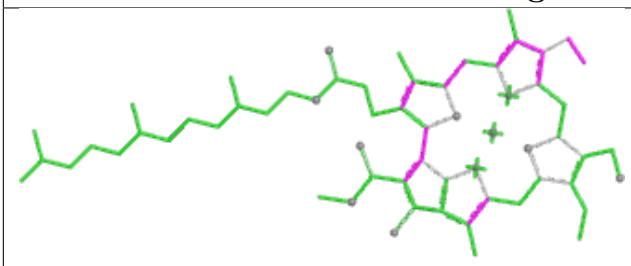


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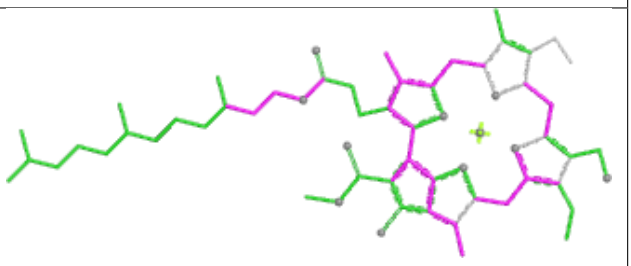


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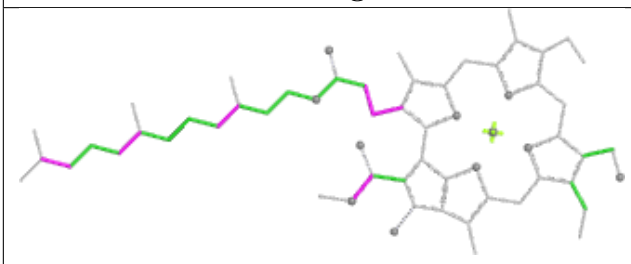
Ligand CHL 6 310



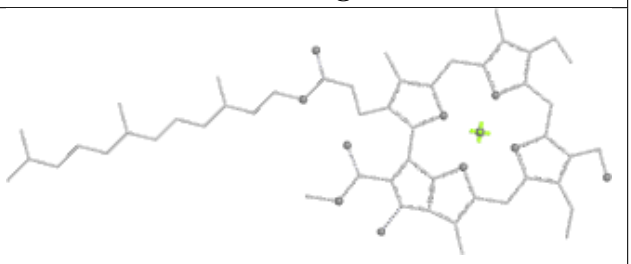
Bond lengths



Bond angles

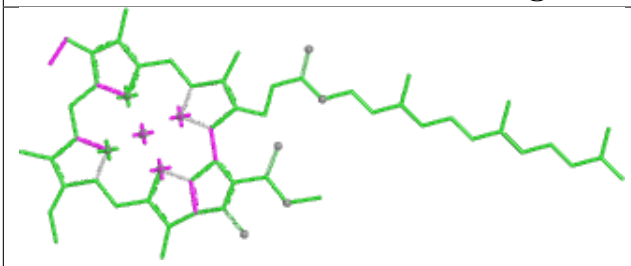


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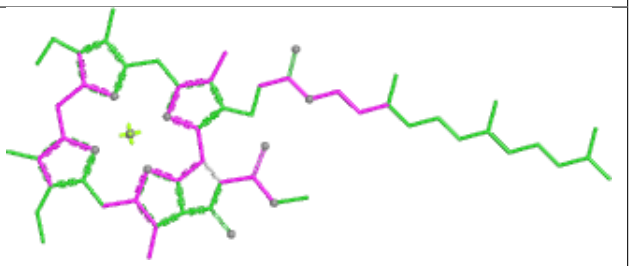


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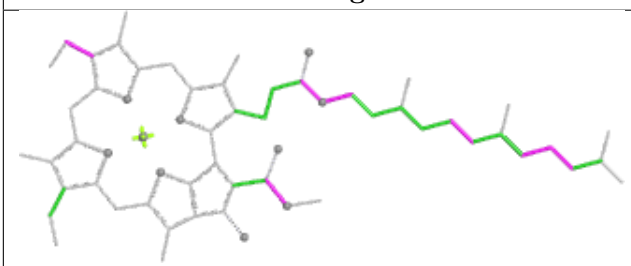
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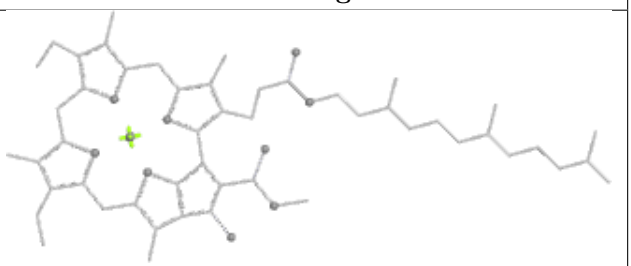
Bond lengths



Bond angles

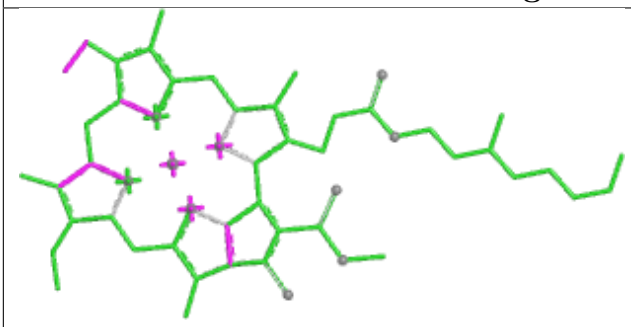


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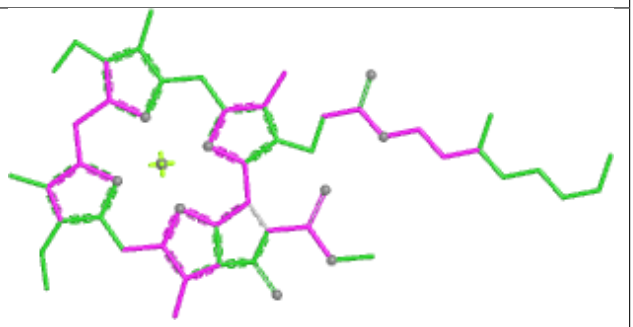


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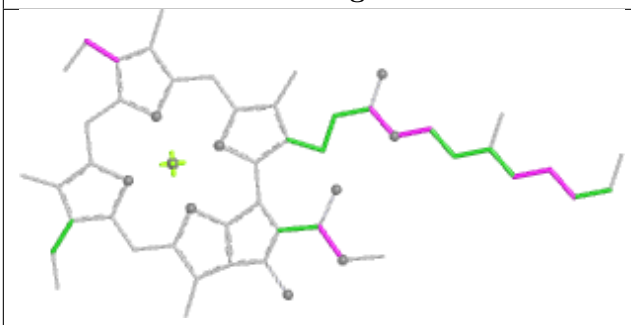
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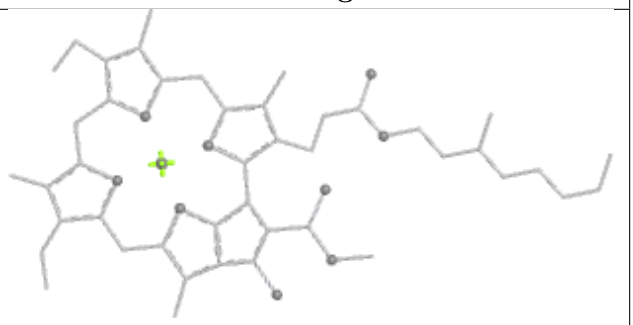
Bond lengths



Bond angles

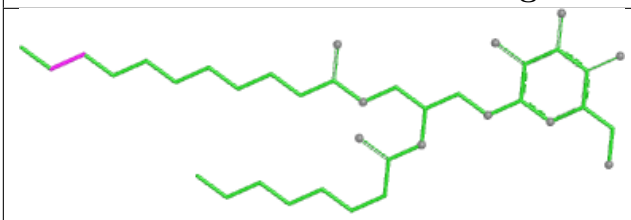


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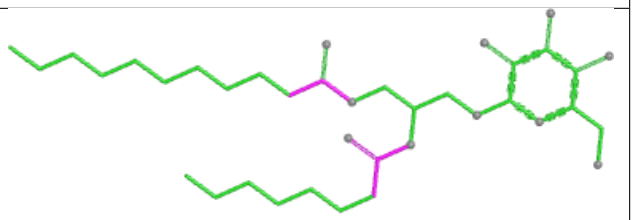


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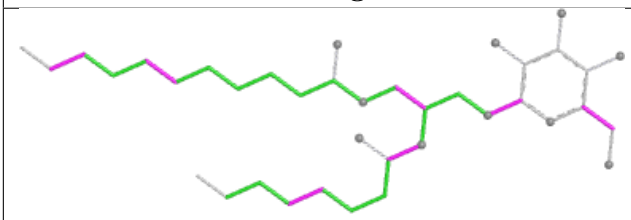
Ligand LMG C 621



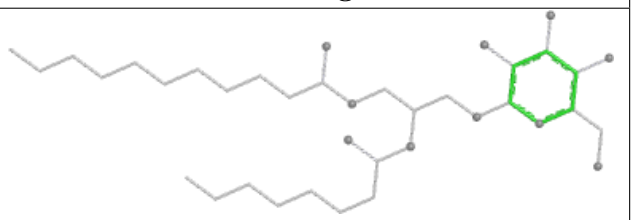
Bond lengths



Bond angles

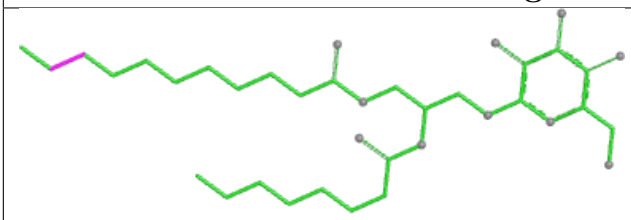


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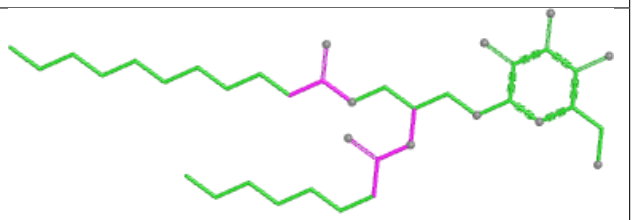


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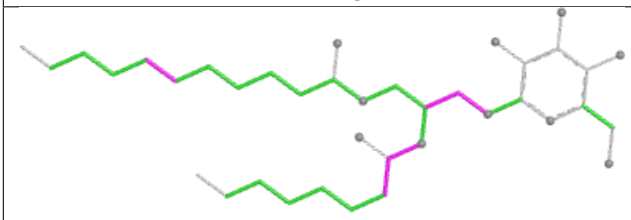
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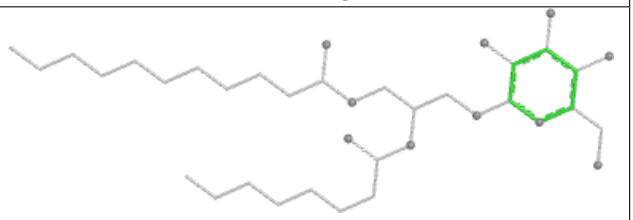
Bond lengths



Bond angles

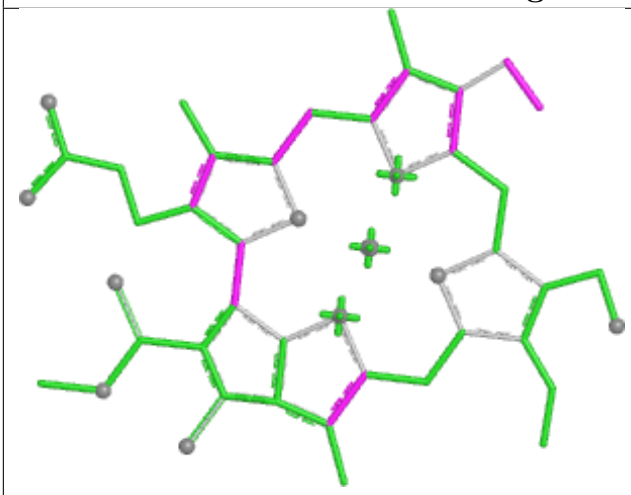


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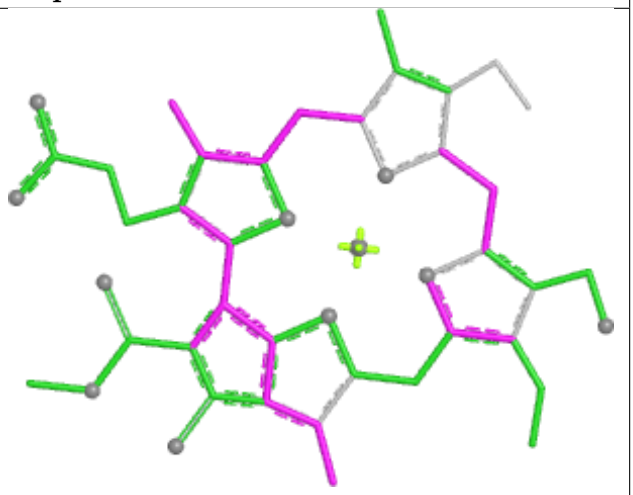


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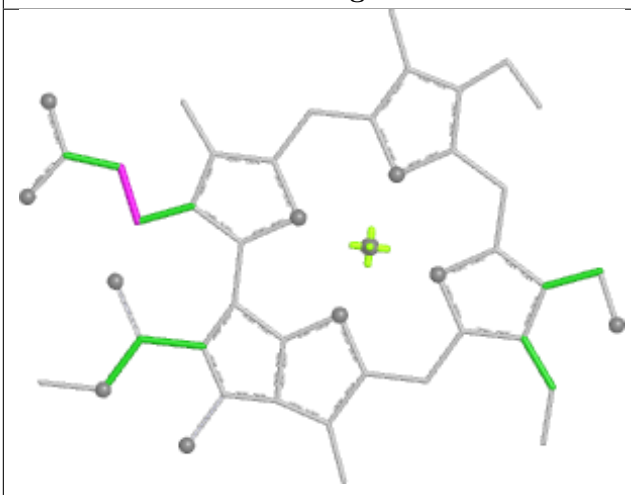
Ligand CHL p 605



Bond lengths



Bond angles

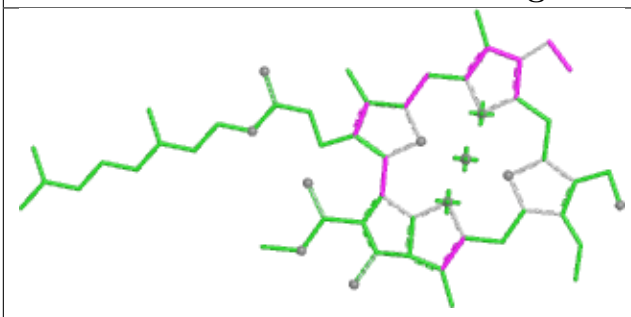


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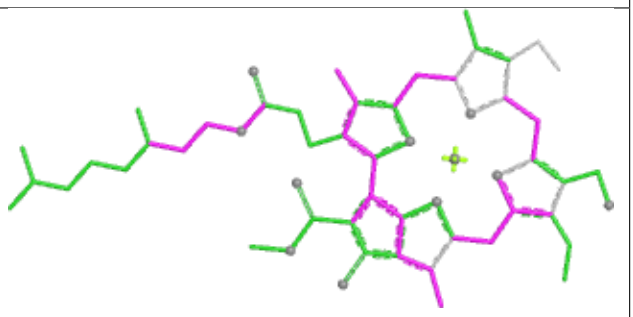


Rings

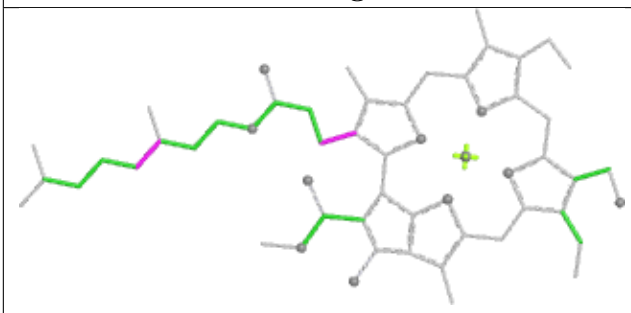
Ligand CHL 6 302



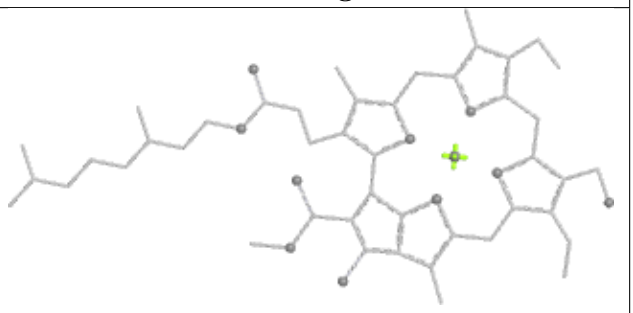
Bond lengths



Bond angles

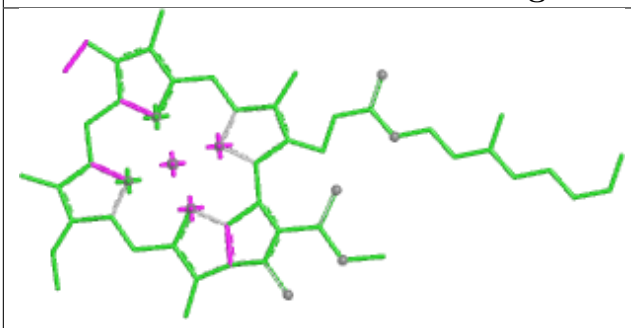


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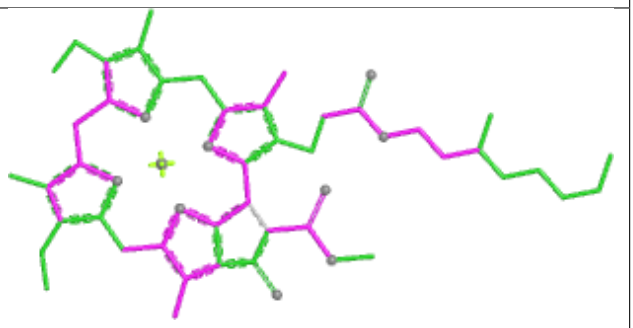


Rings

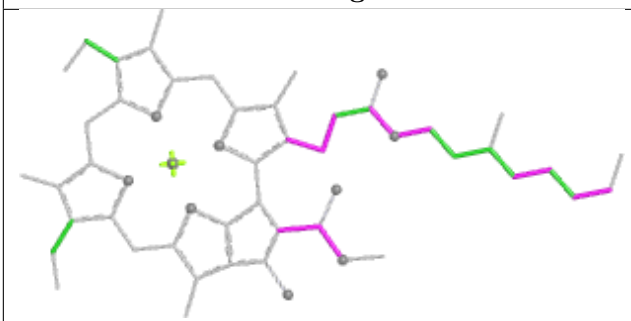
Ligand CLA 2 604



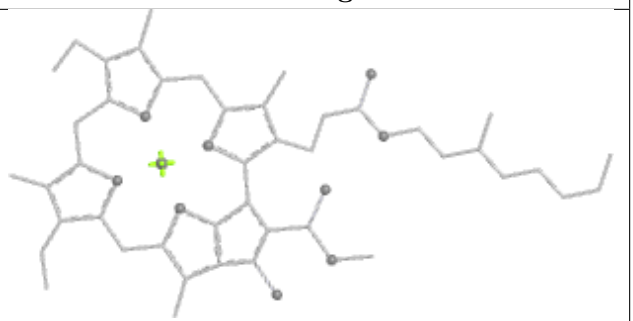
Bond lengths



Bond angles

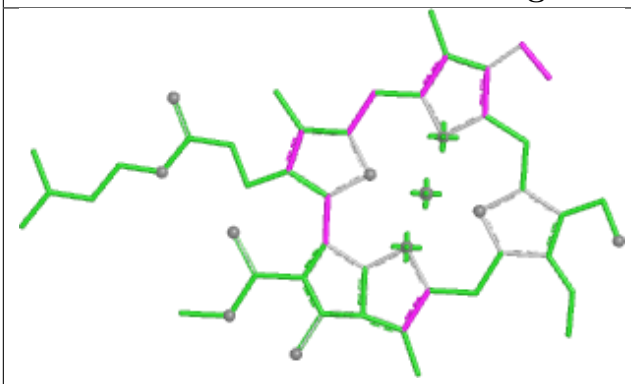


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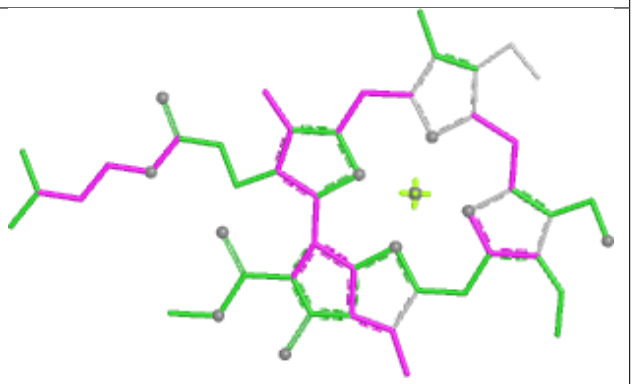


Rings

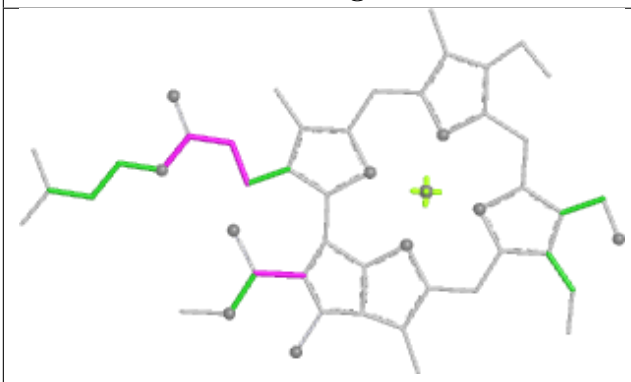
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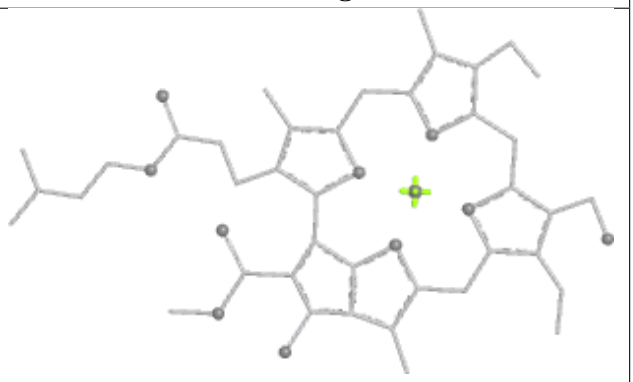
Bond lengths



Bond angles

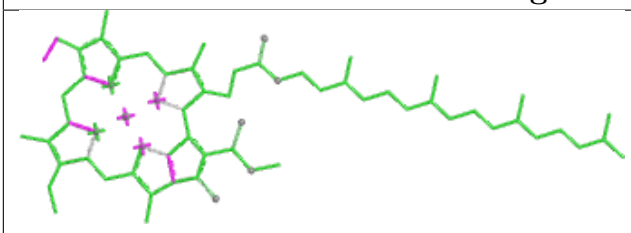


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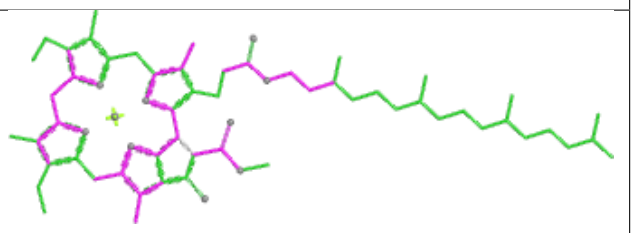


Rings

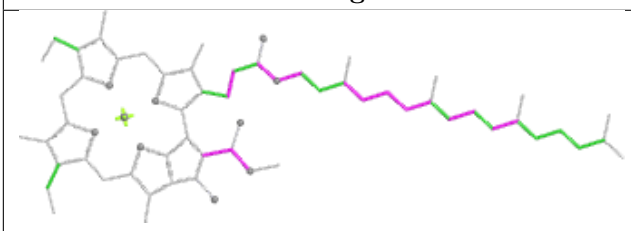
Ligand CLA s 305



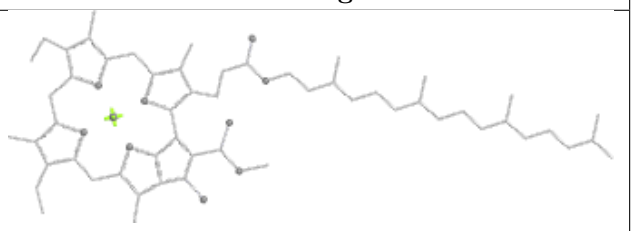
Bond lengths



Bond angles

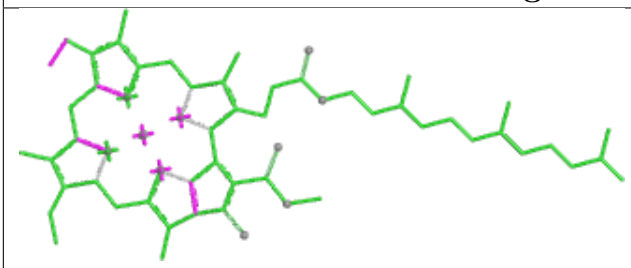


Torsions

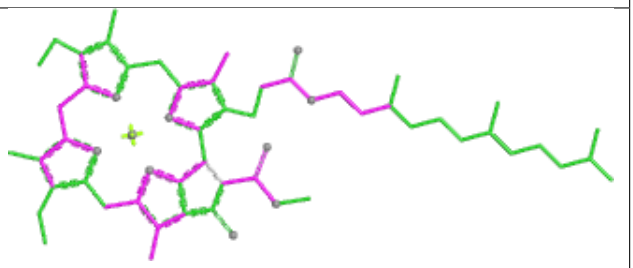


Rings

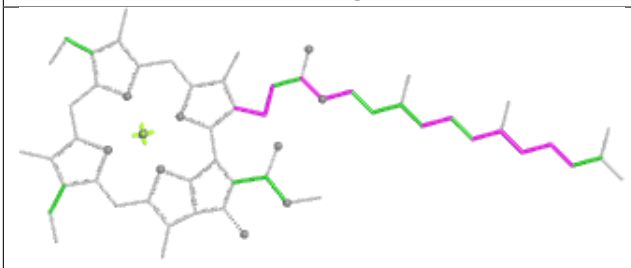
Ligand CLA R 304



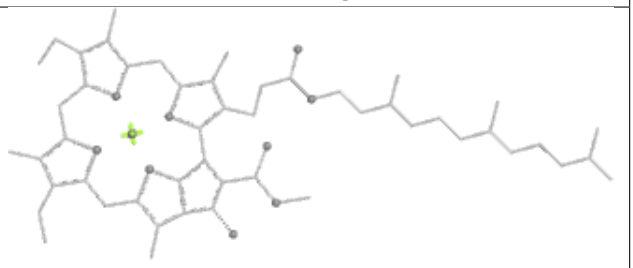
Bond lengths



Bond angles

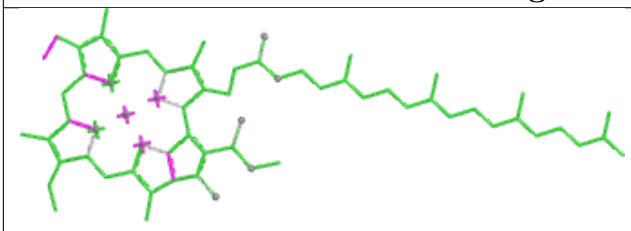


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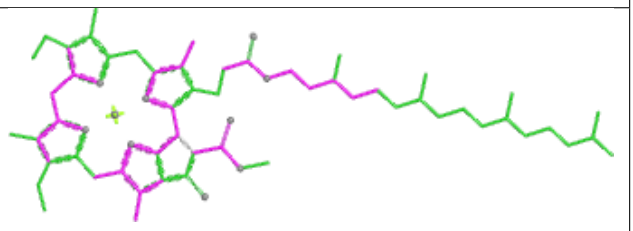


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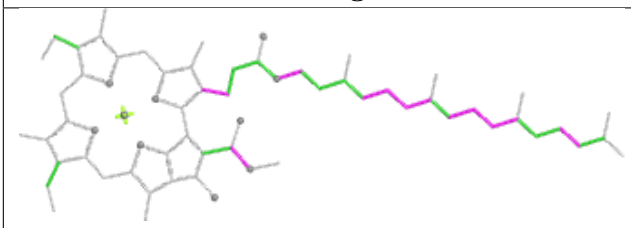
Ligand CLA 8 612



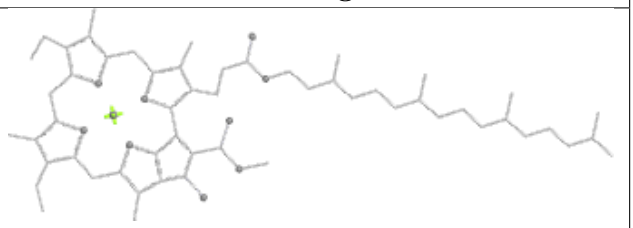
Bond lengths



Bond angles

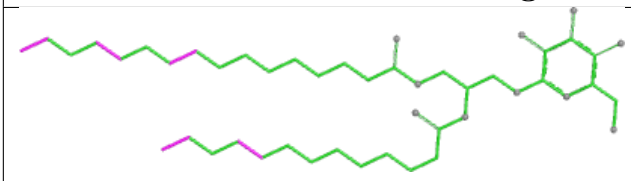


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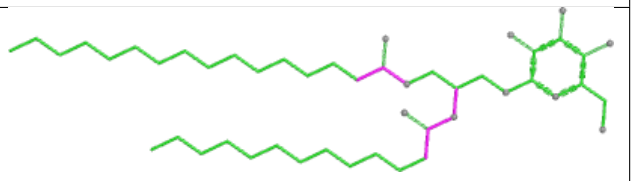


Rings

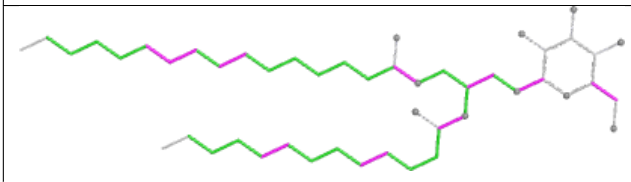
Ligand LMG w 201



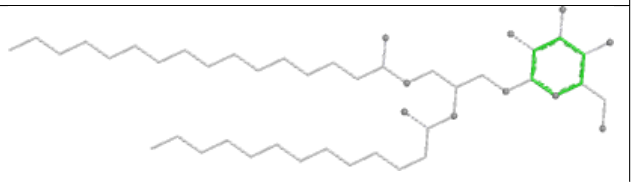
Bond lengths



Bond angles

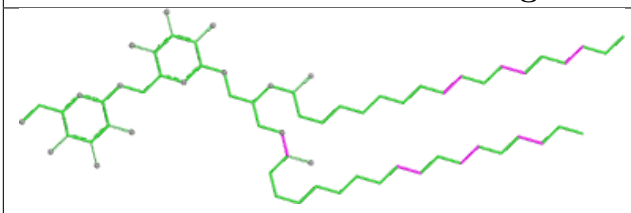


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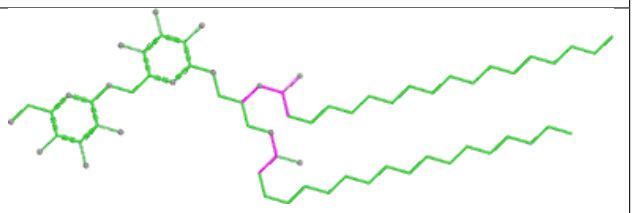


Rings

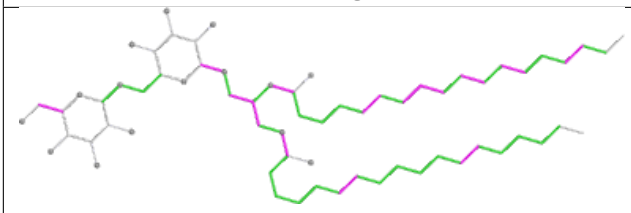
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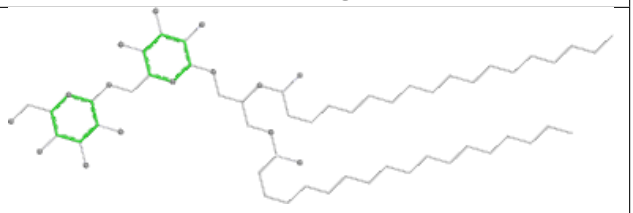
Bond lengths



Bond angles

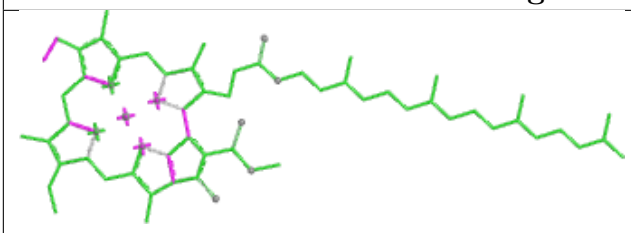


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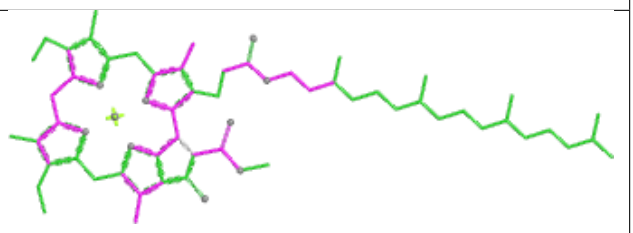


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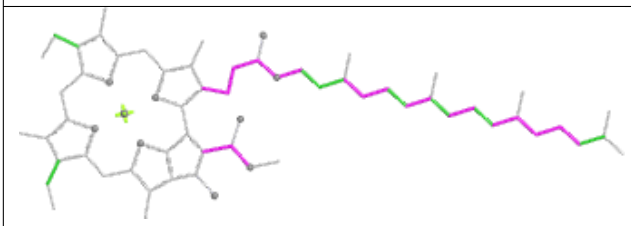
Ligand CLA b 605



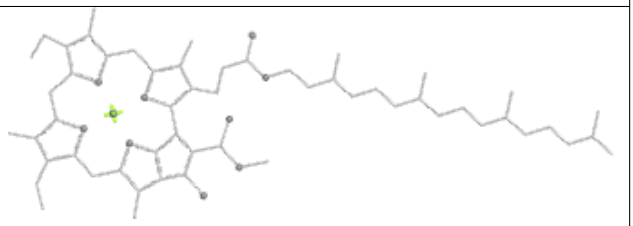
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Bond angles

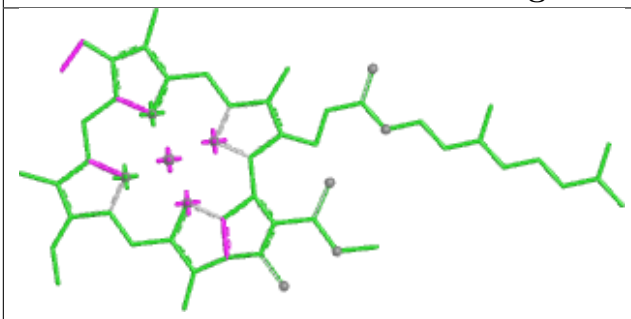


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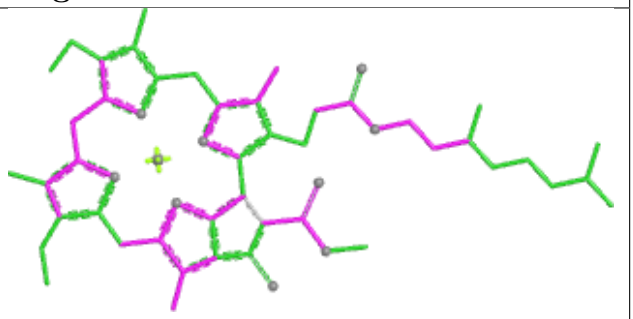


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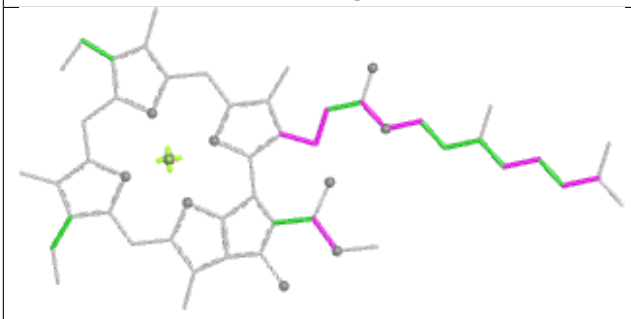
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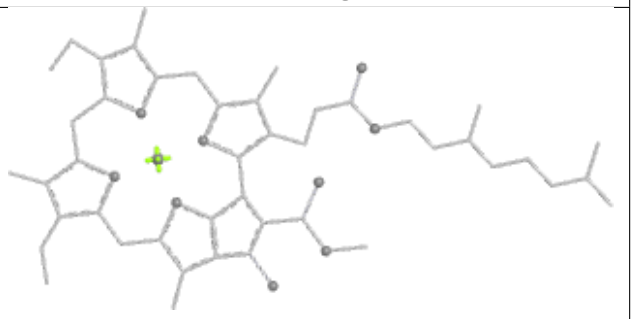
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Bond angles

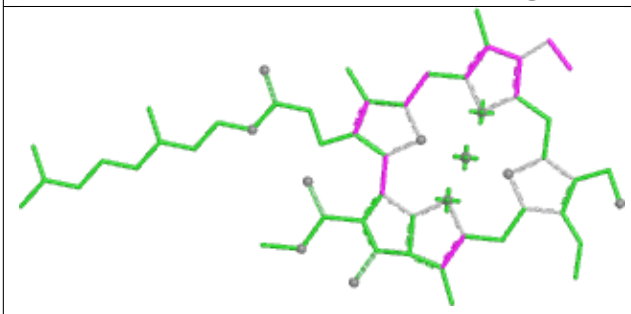


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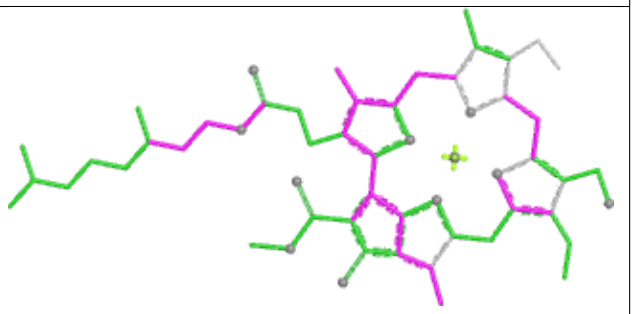


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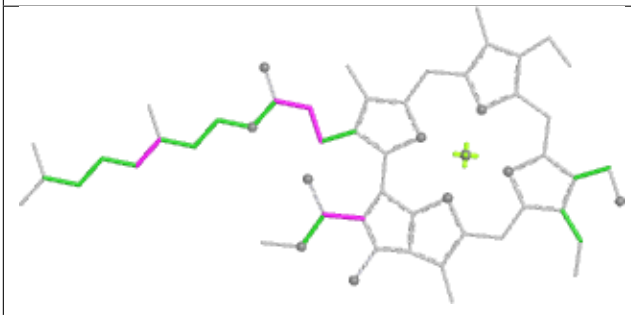
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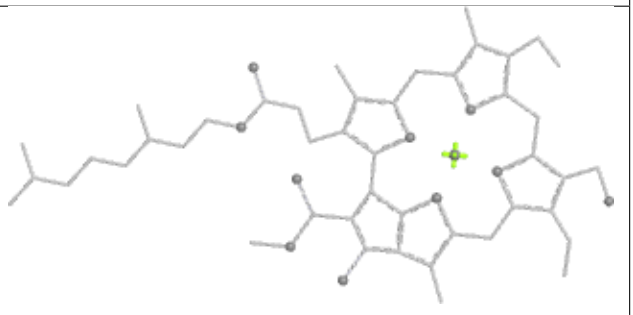
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Bond angles

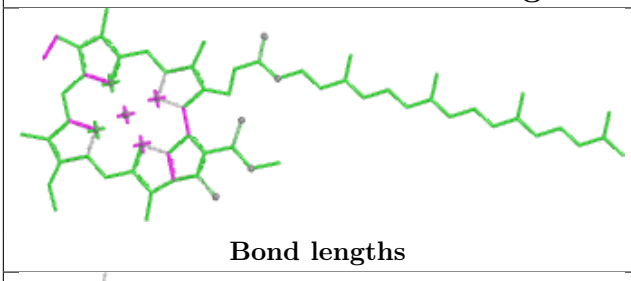


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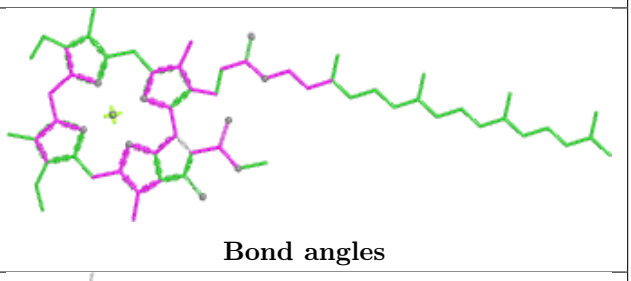


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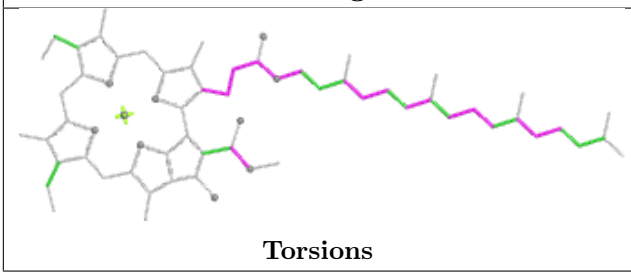
Ligand CLA D 404



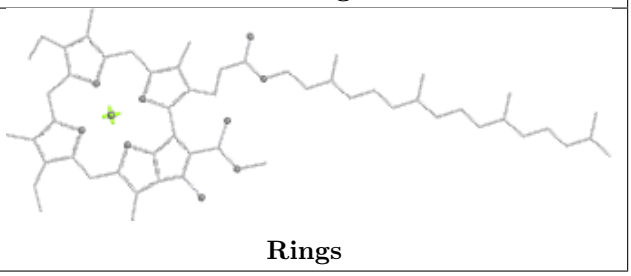
Bond lengths



Bond angles

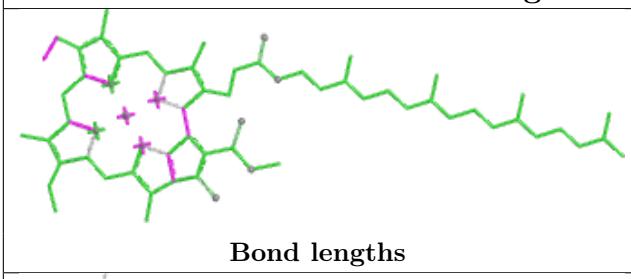


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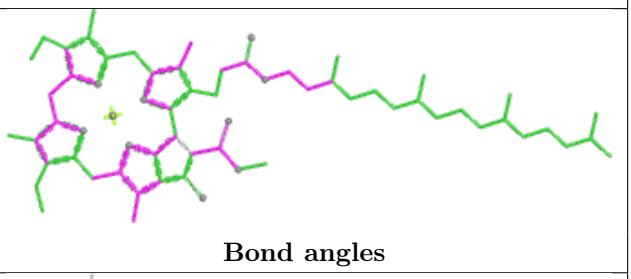


Rings

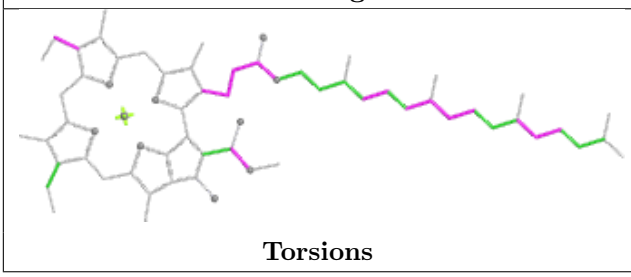
Ligand CLA R 316



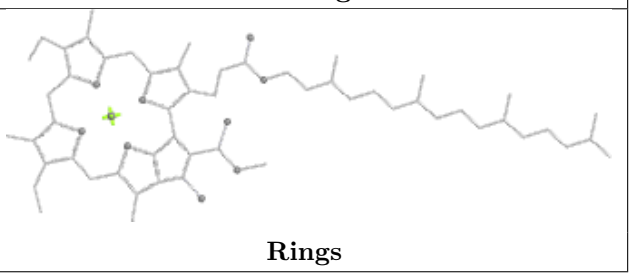
Bond lengths



Bond angles

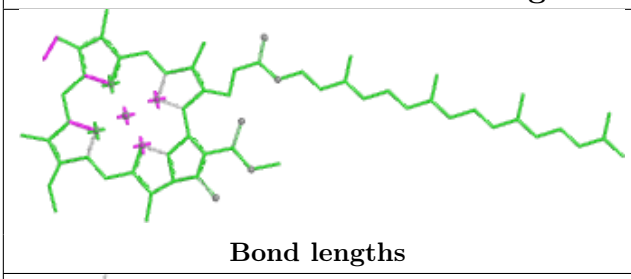


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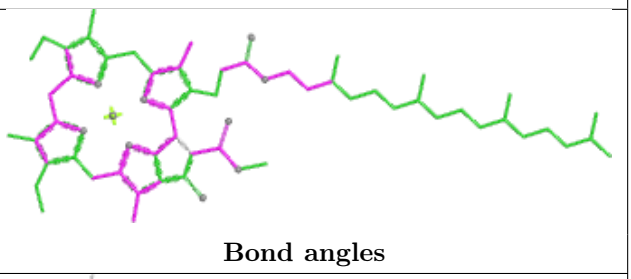


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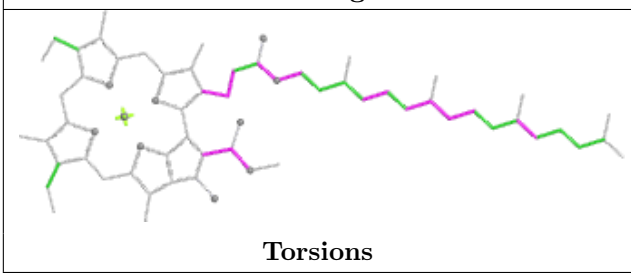
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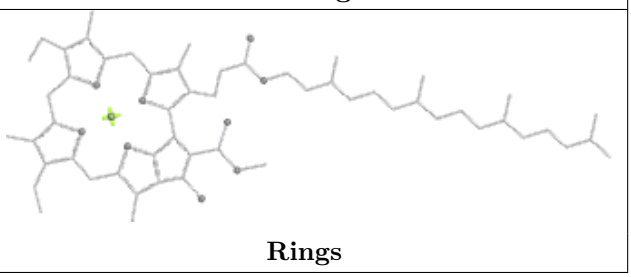
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Bond angles

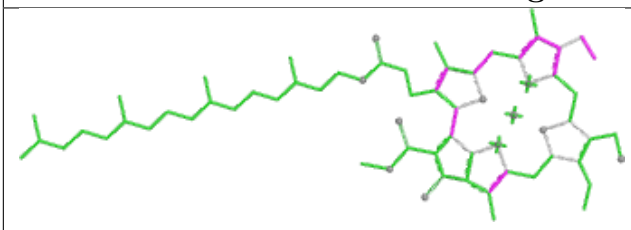


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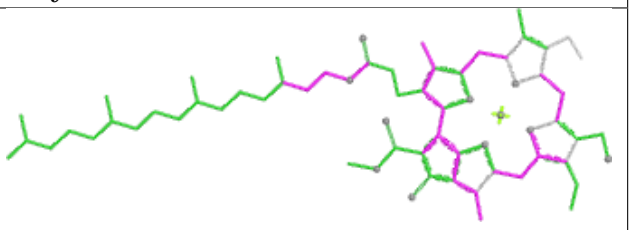


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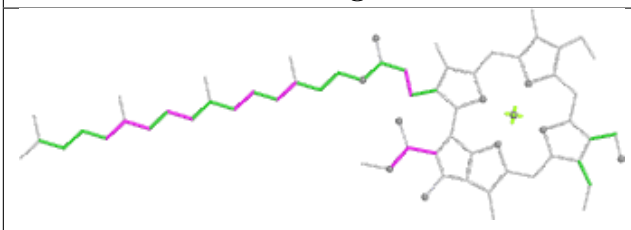
Ligand CHL y 607



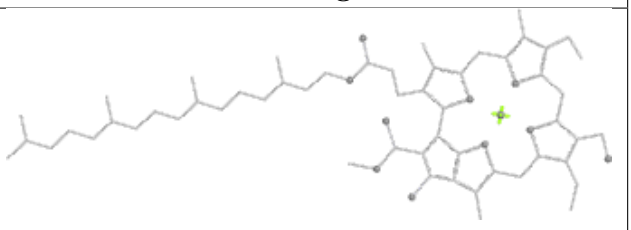
Bond lengths



Bond angles

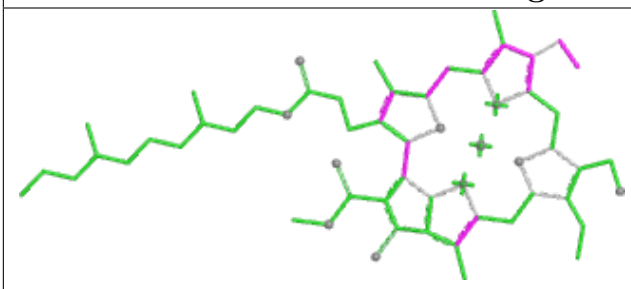


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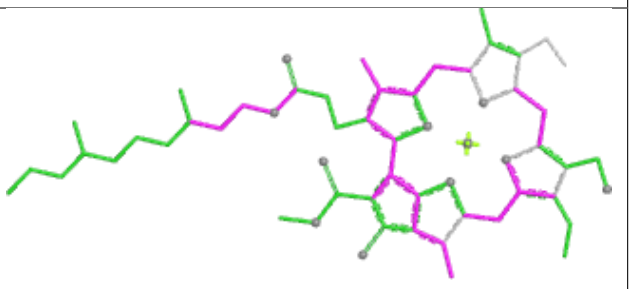


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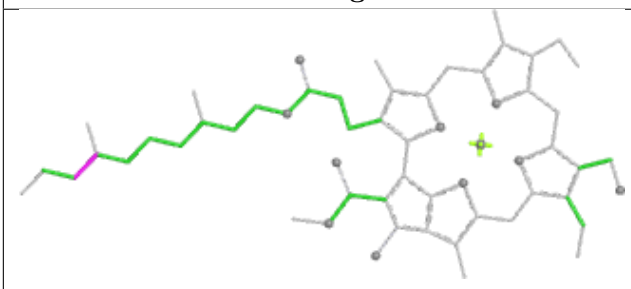
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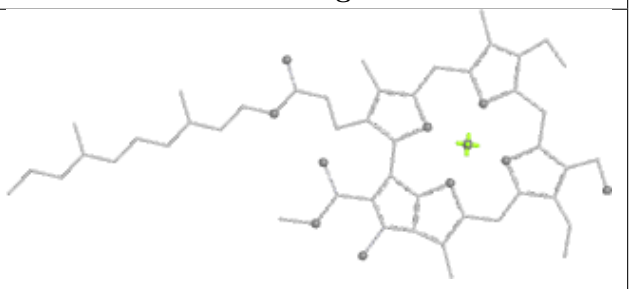
Bond lengths



Bond angles

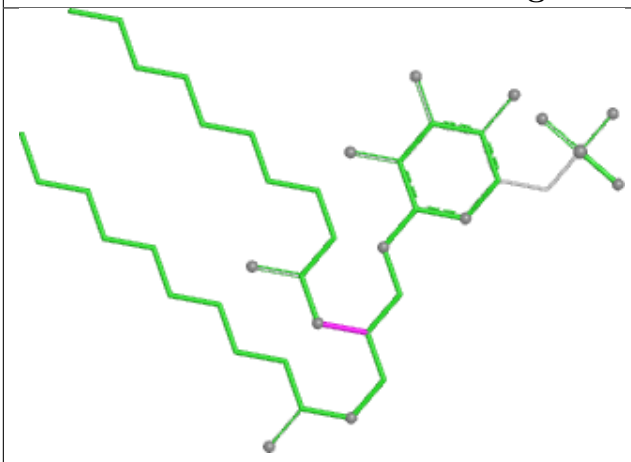


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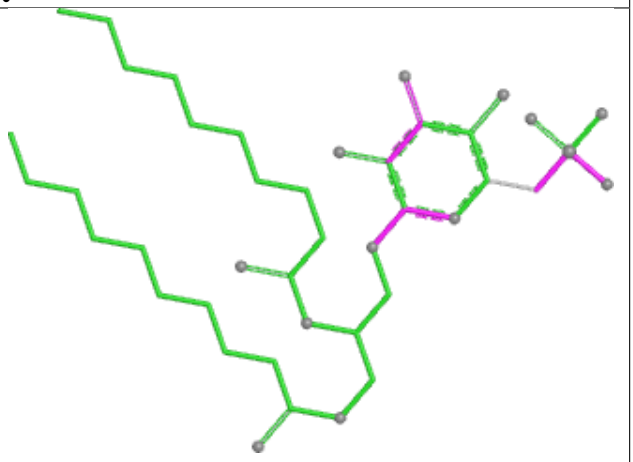


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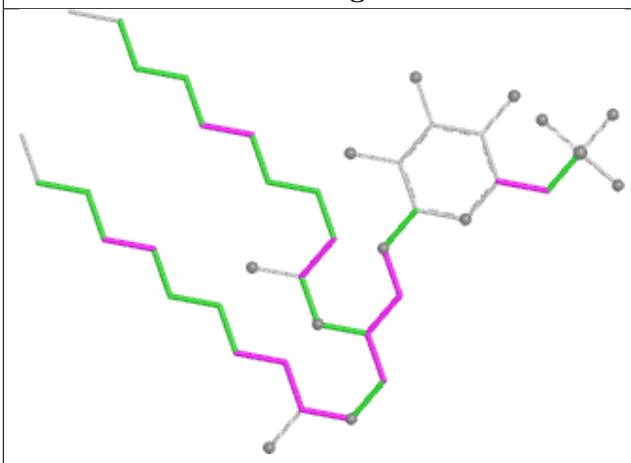
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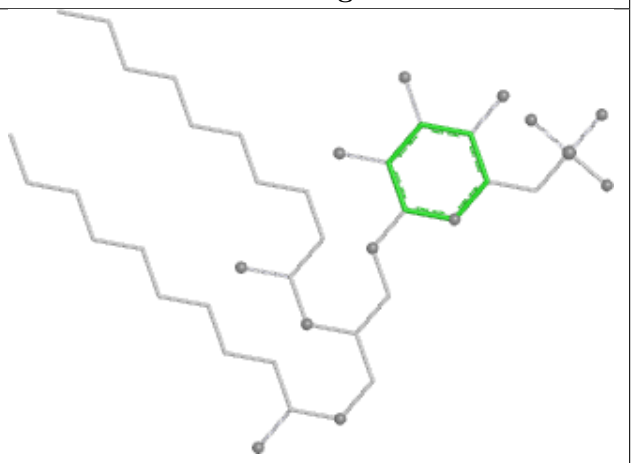
Bond lengths



Bond angles



Torsions

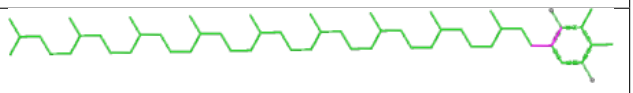


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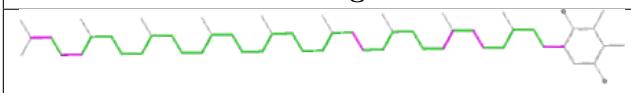
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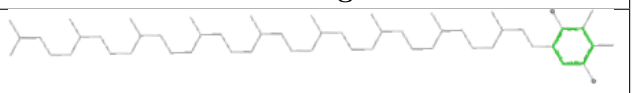
Bond lengths



Bond angles

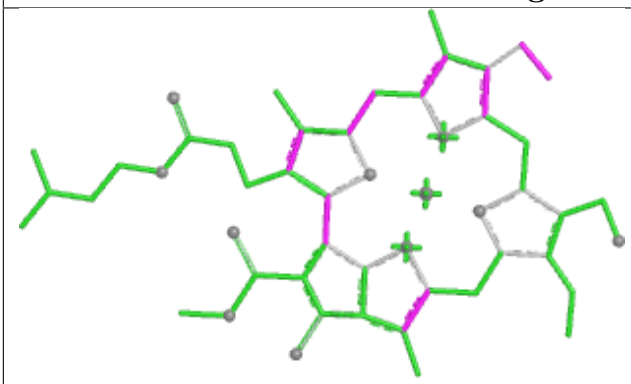


Torsions

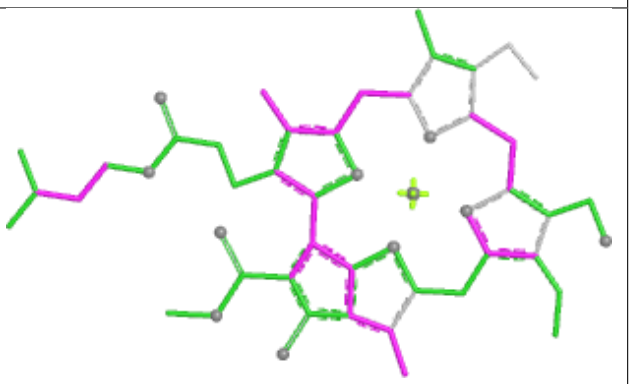


Rings

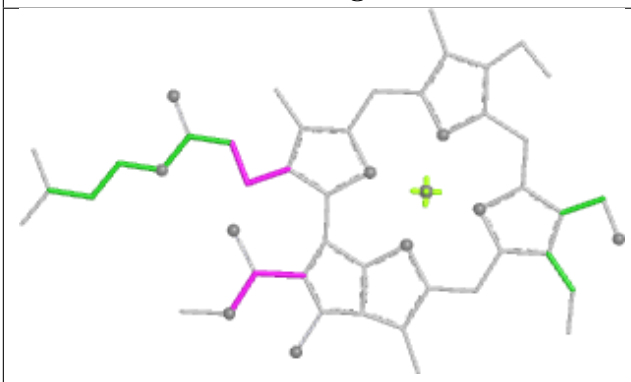
Ligand CHL 6 307



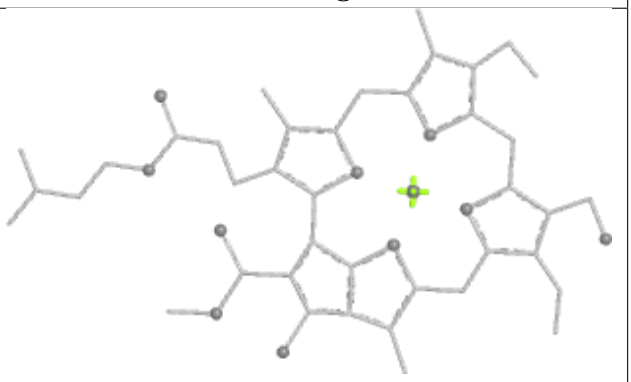
Bond lengths



Bond angles

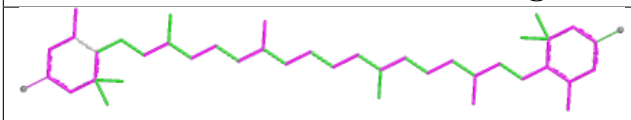


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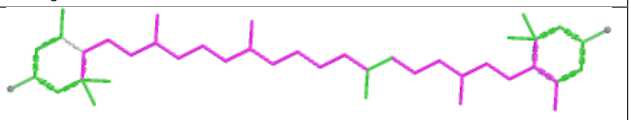


Rings

Ligand LUT y 617



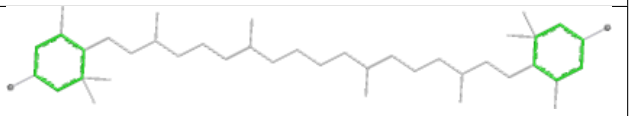
Bond lengths



Bond angles

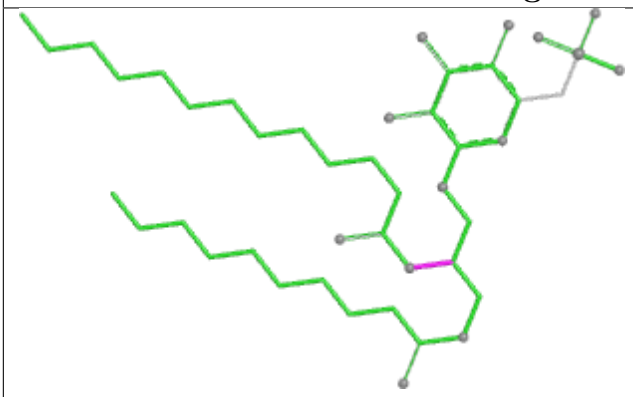


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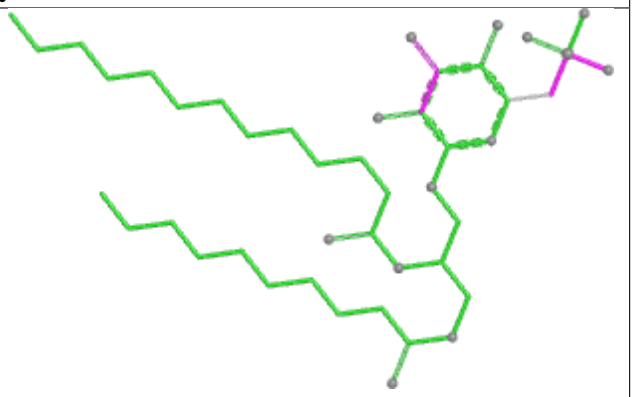


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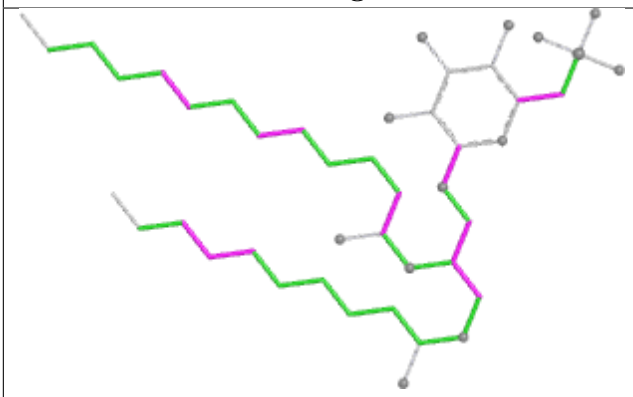
Ligand SQD A 413



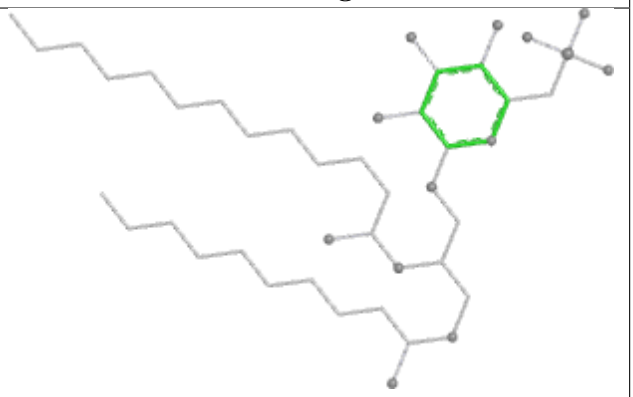
Bond lengths



Bond angles

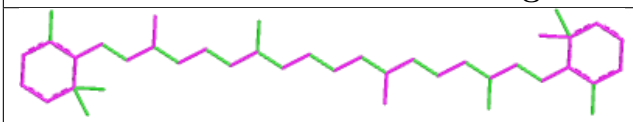


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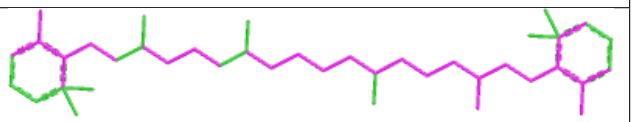


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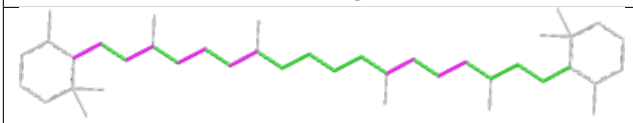
Ligand BCR B 618



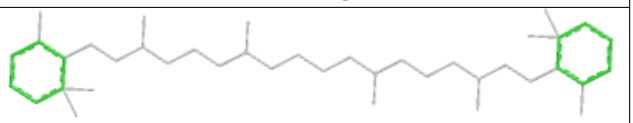
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Bond angles

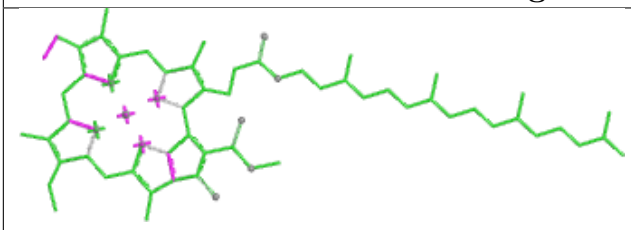


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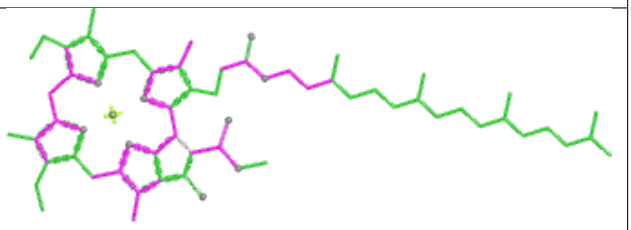


Rings

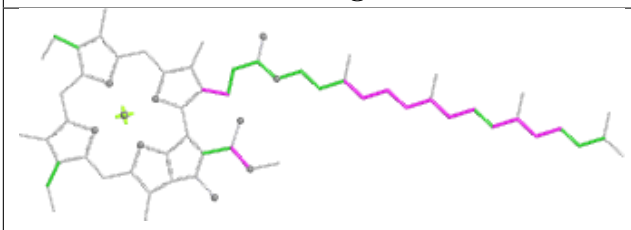
Ligand CLA 1 610



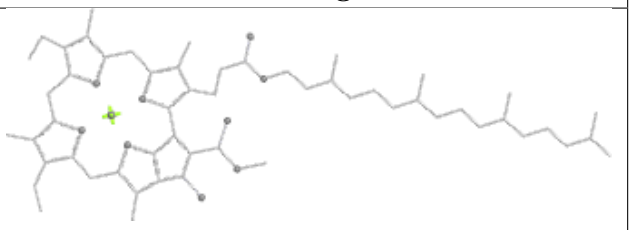
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Bond angles

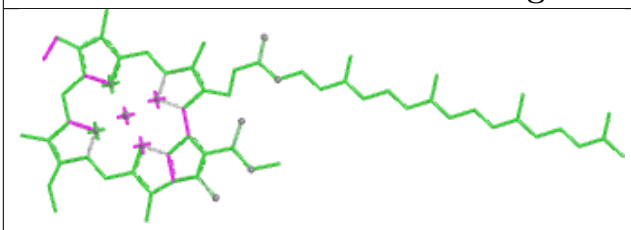


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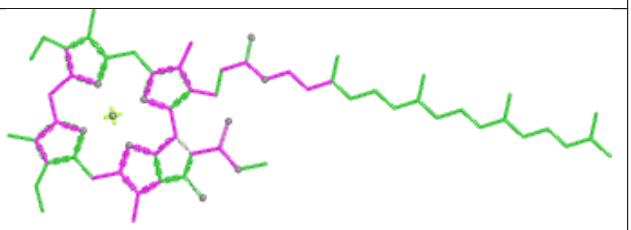


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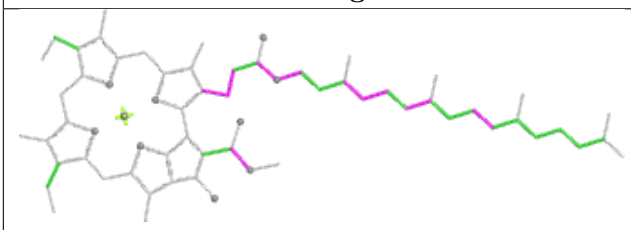
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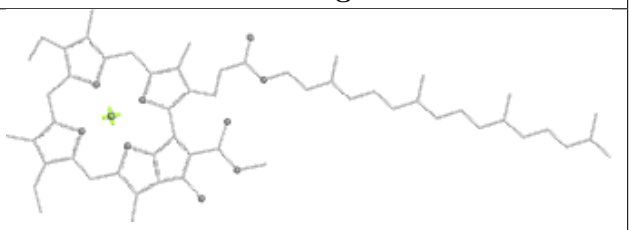
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Bond angles

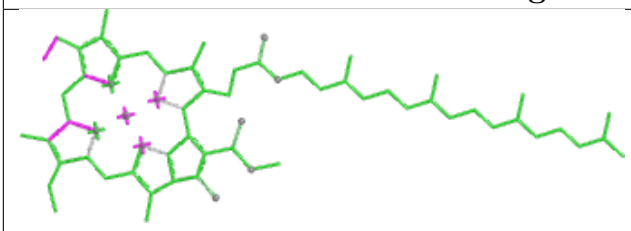


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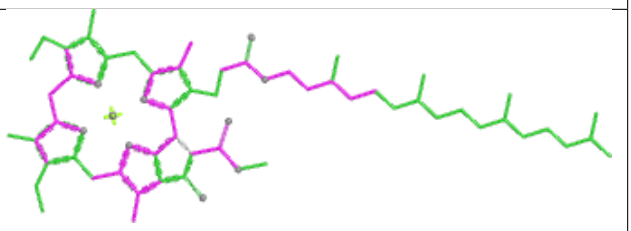


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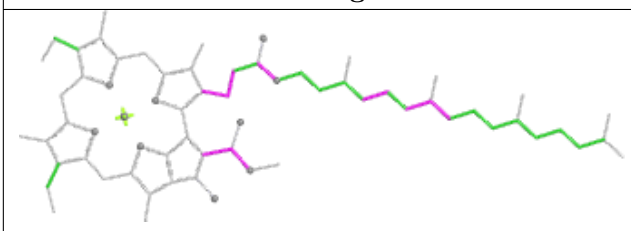
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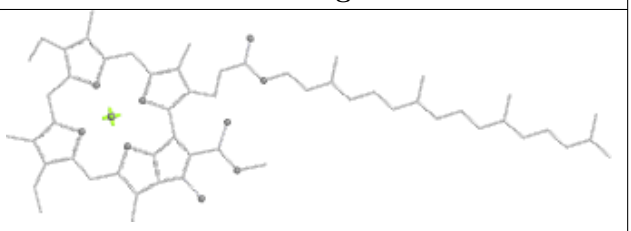
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Bond angles

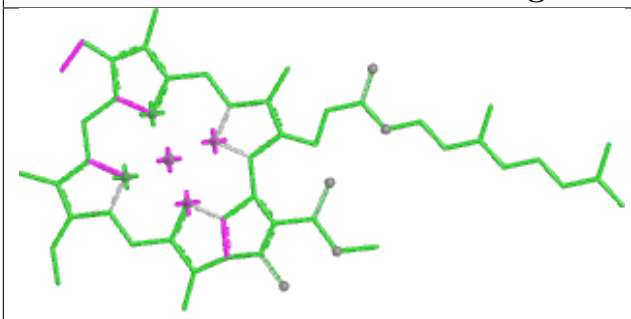


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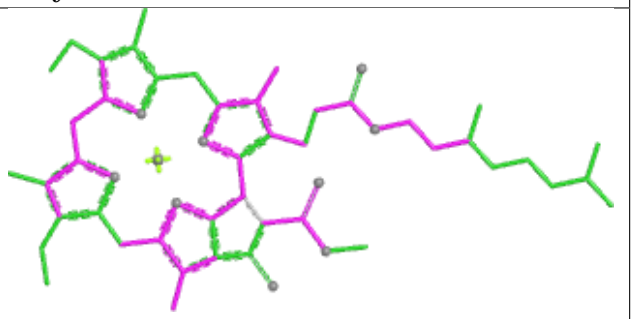


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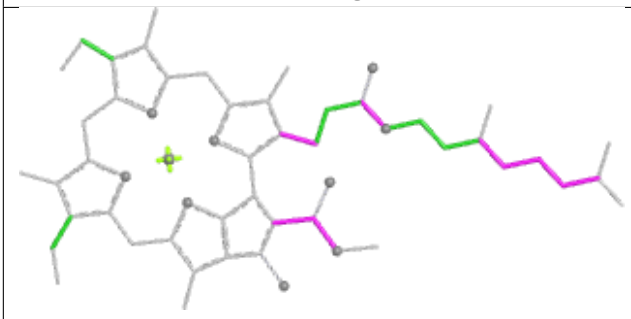
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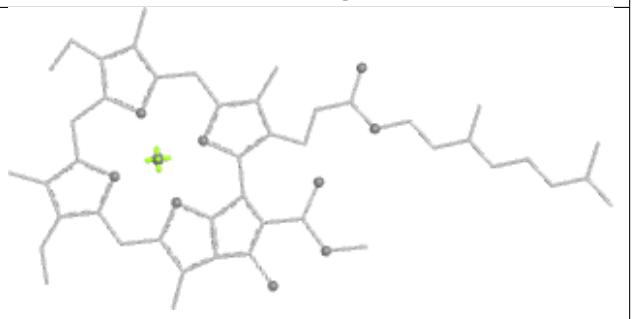
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Bond angles

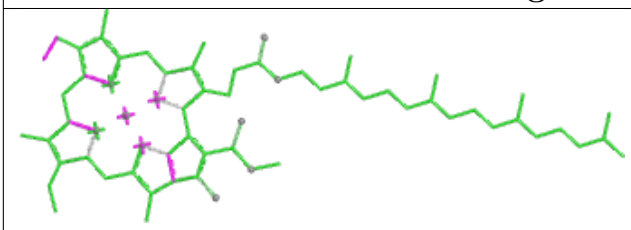


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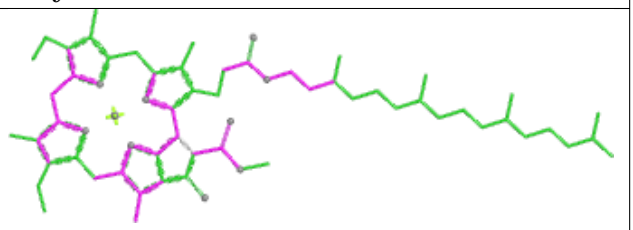


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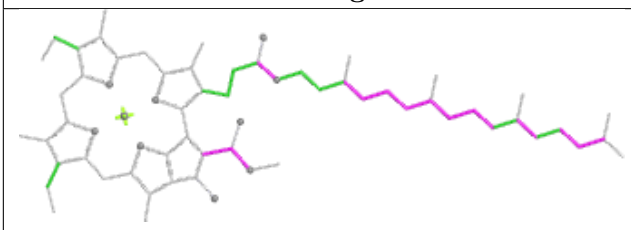
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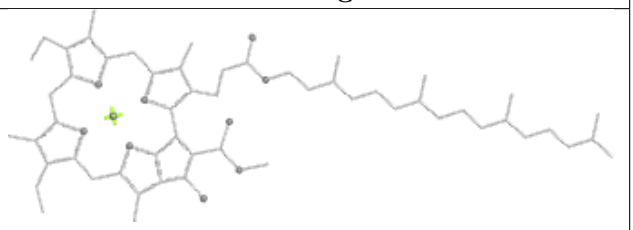
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Bond angles

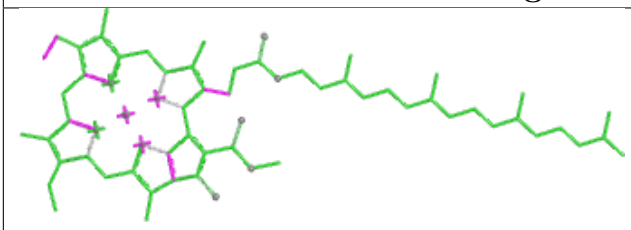


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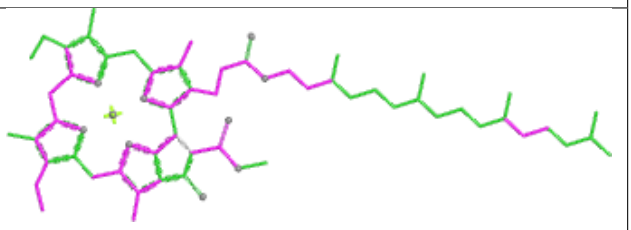


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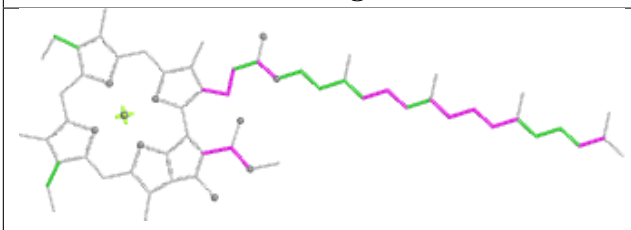
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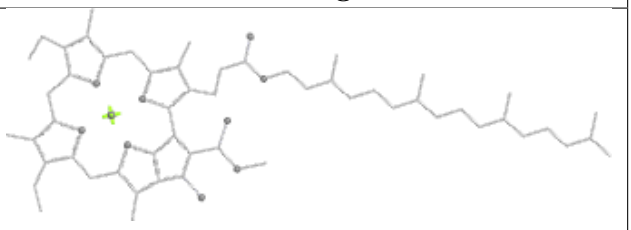
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Bond angles

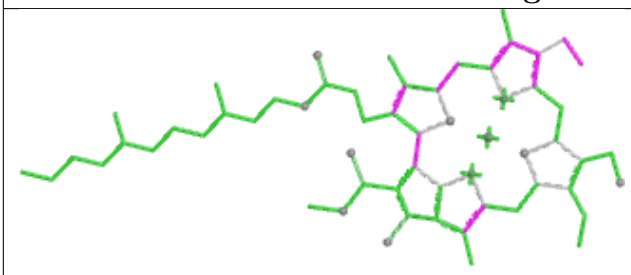


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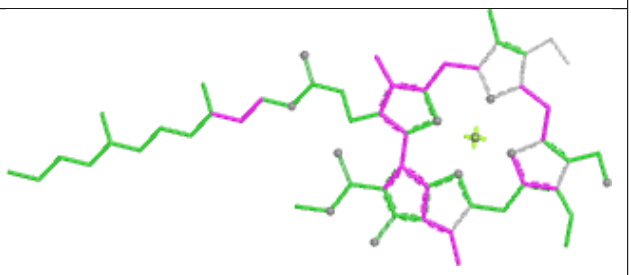


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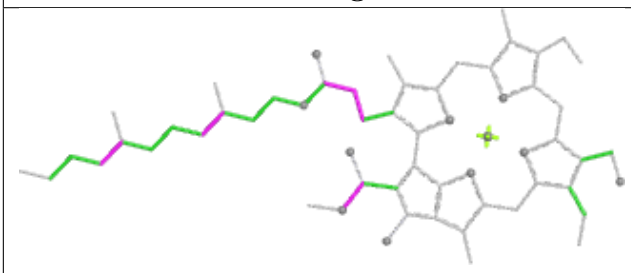
Ligand CHL Y 307



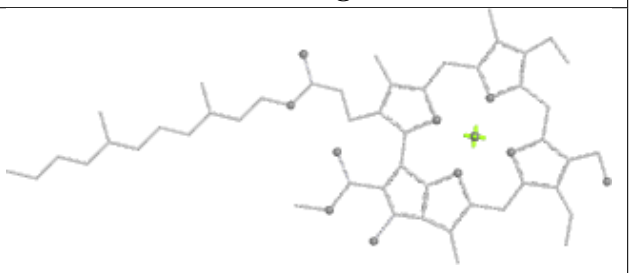
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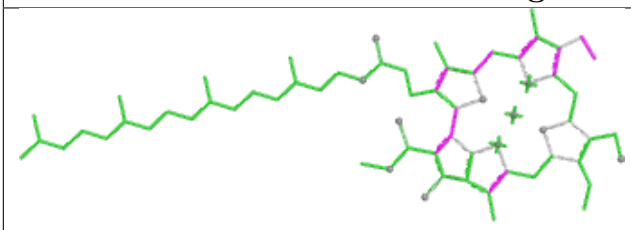


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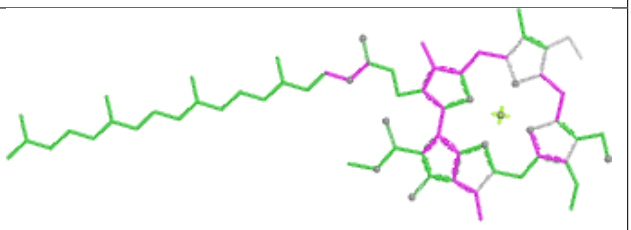


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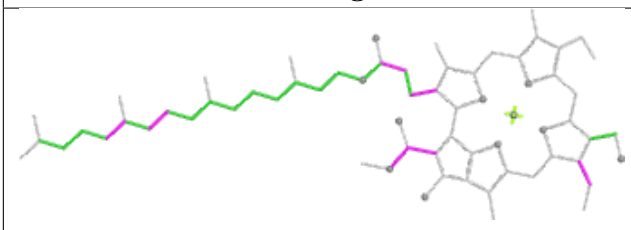
Ligand CHL 8 608



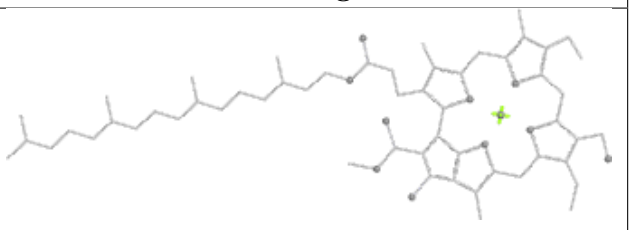
Bond lengths



Bond angles

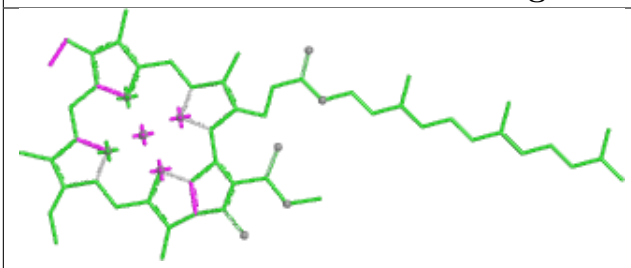


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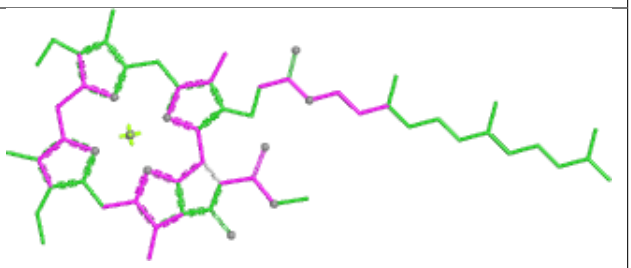


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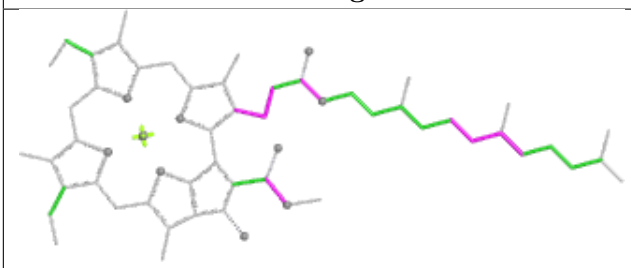
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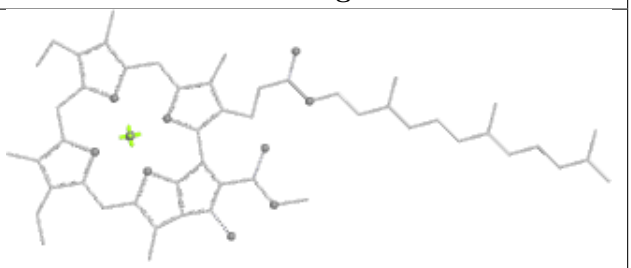
Bond lengths



Bond angles

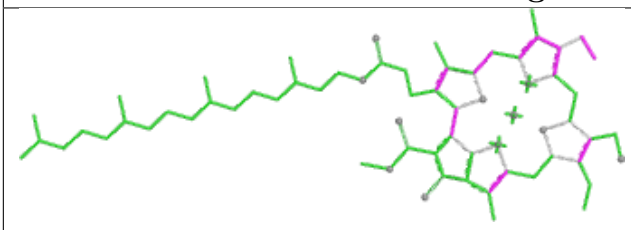


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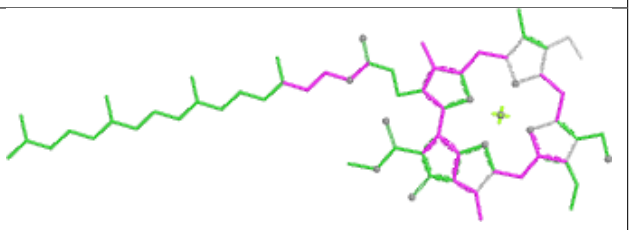


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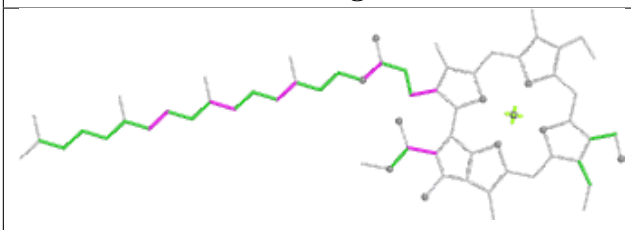
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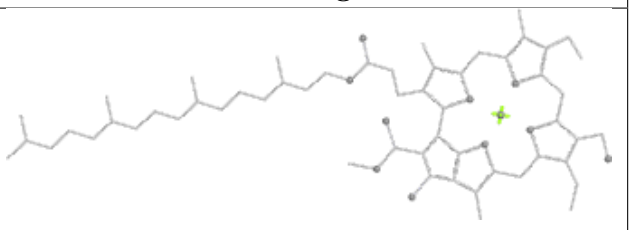
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Bond angles

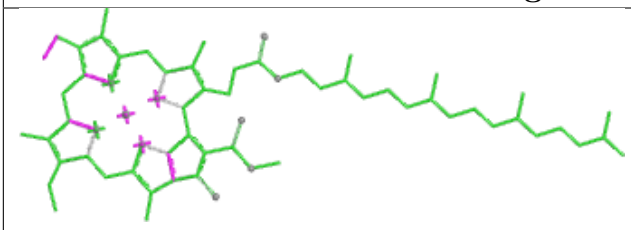


Torsions

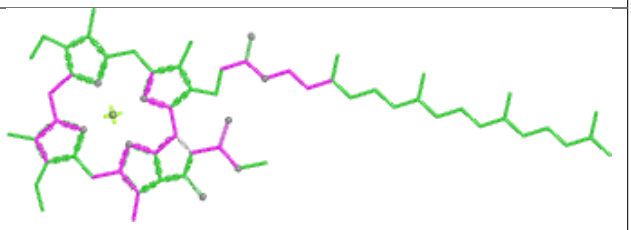


Rings

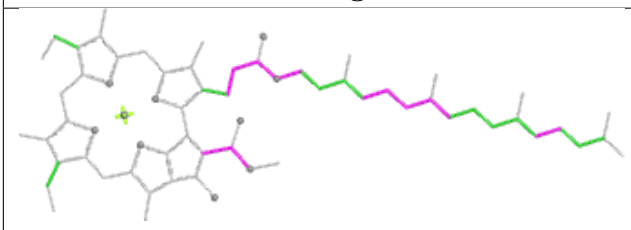
Ligand CLA B 616



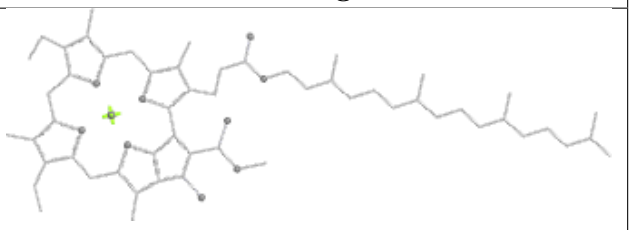
Bond lengths



Bond angles

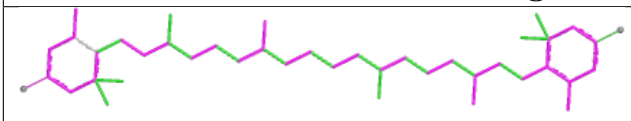


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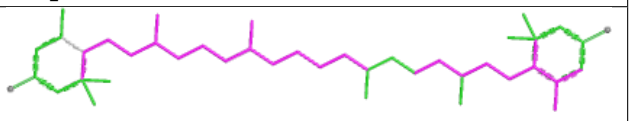


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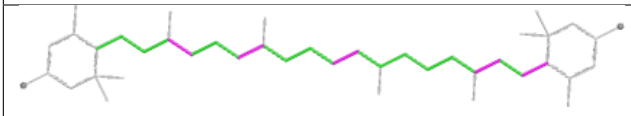
Ligand LUT p 617



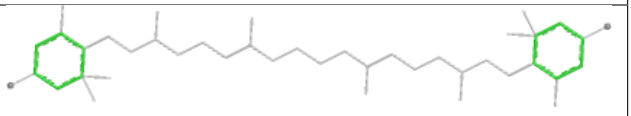
Bond lengths



Bond angles

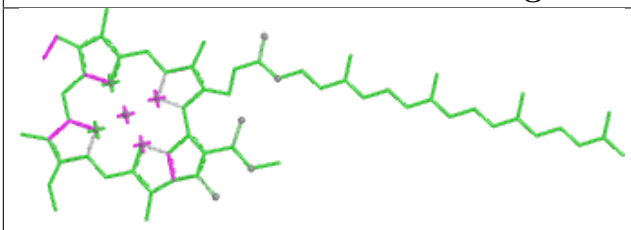


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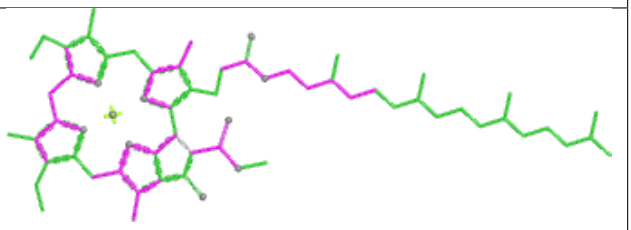


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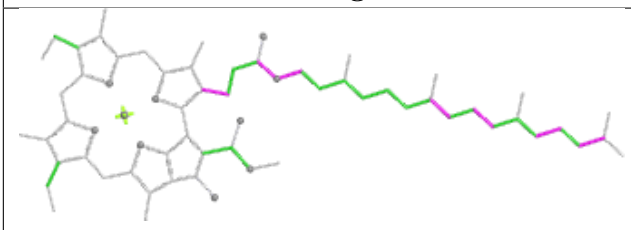
Ligand CLA B 612



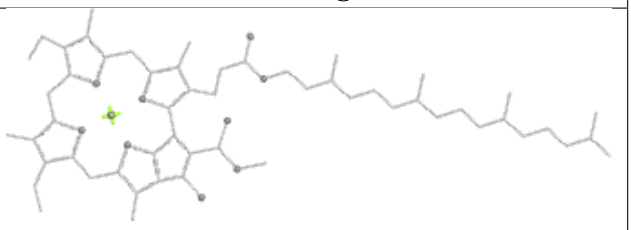
Bond lengths



Bond angles

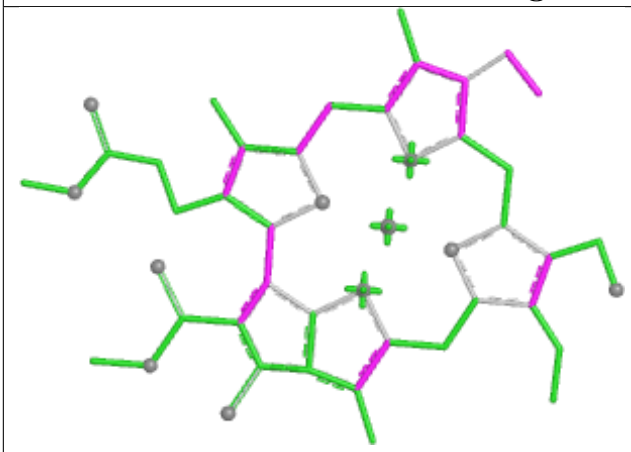


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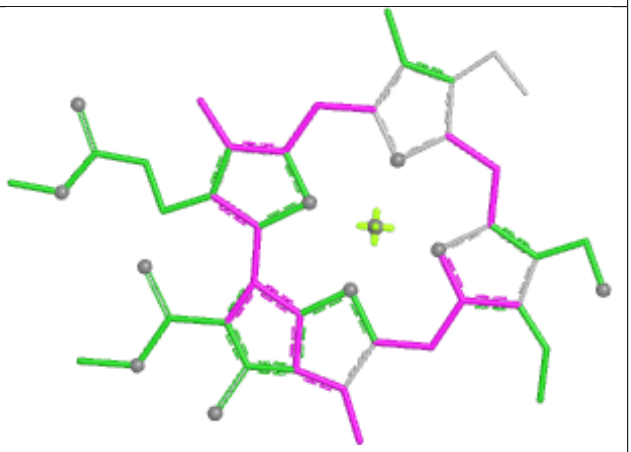


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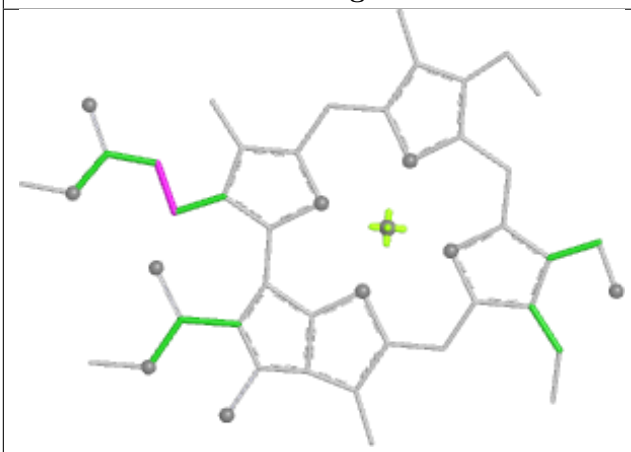
Ligand CHL 3 308



Bond lengths



Bond angles

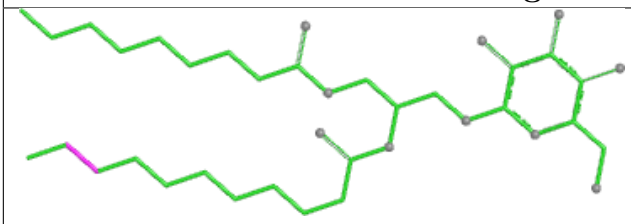


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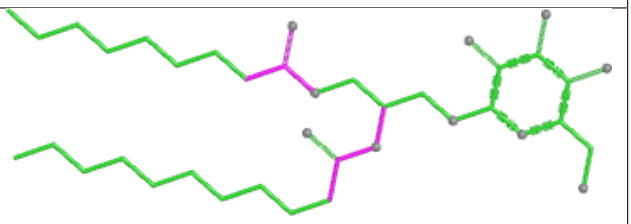


Rings

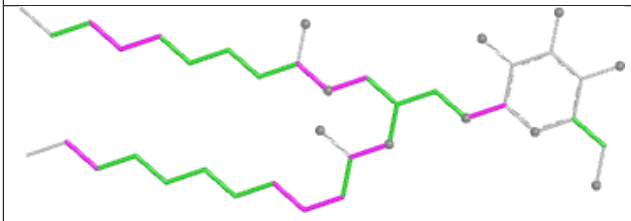
Ligand LMG 6 322



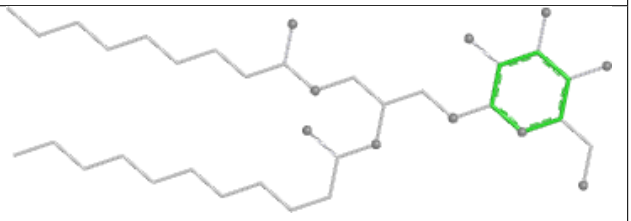
Bond lengths



Bond angles

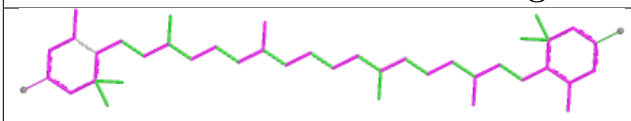


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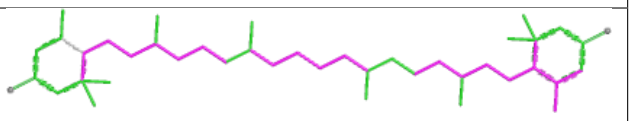


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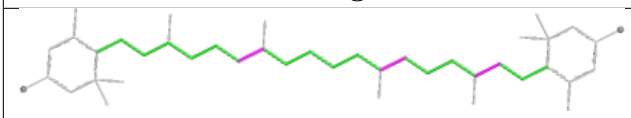
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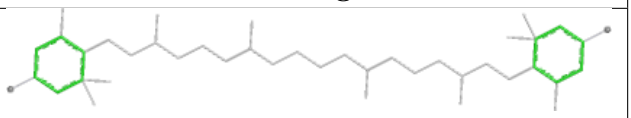
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Bond angles

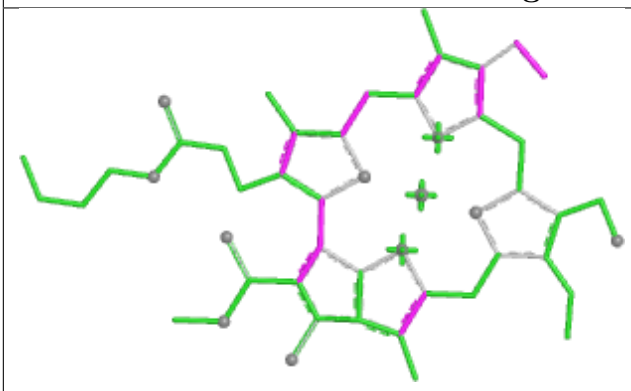


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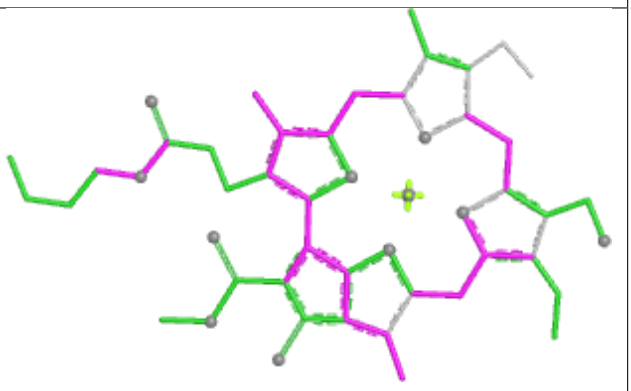


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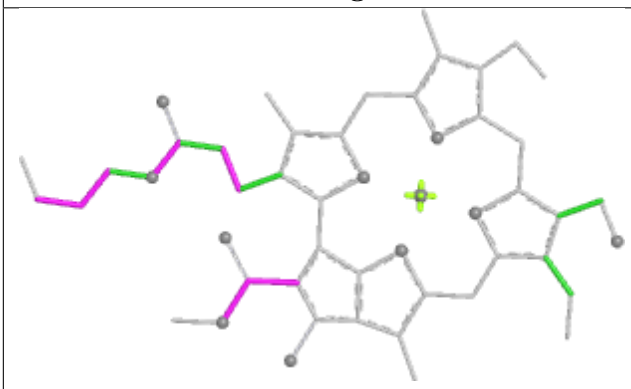
Ligand CHL N 308



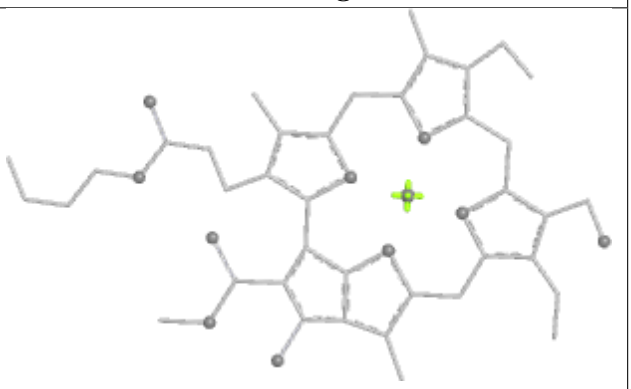
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Bond angles

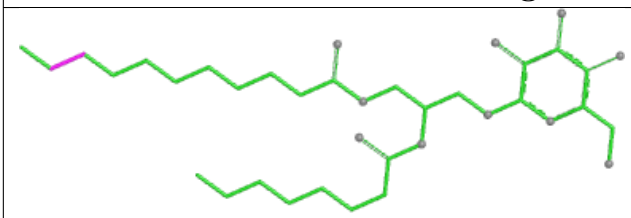


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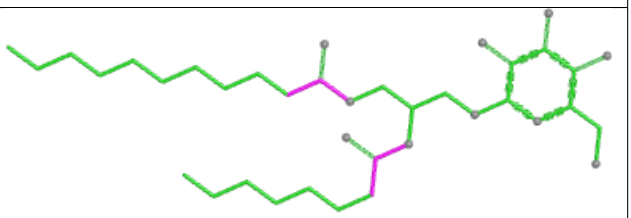


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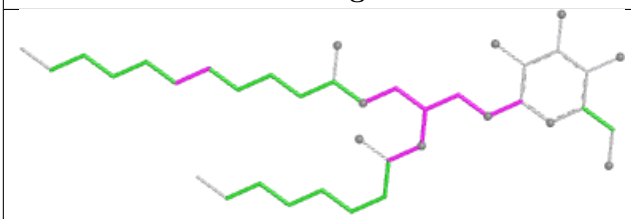
Ligand LMG w 205



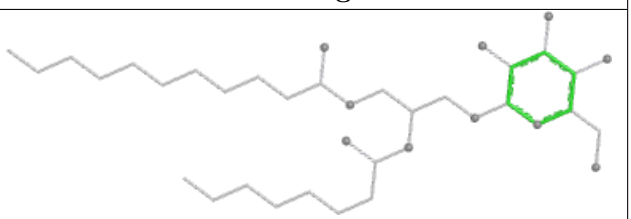
Bond lengths



Bond angles

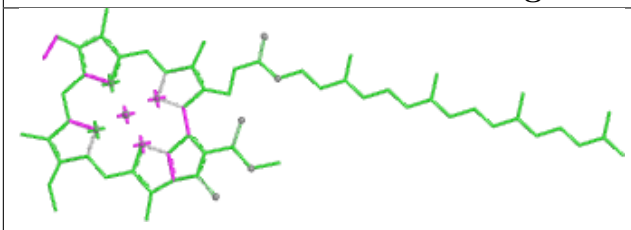


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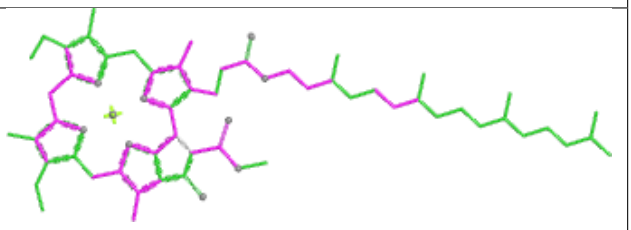


Rings

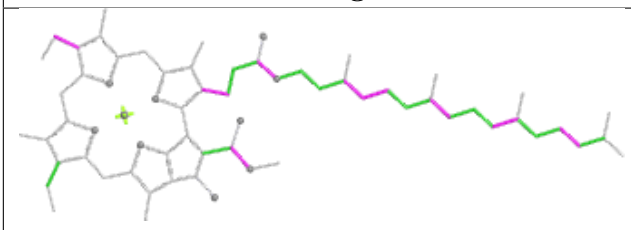
Ligand CLA B 602



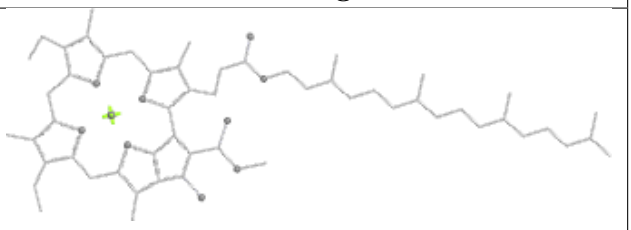
Bond lengths



Bond angles

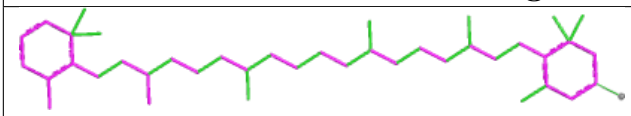


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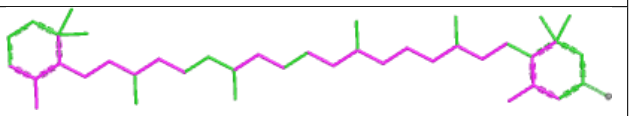


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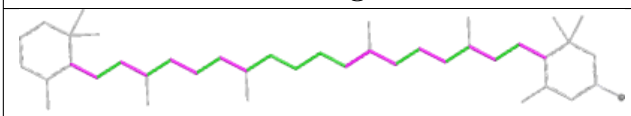
Ligand RRX 4 615



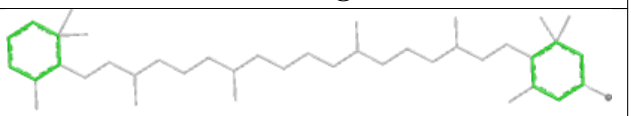
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Bond angles

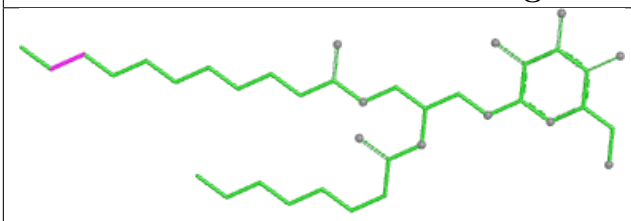


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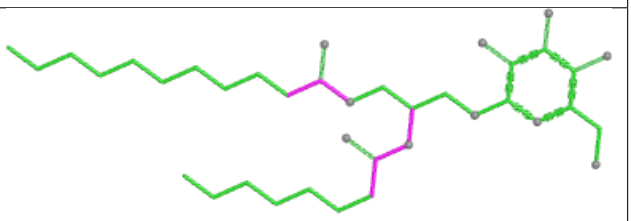


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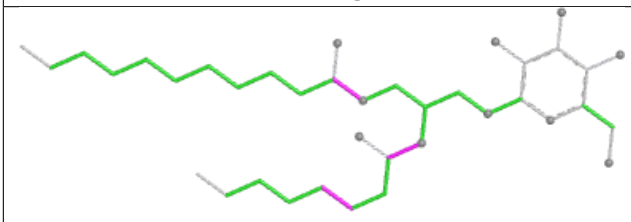
Ligand LMG a 401



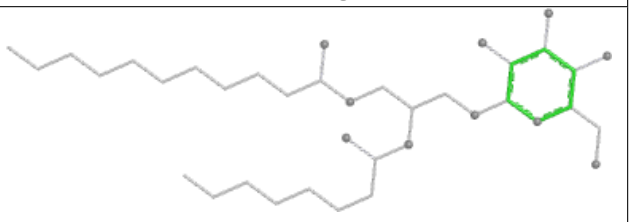
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Bond angles

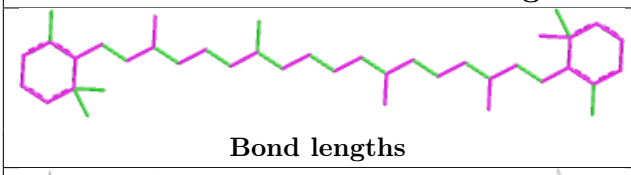


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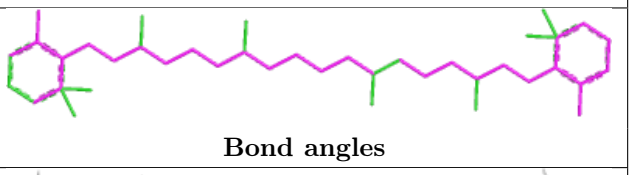


Rings

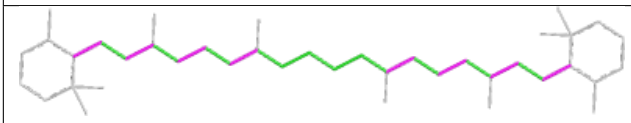
Ligand BCR C 614



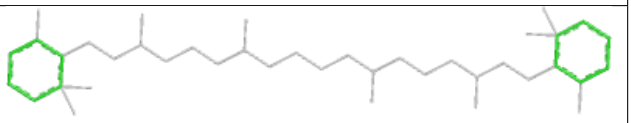
Bond lengths



Bond angles

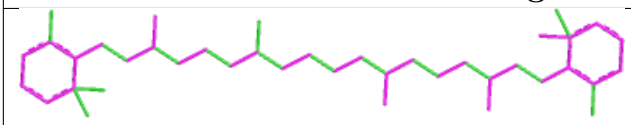


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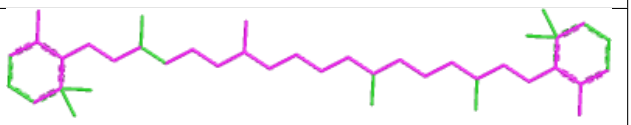


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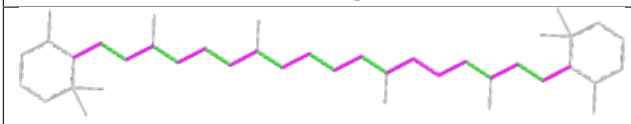
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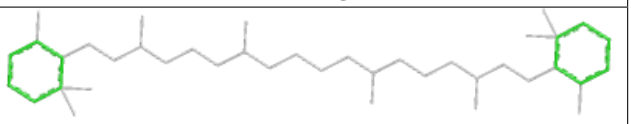
Bond lengths



Bond angles

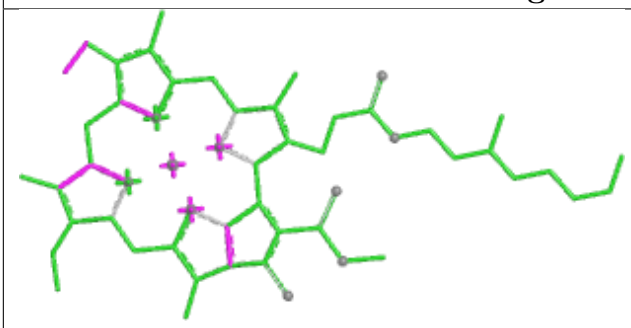


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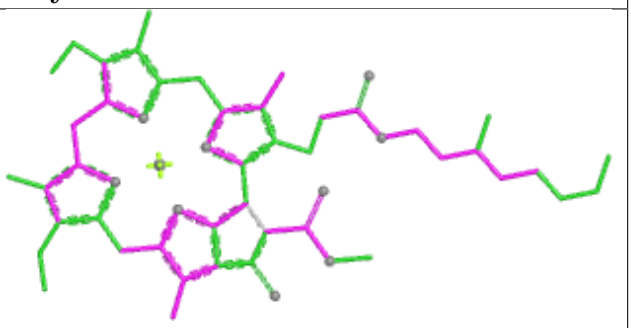


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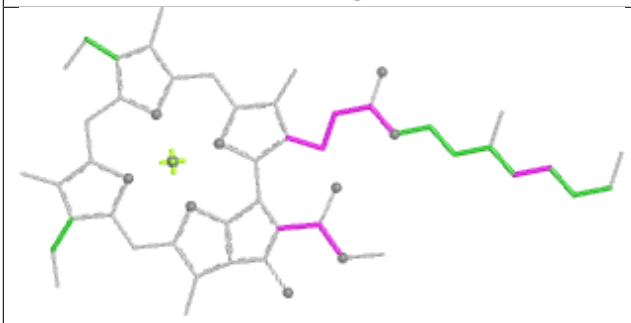
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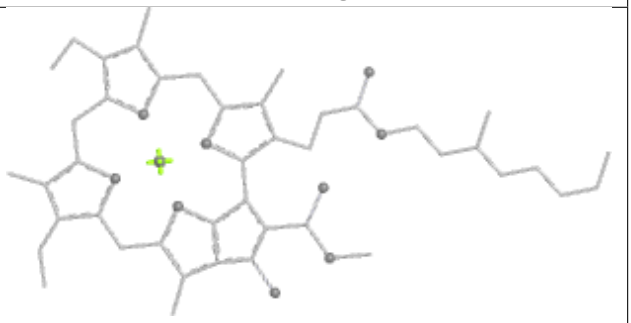
Bond lengths



Bond angles

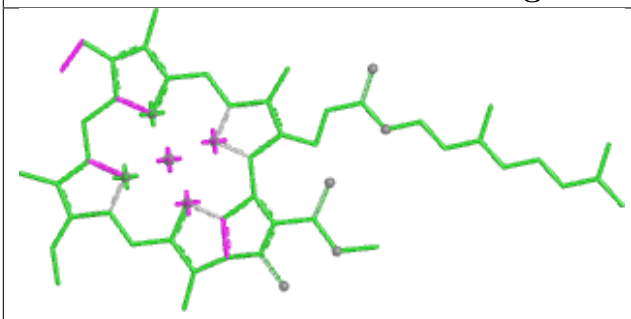


Torsions

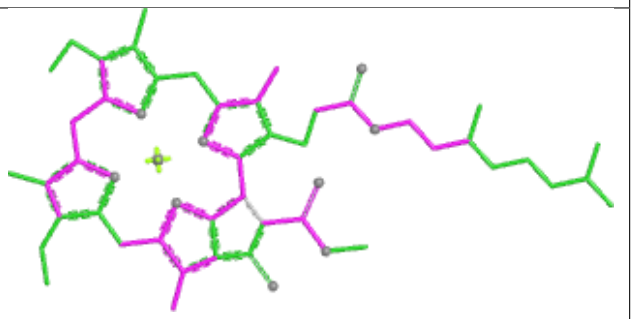


Rings

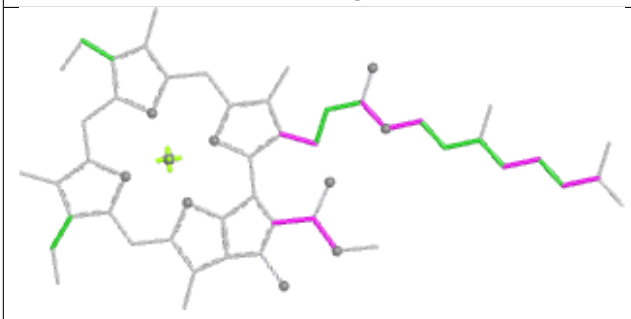
Ligand CLA Y 305



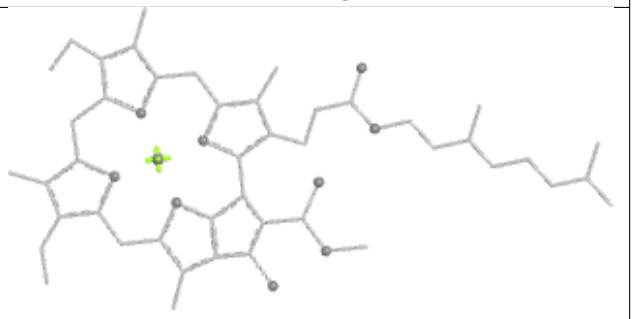
Bond lengths



Bond angles

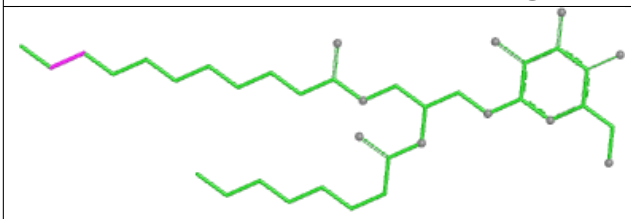


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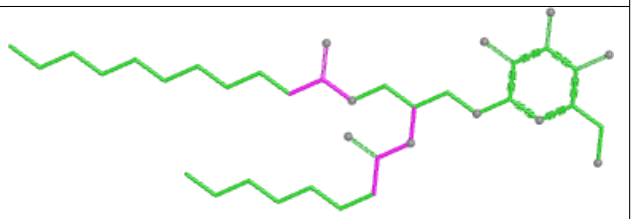


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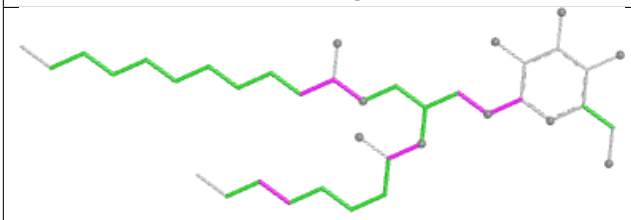
Ligand LMG 9 321



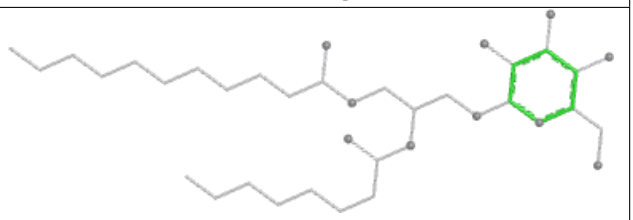
Bond lengths



Bond angles

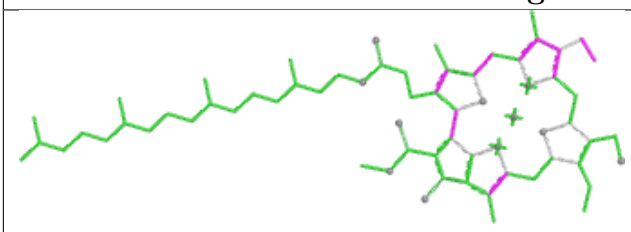


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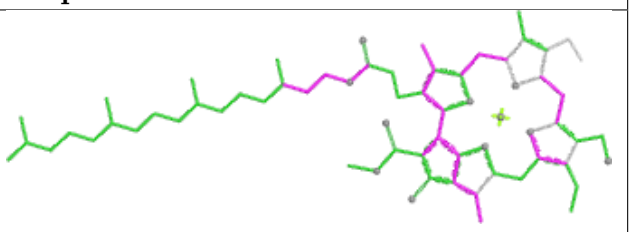


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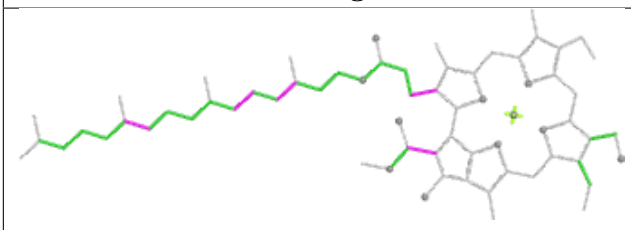
Ligand CHL q 303



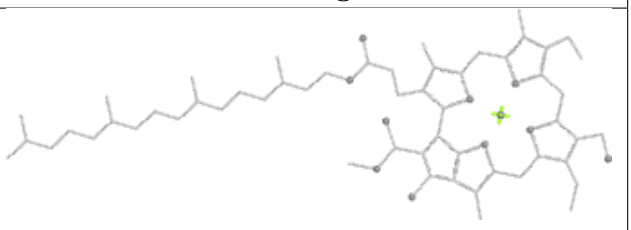
Bond lengths



Bond angles

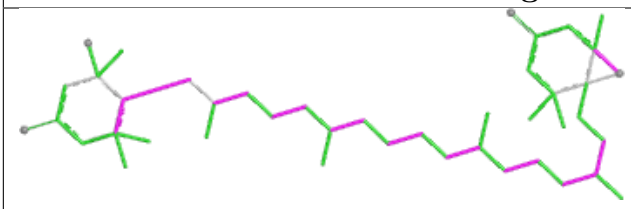


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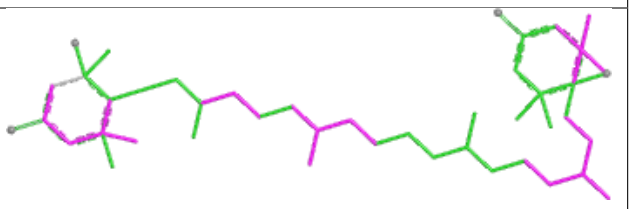


Rings

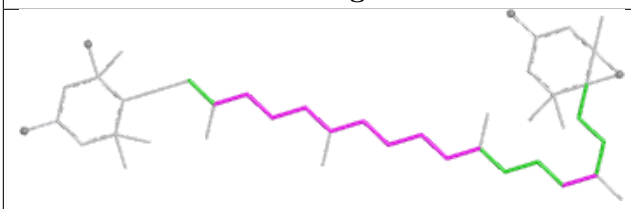
Ligand NEX N 318



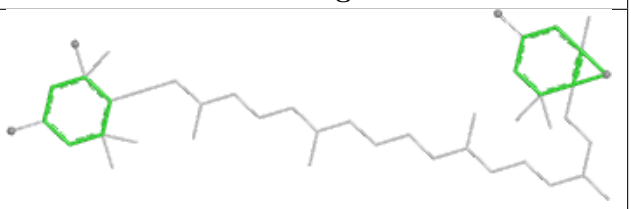
Bond lengths



Bond angles

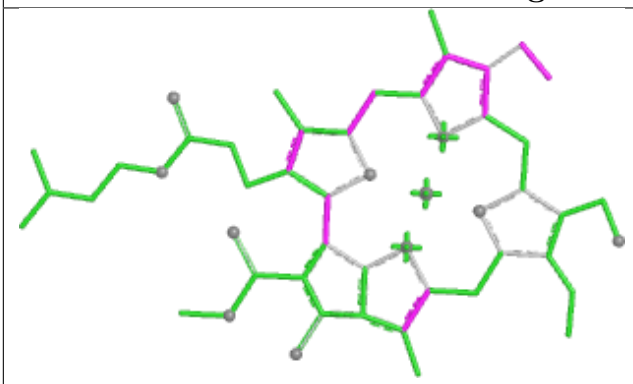


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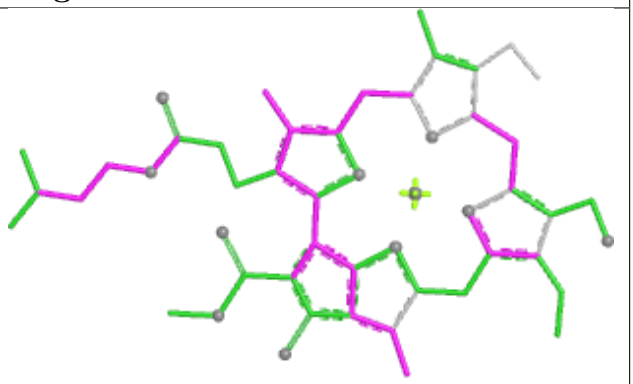


Rings

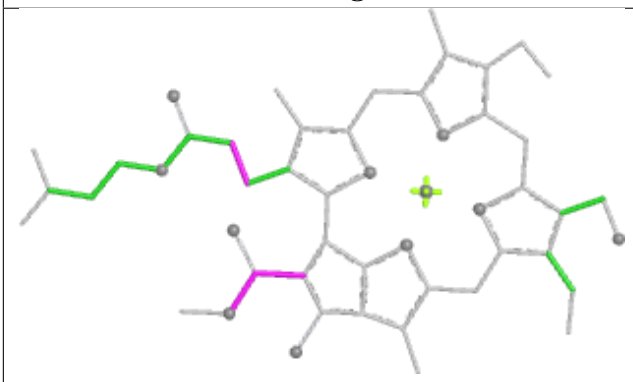
Ligand CHL g 308



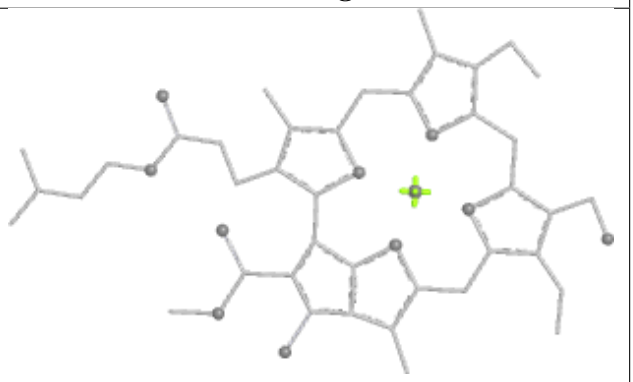
Bond lengths



Bond angles

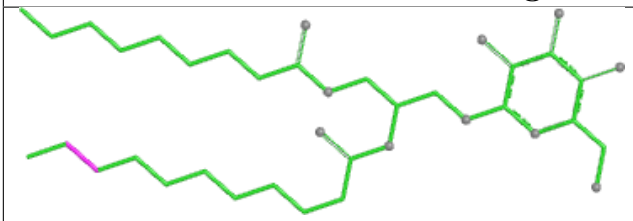


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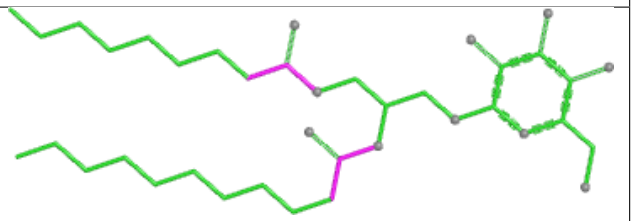


Rings

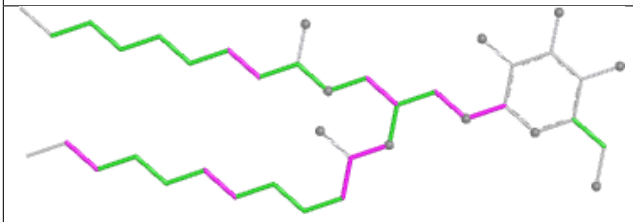
Ligand LMG 7 301



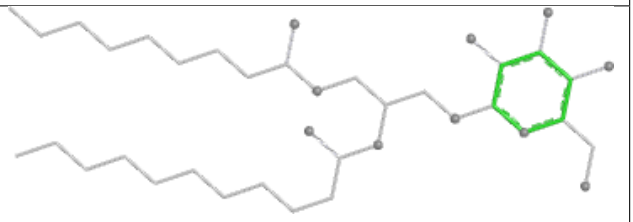
Bond lengths



Bond angles

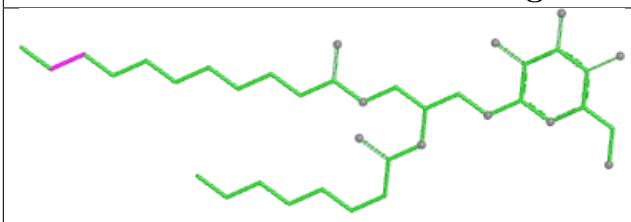


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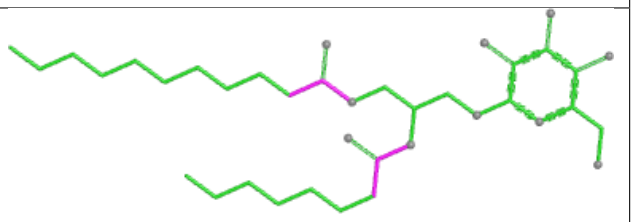


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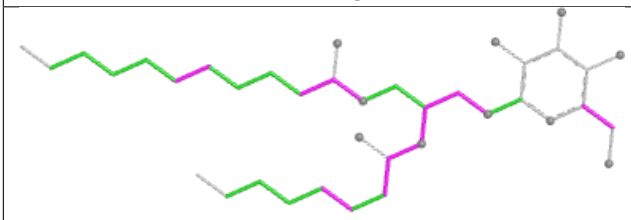
Ligand LMG I 101



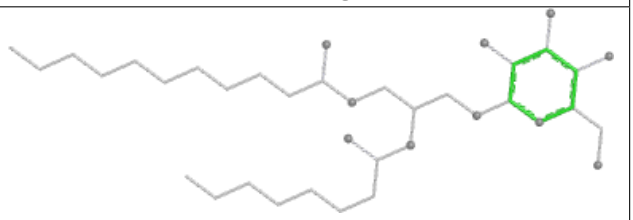
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Bond angles

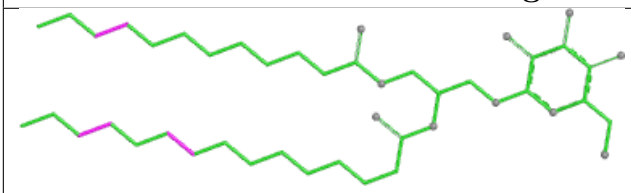


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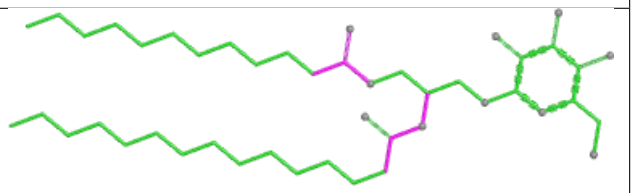


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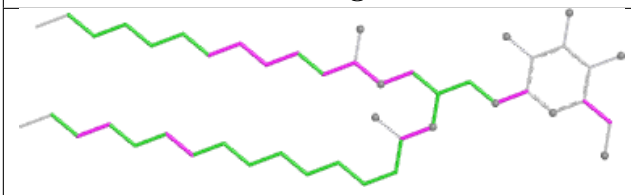
Ligand LMG b 626



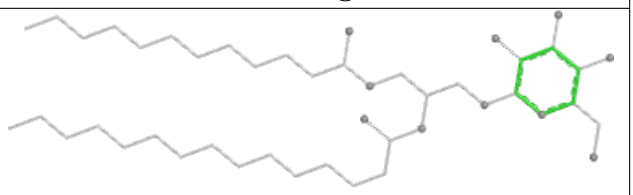
Bond lengths



Bond angles

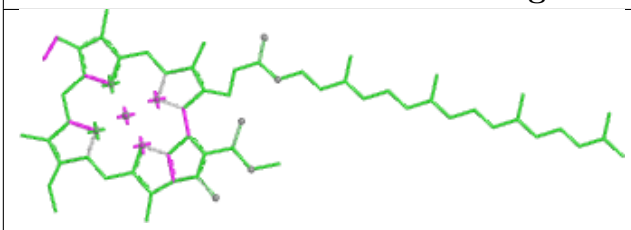


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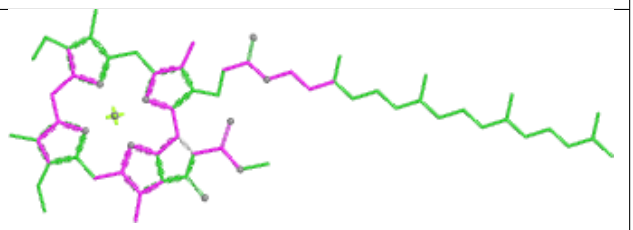


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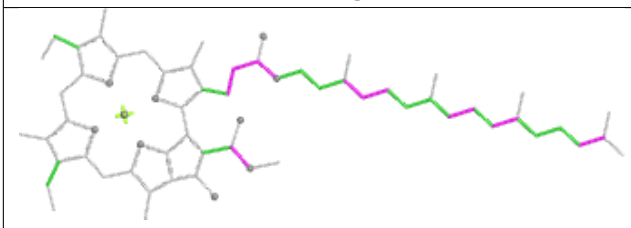
Ligand CLA 2 612



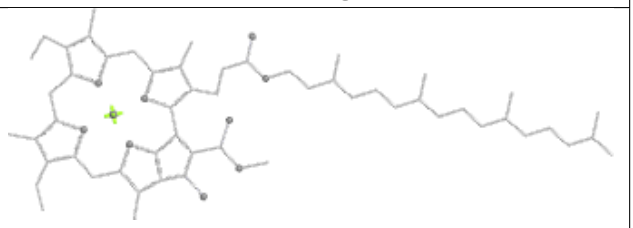
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Bond angles

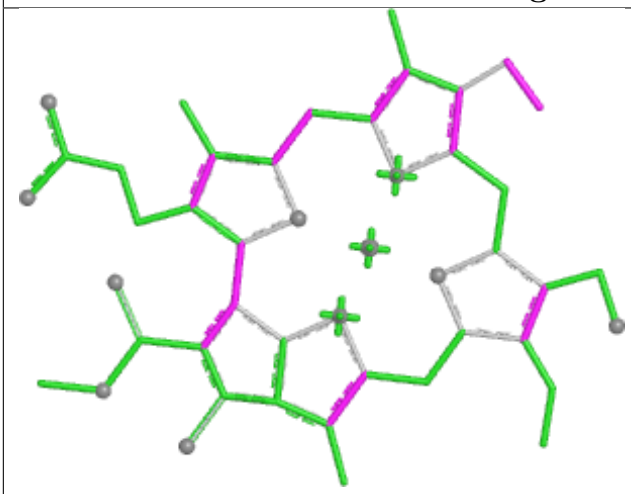


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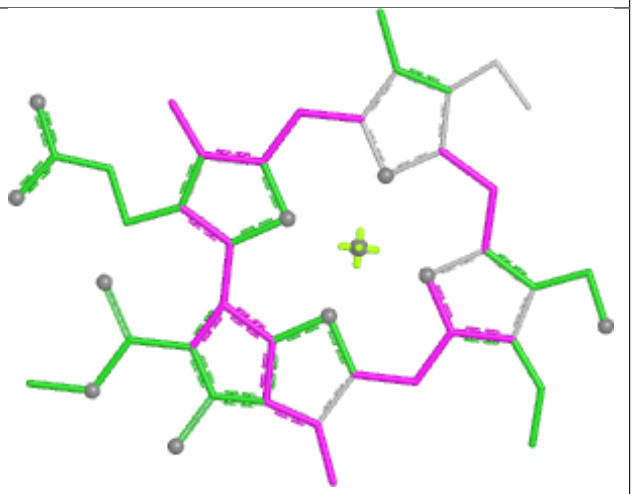


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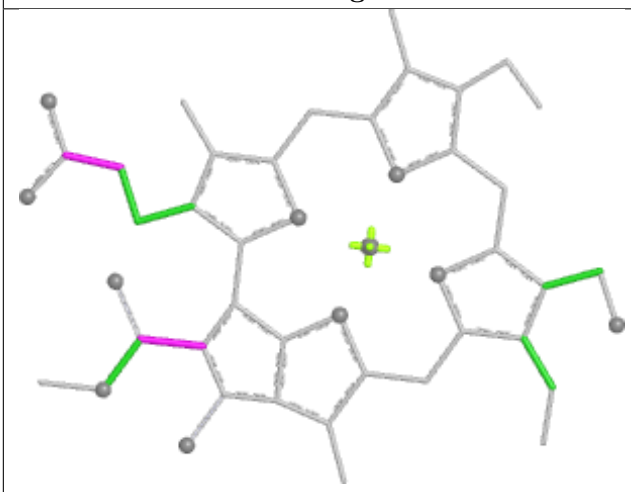
Ligand CHL s 302



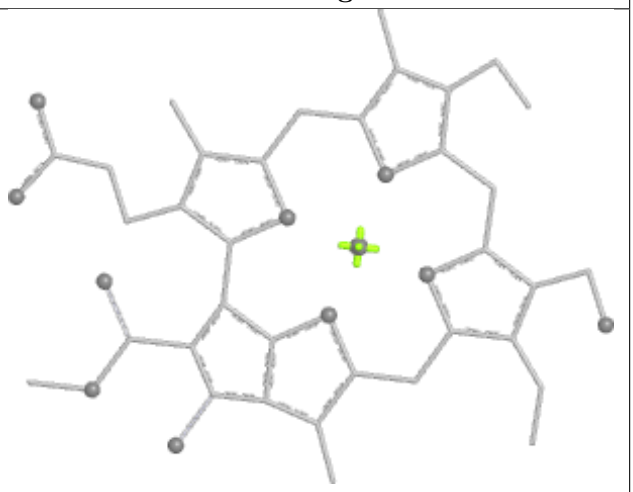
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Bond angles

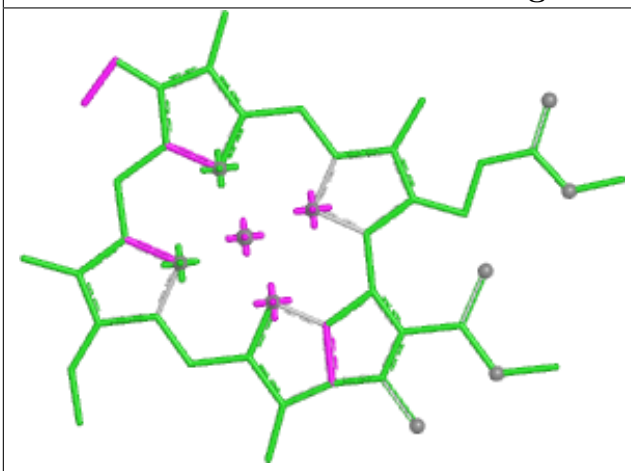


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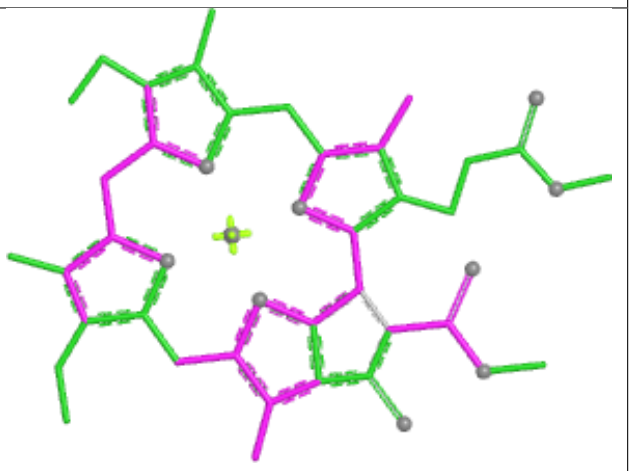


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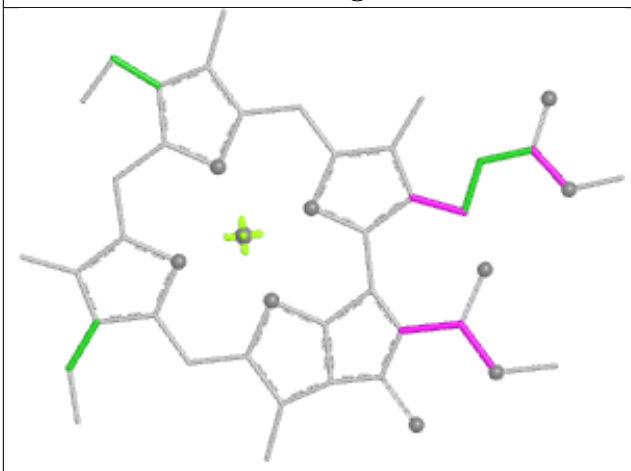
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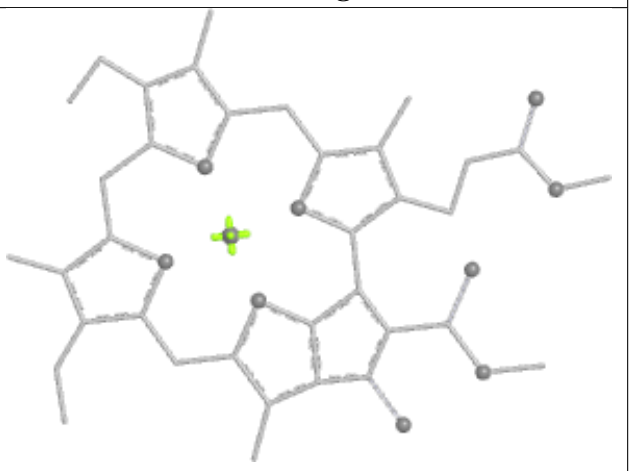
Bond lengths



Bond angles

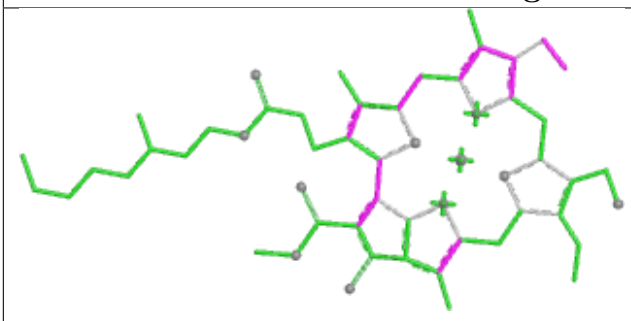


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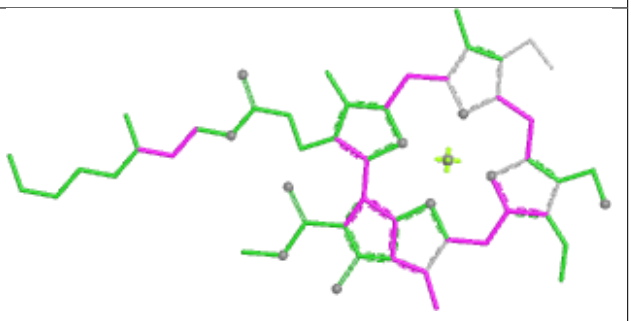


Rings

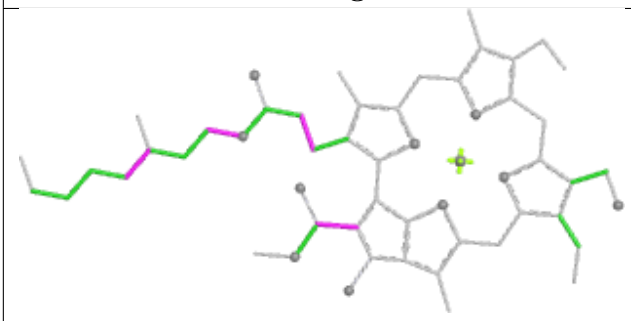
Ligand CHL R 310



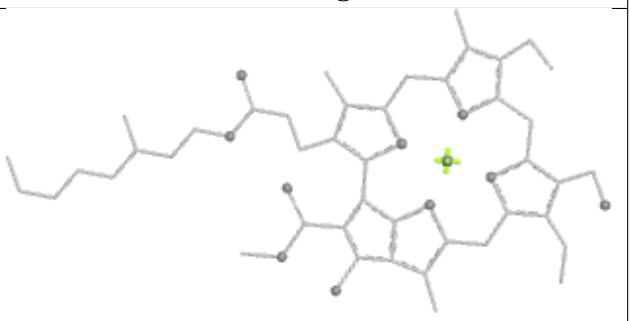
Bond lengths



Bond angles

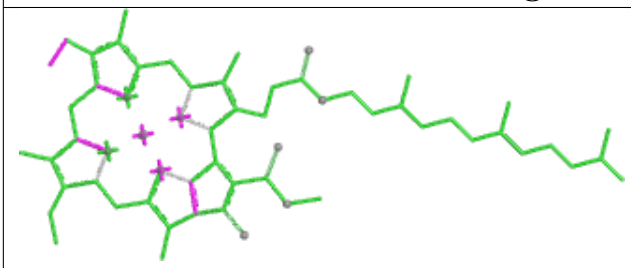


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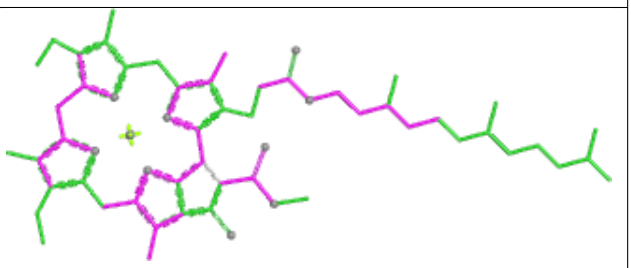


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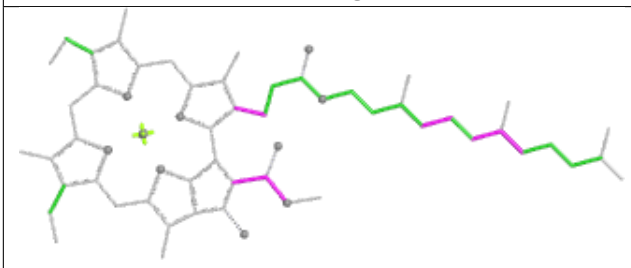
Ligand CLA Y 303



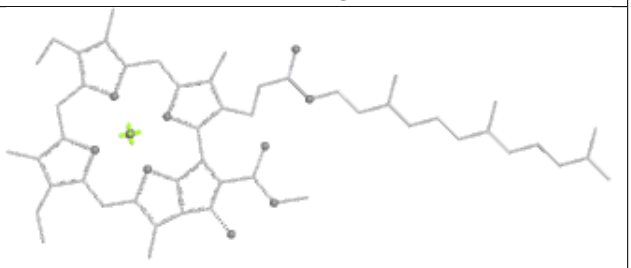
Bond lengths



Bond angles

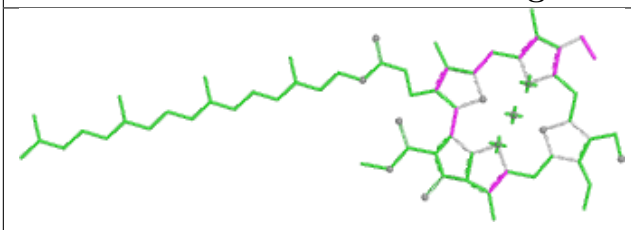


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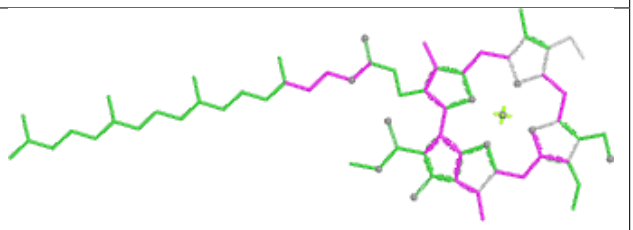


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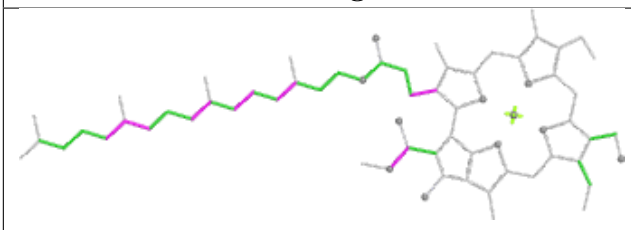
Ligand CHL 1 607



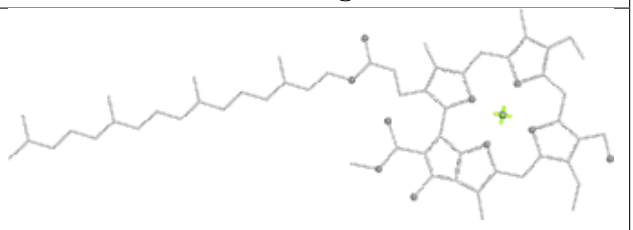
Bond lengths



Bond angles

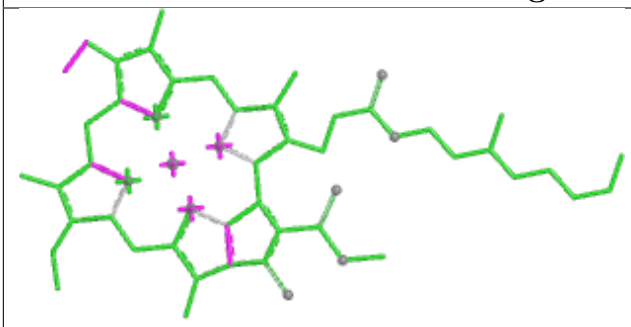


Torsions

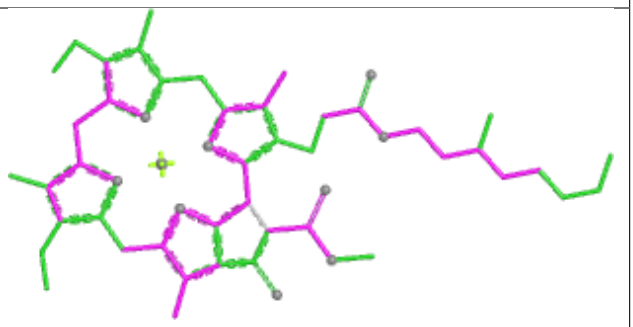


Rings

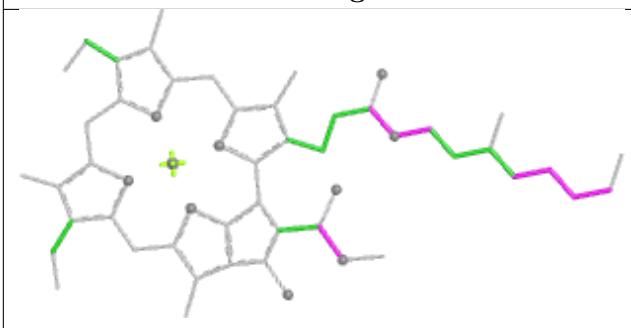
Ligand CLA 8 614



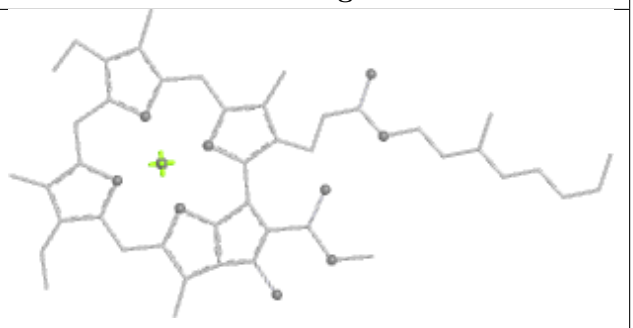
Bond lengths



Bond angles

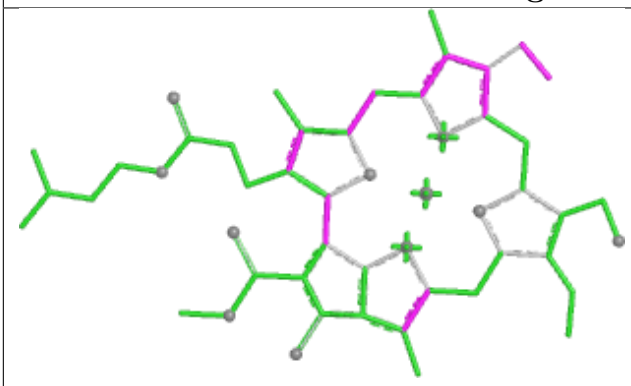


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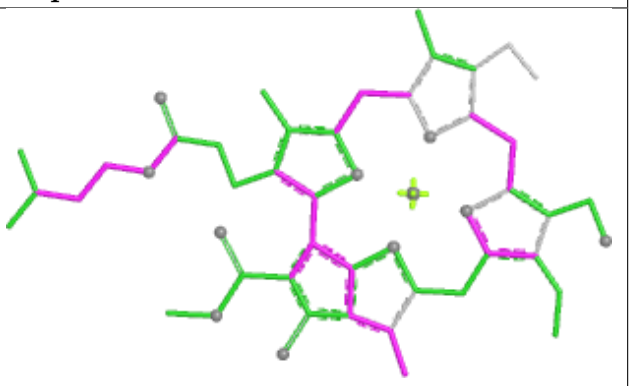


Rings

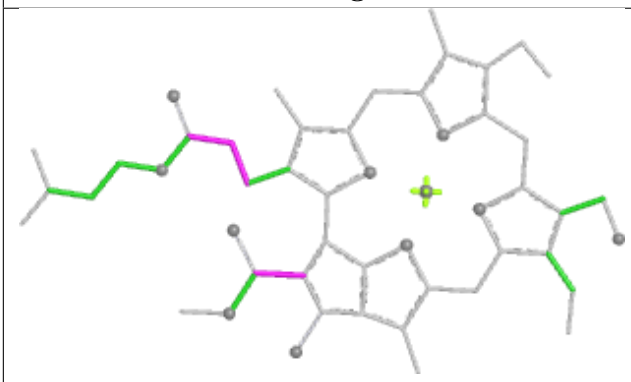
Ligand CHL p 607



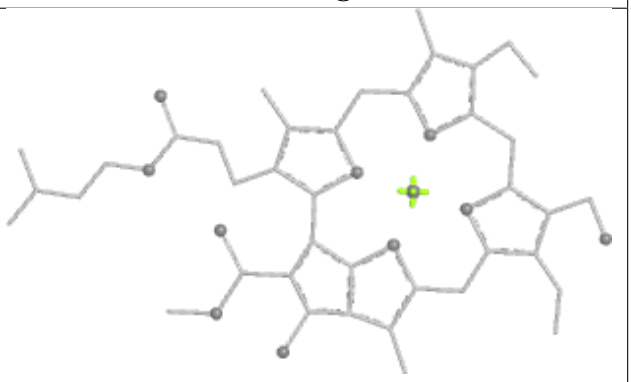
Bond lengths



Bond angles

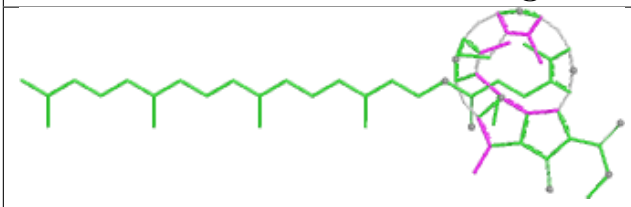


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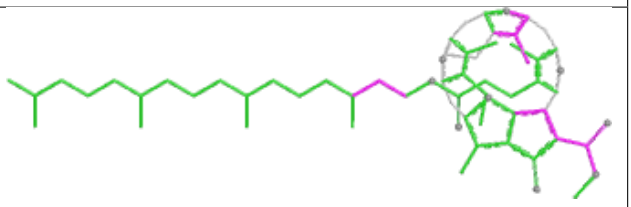


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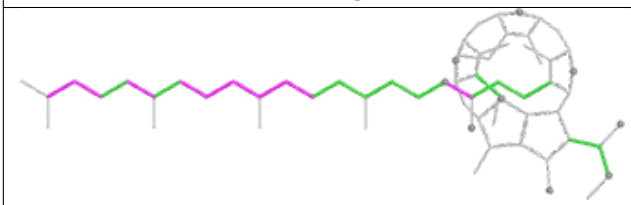
Ligand PHO A 408



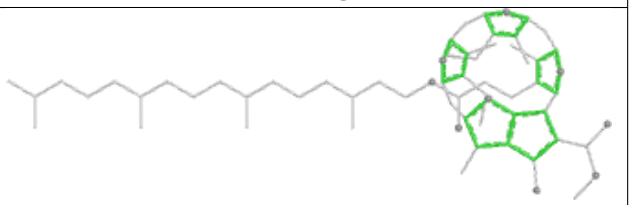
Bond lengths



Bond angles

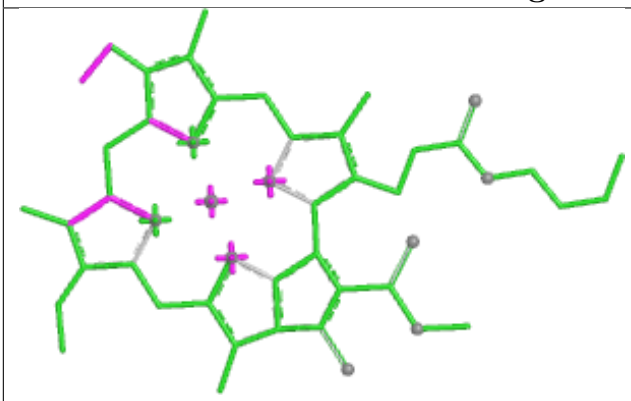


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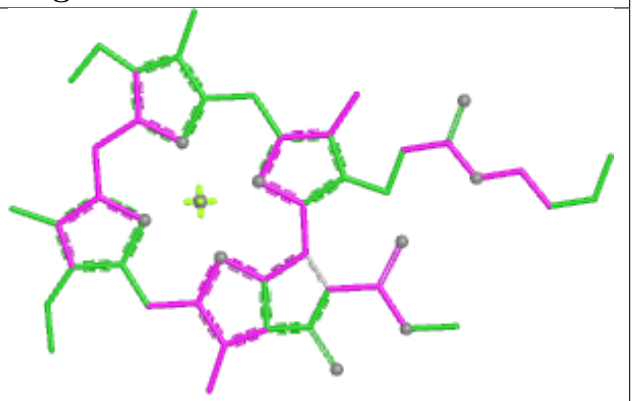


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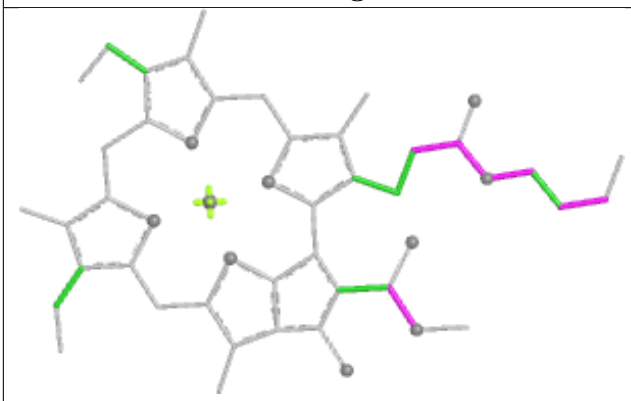
Ligand CLA g 314



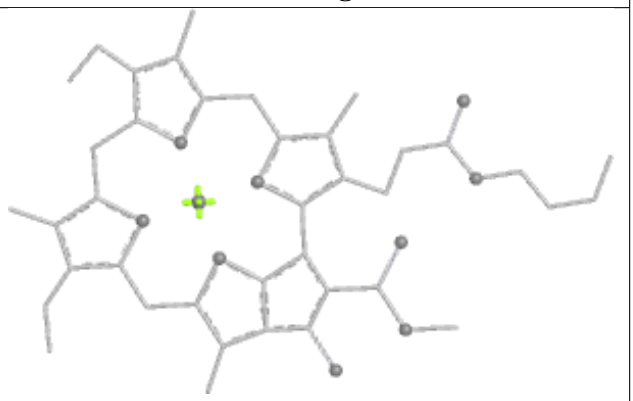
Bond lengths



Bond angles

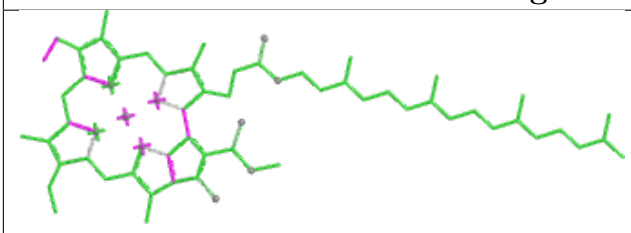


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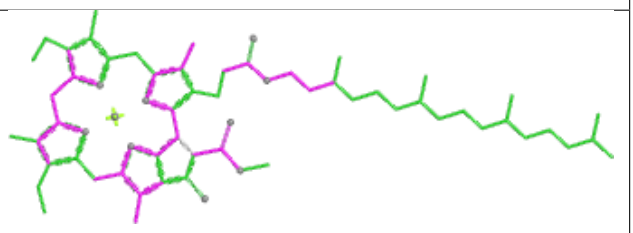


Rings

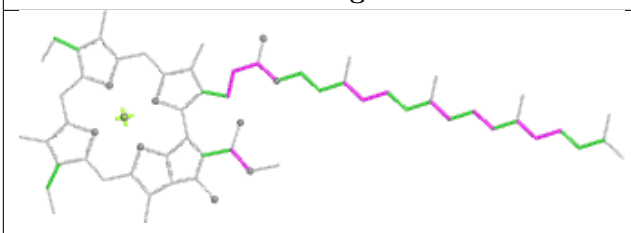
Ligand CLA s 314



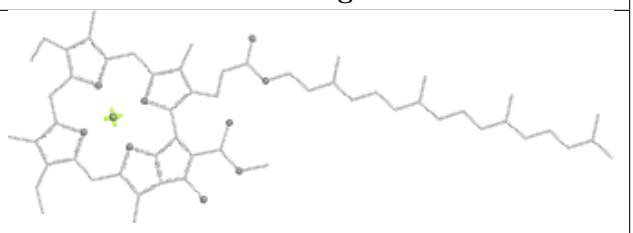
Bond lengths



Bond angles

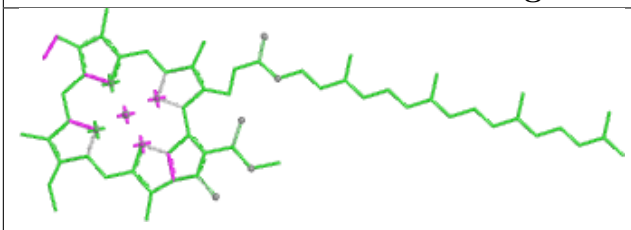


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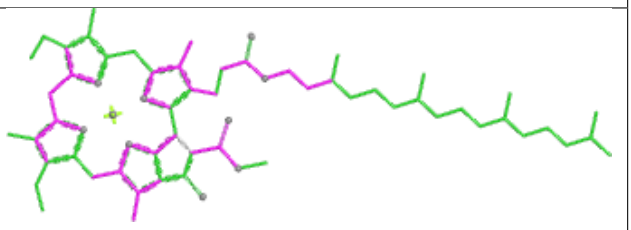


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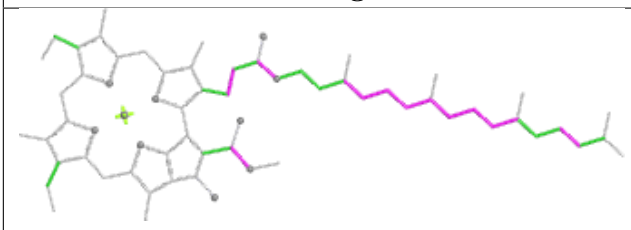
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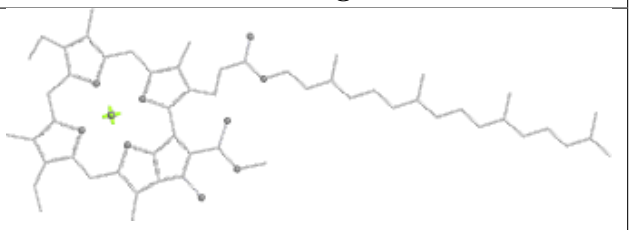
Bond lengths



Bond angles

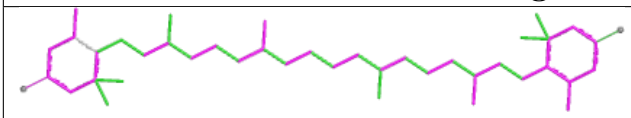


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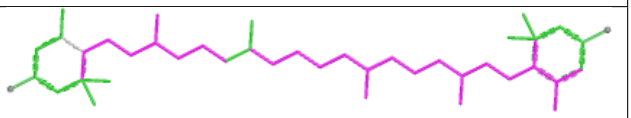


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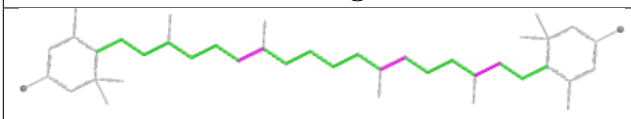
Ligand LUT s 317



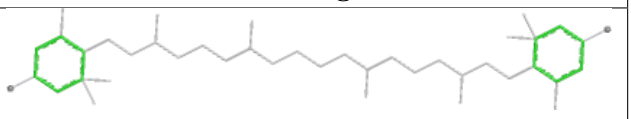
Bond lengths



Bond angles

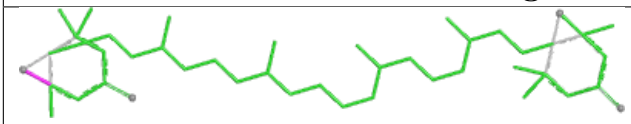


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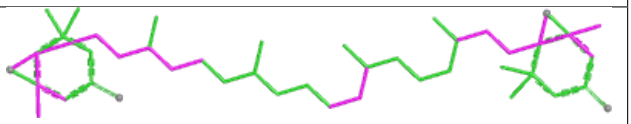


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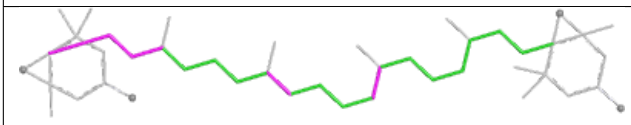
Ligand XAT G 620



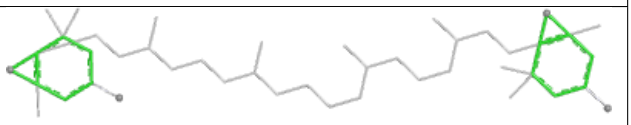
Bond lengths



Bond angles

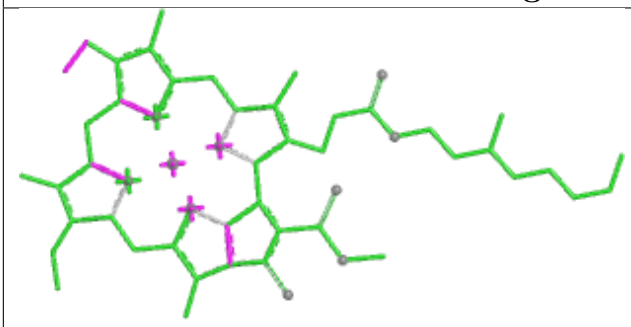


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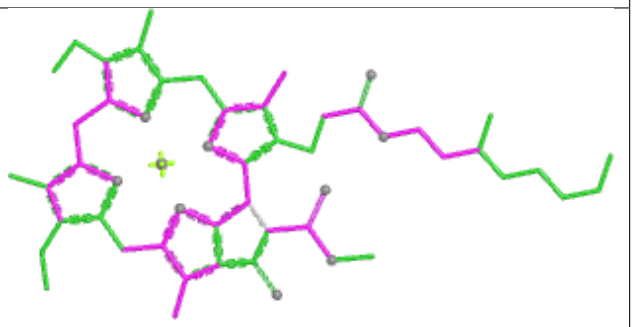


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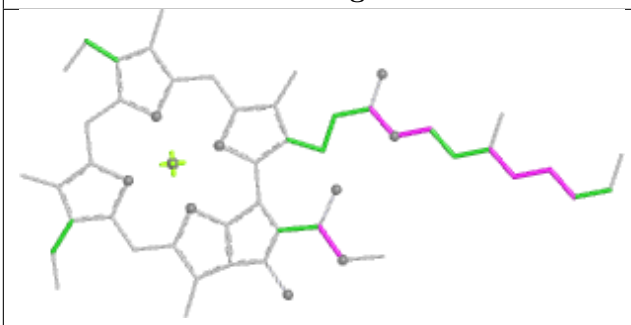
Ligand CLA N 315



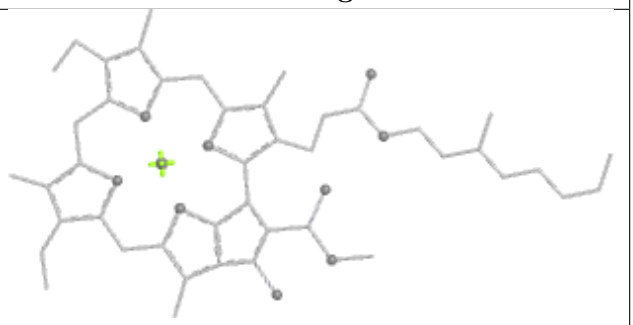
Bond lengths



Bond angles

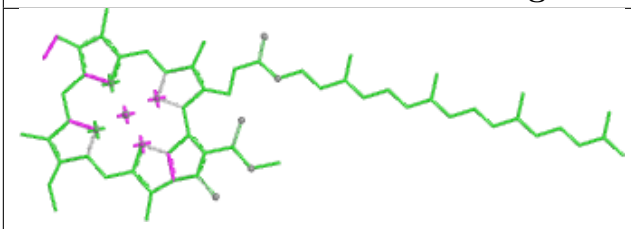


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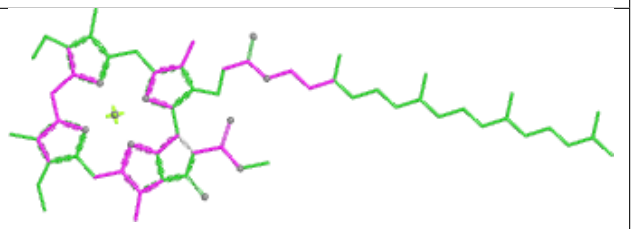


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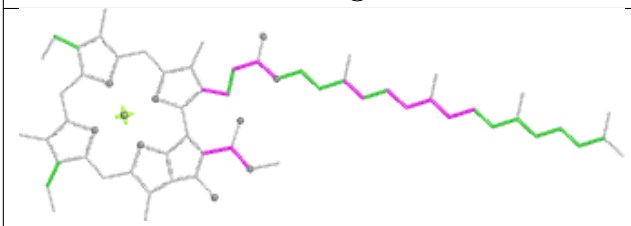
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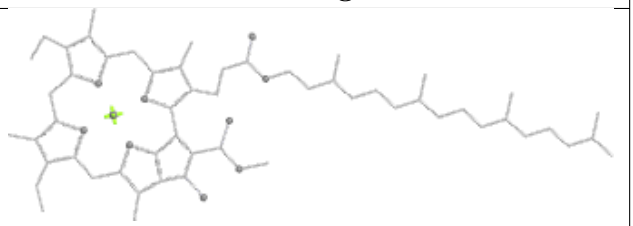
Bond lengths



Bond angles

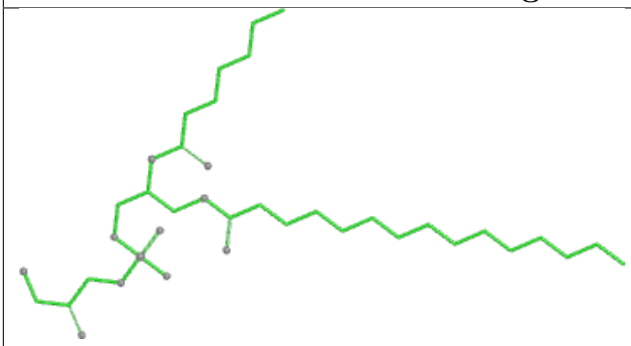


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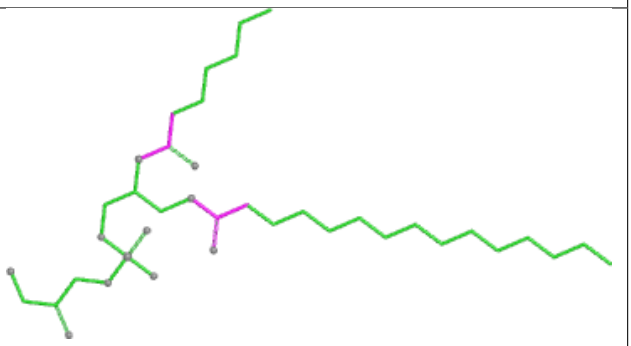


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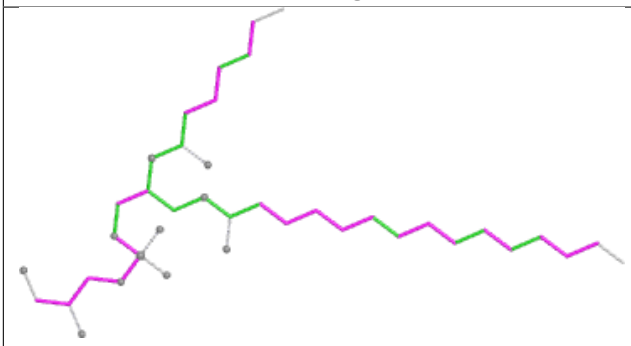
Ligand LHG A 417



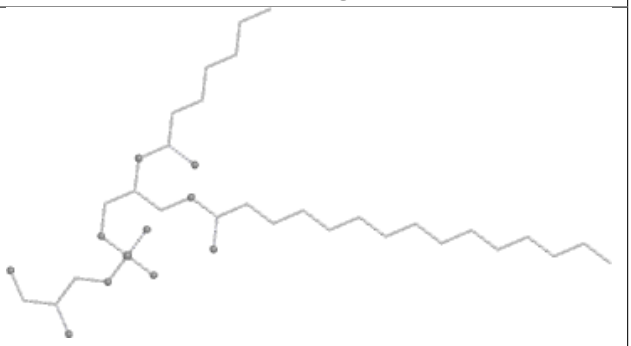
Bond lengths



Bond angles

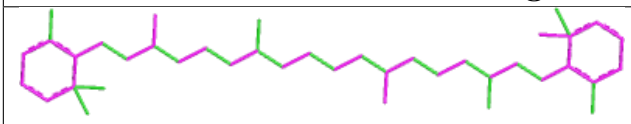


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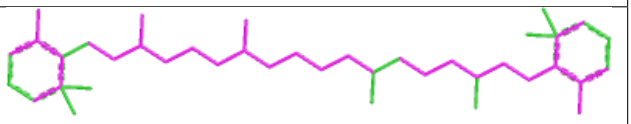


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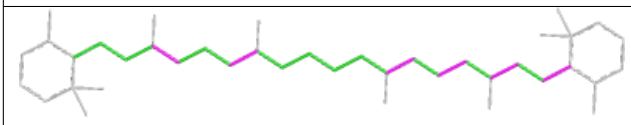
Ligand BCR d 406



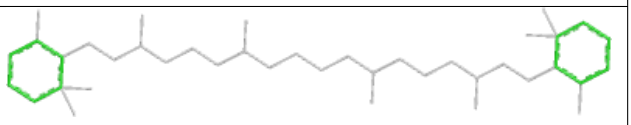
Bond lengths



Bond angles

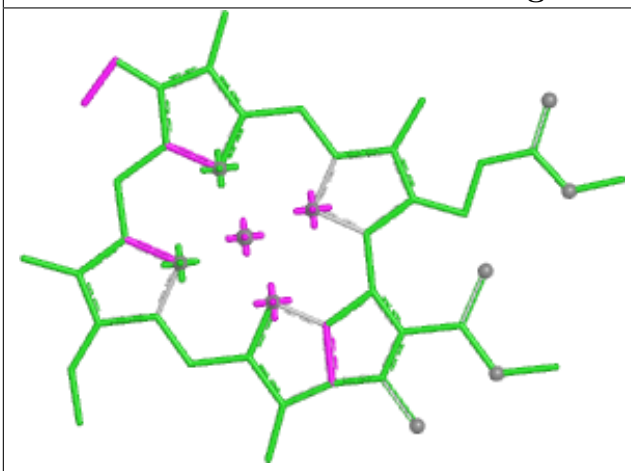


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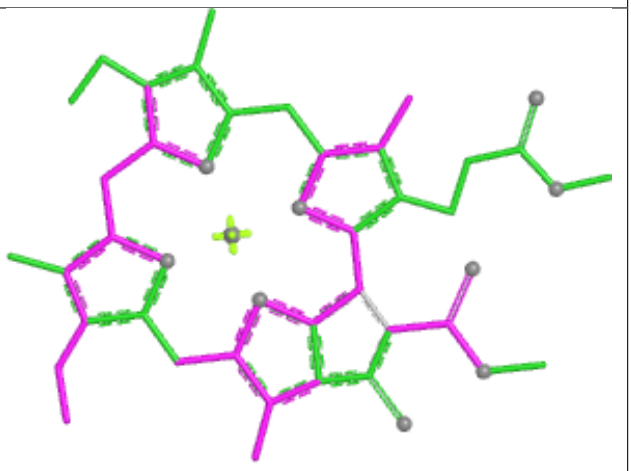


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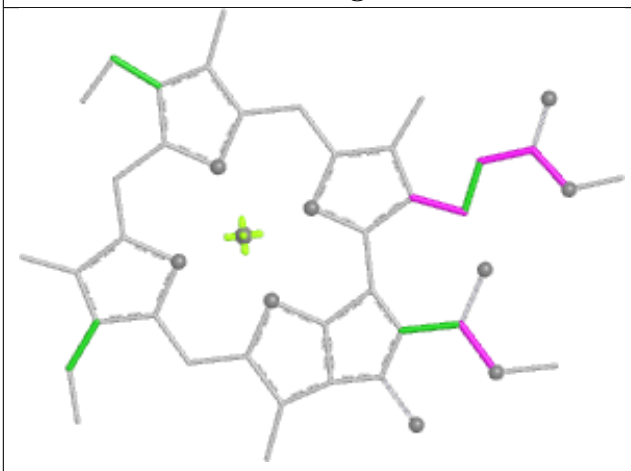
Ligand CLA S 316



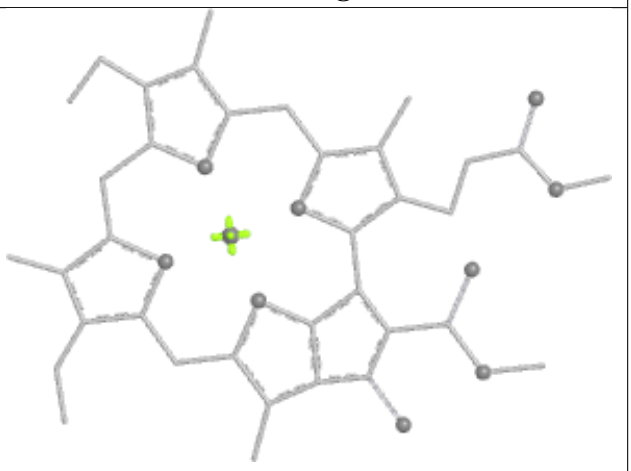
Bond lengths



Bond angles

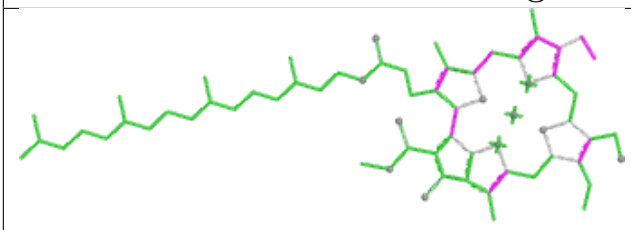


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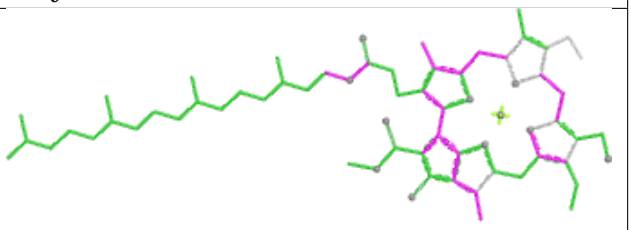


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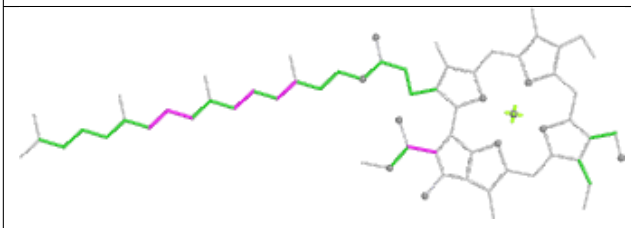
Ligand CHL y 609



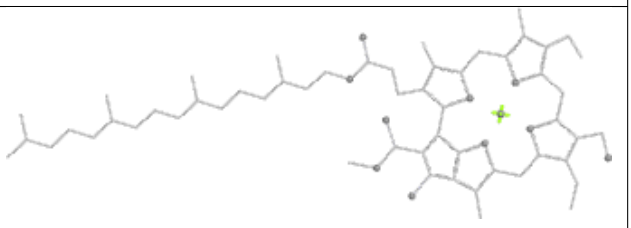
Bond lengths



Bond angles

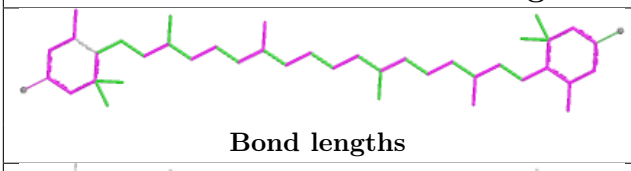


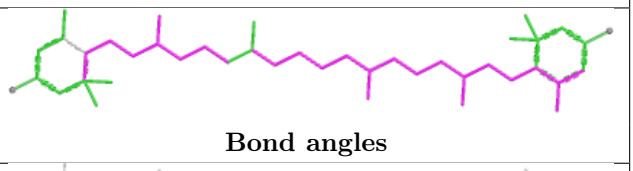
Torsions

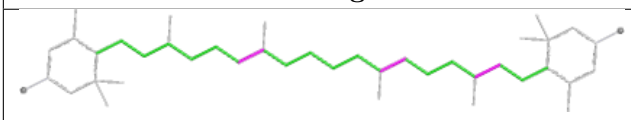


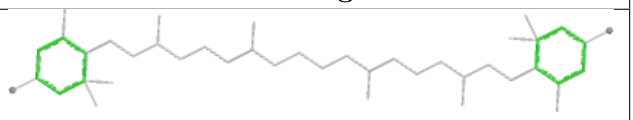
Rings

Ligand LUT n 317

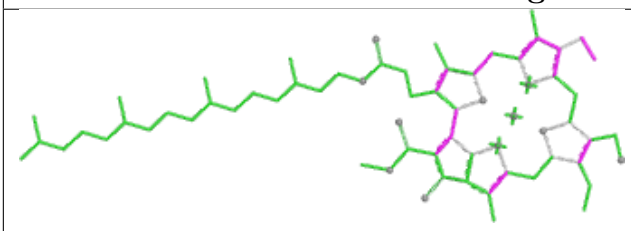

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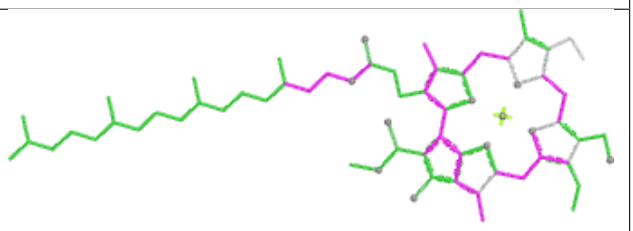

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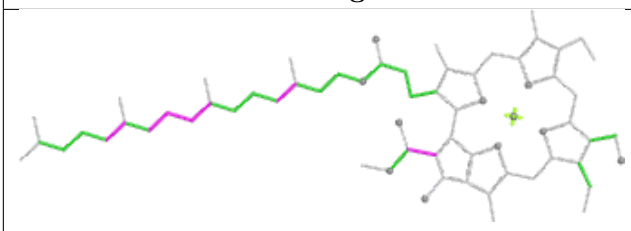

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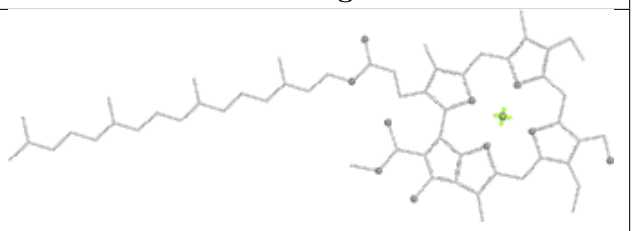

Rings

Ligand CHL 9 303

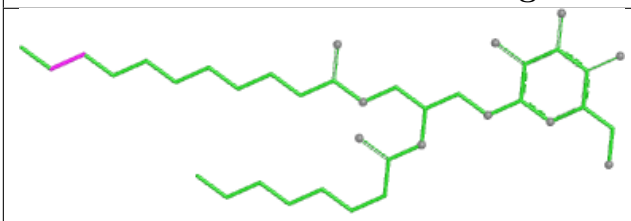

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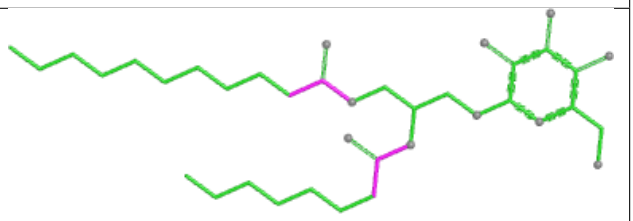

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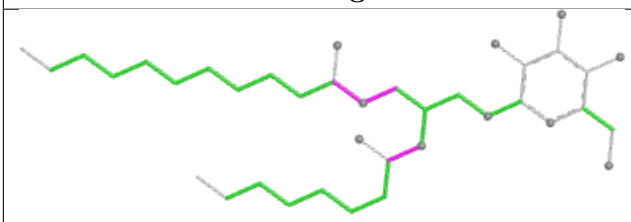

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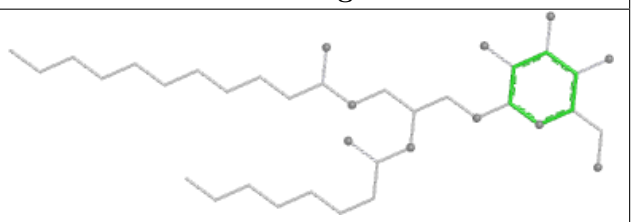

Rings

Ligand LMG X 202

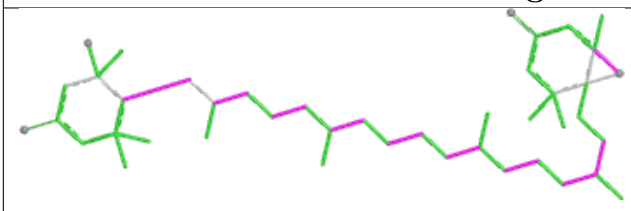

Bond lengths


Bond angles

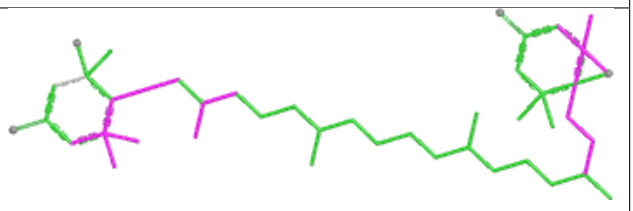

Torsions


Rings

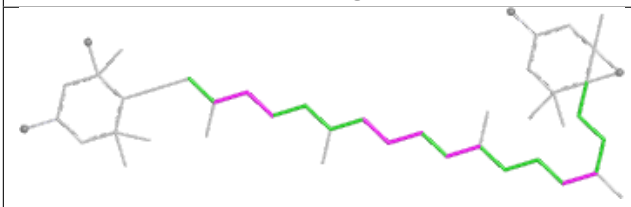
Ligand NEX 3 319



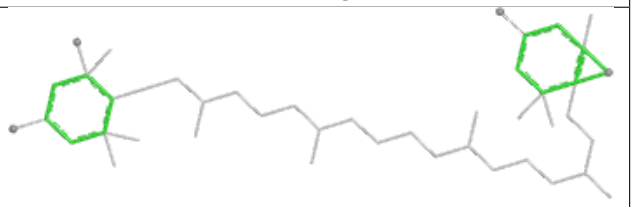
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Bond angles

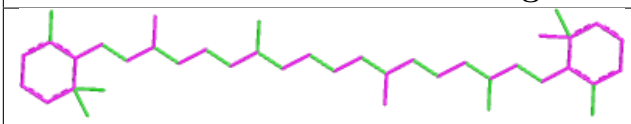


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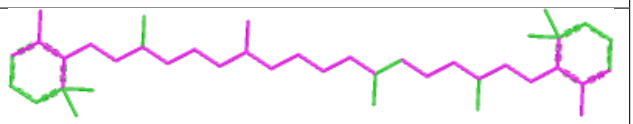


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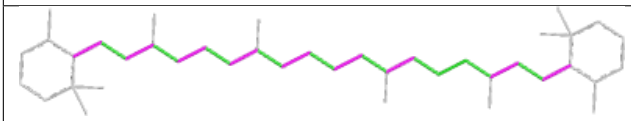
Ligand BCR V 101



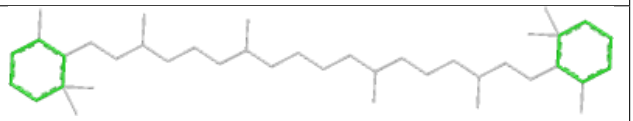
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Bond angles

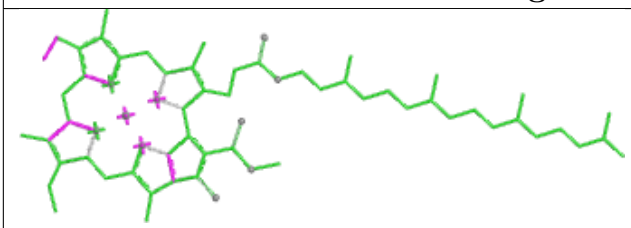


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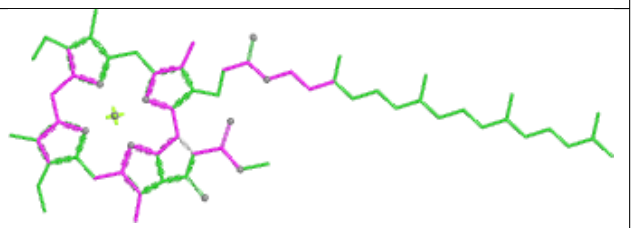


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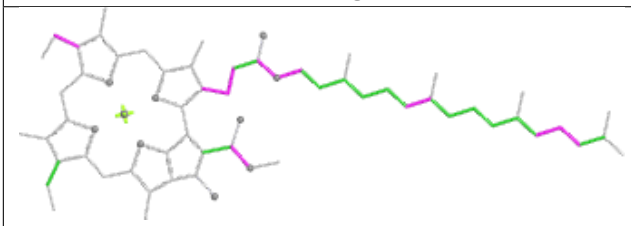
Ligand CLA 3 312



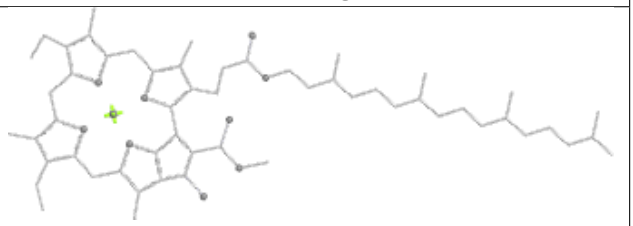
Bond lengths



Bond angles

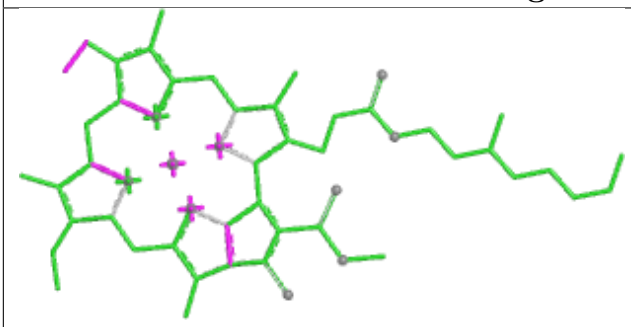


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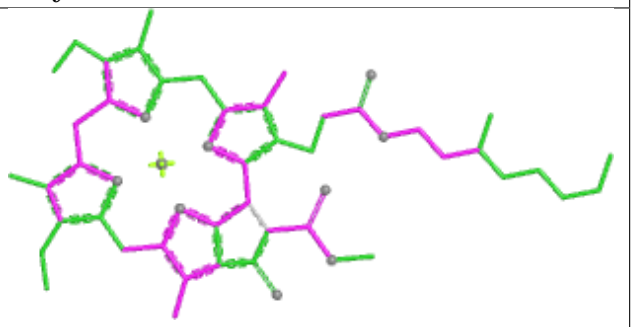


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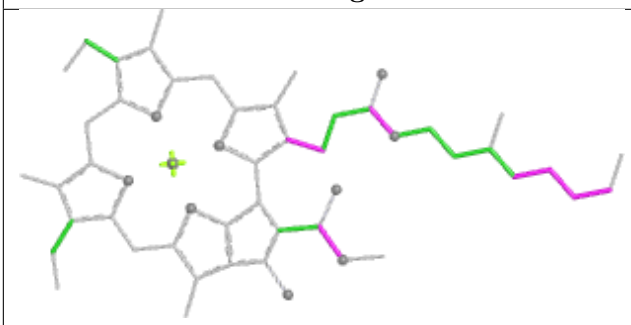
Ligand CLA y 614



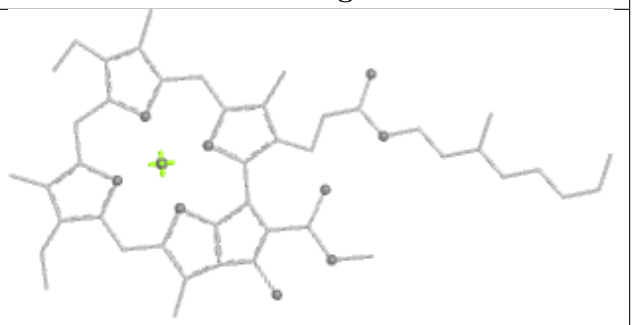
Bond lengths



Bond angles

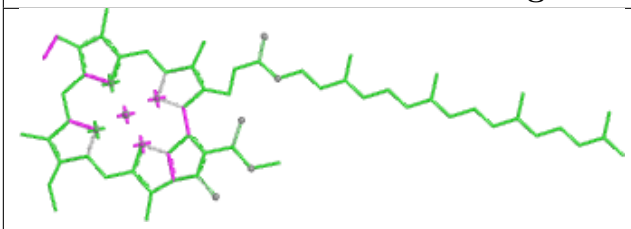


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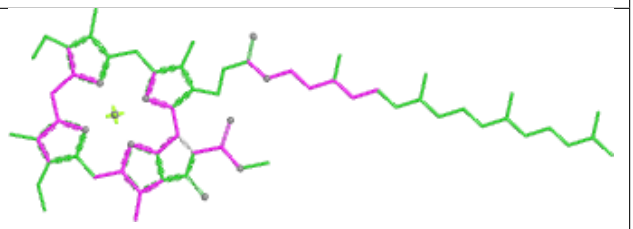


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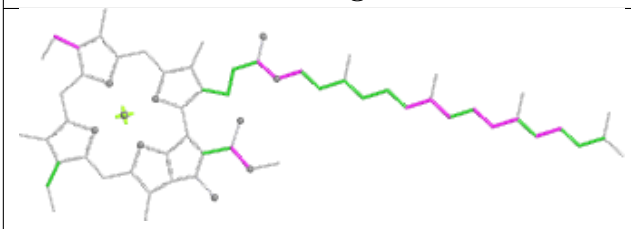
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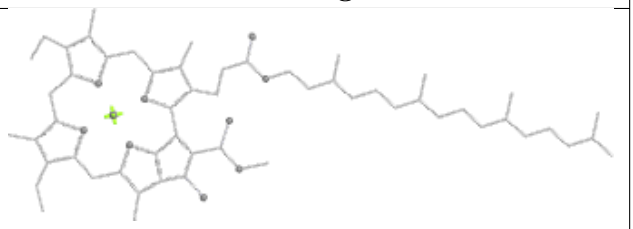
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Bond angles

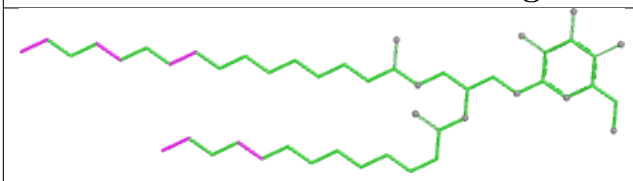


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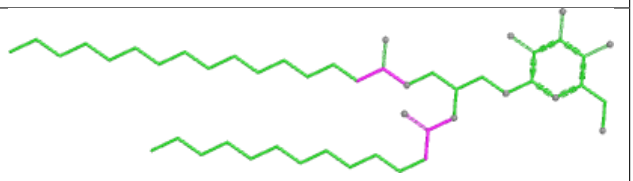


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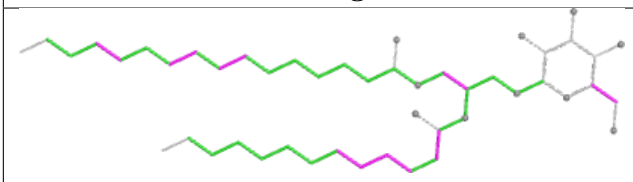
Ligand LMG d 411



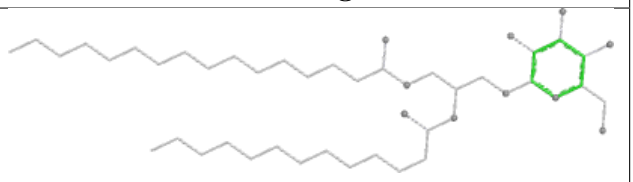
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Bond angles

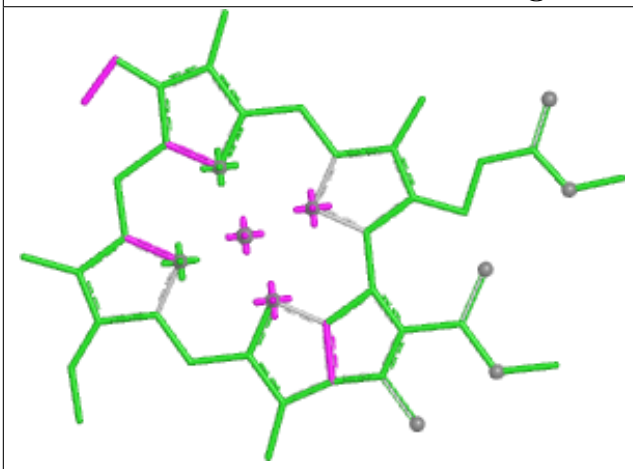


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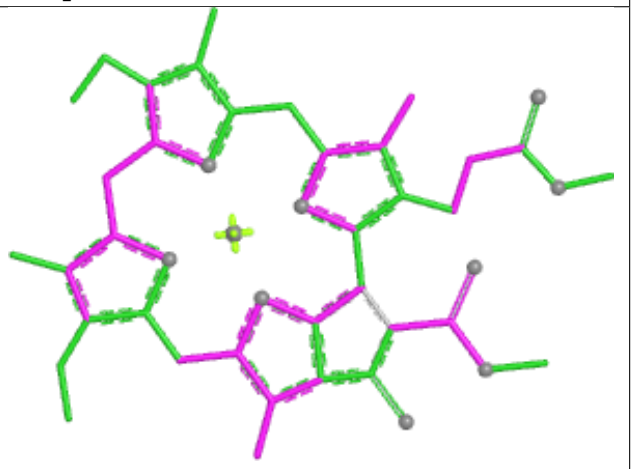


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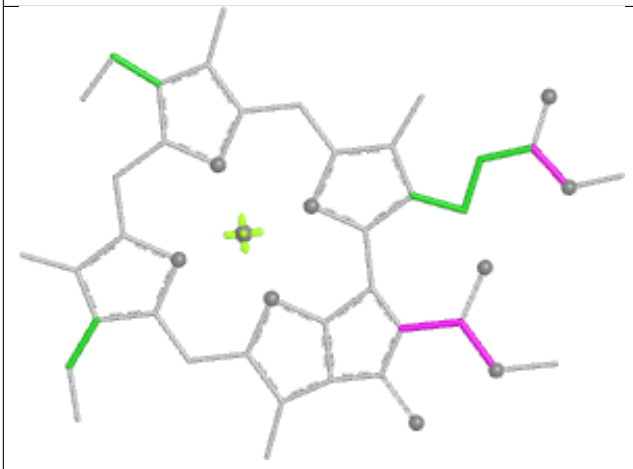
Ligand CLA q 314



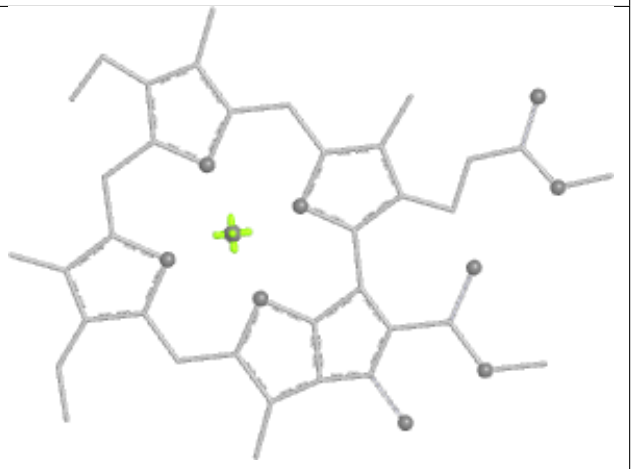
Bond lengths



Bond angles

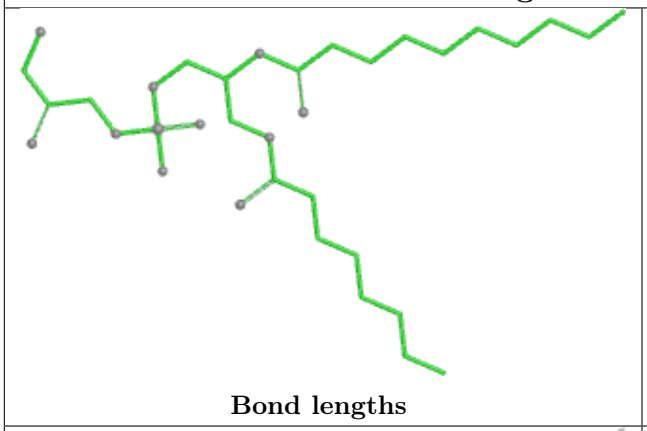


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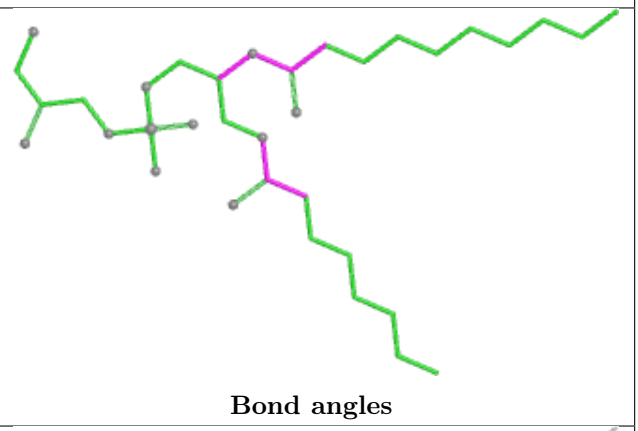


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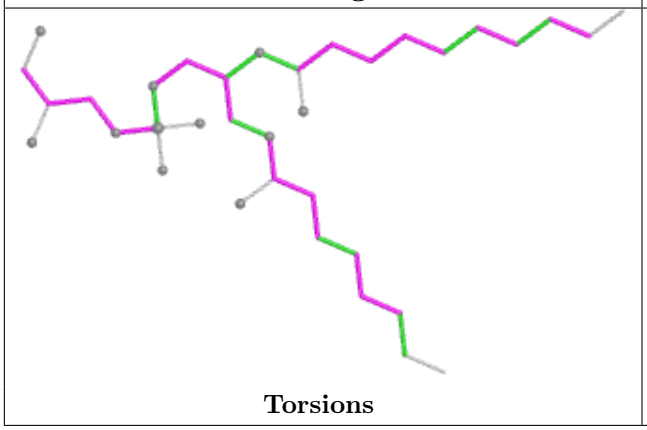
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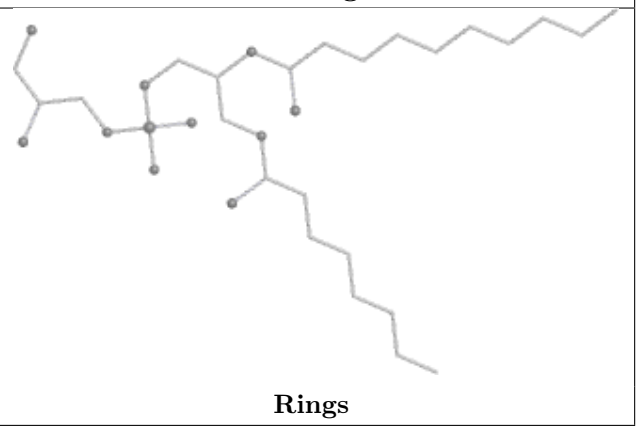
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Bond angles

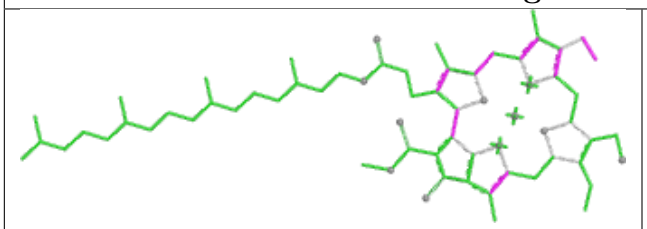


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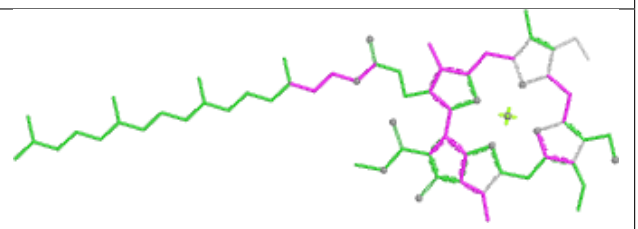


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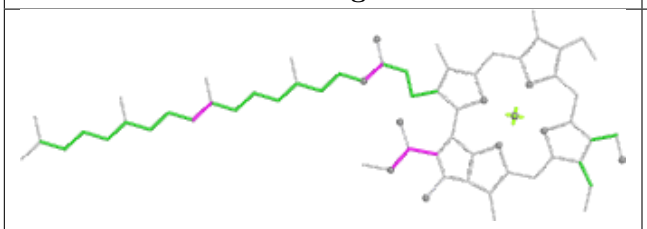
Ligand CHL N 309



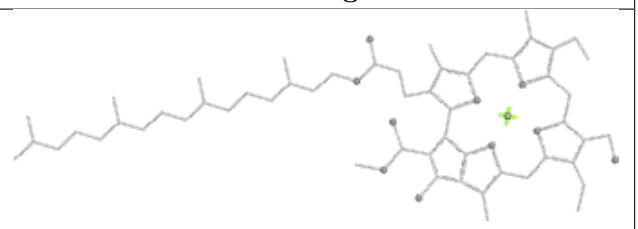
Bond lengths



Bond angles

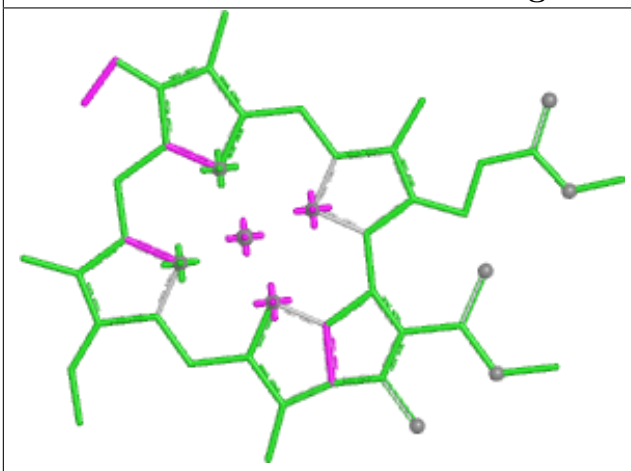


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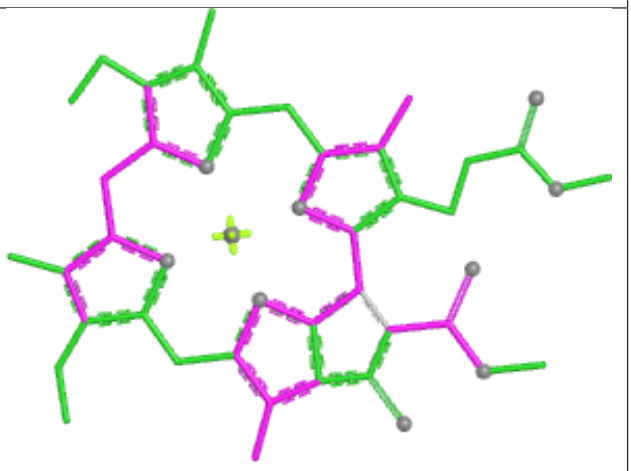


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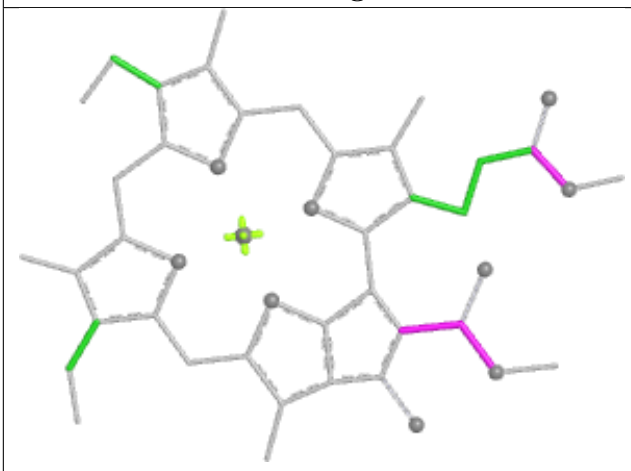
Ligand CLA 4 612



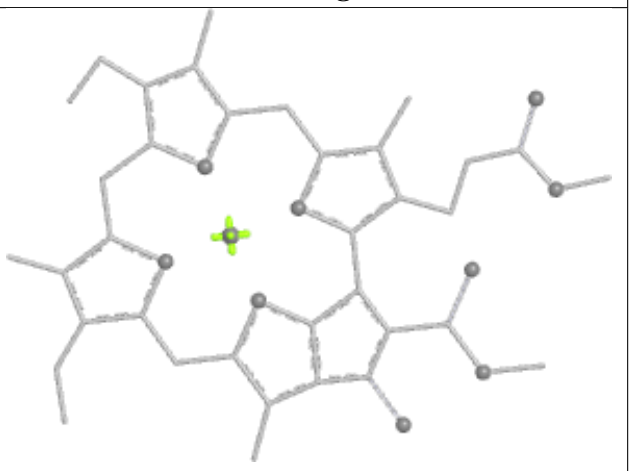
Bond lengths



Bond angles

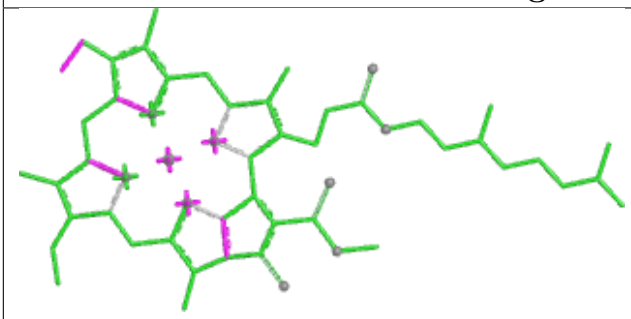


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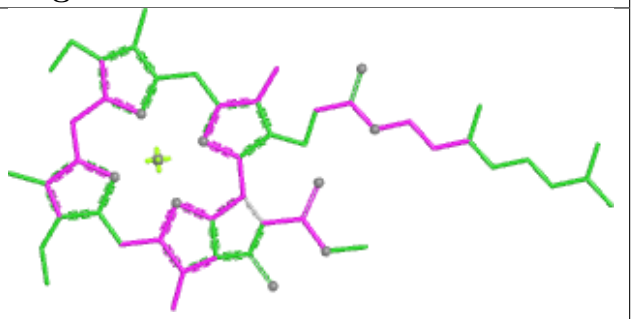


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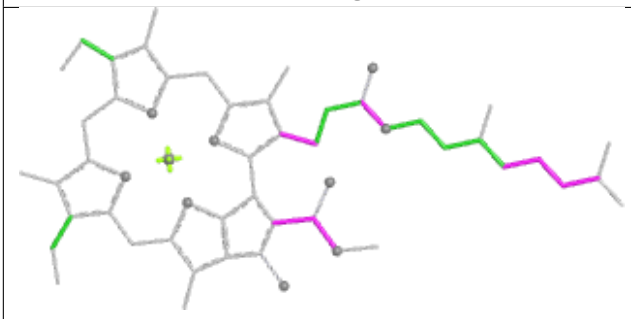
Ligand CLA g 304



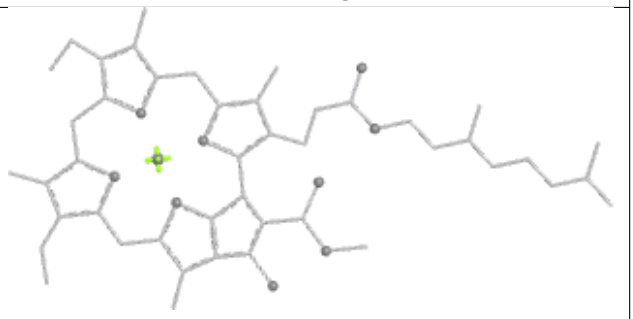
Bond lengths



Bond angles

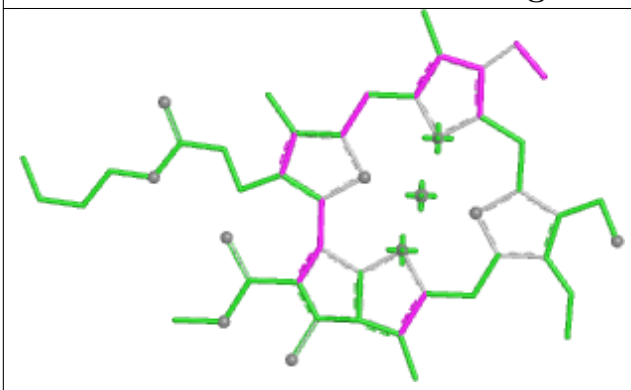


Torsions

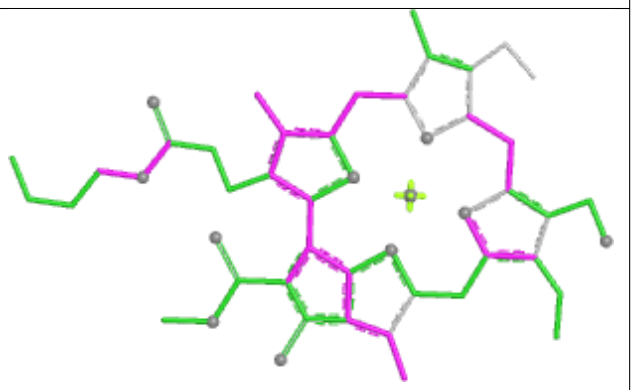


Rings

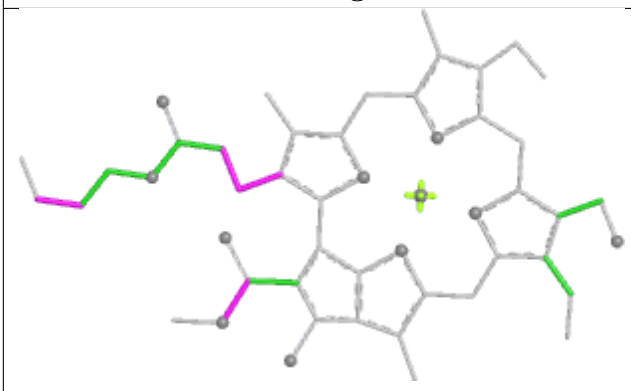
Ligand CHL 2 607



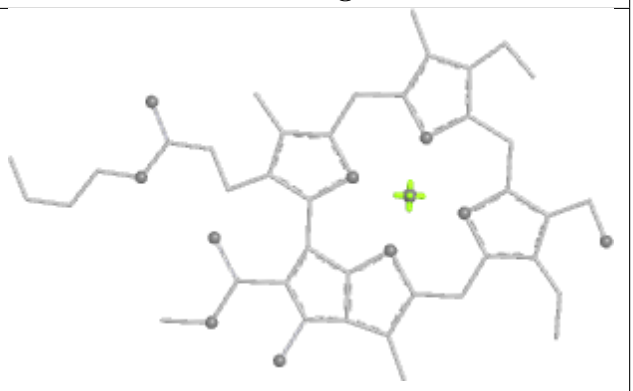
Bond lengths



Bond angles

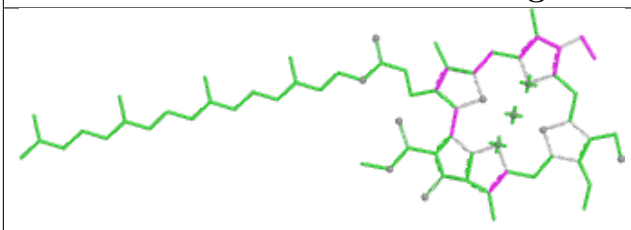


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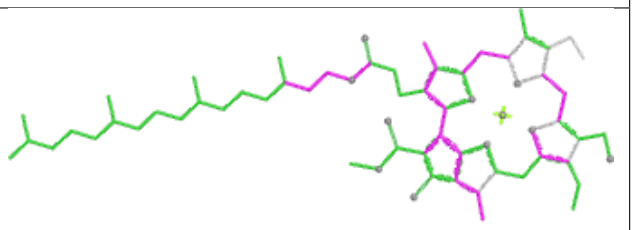


Rings

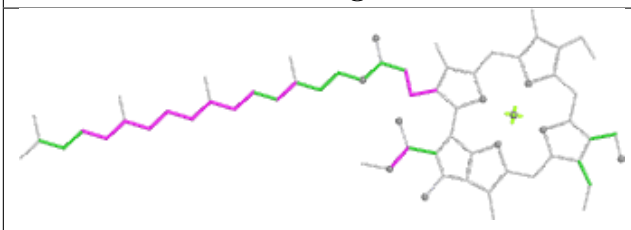
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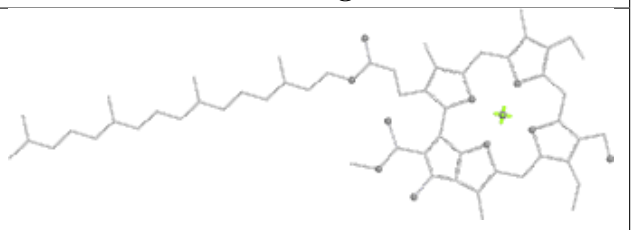
Bond lengths



Bond angles

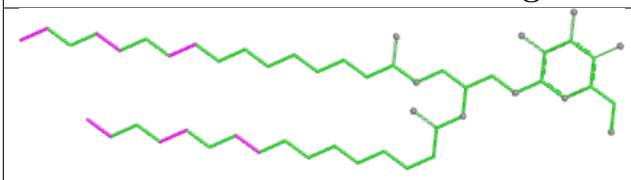


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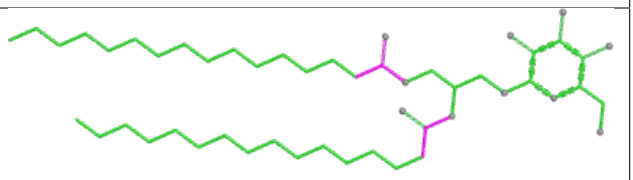


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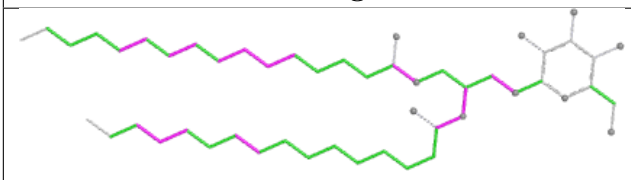
Ligand LMG d 410



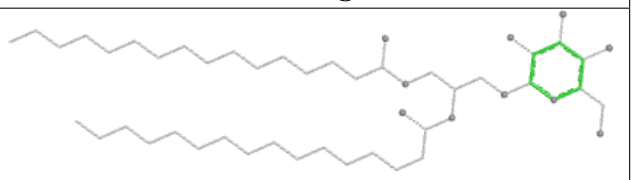
Bond lengths



Bond angles

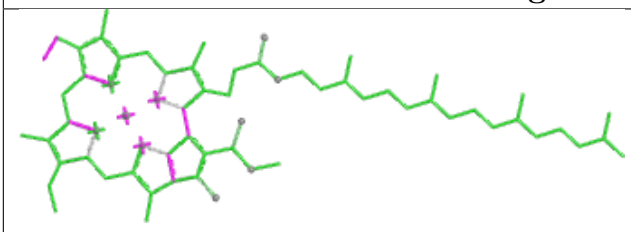


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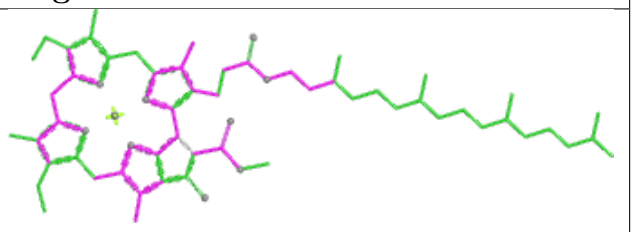


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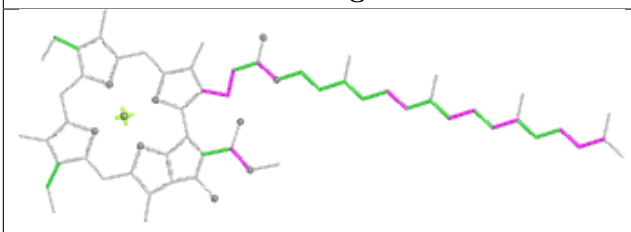
Ligand CLA g 310



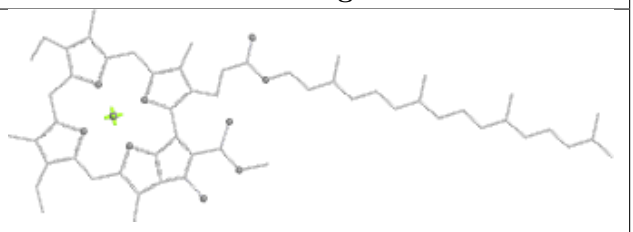
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Bond angles

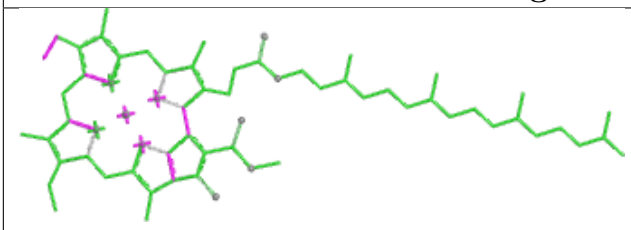


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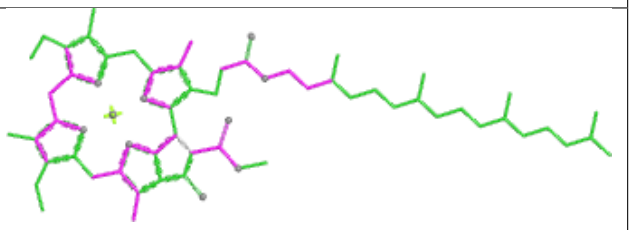


Rings

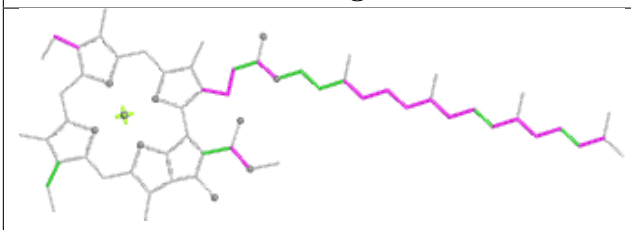
Ligand CLA s 312



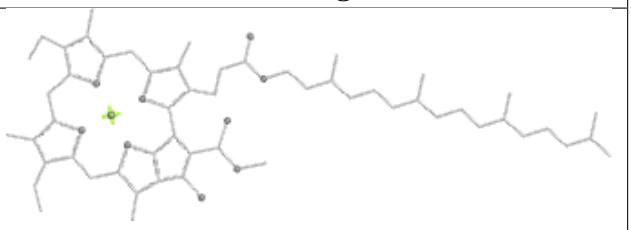
Bond lengths



Bond angles

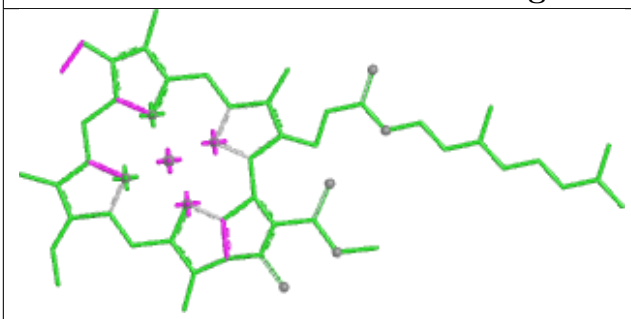


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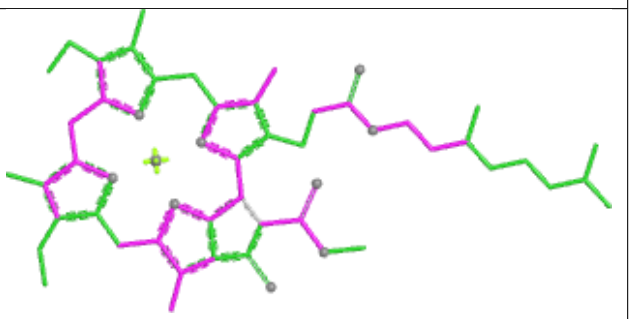


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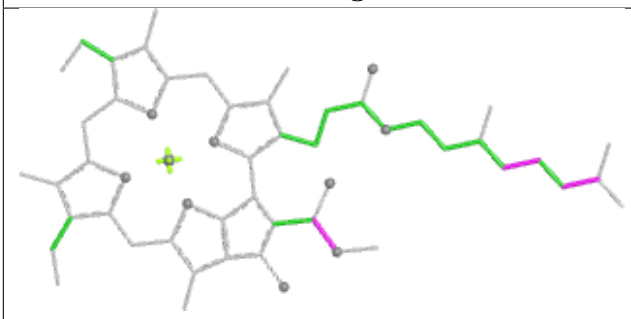
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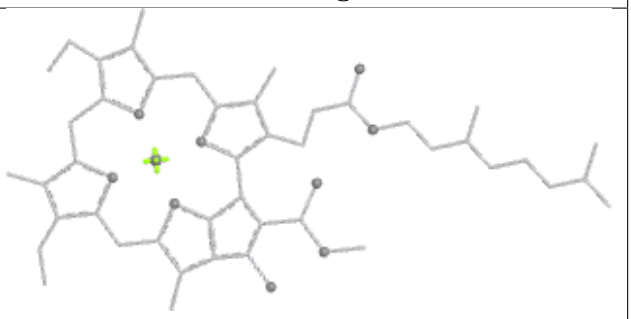
Bond lengths



Bond angles

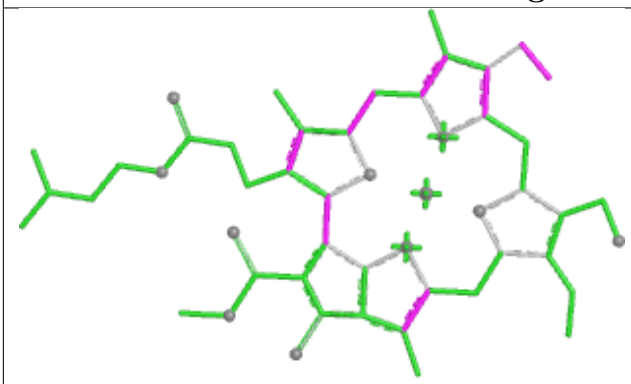


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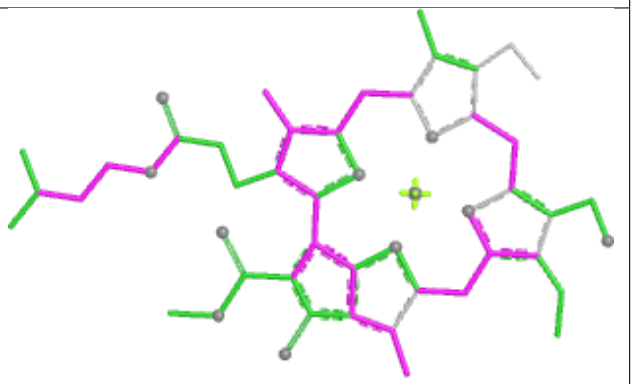


Rings

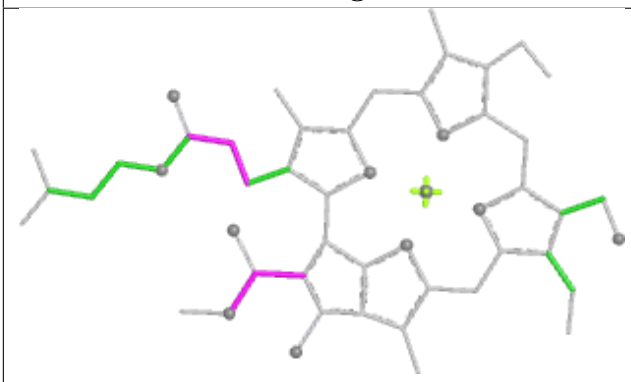
Ligand CHL 4 606



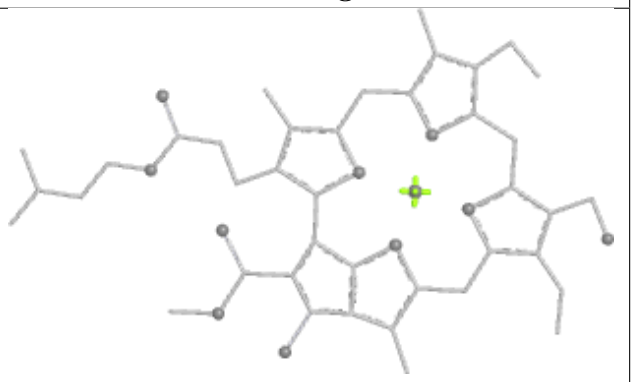
Bond lengths



Bond angles

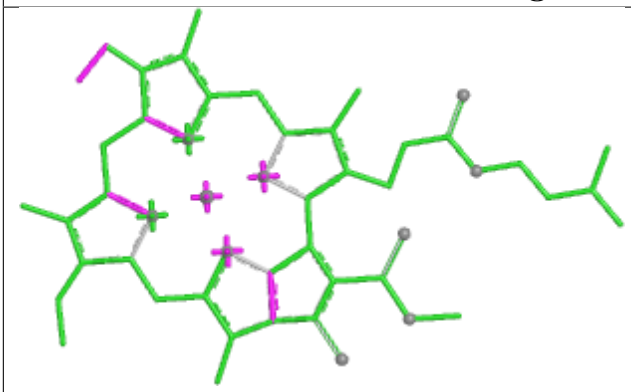


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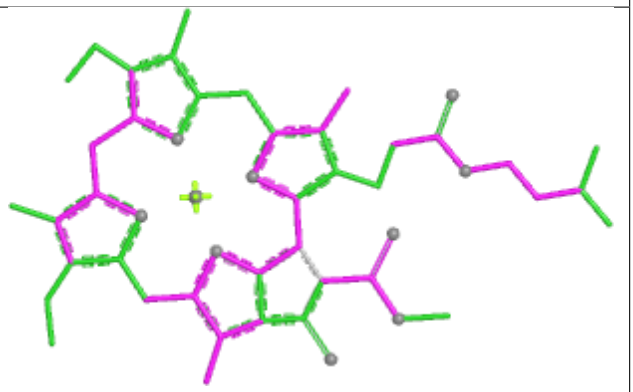


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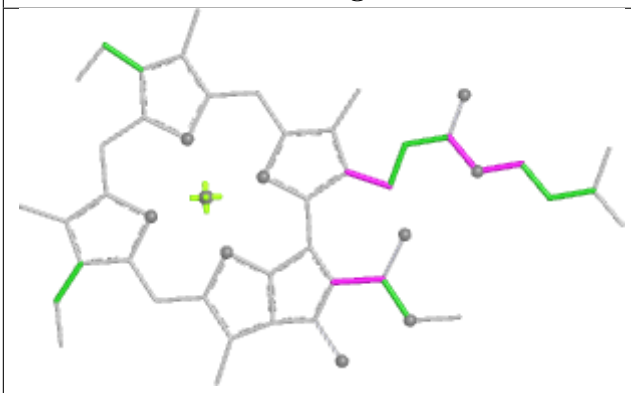
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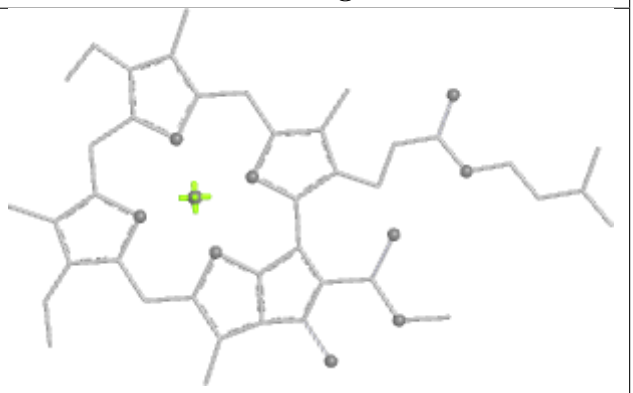
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Bond angles

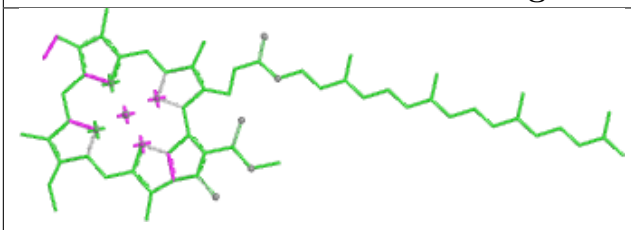


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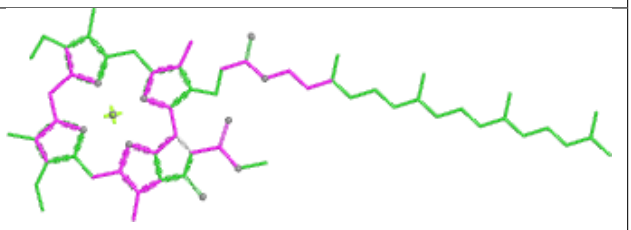


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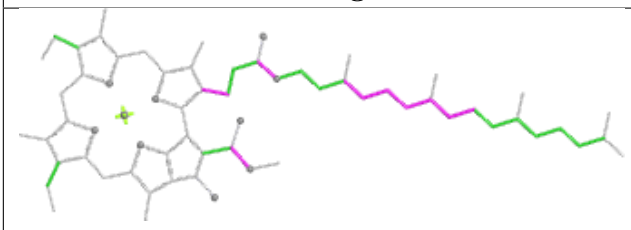
Ligand CLA 0 610



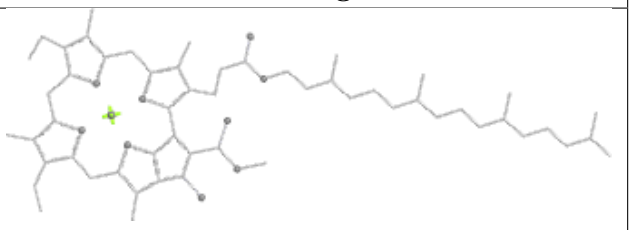
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Bond angles

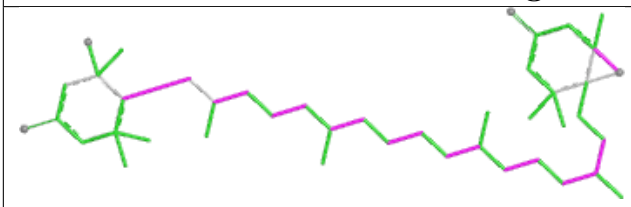


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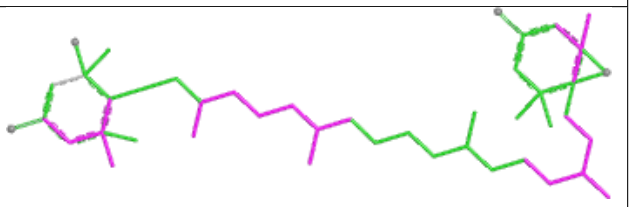


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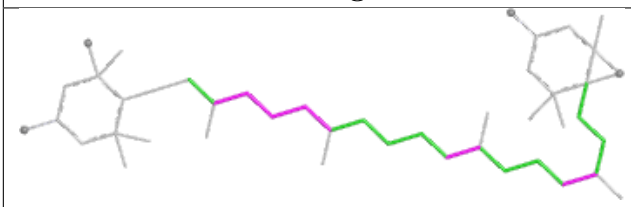
Ligand NEX n 319



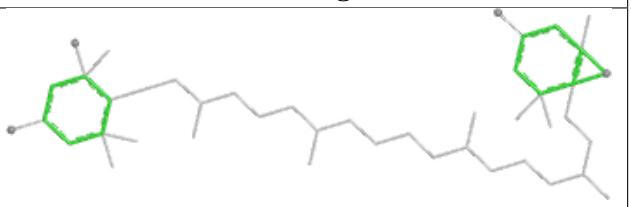
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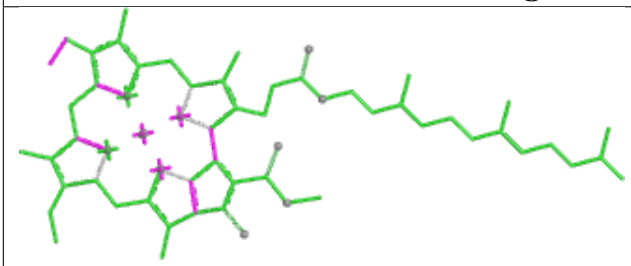


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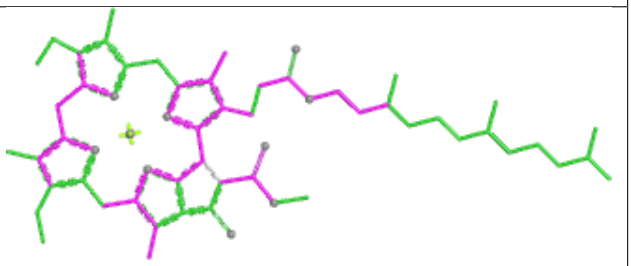


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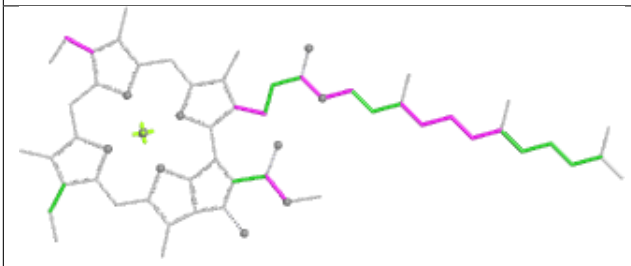
Ligand CLA G 610



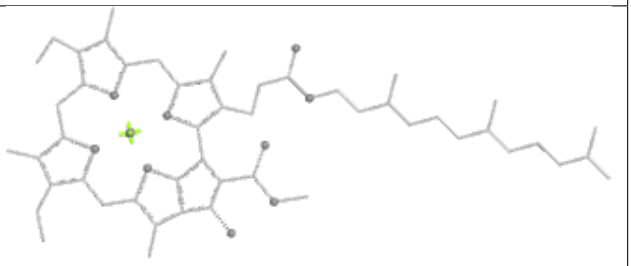
Bond lengths



Bond angles

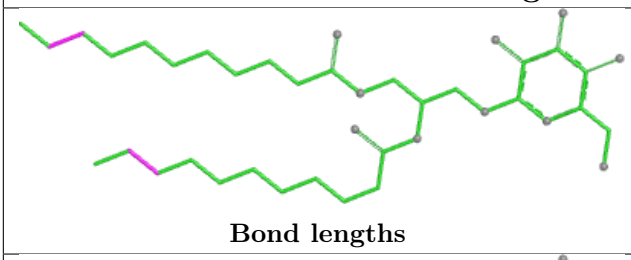


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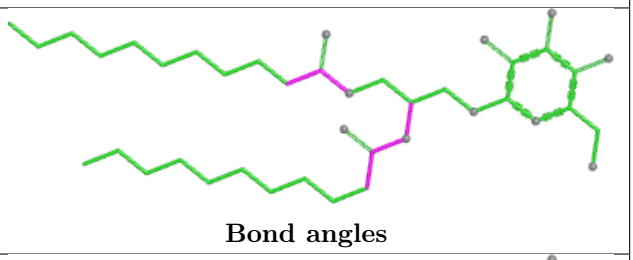


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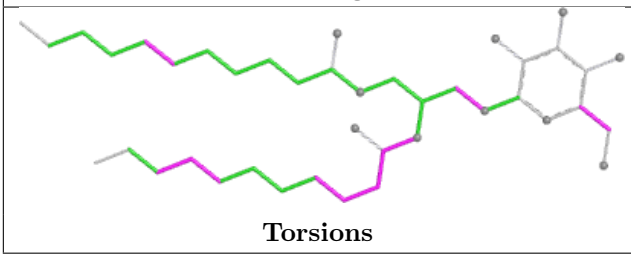
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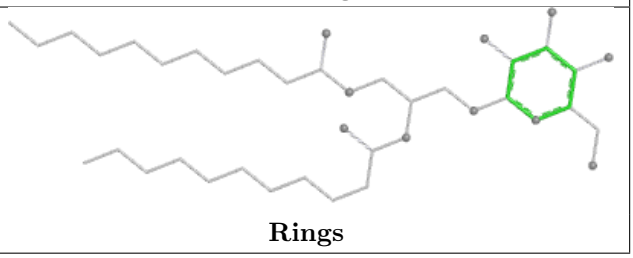
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Bond angles

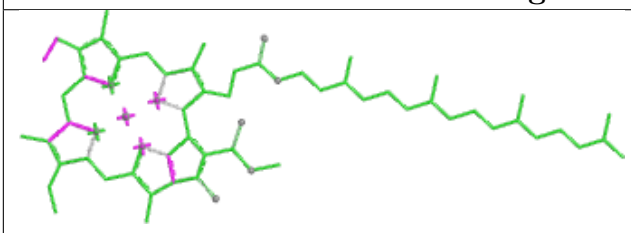


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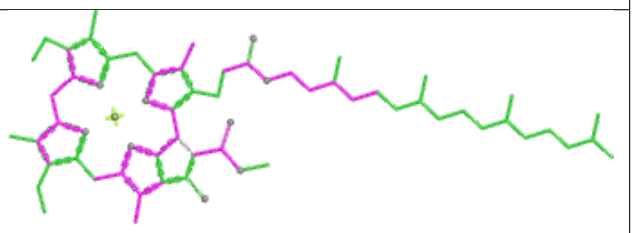


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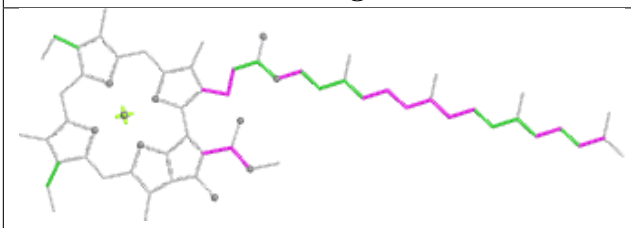
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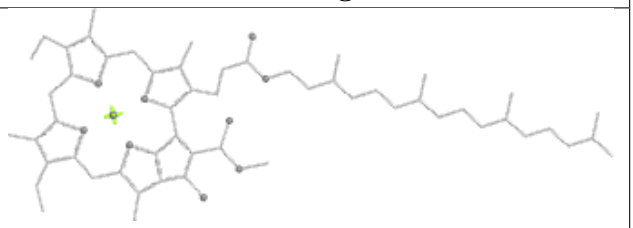
Bond lengths



Bond angles

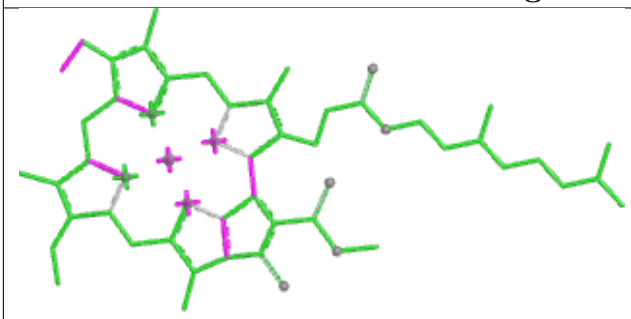


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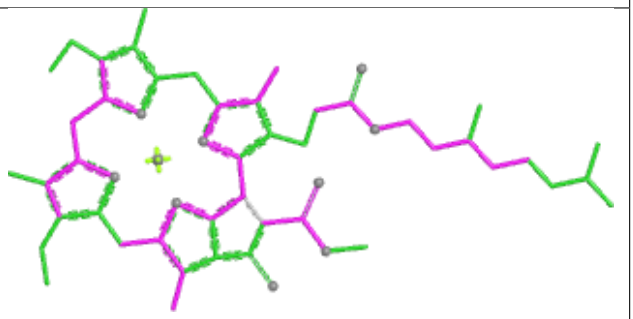


Rings

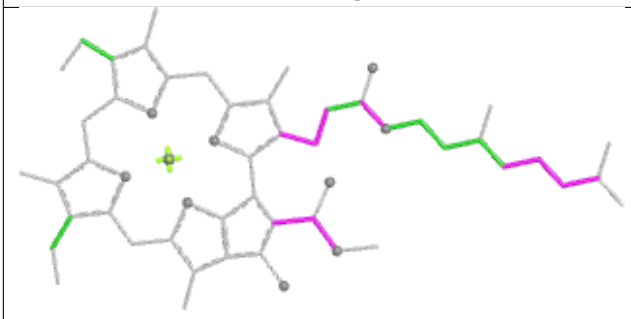
Ligand CLA C 612



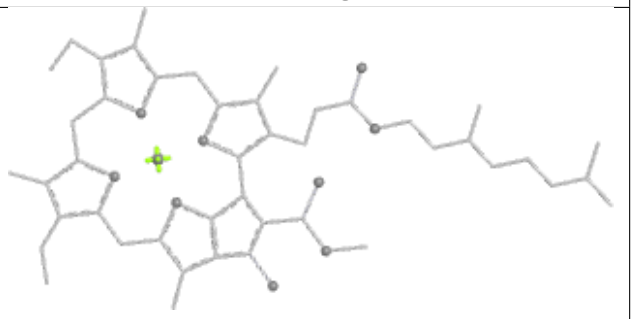
Bond lengths



Bond angles

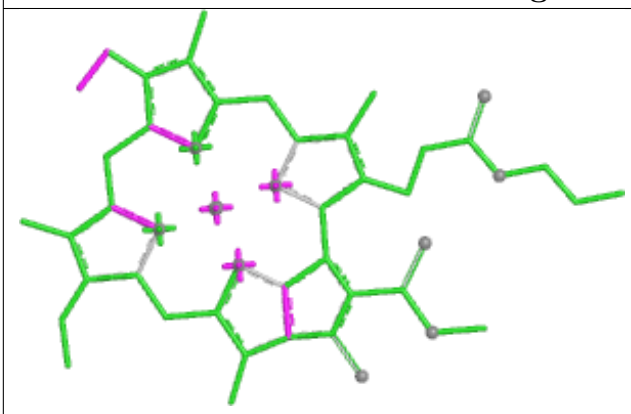


Torsions

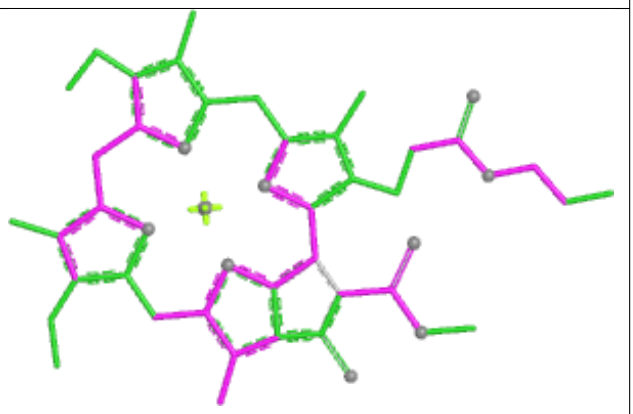


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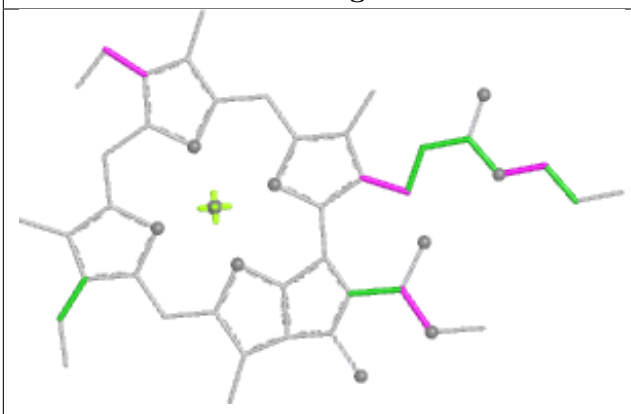
Ligand CLA s 315



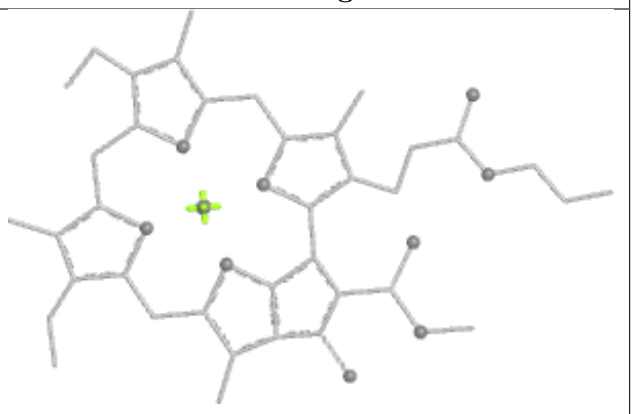
Bond lengths



Bond angles

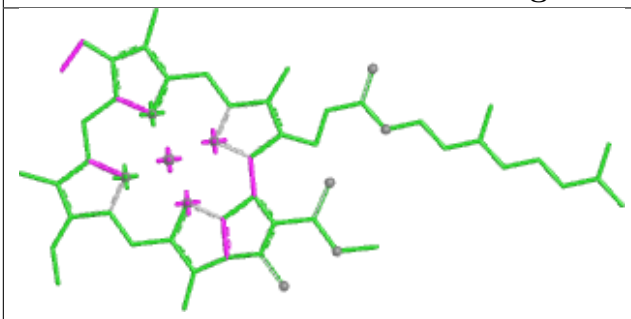


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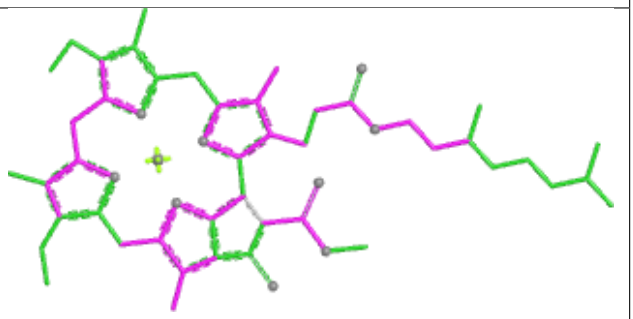


Rings

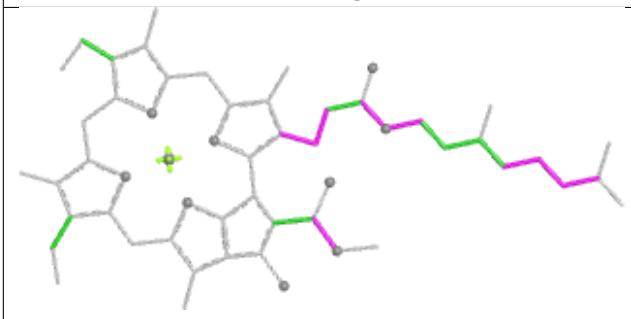
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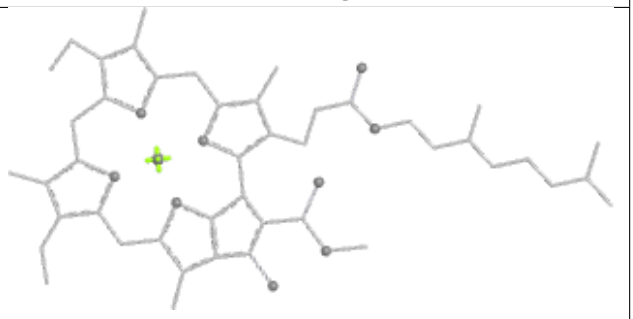
Bond lengths



Bond angles

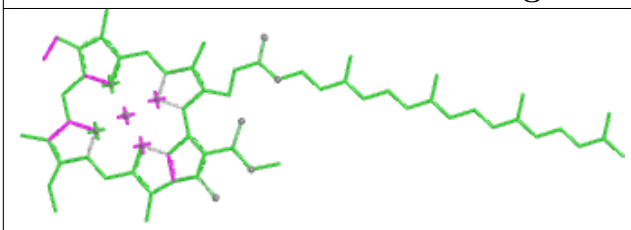


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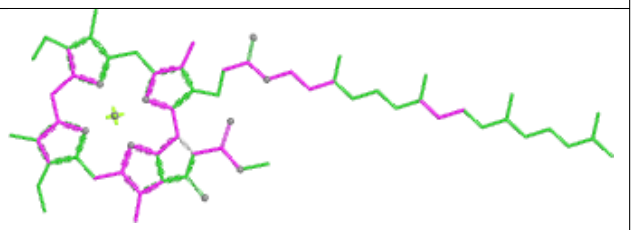


Rings

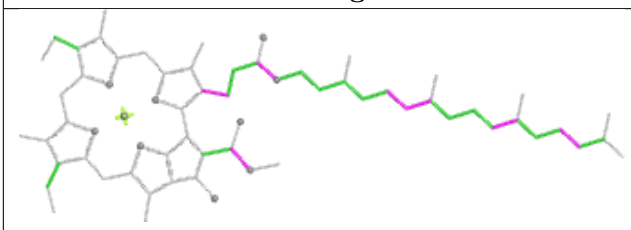
Ligand CLA N 310



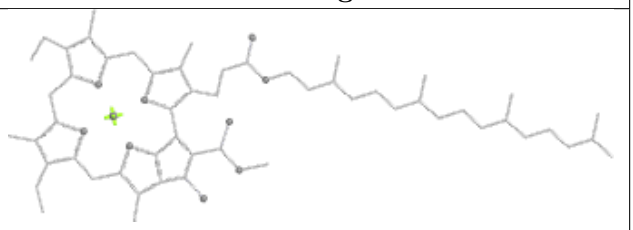
Bond lengths



Bond angles

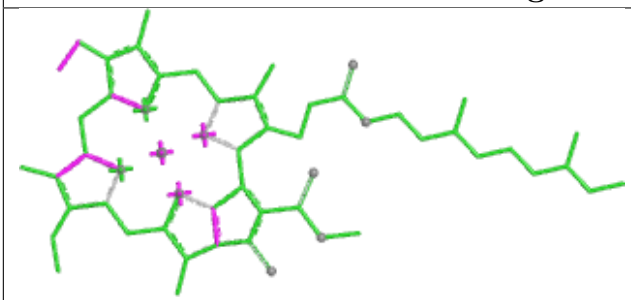


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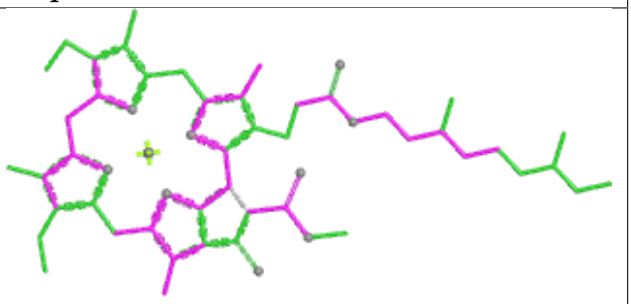


Rings

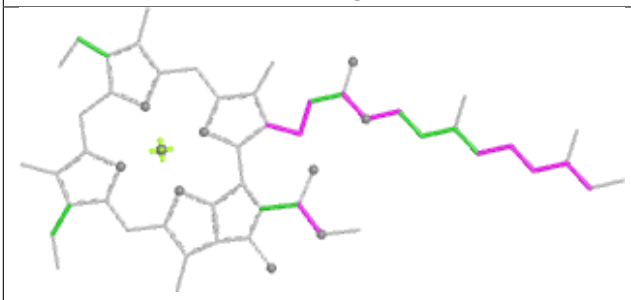
Ligand CLA p 610



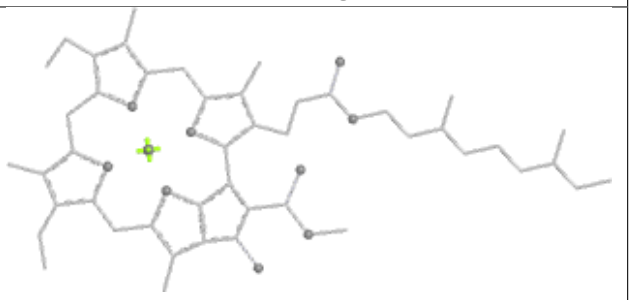
Bond lengths



Bond angles

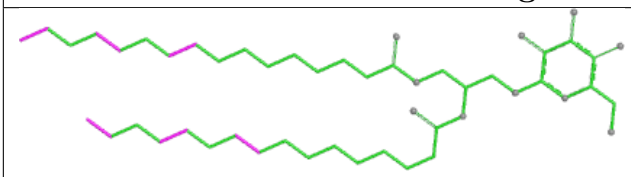


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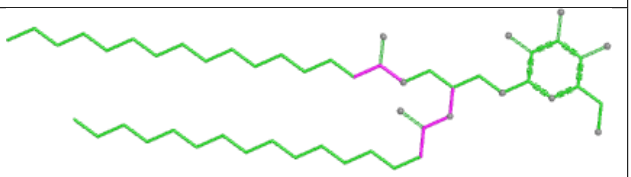


Rings

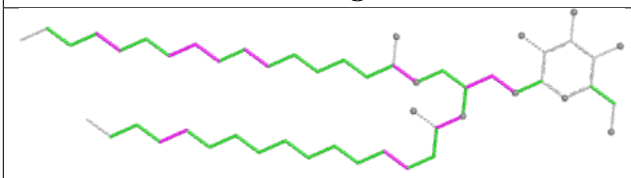
Ligand LMG G 621



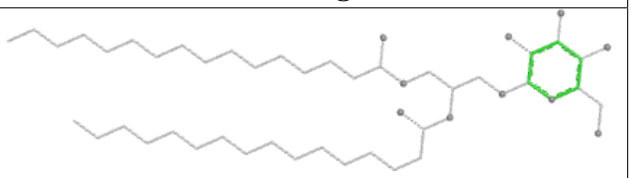
Bond lengths



Bond angles

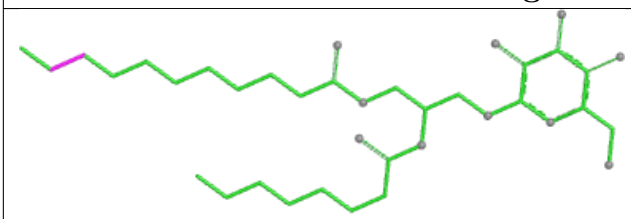


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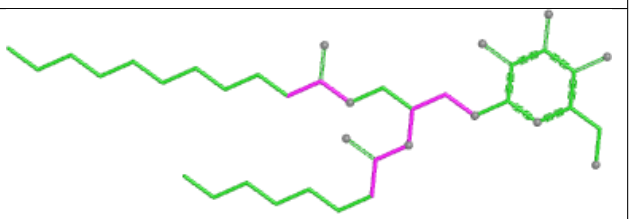


Rings

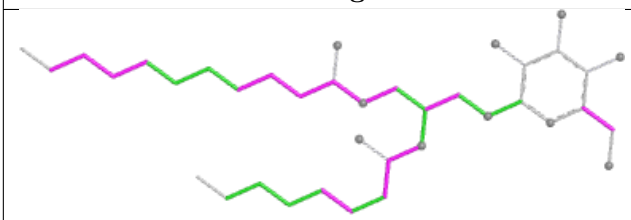
Ligand LMG x 202



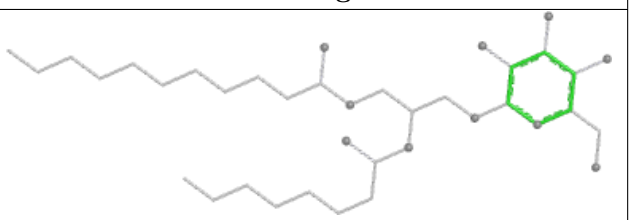
Bond lengths



Bond angles

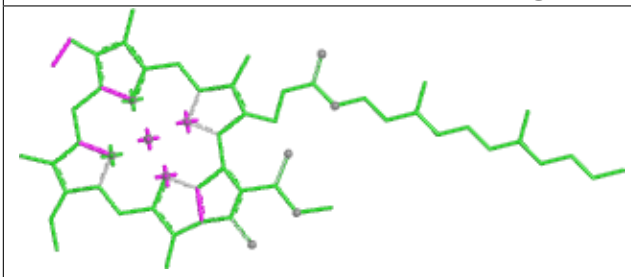


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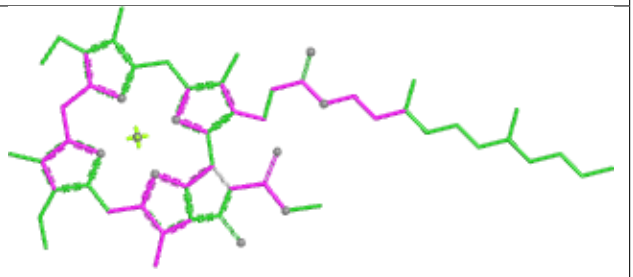


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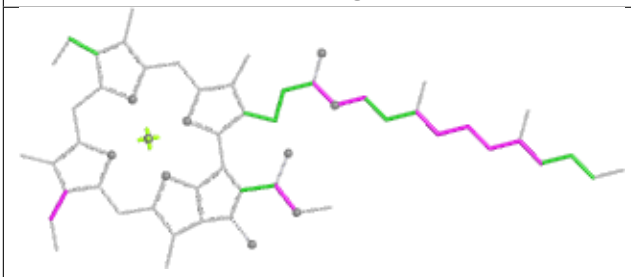
Ligand CLA r 311



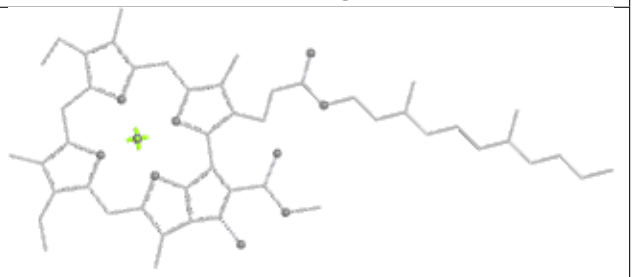
Bond lengths



Bond angles

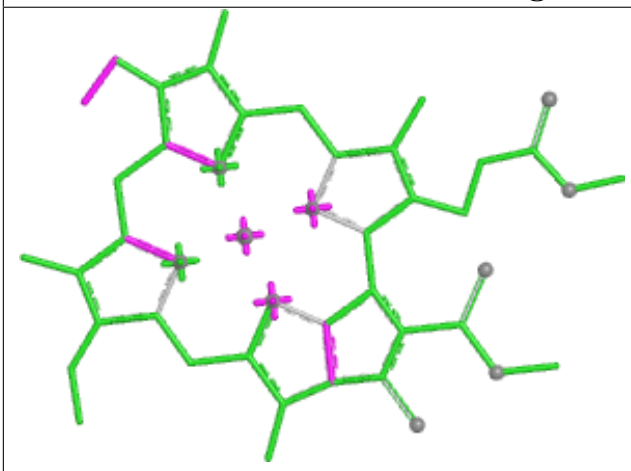


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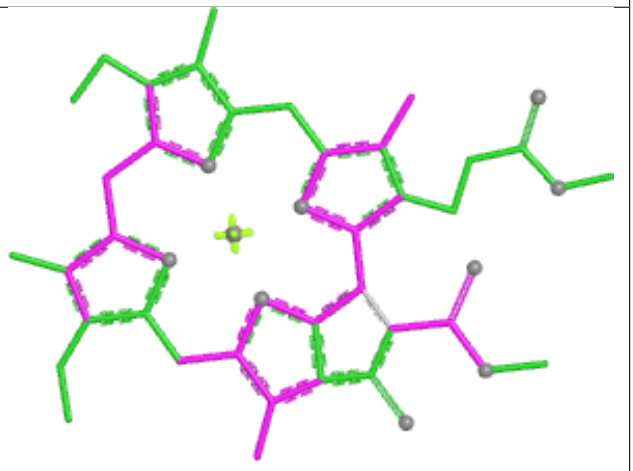


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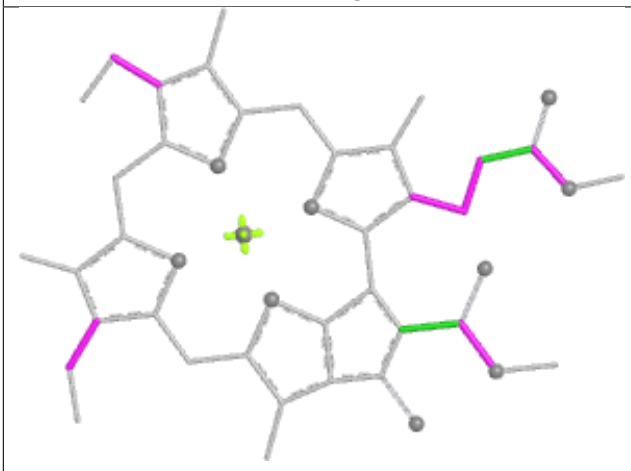
Ligand CLA 5 615



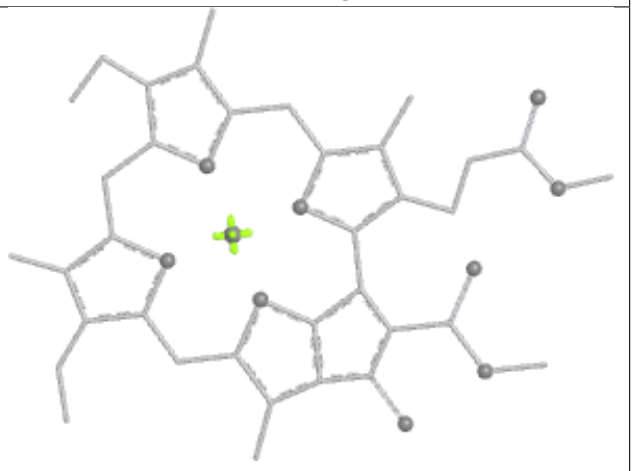
Bond lengths



Bond angles

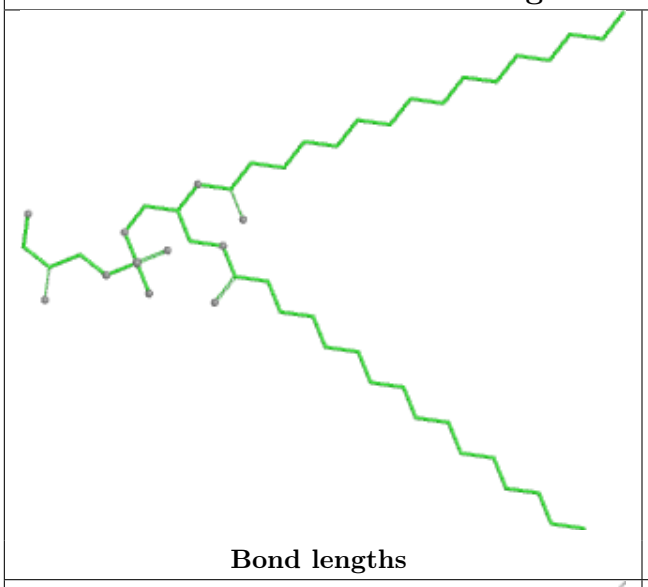


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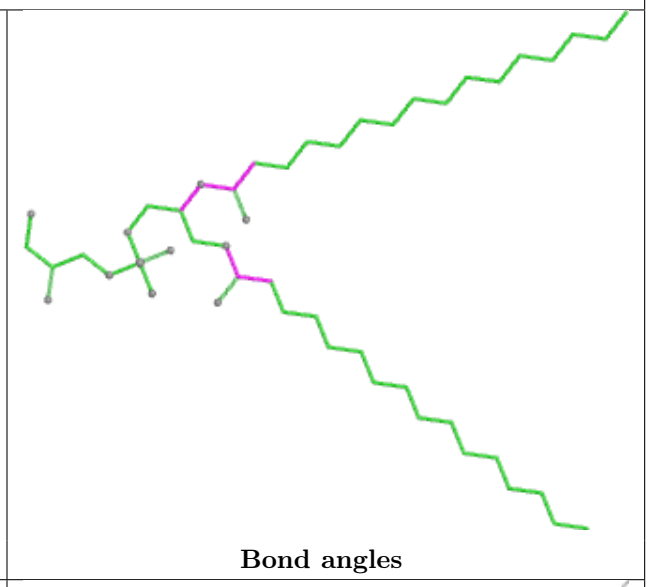


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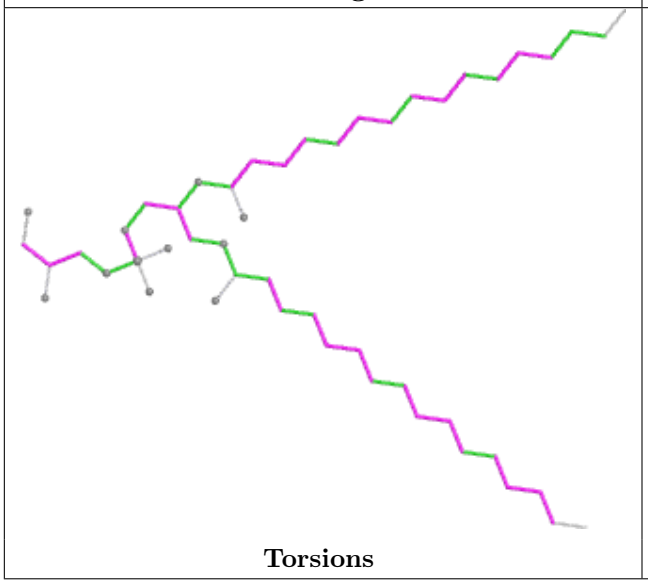
Ligand LHG L 101



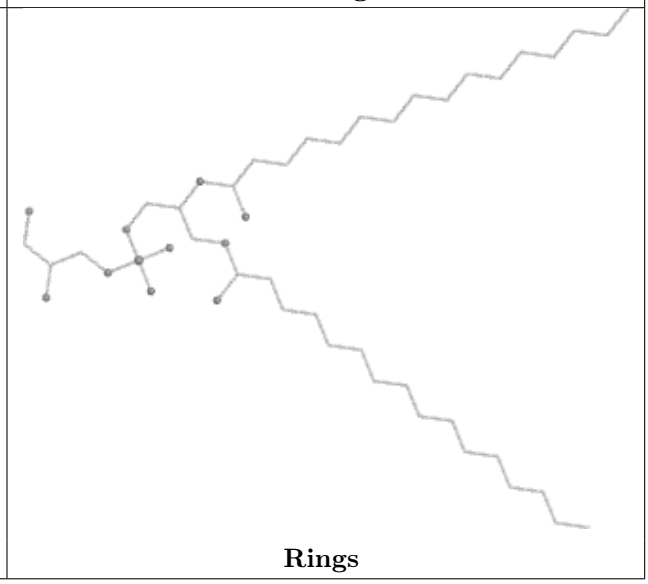
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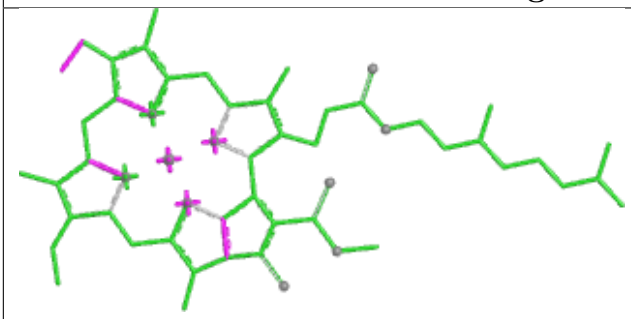


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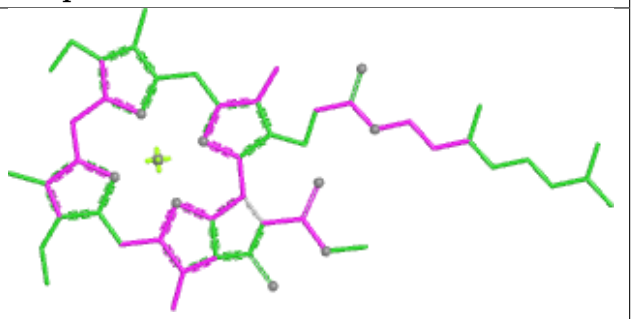


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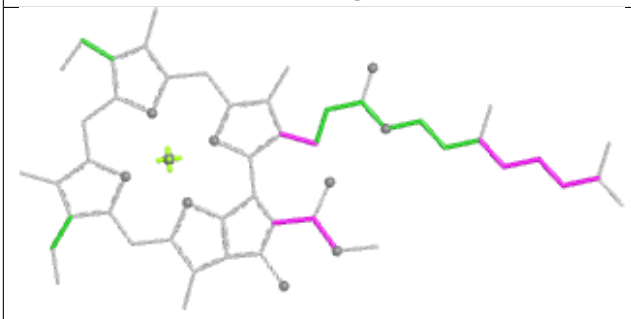
Ligand CLA q 305



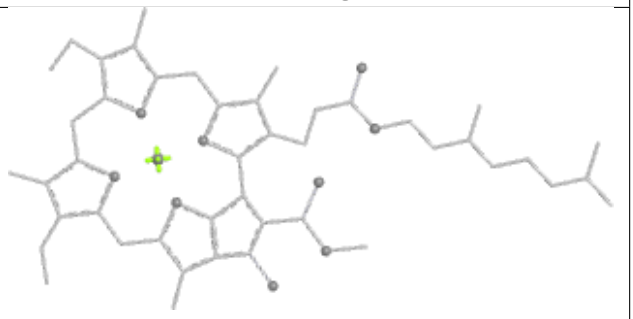
Bond lengths



Bond angles

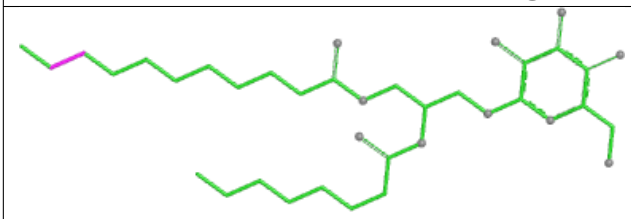


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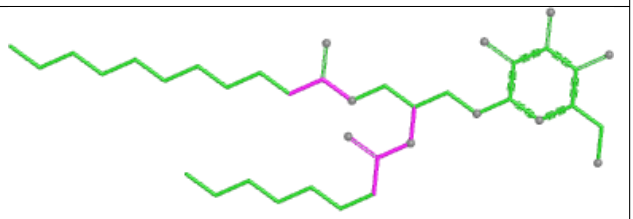


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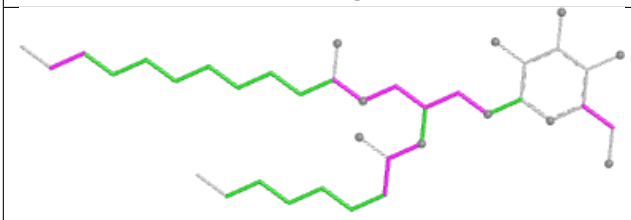
Ligand LMG 2 618



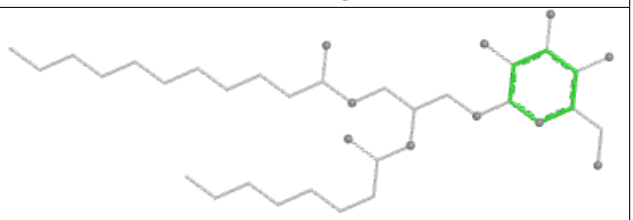
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Bond angles

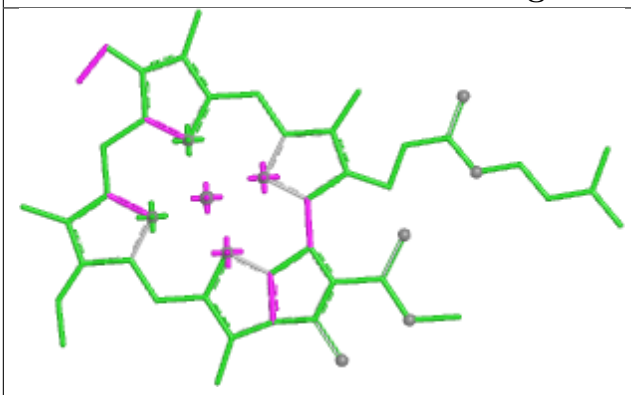


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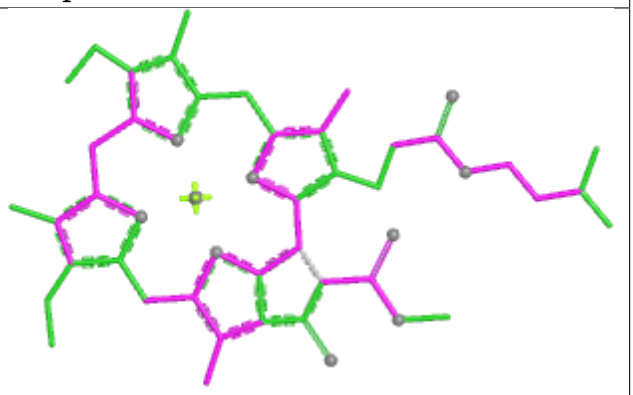


Rings

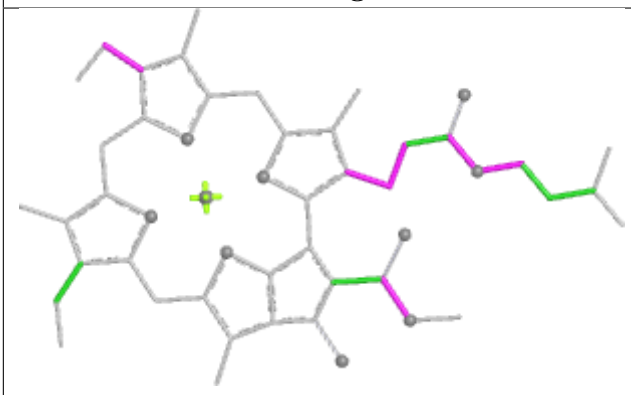
Ligand CLA q 316



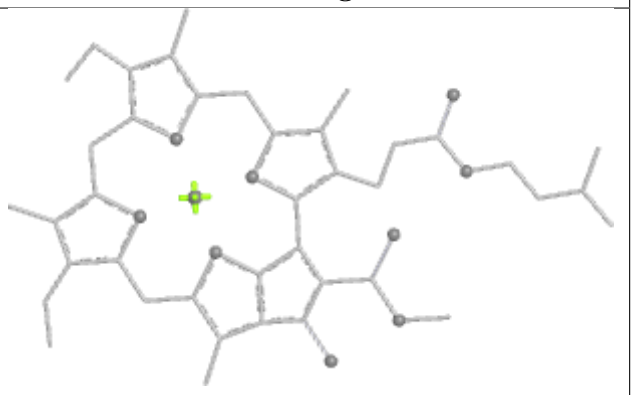
Bond lengths



Bond angles

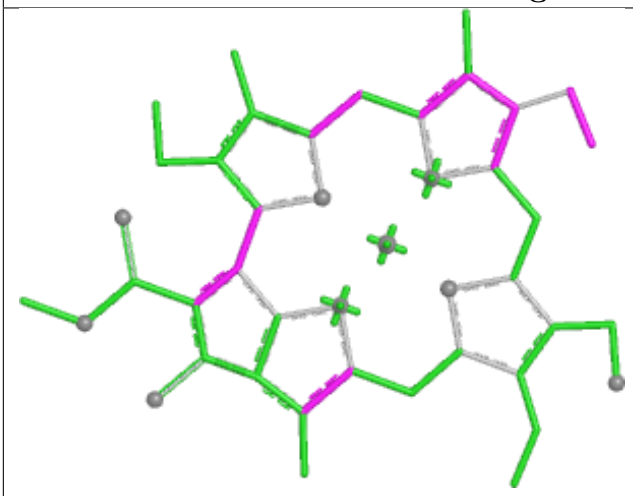


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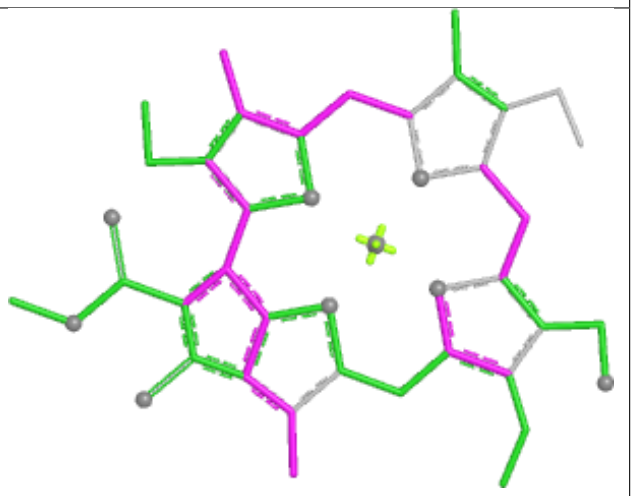


Rings

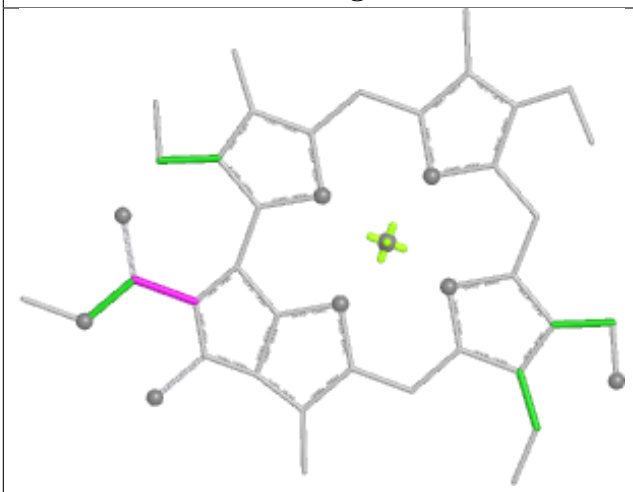
Ligand CHL s 308



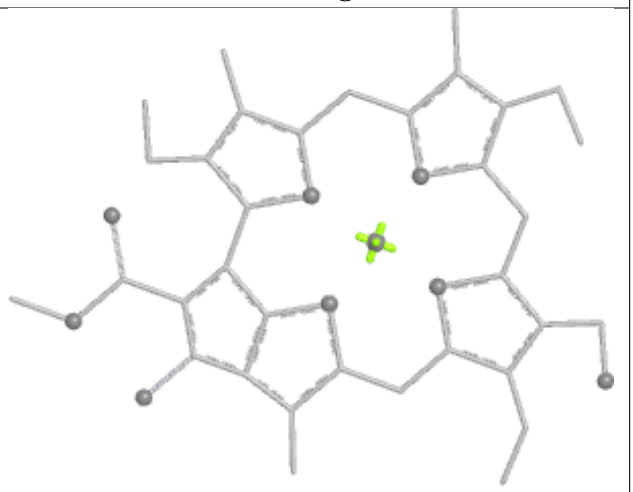
Bond lengths



Bond angles

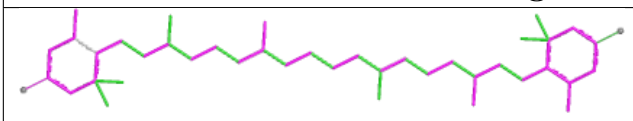


Torsions

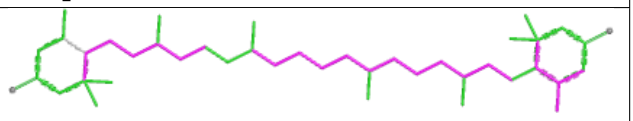


Rings

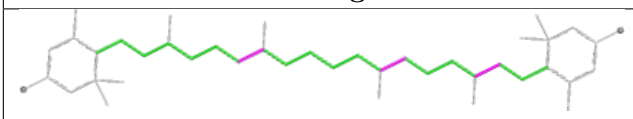
Ligand LUT q 318



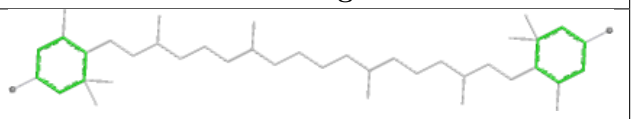
Bond lengths



Bond angles

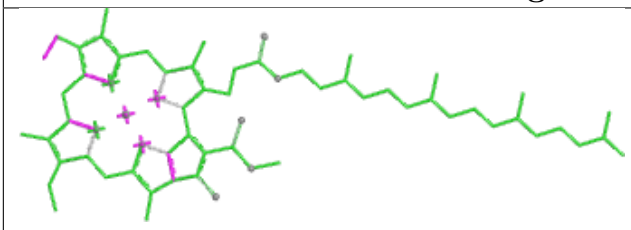


Torsions

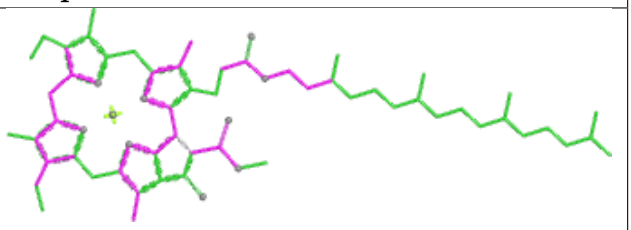


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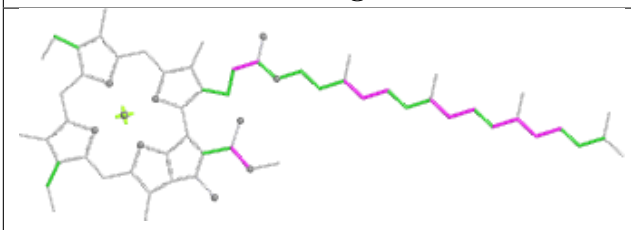
Ligand CLA q 315



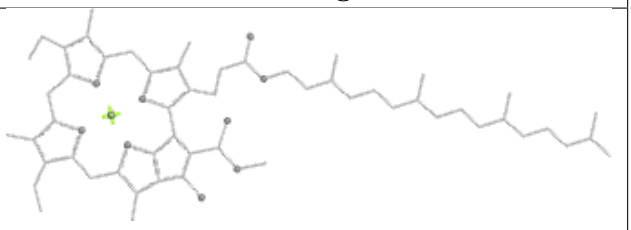
Bond lengths



Bond angles

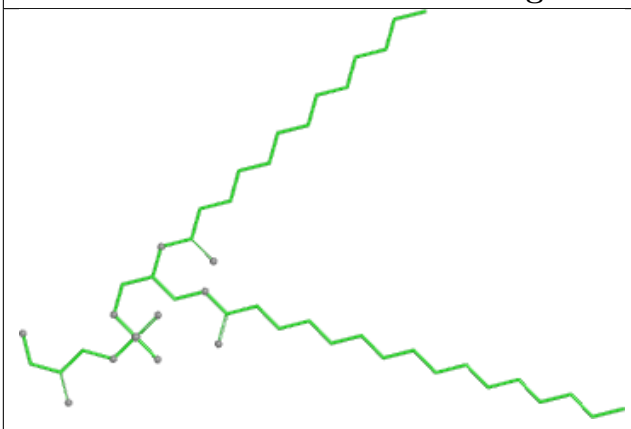


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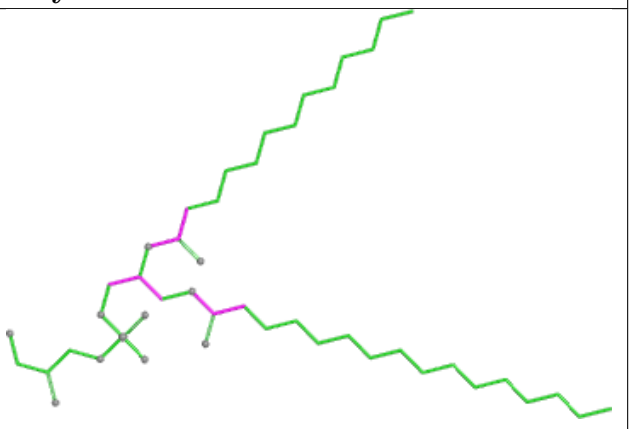


Rings

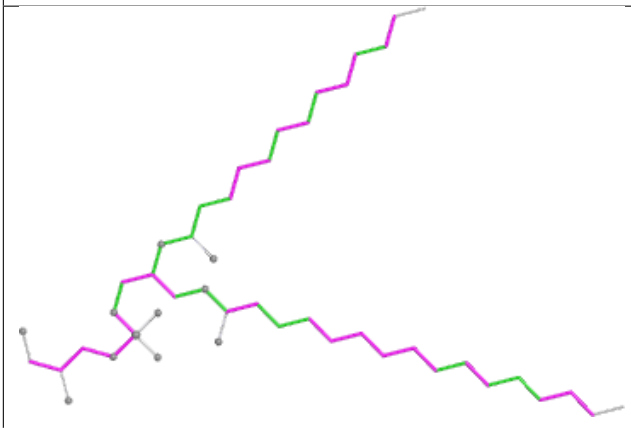
Ligand LHG y 619



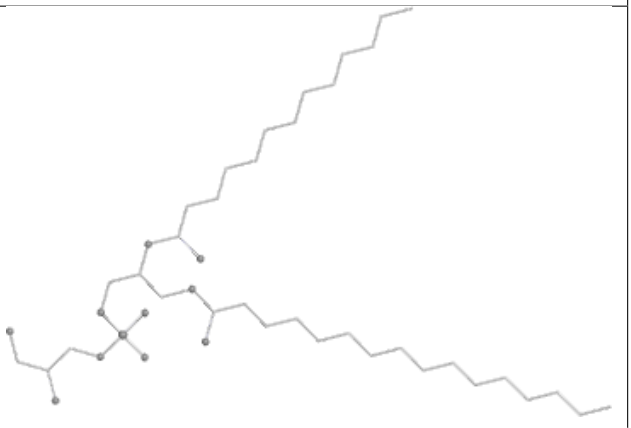
Bond lengths



Bond angles

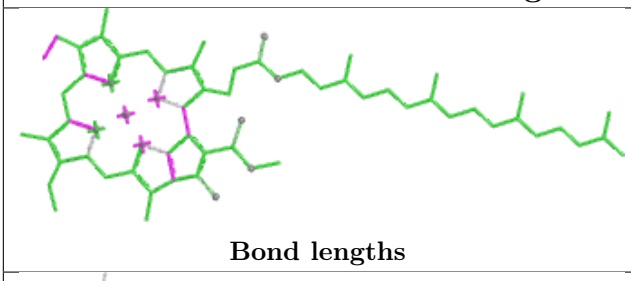


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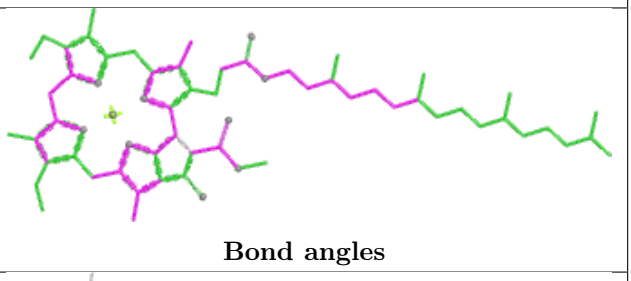


Rings

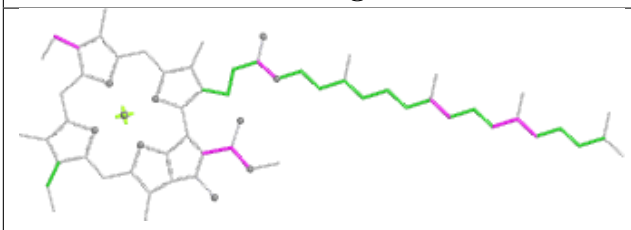
Ligand CLA C 607



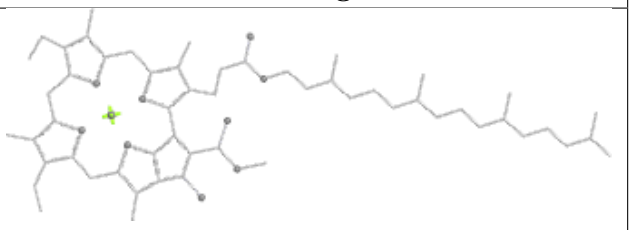
Bond lengths



Bond angles

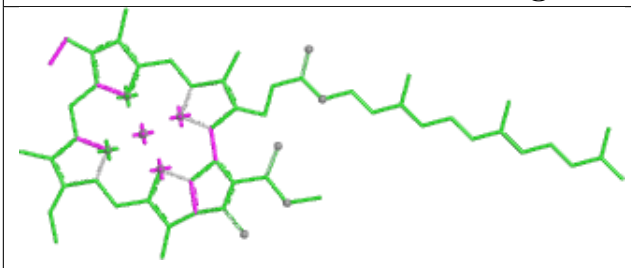


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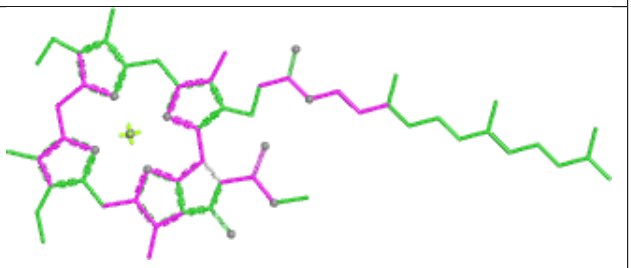


Rings

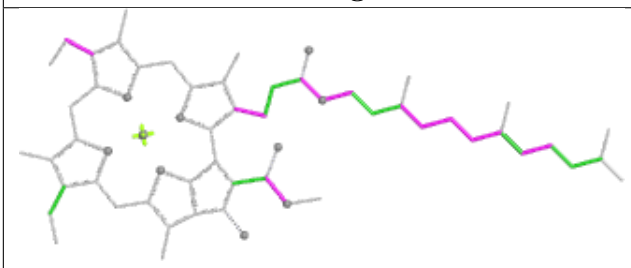
Ligand CLA s 310



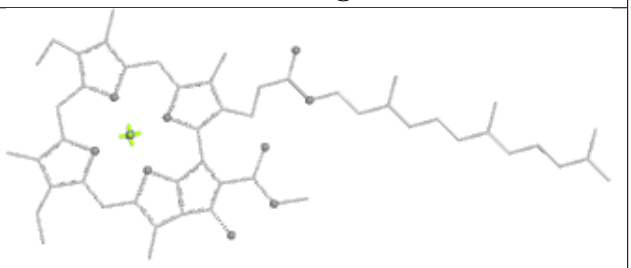
Bond lengths



Bond angles



Torsions



Rings

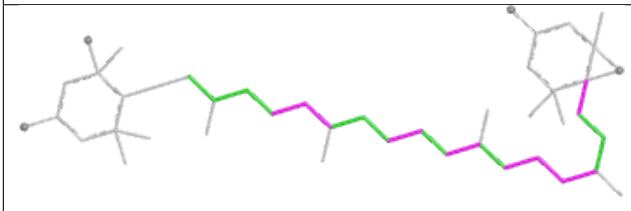
Ligand NEX q 319



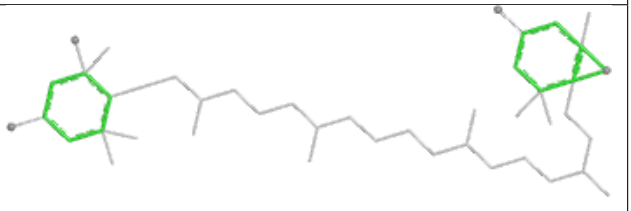
Bond lengths



Bond angles

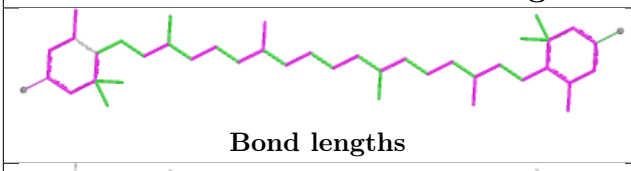


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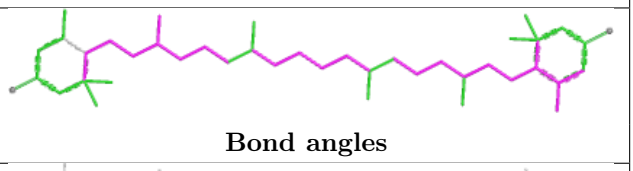


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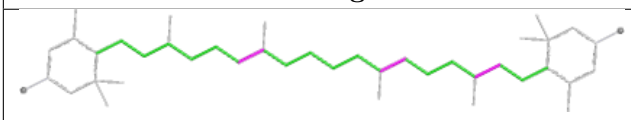
Ligand LUT 8 616



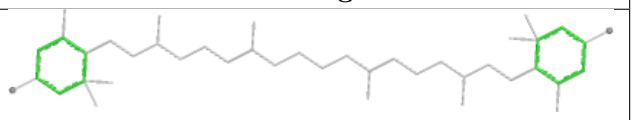
Bond lengths



Bond angles

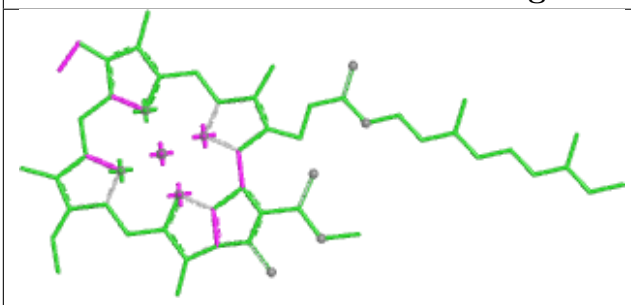


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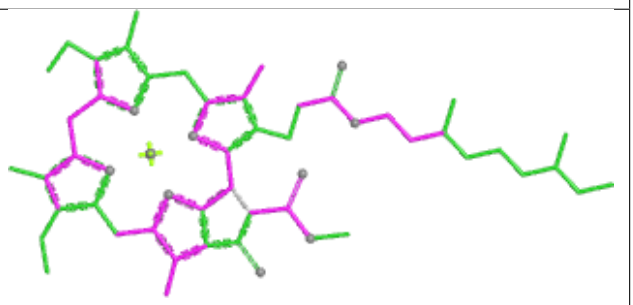


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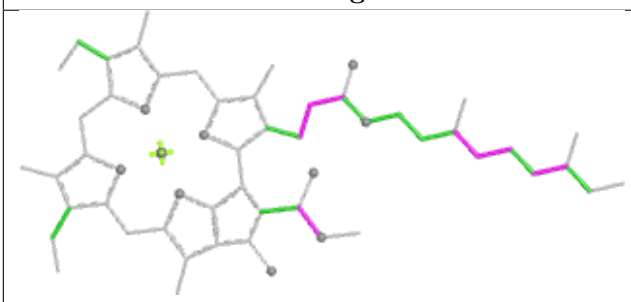
Ligand CLA 0 613



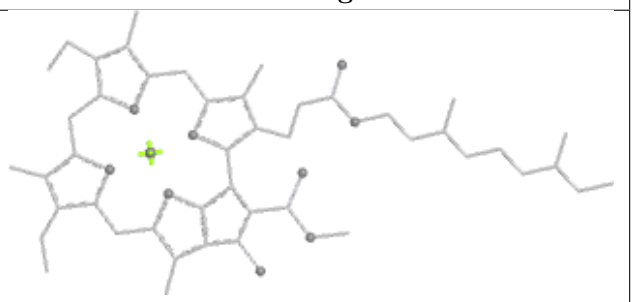
Bond lengths



Bond angles

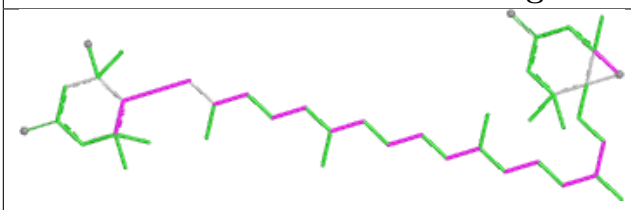


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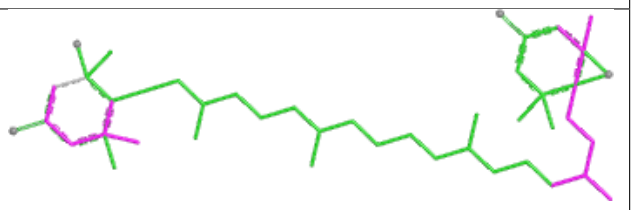


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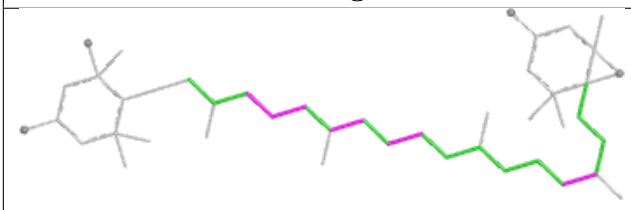
Ligand NEX 9 319



Bond lengths



Bond angles

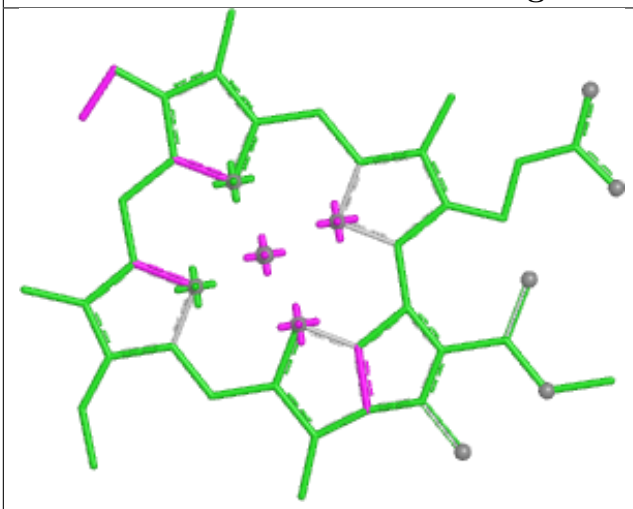


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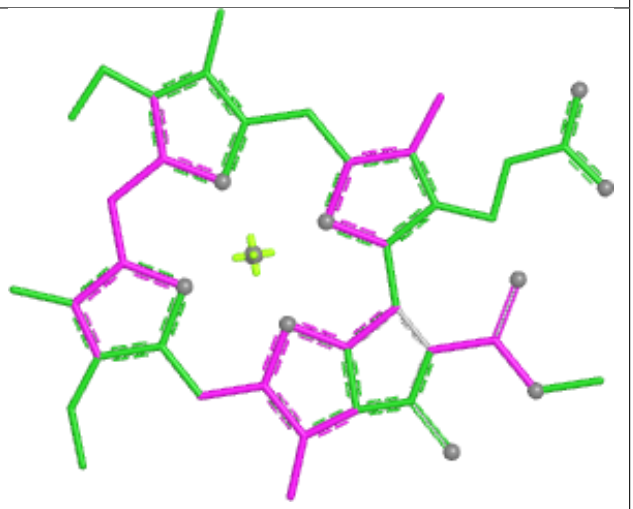


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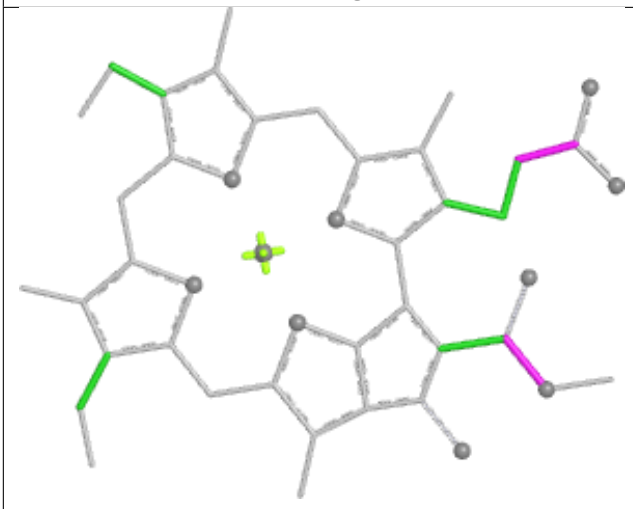
Ligand CLA n 313



Bond lengths



Bond angles

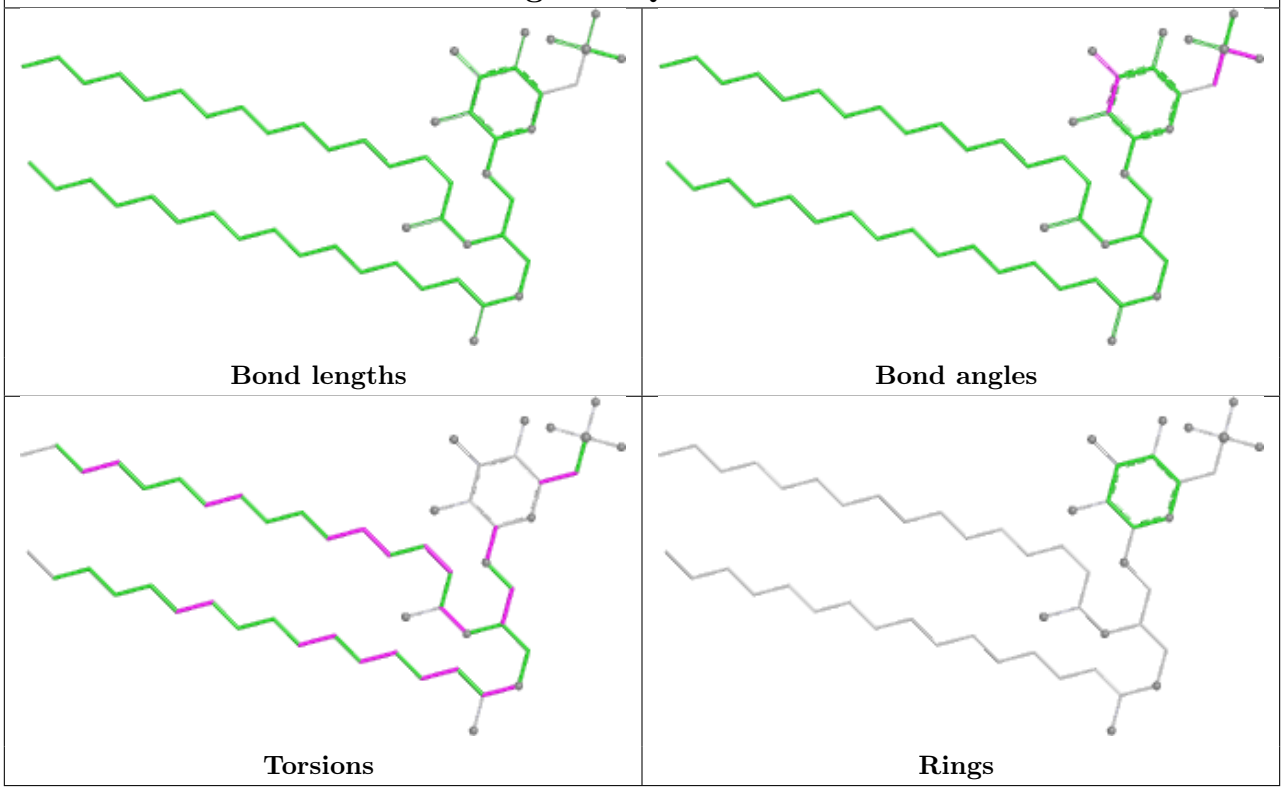


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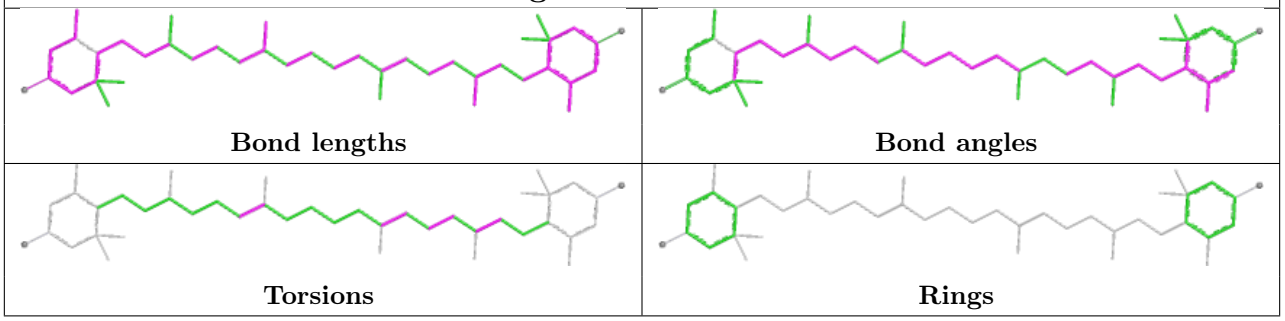


Rings

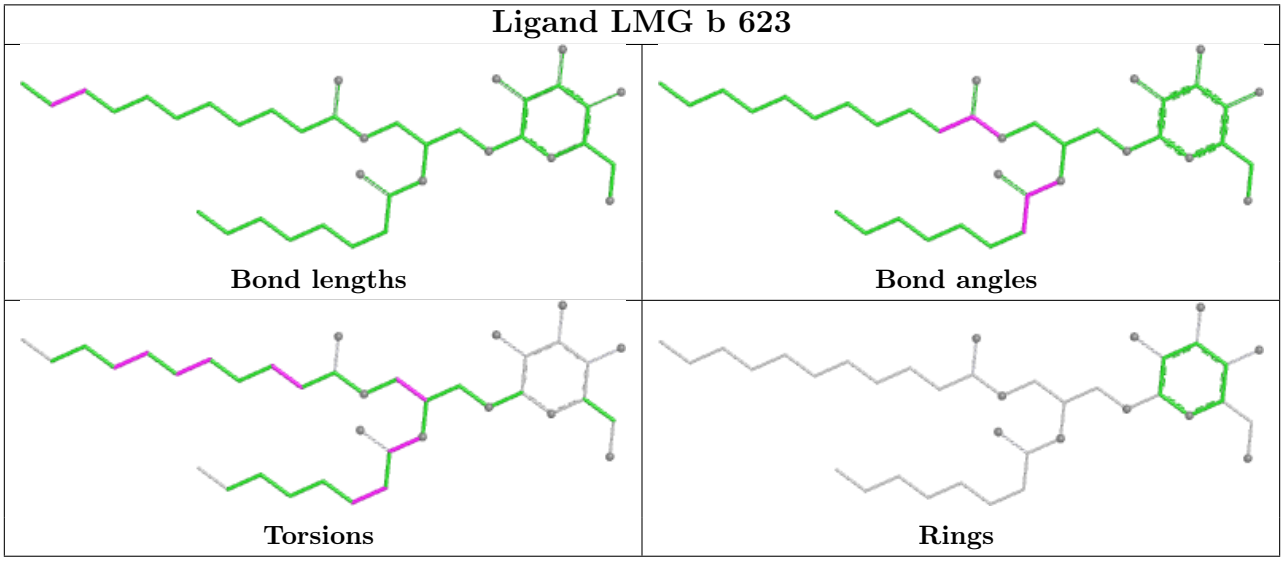
Ligand SQD B 620



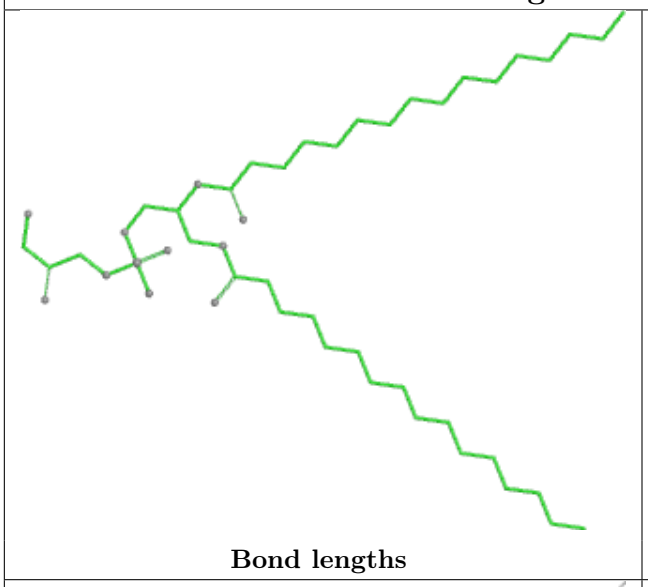
Ligand LUT 3 318



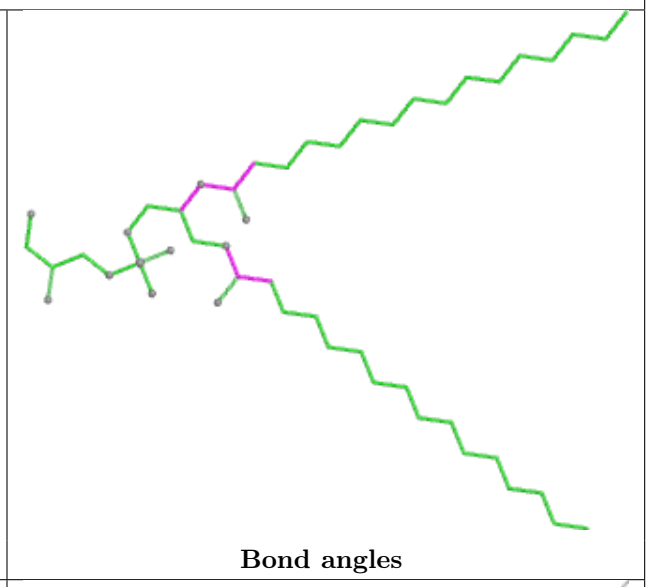
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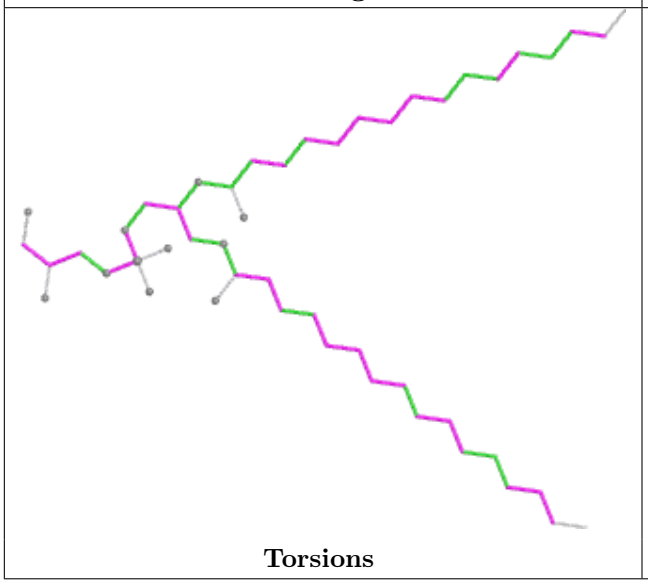
Ligand LHG 2 617



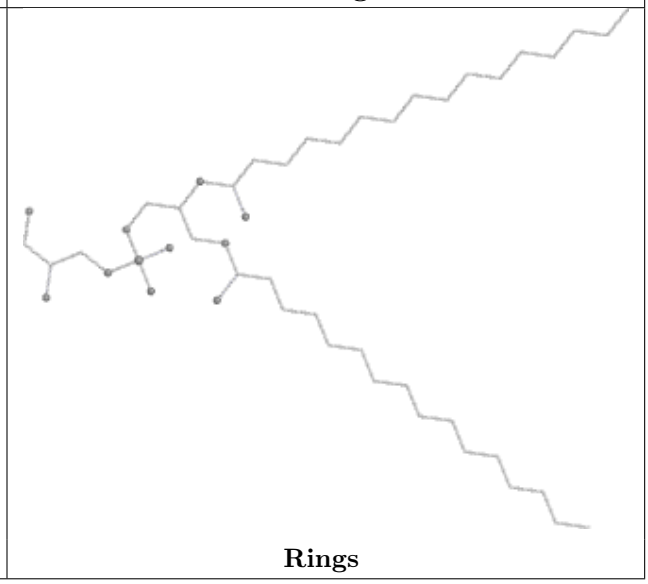
Bond lengths



Bond angles

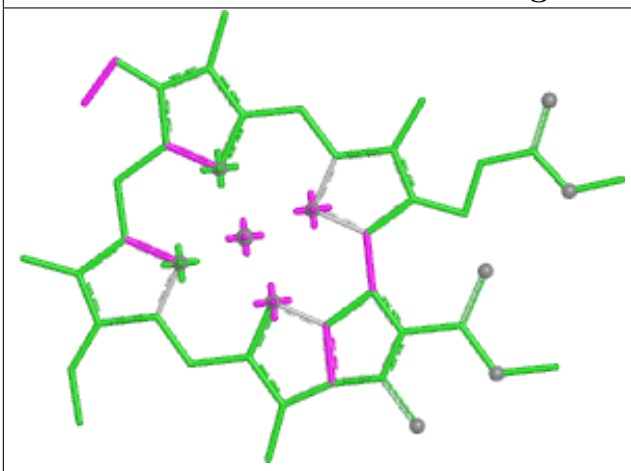


Torsions

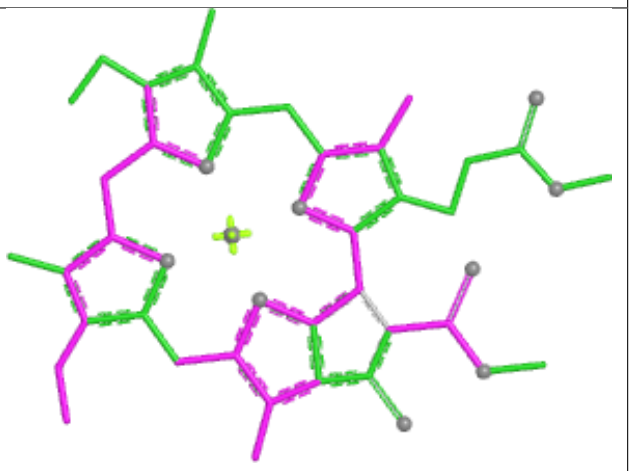


Rings

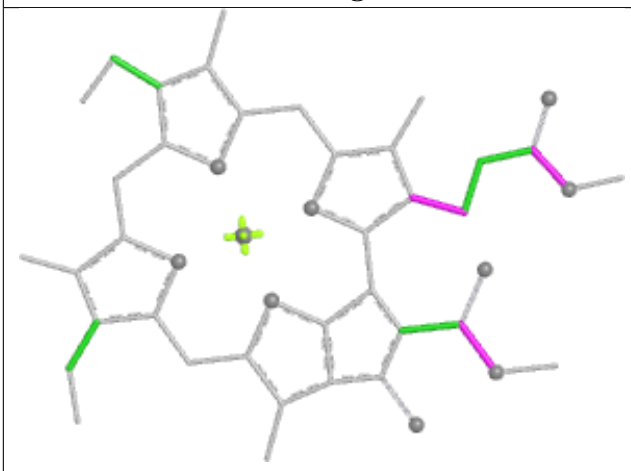
Ligand CLA s 316



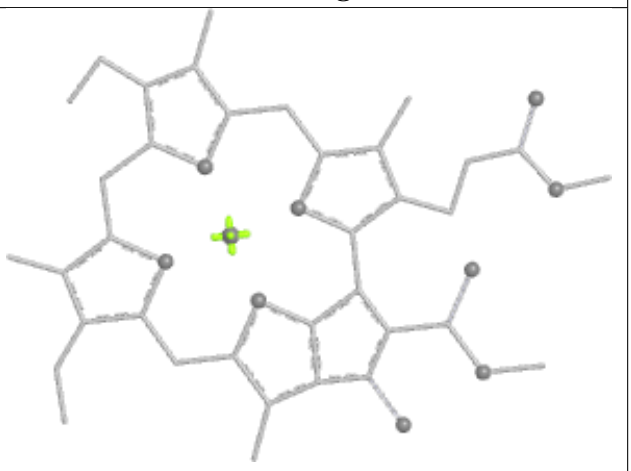
Bond lengths



Bond angles

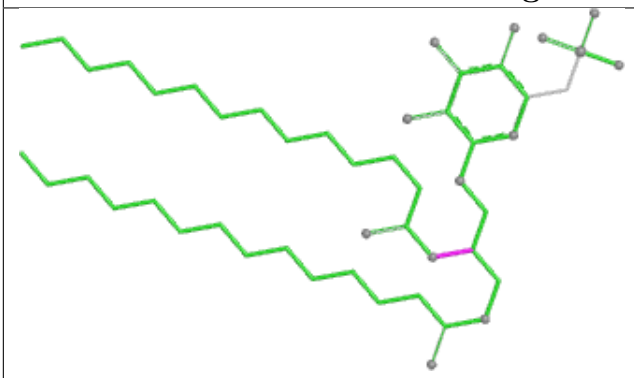


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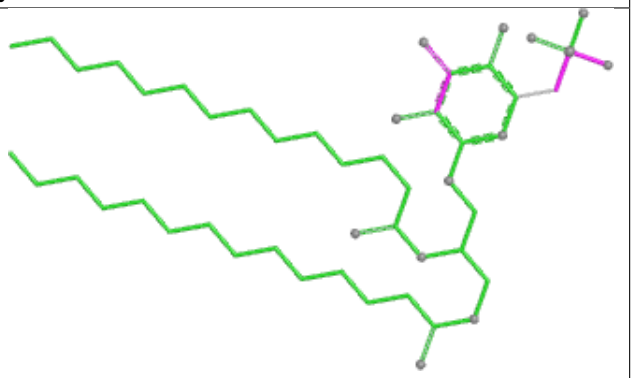


Rings

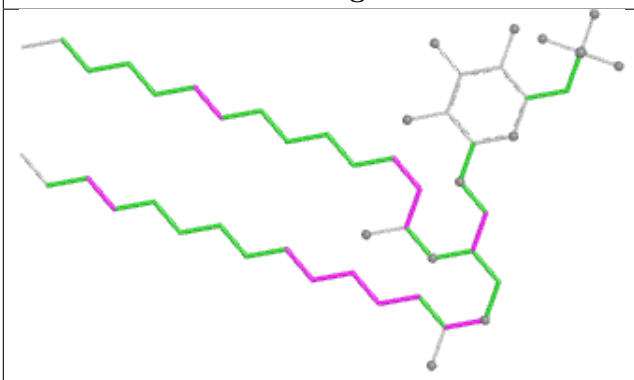
Ligand SQD m 101



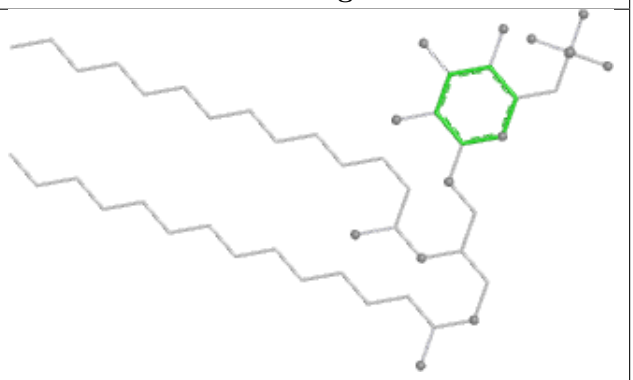
Bond lengths



Bond angles

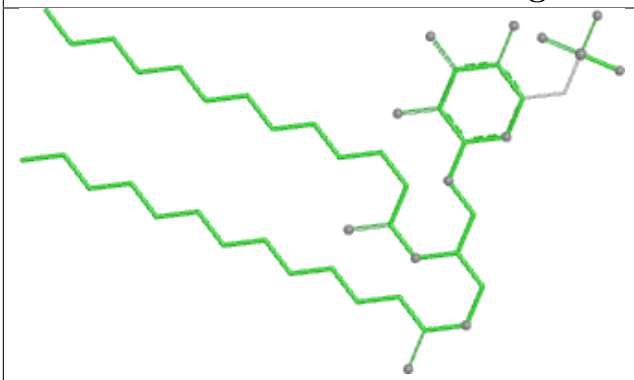


Torsions

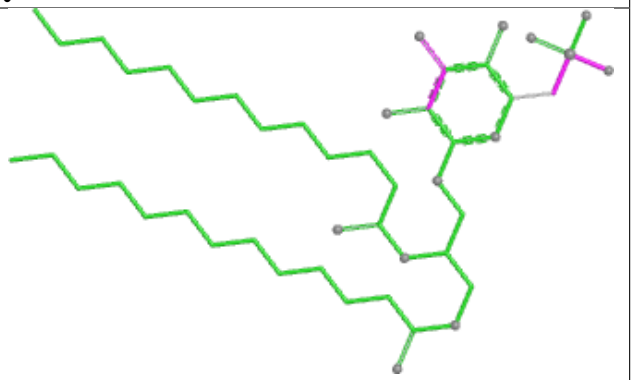


Rings

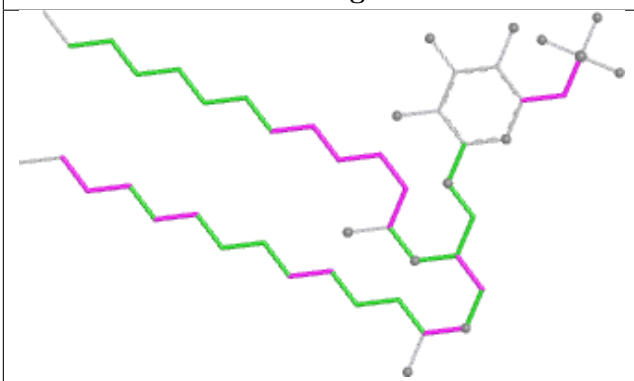
Ligand SQD a 411



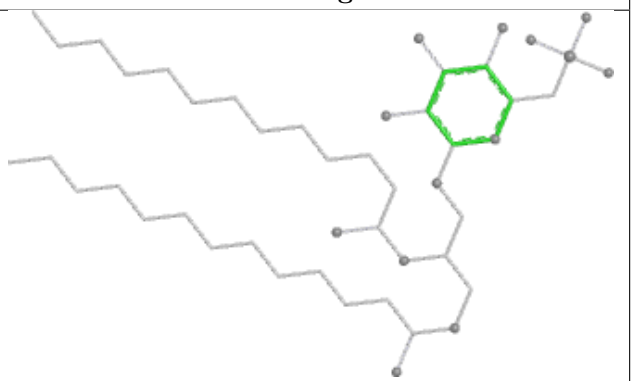
Bond lengths



Bond angles

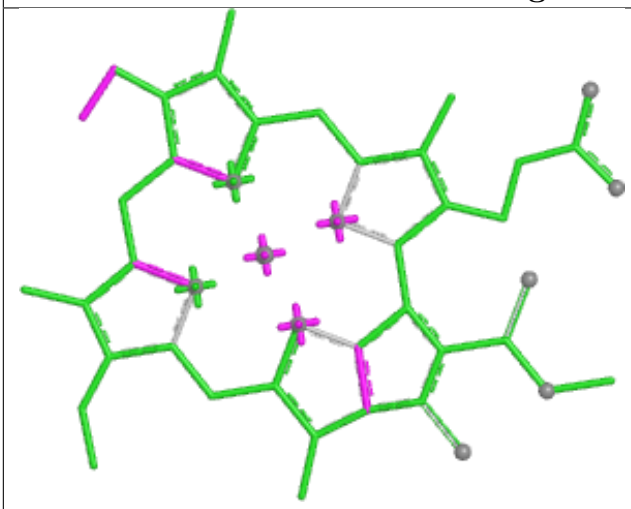


Torsions

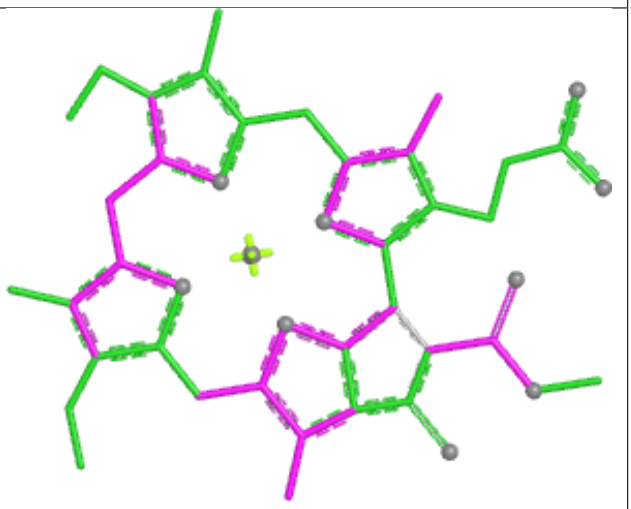


Rings

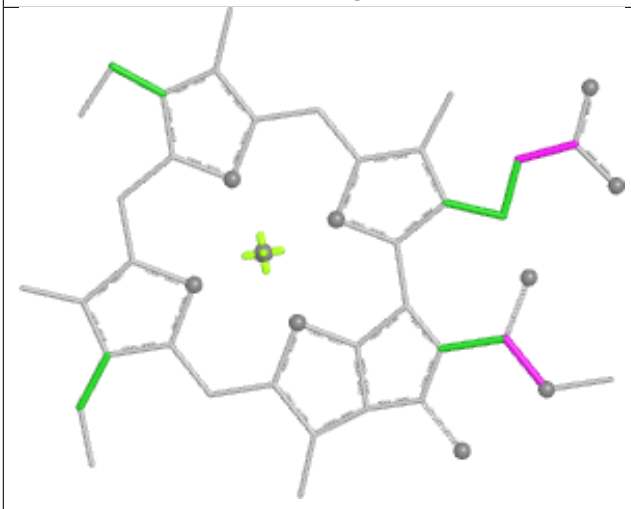
Ligand CLA 8 611



Bond lengths



Bond angles

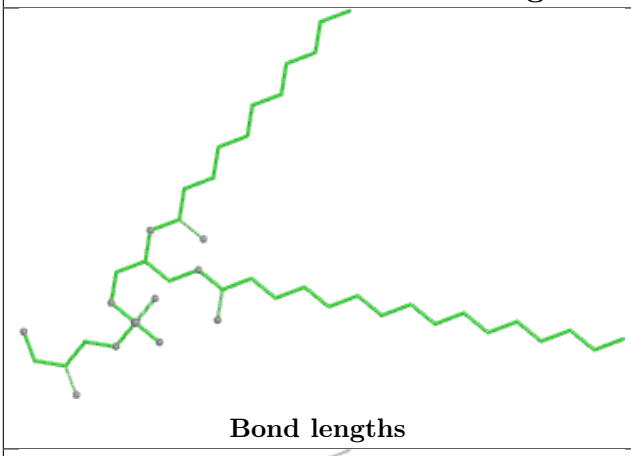


Torsions

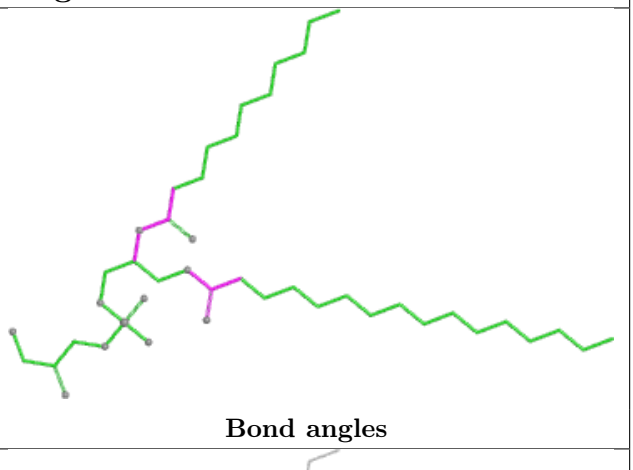


Rings

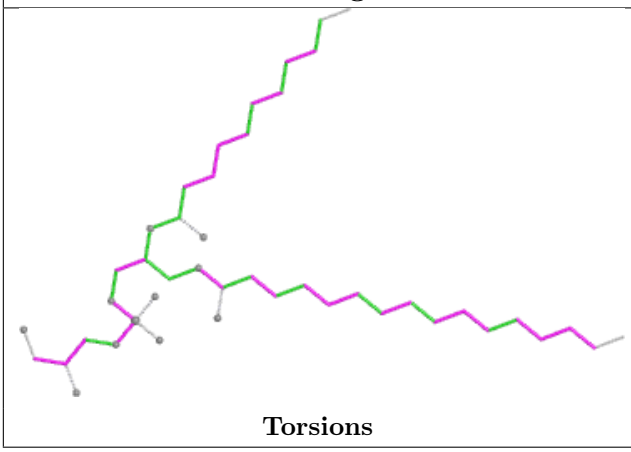
Ligand LHG g 319



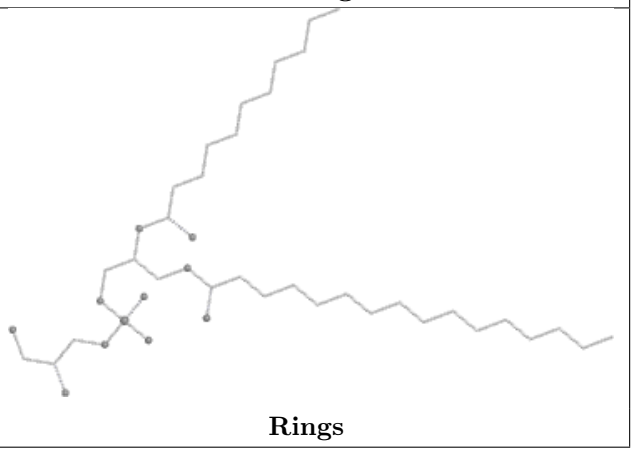
Bond lengths



Bond angles

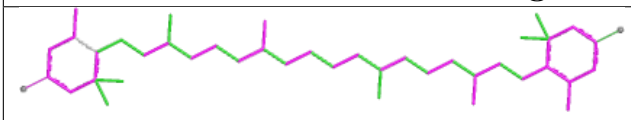


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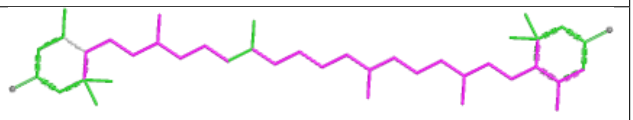


Rings

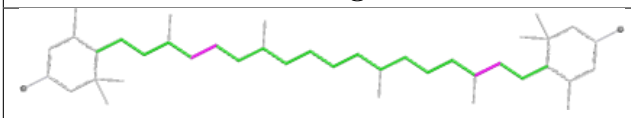
Ligand LUT 1 616



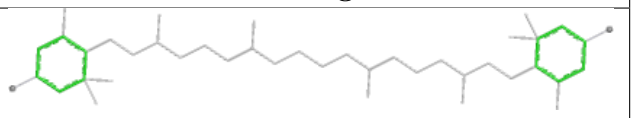
Bond lengths



Bond angles

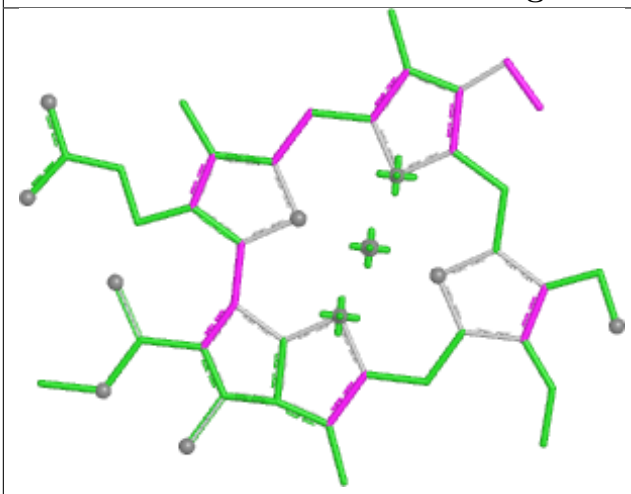


Torsions

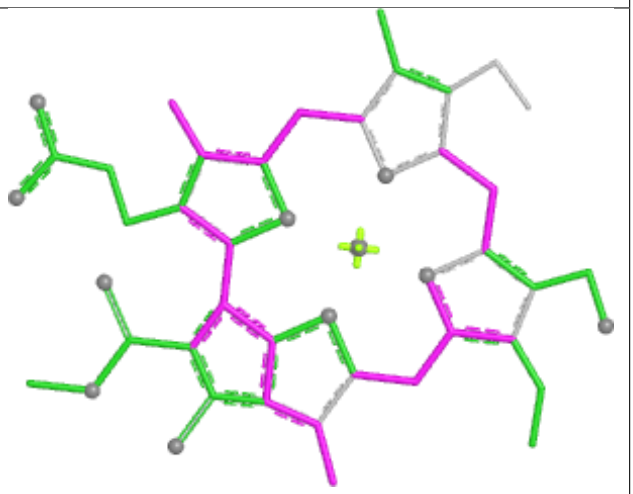


Rings

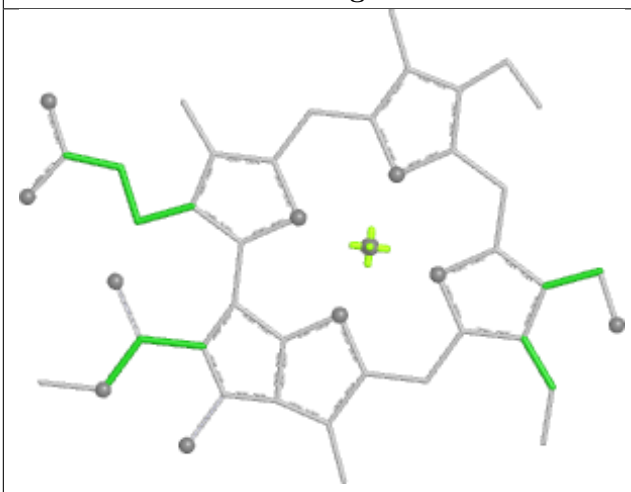
Ligand CHL S 302



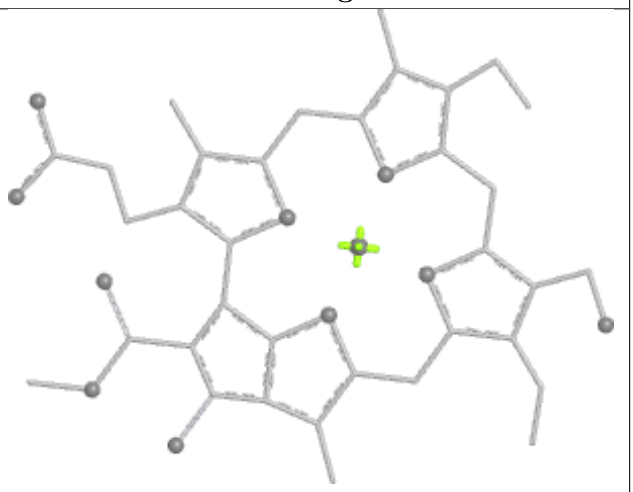
Bond lengths



Bond angles

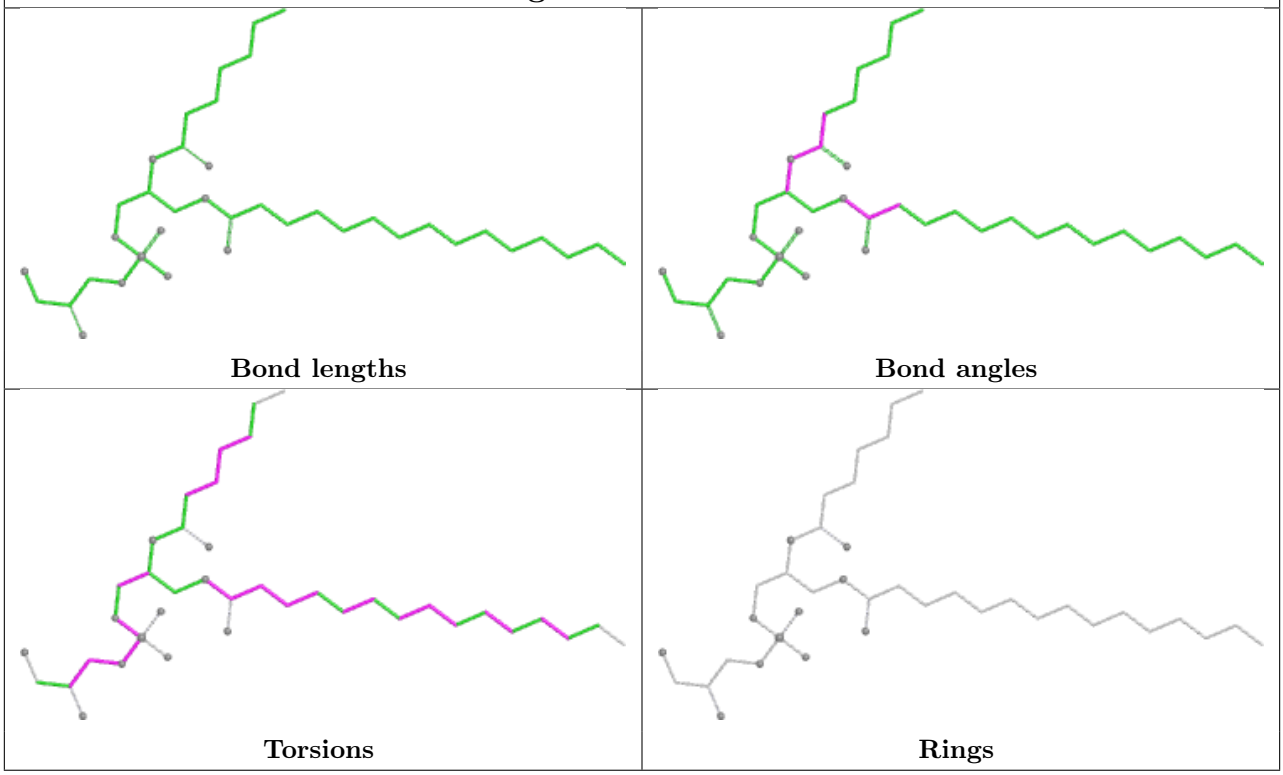


Torsions

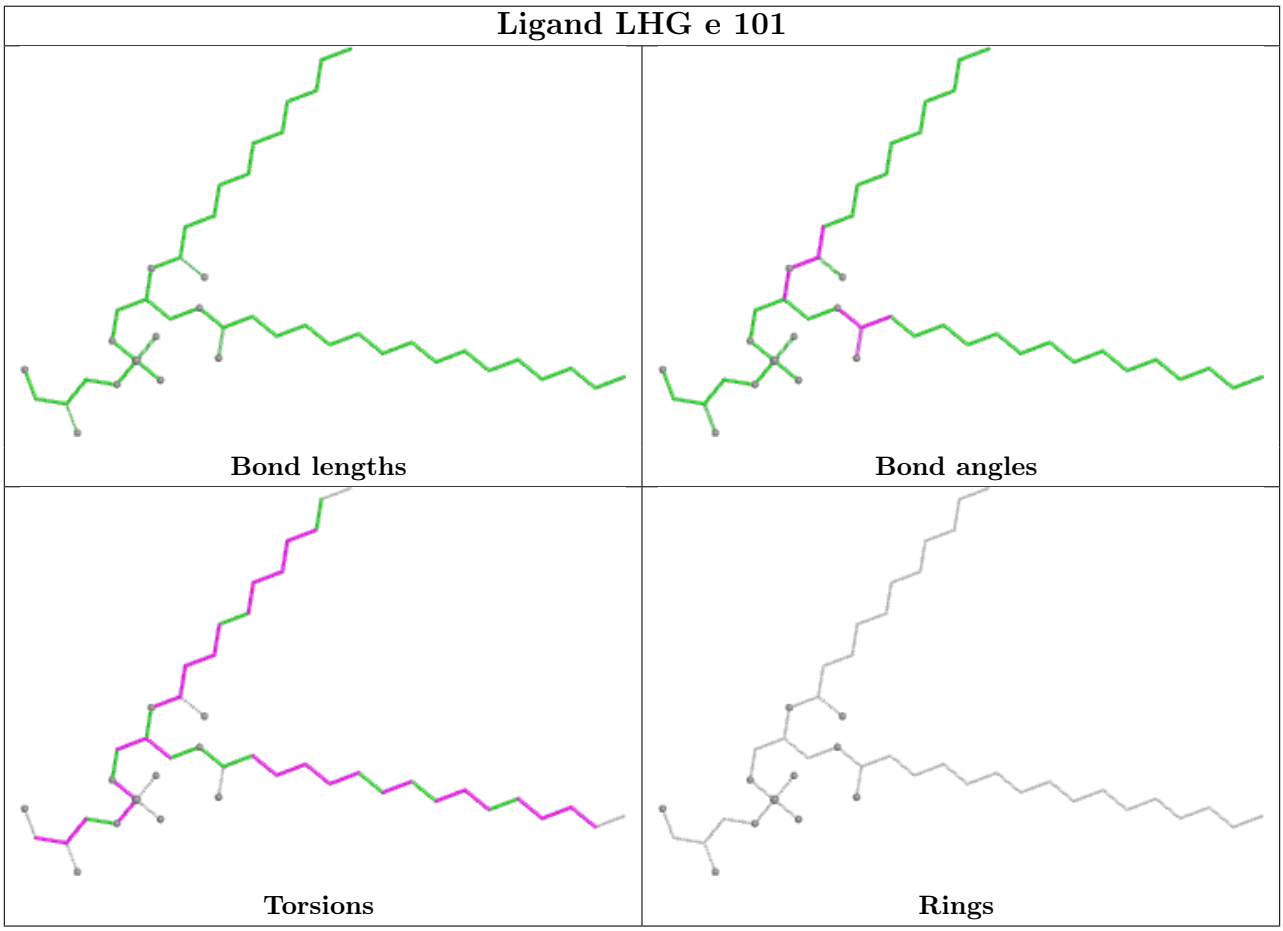


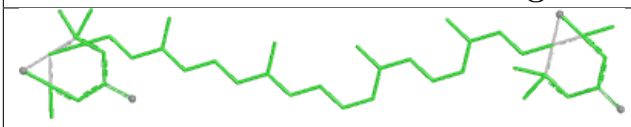
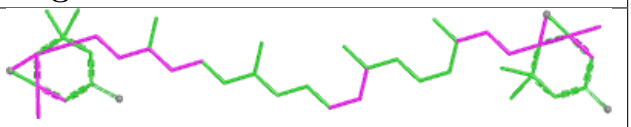
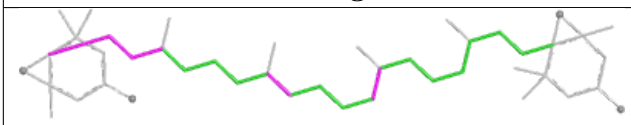
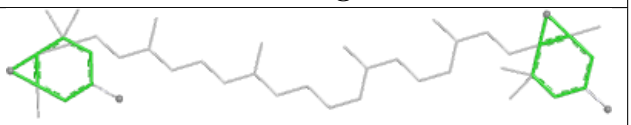
Rings

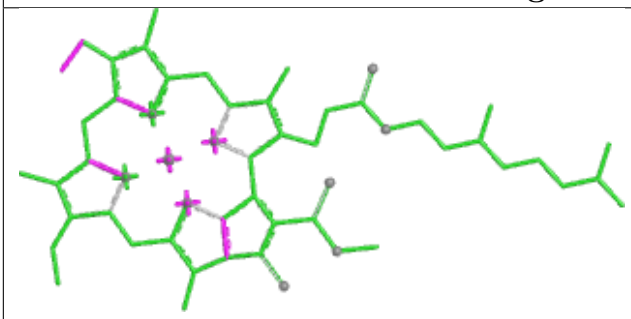
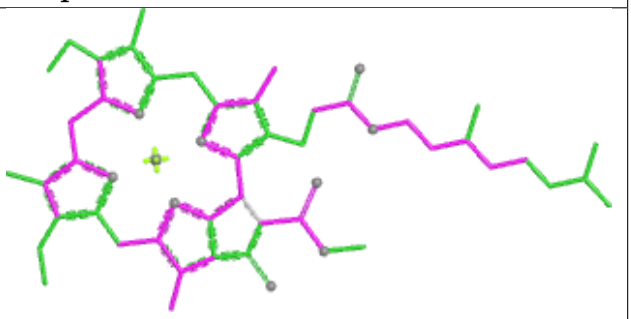
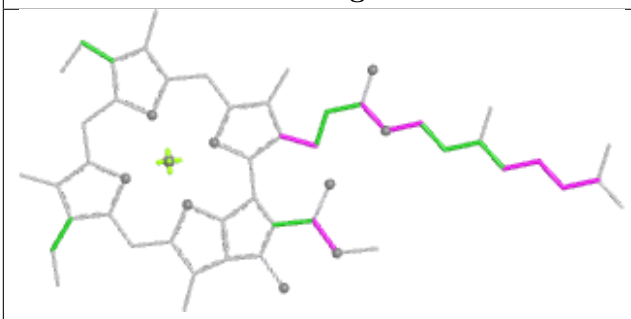
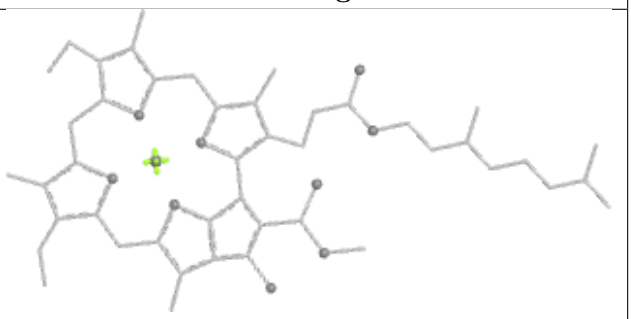
Ligand LHG a 415



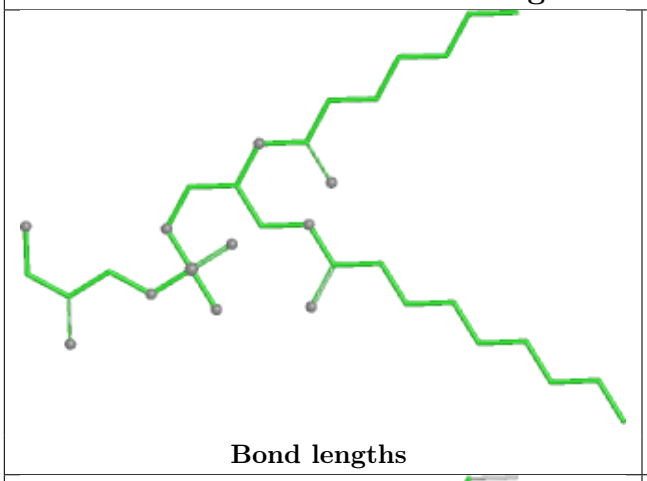
Ligand LHG e 101



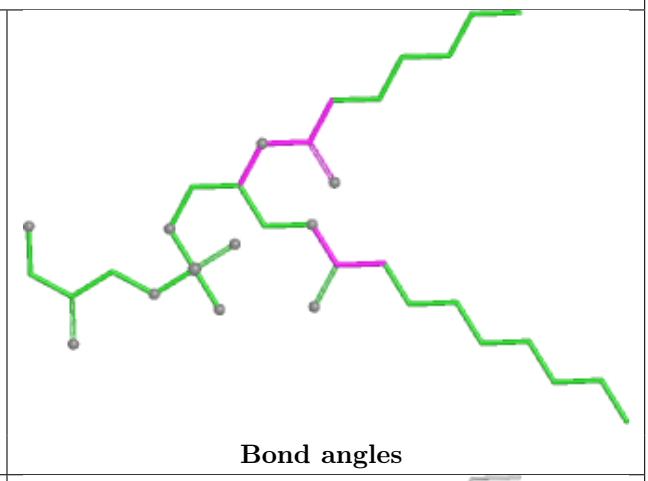
Ligand XAT g 321	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA q 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

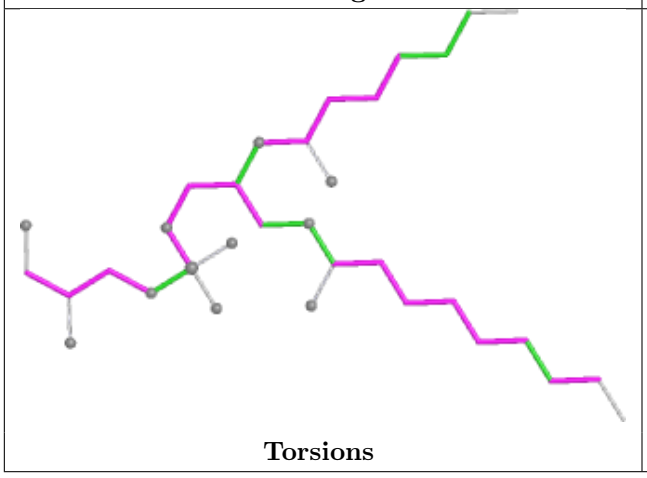
Ligand LHG 9 320



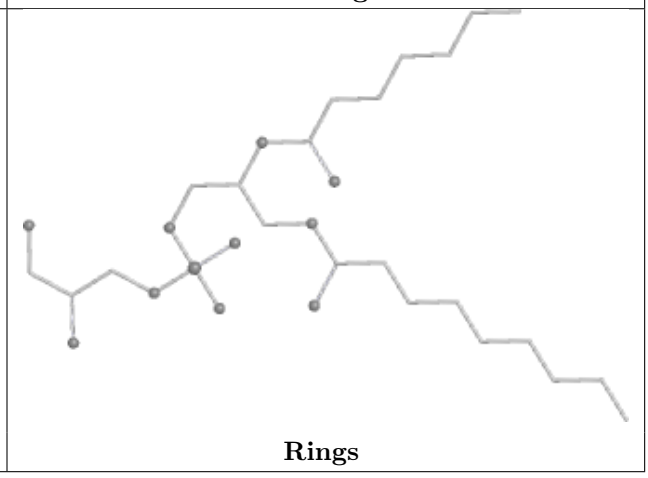
Bond lengths



Bond angles

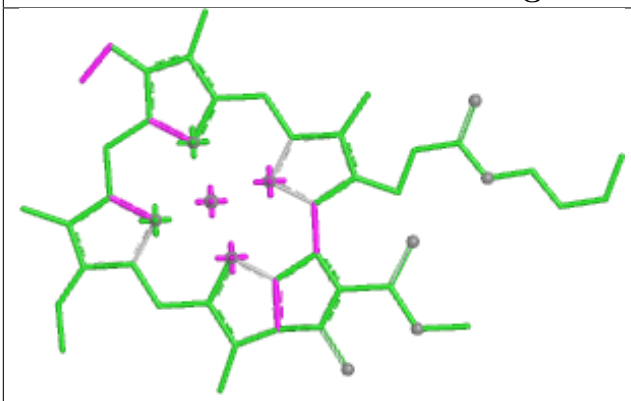


Torsions

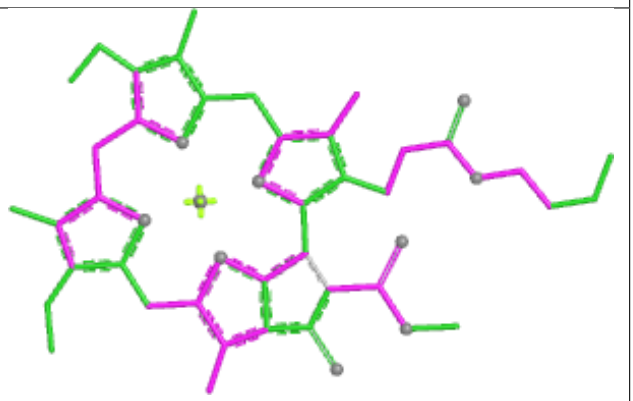


Rings

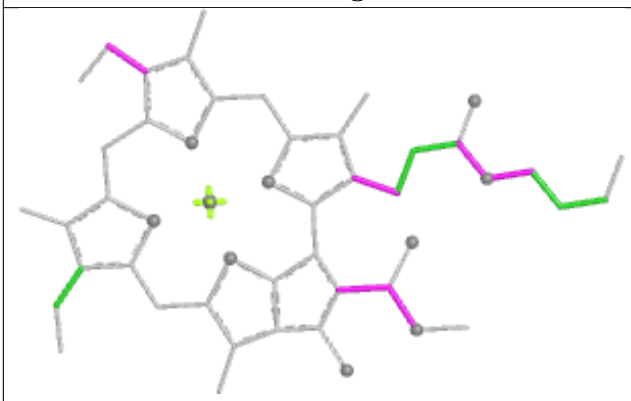
Ligand CLA R 303



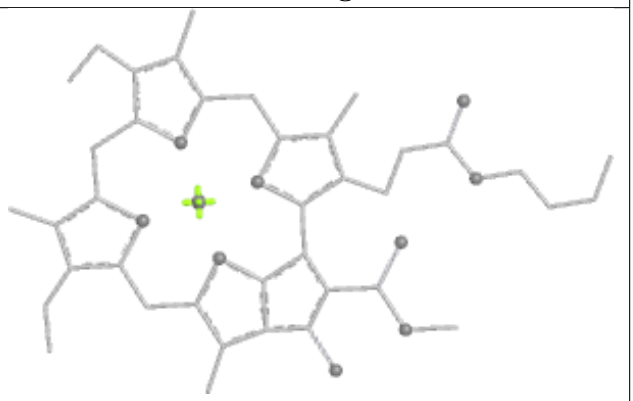
Bond lengths



Bond angles

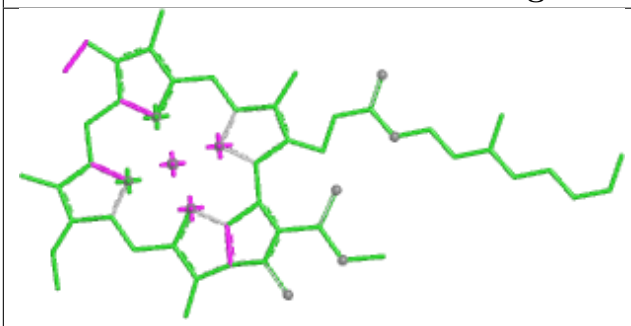


Torsions

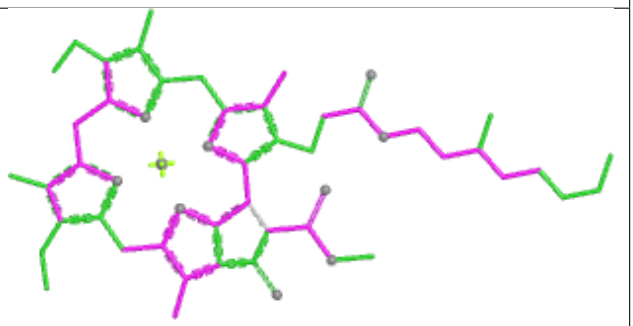


Rings

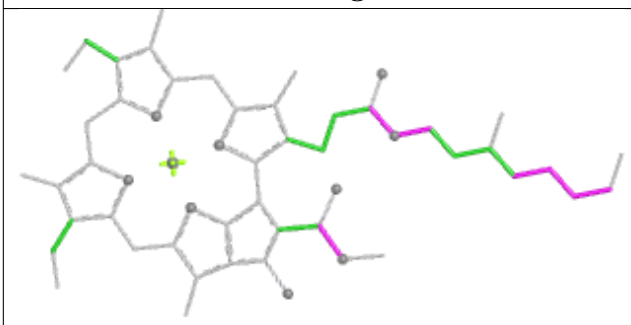
Ligand CLA n 316



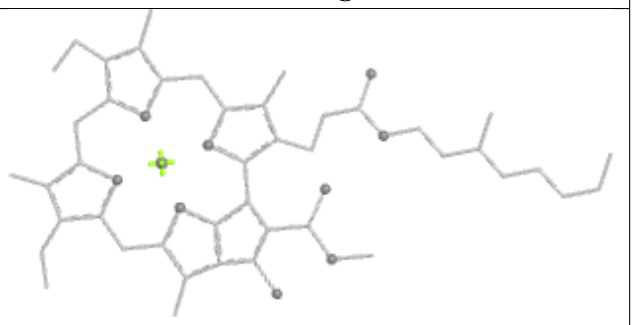
Bond lengths



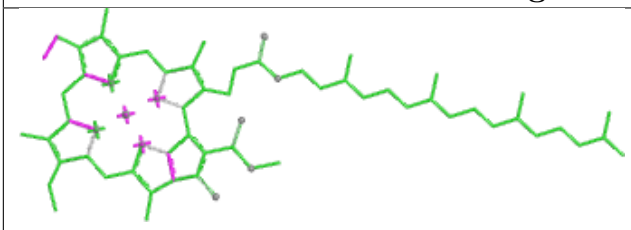
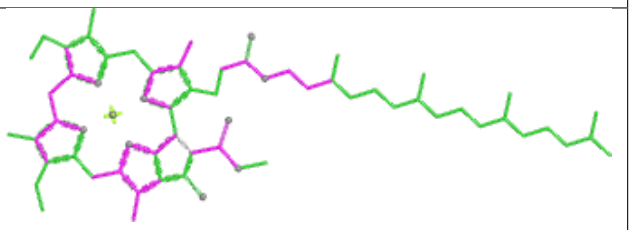
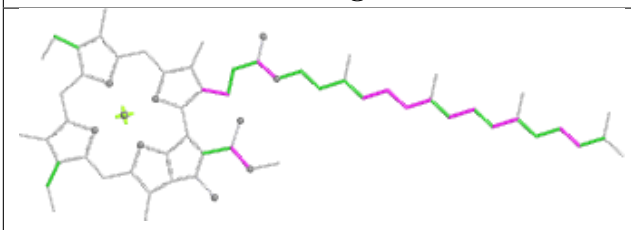
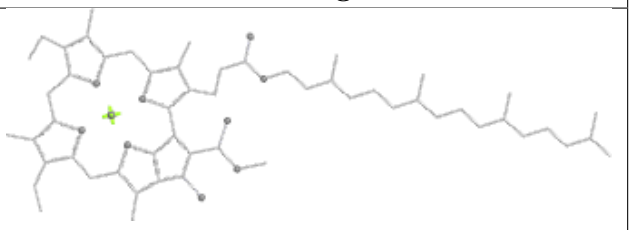
Bond angles

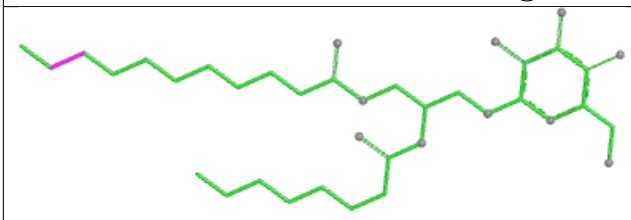
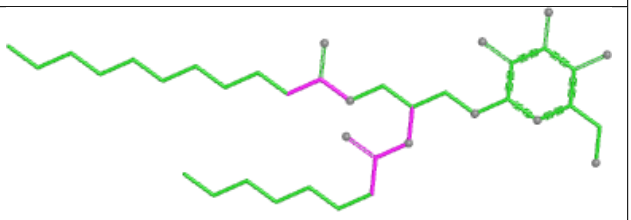
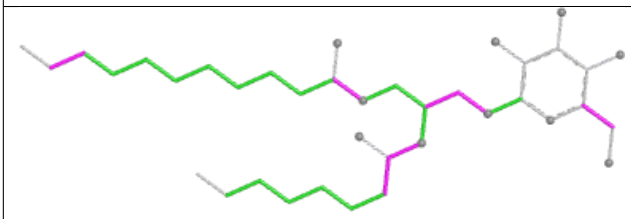
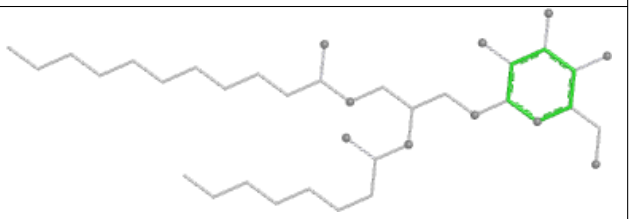


Torsions

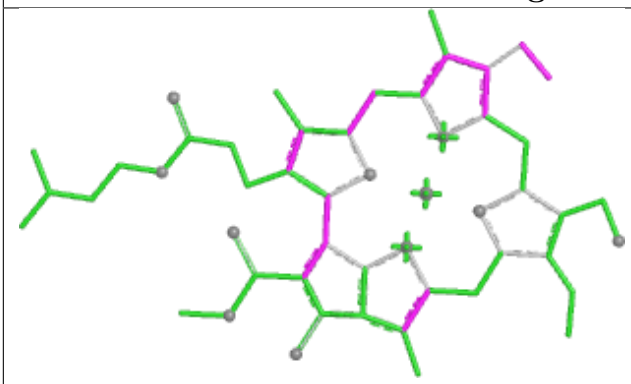


Rings

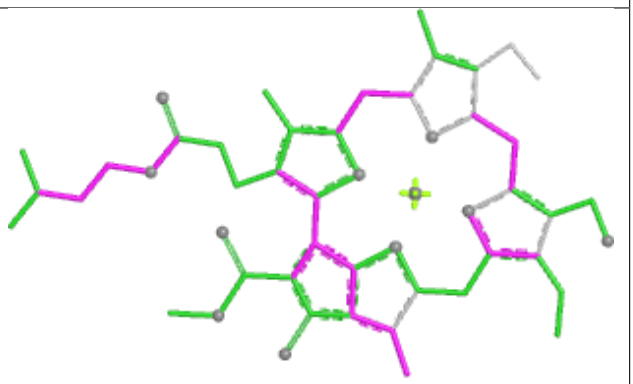
Ligand CLA 6 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG G 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

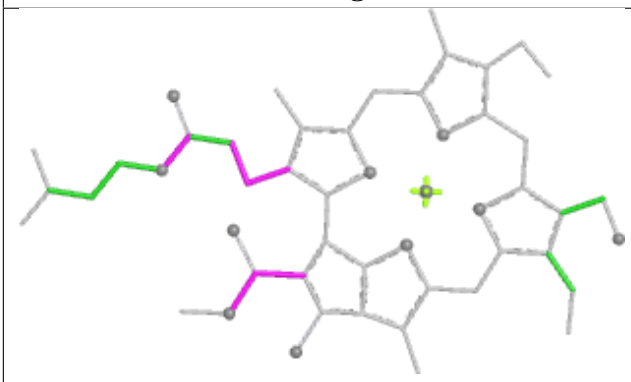
Ligand CHL 5 607



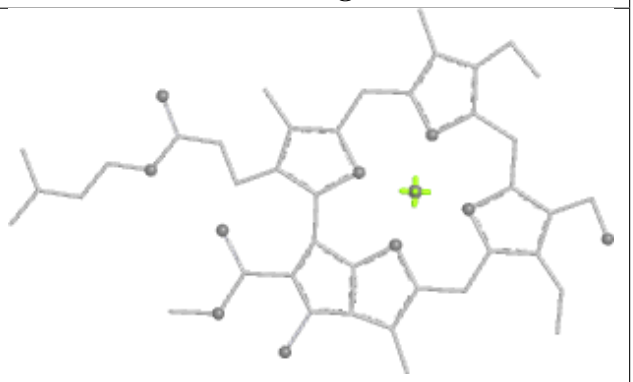
Bond lengths



Bond angles

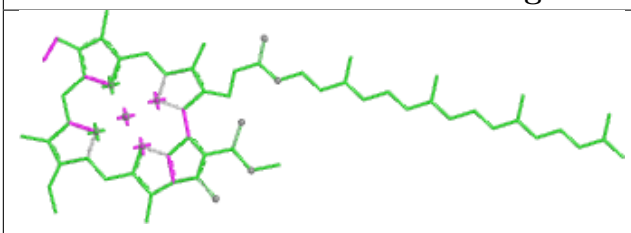


Torsions

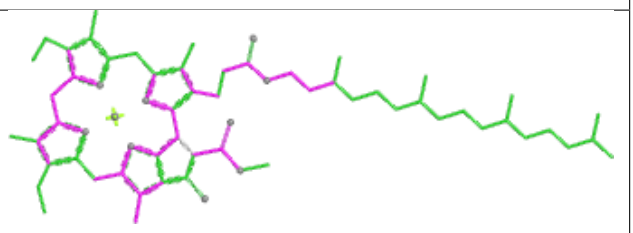


Rings

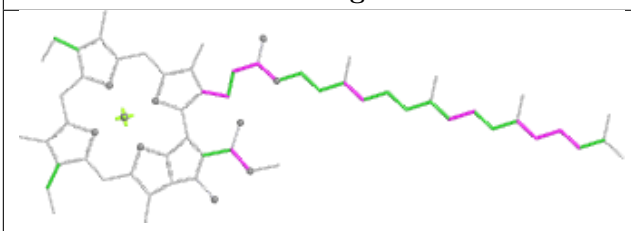
Ligand CLA C 610



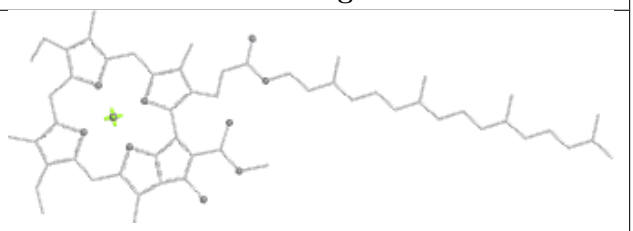
Bond lengths



Bond angles

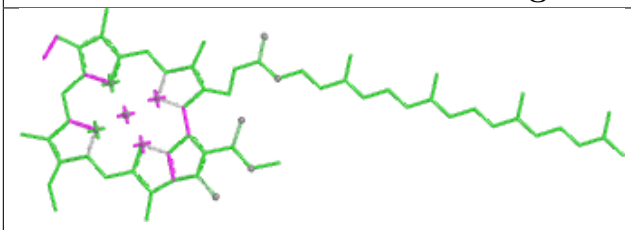


Torsions

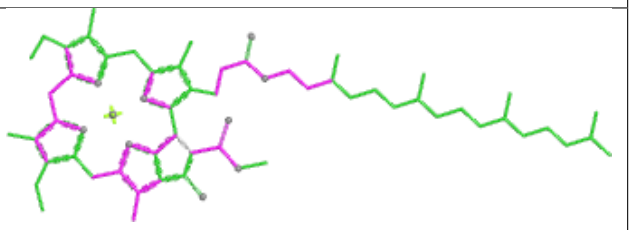


Rings

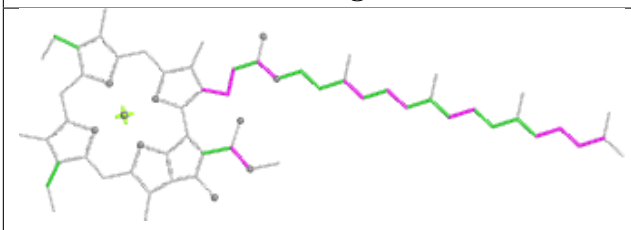
Ligand CLA c 610



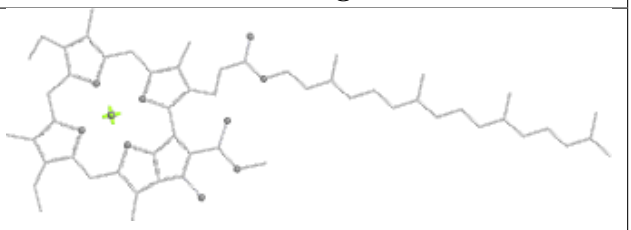
Bond lengths



Bond angles

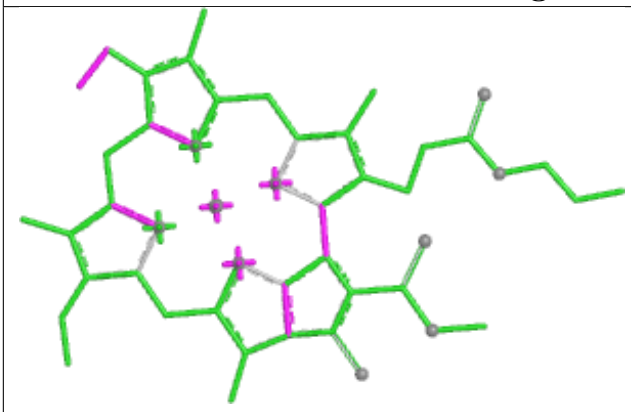


Torsions

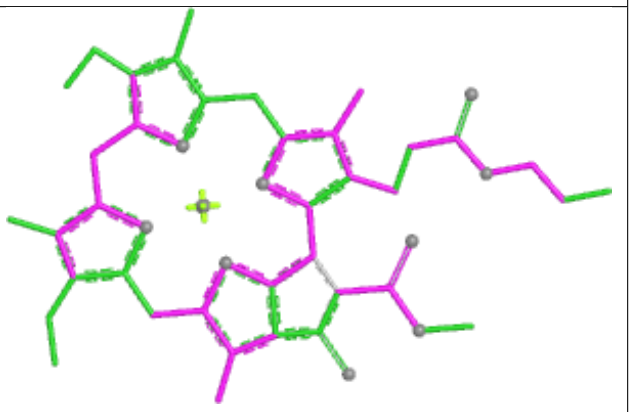


Rings

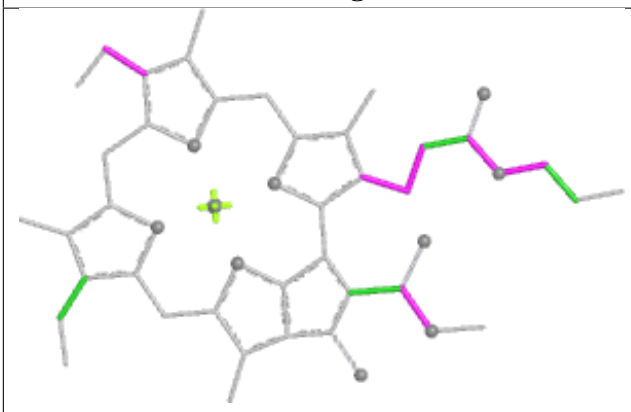
Ligand CLA r 307



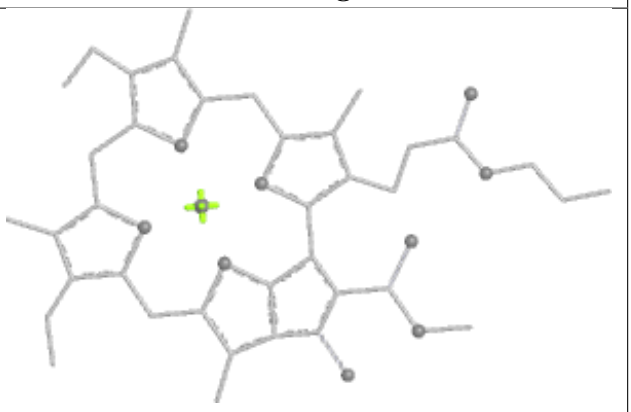
Bond lengths



Bond angles

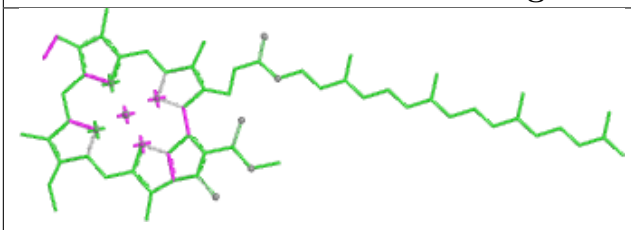


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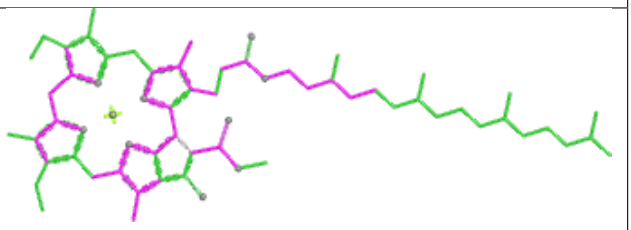


Rings

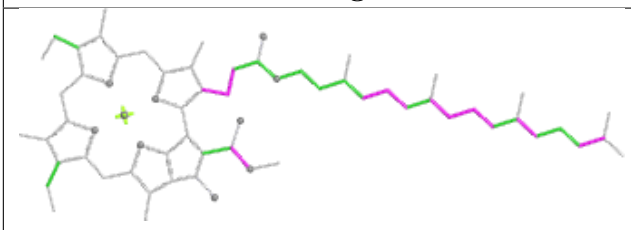
Ligand CLA S 311



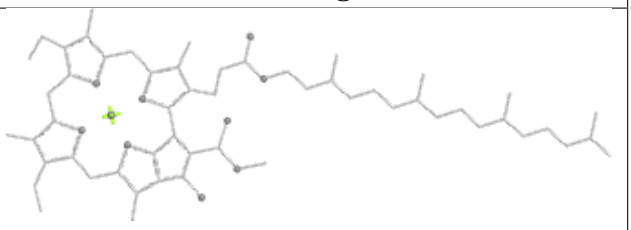
Bond lengths



Bond angles

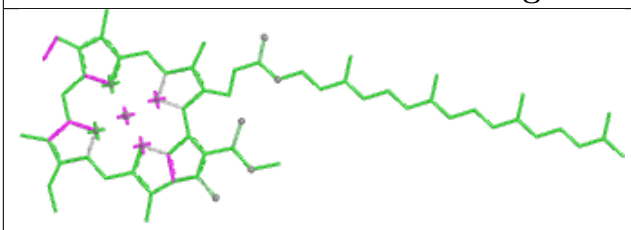


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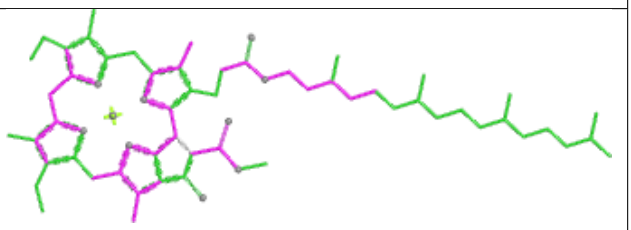


Rings

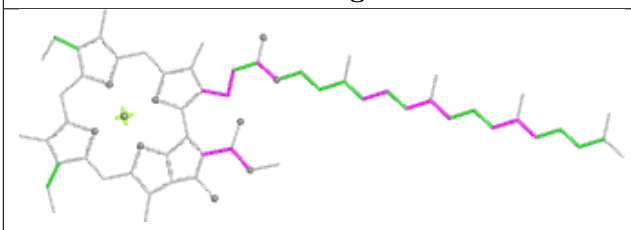
Ligand CLA G 602



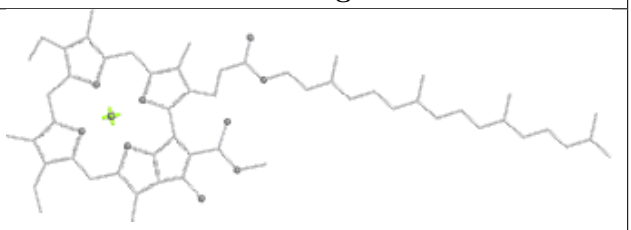
Bond lengths



Bond angles

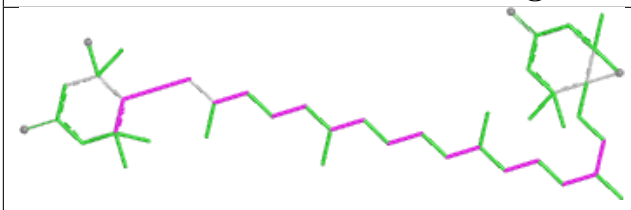


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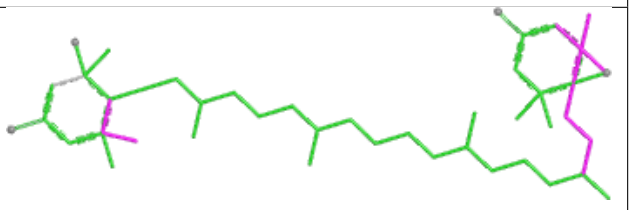


Rings

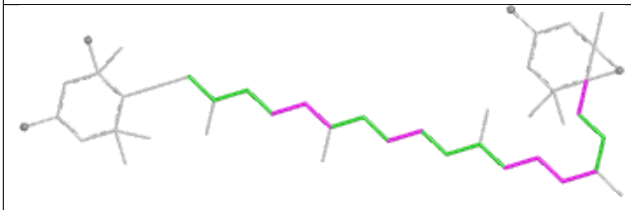
Ligand NEX 5 618



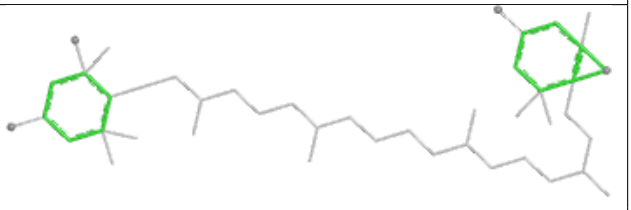
Bond lengths



Bond angles

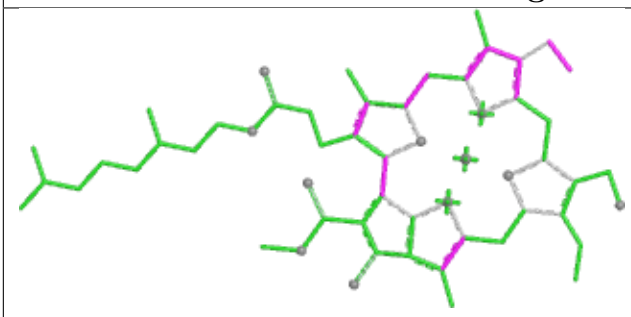


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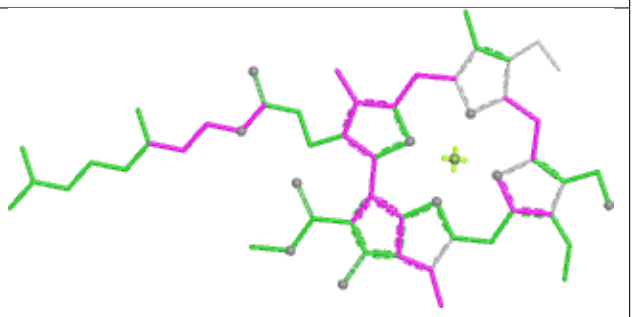


Rings

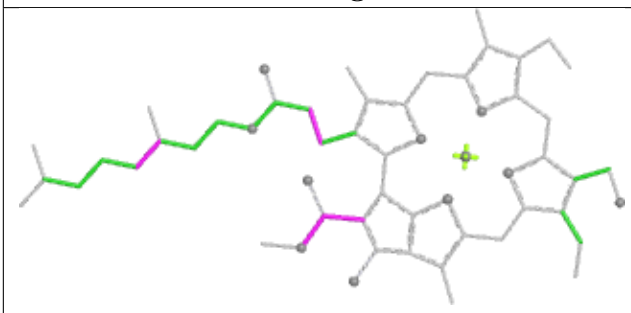
Ligand CHL 8 601



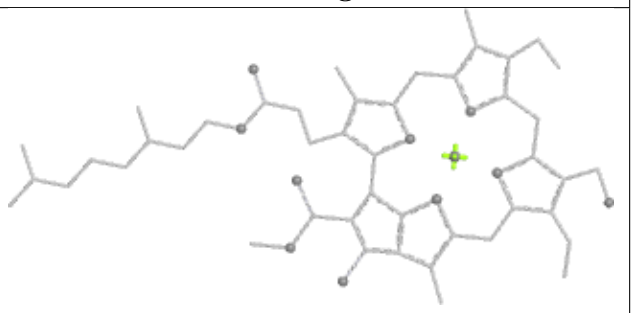
Bond lengths



Bond angles

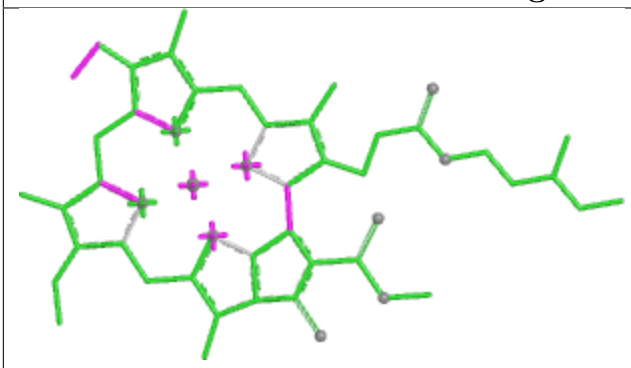


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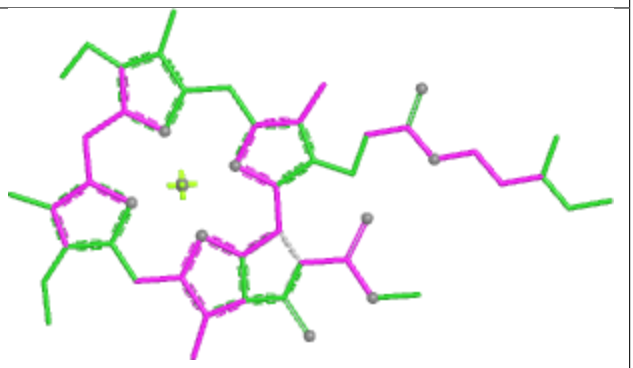


Rings

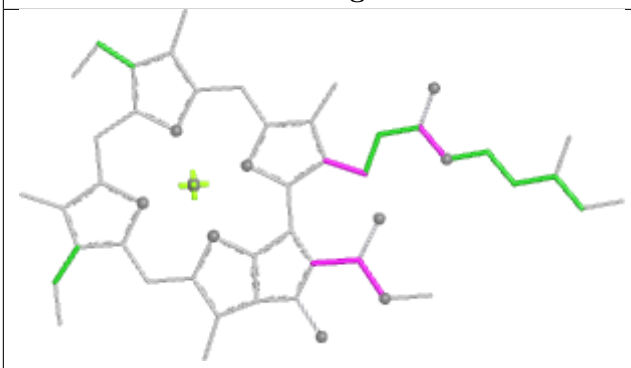
Ligand CLA 5 614



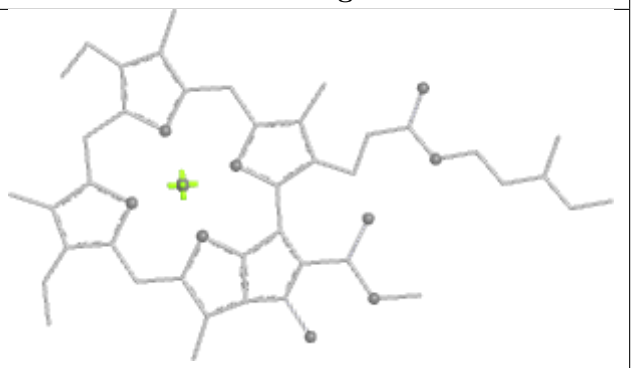
Bond lengths



Bond angles

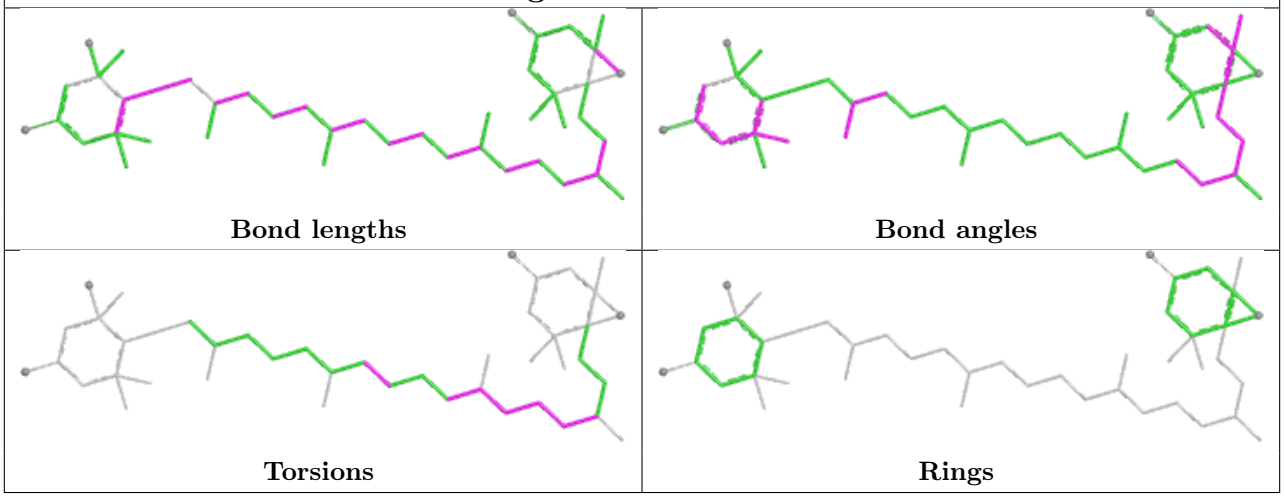


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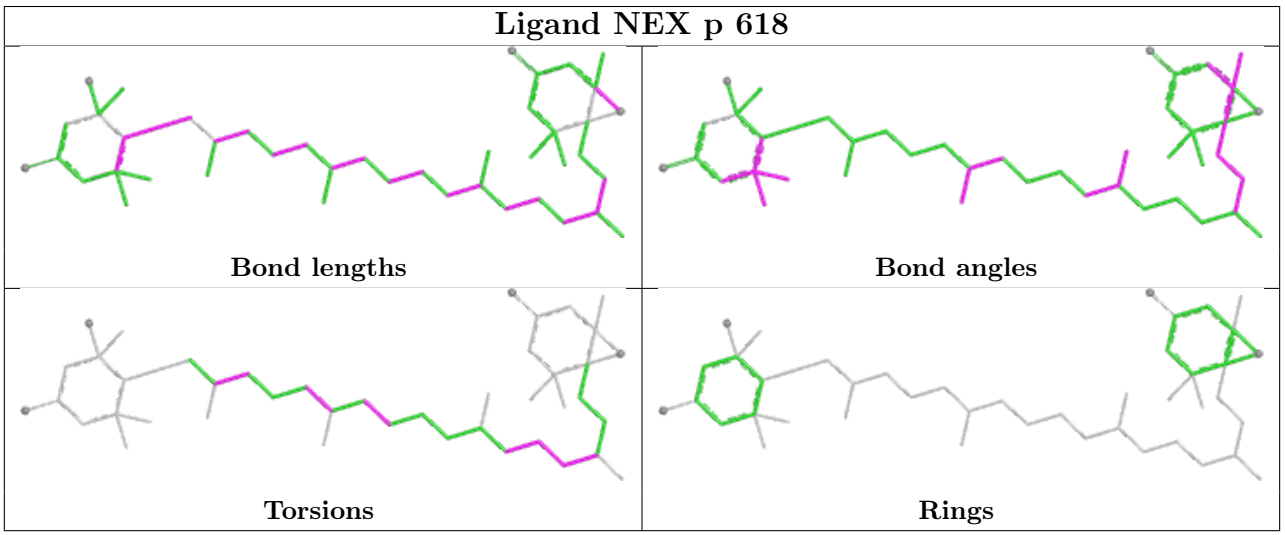


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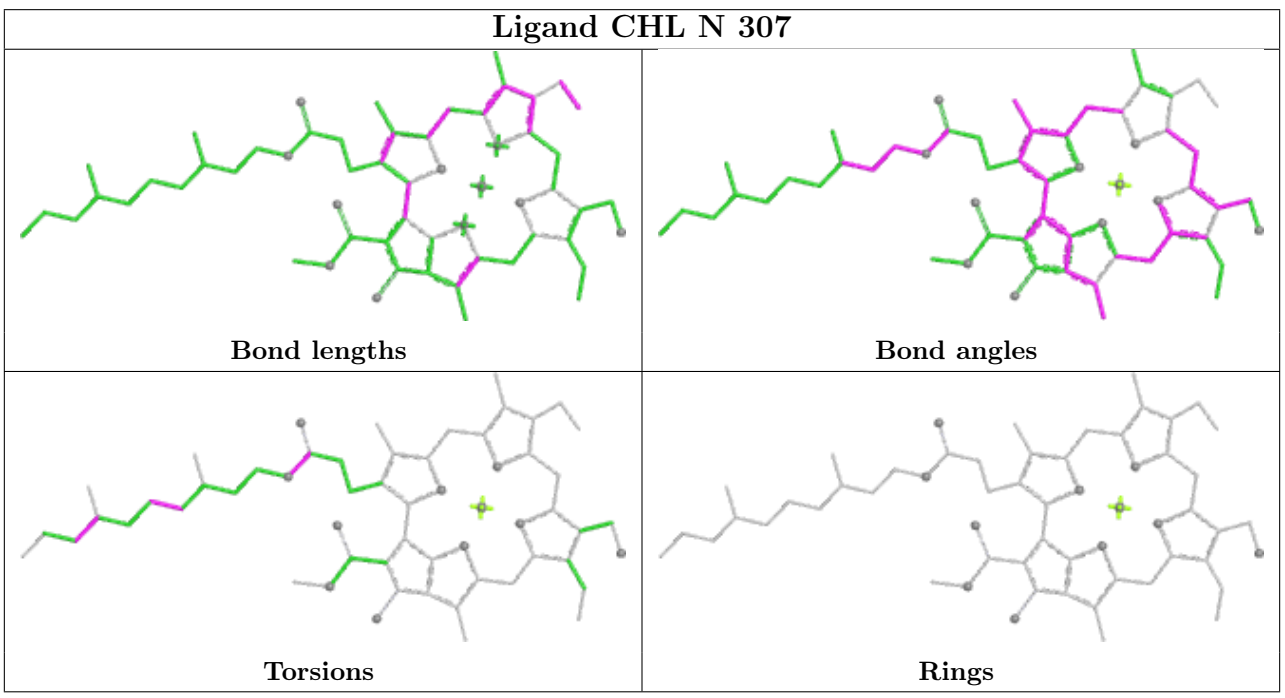
Ligand NEX 6 319



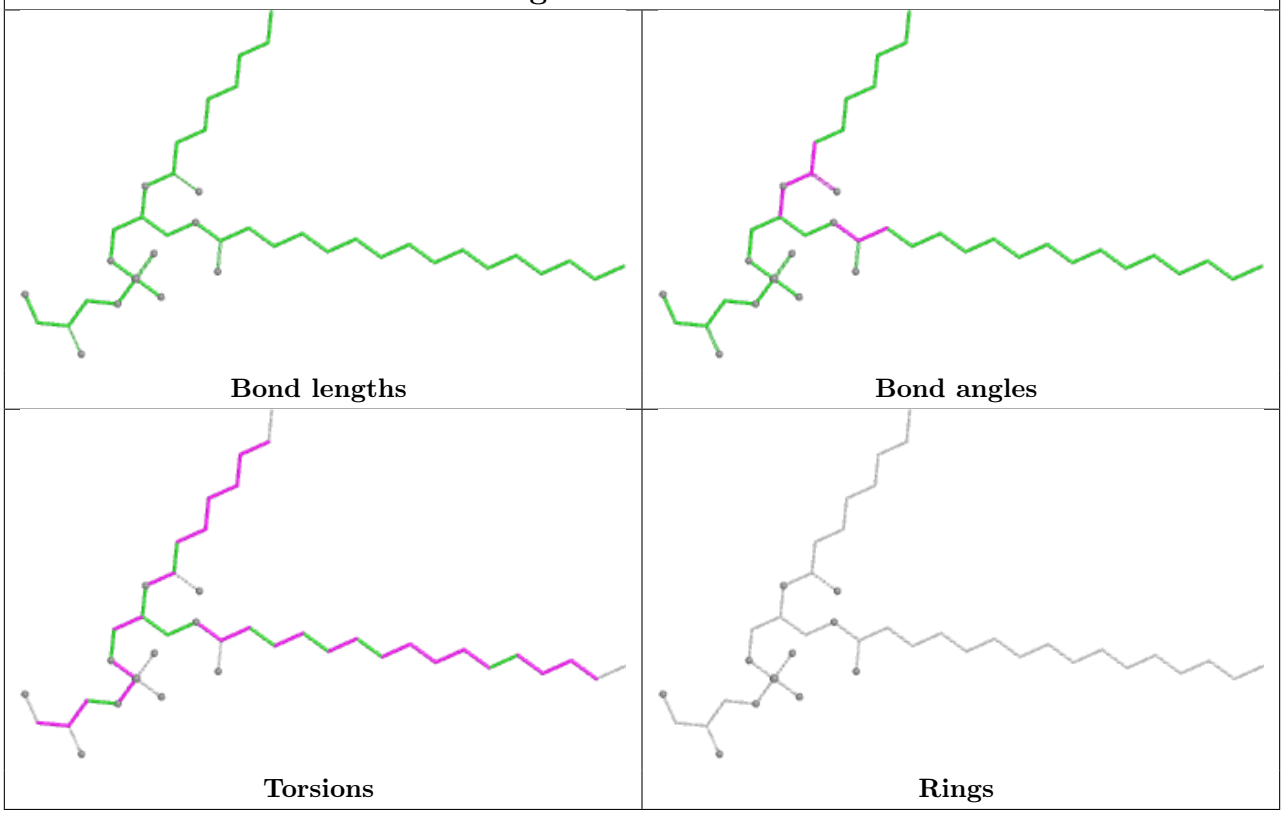
Ligand NEX p 618



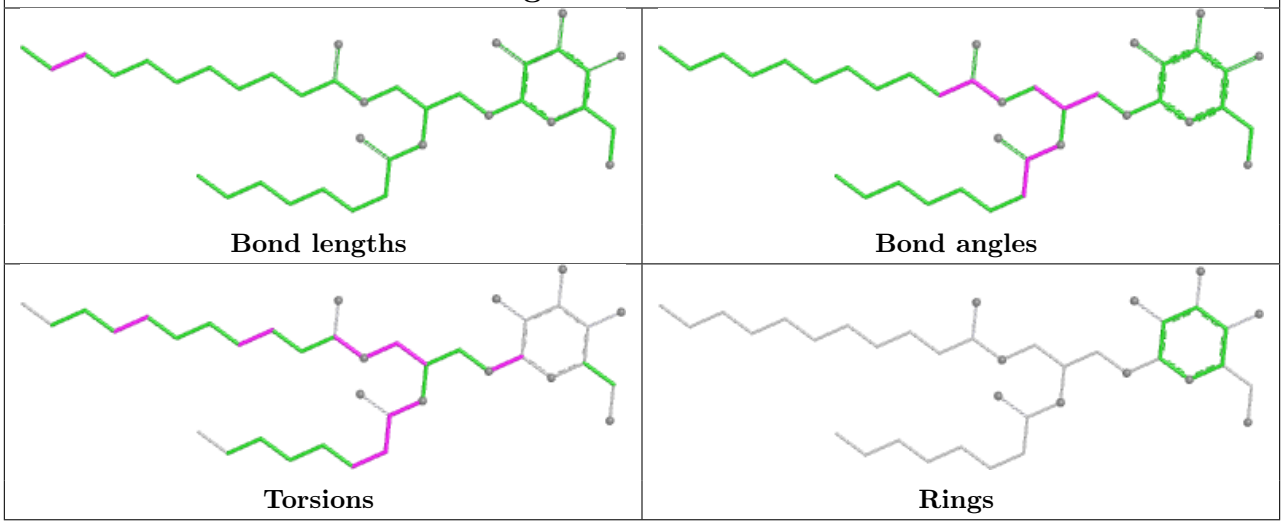
Ligand CHL N 307



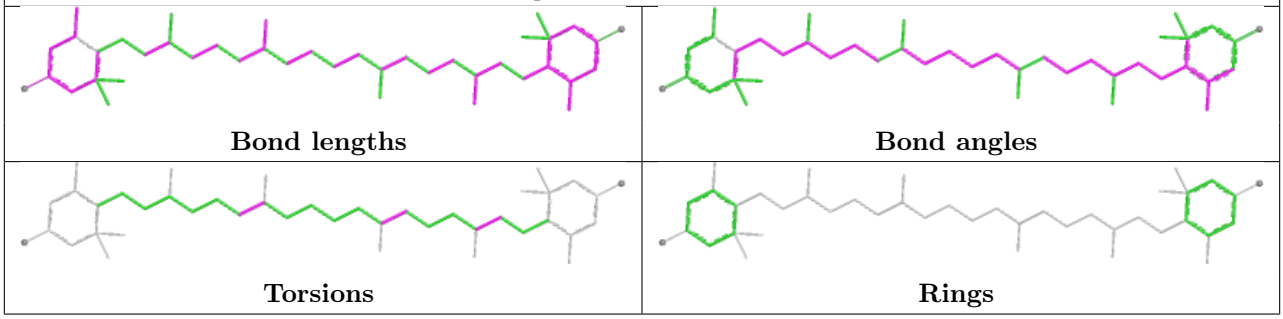
Ligand LHG t 102



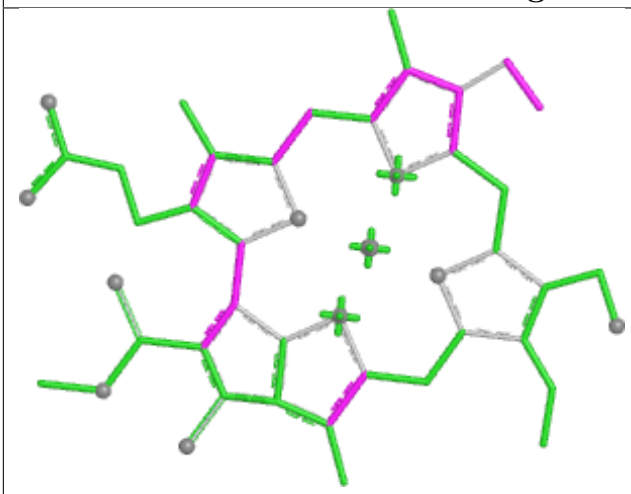
Ligand LMG b 629



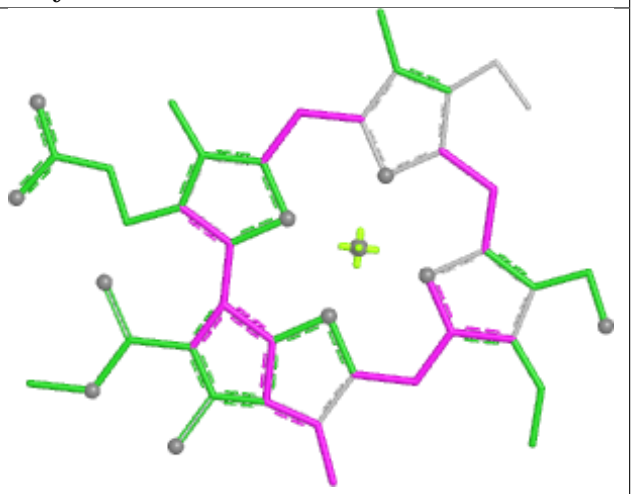
Ligand LUT n 318



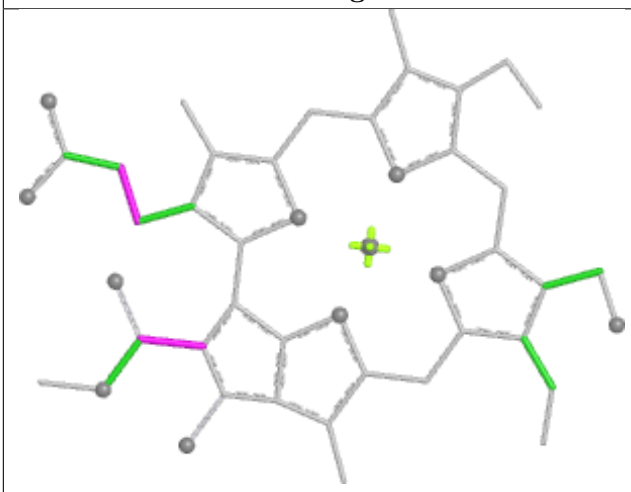
Ligand CHL y 605



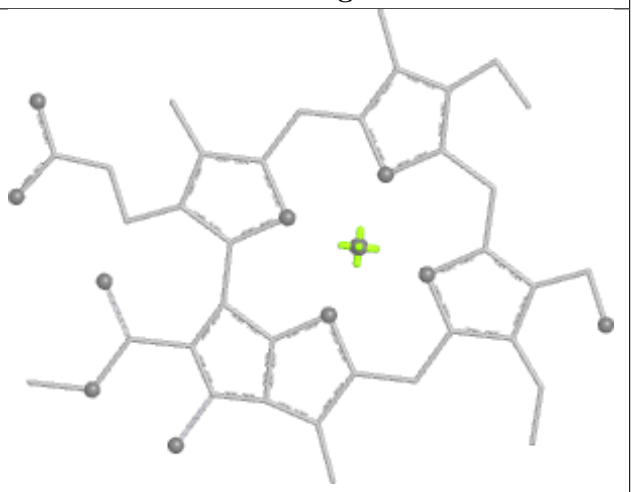
Bond lengths



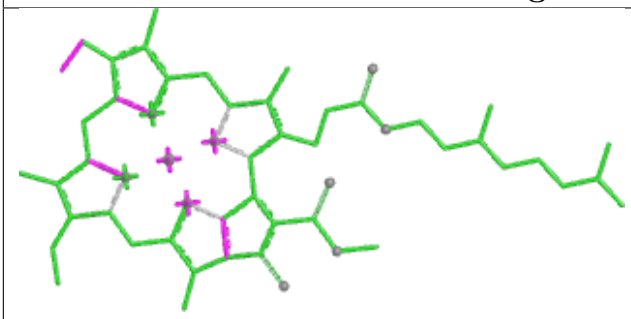
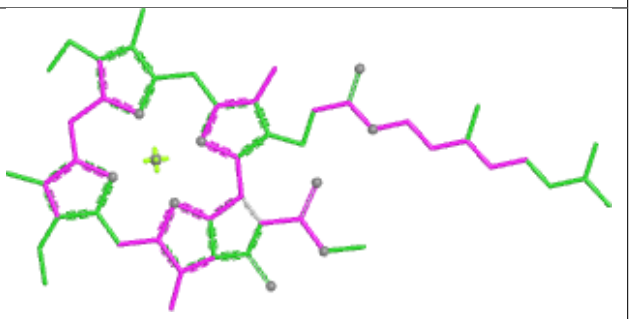
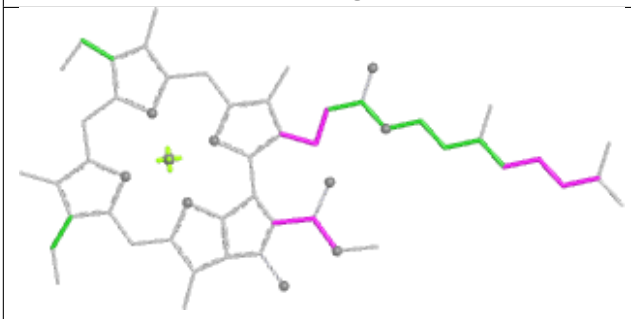
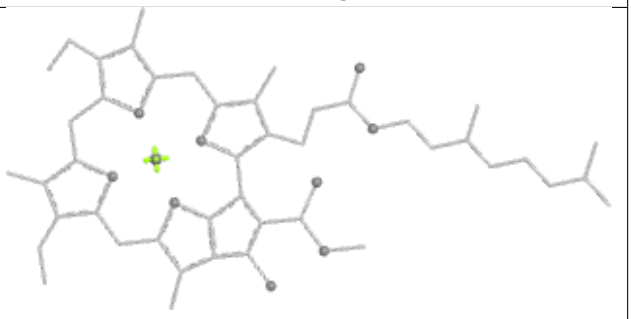
Bond angles

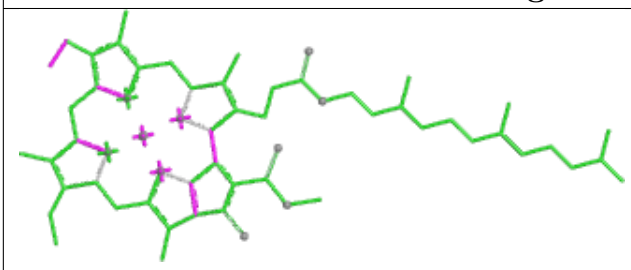
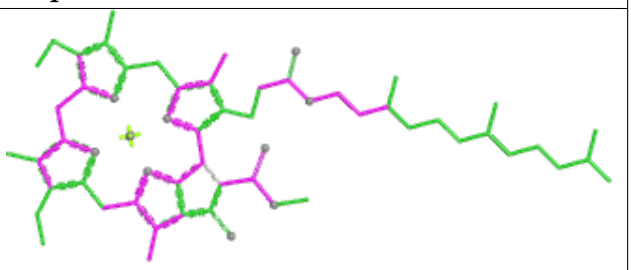
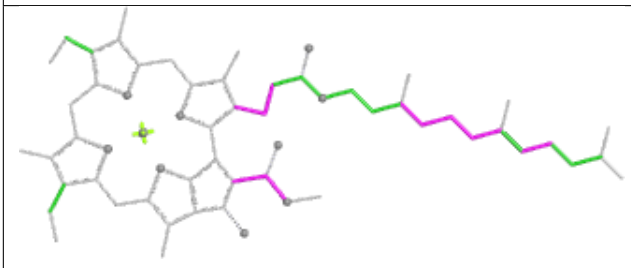
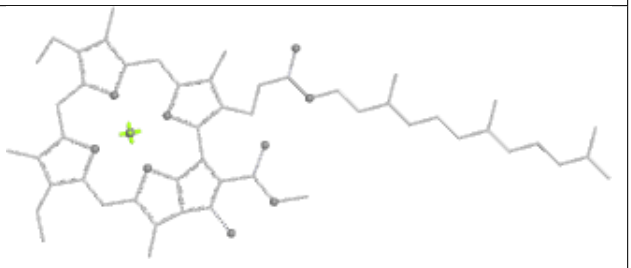


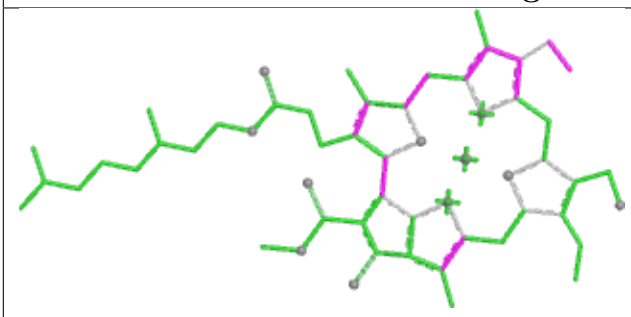
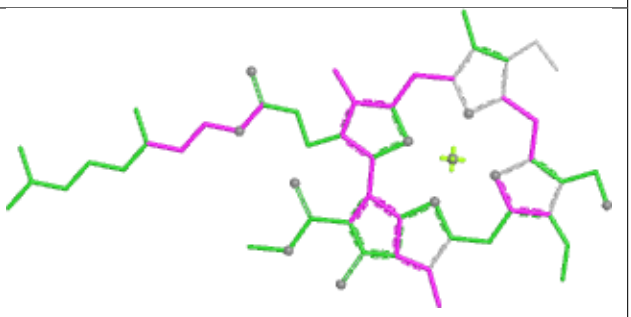
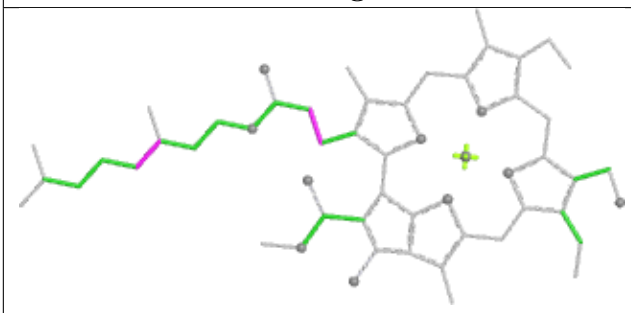
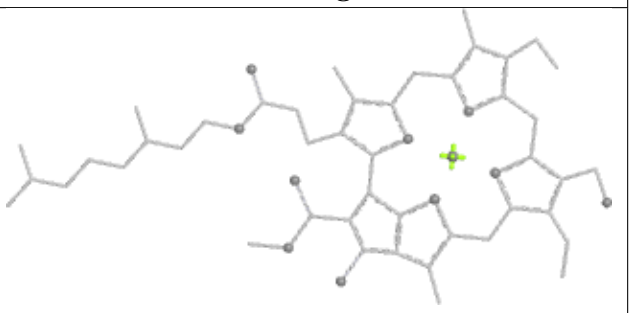
Torsions

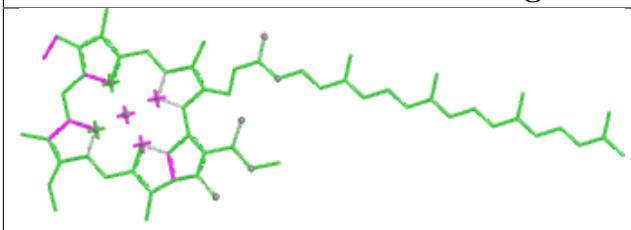
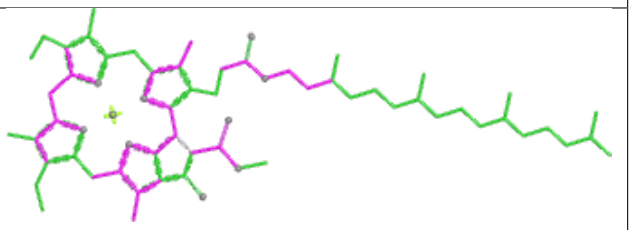
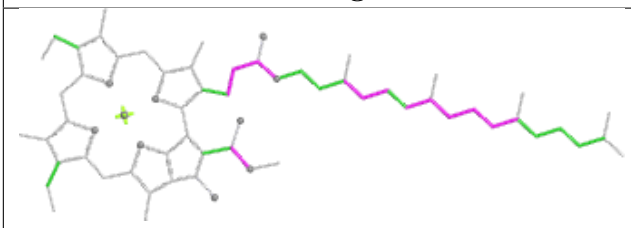
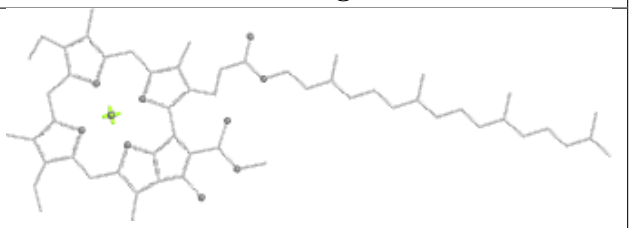


Rings

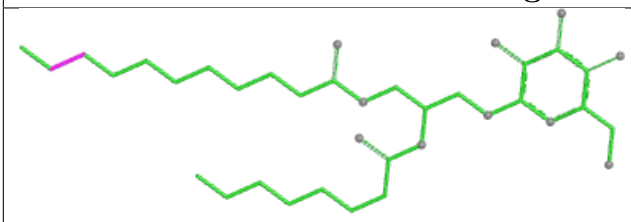
Ligand CLA 3 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA p 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

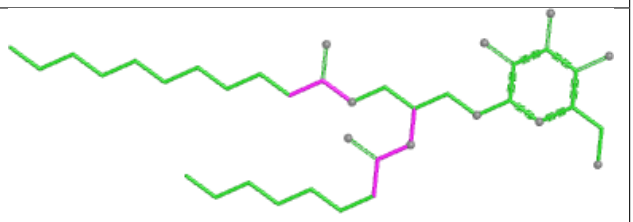
Ligand CHL N 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

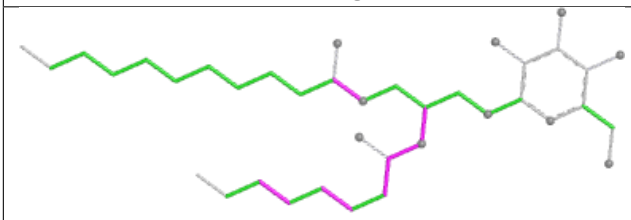
Ligand LMG 1 618



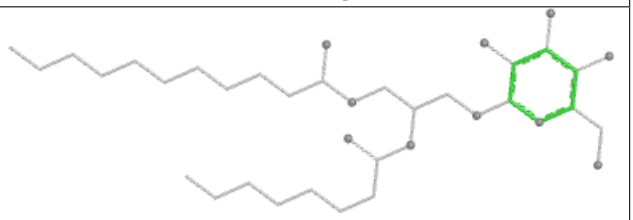
Bond lengths



Bond angles

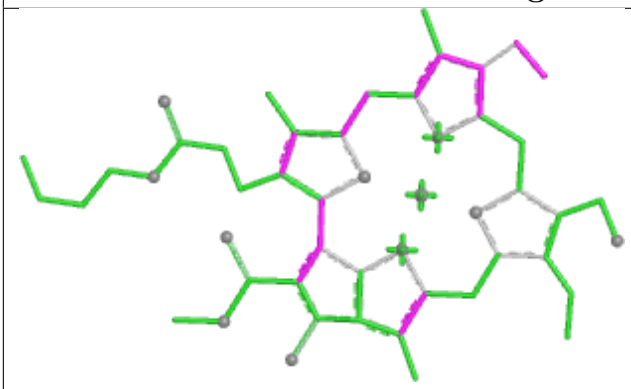


Torsions

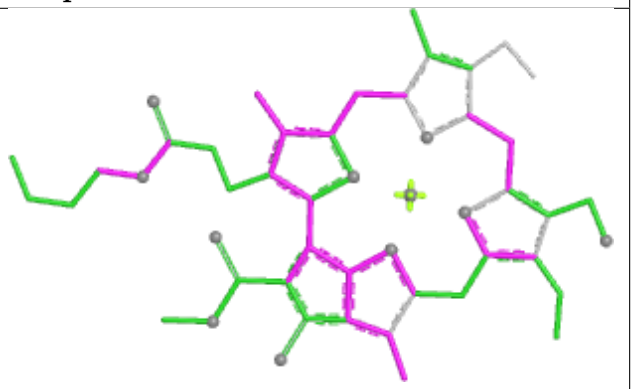


Rings

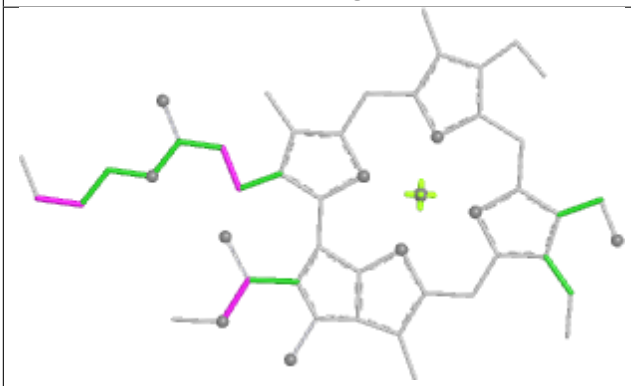
Ligand CHL q 310



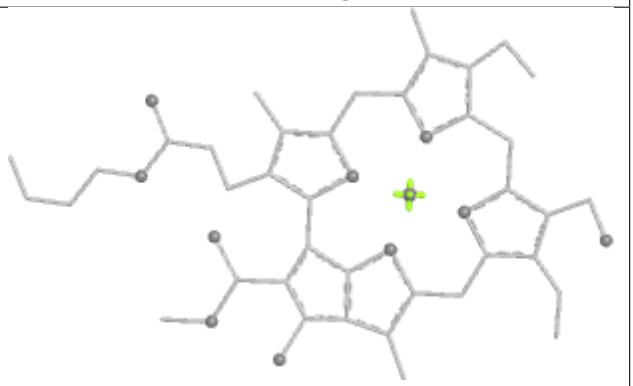
Bond lengths



Bond angles

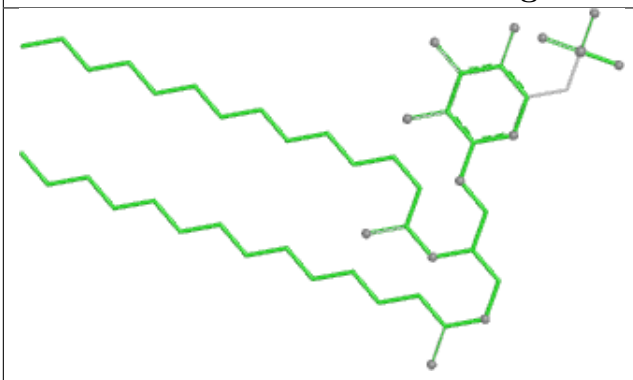


Torsions

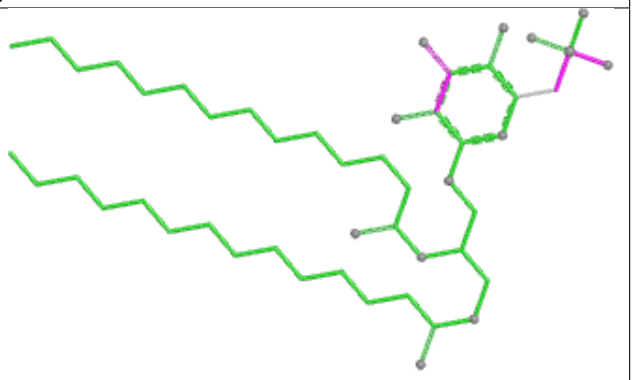


Rings

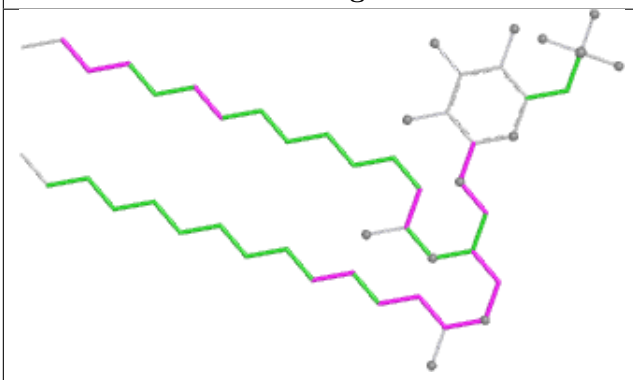
Ligand SQD M 102



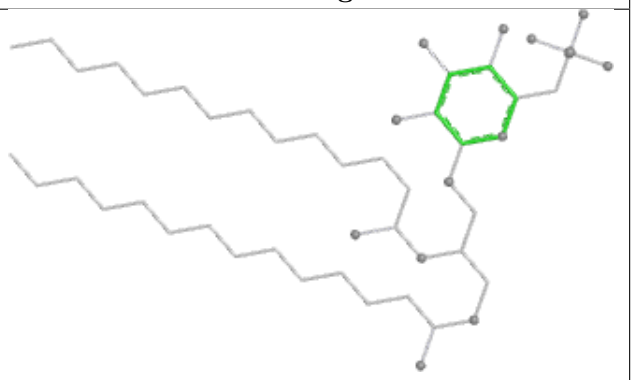
Bond lengths



Bond angles

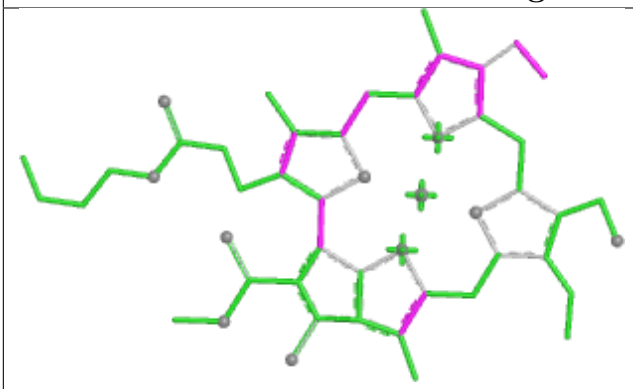


Torsions

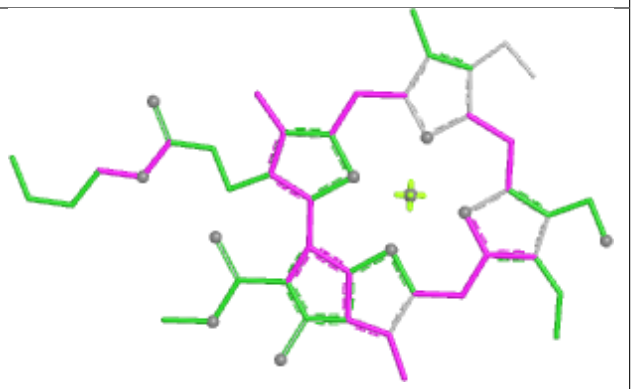


Rings

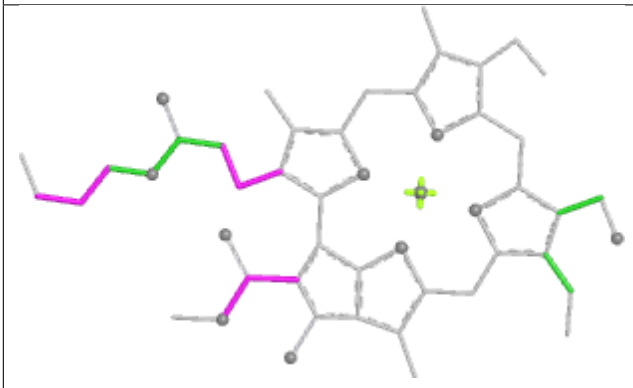
Ligand CHL 9 310



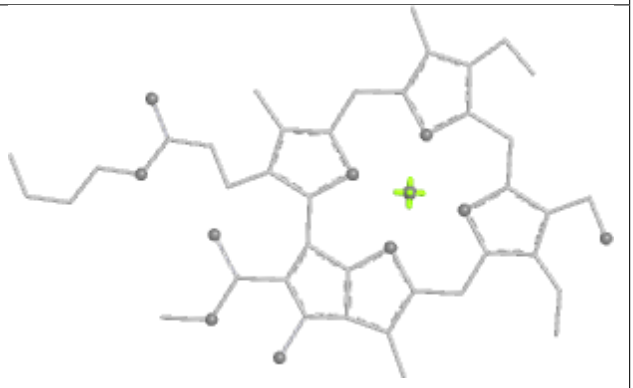
Bond lengths



Bond angles

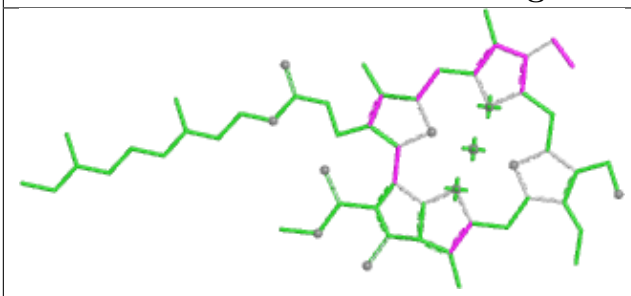


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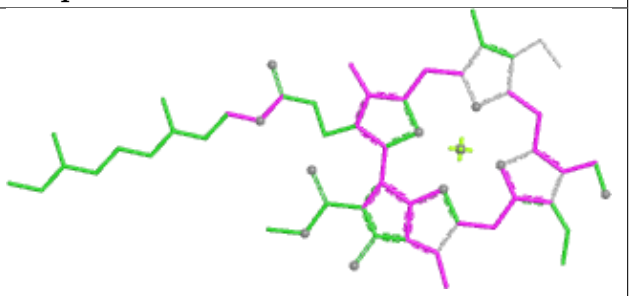


Rings

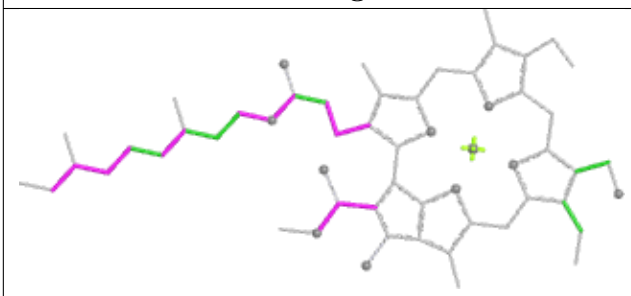
Ligand CHL q 309



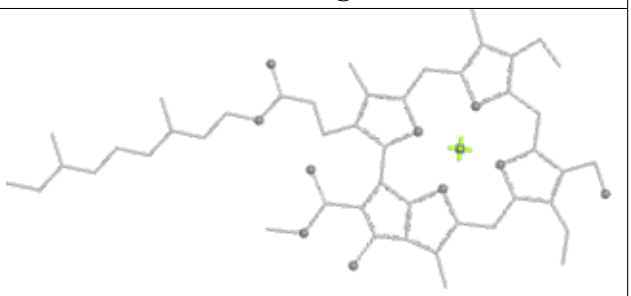
Bond lengths



Bond angles

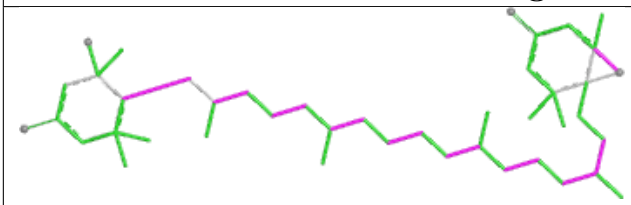


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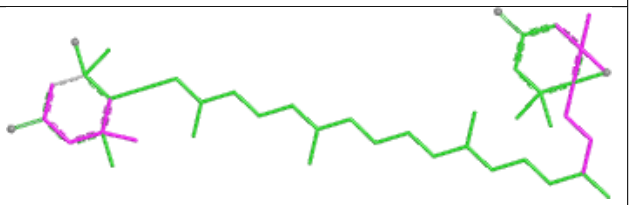


Rings

Ligand NEX s 319



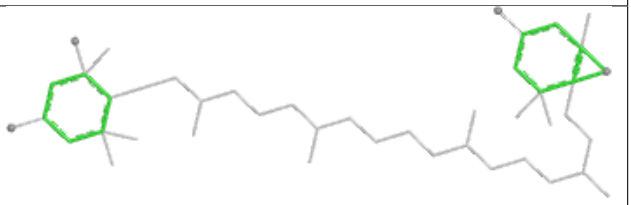
Bond lengths



Bond angles

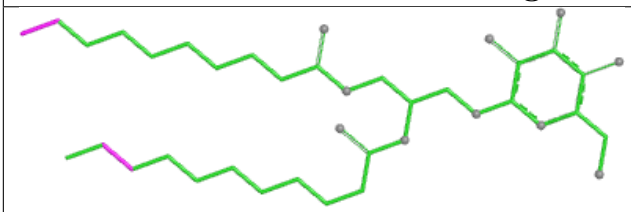


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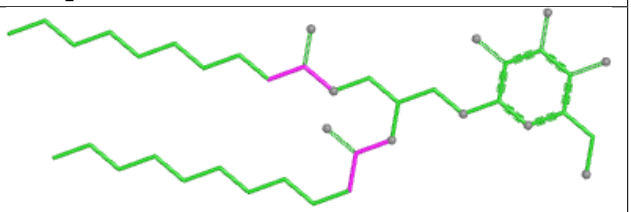


Rings

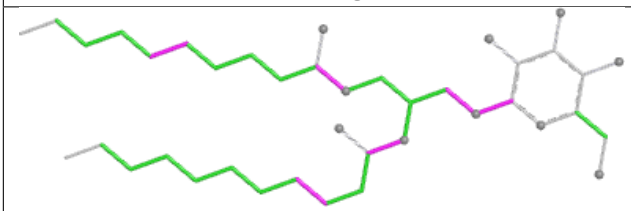
Ligand LMG q 302



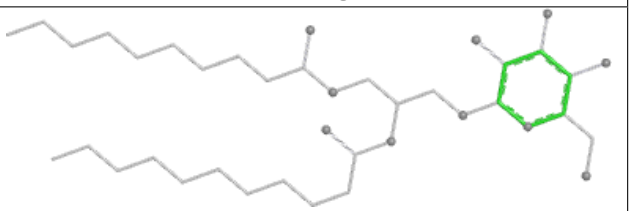
Bond lengths



Bond angles

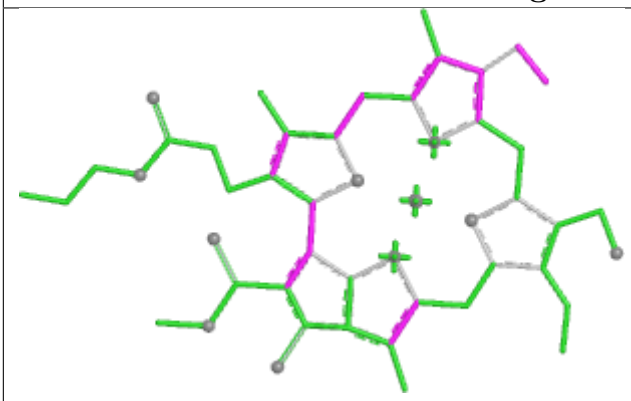


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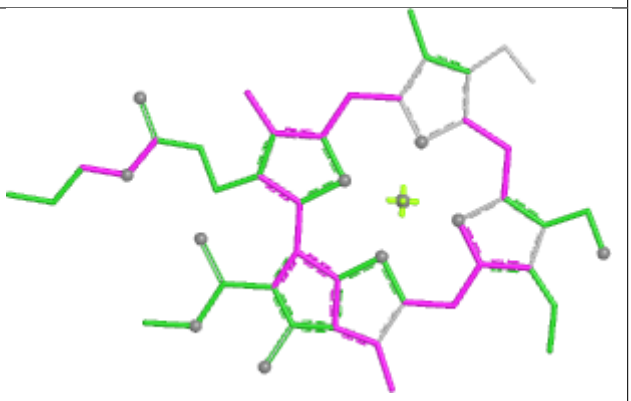


Rings

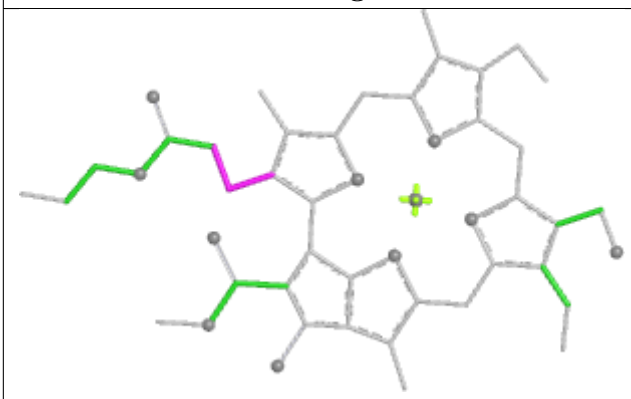
Ligand CHL s 309



Bond lengths



Bond angles

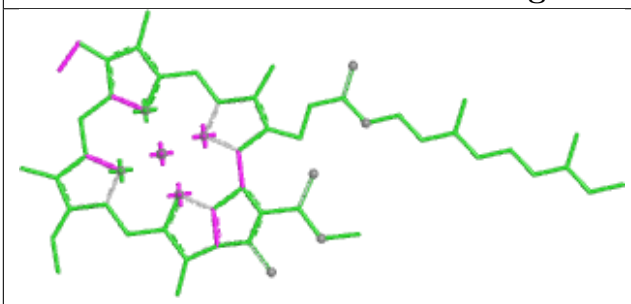


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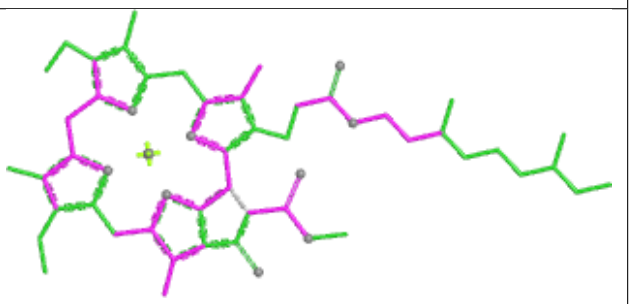


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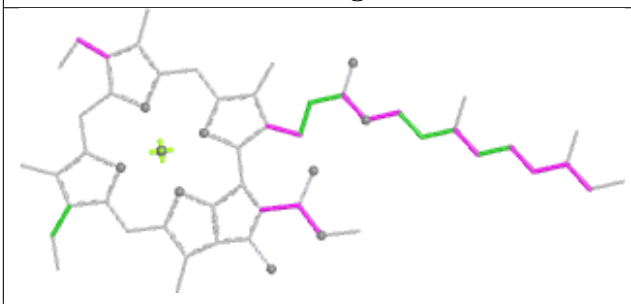
Ligand CLA 0 603



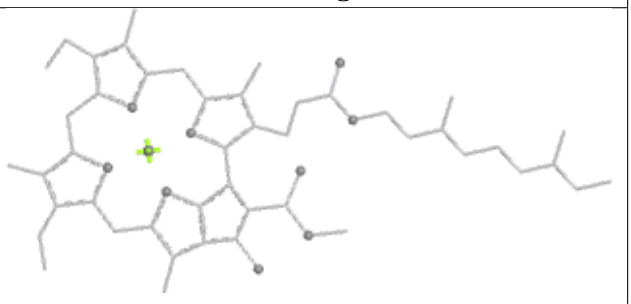
Bond lengths



Bond angles

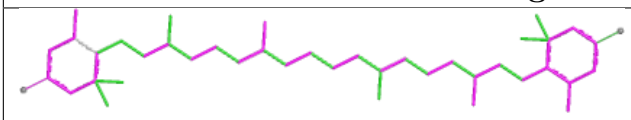


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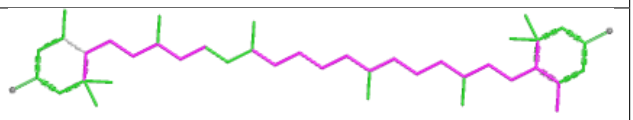


Rings

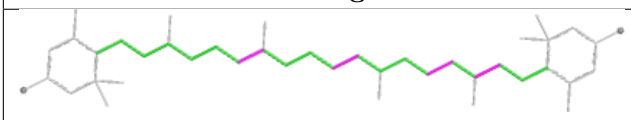
Ligand LUT 4 616



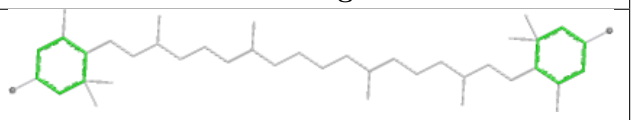
Bond lengths



Bond angles

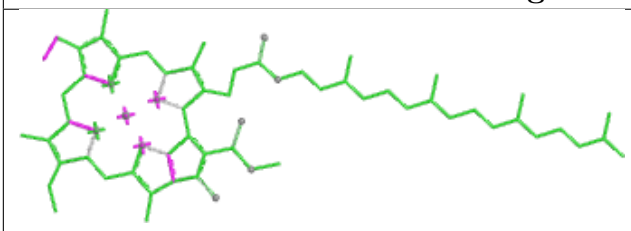


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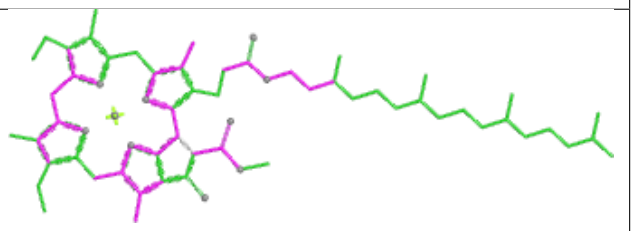


Rings

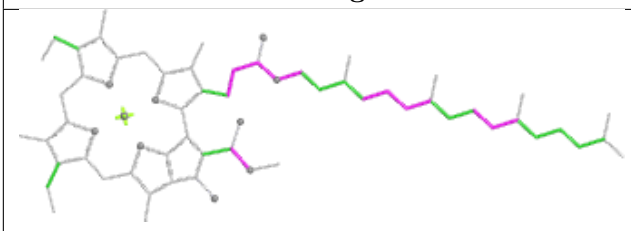
Ligand CLA b 617



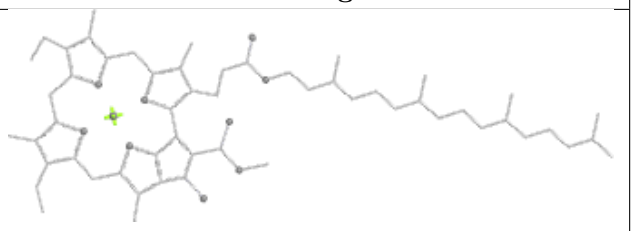
Bond lengths



Bond angles

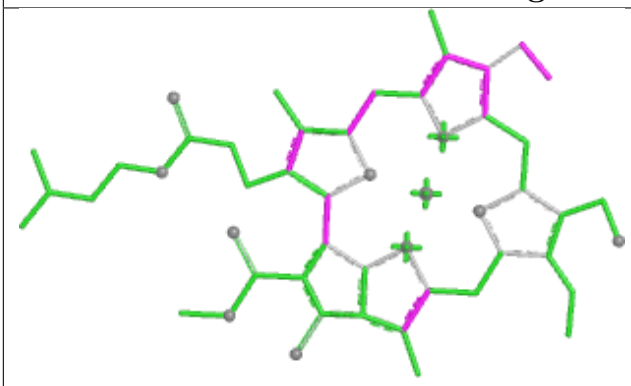


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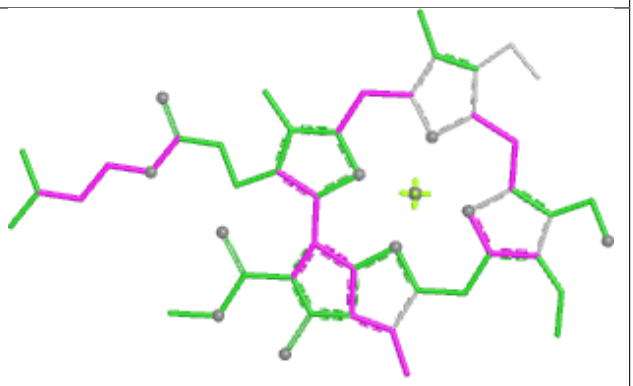


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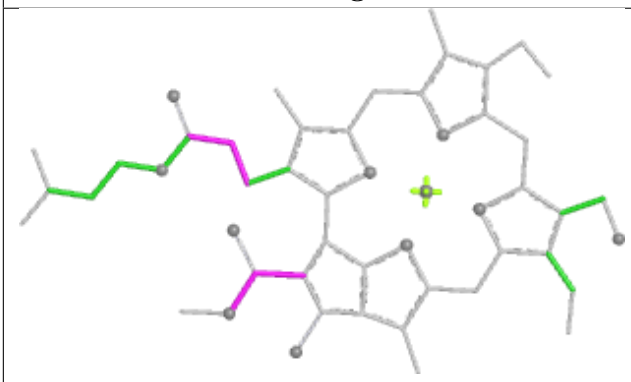
Ligand CHL 5 601



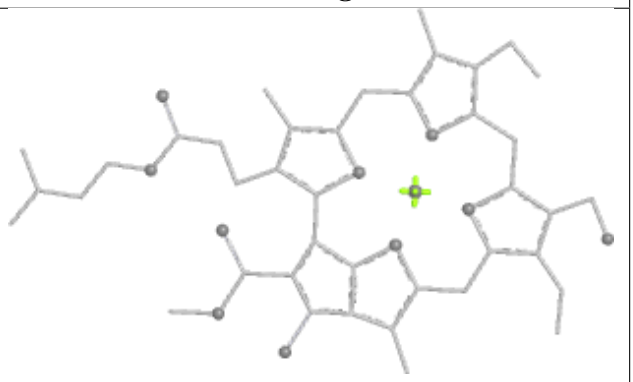
Bond lengths



Bond angles

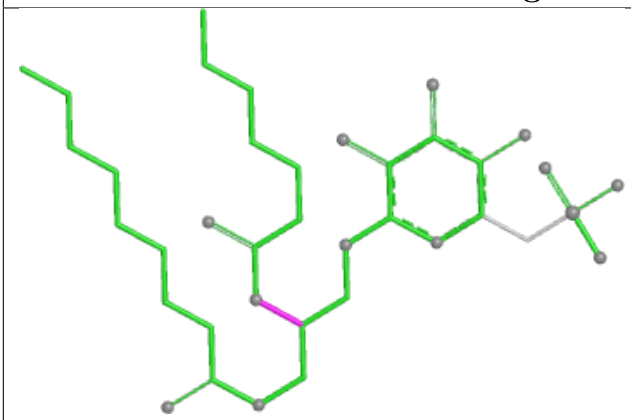


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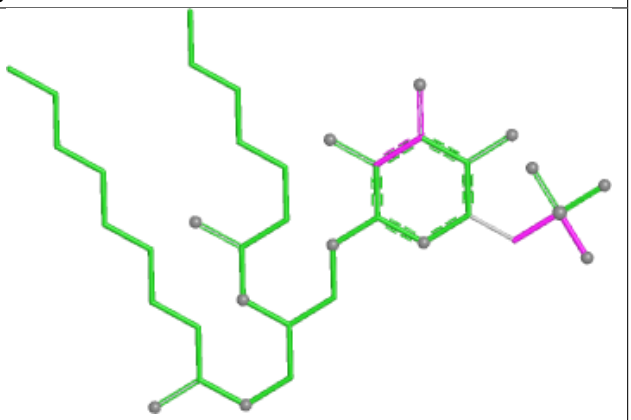


Rings

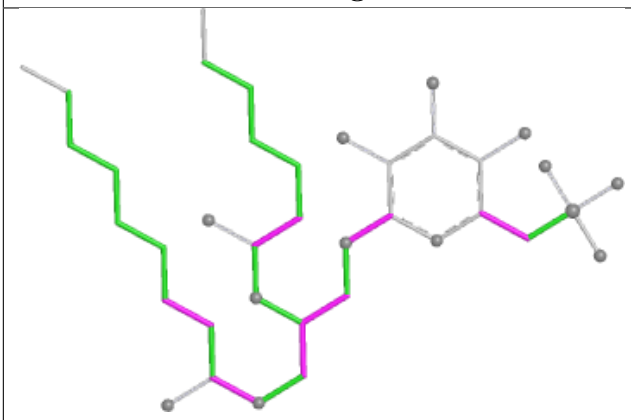
Ligand SQD G 624



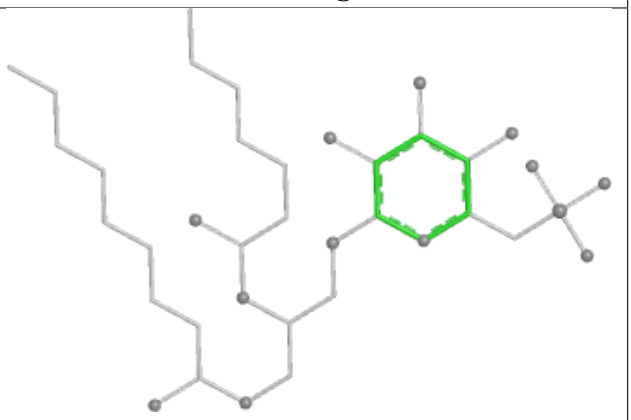
Bond lengths



Bond angles

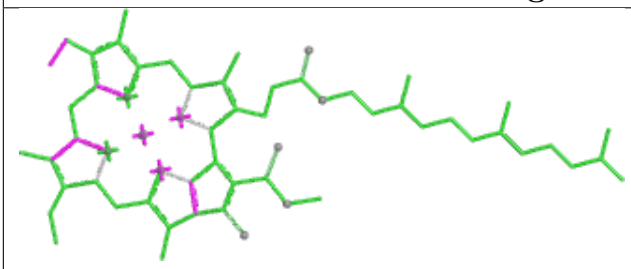


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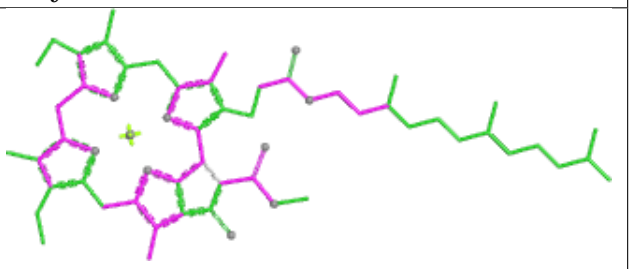


Rings

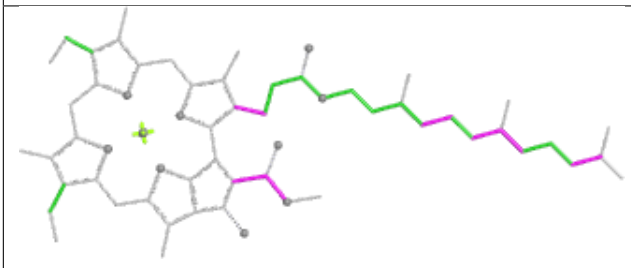
Ligand CLA y 602



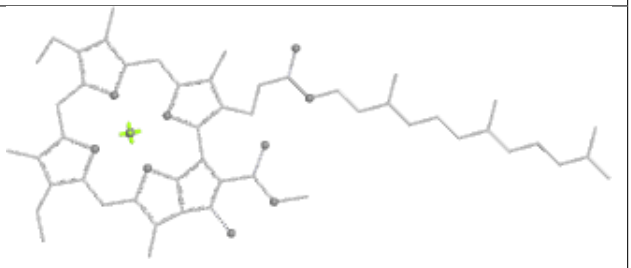
Bond lengths



Bond angles

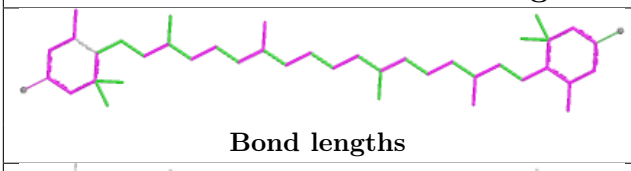


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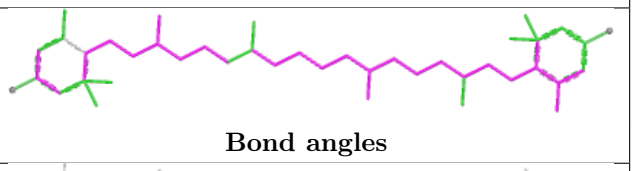


Rings

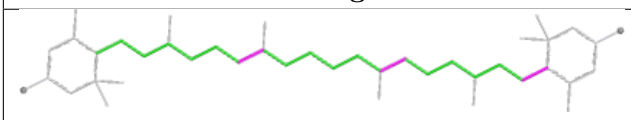
Ligand LUT s 318



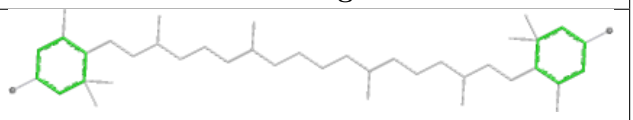
Bond lengths



Bond angles

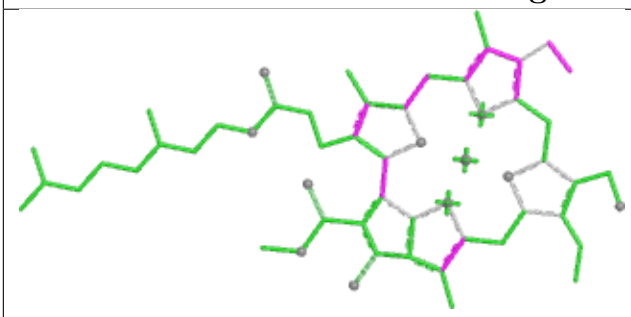


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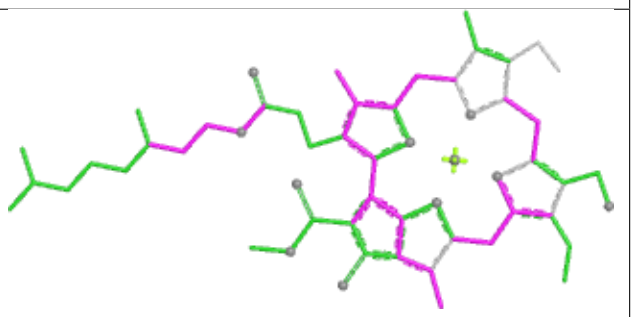


Rings

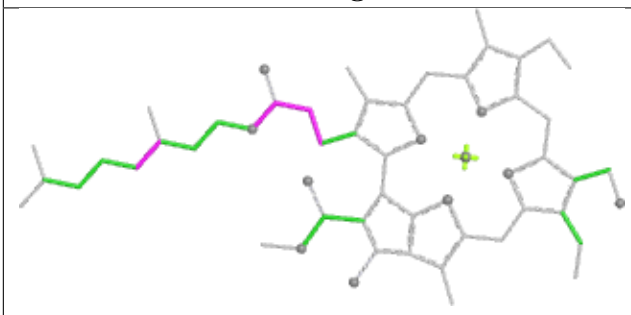
Ligand CHL r 308



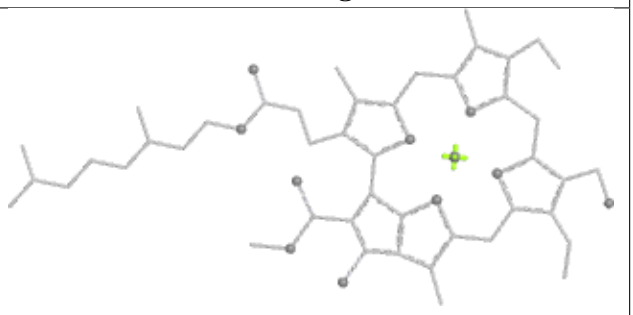
Bond lengths



Bond angles

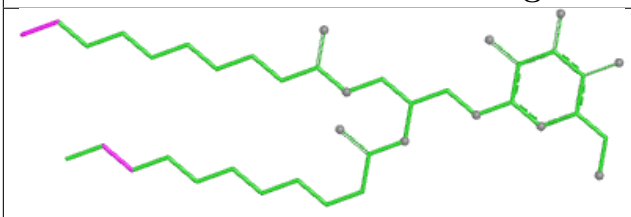


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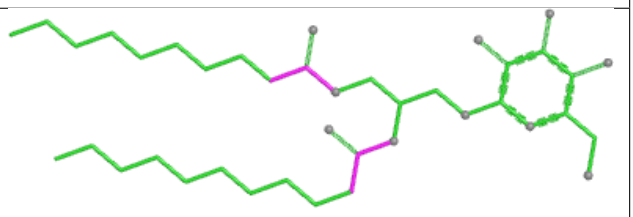


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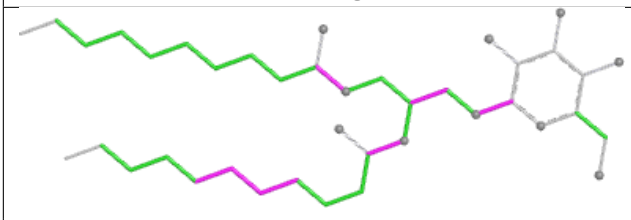
Ligand LMG 4 621



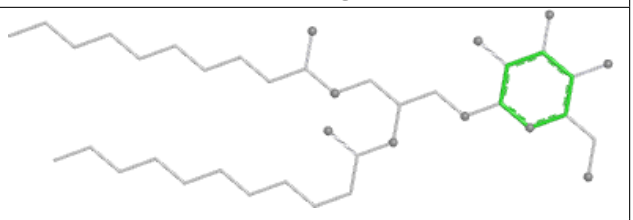
Bond lengths



Bond angles

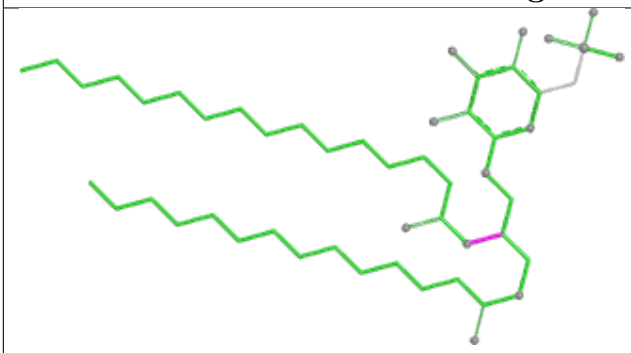


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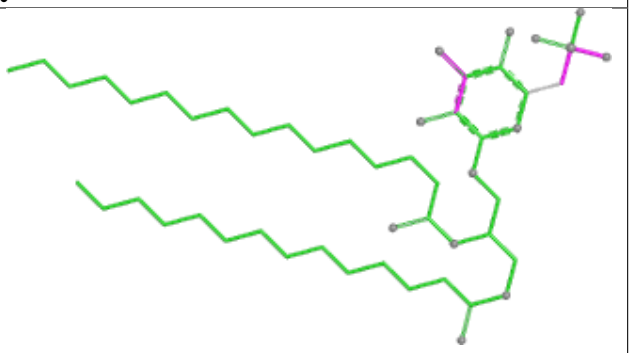


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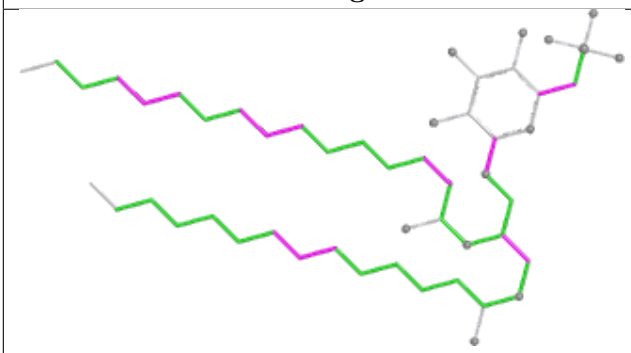
Ligand SQD b 627



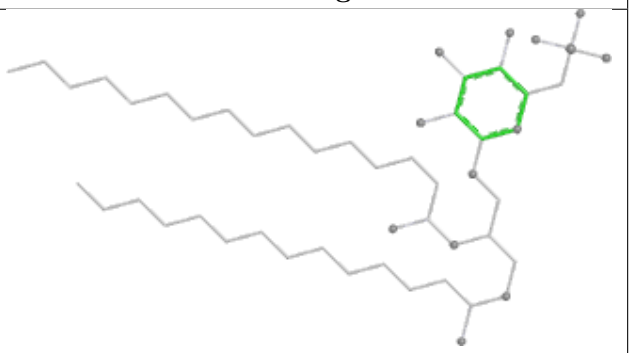
Bond lengths



Bond angles

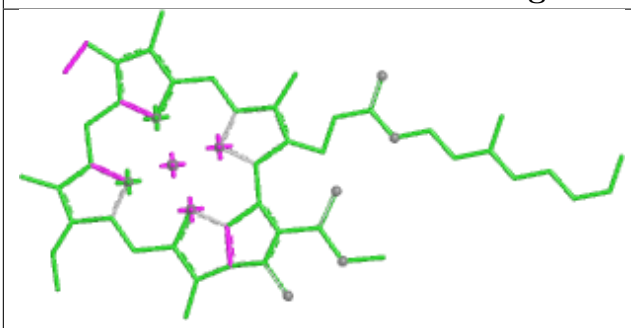


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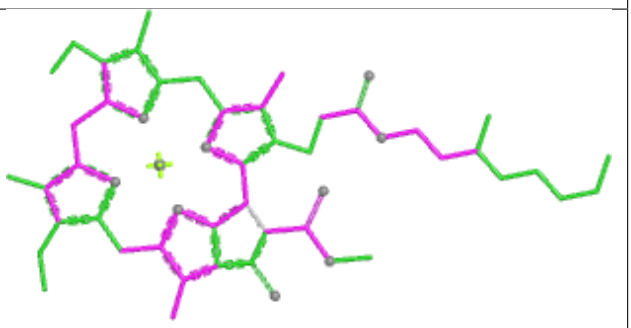


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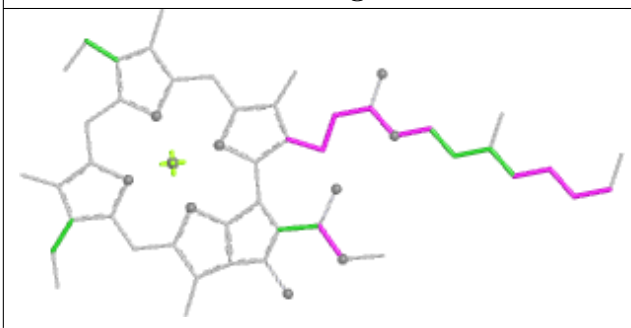
Ligand CLA 2 613



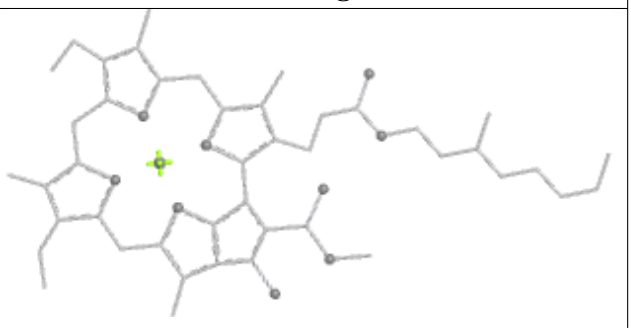
Bond lengths



Bond angles

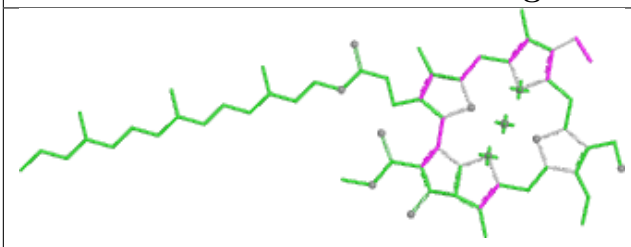


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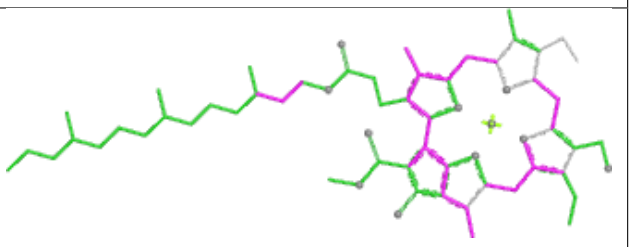


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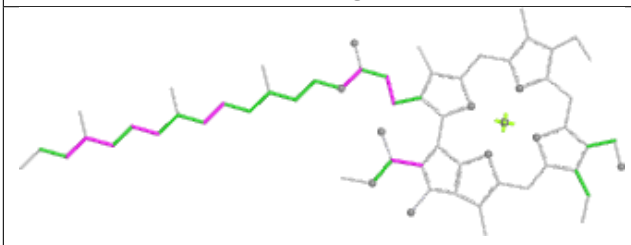
Ligand CHL Y 301



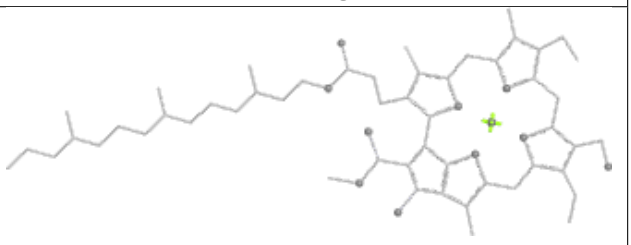
Bond lengths



Bond angles

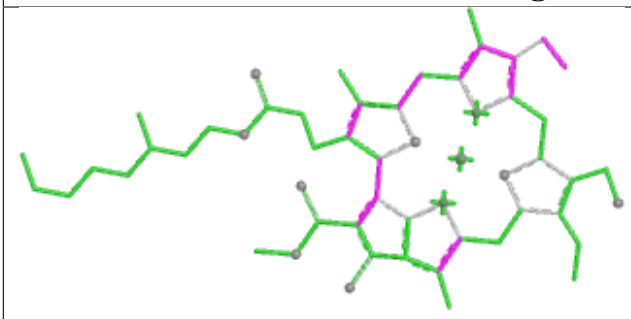


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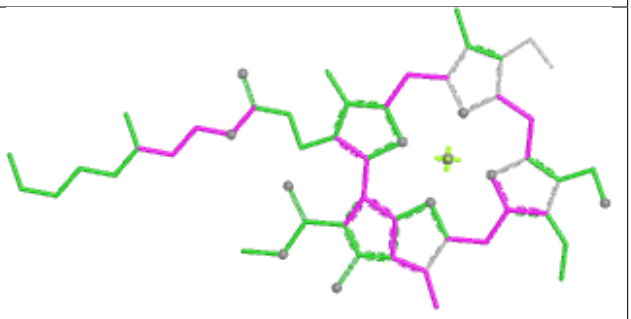


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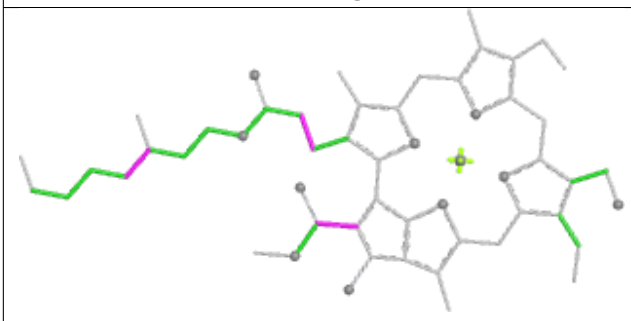
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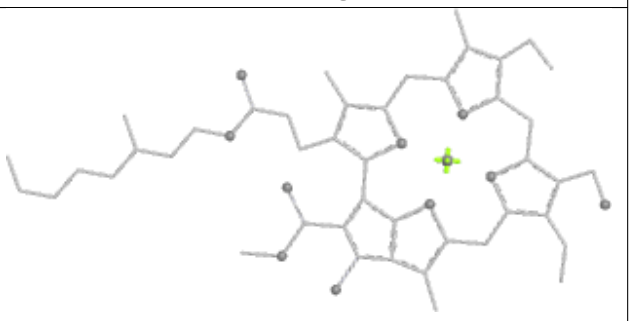
Bond lengths



Bond angles

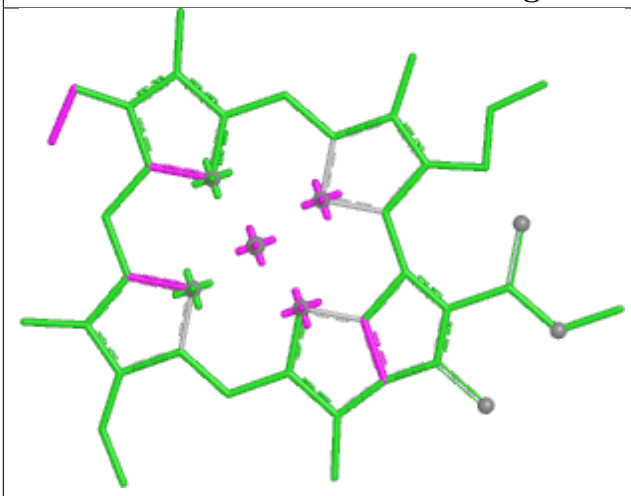


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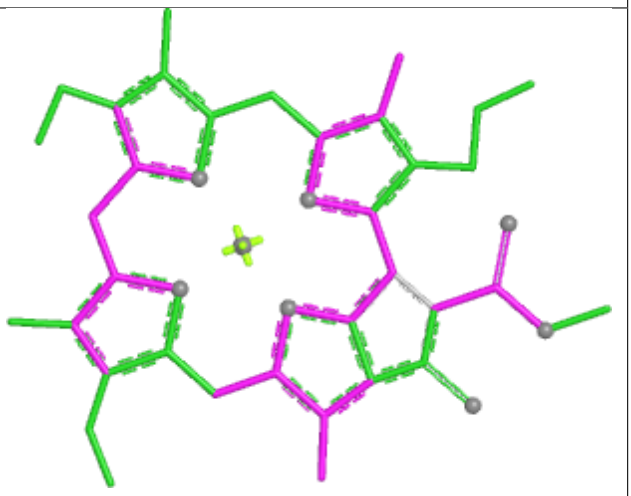


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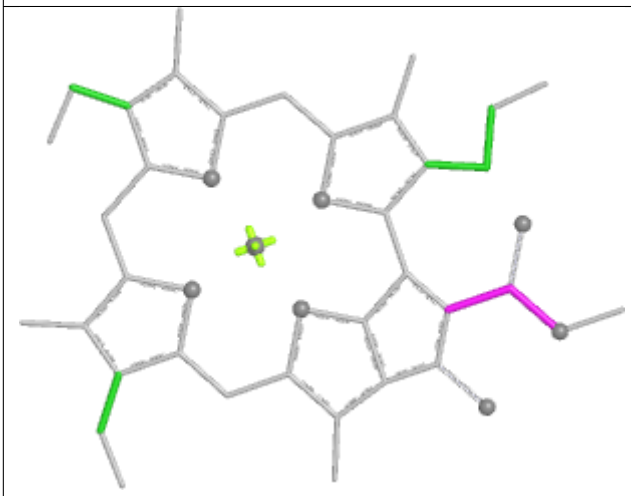
Ligand CLA G 611



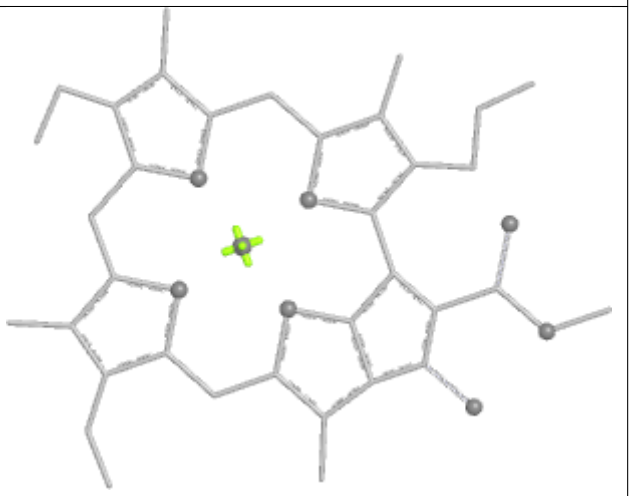
Bond lengths



Bond angles

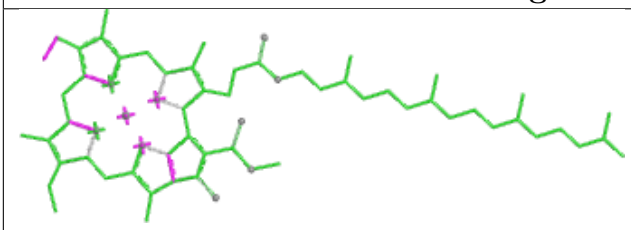


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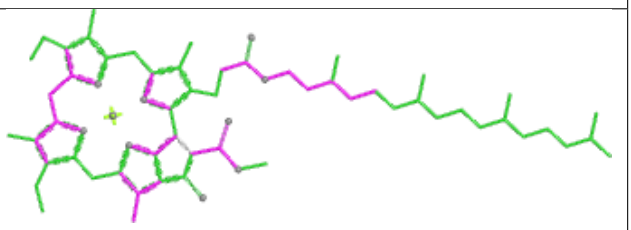


Rings

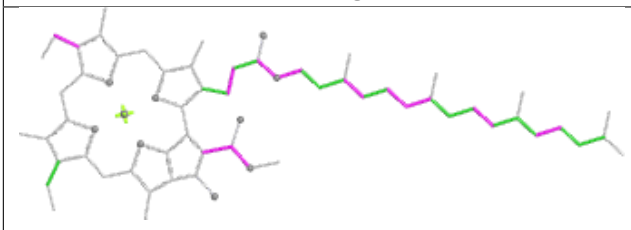
Ligand CLA c 605



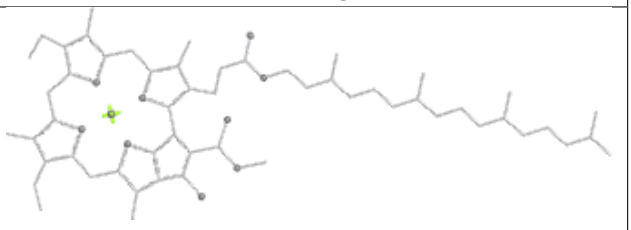
Bond lengths



Bond angles

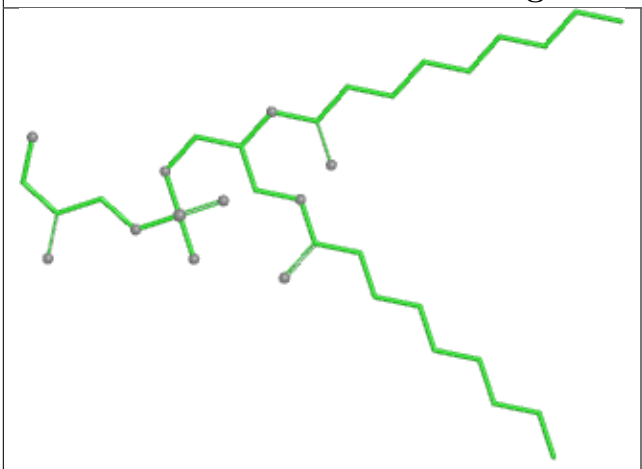


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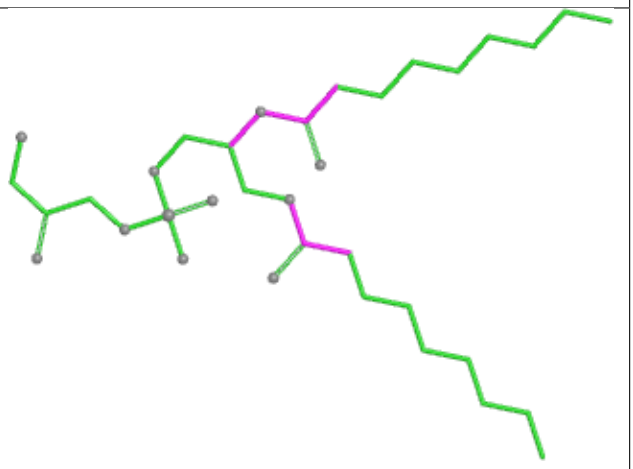


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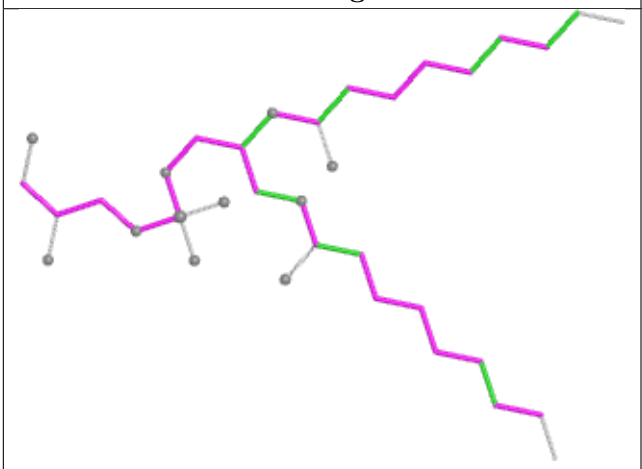
Ligand LHG 5 619



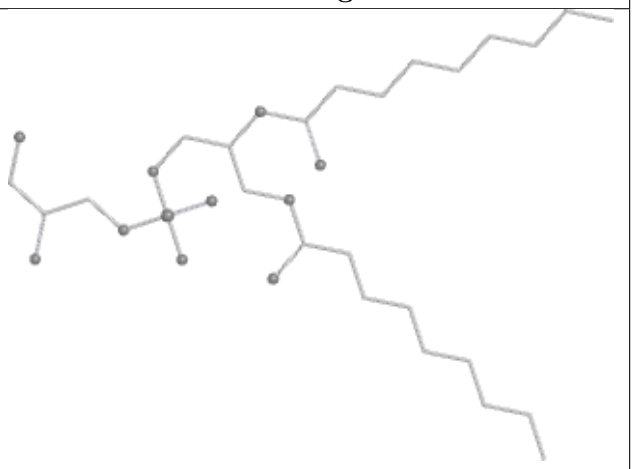
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Bond angles

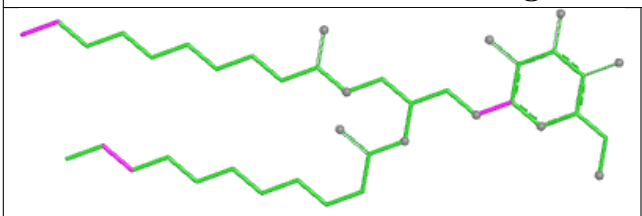


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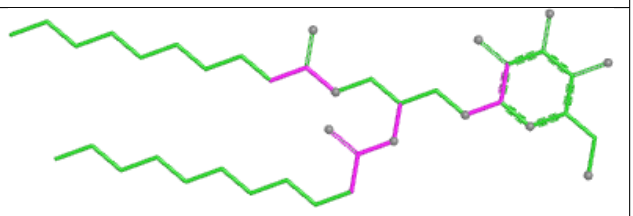


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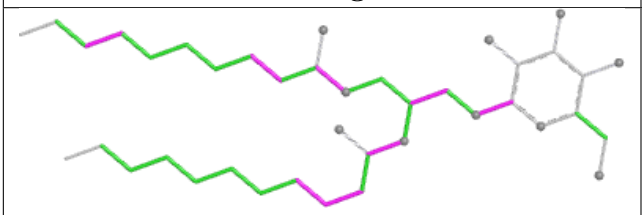
Ligand LMG n 322



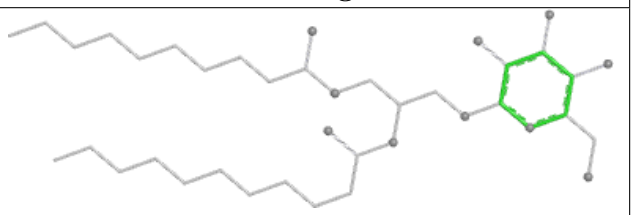
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Bond angles

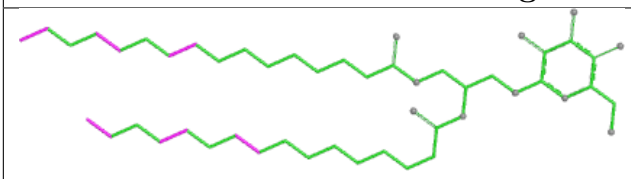


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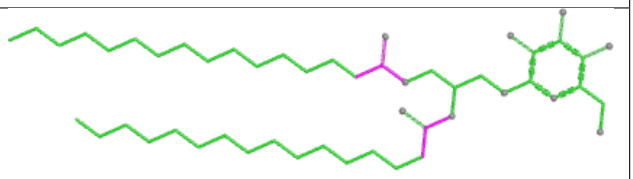


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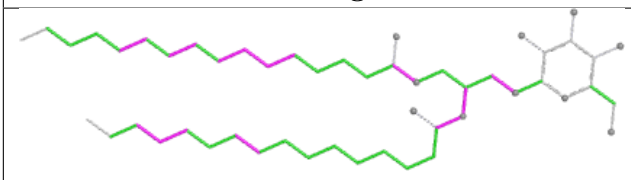
Ligand LMG D 411



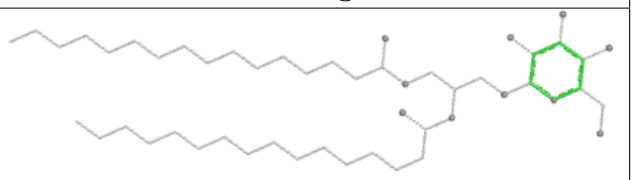
Bond lengths



Bond angles

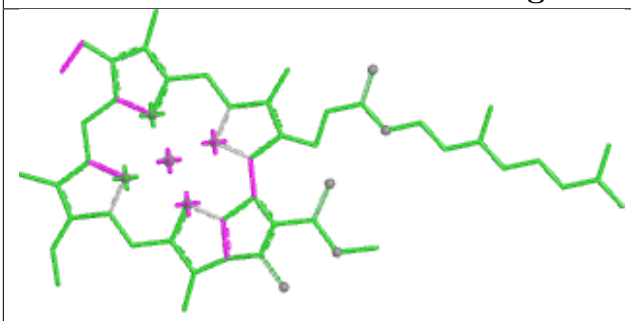


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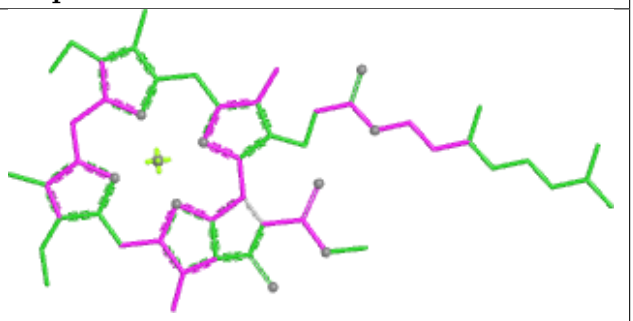


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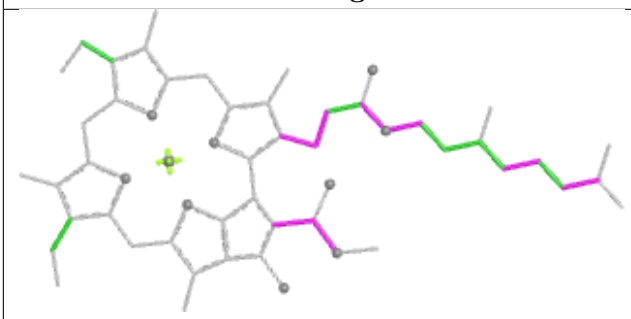
Ligand CLA p 603



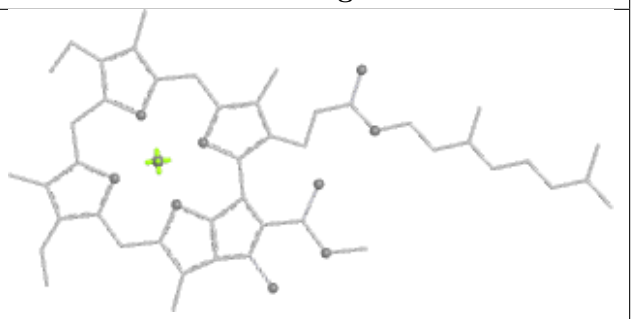
Bond lengths



Bond angles



Torsions



Rings

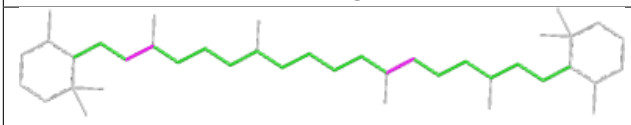
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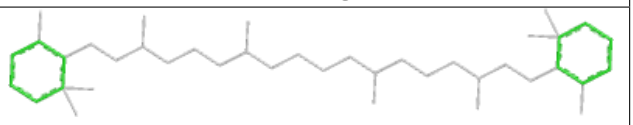
Bond lengths



Bond angles

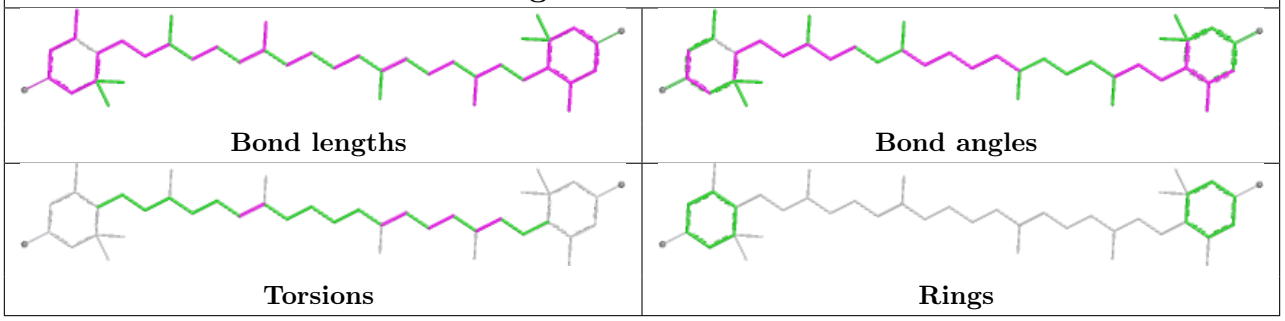


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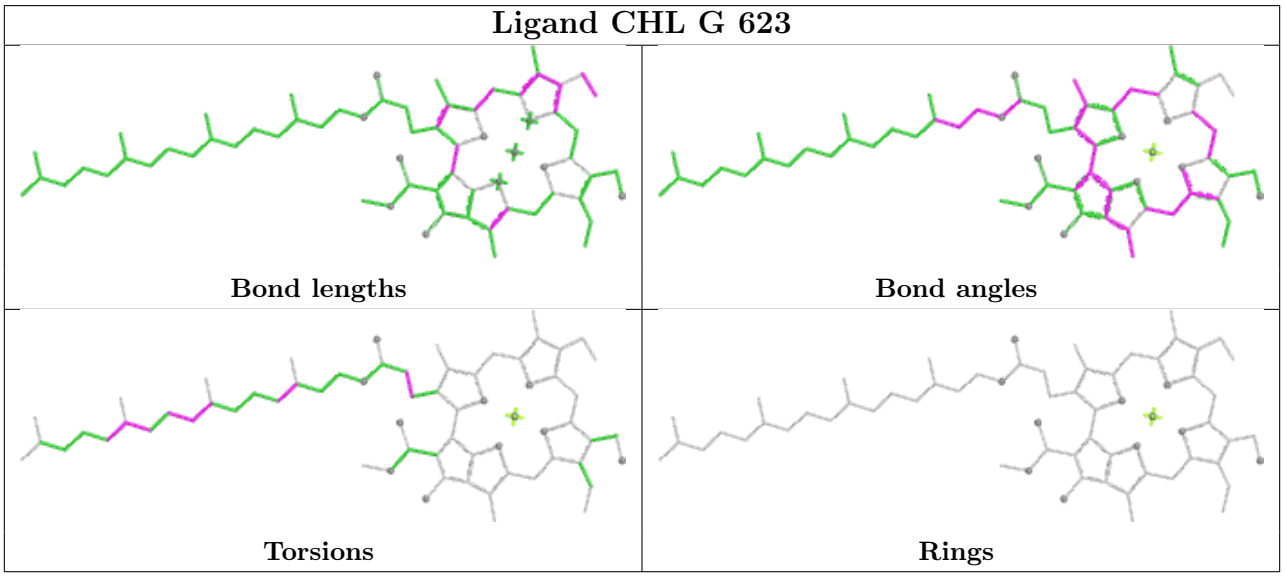


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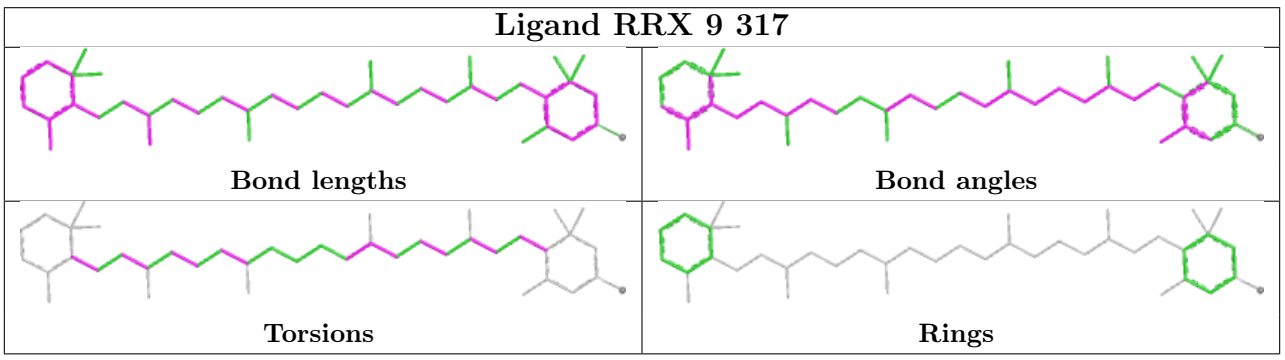
Ligand LUT 5 617



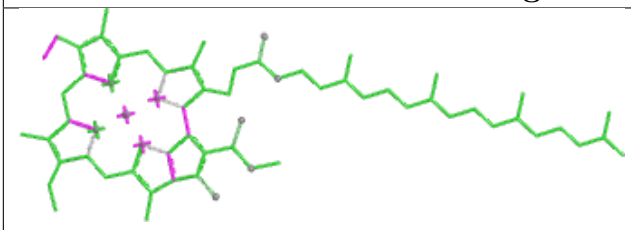
Ligand CHL G 623



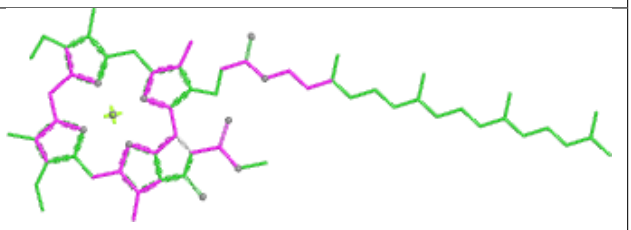
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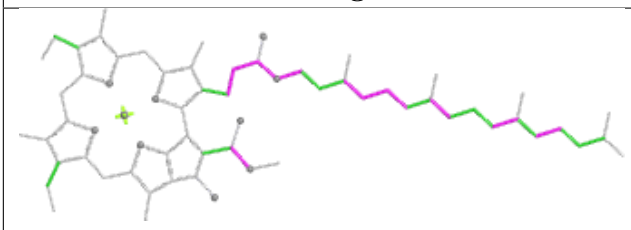
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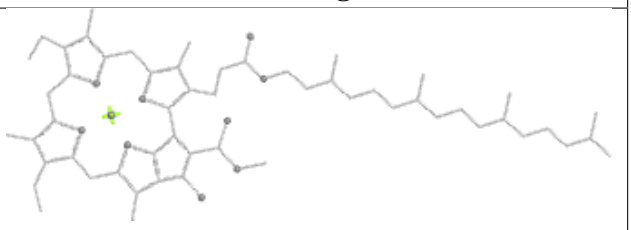
Bond lengths



Bond angles

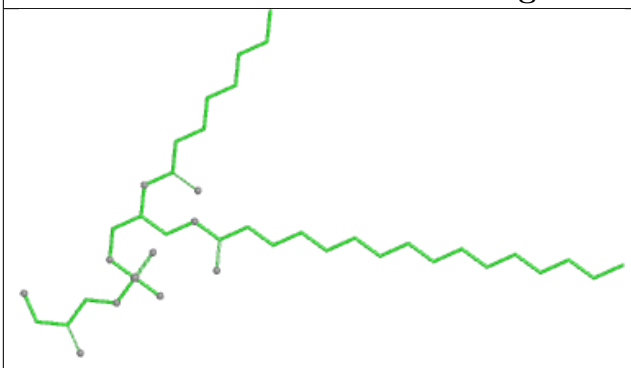


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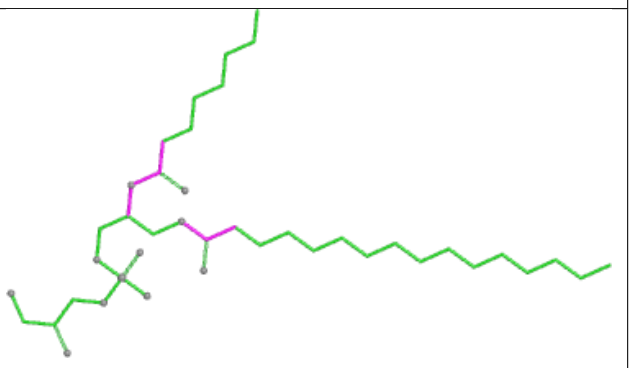


Rings

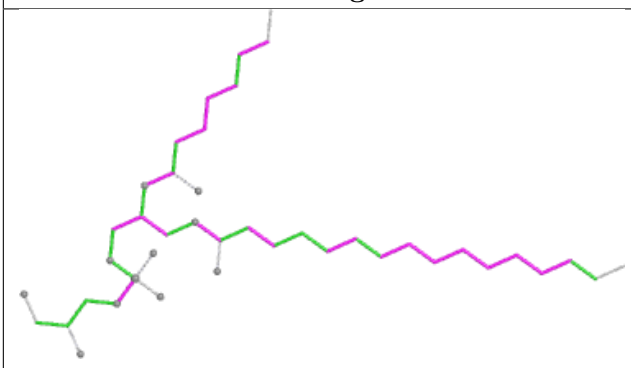
Ligand LHG M 101



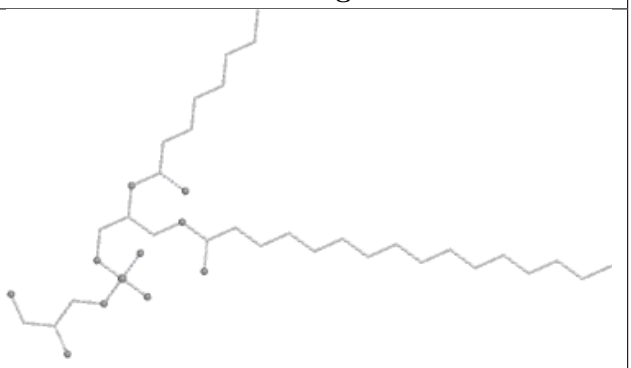
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Bond angles

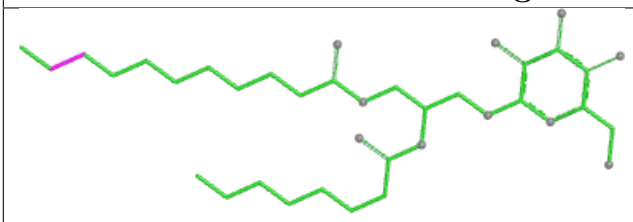


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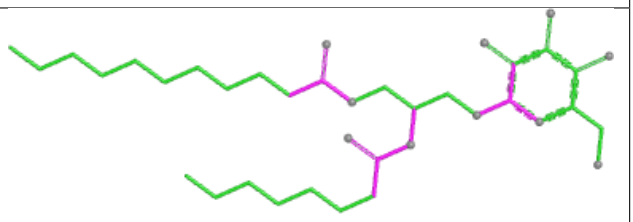


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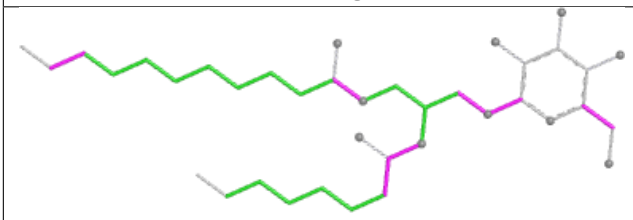
Ligand LMG W 202



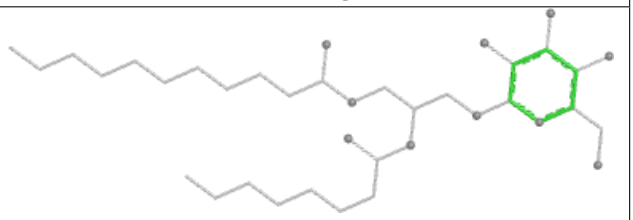
Bond lengths



Bond angles



Torsions

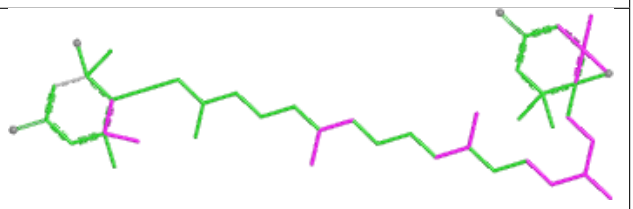


Rings

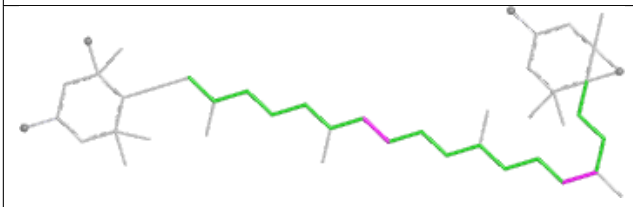
Ligand NEX R 301



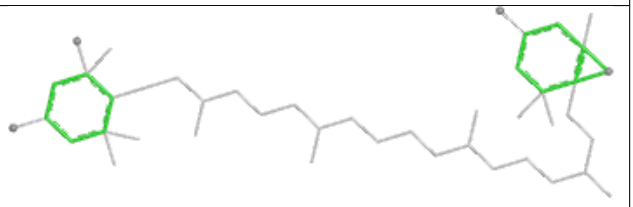
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Bond angles

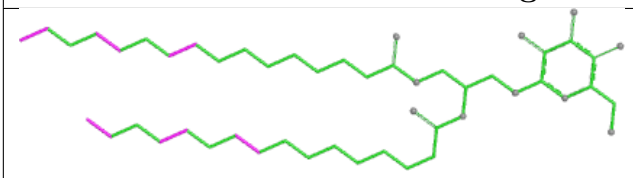


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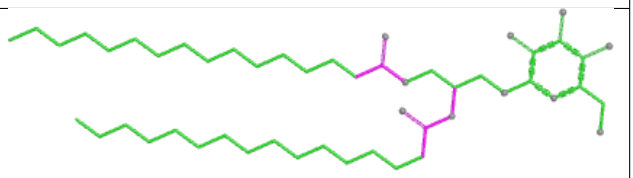


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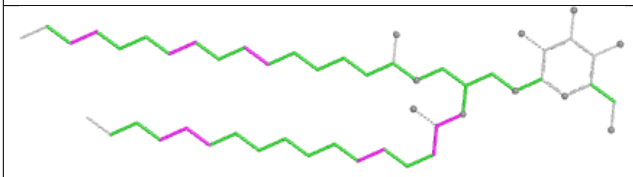
Ligand LMG C 619



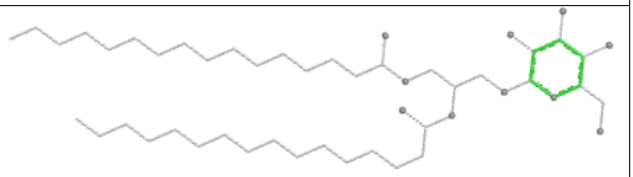
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Bond angles

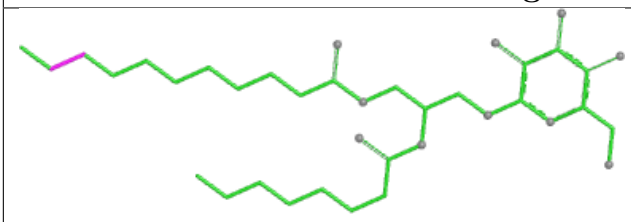


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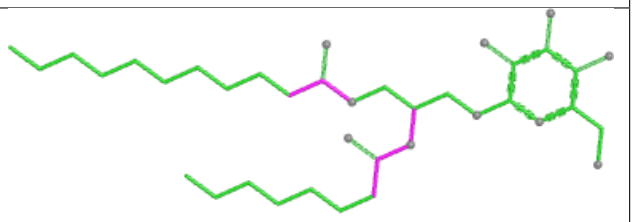


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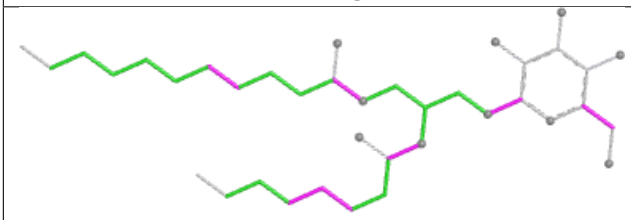
Ligand LMG k 102



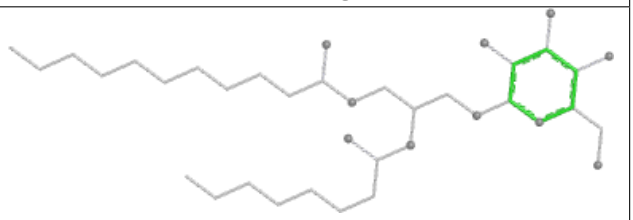
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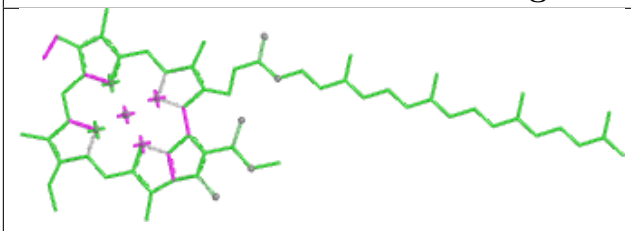


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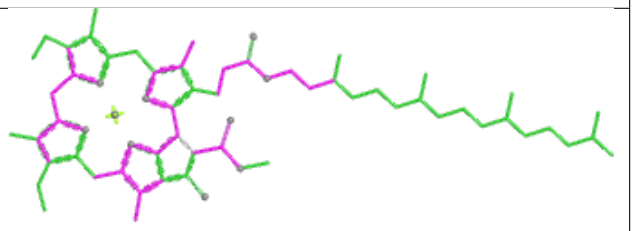


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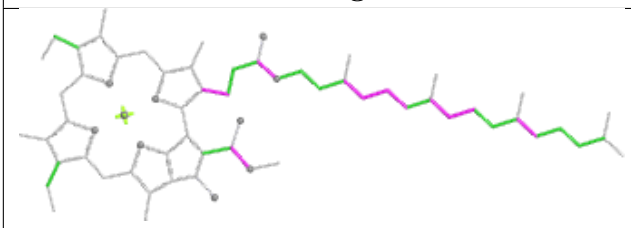
Ligand CLA c 611



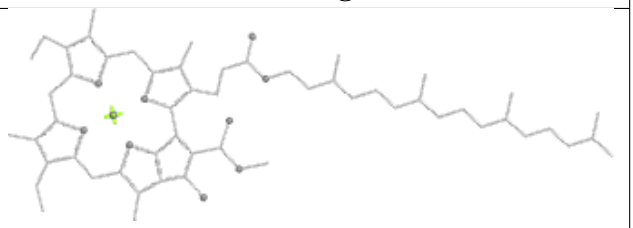
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Bond angles

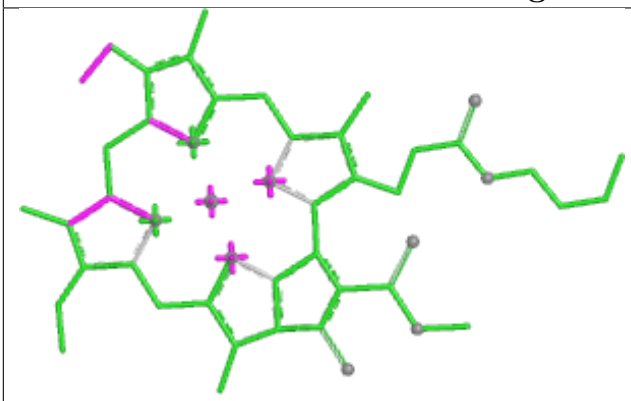


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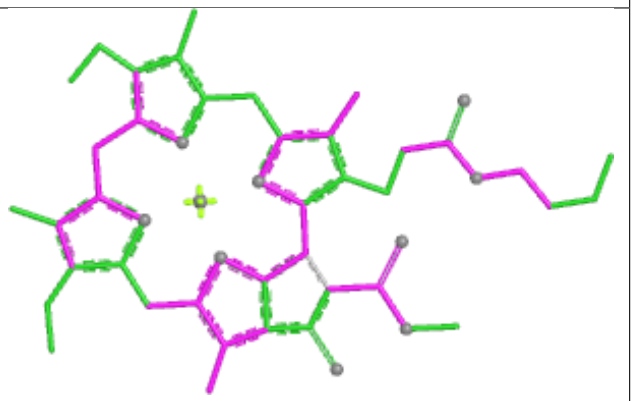


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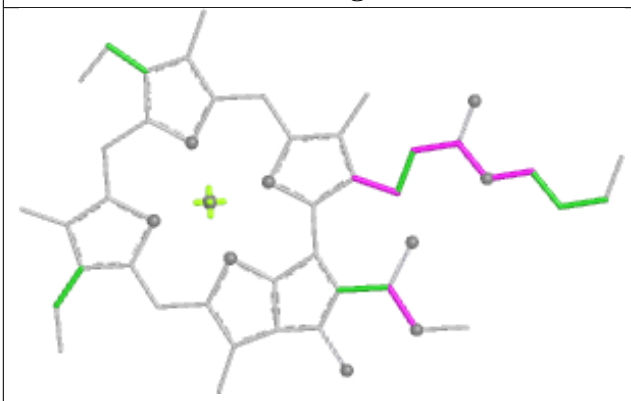
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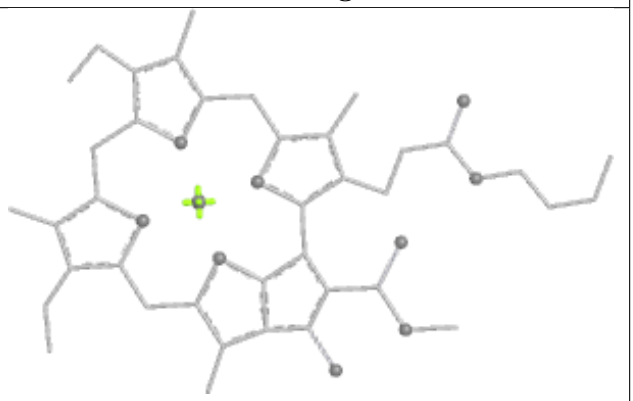
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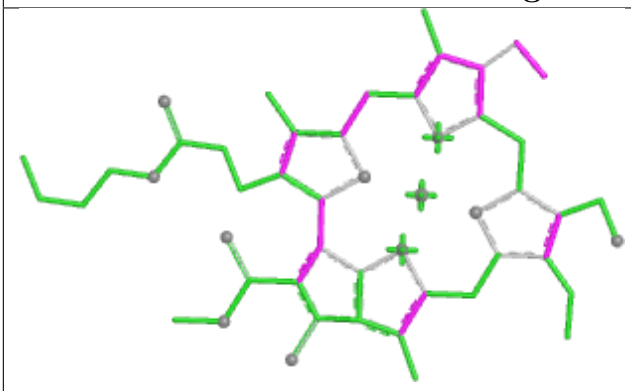


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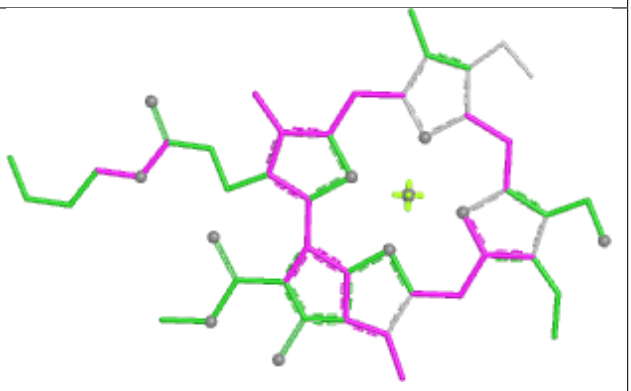


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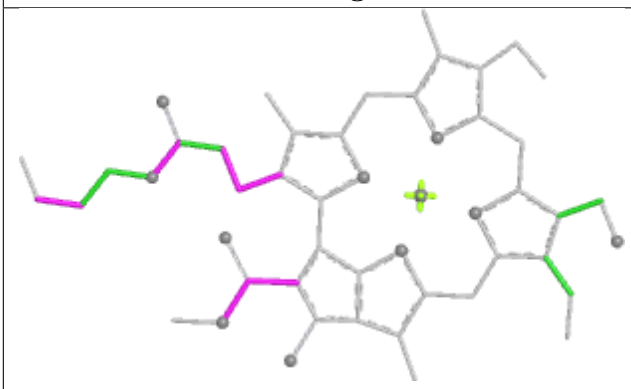
Ligand CHL Y 308



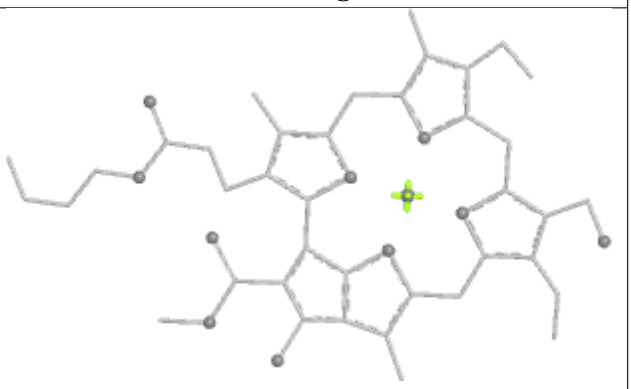
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Bond angles

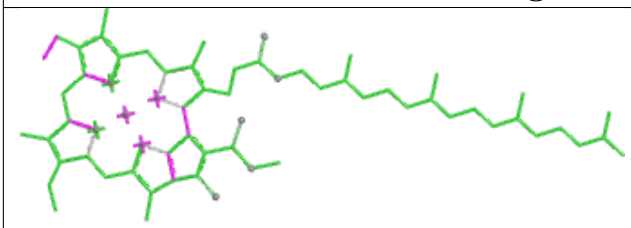


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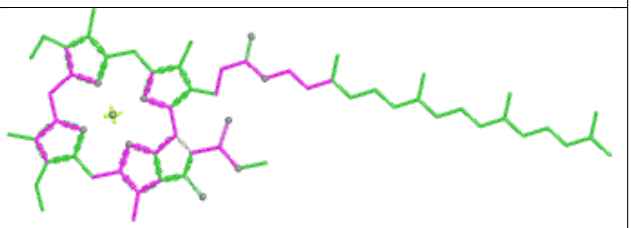


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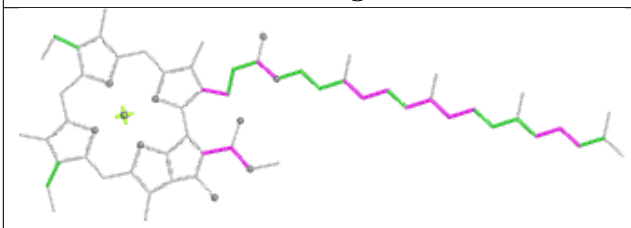
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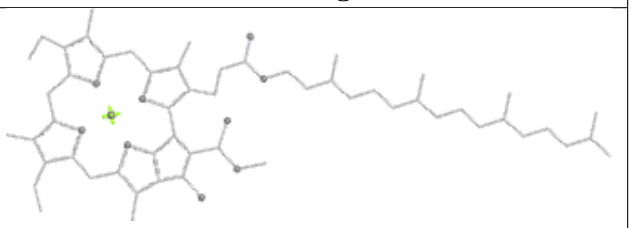
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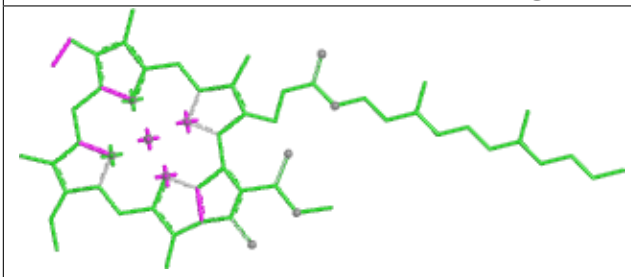


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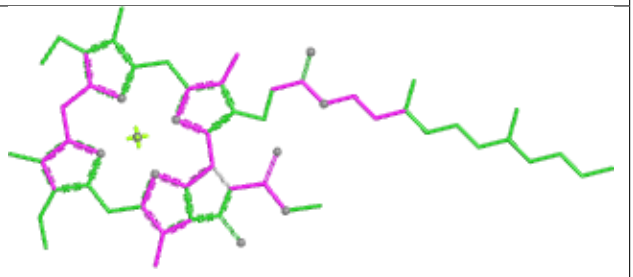


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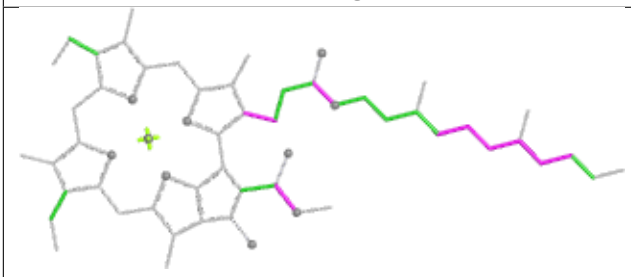
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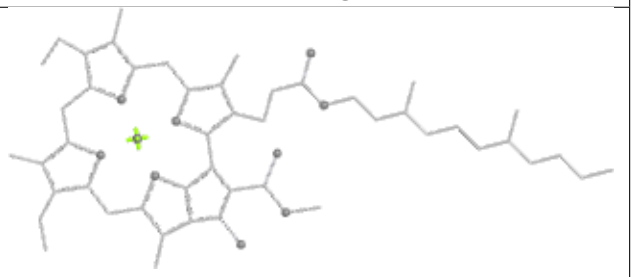
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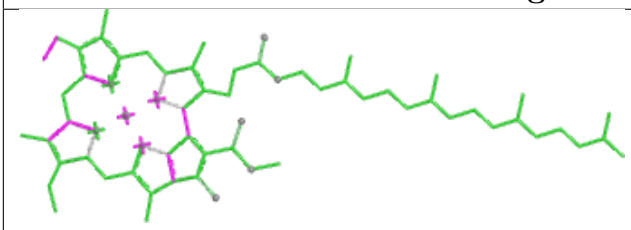


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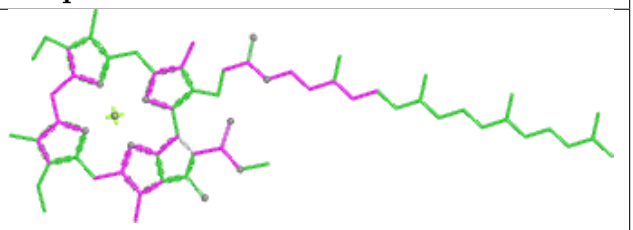


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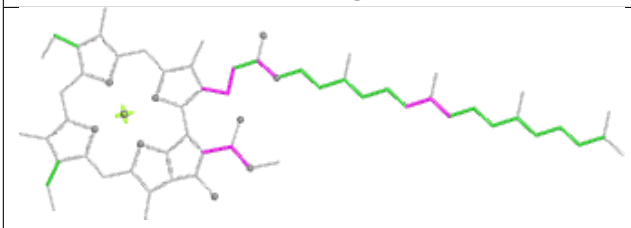
Ligand CLA q 304



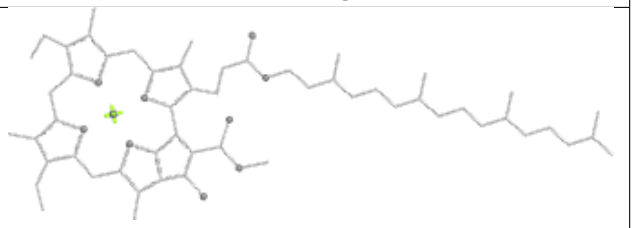
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Bond angles

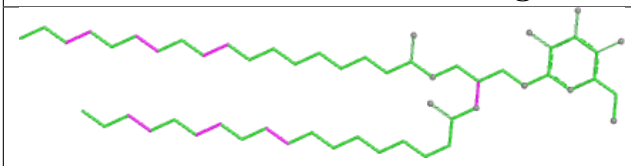


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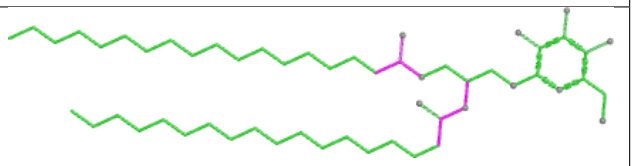


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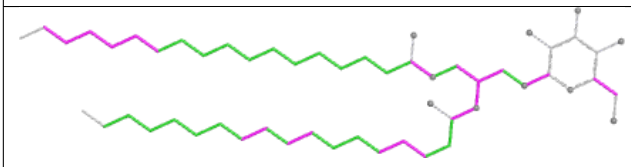
Ligand LMG W 201



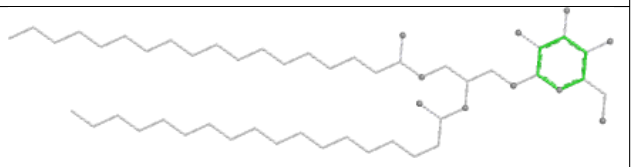
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Bond angles

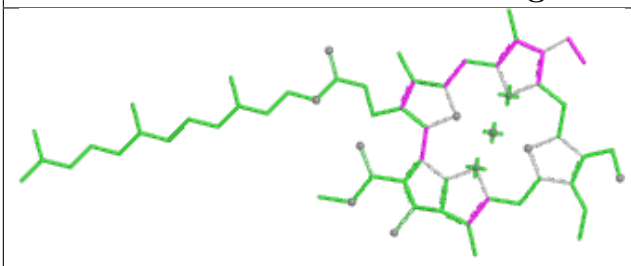


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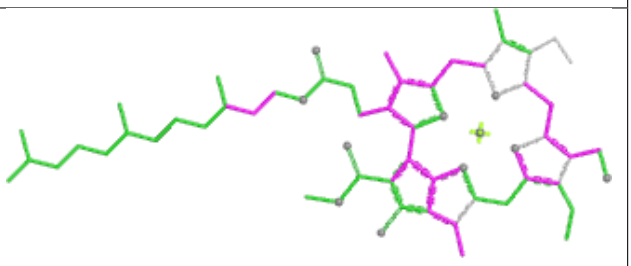


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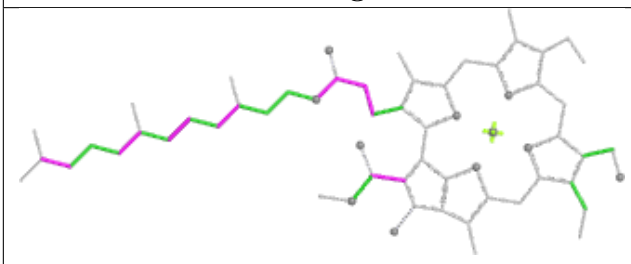
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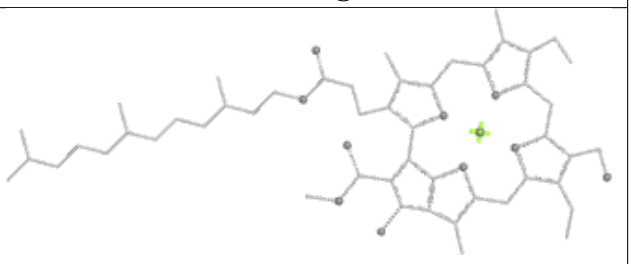
Bond lengths



Bond angles

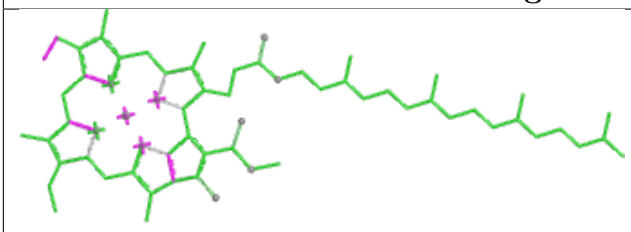


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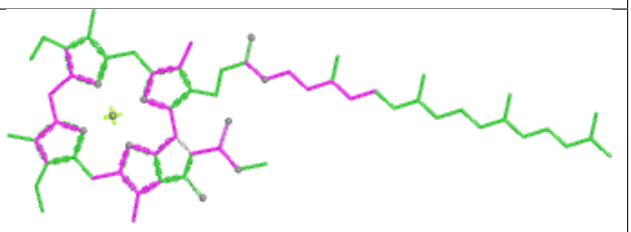


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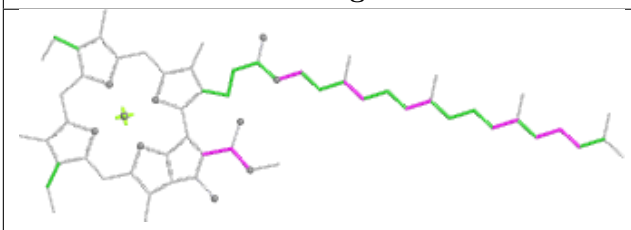
Ligand CLA C 602



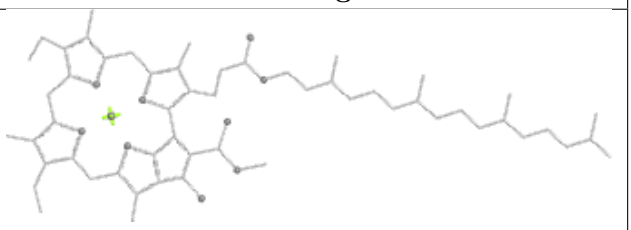
Bond lengths



Bond angles

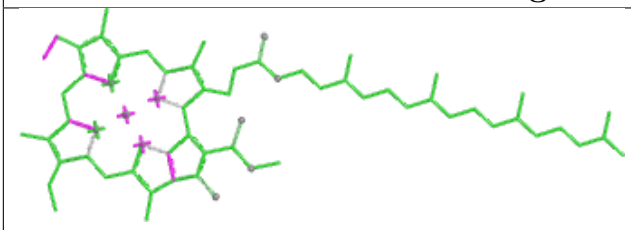


Torsions

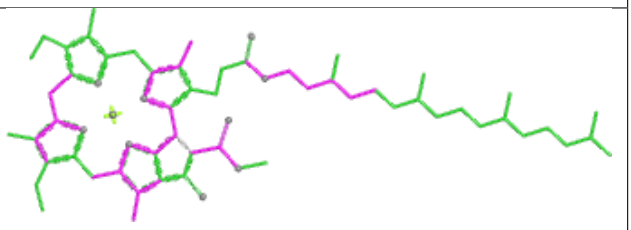


Rings

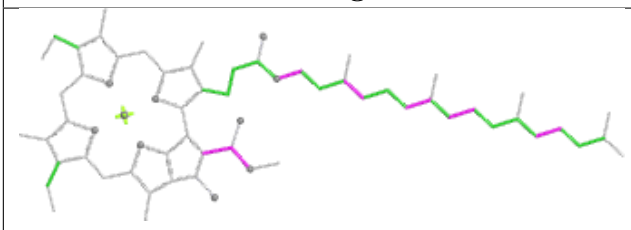
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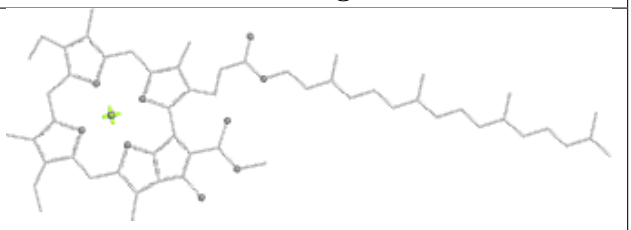
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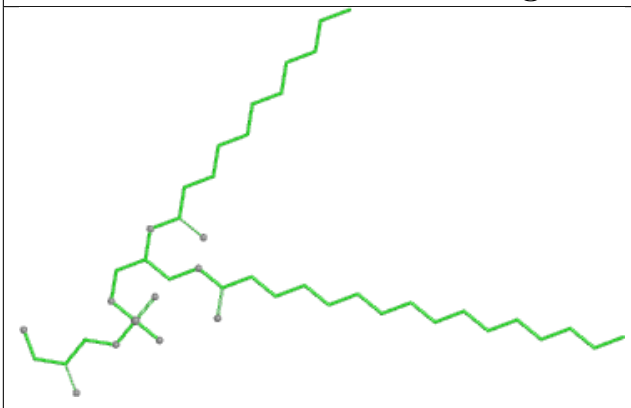


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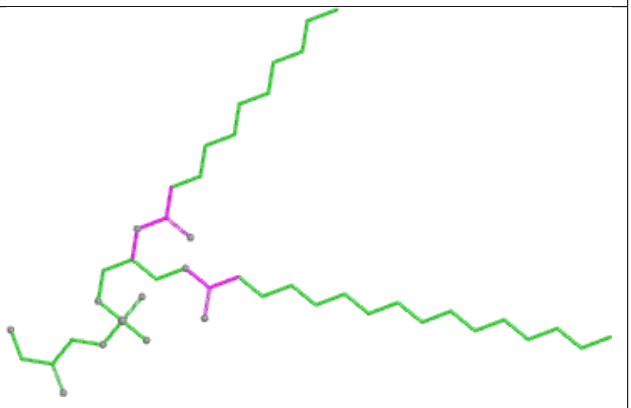


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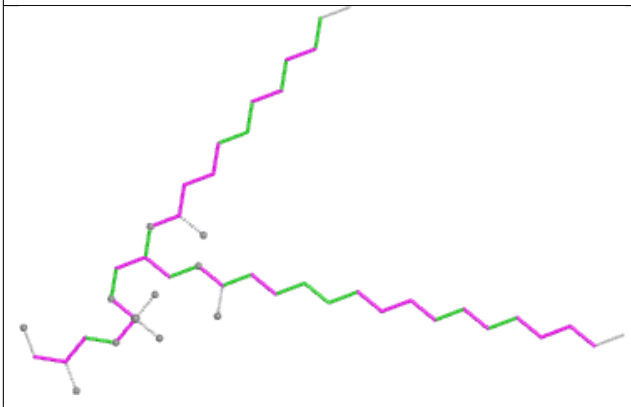
Ligand LHG A 415



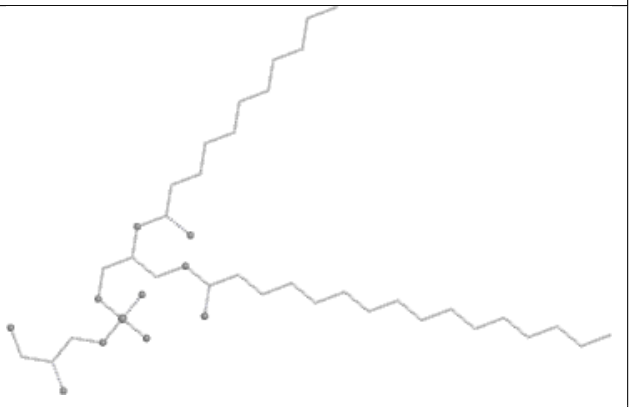
Bond lengths



Bond angles

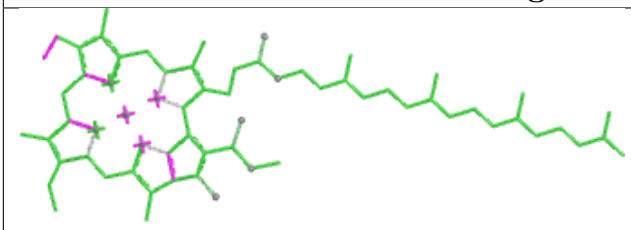


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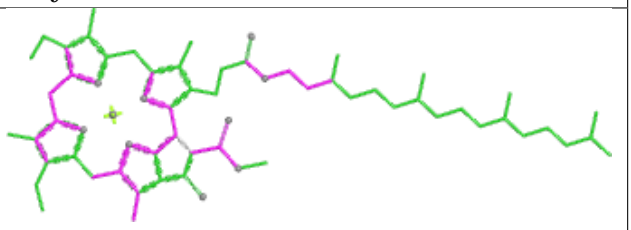


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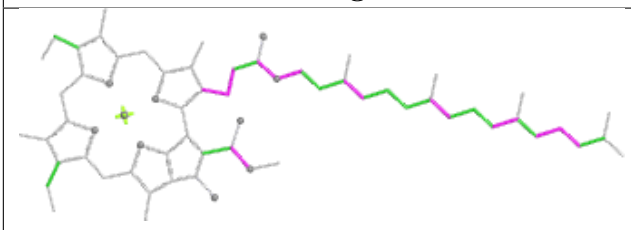
Ligand CLA y 611



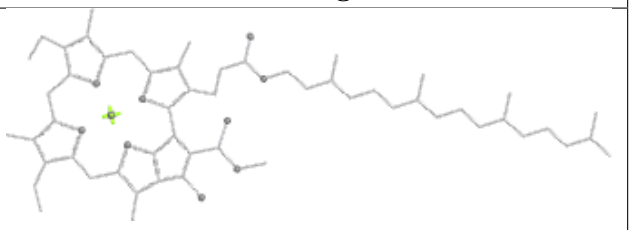
Bond lengths



Bond angles

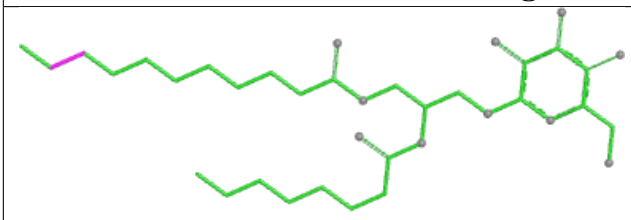


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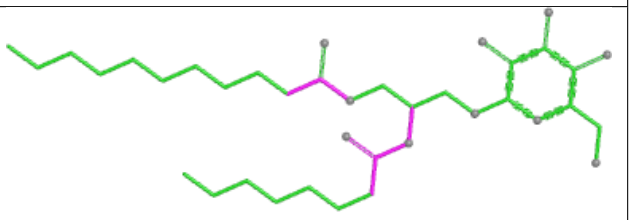


Rings

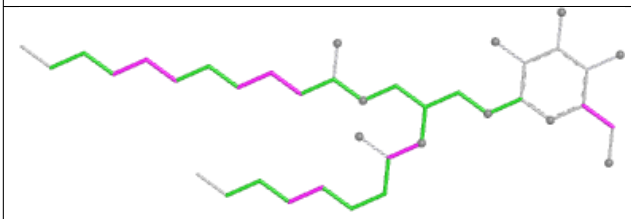
Ligand LMG B 622



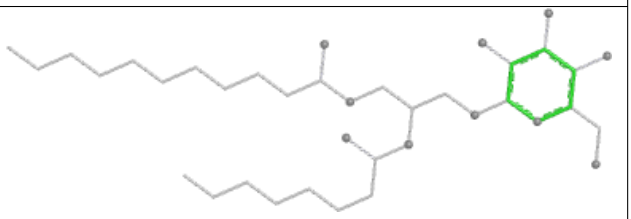
Bond lengths



Bond angles

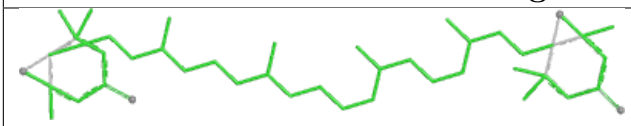


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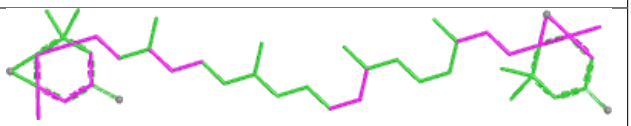


Rings

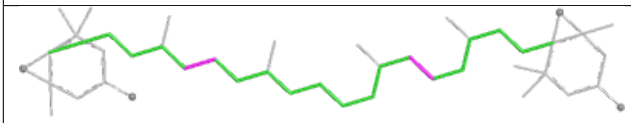
Ligand XAT r 318



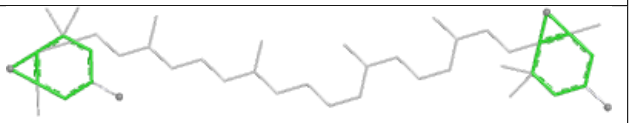
Bond lengths



Bond angles

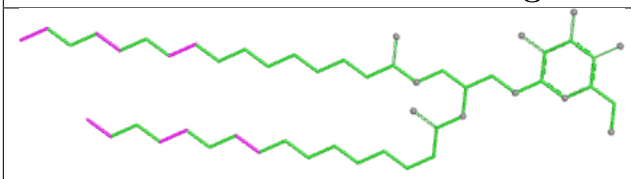


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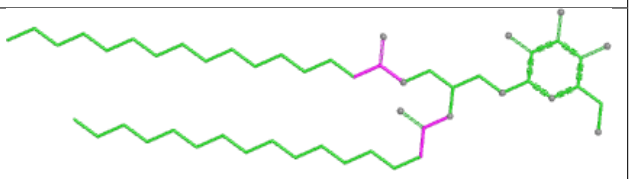


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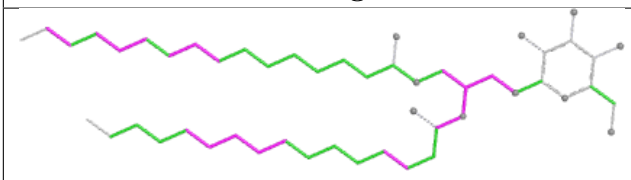
Ligand LMG 2 620



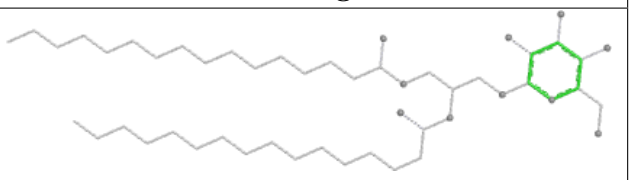
Bond lengths



Bond angles

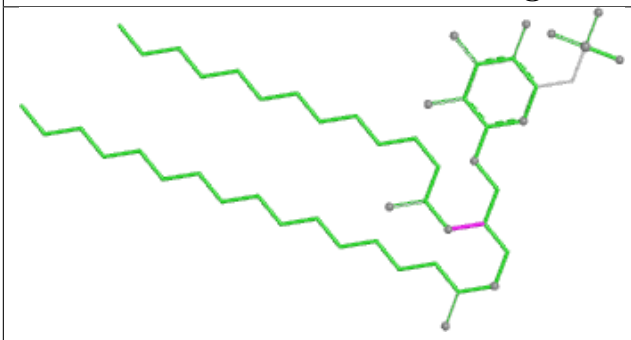


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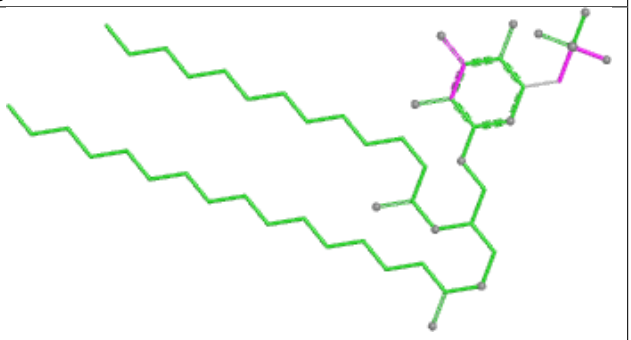


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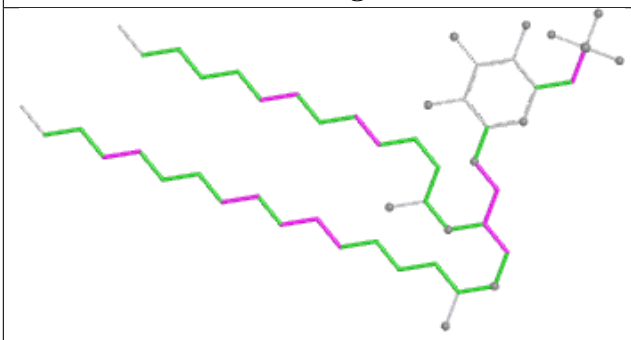
Ligand SQD A 411



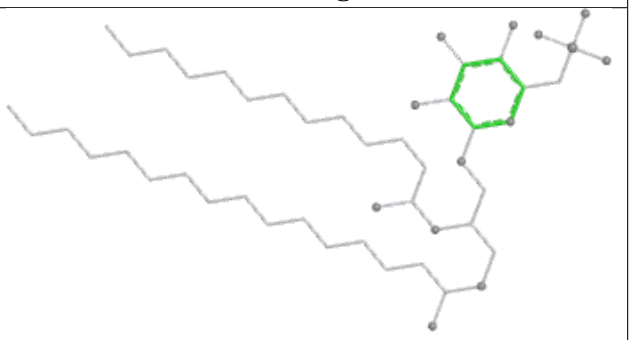
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Bond angles

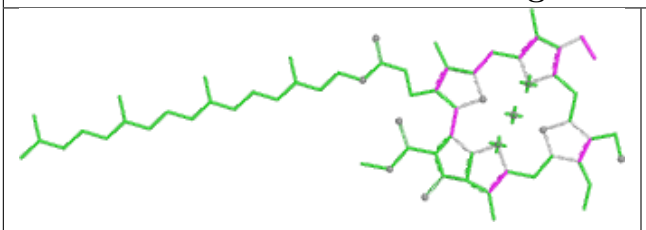


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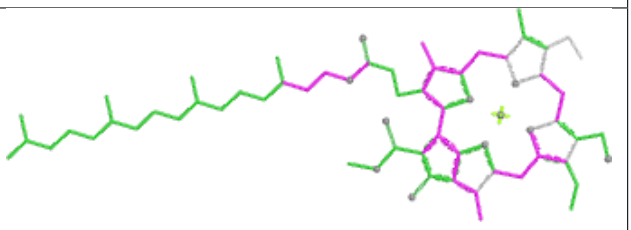


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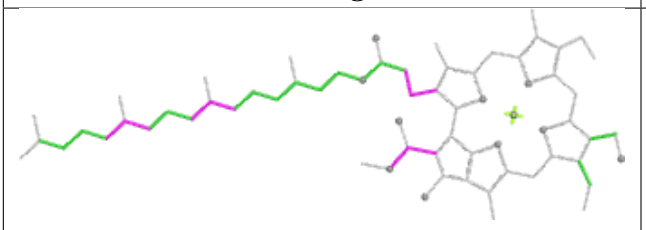
Ligand CHL 7 306



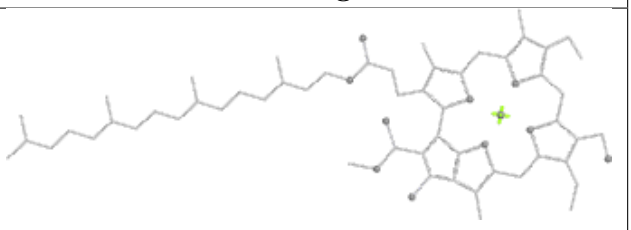
Bond lengths



Bond angles

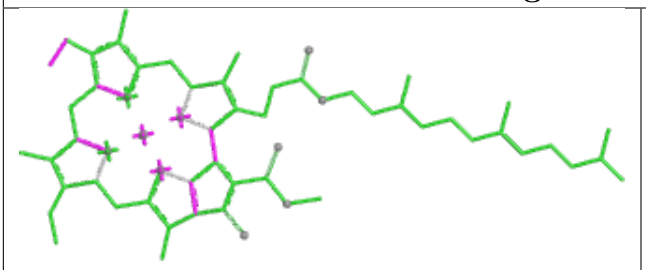


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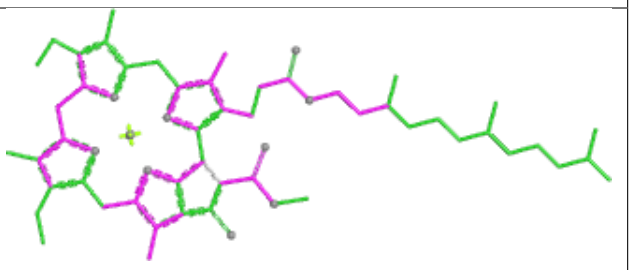


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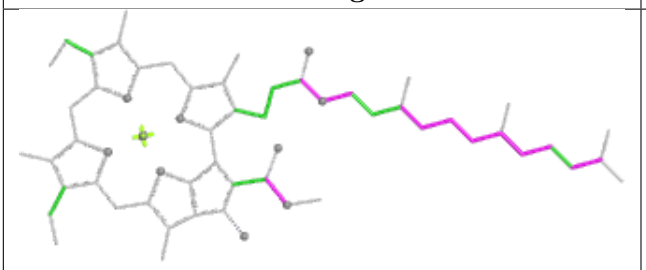
Ligand CLA A 409



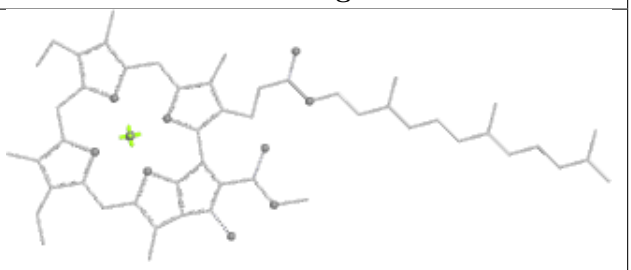
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Bond angles

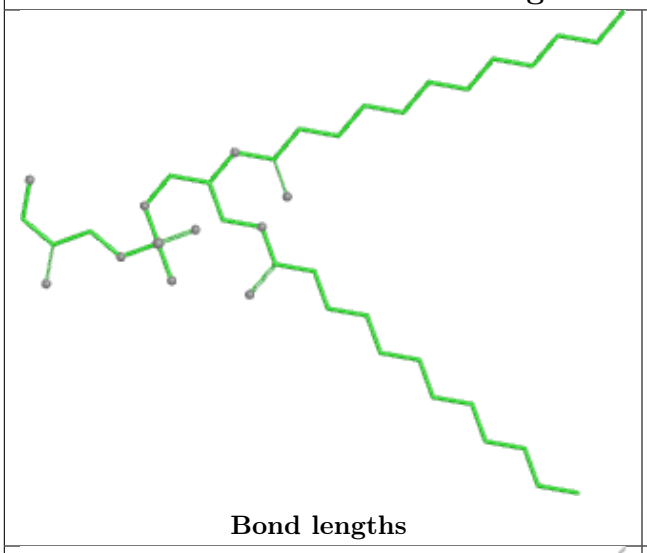


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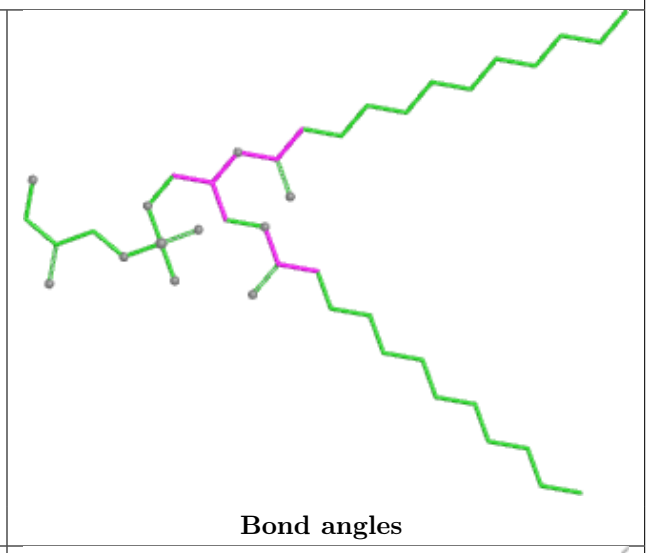


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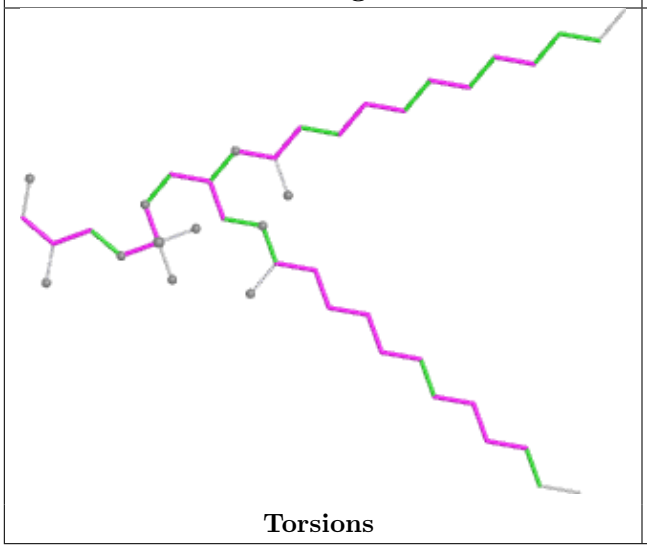
Ligand LHG S 320



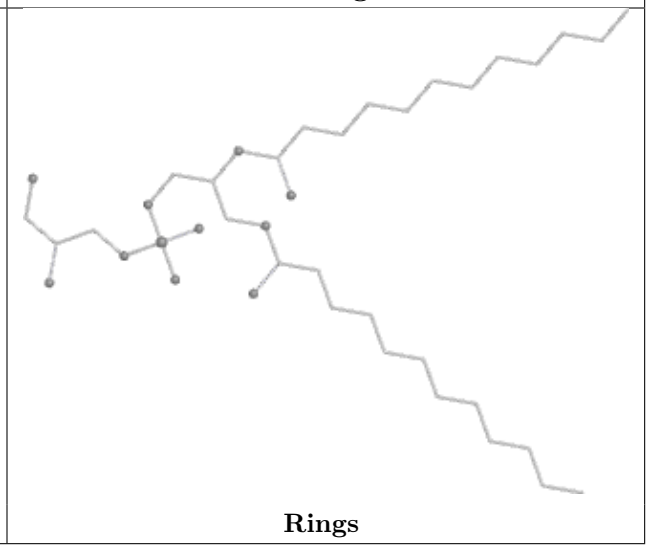
Bond lengths



Bond angles

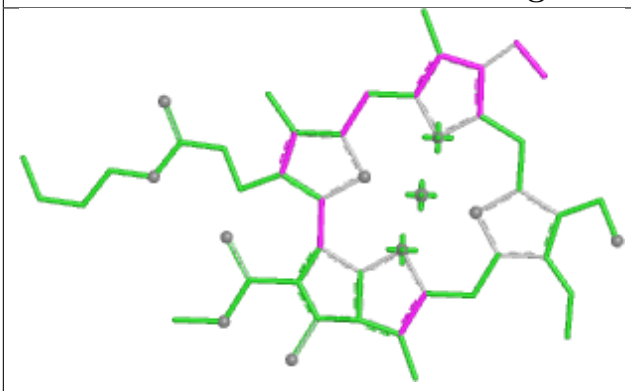


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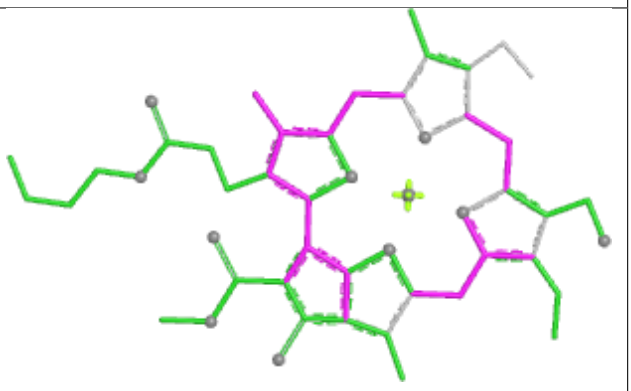


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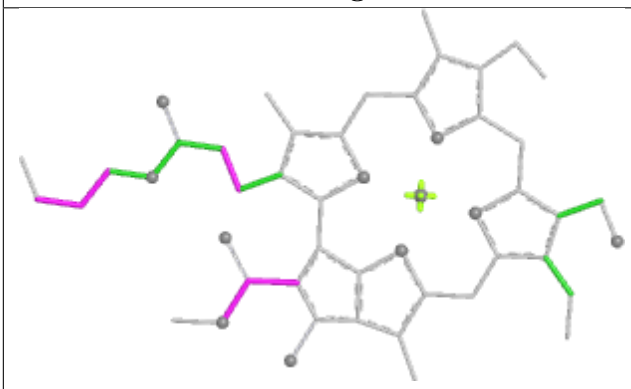
Ligand CHL 1 608



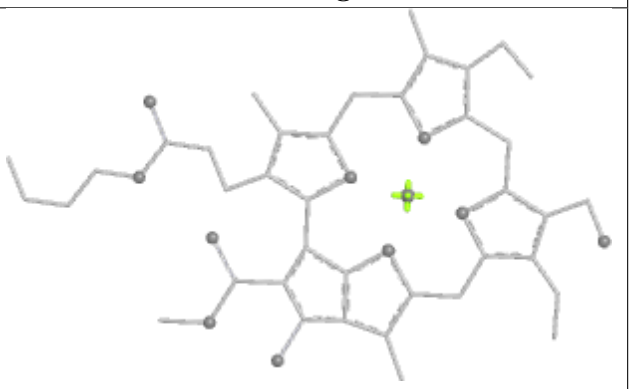
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Bond angles

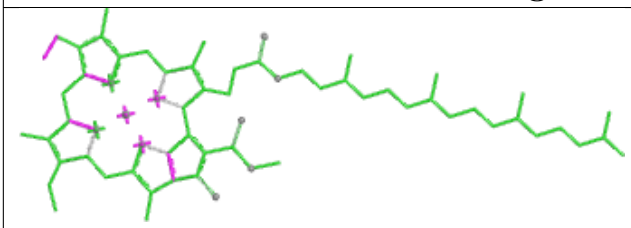


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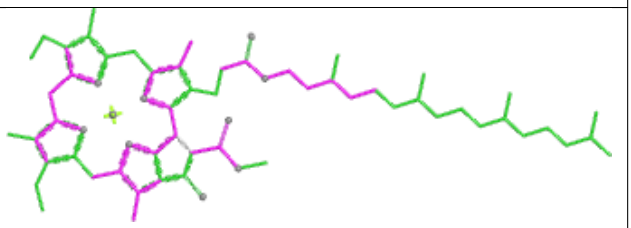


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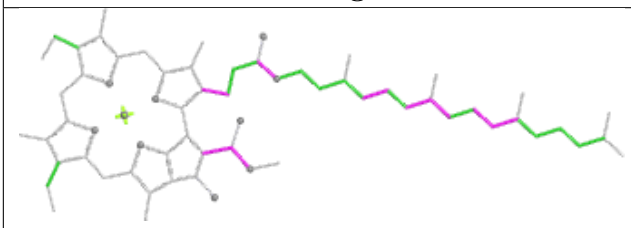
Ligand CLA 6 303



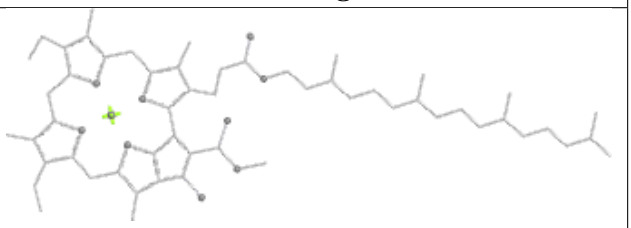
Bond lengths



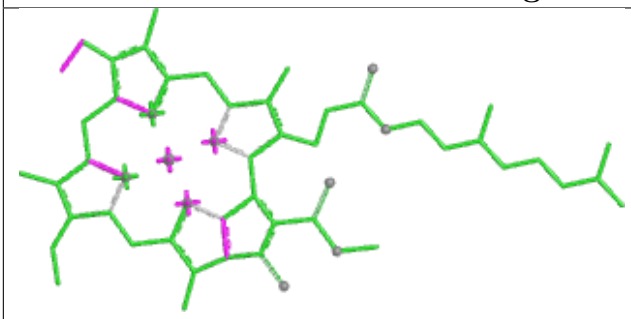
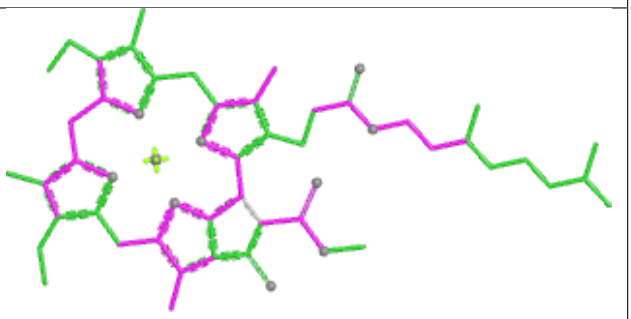
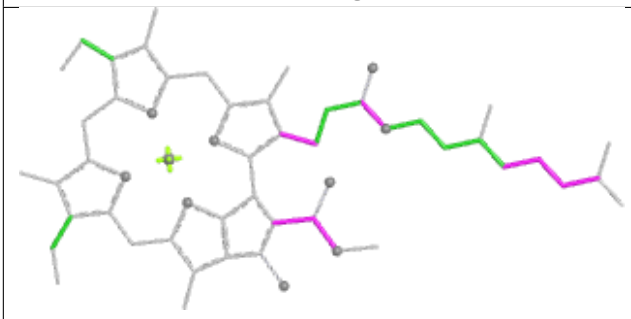
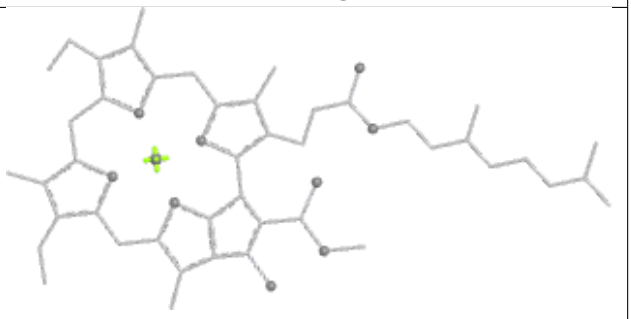
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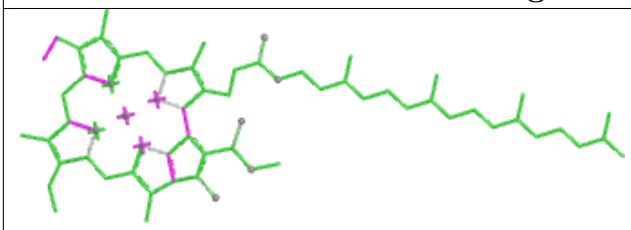
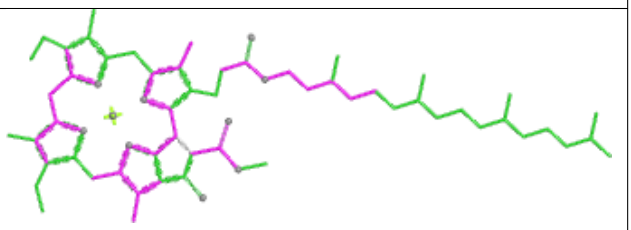
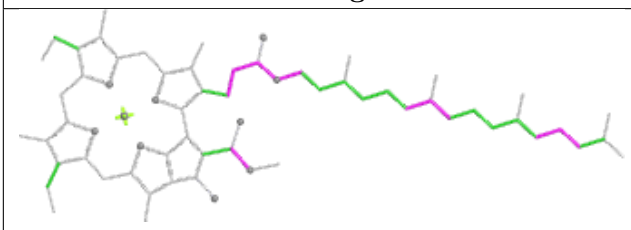
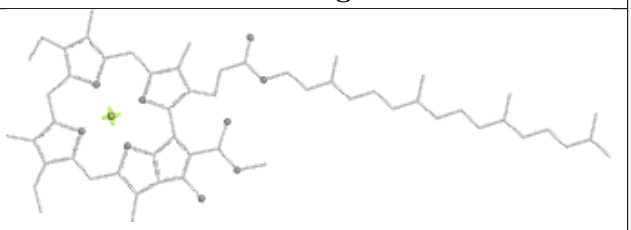


Torsions

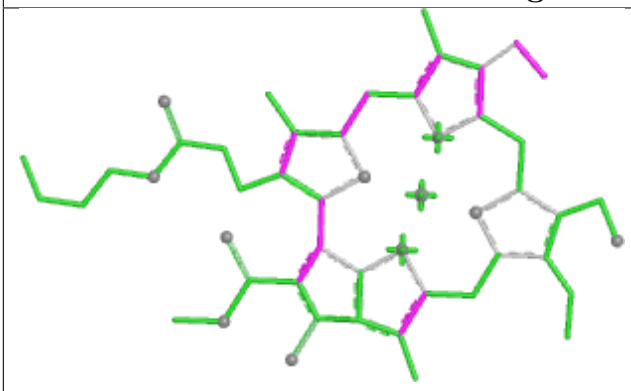


Rings

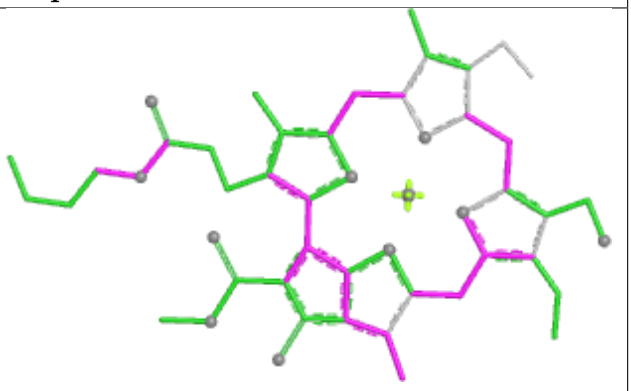
Ligand CLA G 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

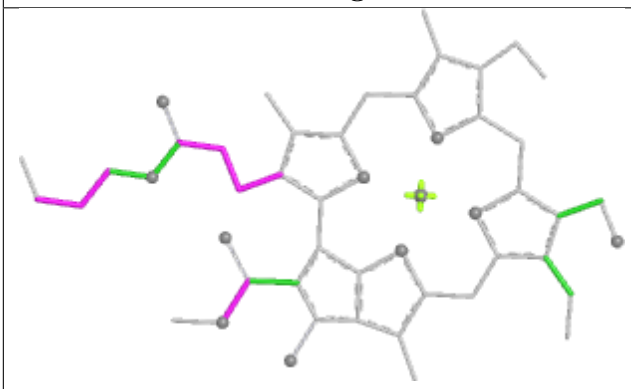
Ligand CHL p 608



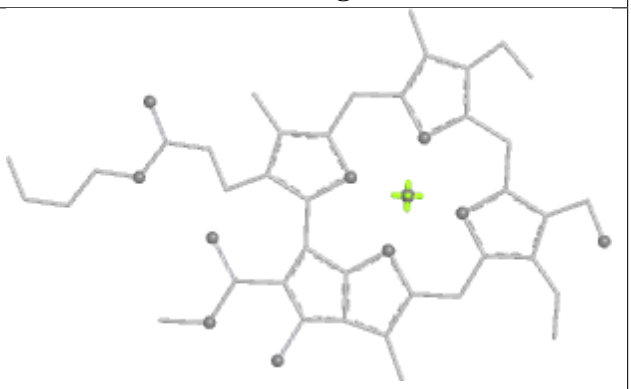
Bond lengths



Bond angles

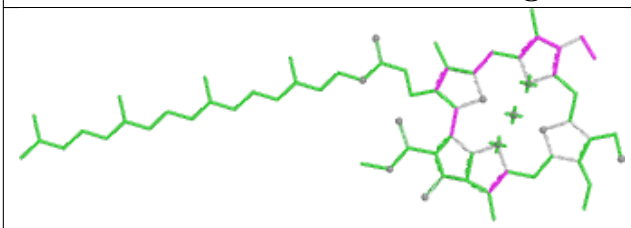


Torsions

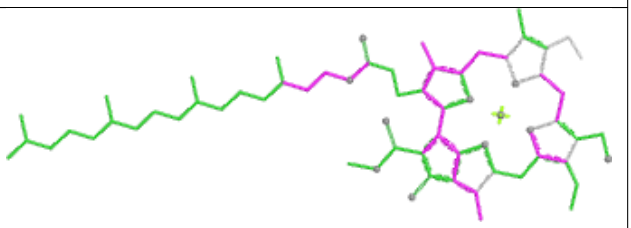


Rings

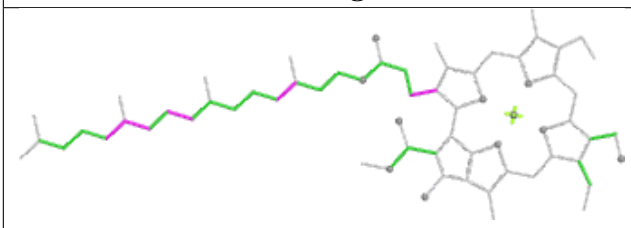
Ligand CHL G 601



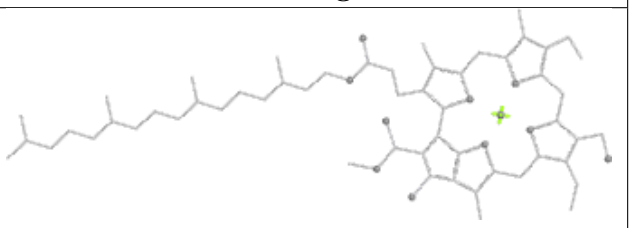
Bond lengths



Bond angles

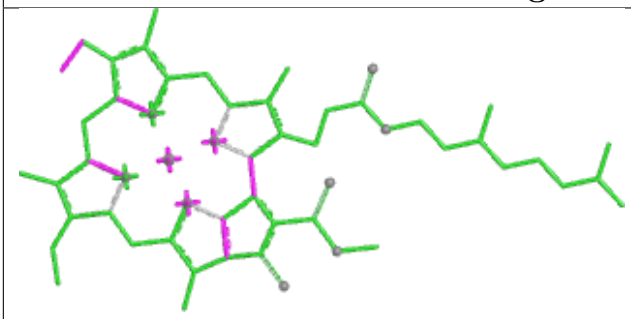


Torsions

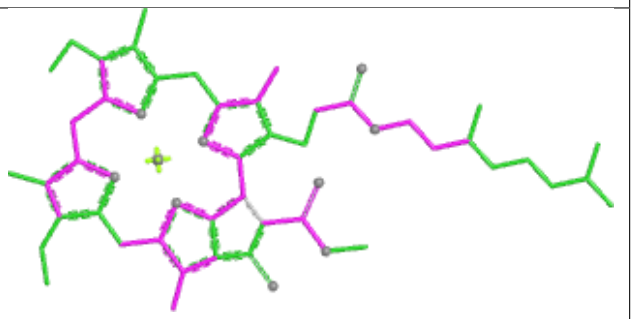


Rings

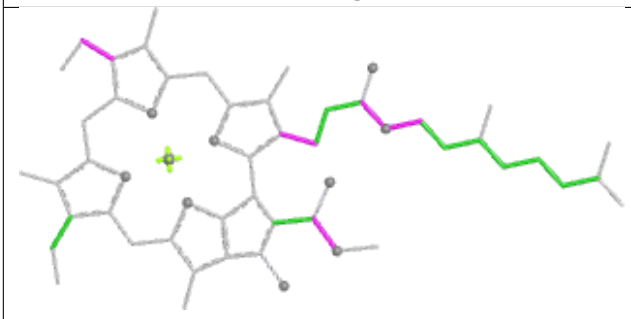
Ligand CLA 1 603



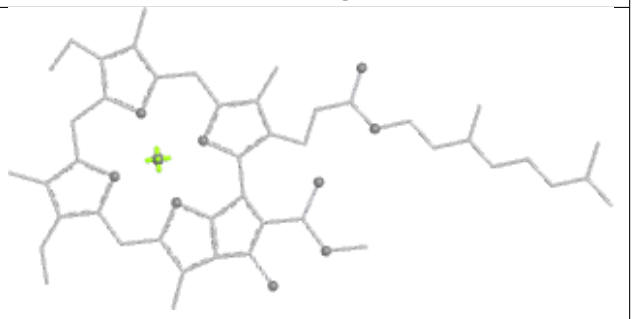
Bond lengths



Bond angles

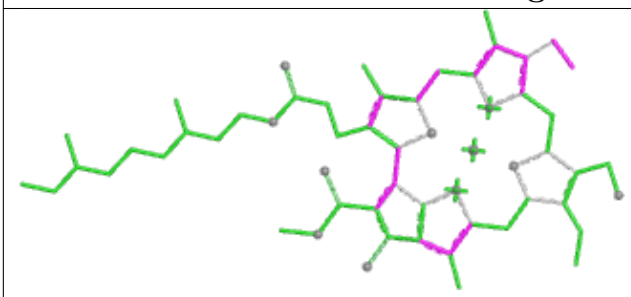


Torsions

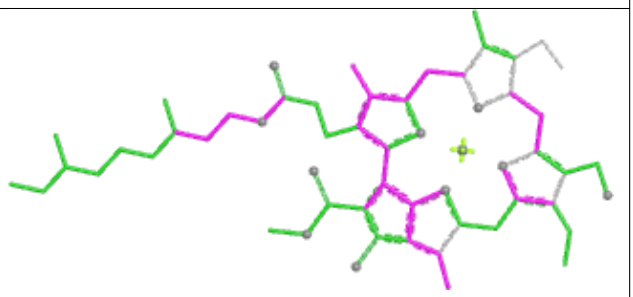


Rings

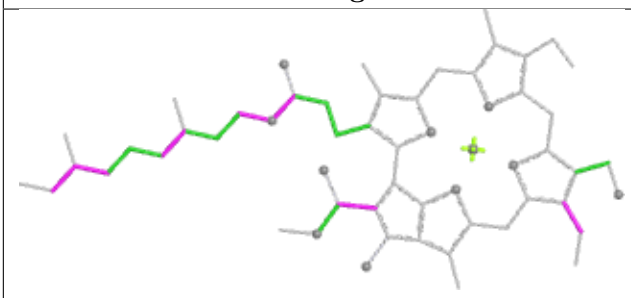
Ligand CHL 3 302



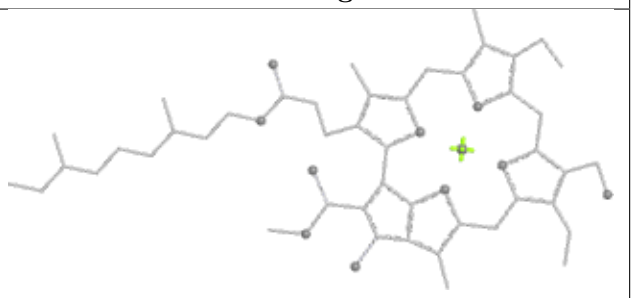
Bond lengths



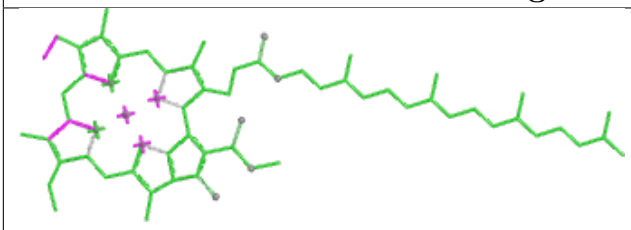
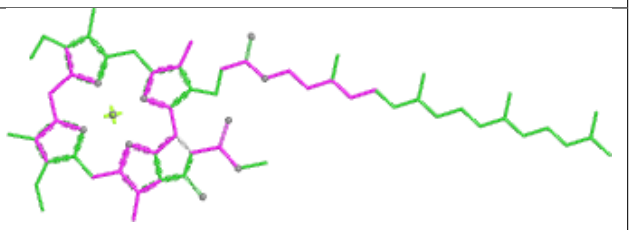
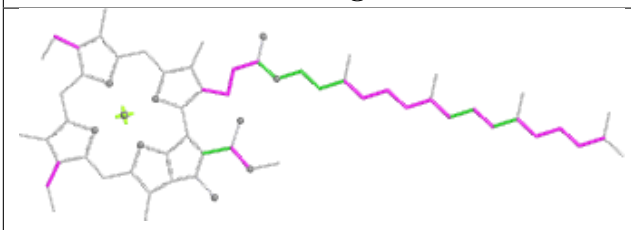
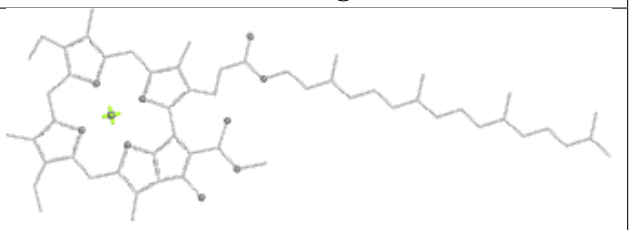
Bond angles

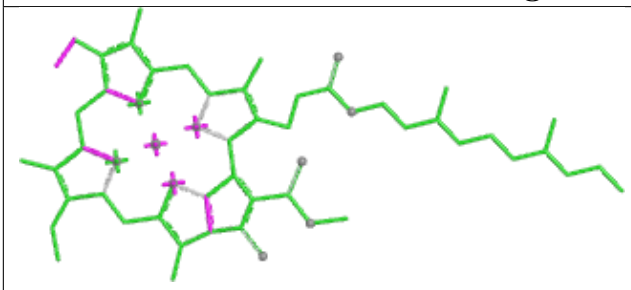
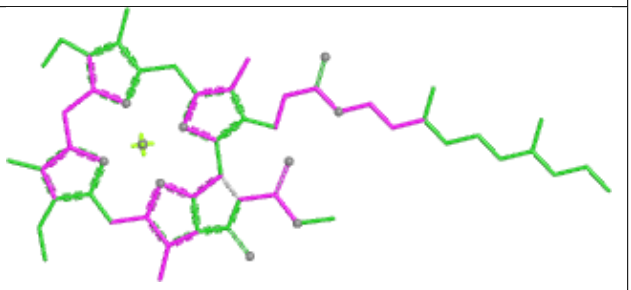
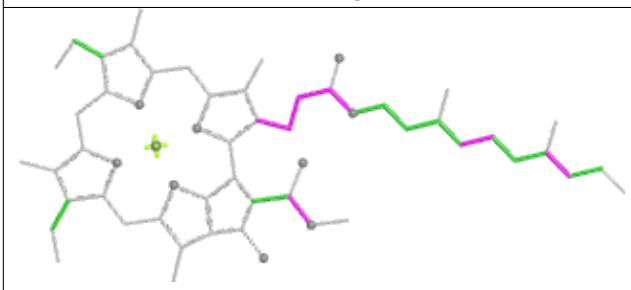
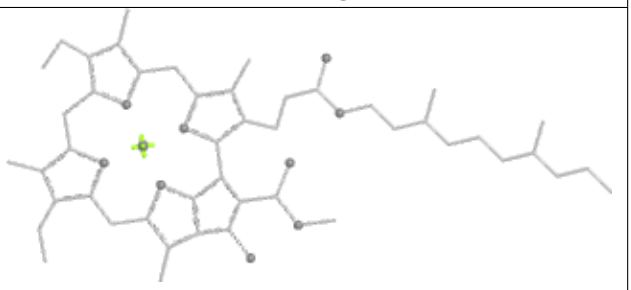


Torsions

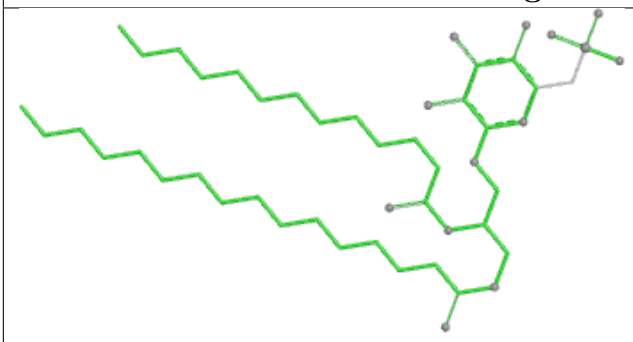


Rings

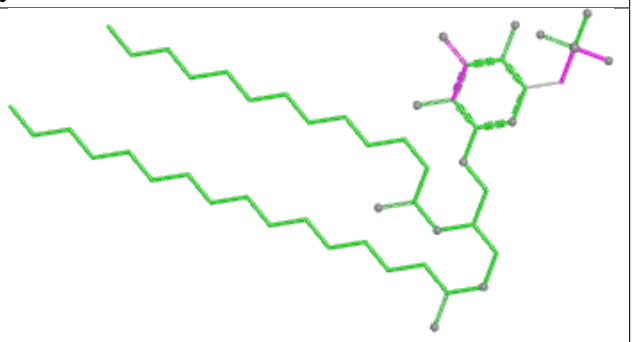
Ligand CLA 2 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

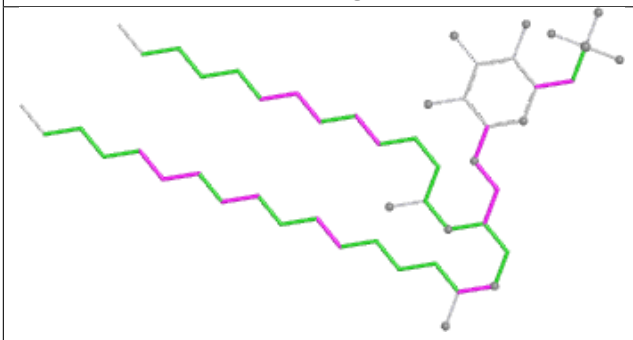
Ligand SQD R 322



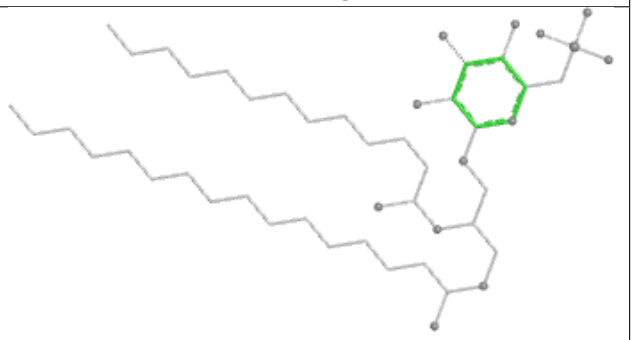
Bond lengths



Bond angles

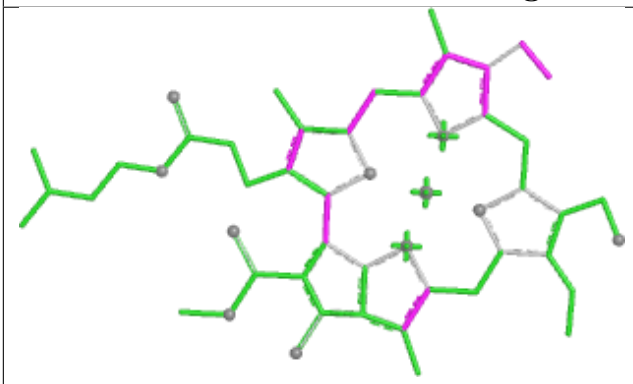


Torsions

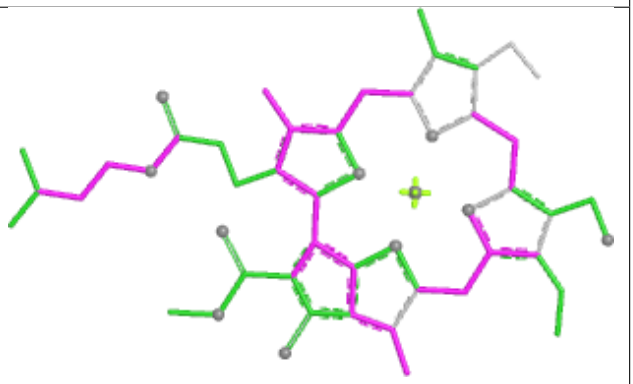


Rings

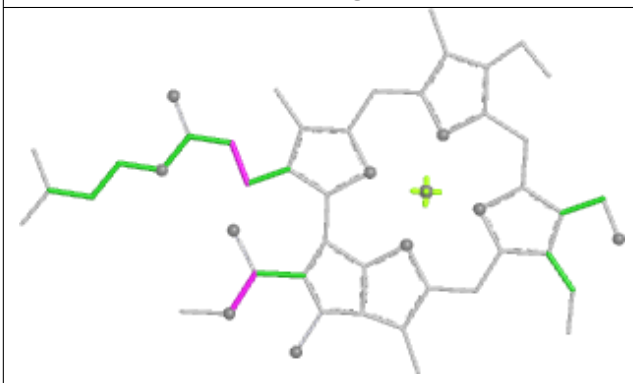
Ligand CHL G 607



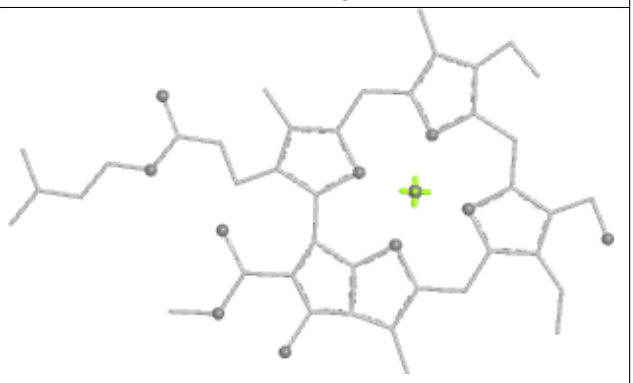
Bond lengths



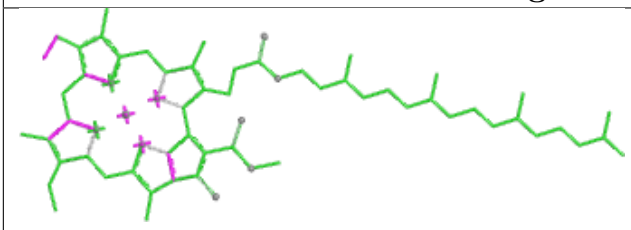
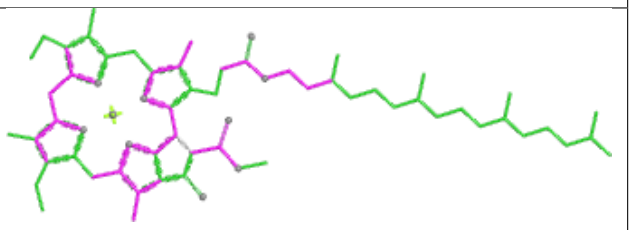
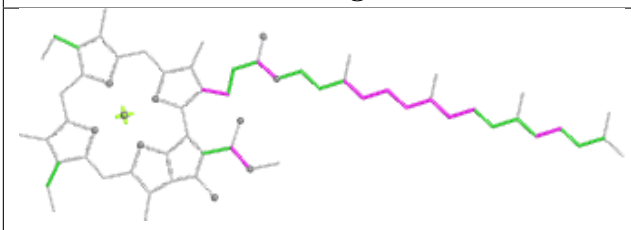
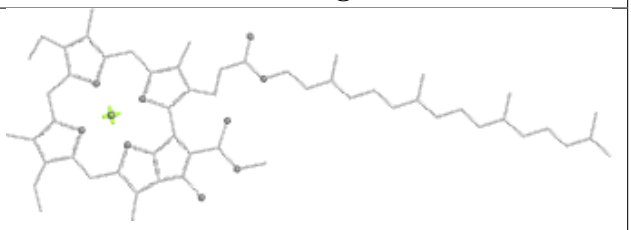
Bond angles

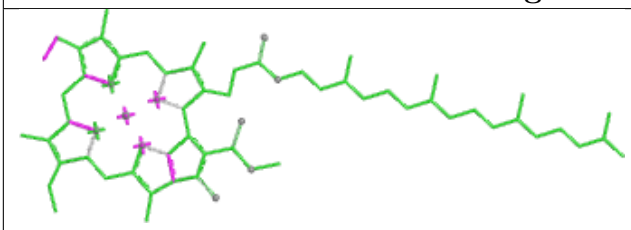
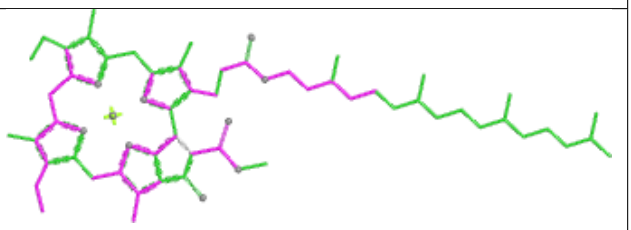
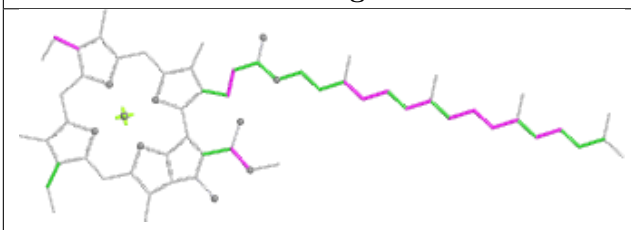
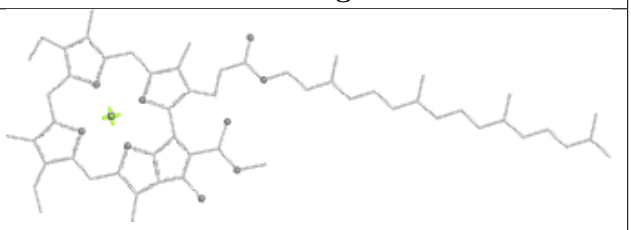


Torsions

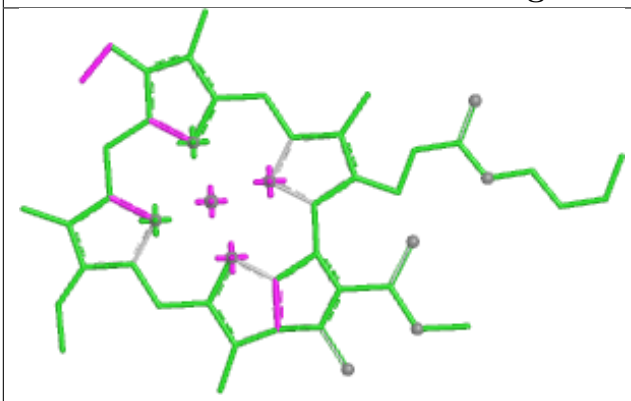


Rings

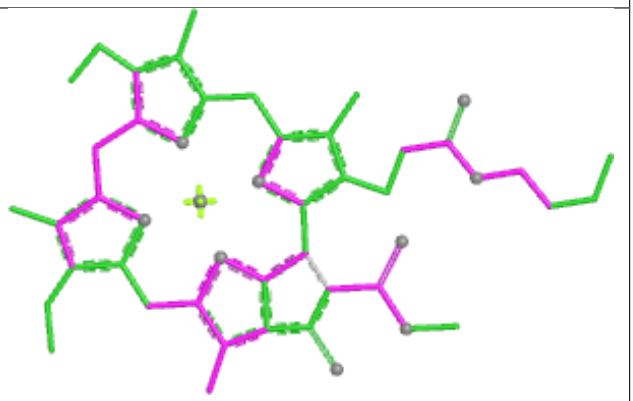
Ligand CLA 7 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

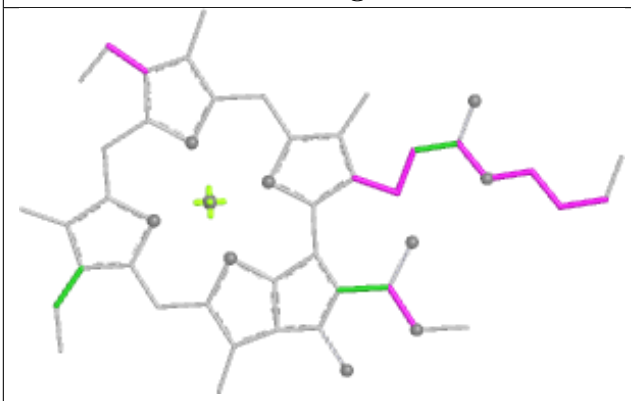
Ligand CLA b 602



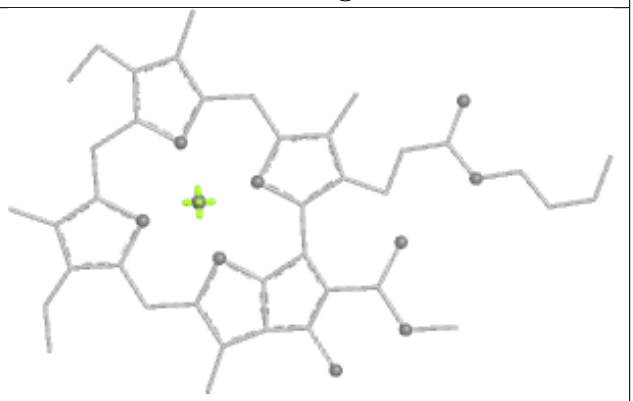
Bond lengths



Bond angles

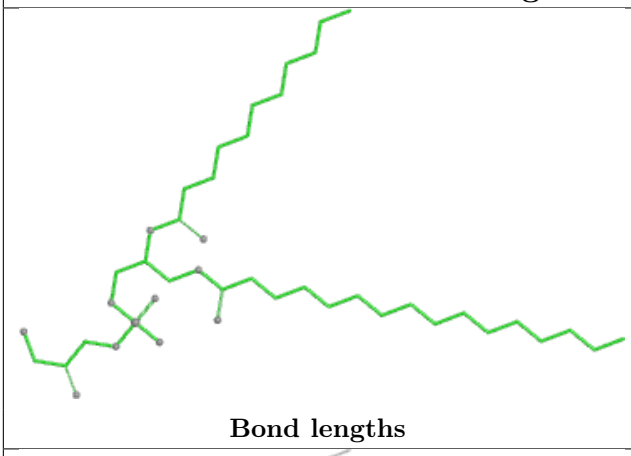


Torsions

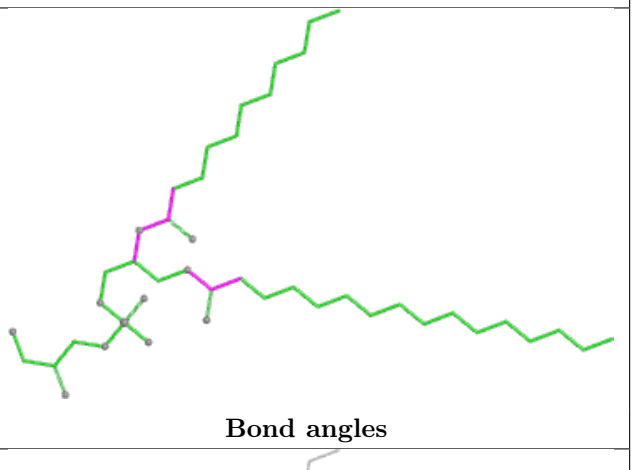


Rings

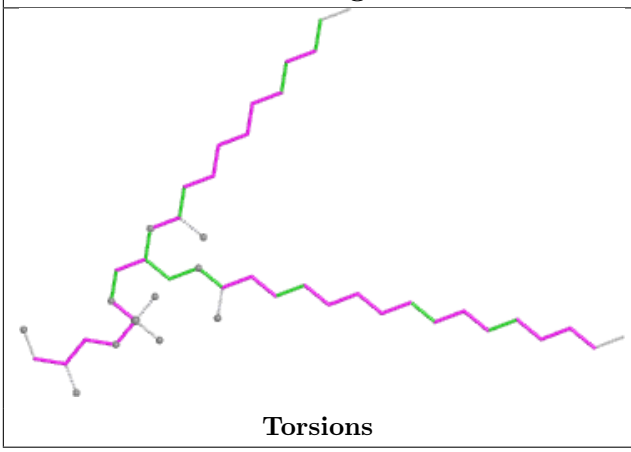
Ligand LHG D 407



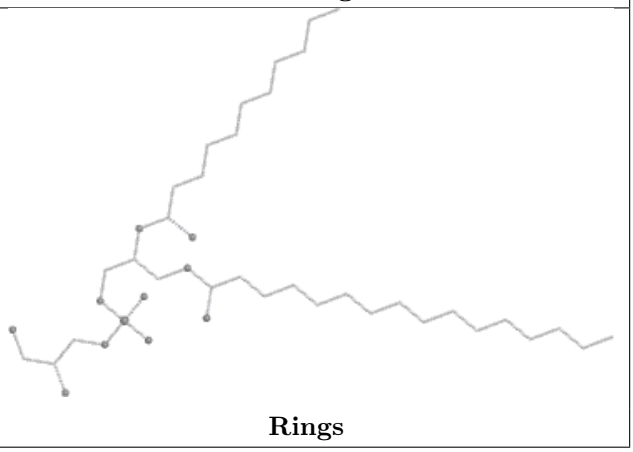
Bond lengths



Bond angles

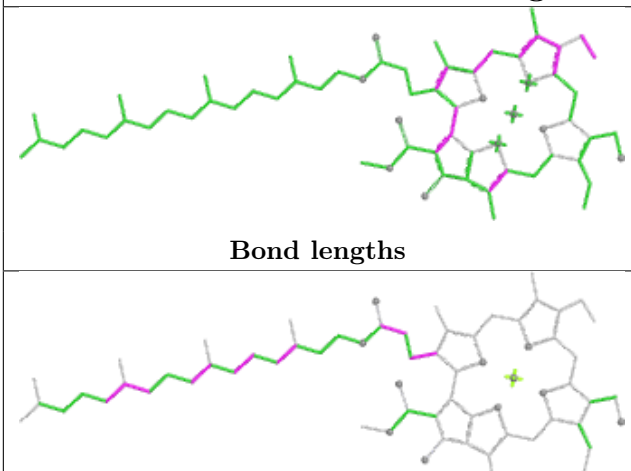


Torsions

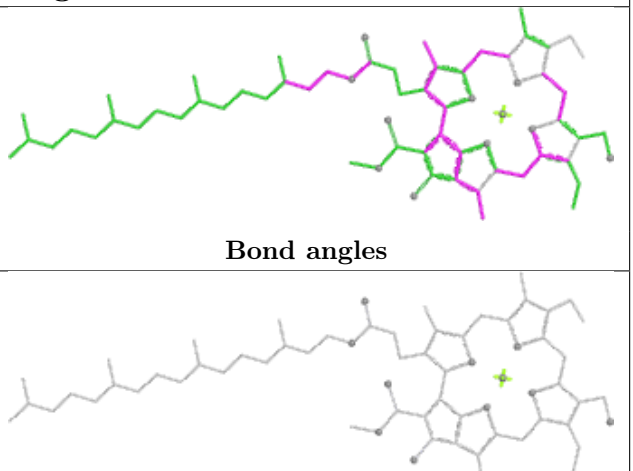


Rings

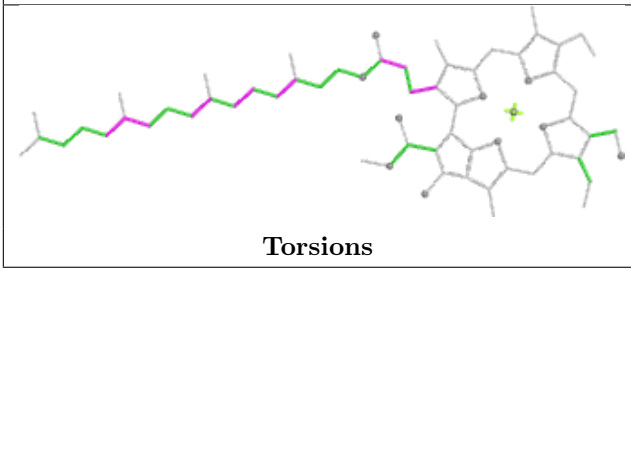
Ligand CHL g 302



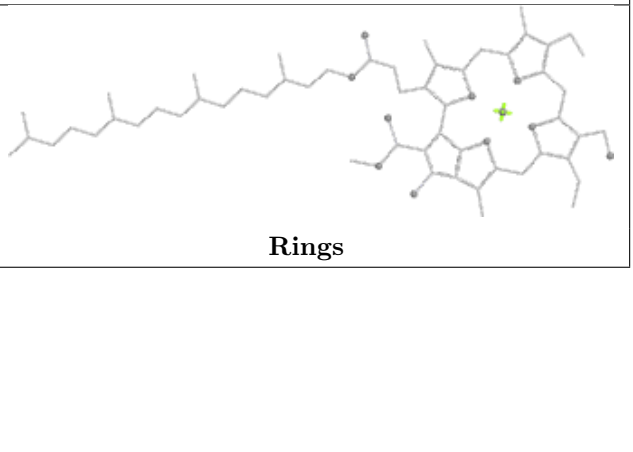
Bond lengths



Bond angles

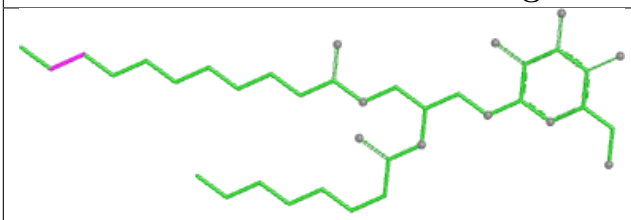


Torsions

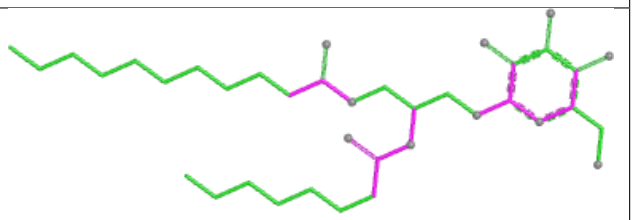


Rings

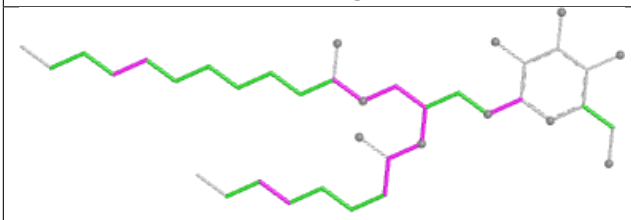
Ligand LMG b 624



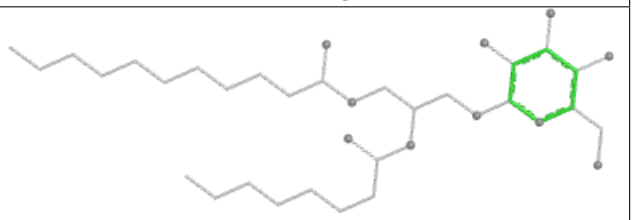
Bond lengths



Bond angles

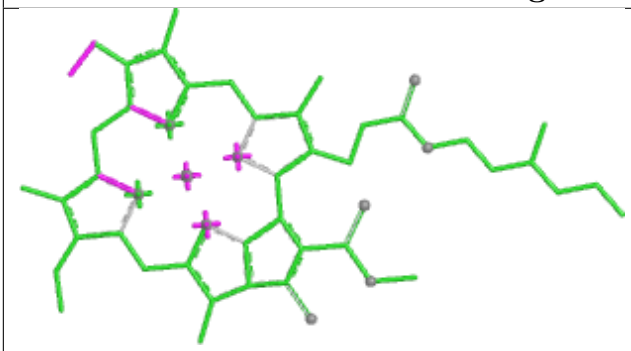


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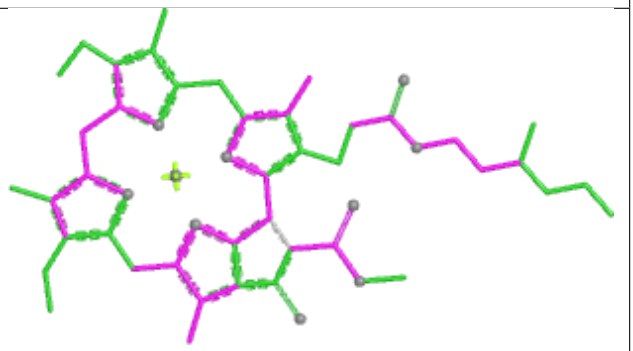


Rings

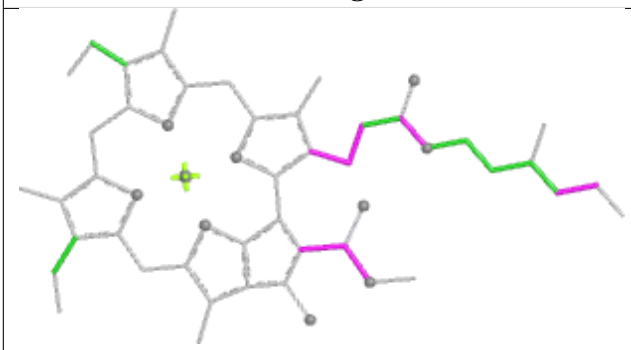
Ligand CLA 5 603



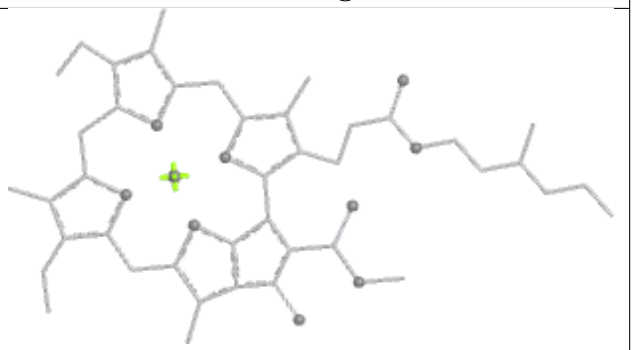
Bond lengths



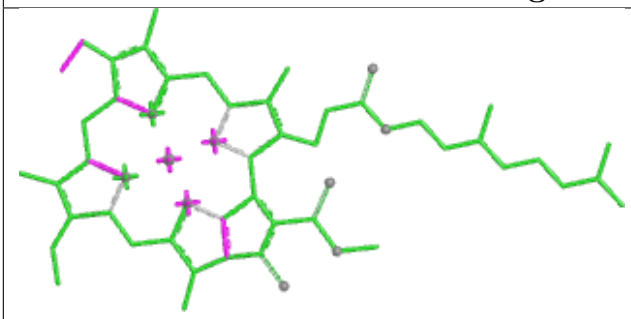
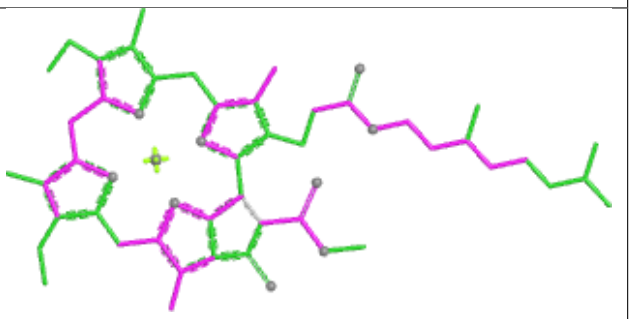
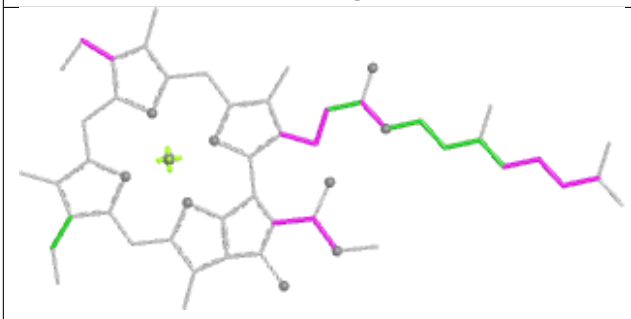
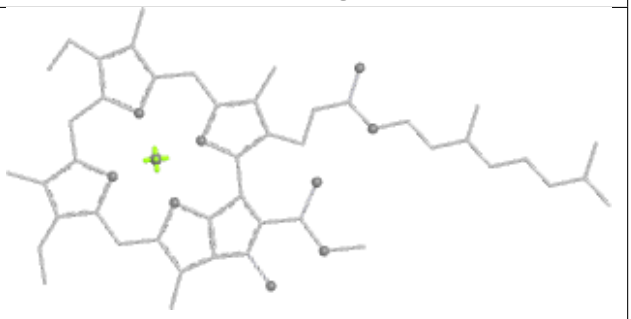
Bond angles

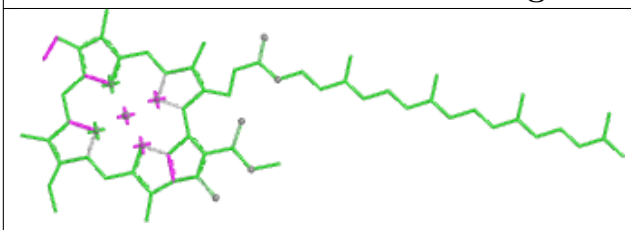
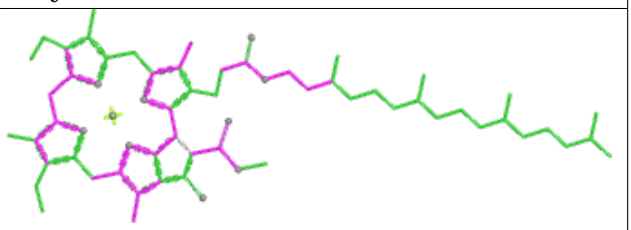
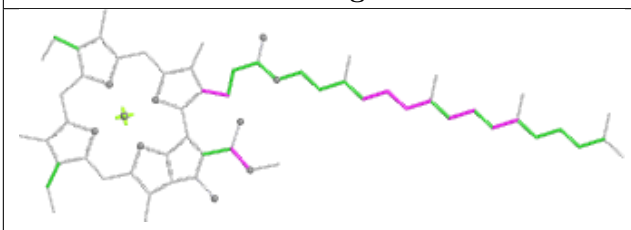
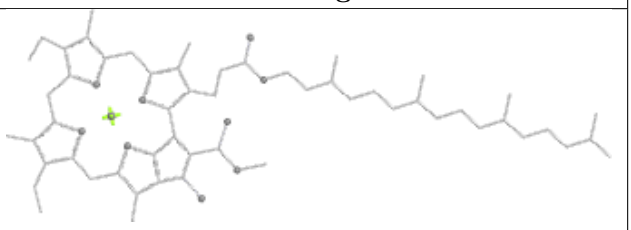


Torsions

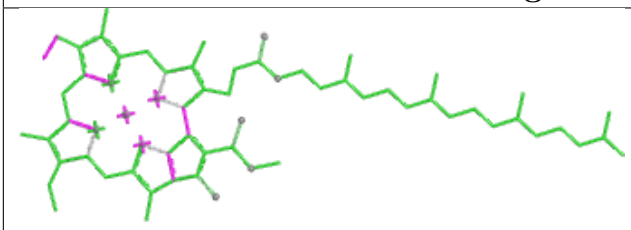


Rings

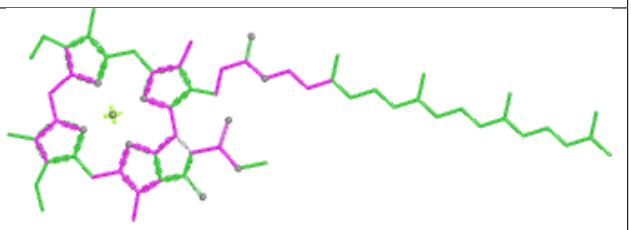
Ligand CLA 6 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA y 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

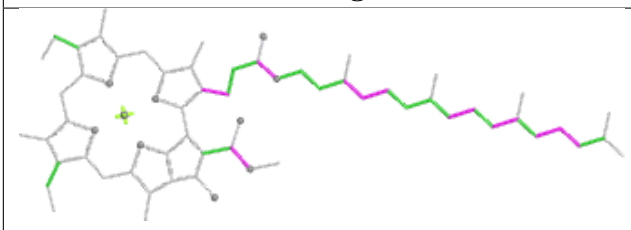
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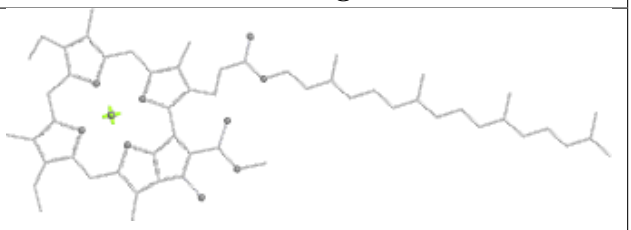
Bond lengths



Bond angles

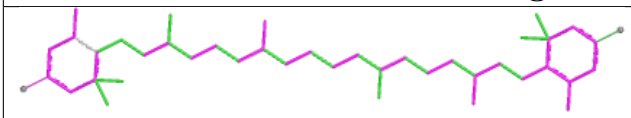


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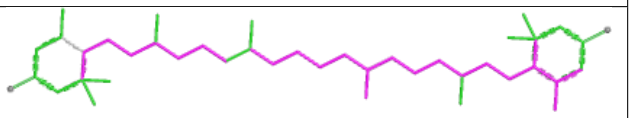


Rings

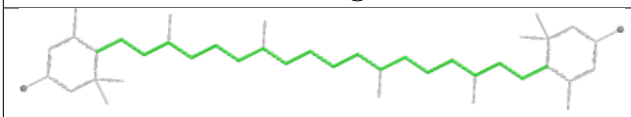
Ligand LUT 0 617



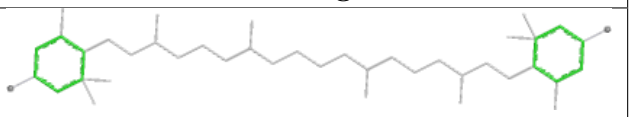
Bond lengths



Bond angles

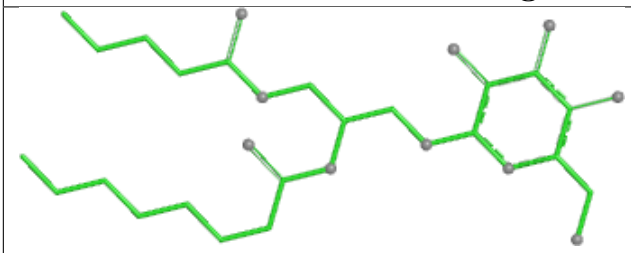


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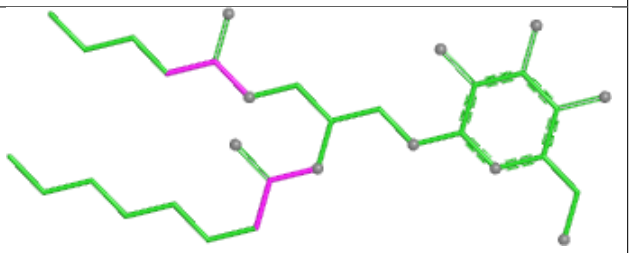


Rings

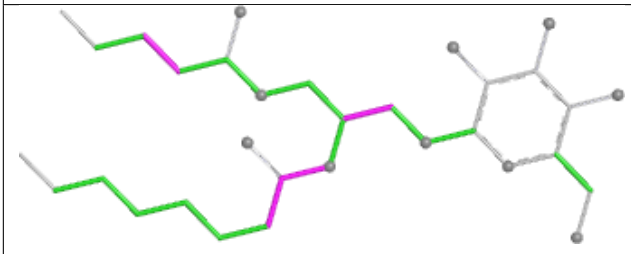
Ligand LMG C 622



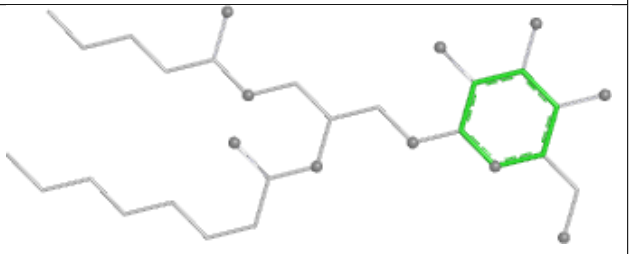
Bond lengths



Bond angles

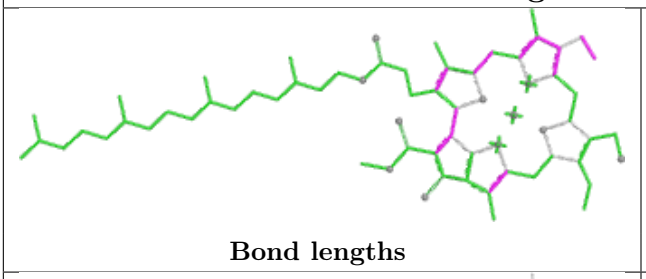


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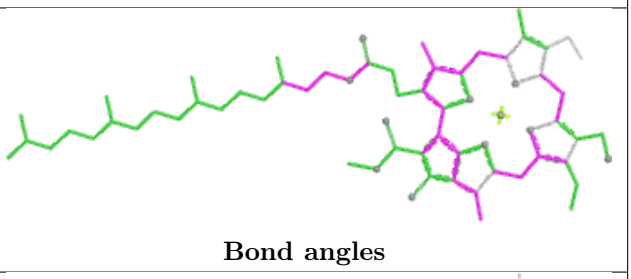


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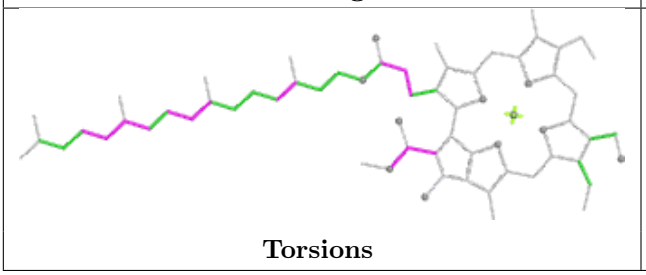
Ligand CHL 8 605



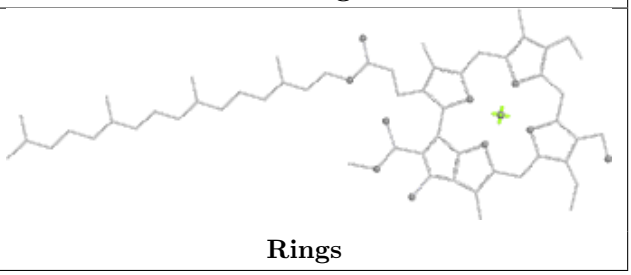
Bond lengths



Bond angles

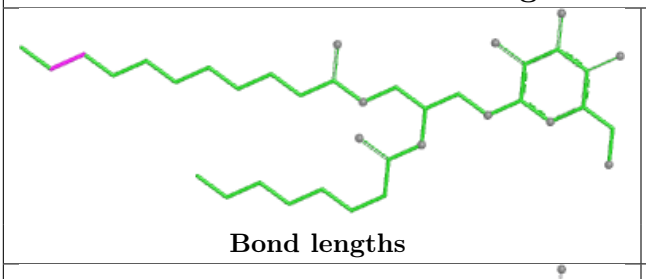


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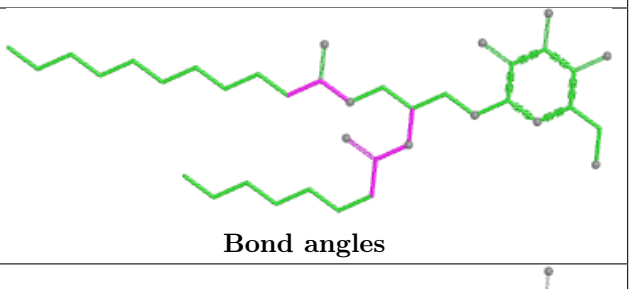


Rings

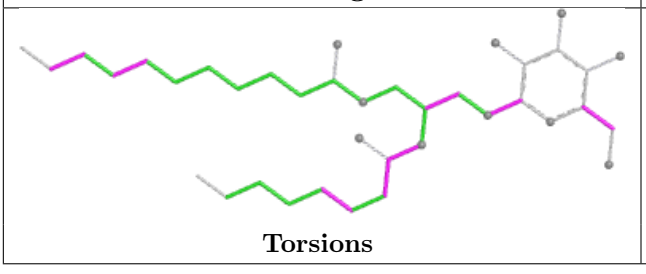
Ligand LMG w 204



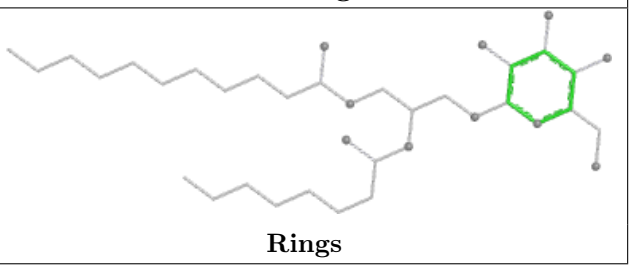
Bond lengths



Bond angles

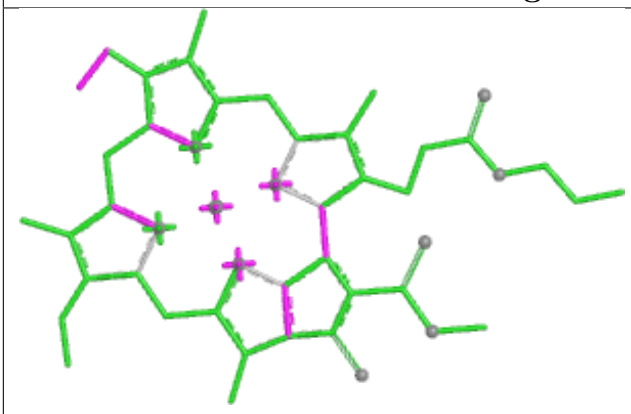


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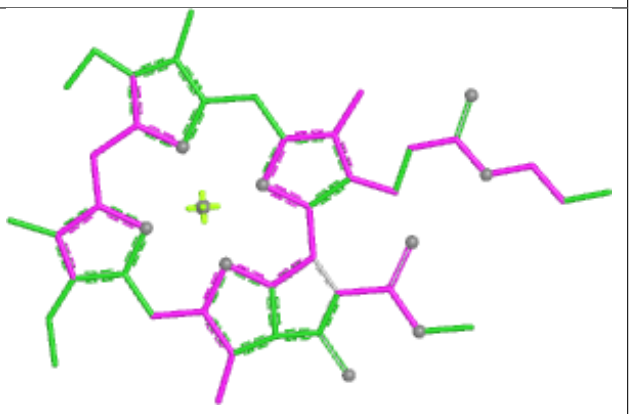


Rings

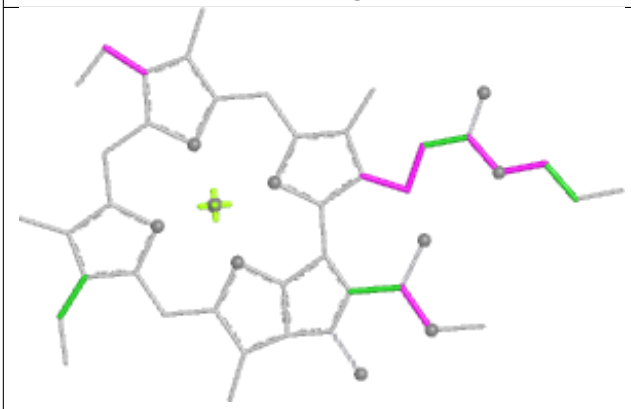
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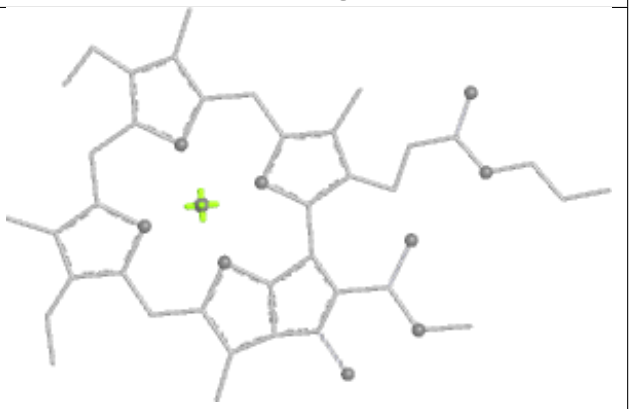
Bond lengths



Bond angles

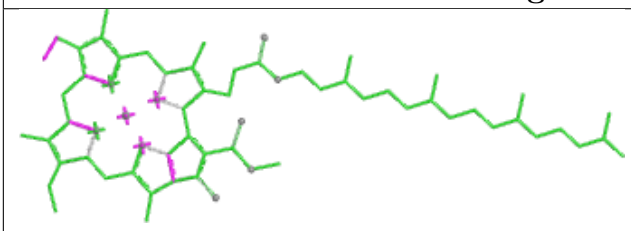


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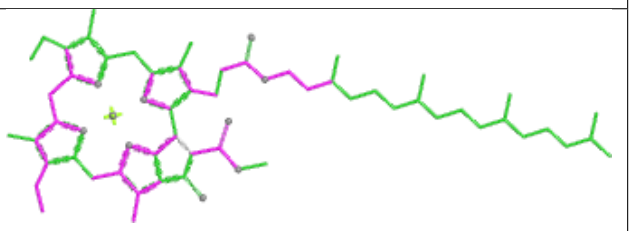


Rings

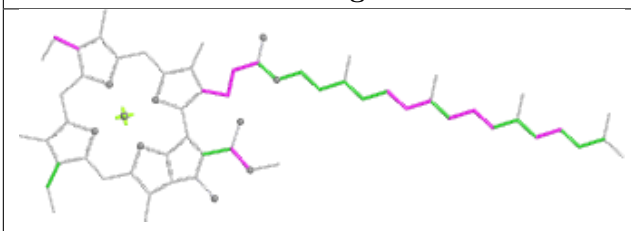
Ligand CLA b 607



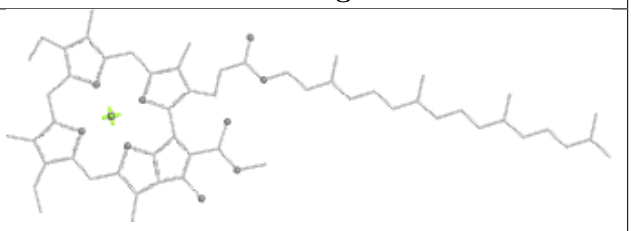
Bond lengths



Bond angles

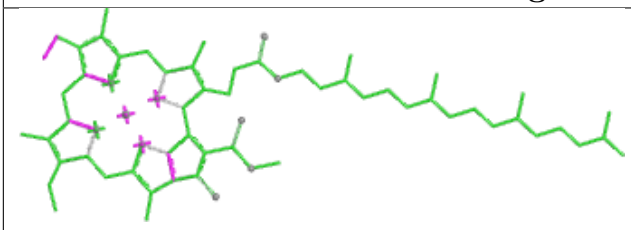


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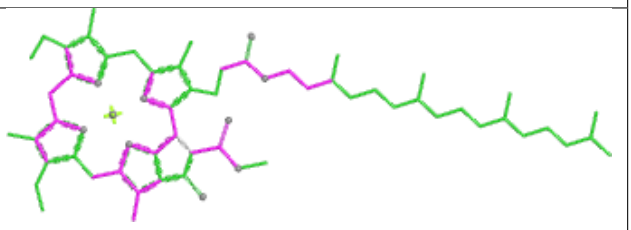


Rings

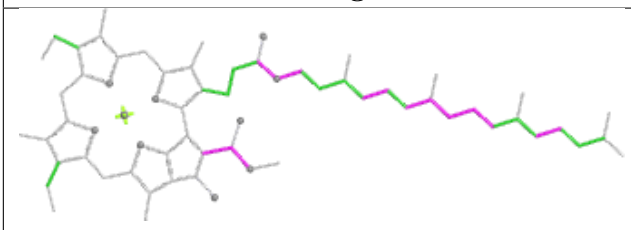
Ligand CLA 1 604



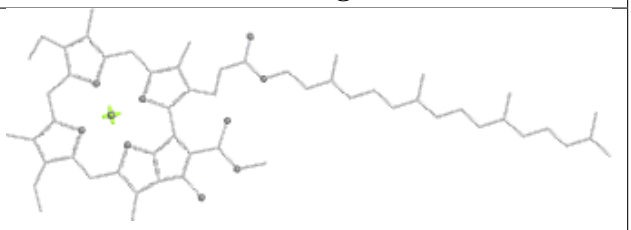
Bond lengths



Bond angles

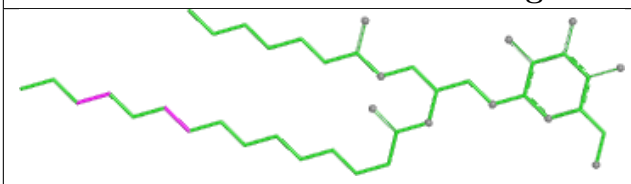


Torsions

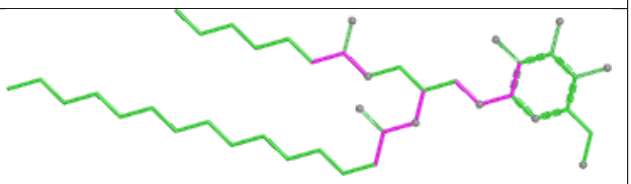


Rings

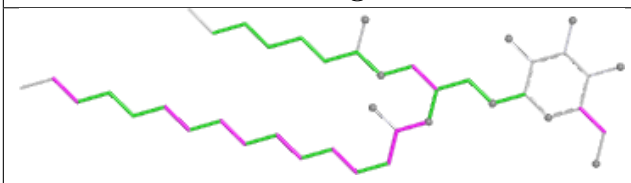
Ligand LMG s 321



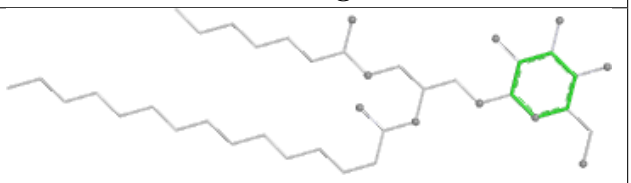
Bond lengths



Bond angles

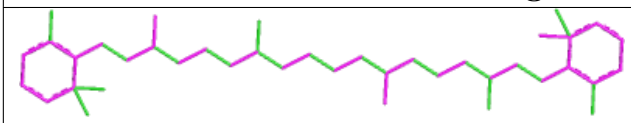


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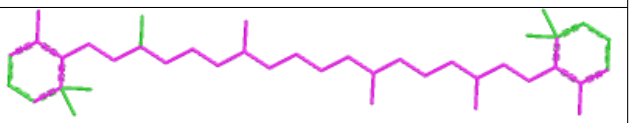


Rings

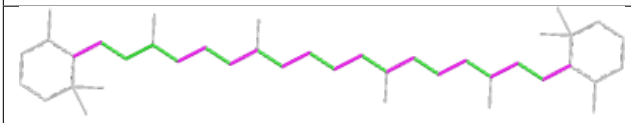
Ligand BCR b 618



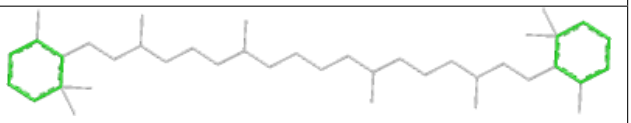
Bond lengths



Bond angles

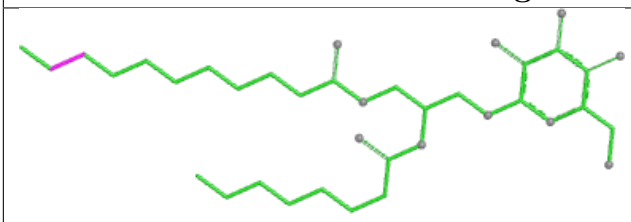


Torsions

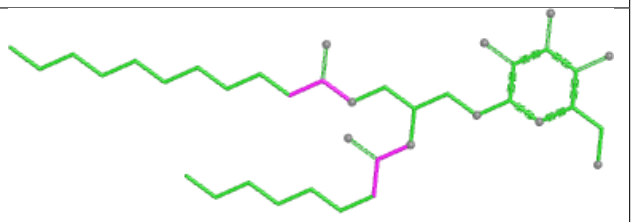


Rings

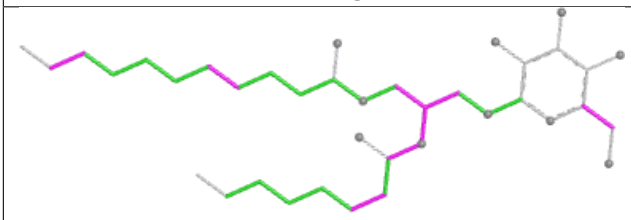
Ligand LMG W 203



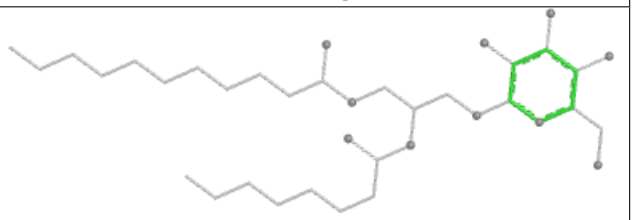
Bond lengths



Bond angles

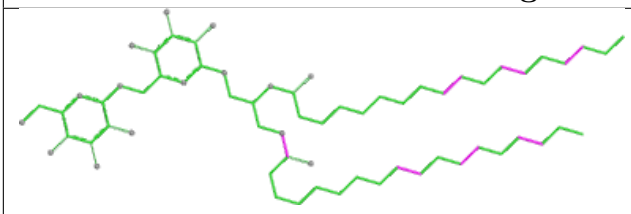


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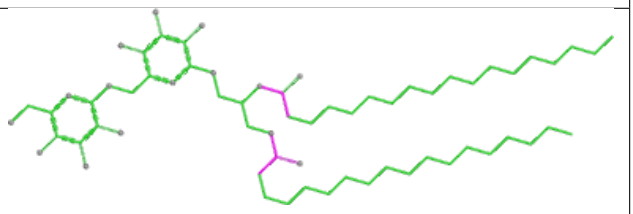


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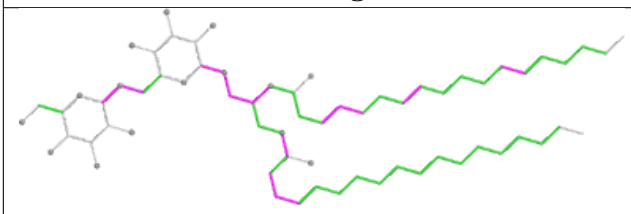
Ligand DGD C 617



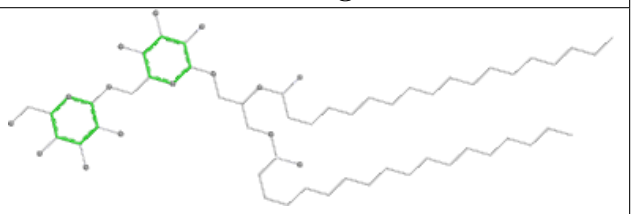
Bond lengths



Bond angles

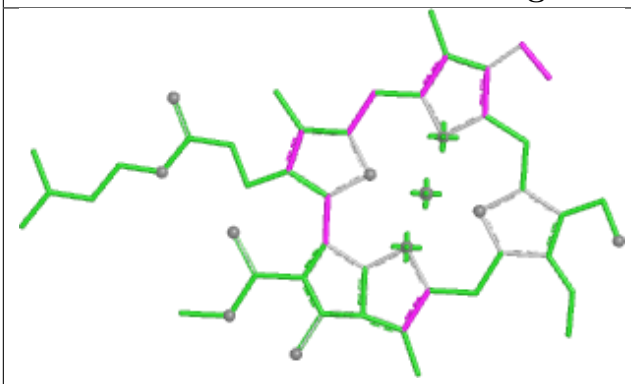


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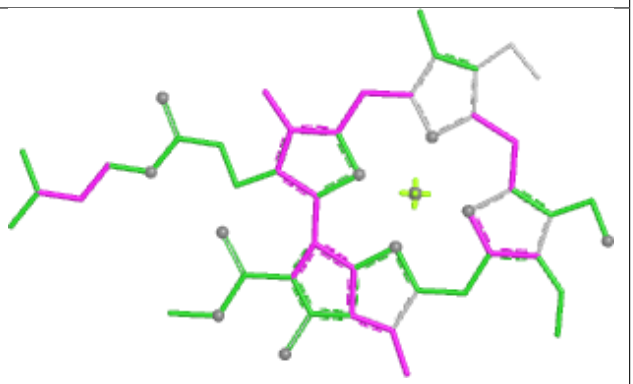


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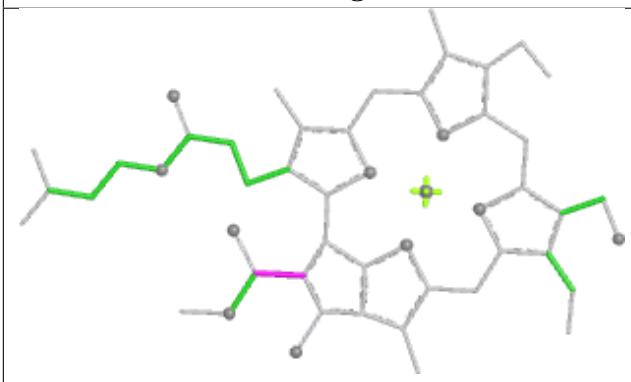
Ligand CHL 5 606



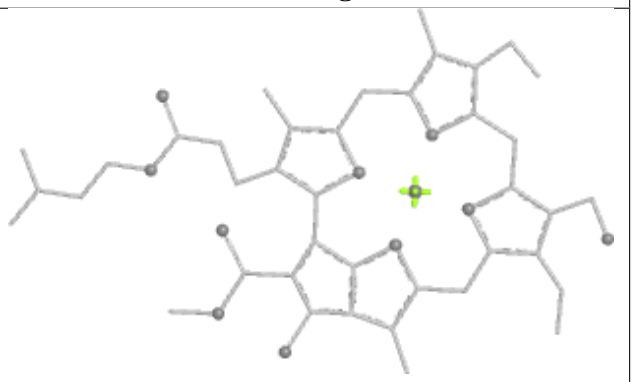
Bond lengths



Bond angles

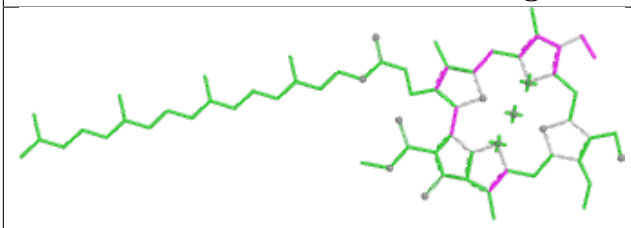


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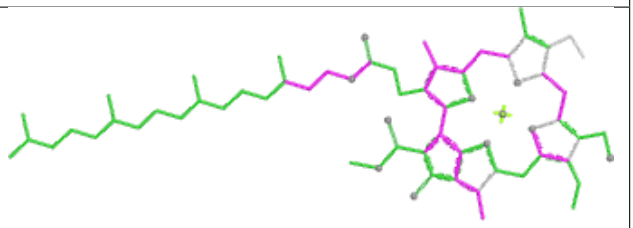


Rings

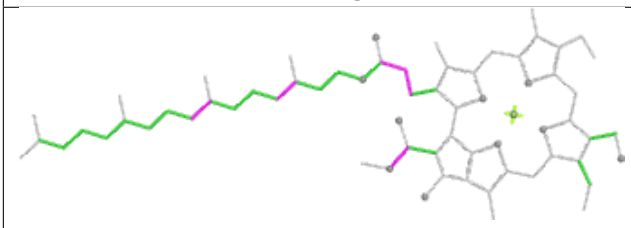
Ligand CHL N 306



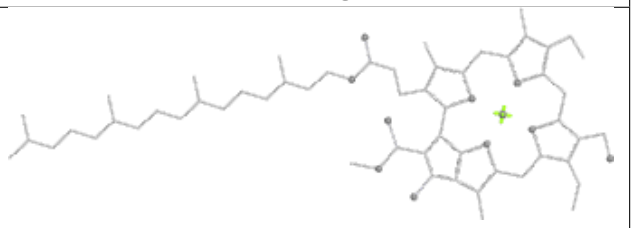
Bond lengths



Bond angles

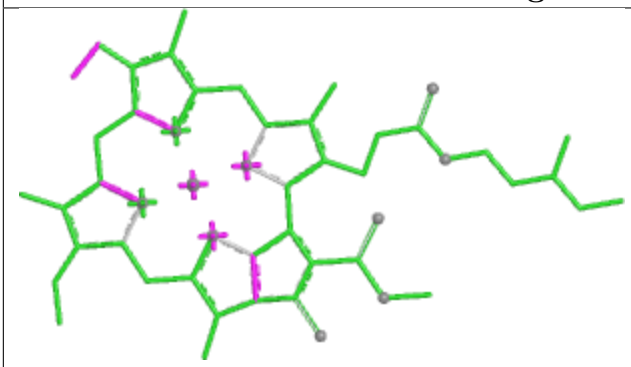


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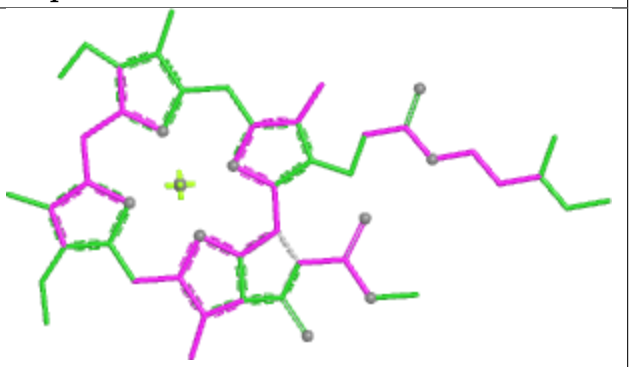


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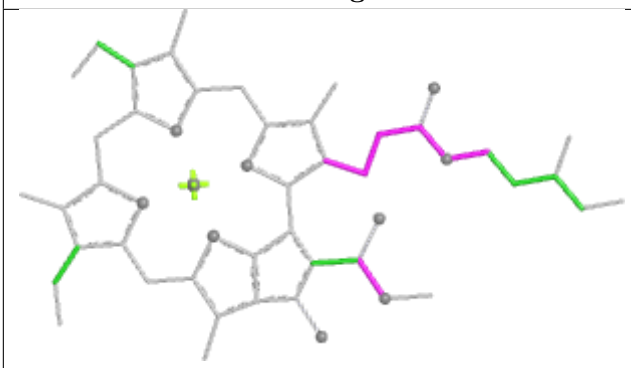
Ligand CLA p 614



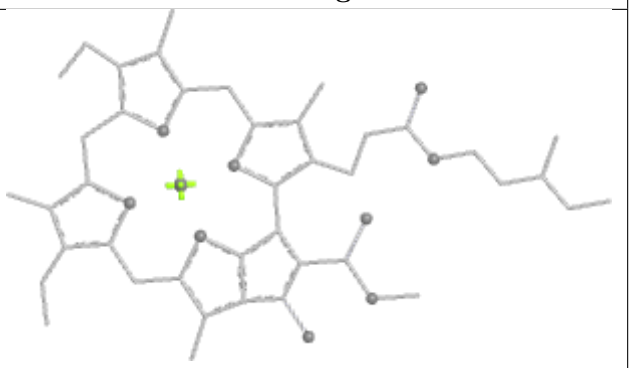
Bond lengths



Bond angles

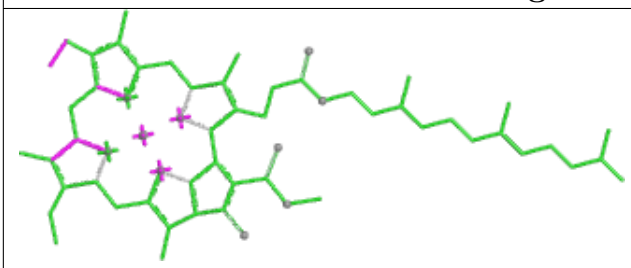


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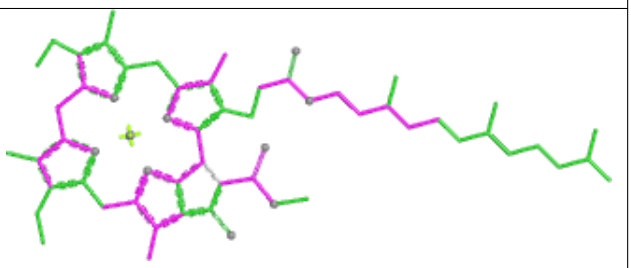


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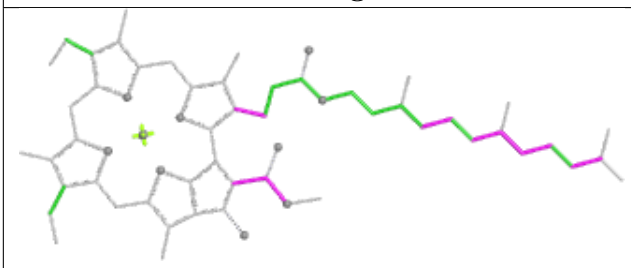
Ligand CLA 3 304



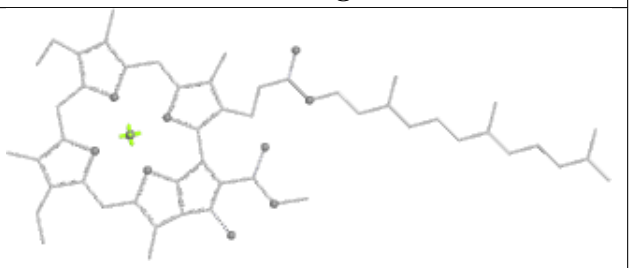
Bond lengths



Bond angles

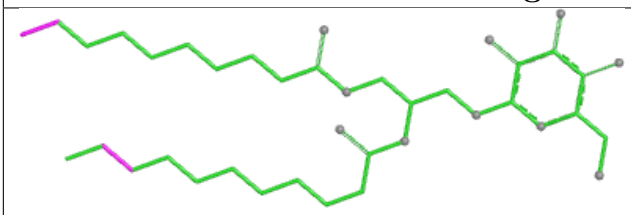


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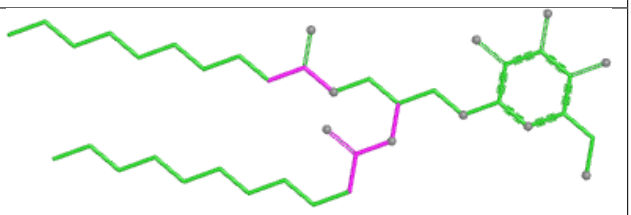


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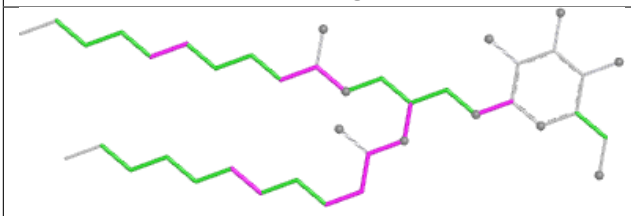
Ligand LMG 9 302



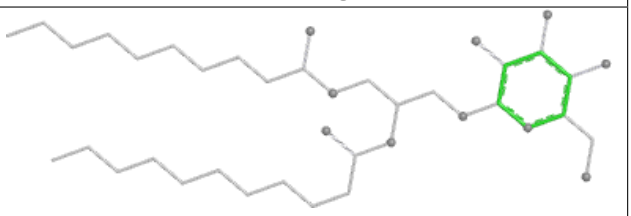
Bond lengths



Bond angles

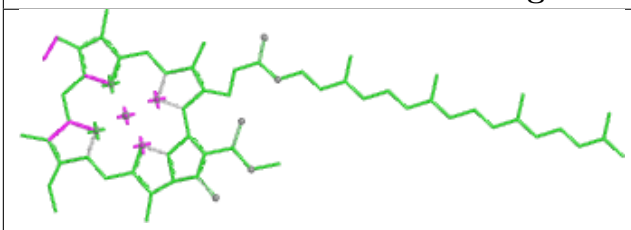


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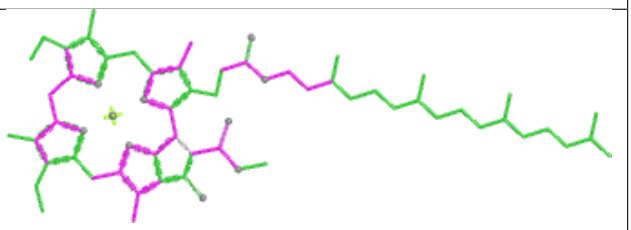


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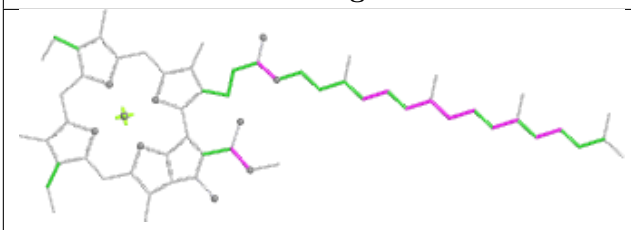
Ligand CLA b 612



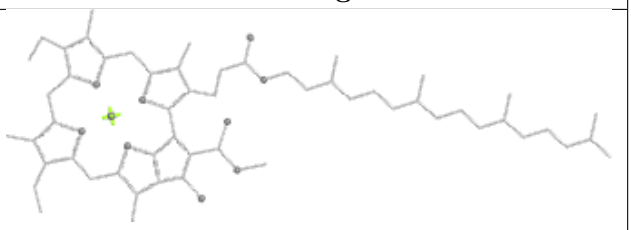
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Bond angles

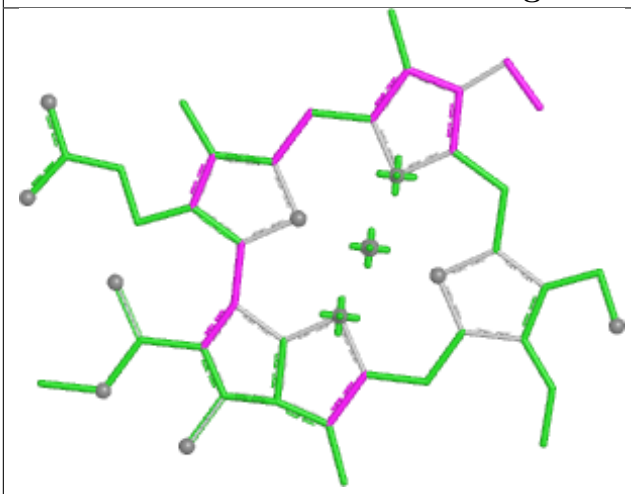


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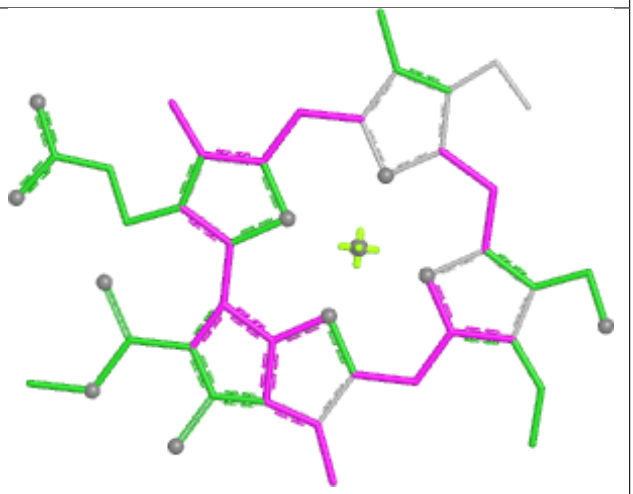


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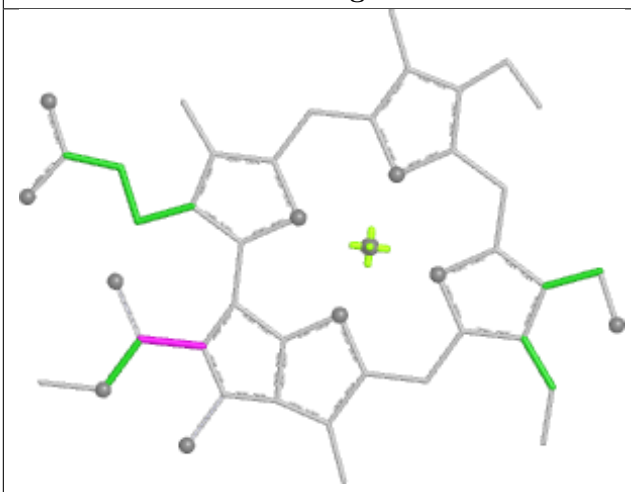
Ligand CHL Y 306



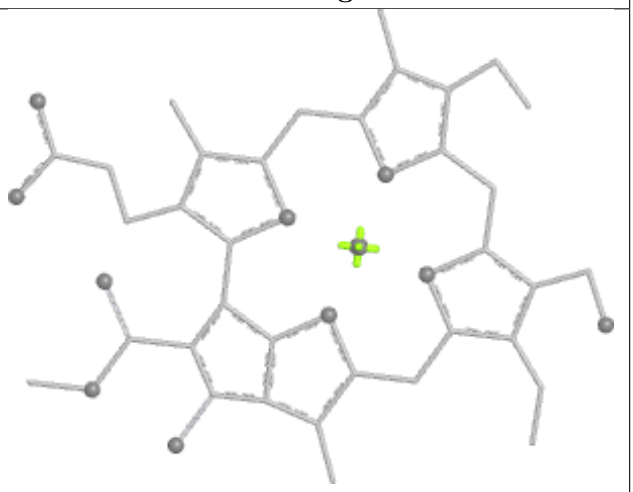
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Bond angles

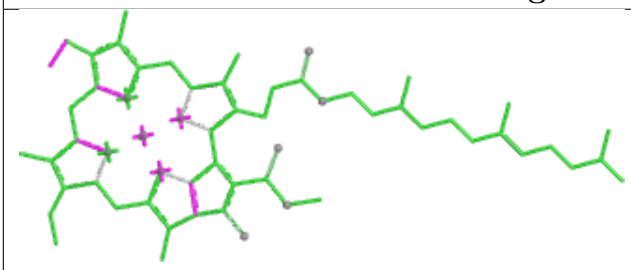


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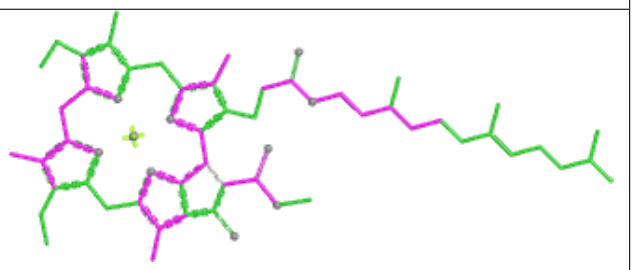


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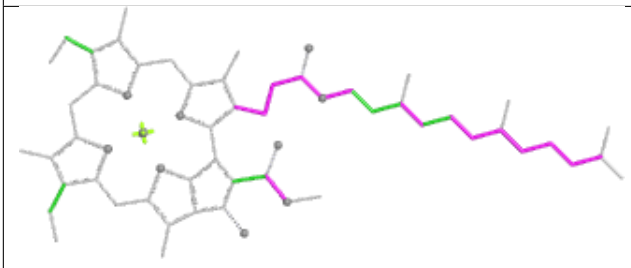
Ligand CLA 4 610



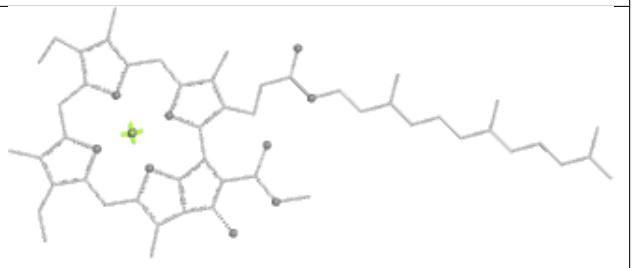
Bond lengths



Bond angles

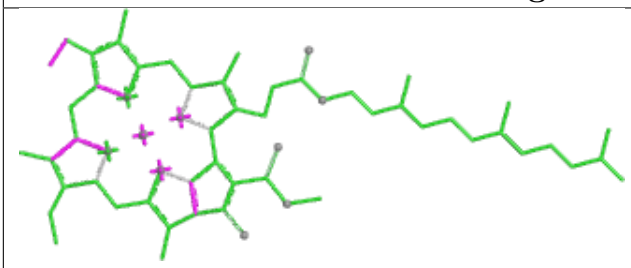


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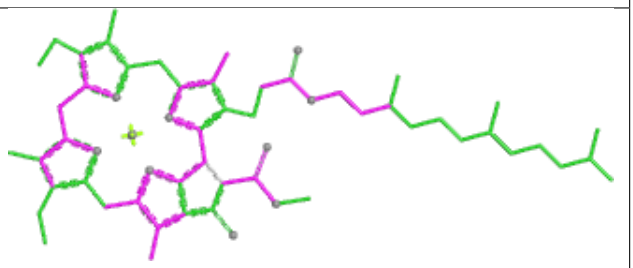


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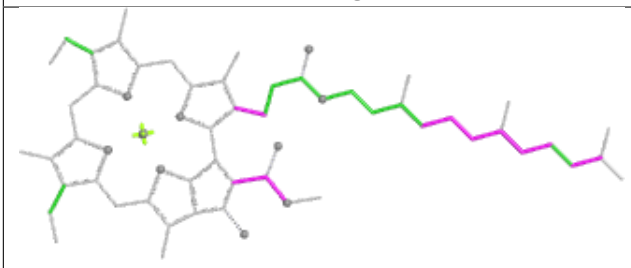
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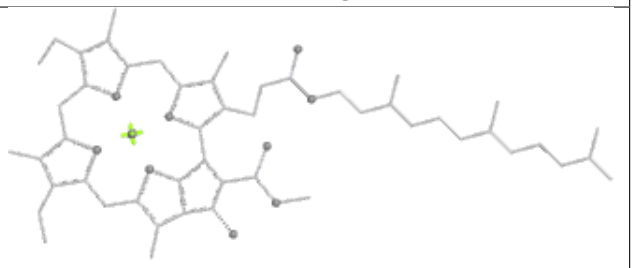
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Bond angles

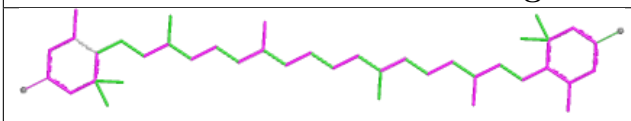


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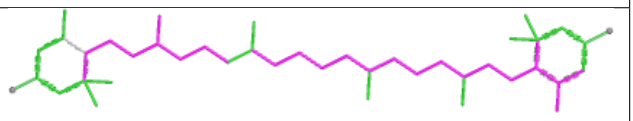


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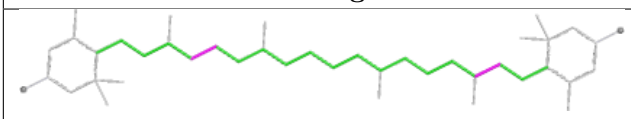
Ligand LUT Y 316



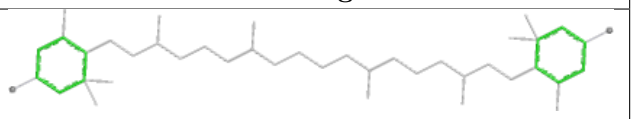
Bond lengths



Bond angles

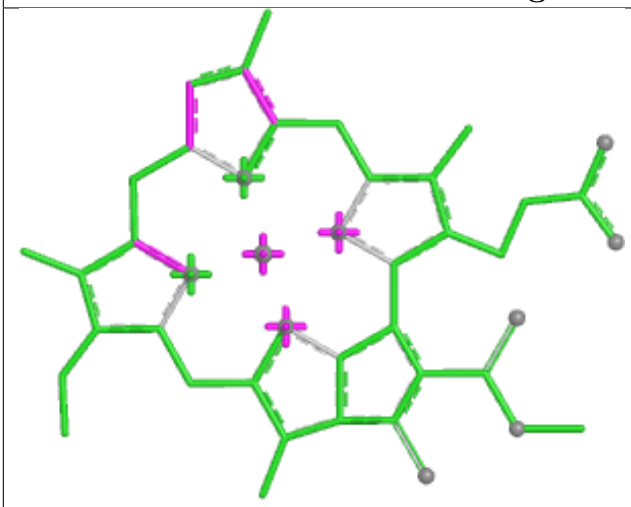


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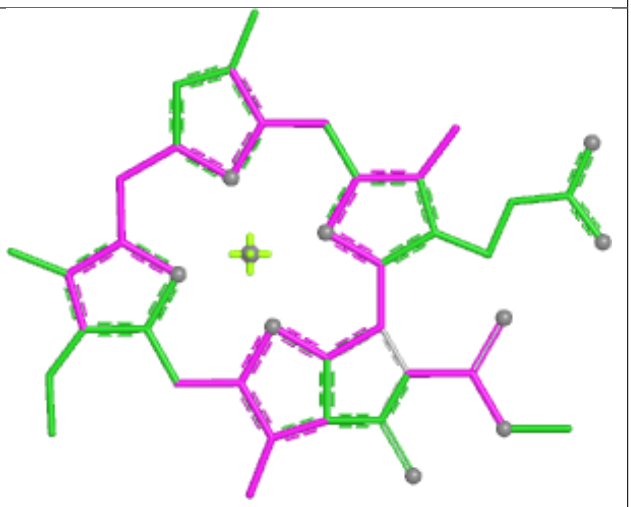


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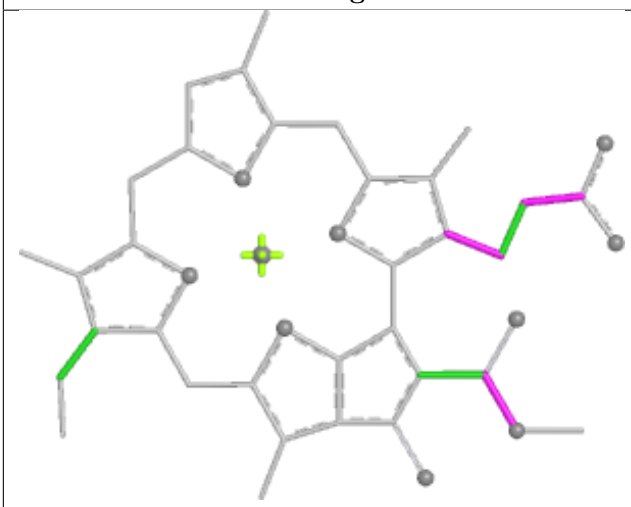
Ligand CLA 4 611



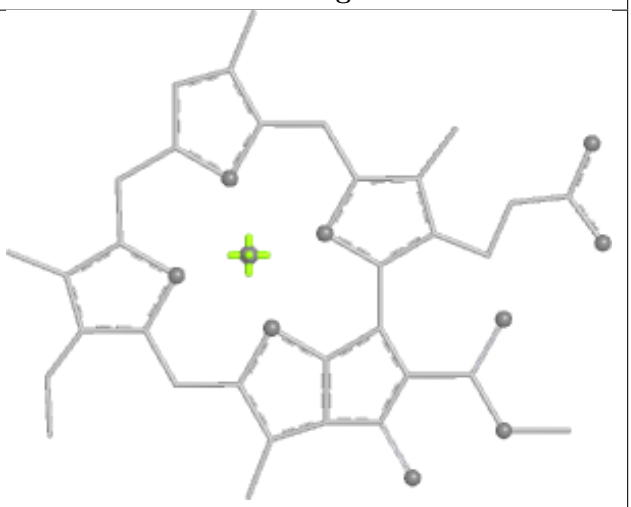
Bond lengths



Bond angles

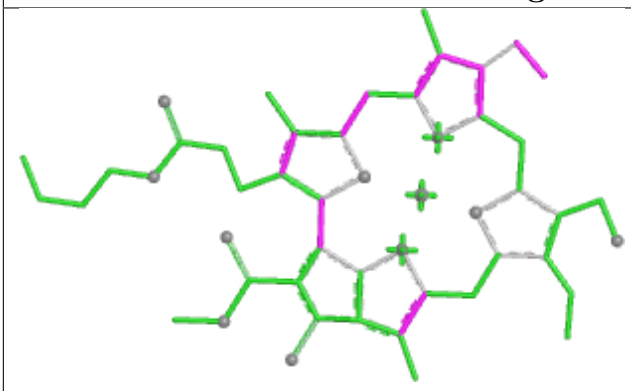


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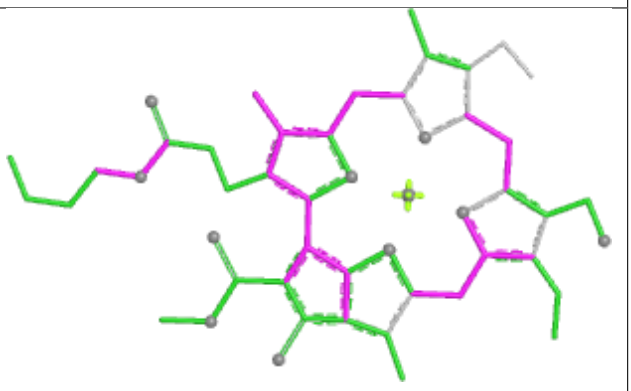


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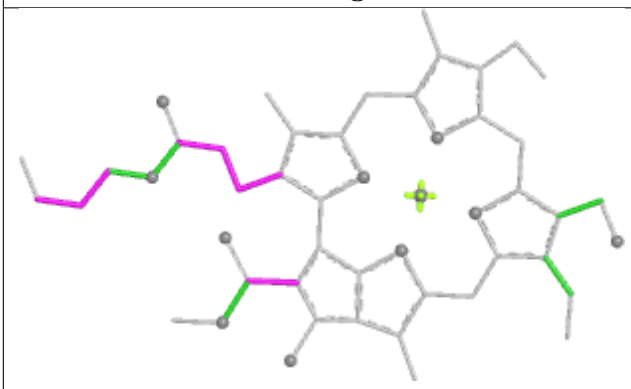
Ligand CHL 7 309



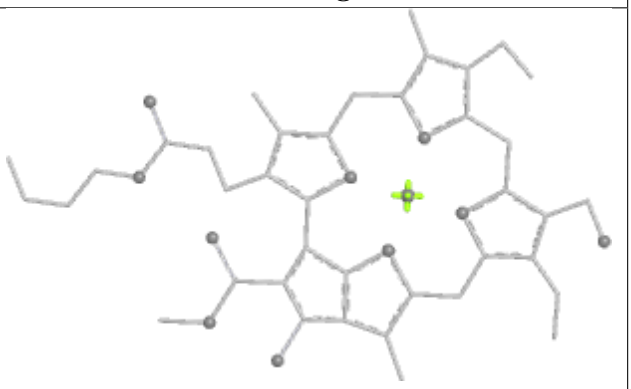
Bond lengths



Bond angles

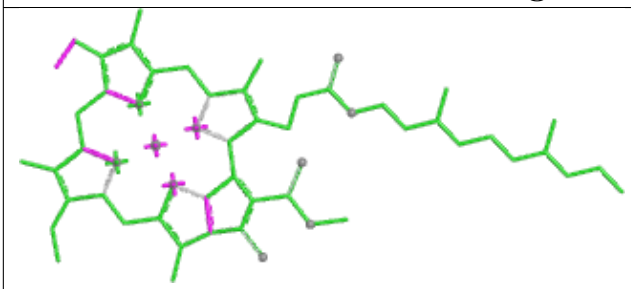


Torsions

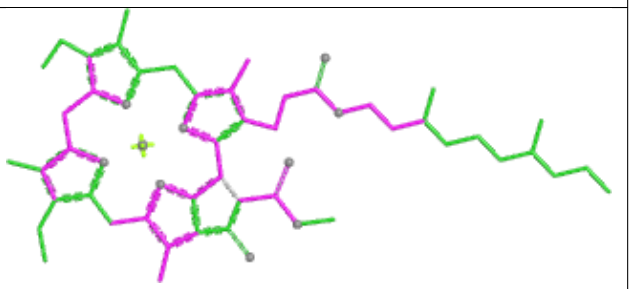


Rings

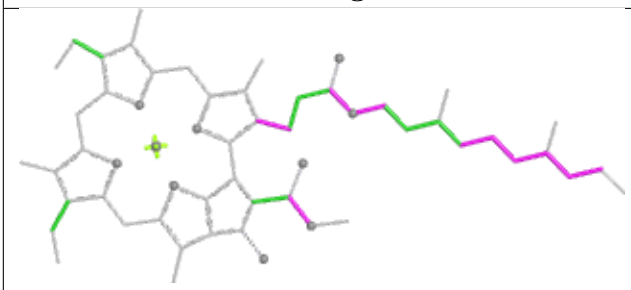
Ligand CLA 3 316



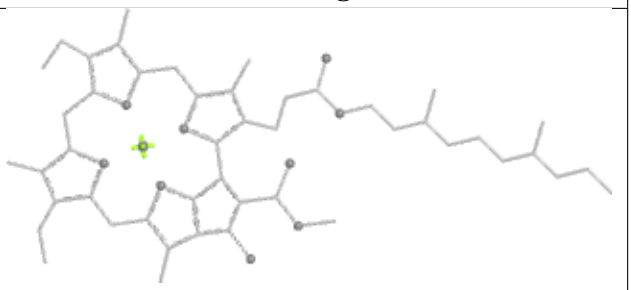
Bond lengths



Bond angles

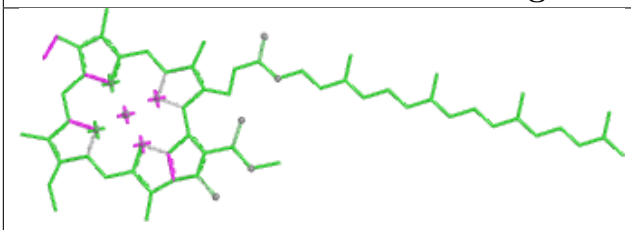


Torsions

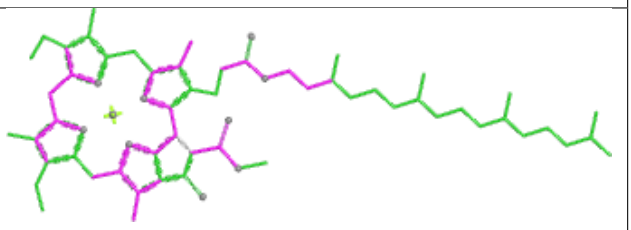


Rings

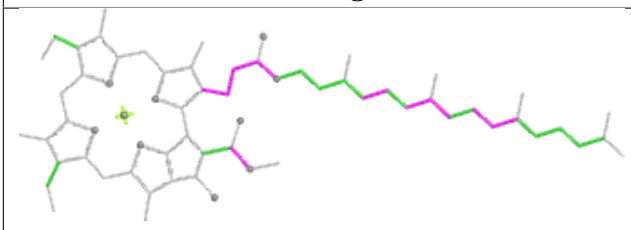
Ligand CLA 7 312



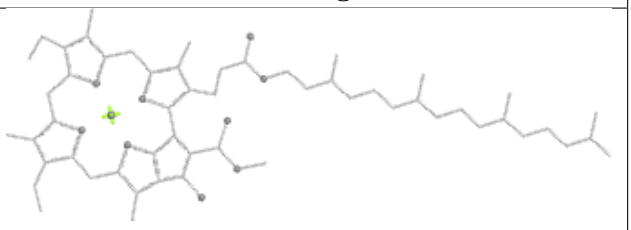
Bond lengths



Bond angles

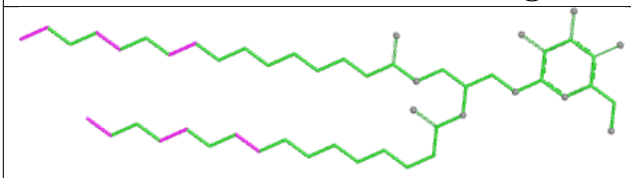


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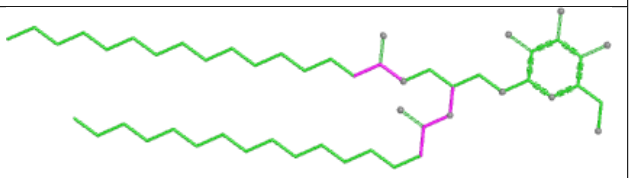


Rings

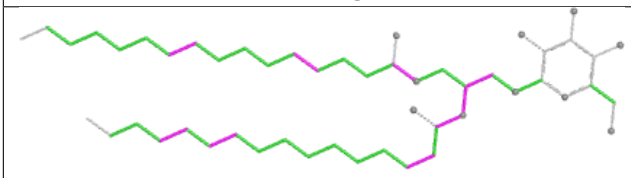
Ligand LMG J 101



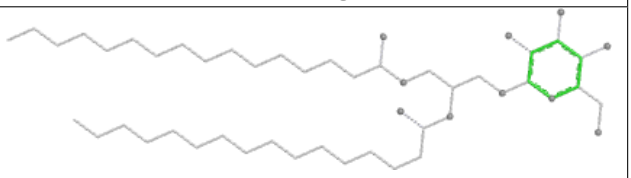
Bond lengths



Bond angles

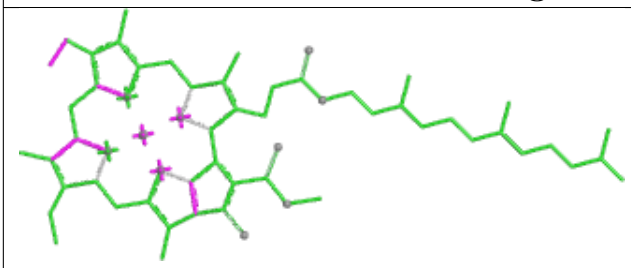


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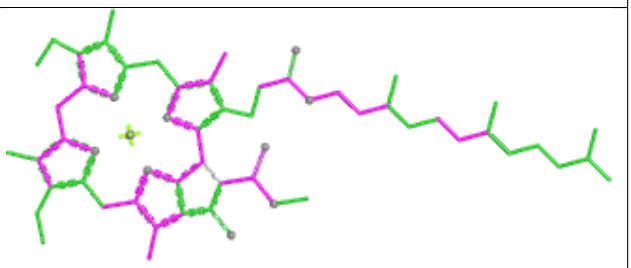


Rings

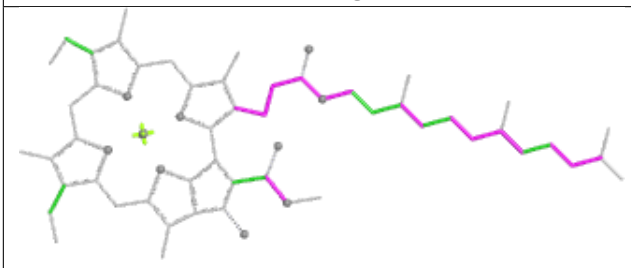
Ligand CLA 2 609



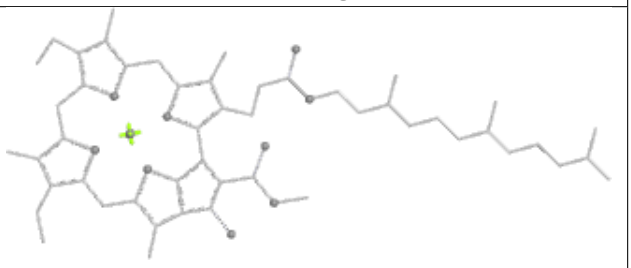
Bond lengths



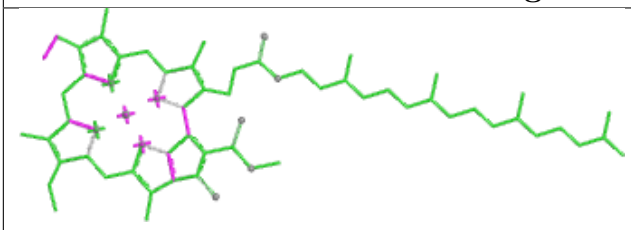
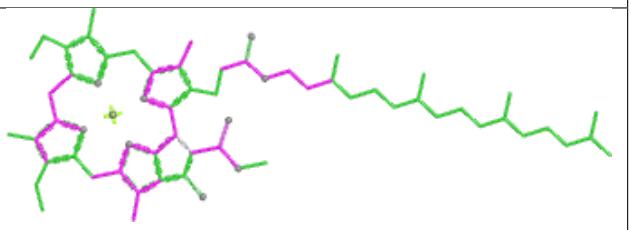
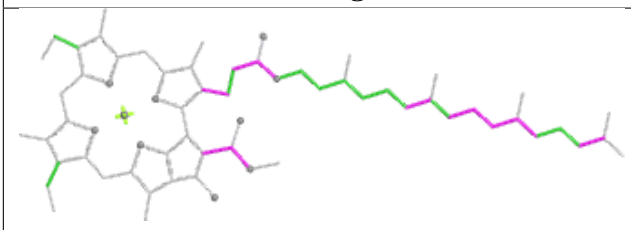
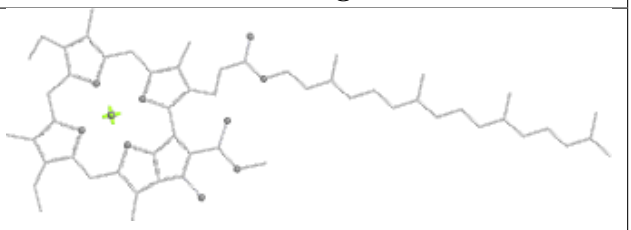
Bond angles

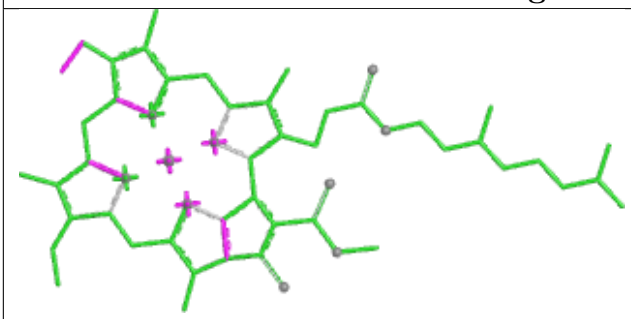
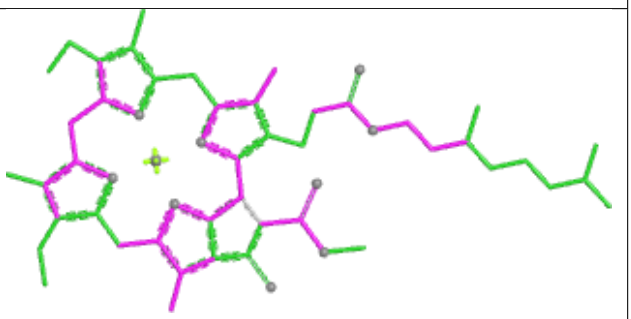
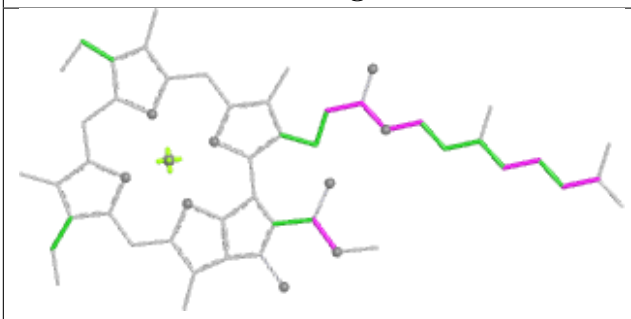
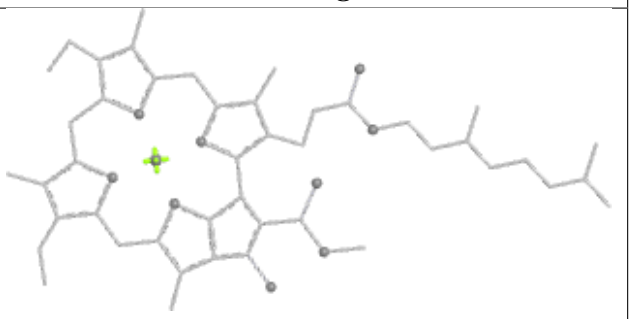


Torsions

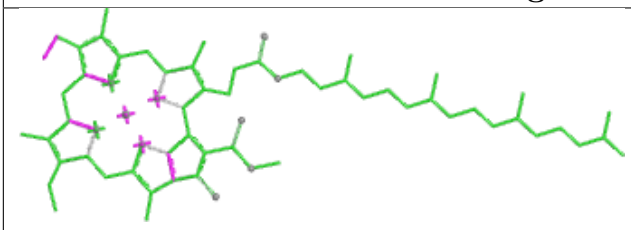


Rings

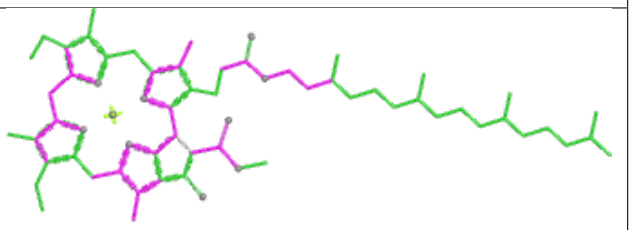
Ligand CLA C 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

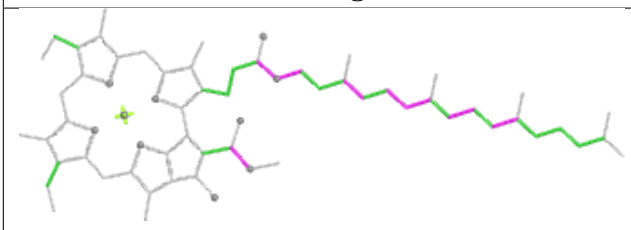
Ligand CLA b 614



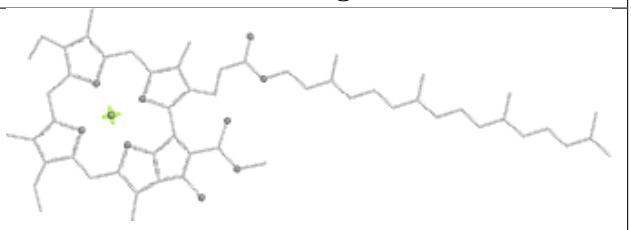
Bond lengths



Bond angles

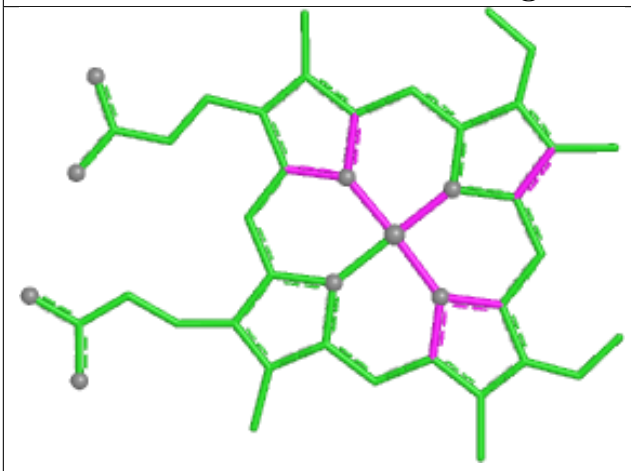


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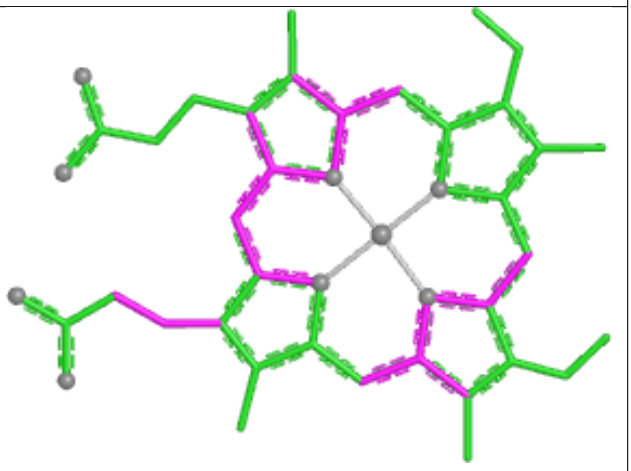


Rings

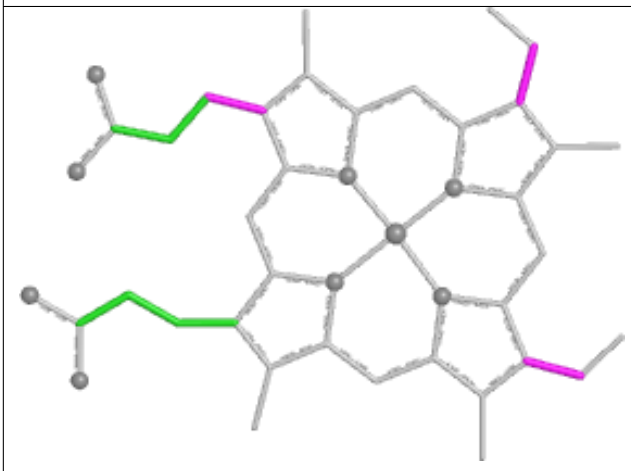
Ligand HEM E 101



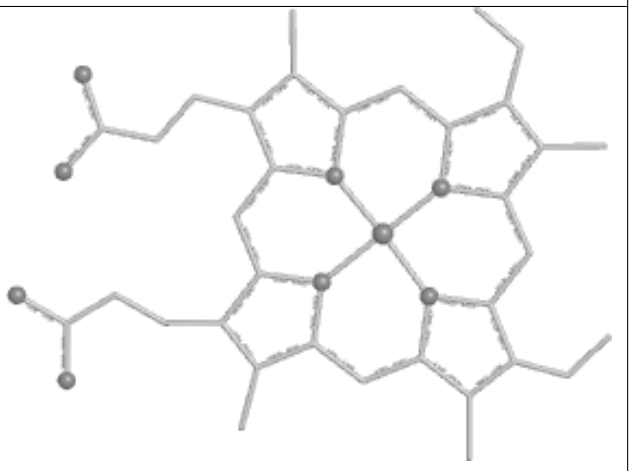
Bond lengths



Bond angles

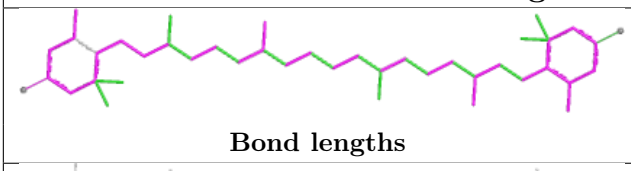


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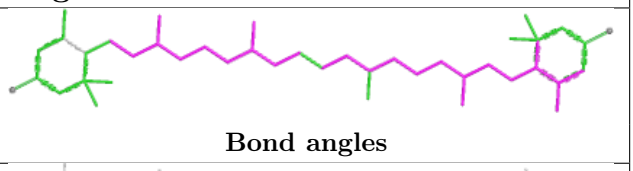


Rings

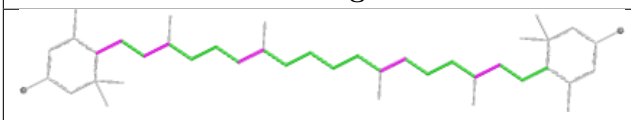
Ligand LUT g 316



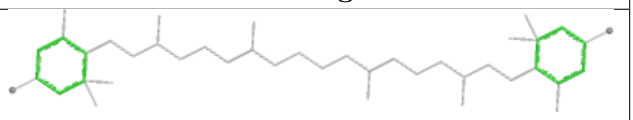
Bond lengths



Bond angles

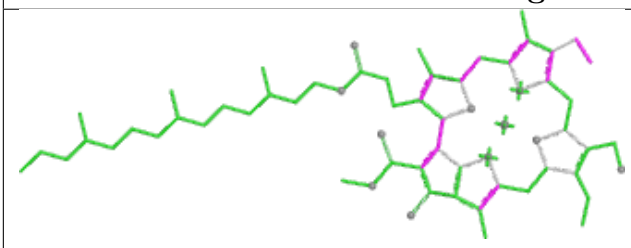


Torsions

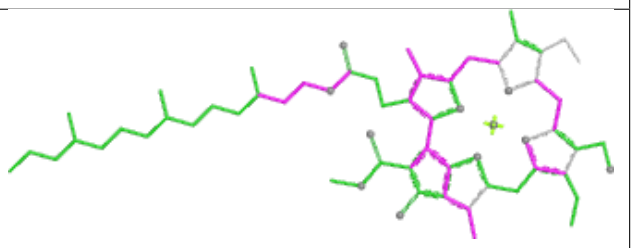


Rings

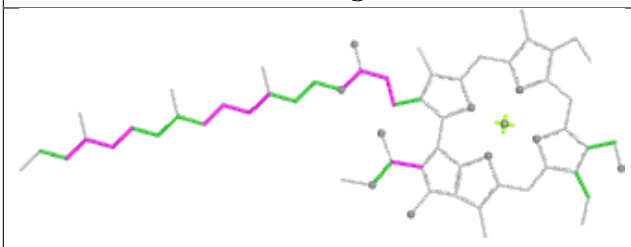
Ligand CHL 7 321



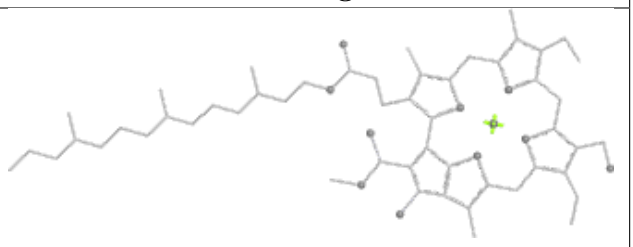
Bond lengths



Bond angles

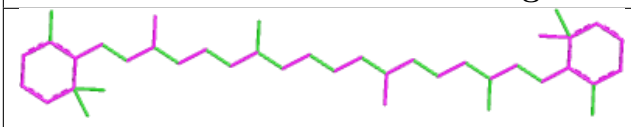


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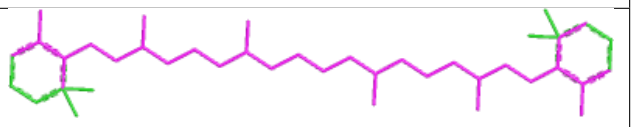


Rings

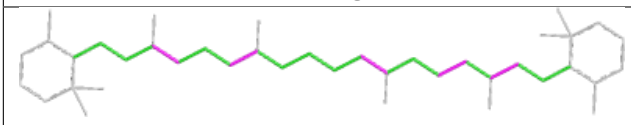
Ligand BCR C 615



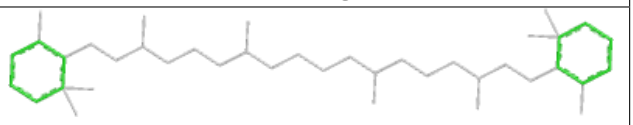
Bond lengths



Bond angles

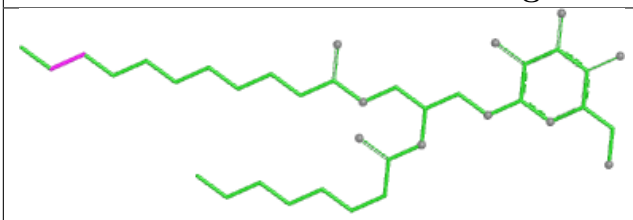


Torsions

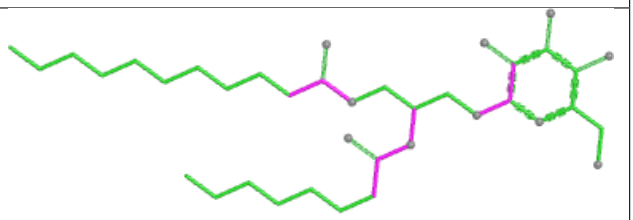


Rings

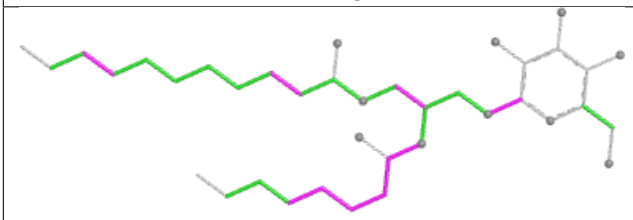
Ligand LMG n 321



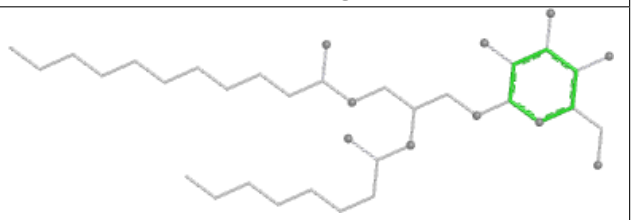
Bond lengths



Bond angles

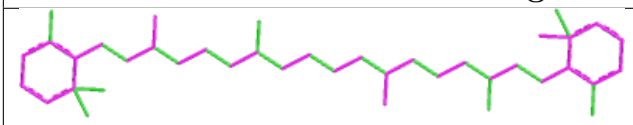


Torsions

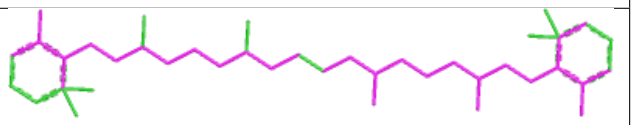


Rings

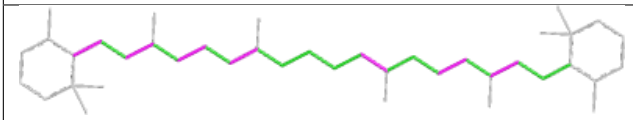
Ligand BCR c 615



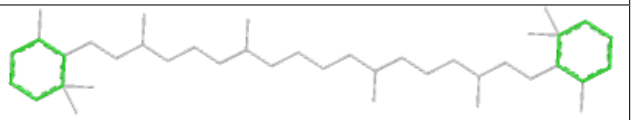
Bond lengths



Bond angles

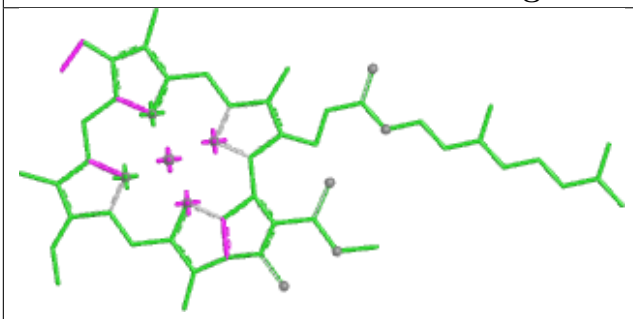


Torsions

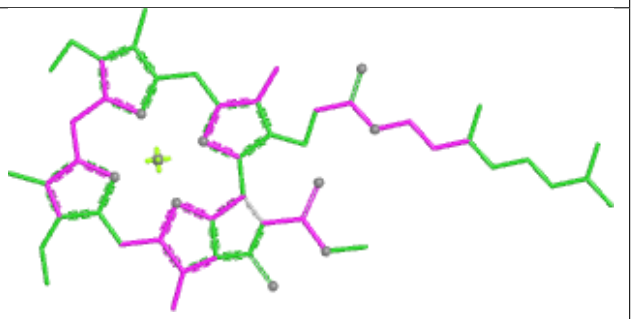


Rings

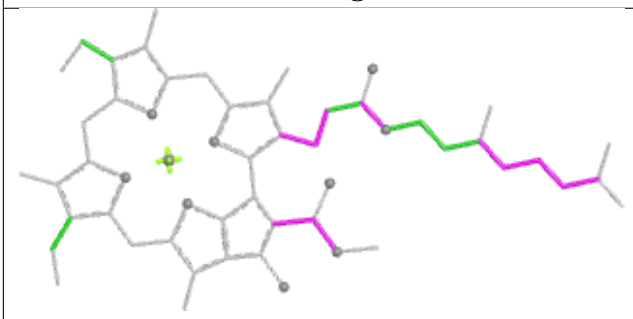
Ligand CLA G 604



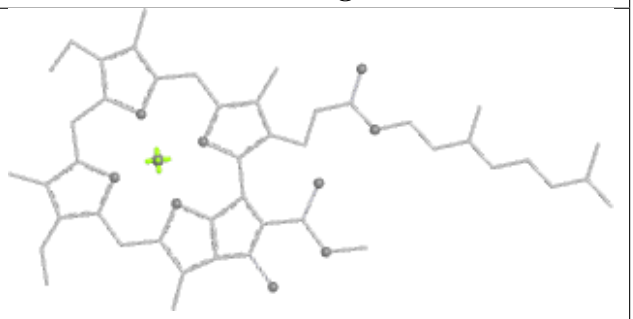
Bond lengths



Bond angles

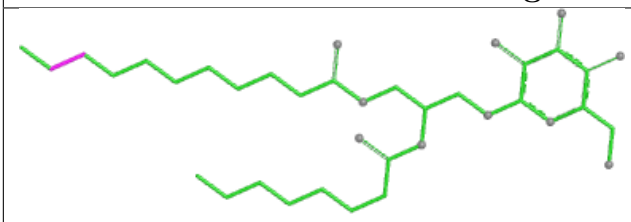


Torsions

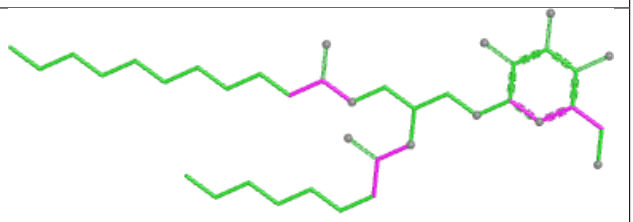


Rings

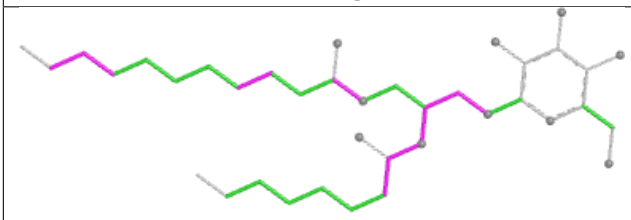
Ligand LMG 6 323



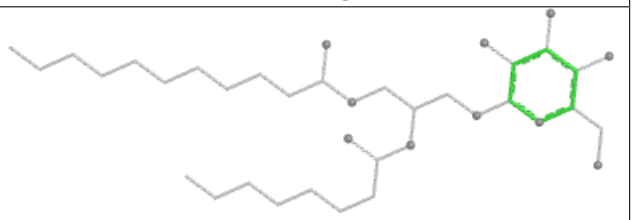
Bond lengths



Bond angles

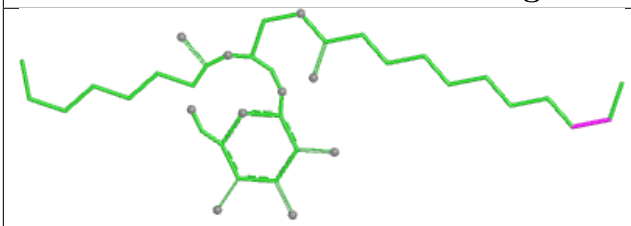


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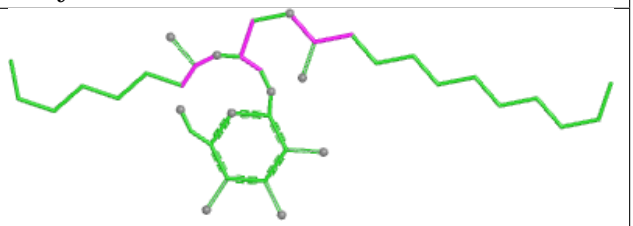


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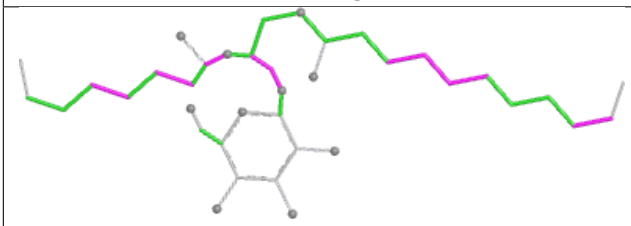
Ligand LMG y 620



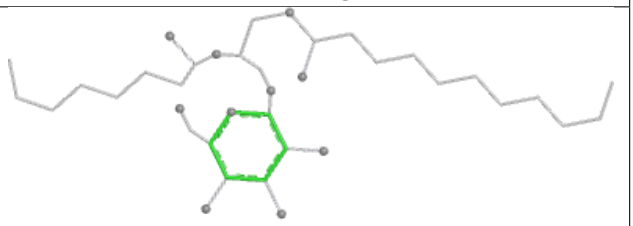
Bond lengths



Bond angles

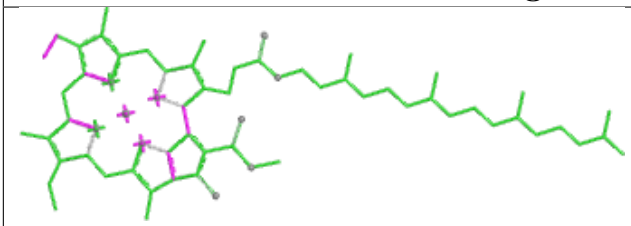


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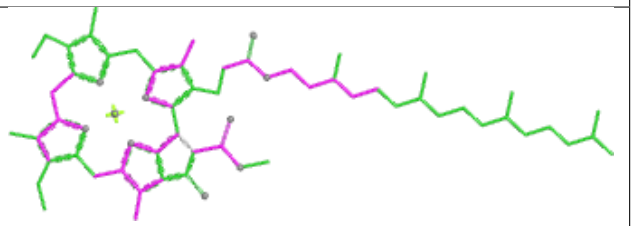


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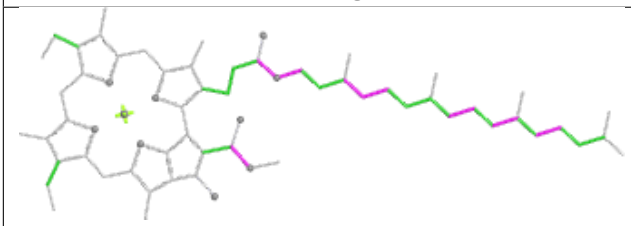
Ligand CLA C 609



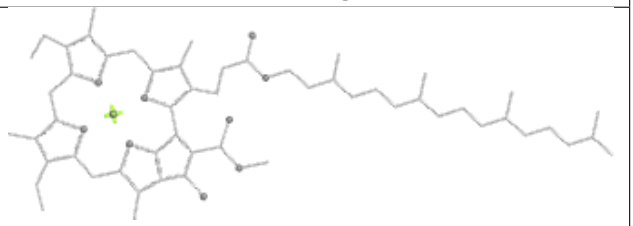
Bond lengths



Bond angles

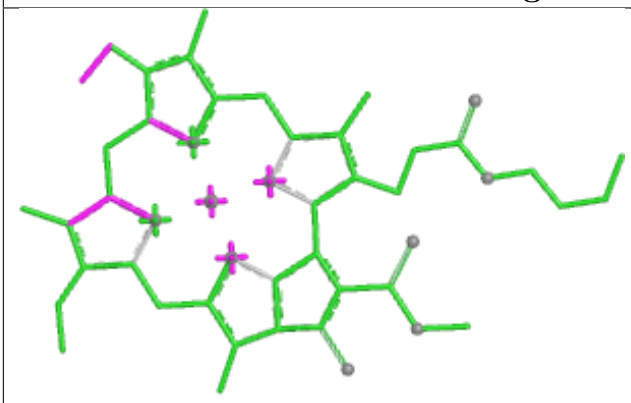


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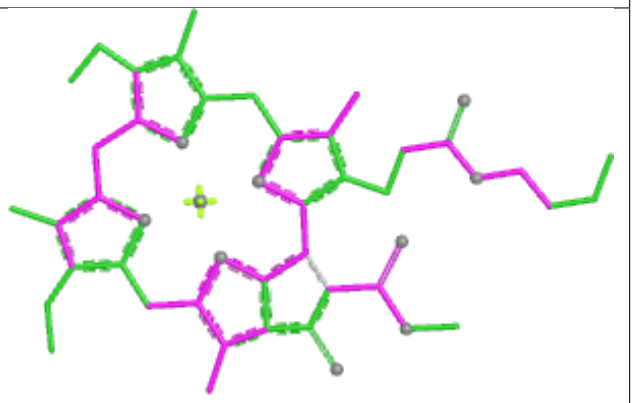


Rings

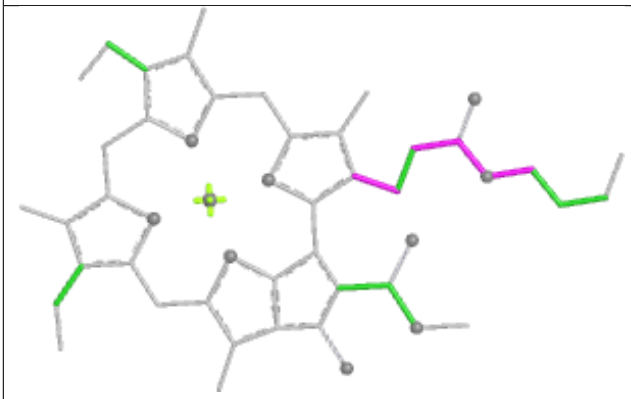
Ligand CLA N 314



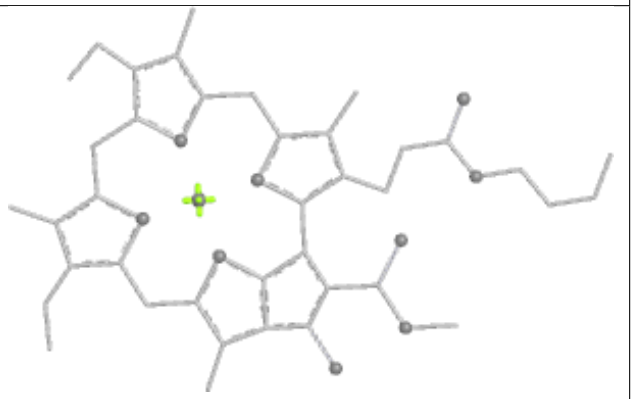
Bond lengths



Bond angles

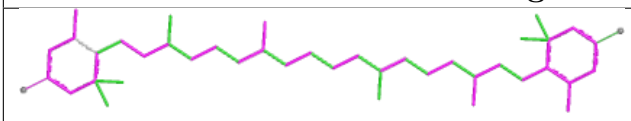


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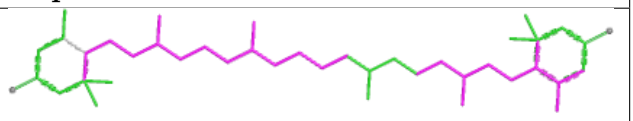


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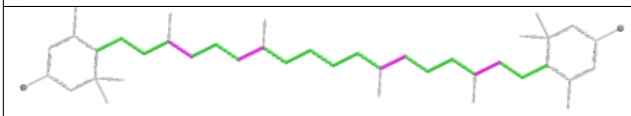
Ligand LUT p 616



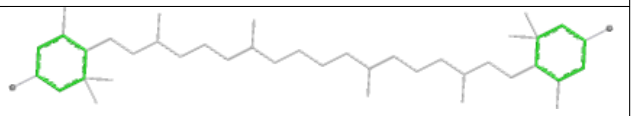
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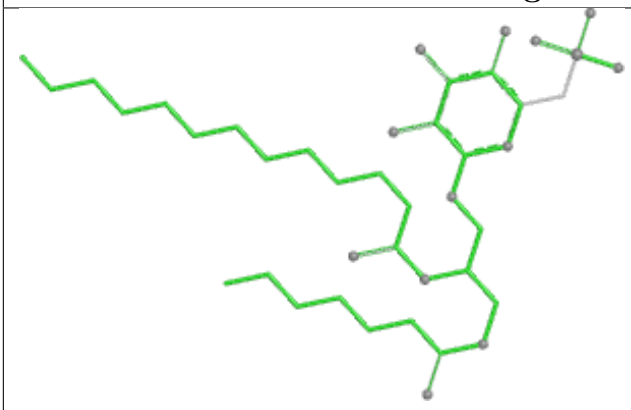


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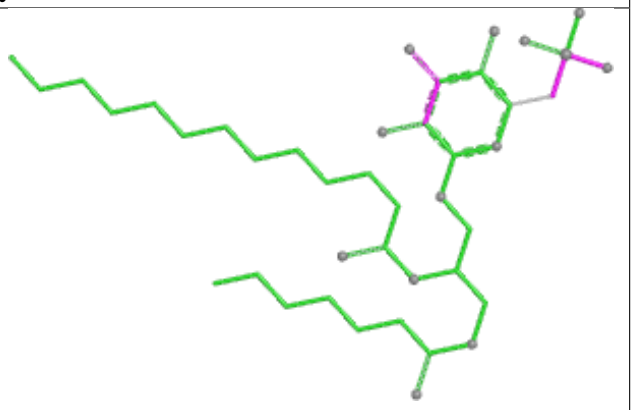


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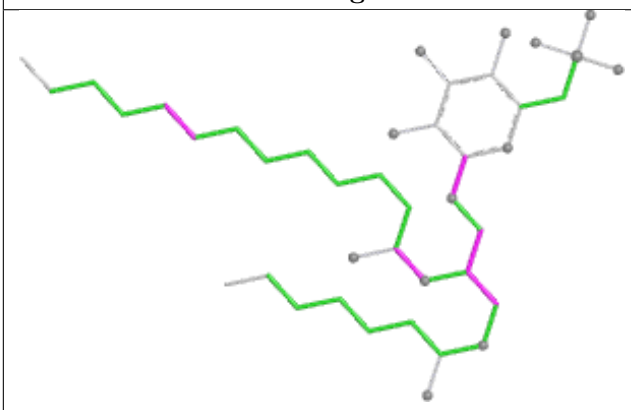
Ligand SQD Y 320



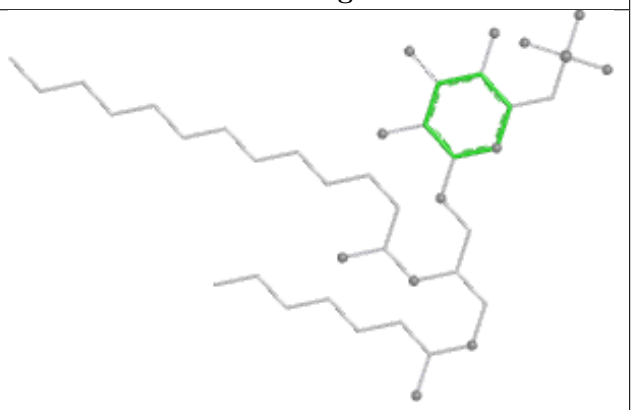
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Bond angles

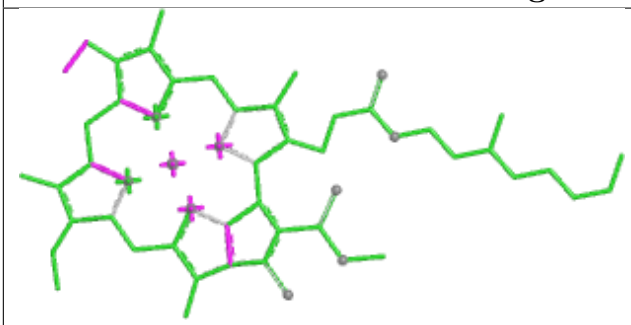


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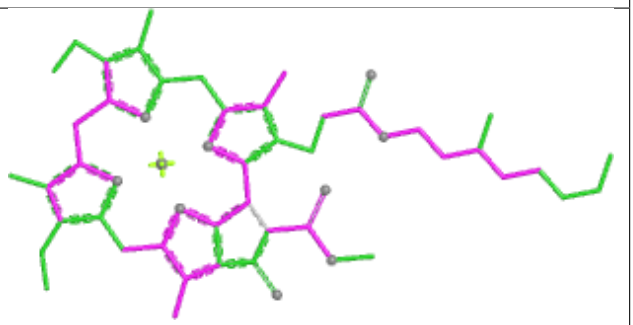


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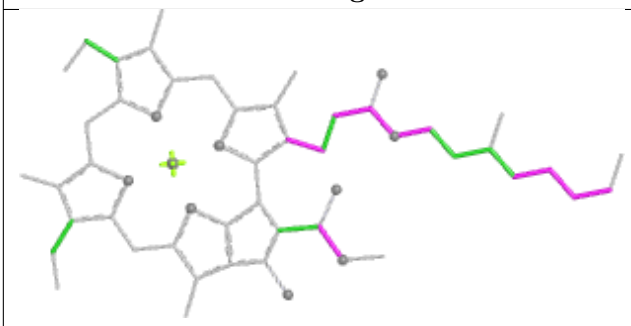
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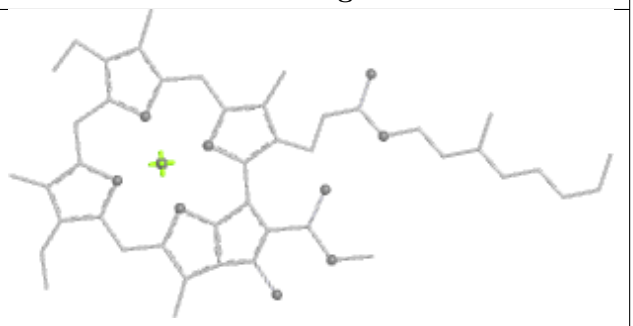
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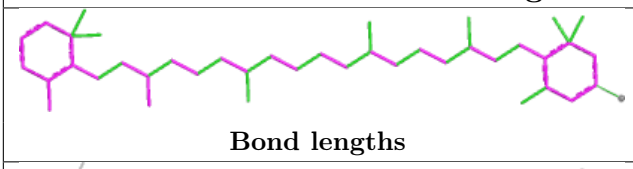


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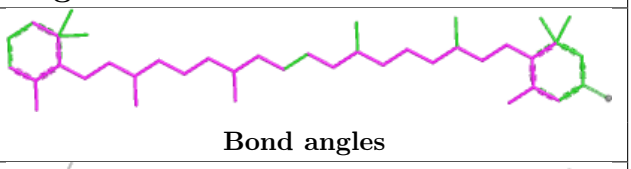


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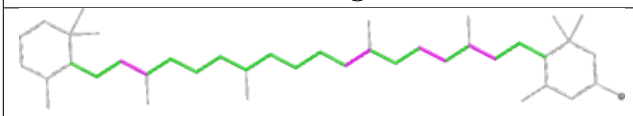
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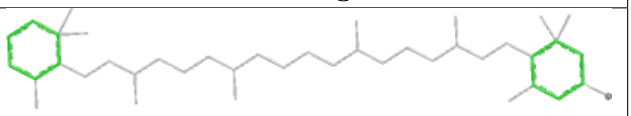
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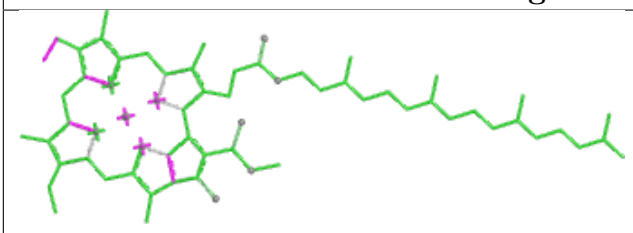


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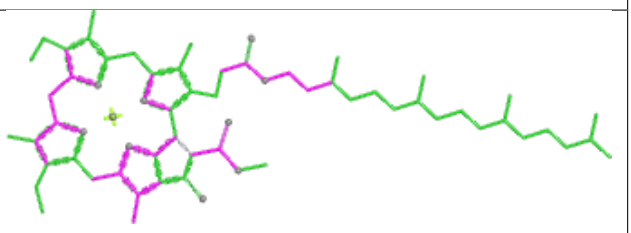


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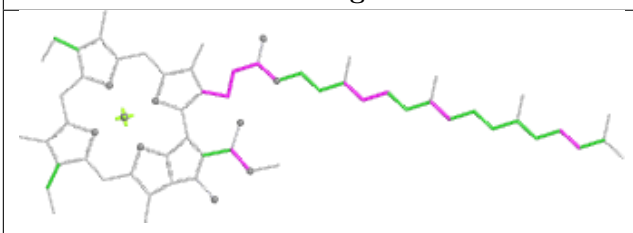
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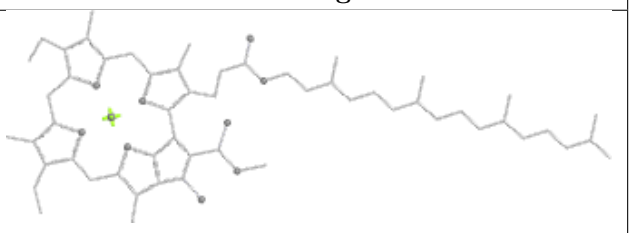
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Bond angles

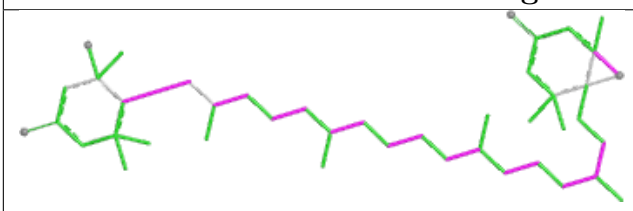


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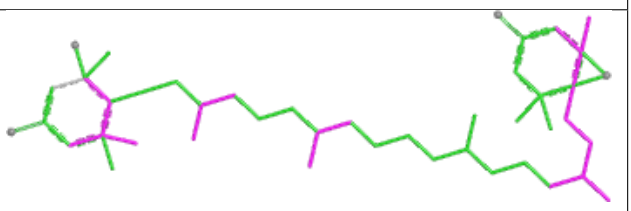


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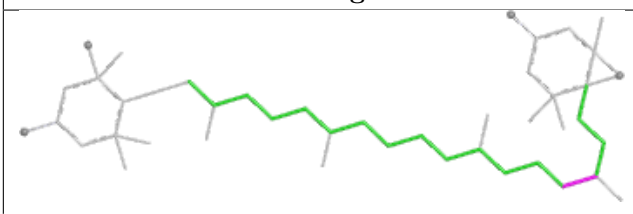
Ligand NEX G 616



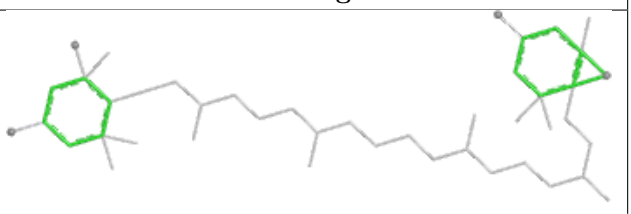
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Bond angles

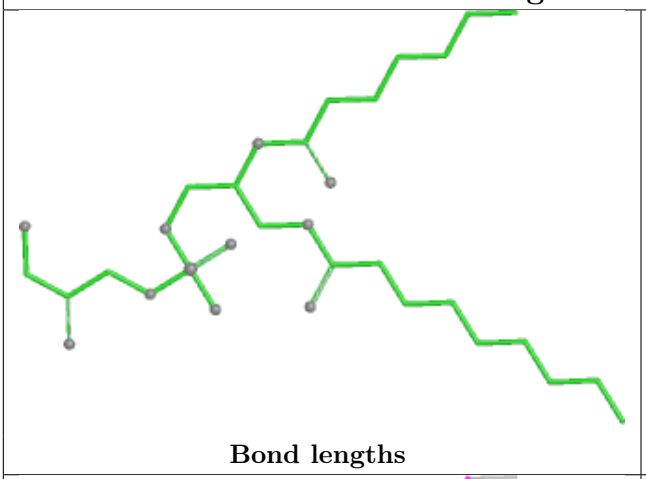


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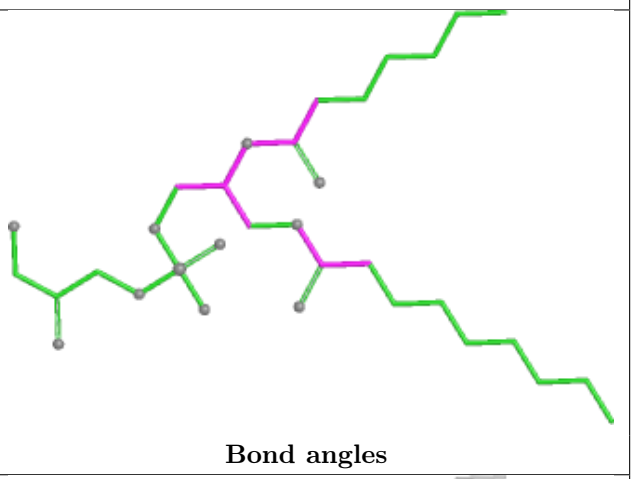


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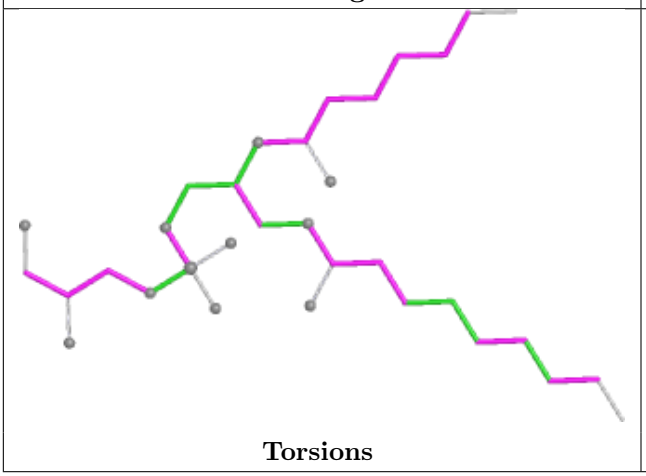
Ligand LHG 3 320



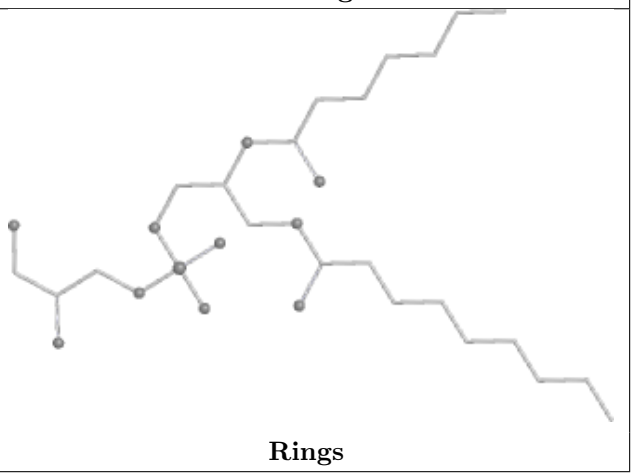
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Bond angles

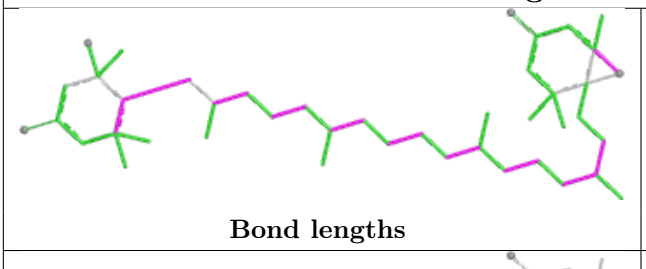


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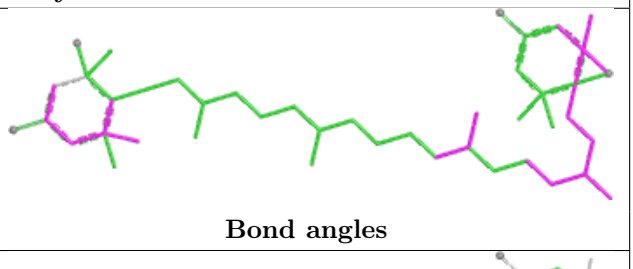


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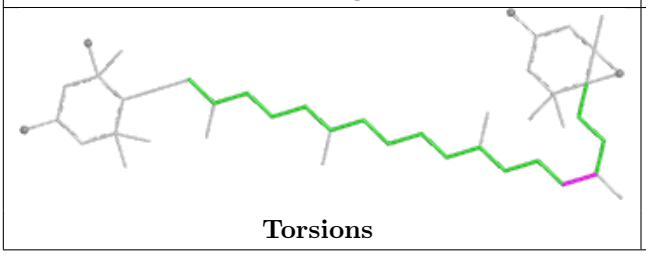
Ligand NEX y 618



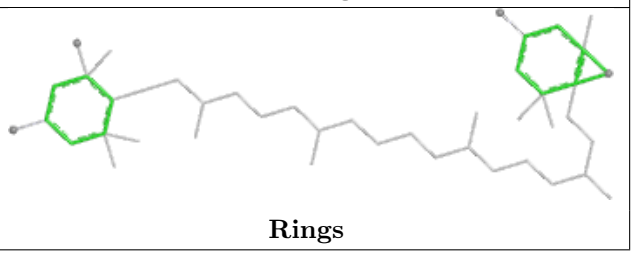
Bond lengths



Bond angles

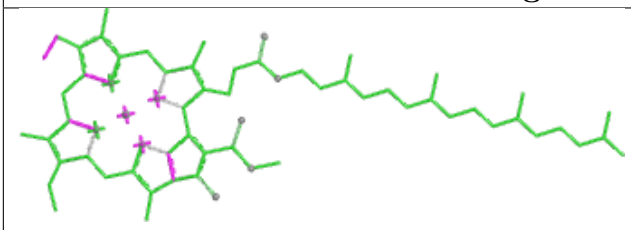


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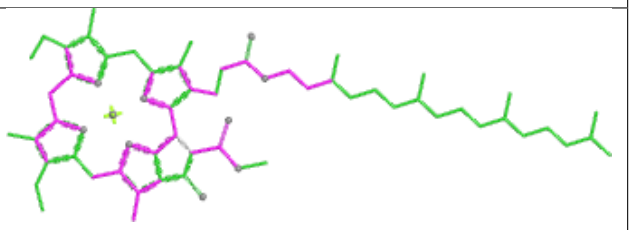


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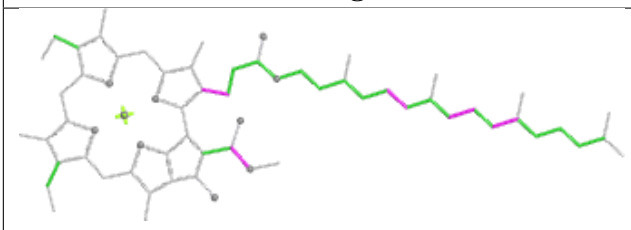
Ligand CLA G 609



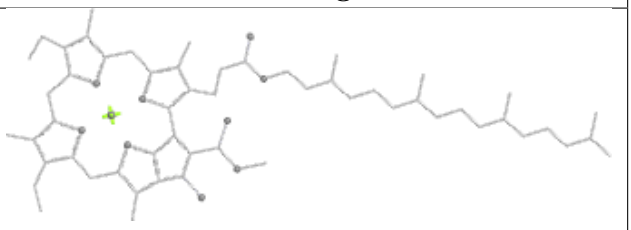
Bond lengths



Bond angles

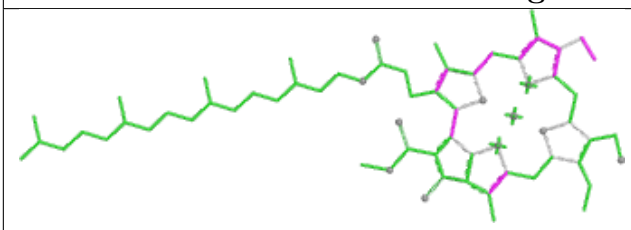


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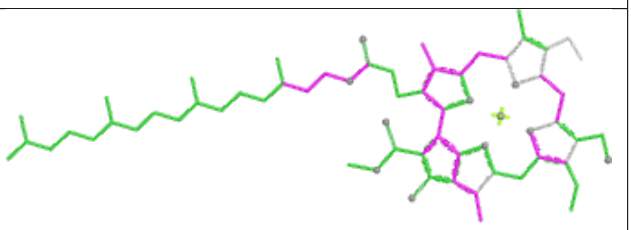


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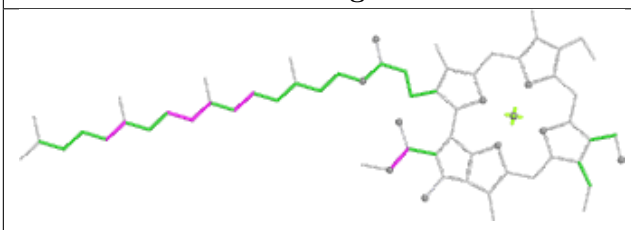
Ligand CHL 7 307



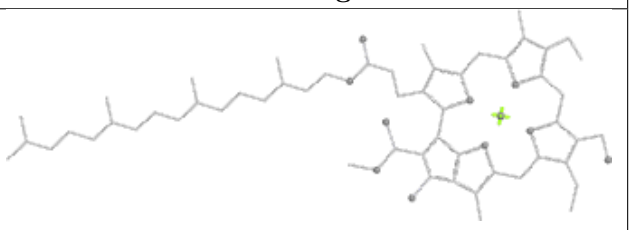
Bond lengths



Bond angles

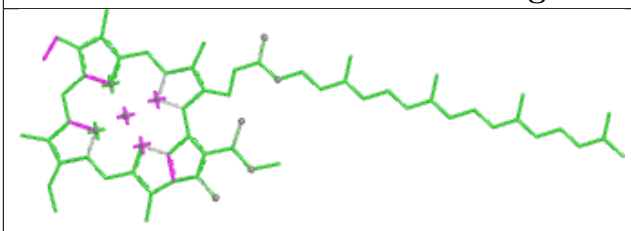


Torsions

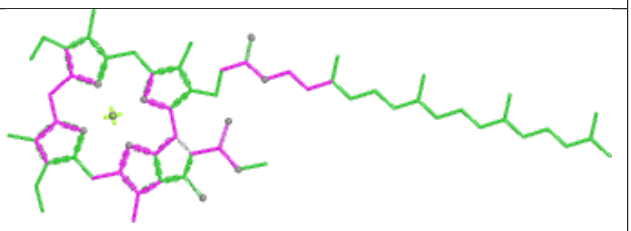


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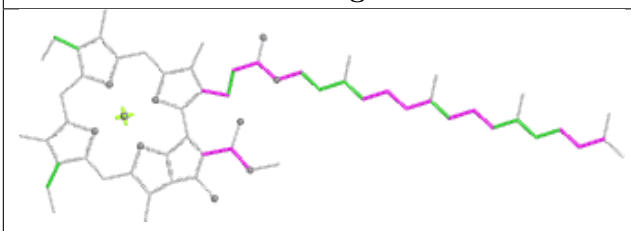
Ligand CLA 1 612



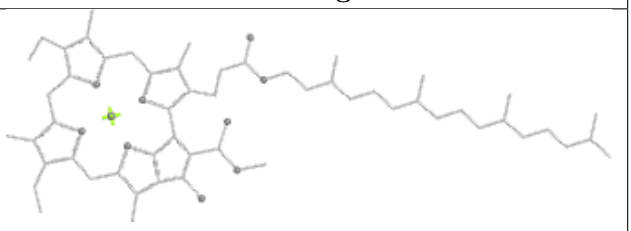
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Bond angles

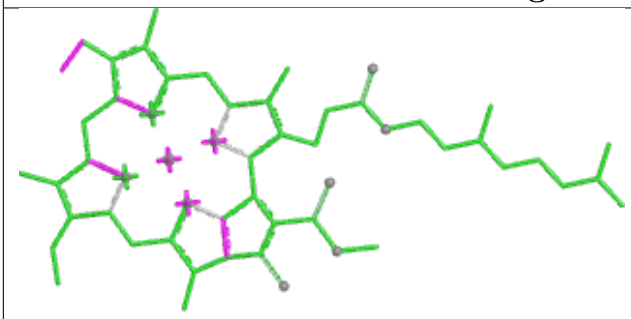


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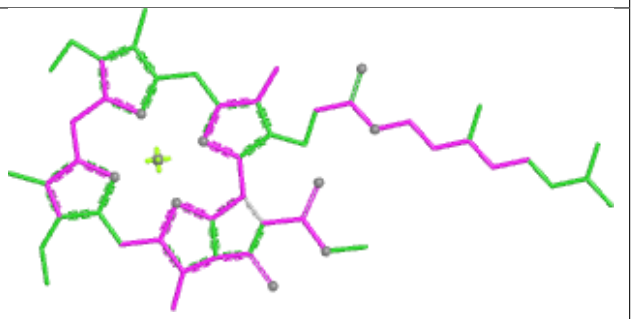


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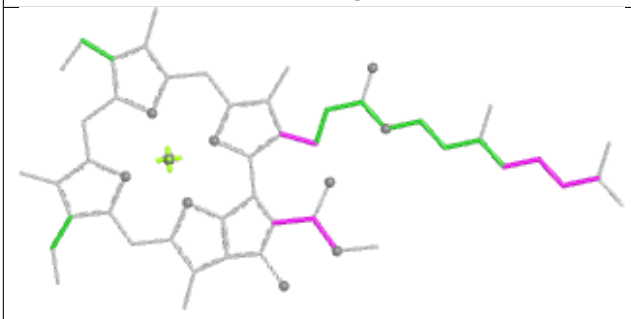
Ligand CLA 4 603



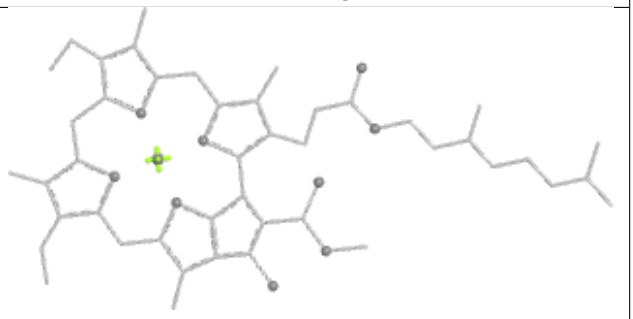
Bond lengths



Bond angles

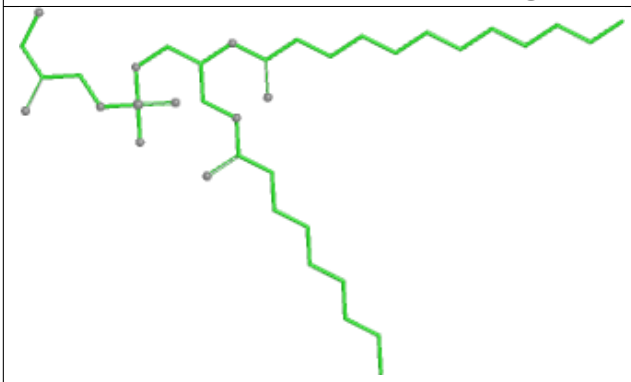


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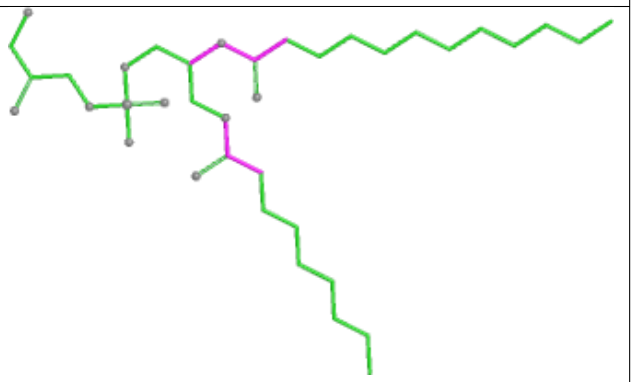


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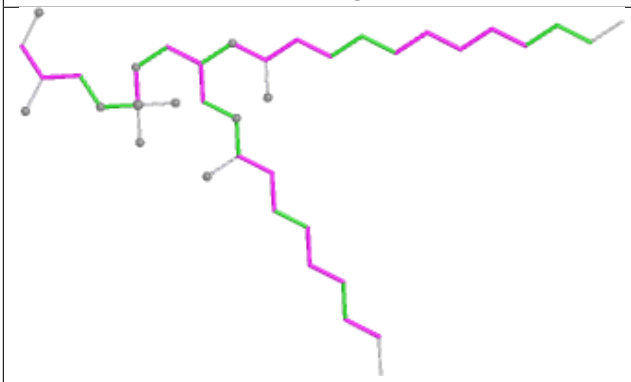
Ligand LHG R 320



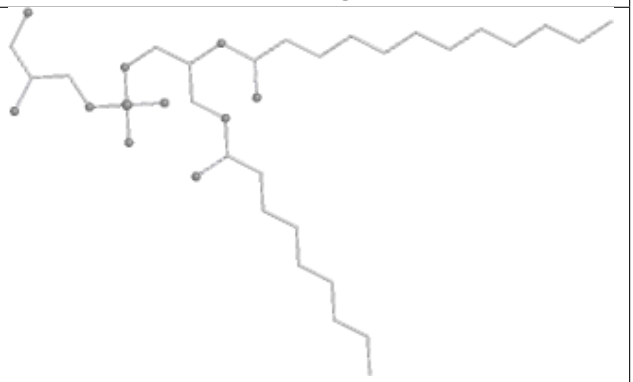
Bond lengths



Bond angles

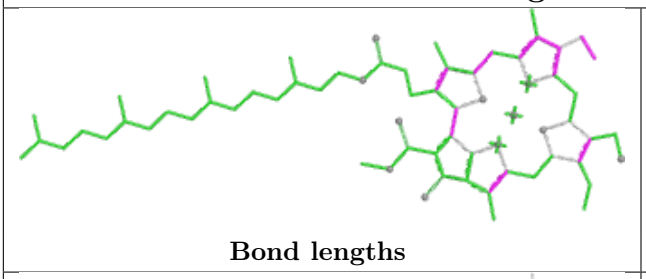


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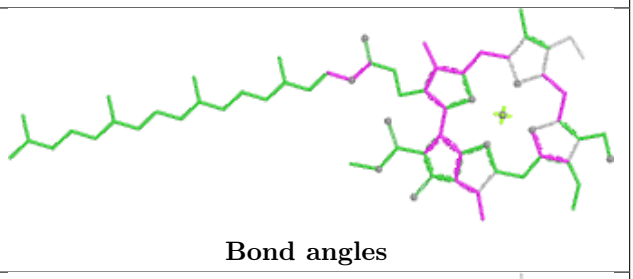


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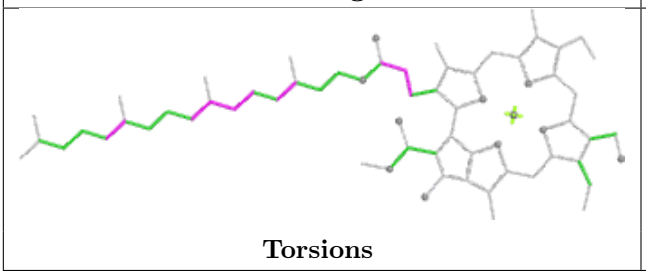
Ligand CHL 1 605



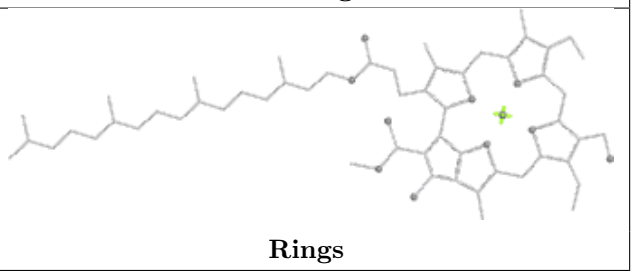
Bond lengths



Bond angles

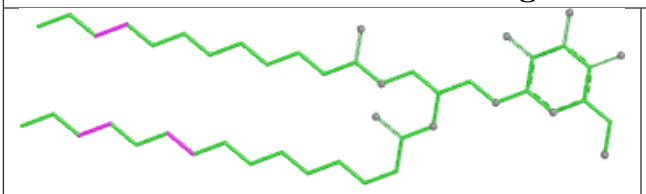


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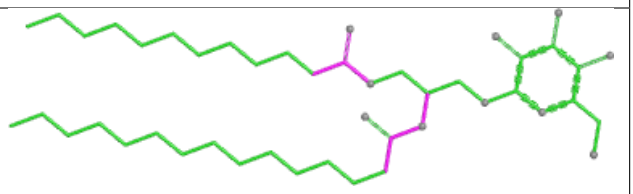


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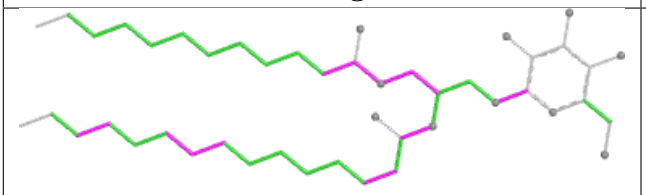
Ligand LMG D 410



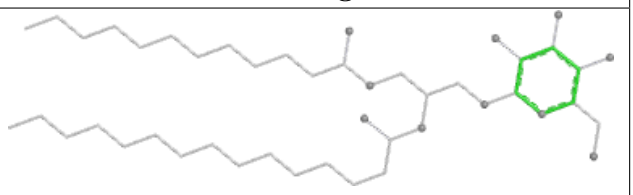
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Bond angles

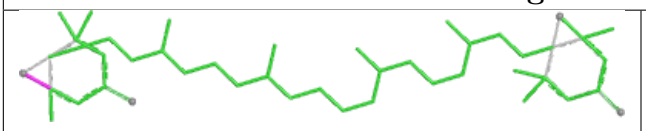


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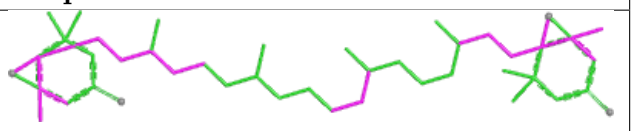


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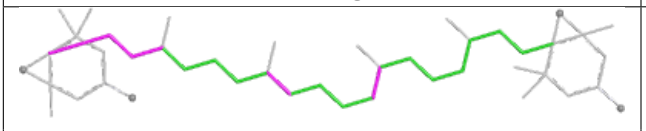
Ligand XAT q 321



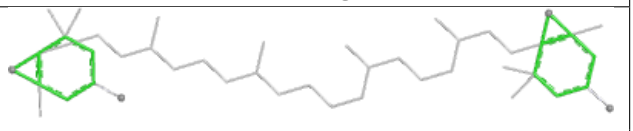
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Bond angles

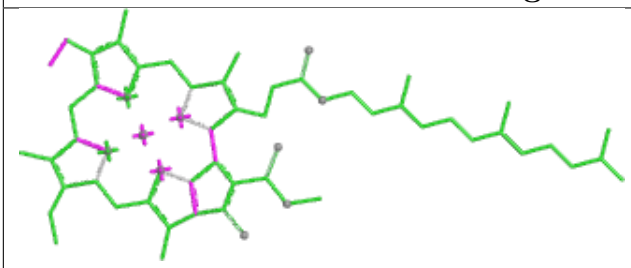


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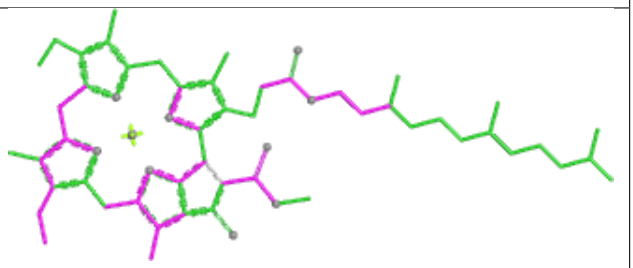


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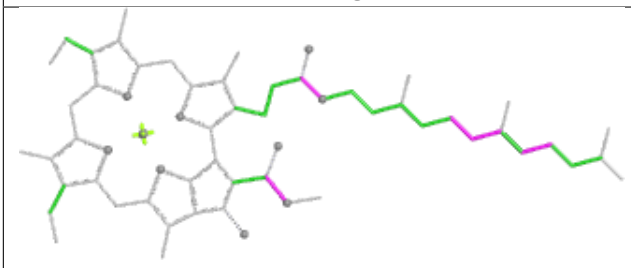
Ligand CLA R 305



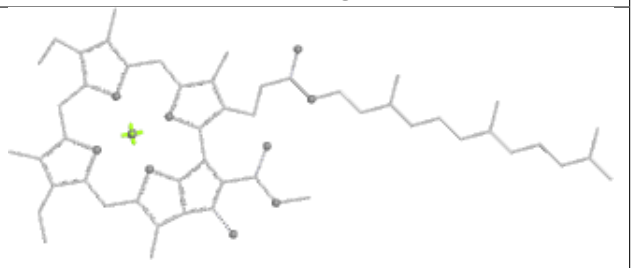
Bond lengths



Bond angles

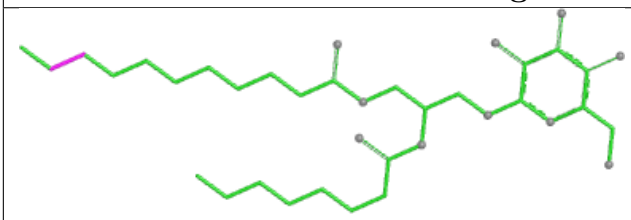


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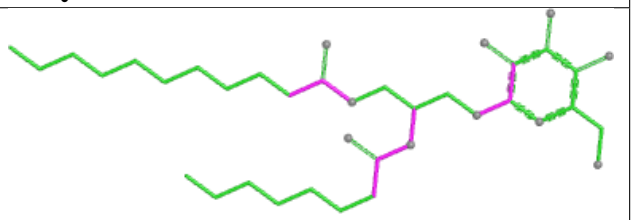


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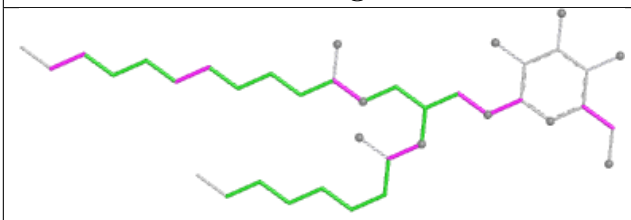
Ligand LMG Q1 101



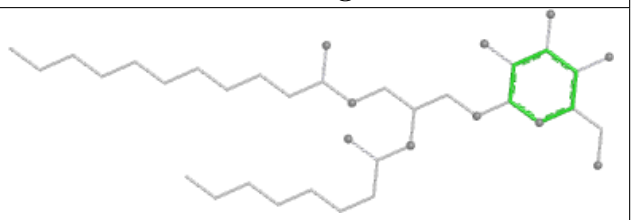
Bond lengths



Bond angles

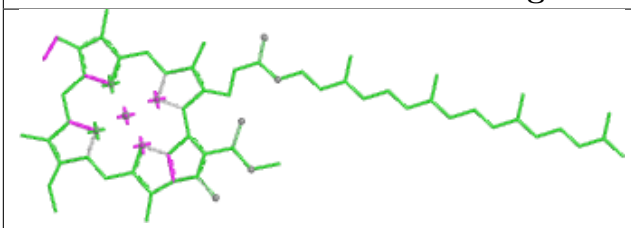


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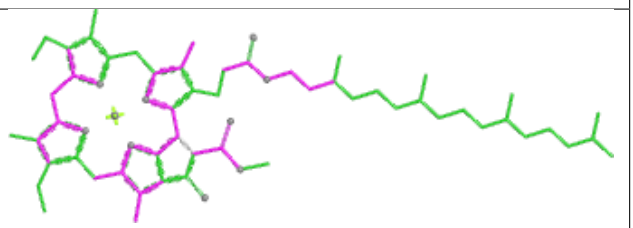


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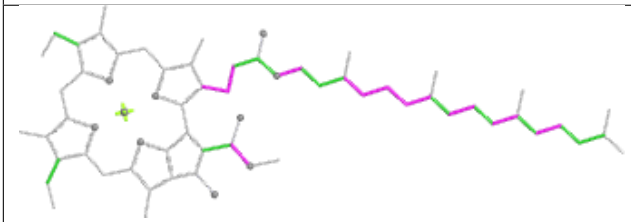
Ligand CLA b 604



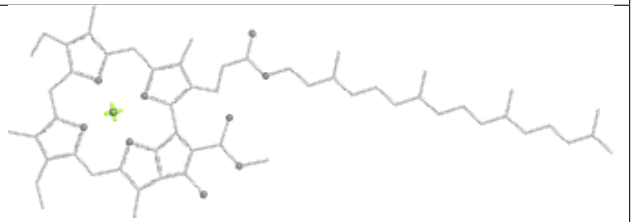
Bond lengths



Bond angles

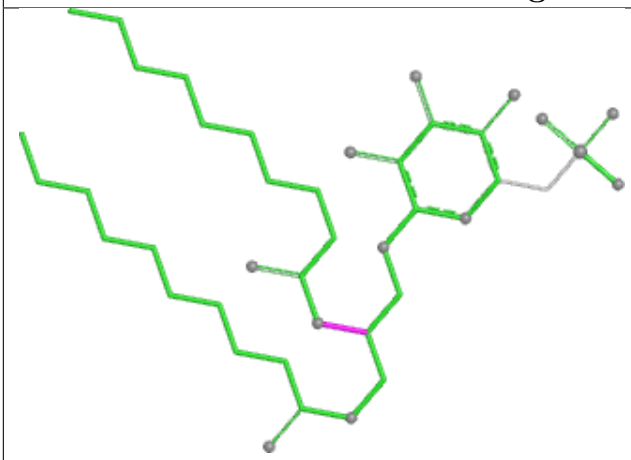


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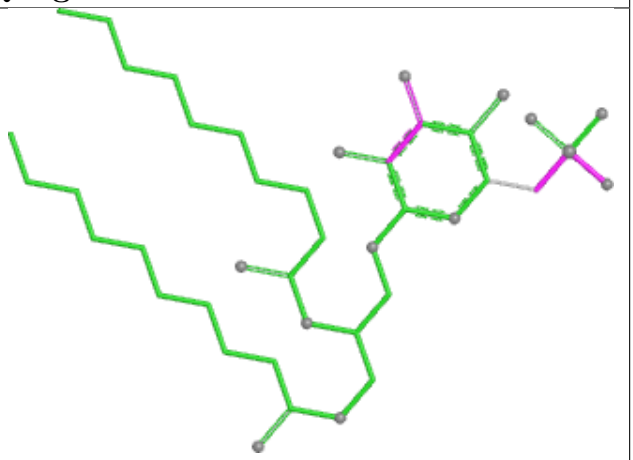


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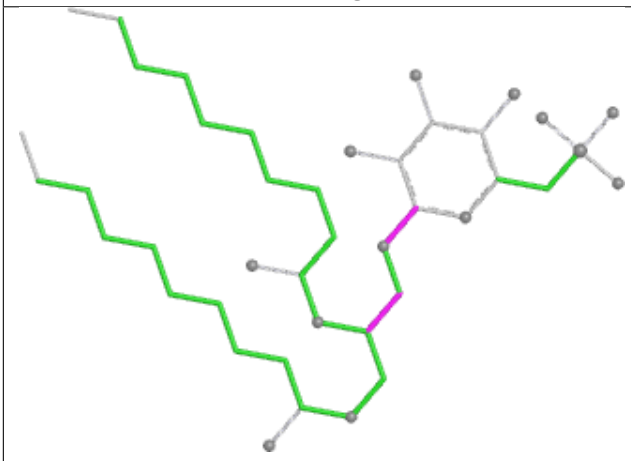
Ligand SQD g 318



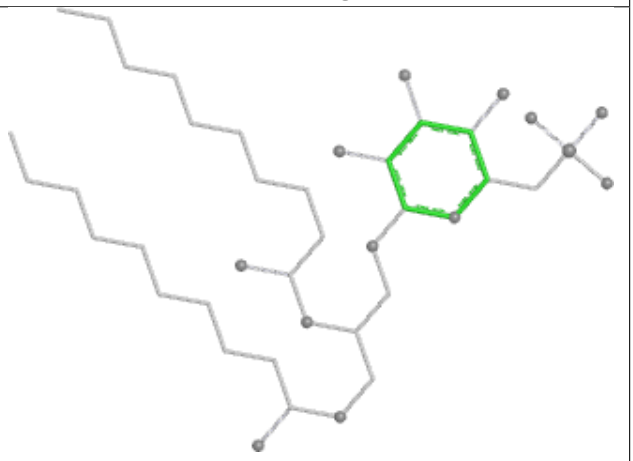
Bond lengths



Bond angles

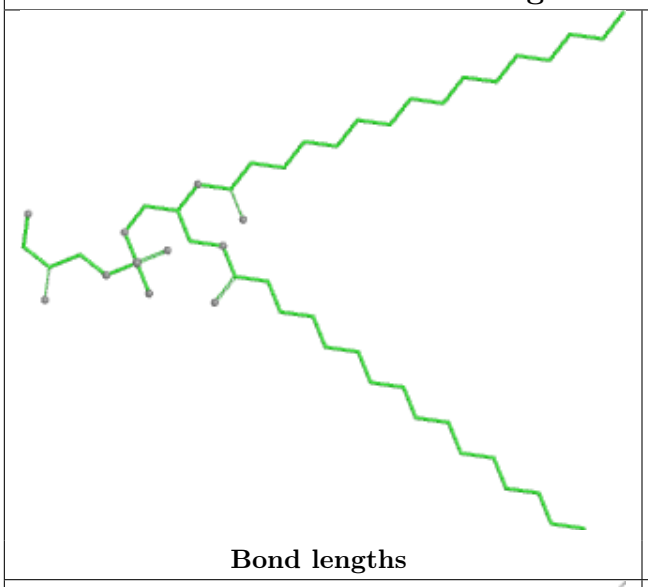


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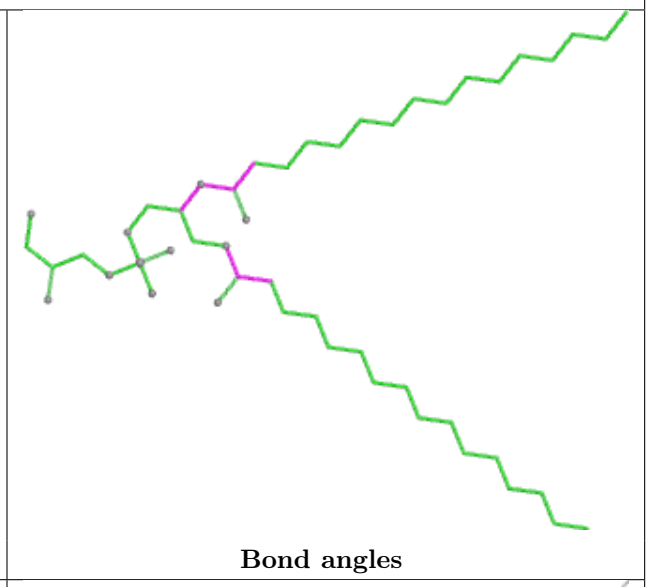


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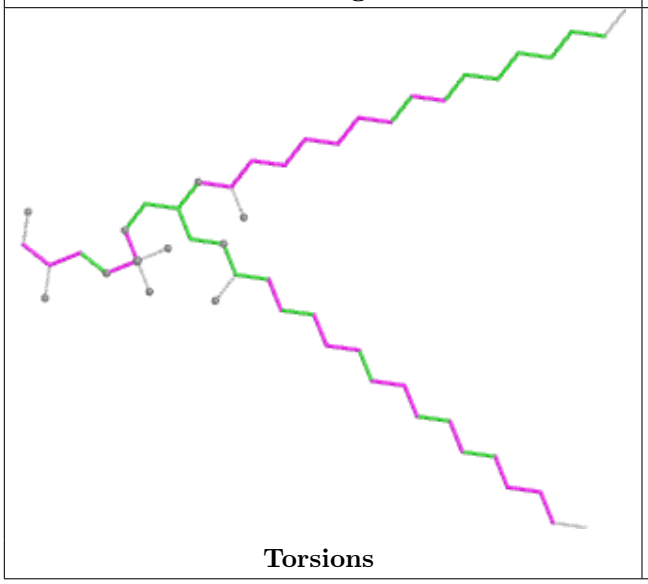
Ligand LHG d 408



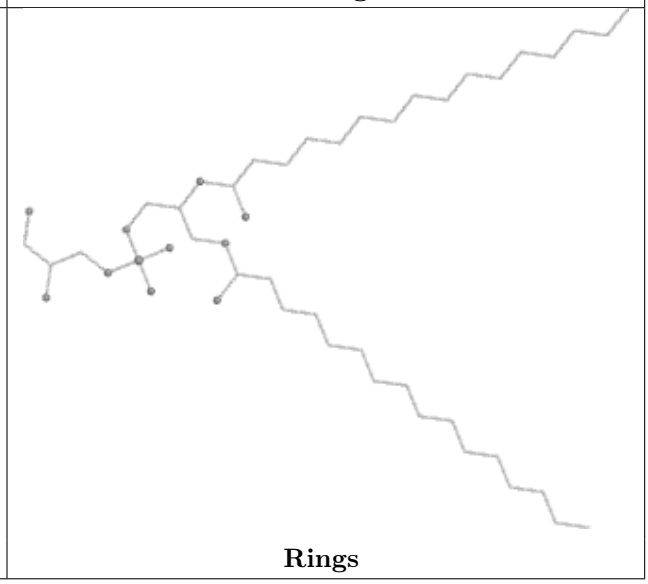
Bond lengths



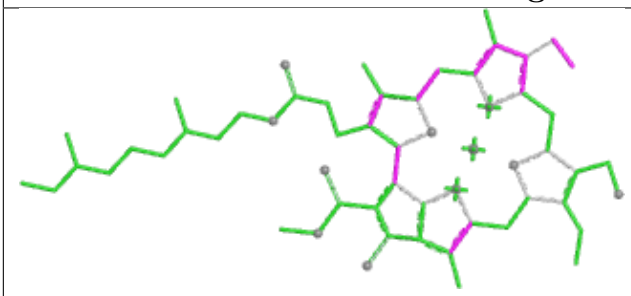
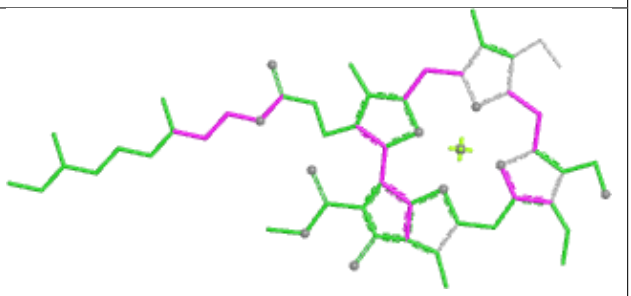
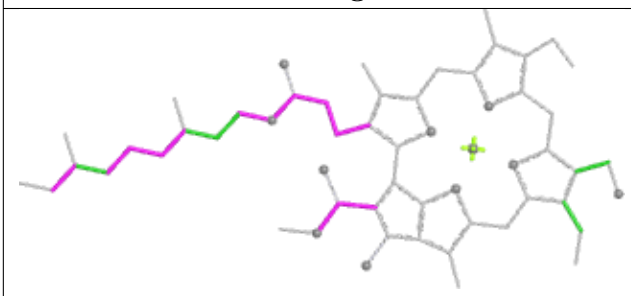
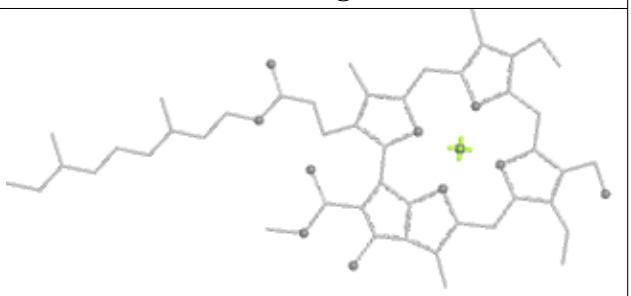
Bond angles

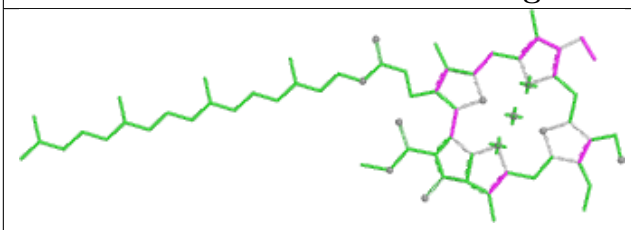
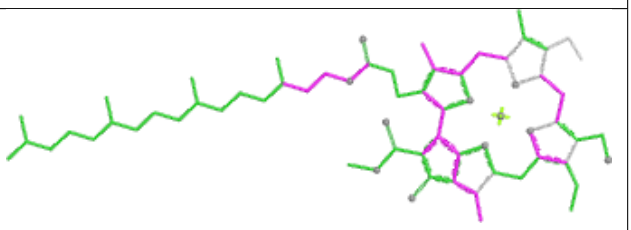
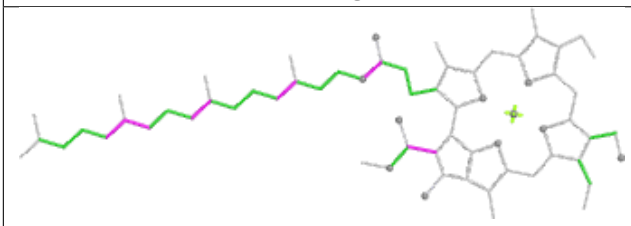
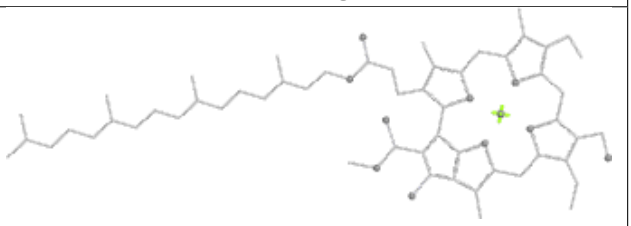


Torsions

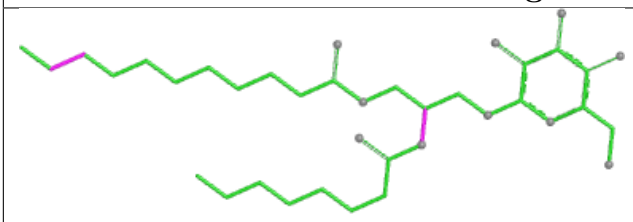


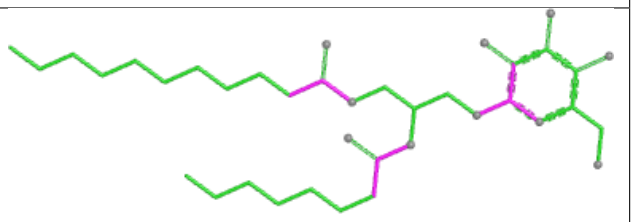
Rings

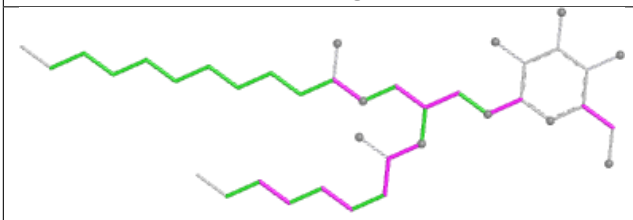
Ligand CHL 4 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

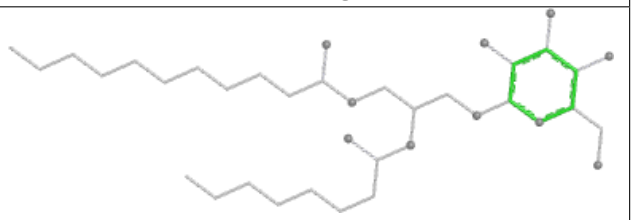
Ligand CHL Y 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG r 321


Bond lengths

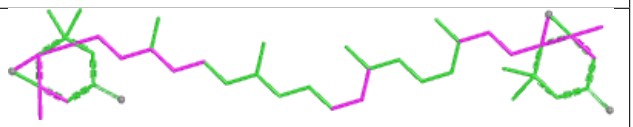

Bond angles

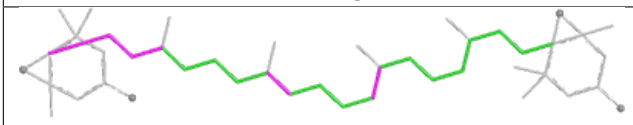

Torsions

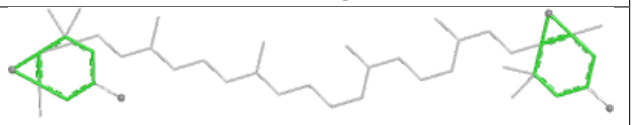

Rings

Ligand XAT 4 619

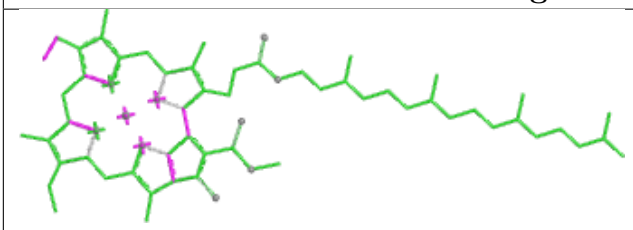

Bond lengths

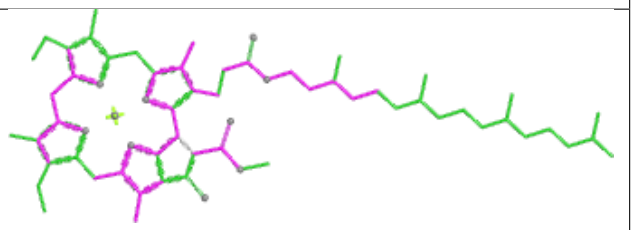

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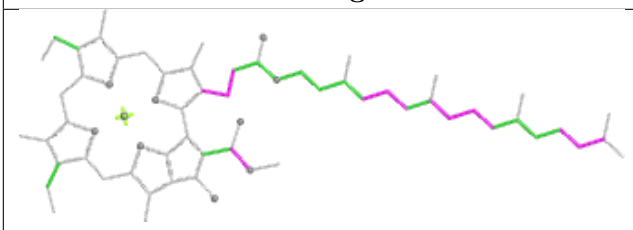

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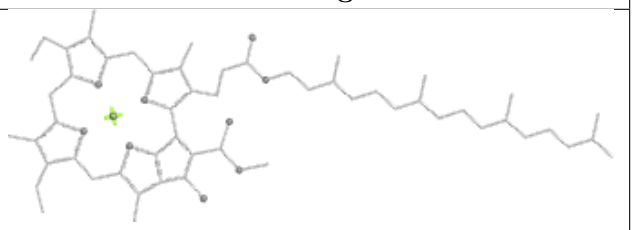

Rings

Ligand CLA s 311

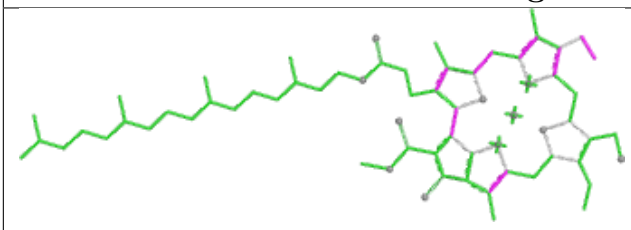

Bond lengths


Bond angles

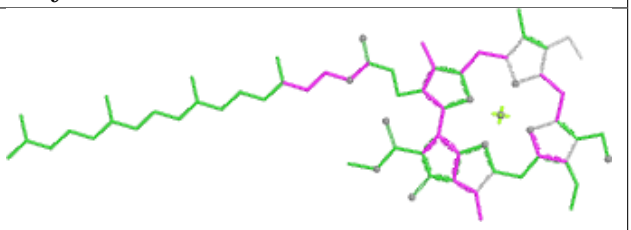

Torsions


Rings

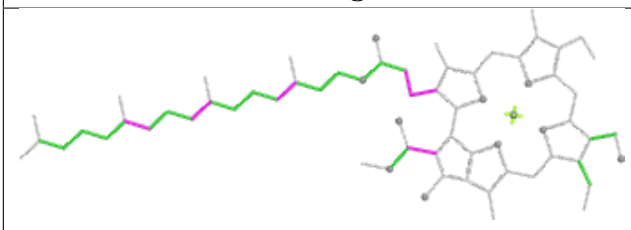
Ligand CHL y 601



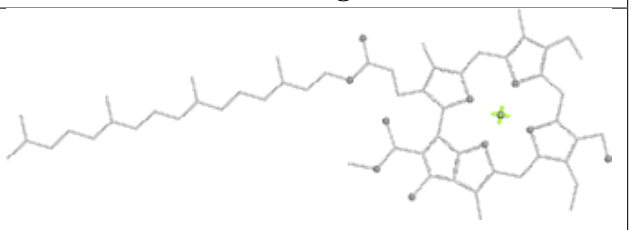
Bond lengths



Bond angles

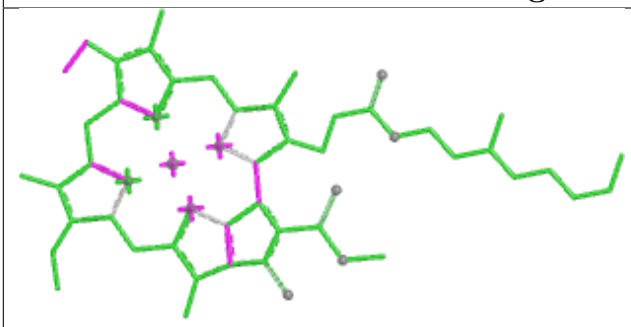


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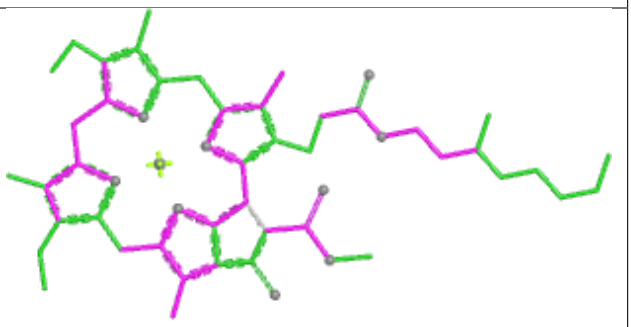


Rings

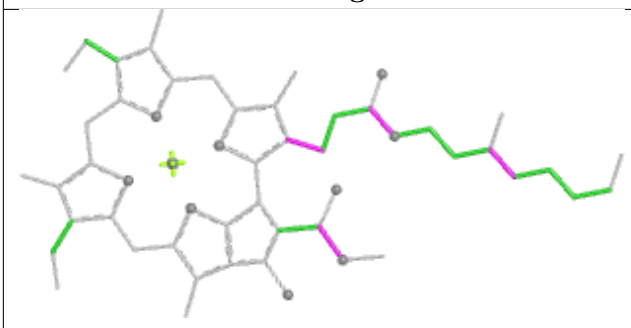
Ligand CLA 4 614



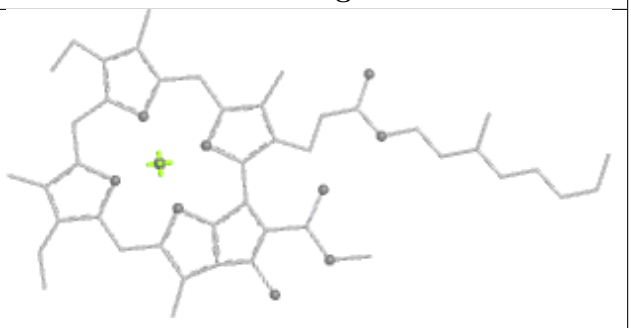
Bond lengths



Bond angles

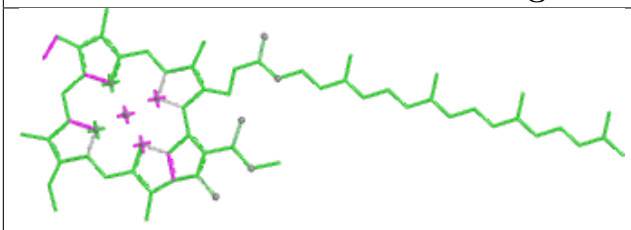


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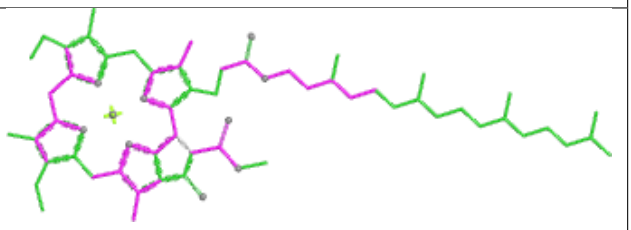


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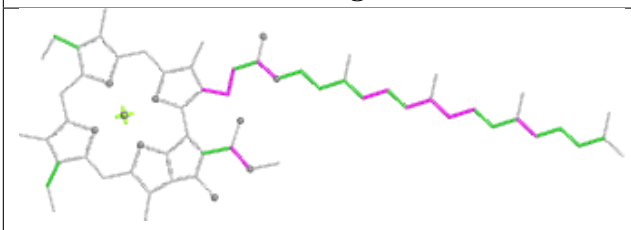
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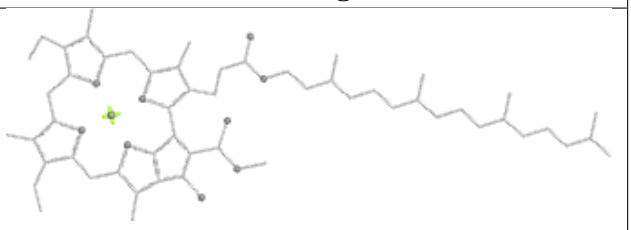
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Bond angles

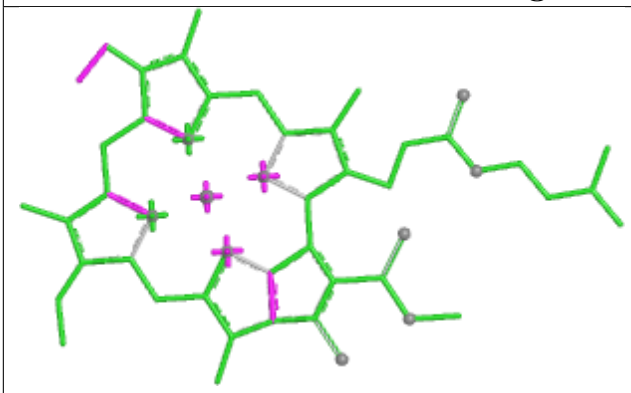


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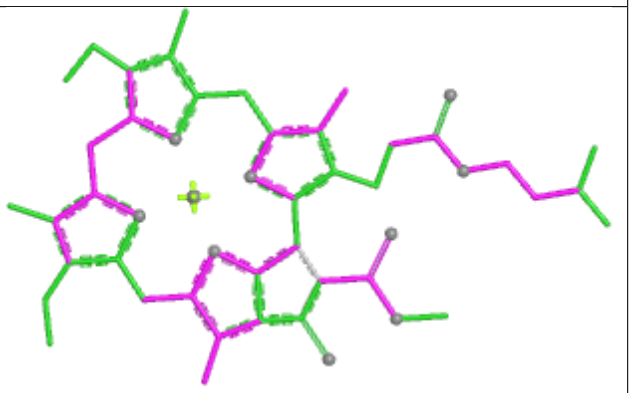


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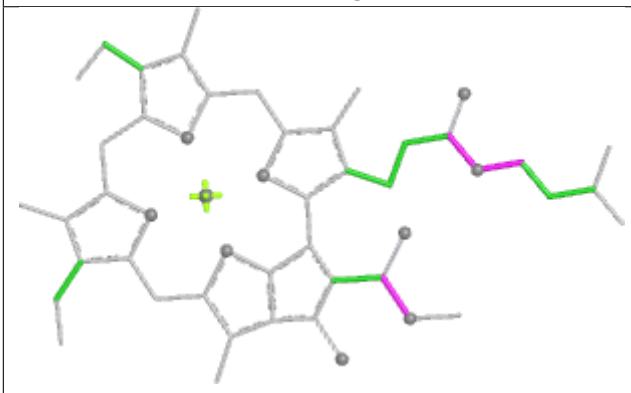
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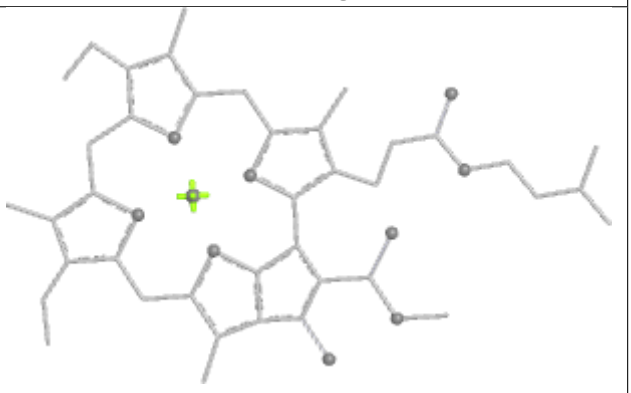
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Bond angles

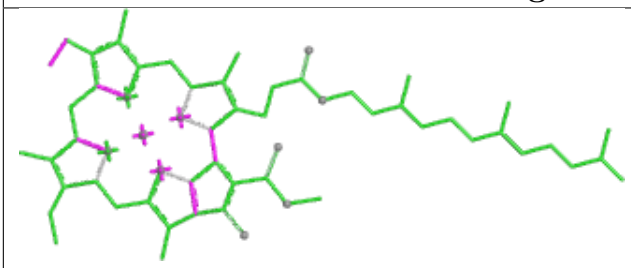


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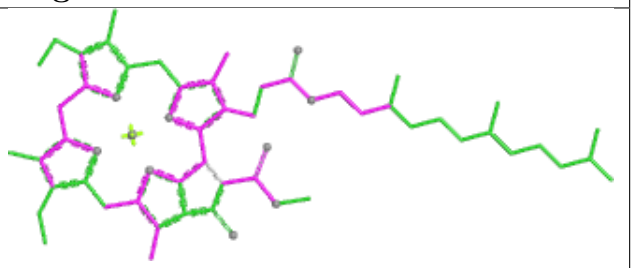


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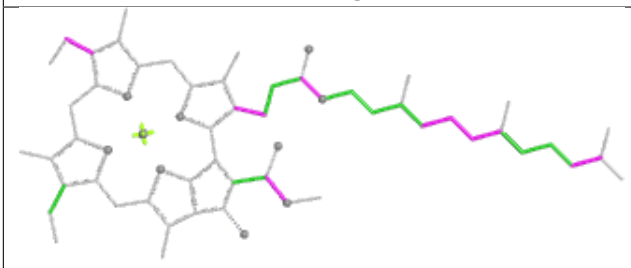
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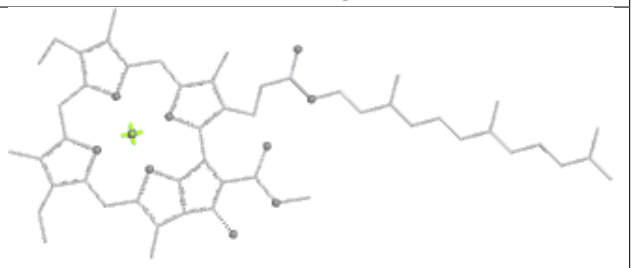
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Bond angles

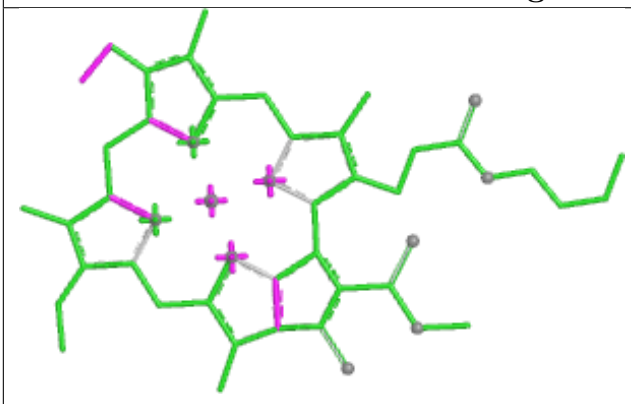


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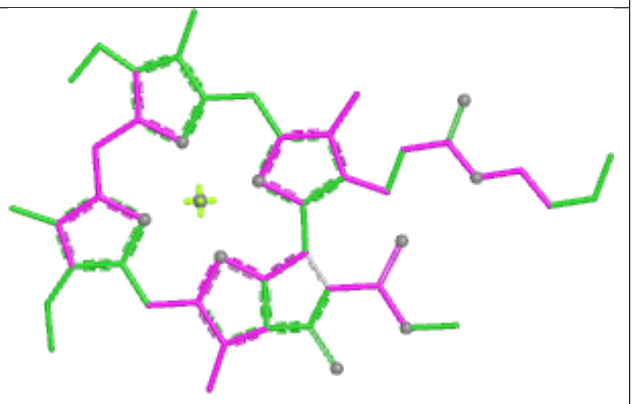


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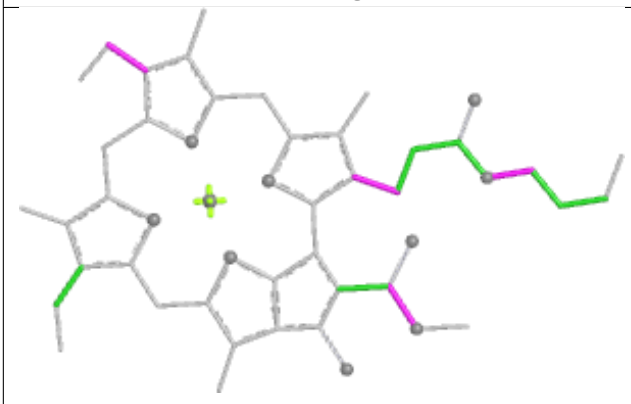
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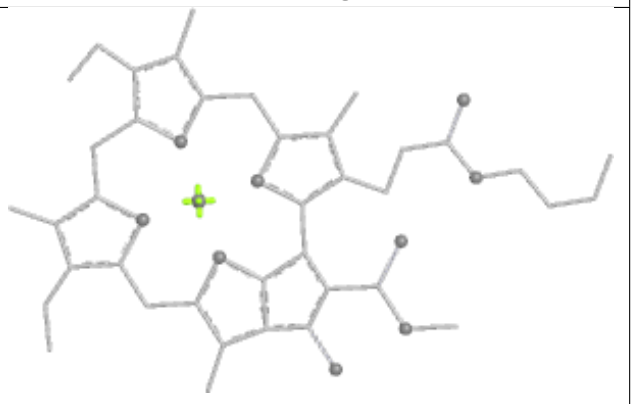
Bond lengths



Bond angles

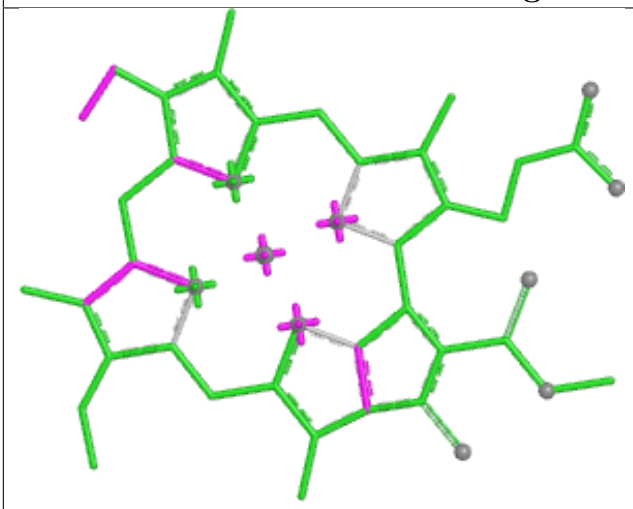


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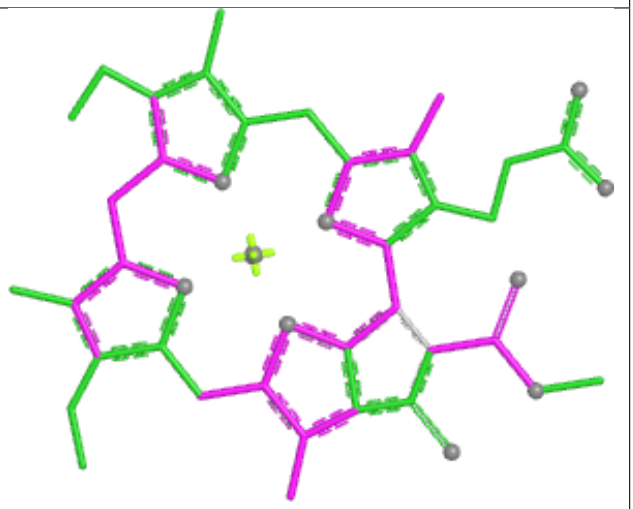


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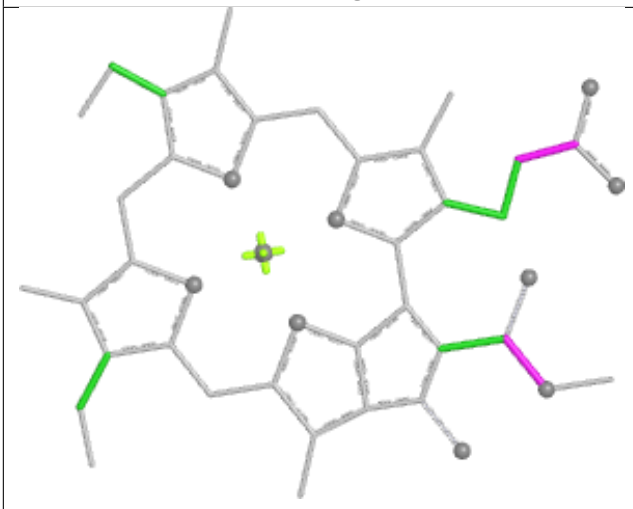
Ligand CLA N 312



Bond lengths



Bond angles

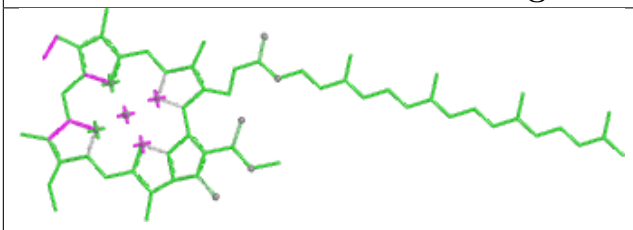


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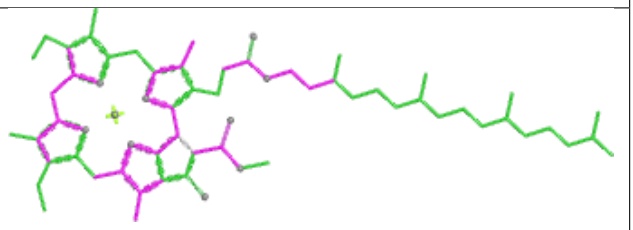


Rings

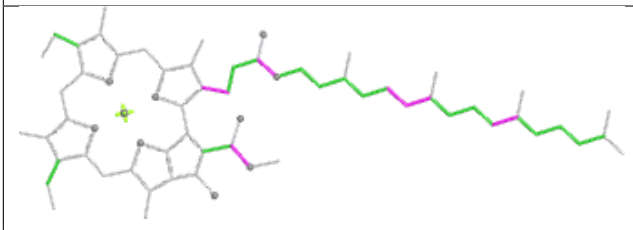
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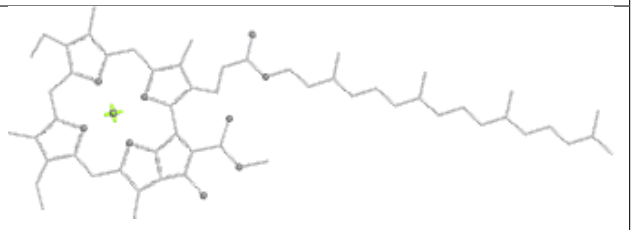
Bond lengths



Bond angles

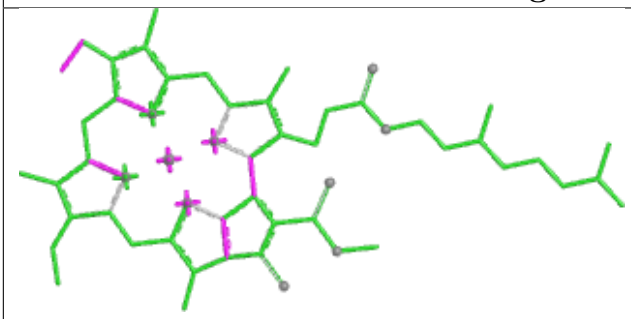


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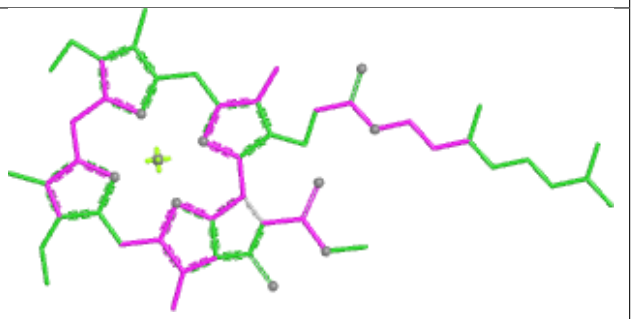


Rings

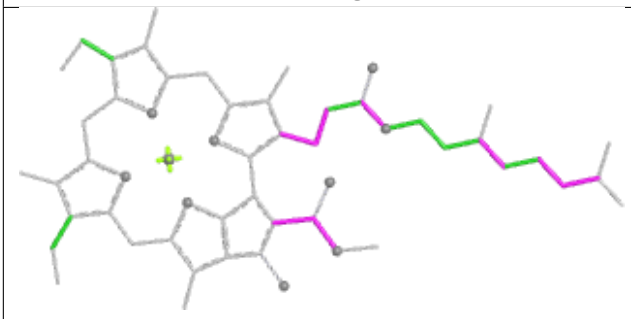
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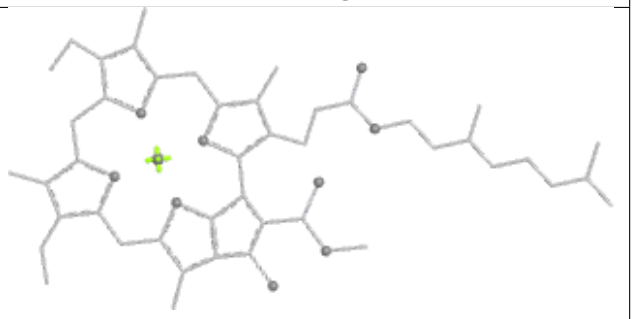
Bond lengths



Bond angles

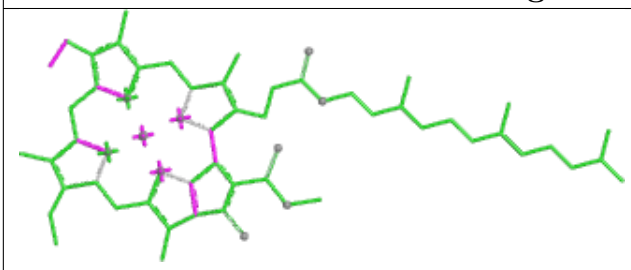


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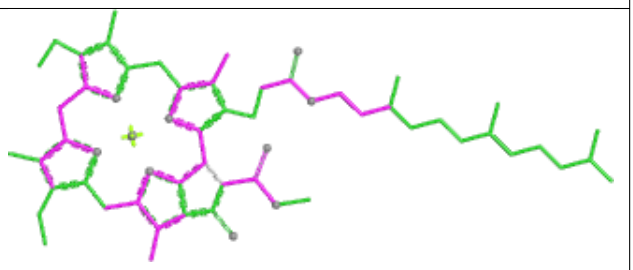


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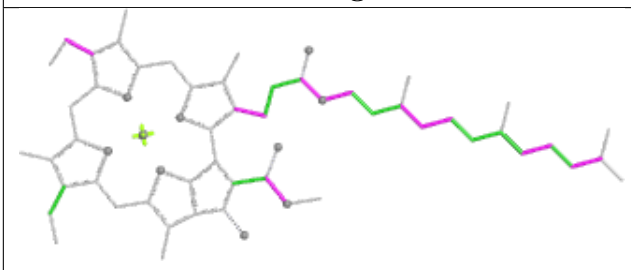
Ligand CLA S 310



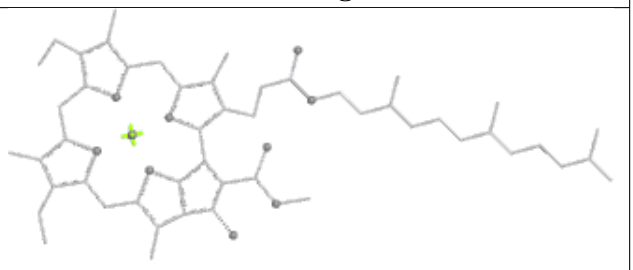
Bond lengths



Bond angles

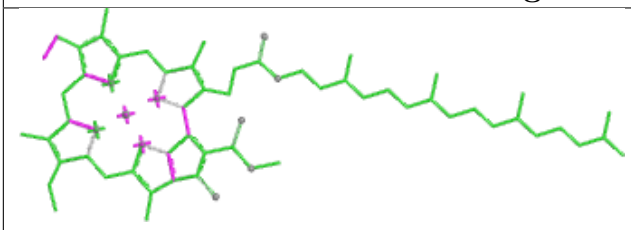


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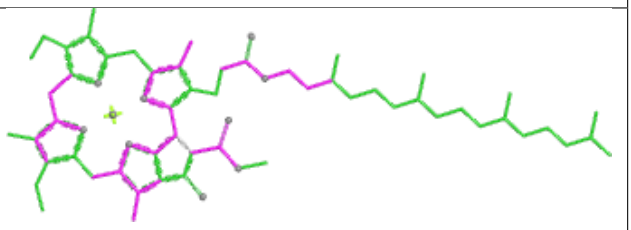


Rings

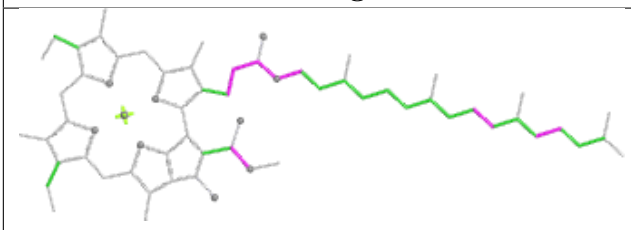
Ligand CLA Y 313



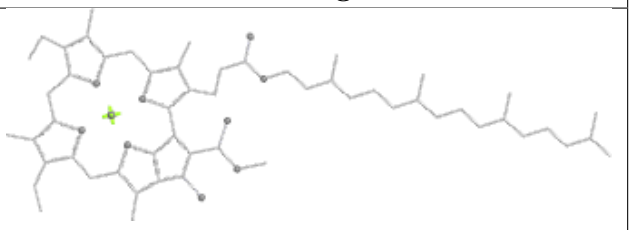
Bond lengths



Bond angles

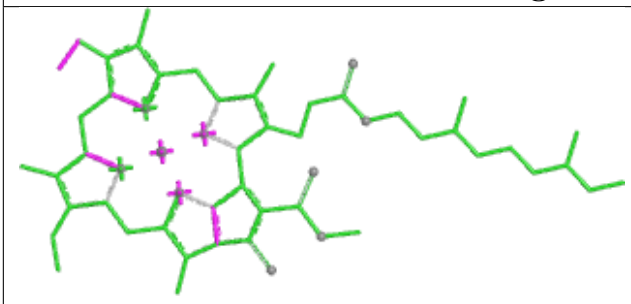


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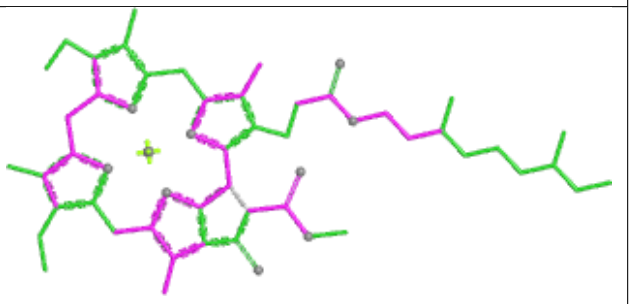


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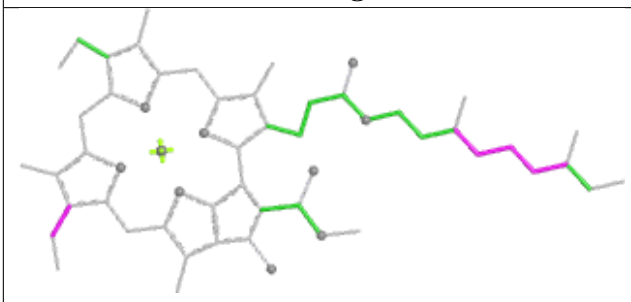
Ligand CLA s 313



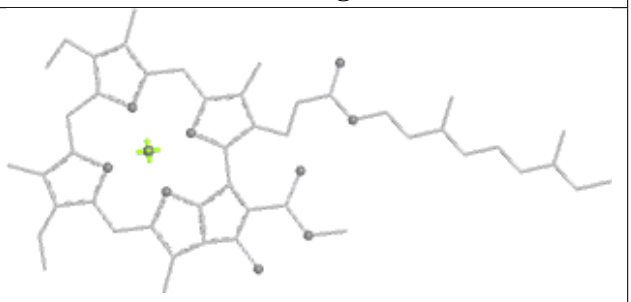
Bond lengths



Bond angles

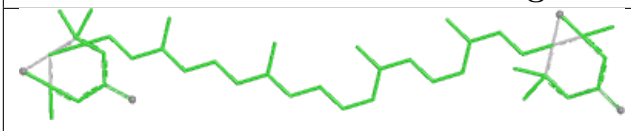


Torsions

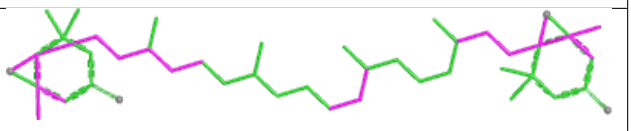


Rings

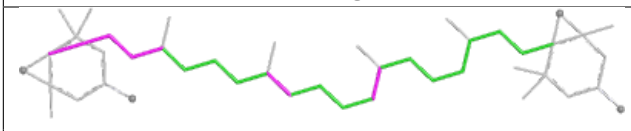
Ligand XAT 2 619



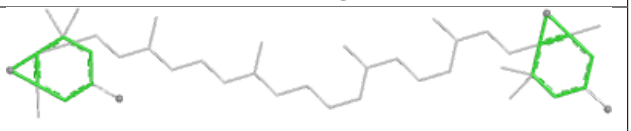
Bond lengths



Bond angles

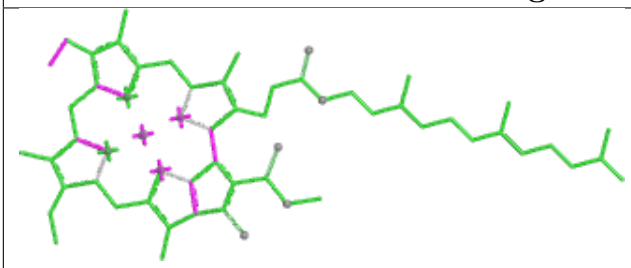


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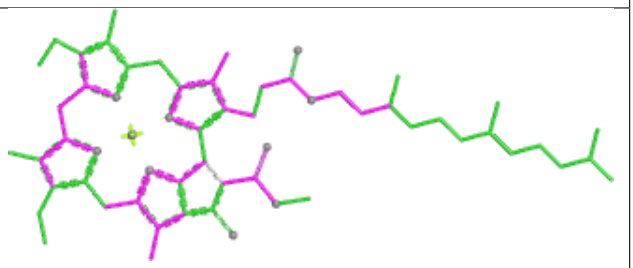


Rings

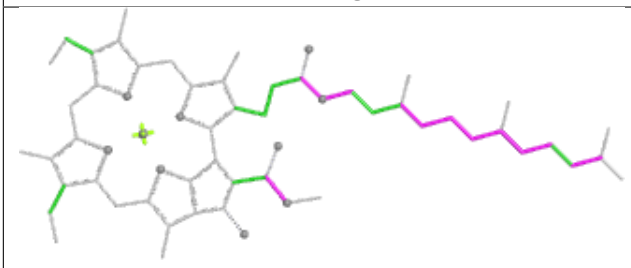
Ligand CLA a 409



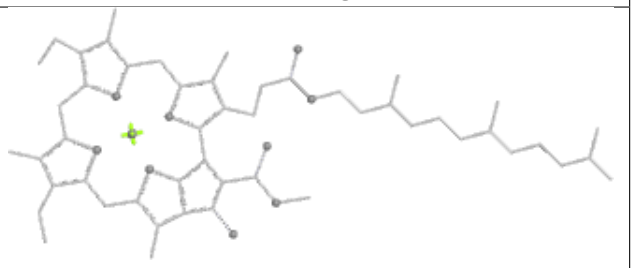
Bond lengths



Bond angles

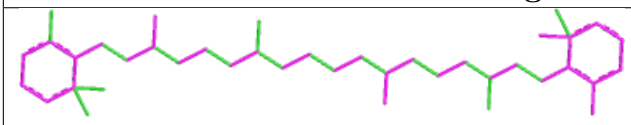


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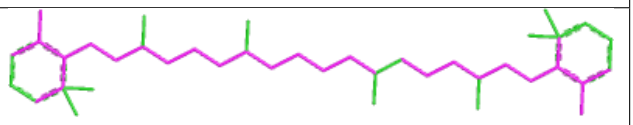


Rings

Ligand BCR Z 101



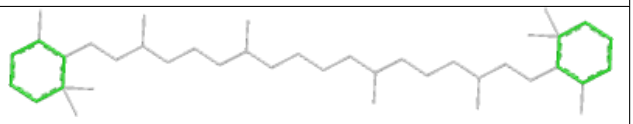
Bond lengths



Bond angles

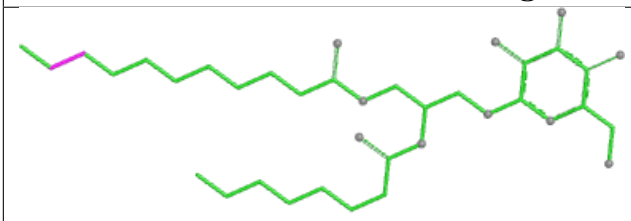


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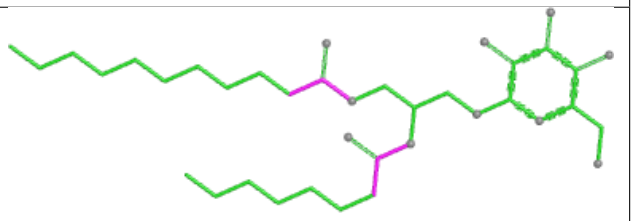


Rings

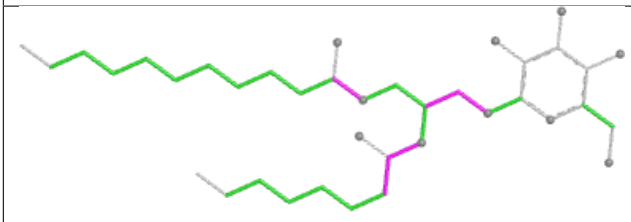
Ligand LMG N 320



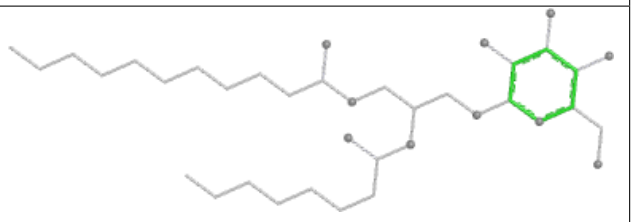
Bond lengths



Bond angles

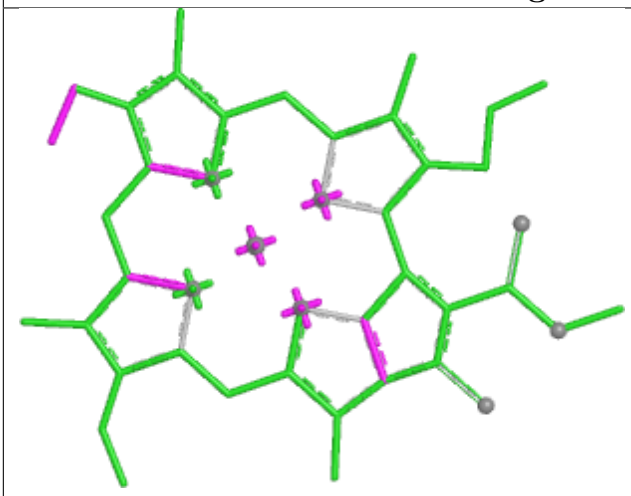


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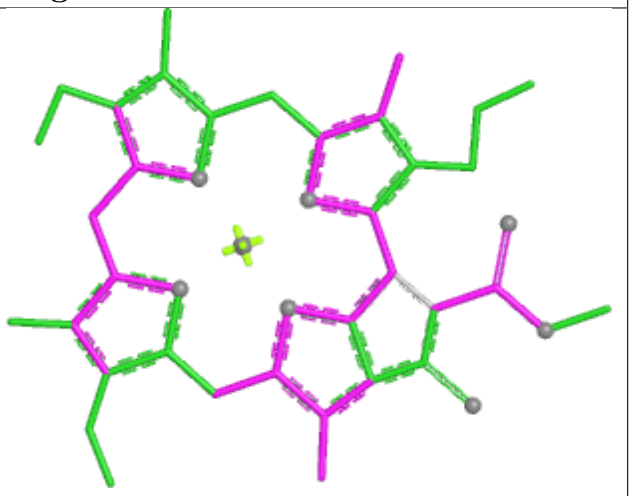


Rings

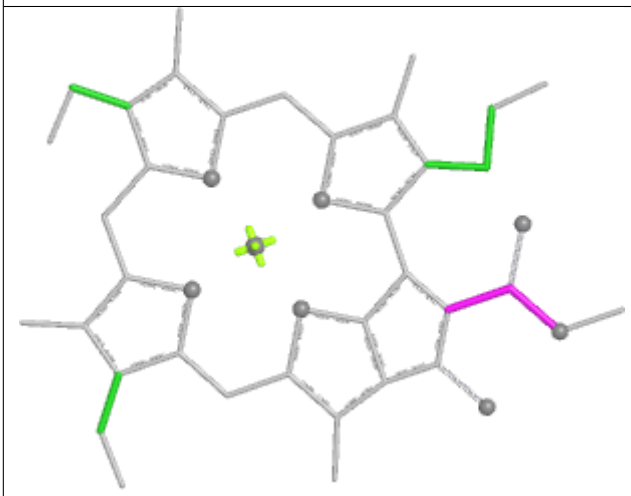
Ligand CLA g 312



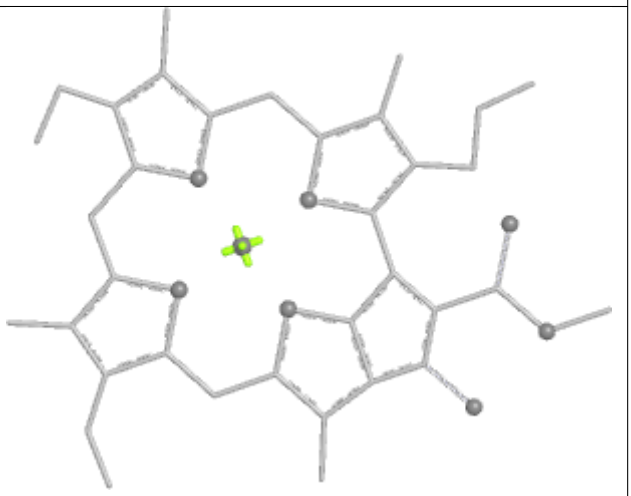
Bond lengths



Bond angles

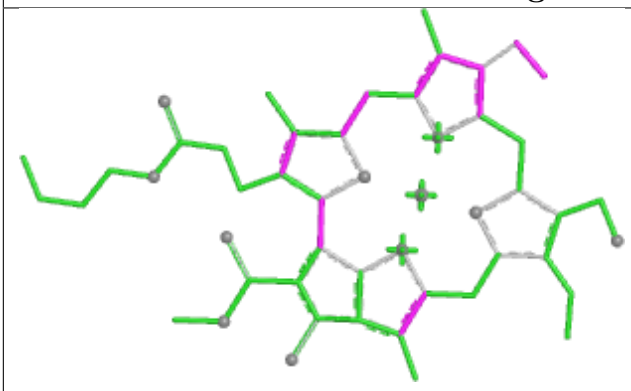


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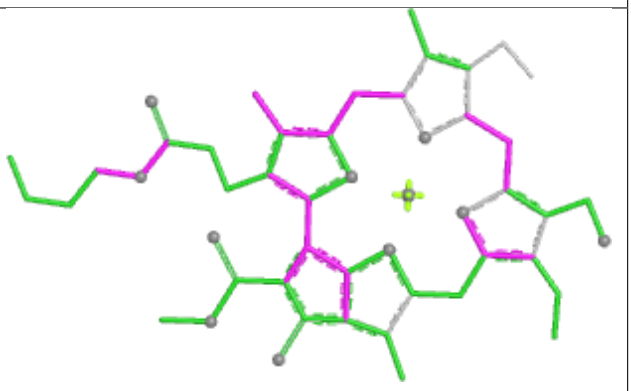


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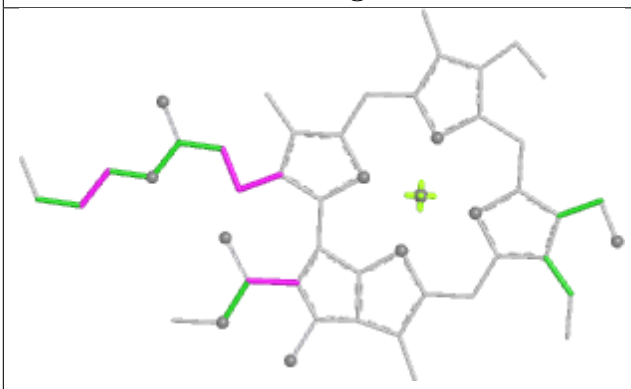
Ligand CHL 4 608



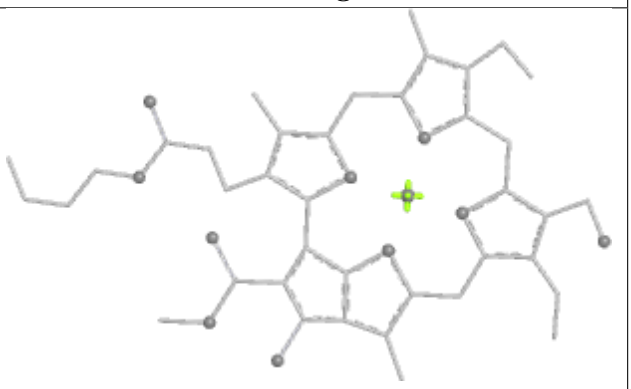
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Bond angles

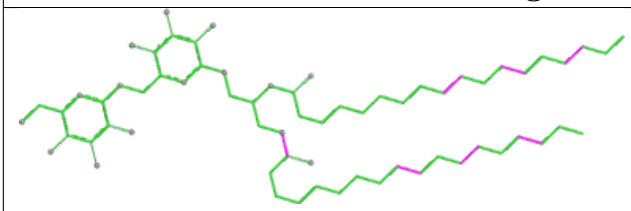


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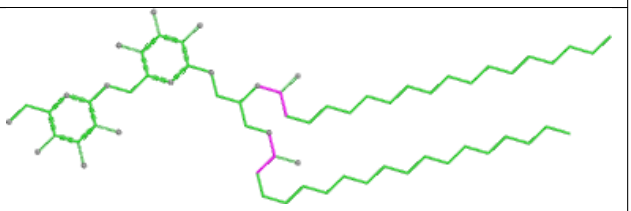


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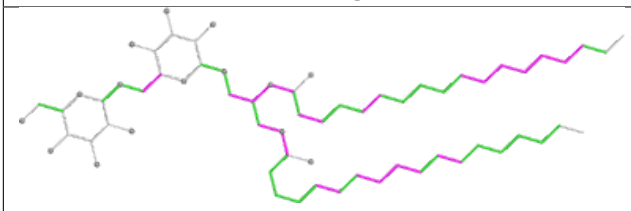
Ligand DGD c 616



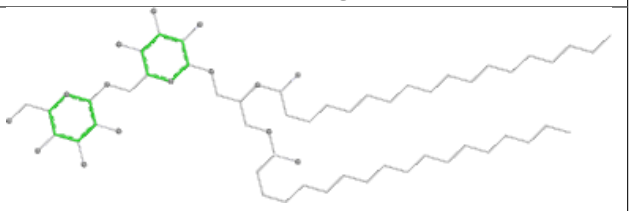
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Bond angles

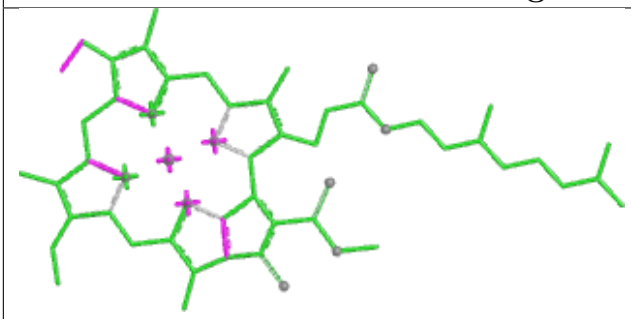


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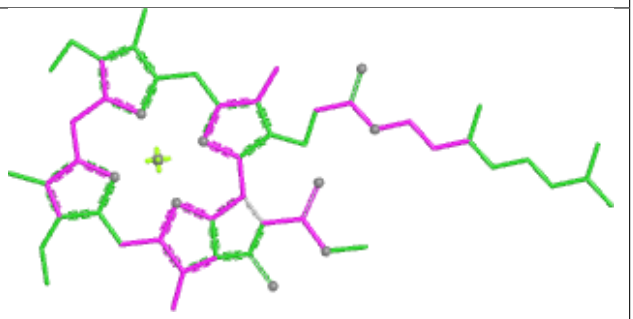


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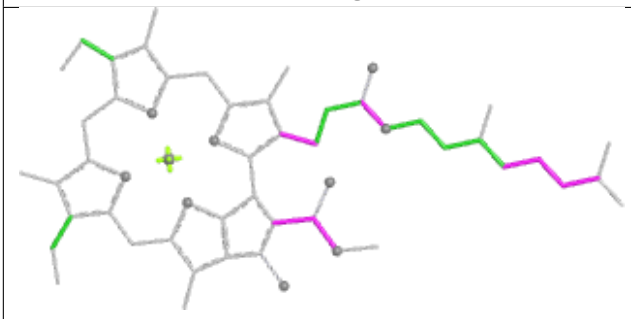
Ligand CLA n 304



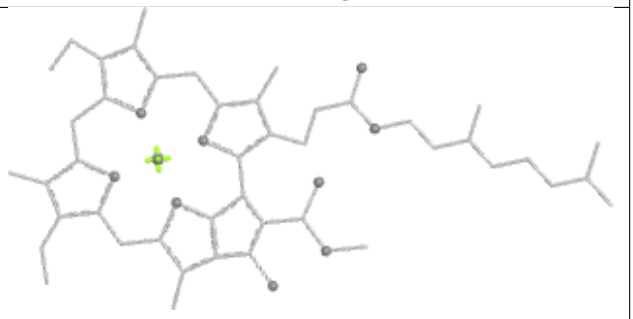
Bond lengths



Bond angles

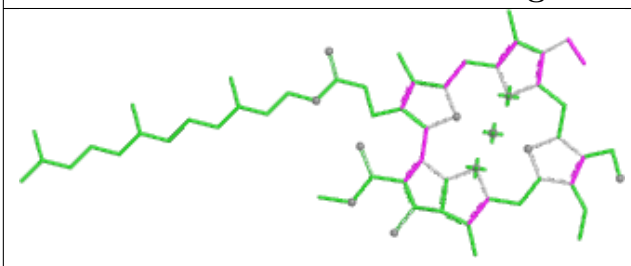


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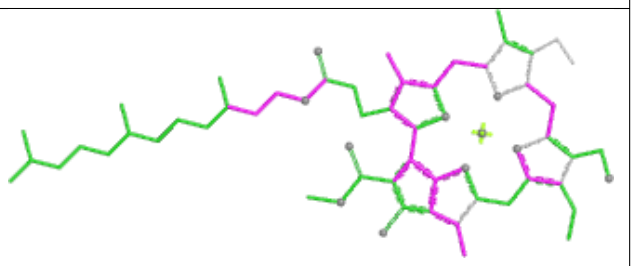


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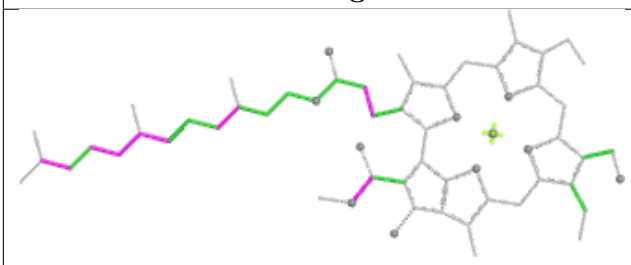
Ligand CHL 9 311



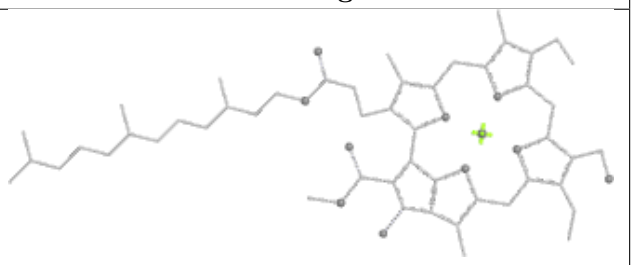
Bond lengths



Bond angles

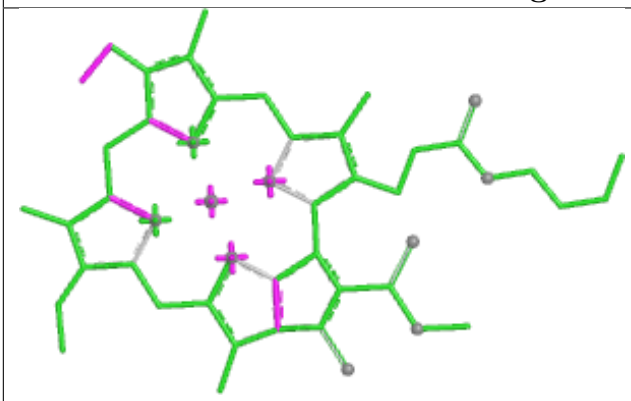


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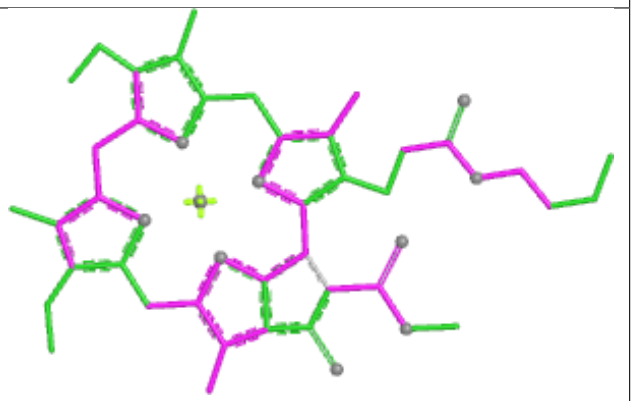


Rings

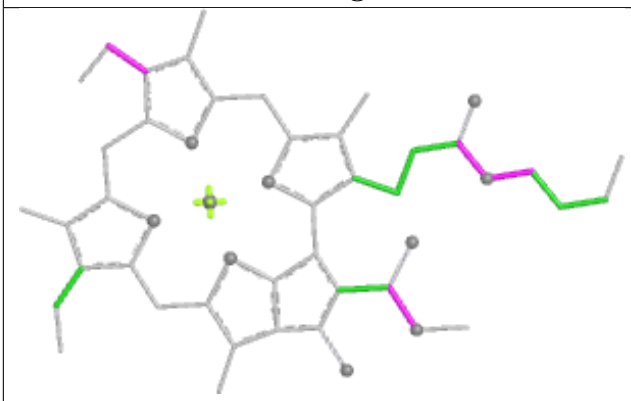
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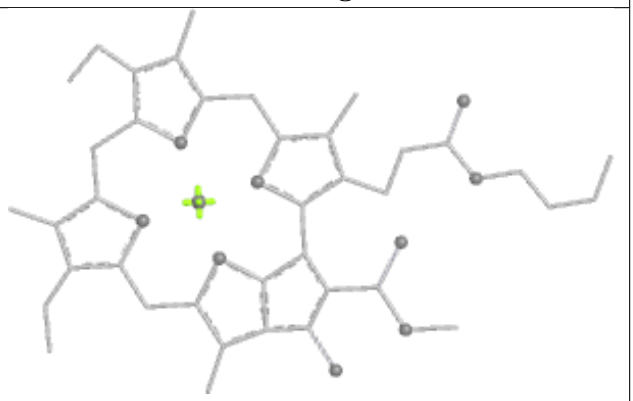
Bond lengths



Bond angles

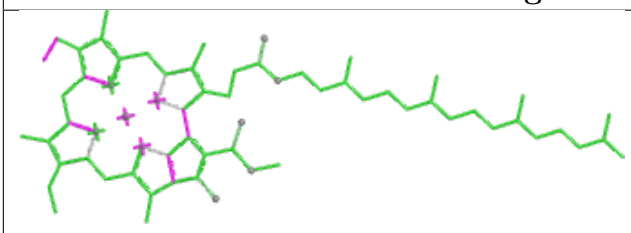


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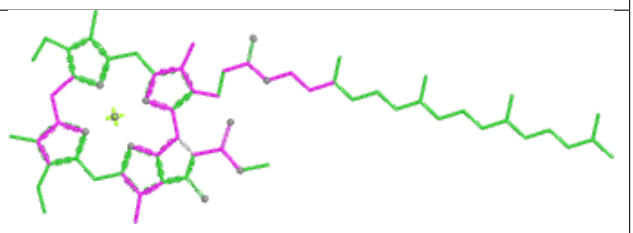


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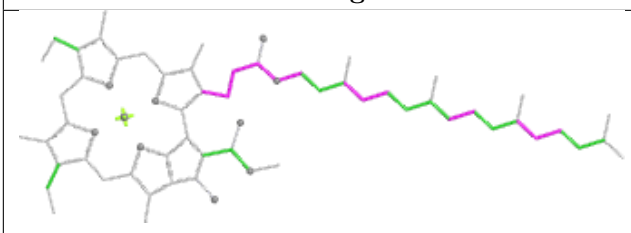
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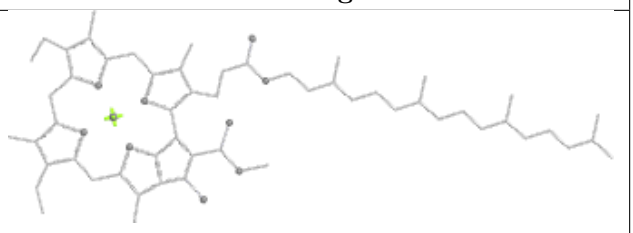
Bond lengths



Bond angles

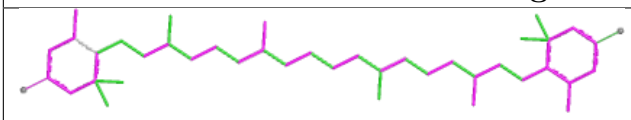


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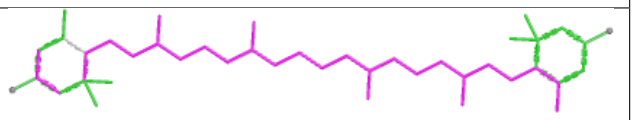


Rings

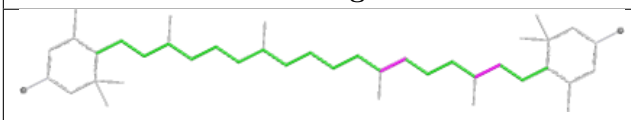
Ligand LUT r 317



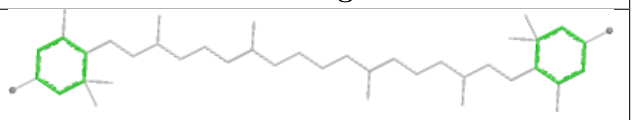
Bond lengths



Bond angles

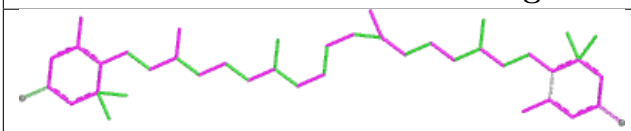


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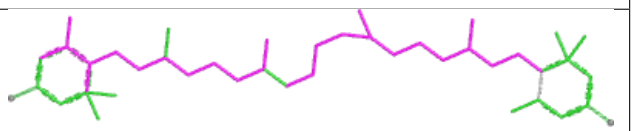


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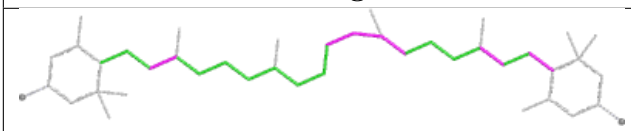
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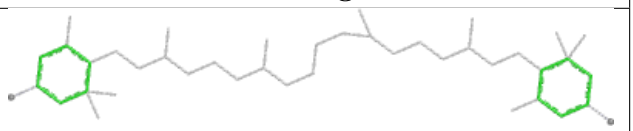
Bond lengths



Bond angles

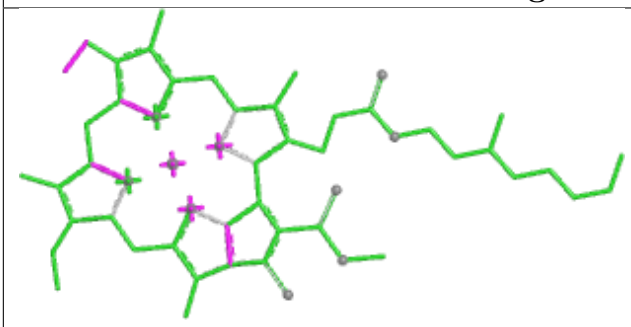


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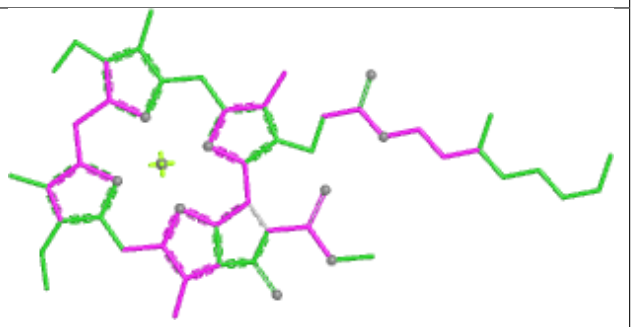


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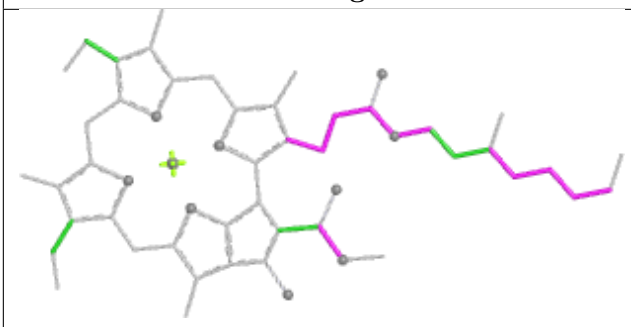
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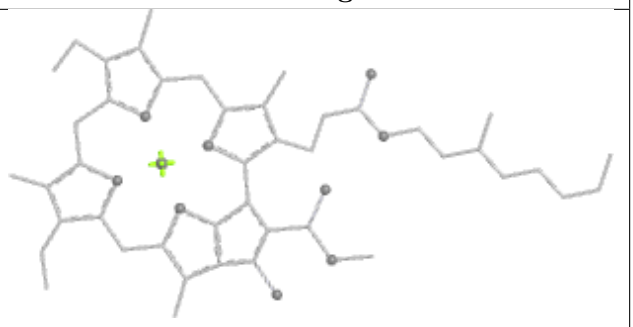
Bond lengths



Bond angles

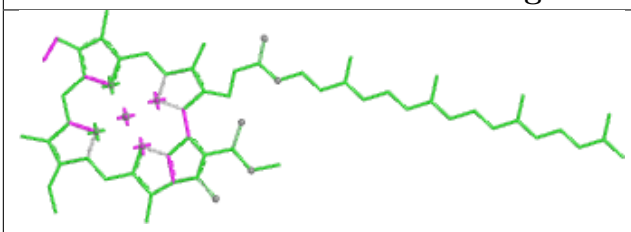


Torsions

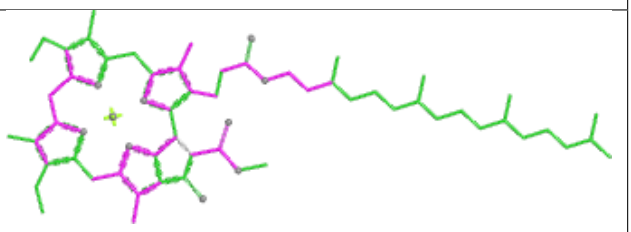


Rings

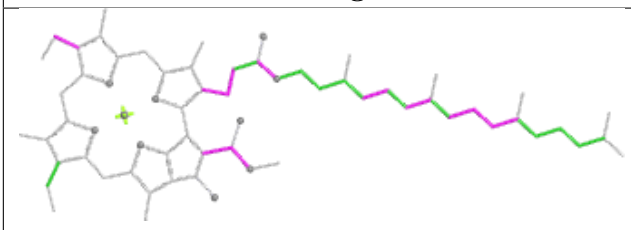
Ligand CLA C 601



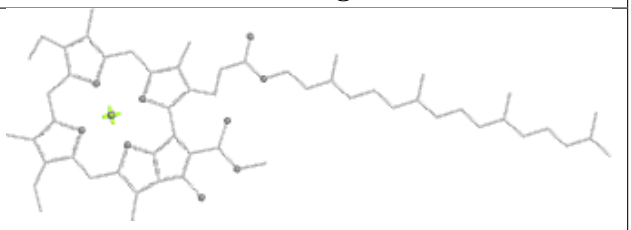
Bond lengths



Bond angles

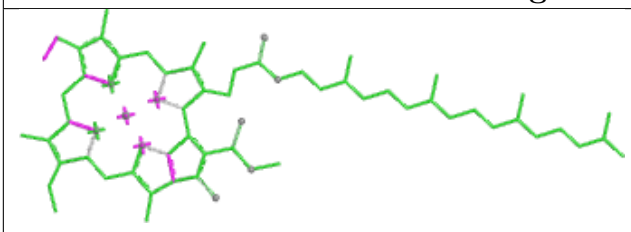


Torsions

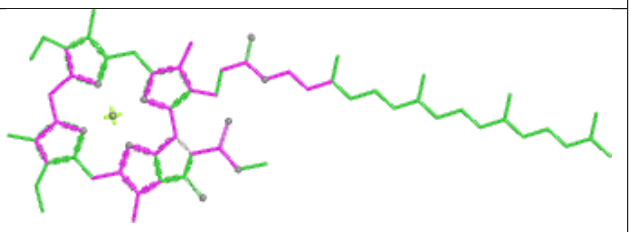


Rings

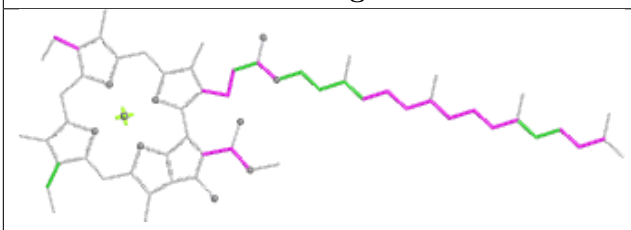
Ligand CLA c 601



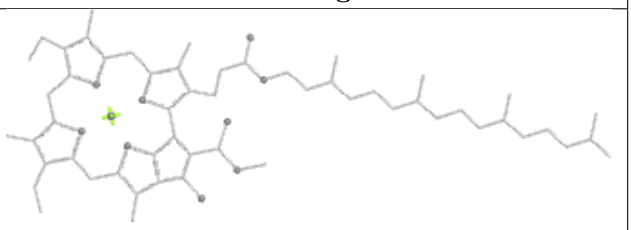
Bond lengths



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.

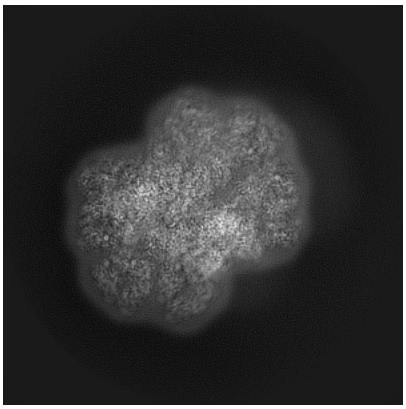
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15973. These allow visual inspection of the internal detail of the map and identification of artifacts.

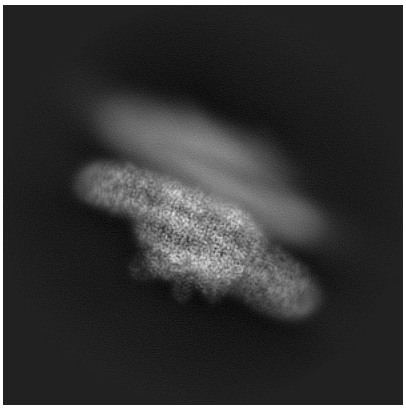
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

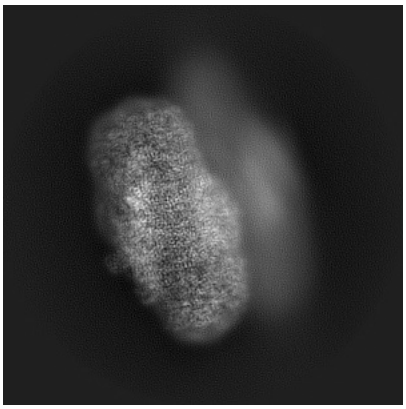
6.1.1 Primary map



X

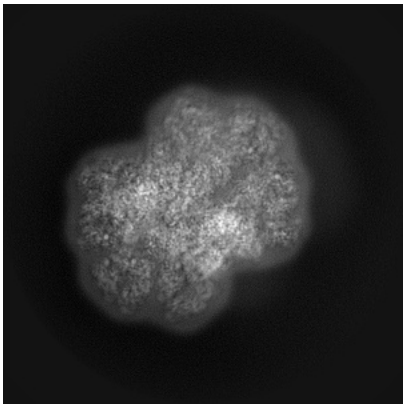


Y

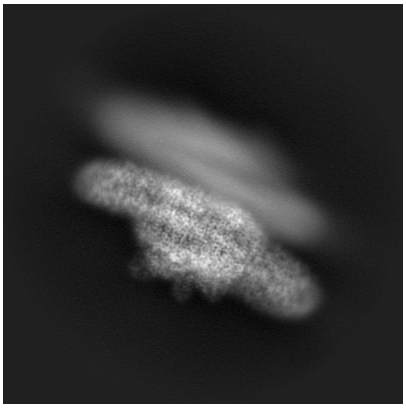


Z

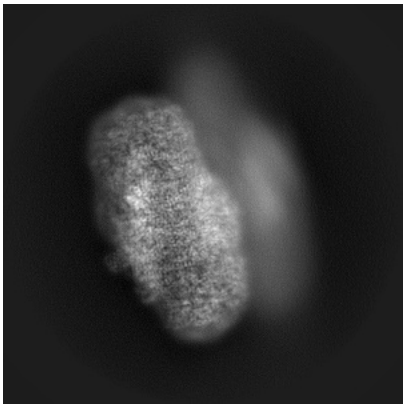
6.1.2 Raw map



X



Y

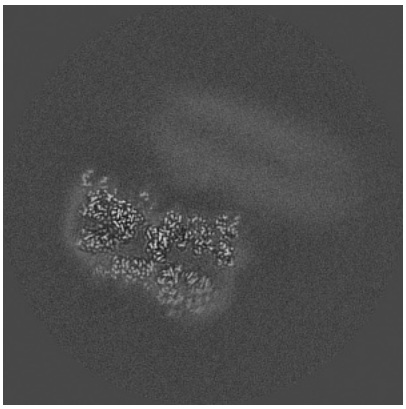


Z

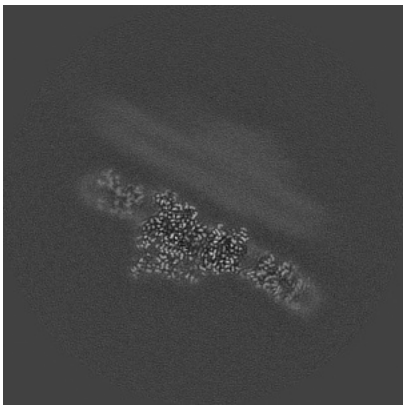
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

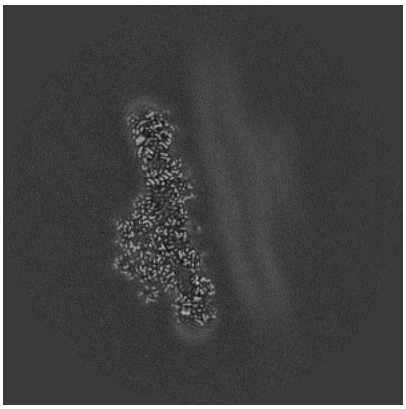
6.2.1 Primary map



X Index: 250

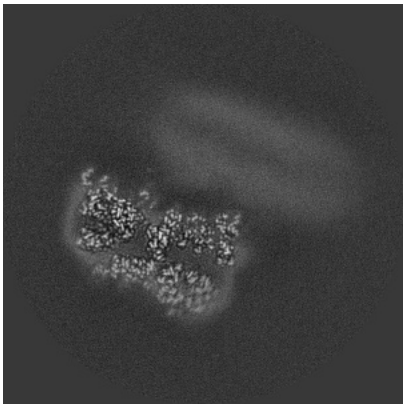


Y Index: 250

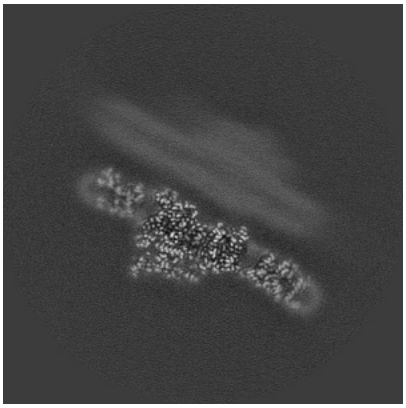


Z Index: 250

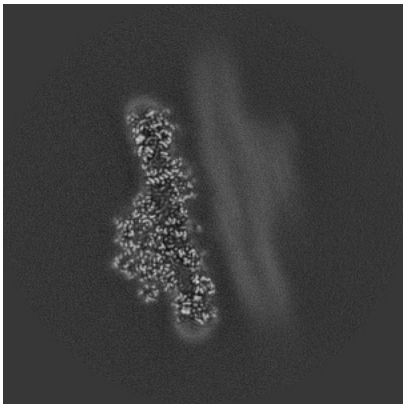
6.2.2 Raw map



X Index: 250



Y Index: 250

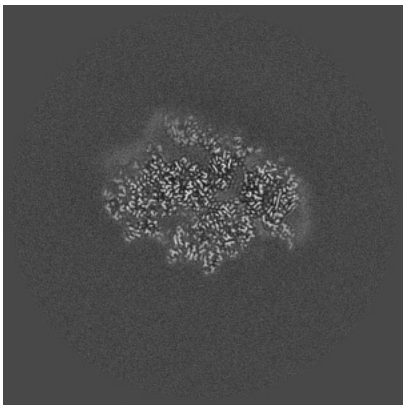


Z Index: 250

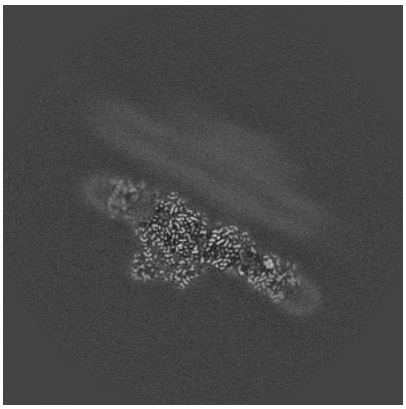
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

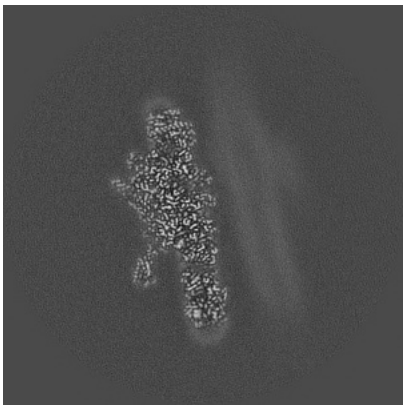
6.3.1 Primary map



X Index: 183

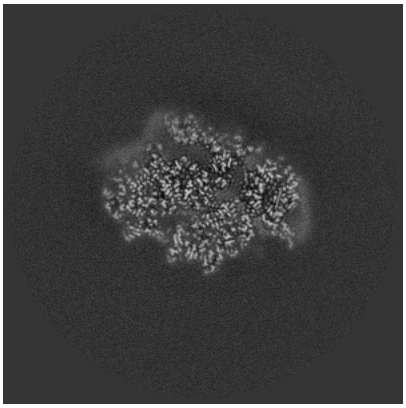


Y Index: 257

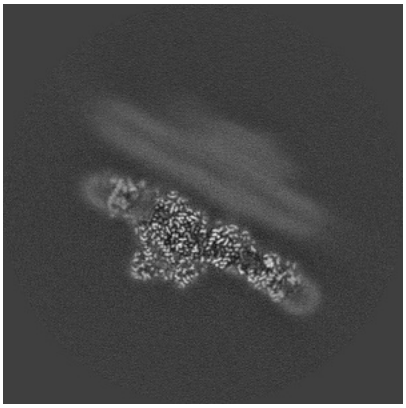


Z Index: 213

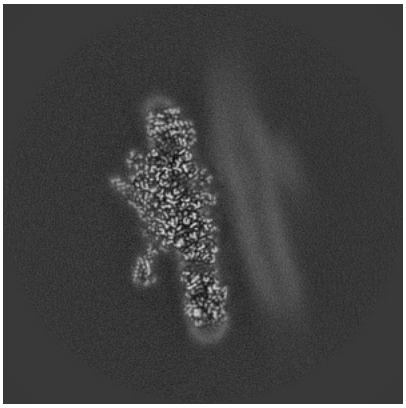
6.3.2 Raw map



X Index: 183



Y Index: 257

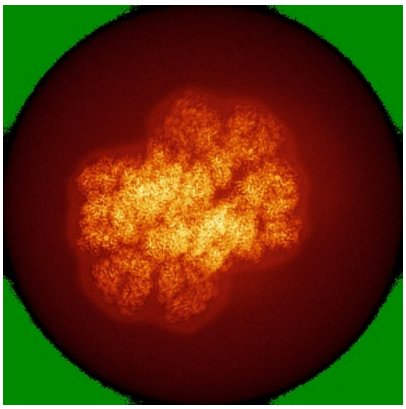


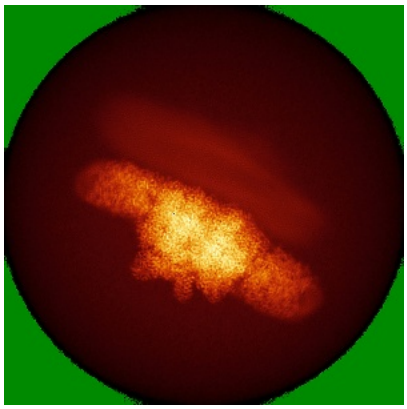
Z Index: 213

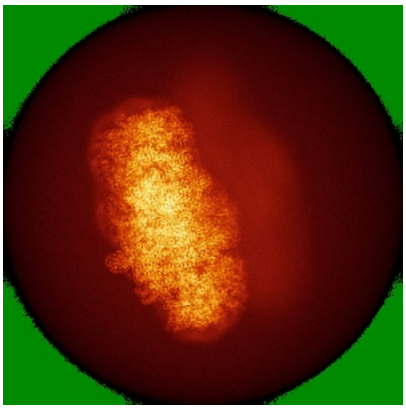
The images above show the largest variance slices of the map in three orthogonal directions.

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

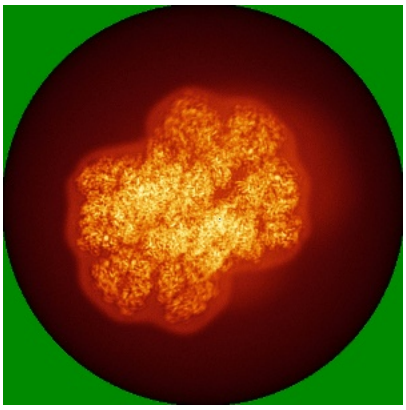
6.4.1 Primary map

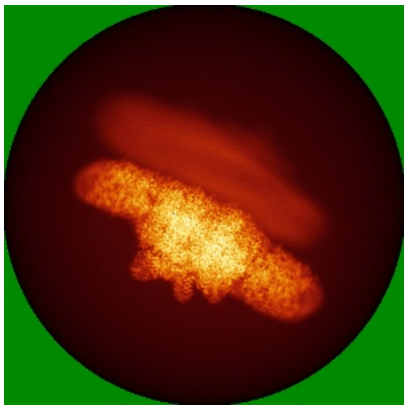

X

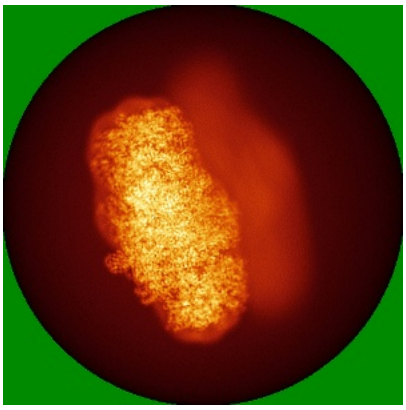

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

This section was not generated.

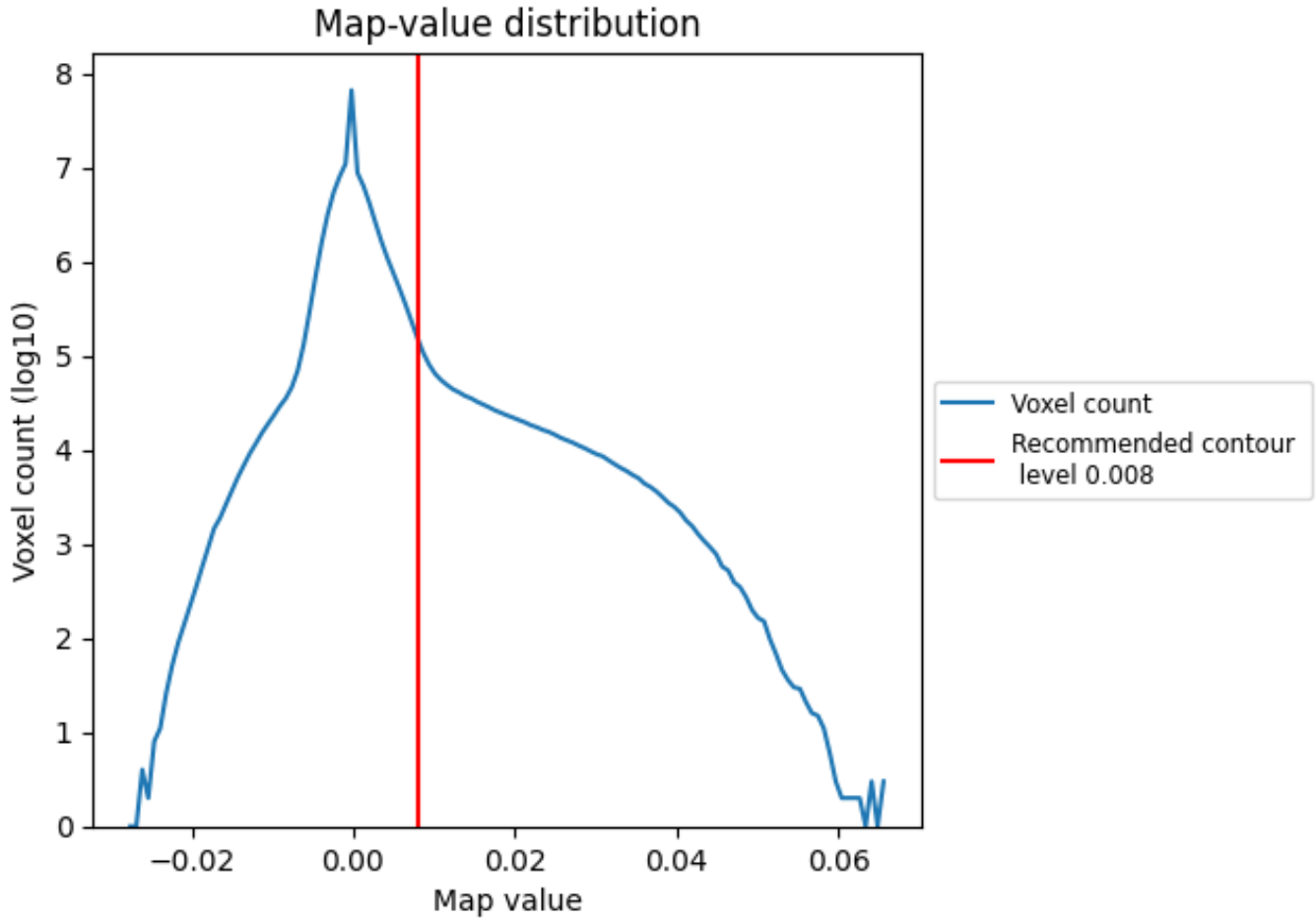
6.6 Mask visualisation (i)

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

7 Map analysis

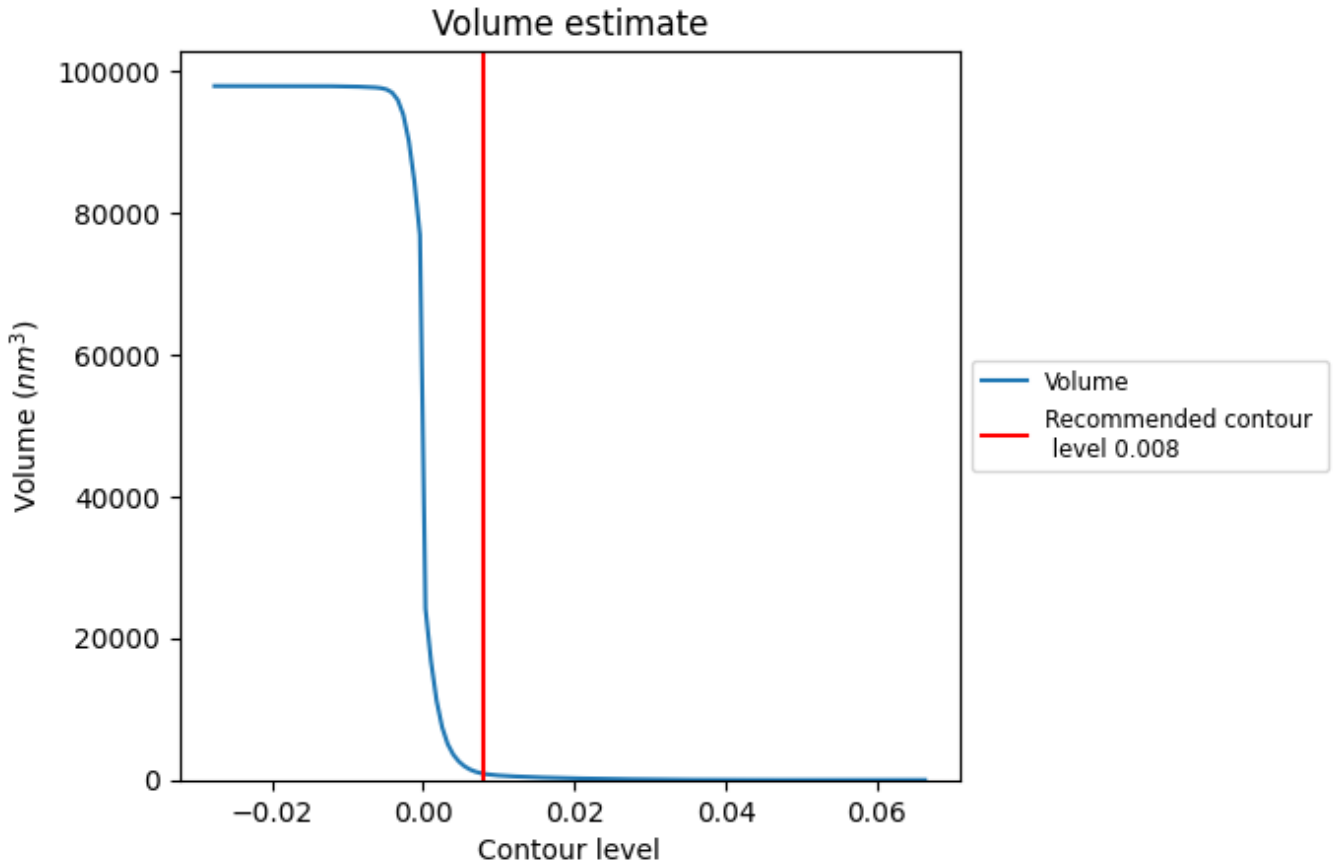
This section contains the results of statistical analysis of the map.

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.

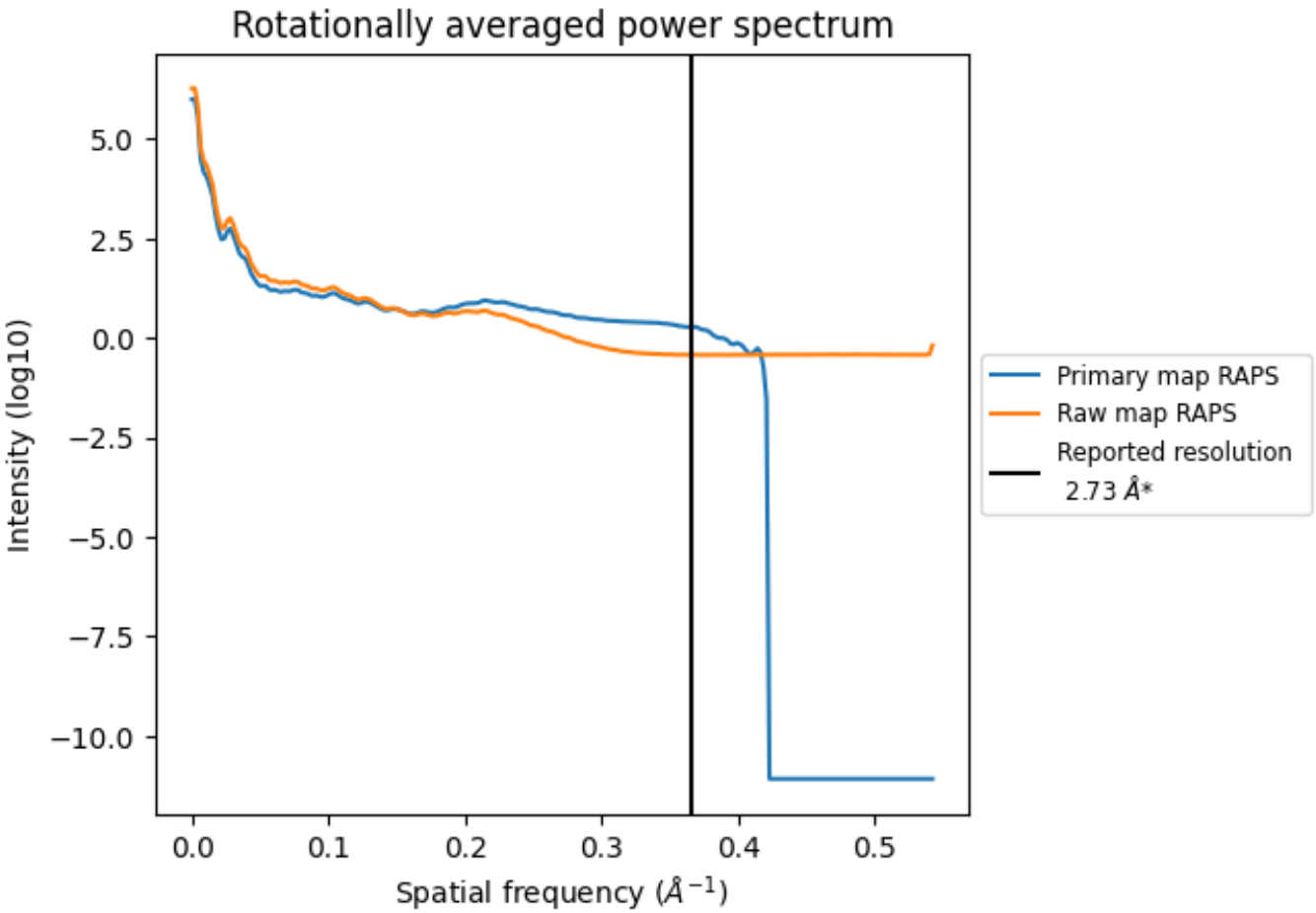
7.2 Volume estimate



The volume at the recommended contour level is 885 nm^3; this corresponds to an approximate mass of 799 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)

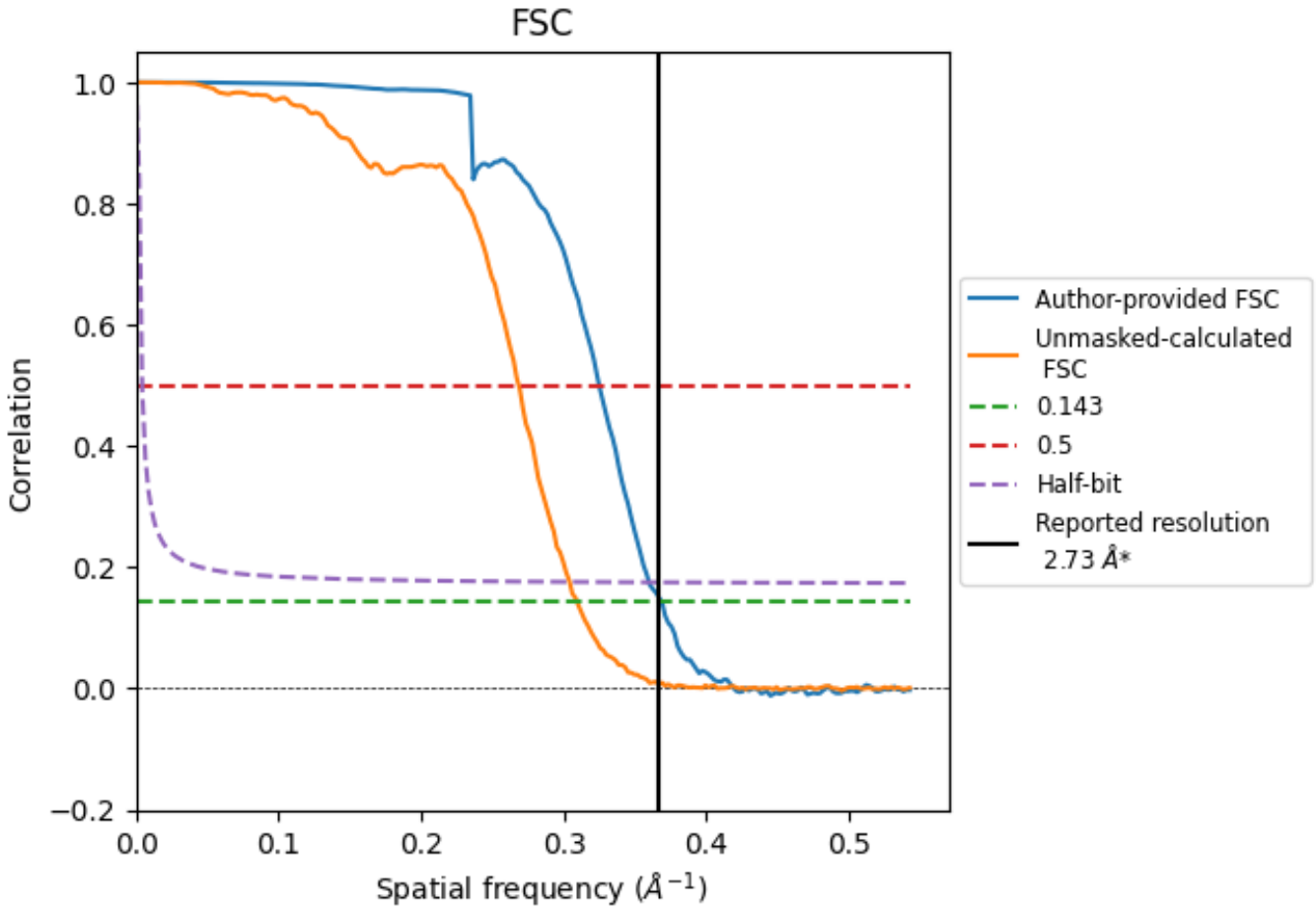


*Reported resolution corresponds to spatial frequency of 0.366 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.366 Å^{-1}

8.2 Resolution estimates (i)

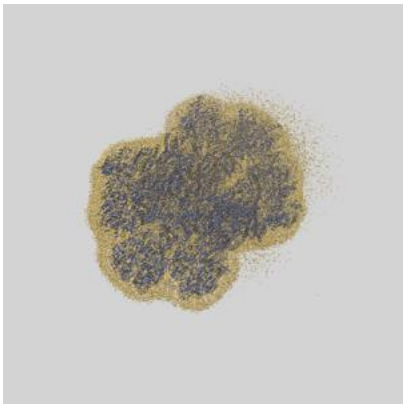
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.71	3.08	2.78
Unmasked-calculated*	3.23	3.73	3.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.23 differs from the reported value 2.73 by more than 10 %

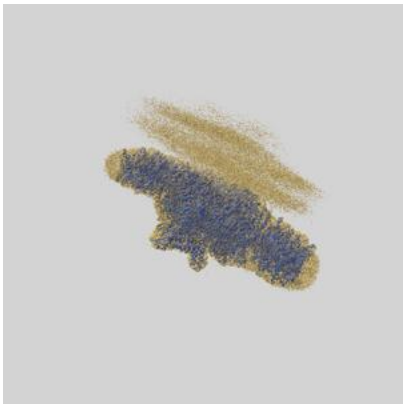
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15973 and PDB model 8BD3. Per-residue inclusion information can be found in section 3 on page 66.

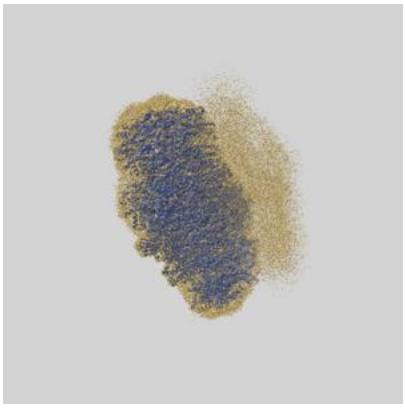
9.1 Map-model overlay



X



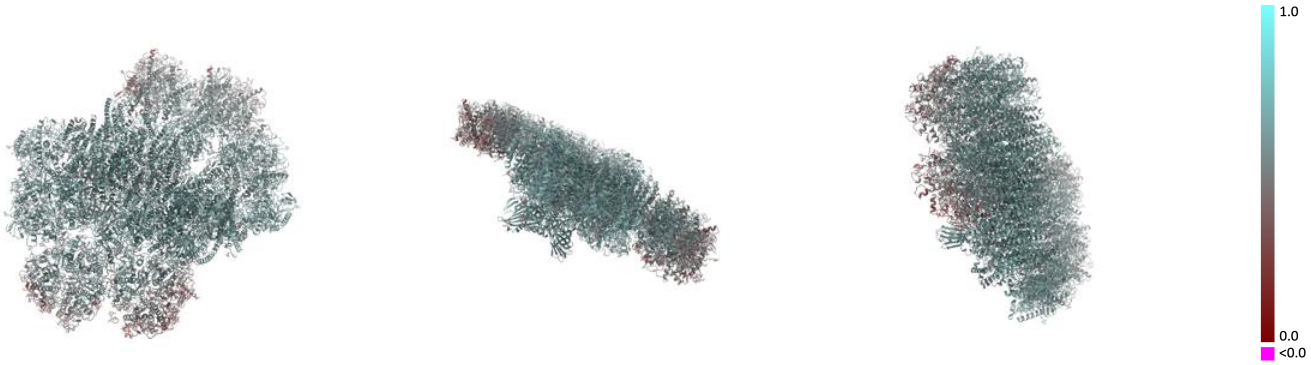
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



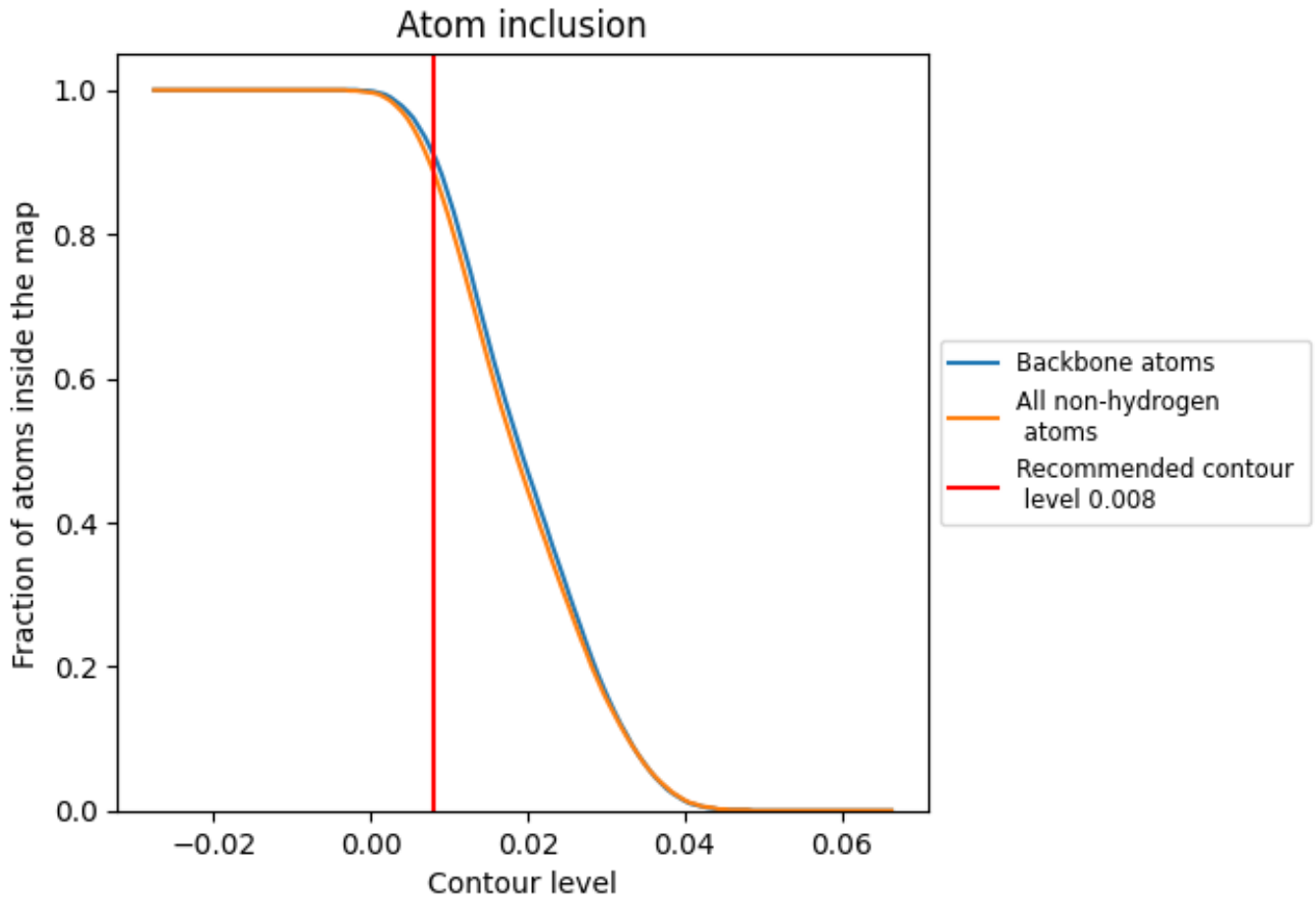
X Y Z

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

9.3 Atom inclusion mapped to coordinate model

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 89% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8870	0.5740
0	0.8560	0.5540
1	0.8750	0.5670
2	0.8000	0.5010
3	0.8160	0.4830
4	0.7510	0.4600
5	0.7340	0.4100
6	0.8510	0.5480
7	0.8590	0.5610
8	0.7870	0.4560
9	0.7940	0.4860
A	0.9550	0.6360
B	0.9450	0.6280
C	0.9450	0.6240
D	0.9590	0.6370
E	0.9350	0.6170
F	0.9590	0.6310
F1	0.9210	0.5910
G	0.8990	0.5780
H	0.9560	0.6210
I	0.9350	0.6110
J	0.8950	0.6030
K	0.8510	0.5810
L	0.9280	0.6150
M	0.7890	0.5400
N	0.9150	0.5880
O	0.8970	0.5770
P1	0.8790	0.5930
Q1	0.7590	0.5390
R	0.9020	0.6000
S	0.8980	0.5830
T	0.9070	0.6020
U	0.8870	0.5770
V	0.8380	0.5670
W	0.8310	0.5780



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
X	0.8580	0.5780
Y	0.9280	0.6150
Z	0.9200	0.5810
a	0.9540	0.6320
b	0.9410	0.6240
c	0.9370	0.6190
d	0.9640	0.6400
e	0.9260	0.6050
f	0.9310	0.6210
f1	0.9180	0.5860
g	0.8950	0.5790
h	0.9580	0.6240
i	0.9740	0.6400
j	0.8940	0.5880
k	0.9420	0.6090
l	0.9340	0.6190
m	0.8210	0.5590
n	0.9170	0.5890
o	0.8930	0.5850
p	0.7040	0.4150
p1	0.8800	0.5840
q	0.7420	0.4650
q1	0.7490	0.5230
r	0.9090	0.6030
s	0.9000	0.5820
t	0.8760	0.5990
u	0.8940	0.5850
v	0.8520	0.5680
w	0.8480	0.5680
x	0.8280	0.5630
y	0.9350	0.6170
z	0.8880	0.5610